Supporting Information

Electrochemical Reductive Cascade Cyclizations of *o*-Alkynylated Derivatives for Saturated Amides/Amines

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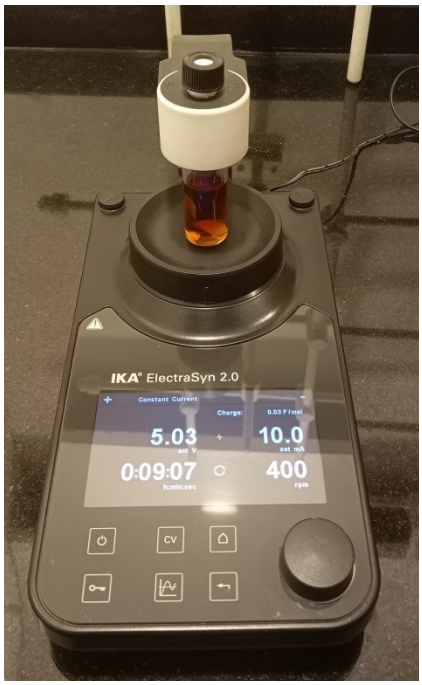
1. General considerations

The ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ solvent on Bruker Spectrometers 300, 400, 500 MHz (300, 400, 500 for ^{1}H NMR and 75, 101, 125 MHz for ^{13}C NMR), respectively with TMS as an internal standard. Mass spectra were recorded on Xevo G2S Q-TOF spectrometer. TLC was performed using Merck pre-coated TLC plates (Merck 60 F254) and detected under UV light. Column chromatography was carried out with silica gel (100-200 mesh). Reagents and solvents were purified as per the standard procedures. IKA Electrasyn 2.0 was used to perform electrochemical reactions.

a) Electrodes

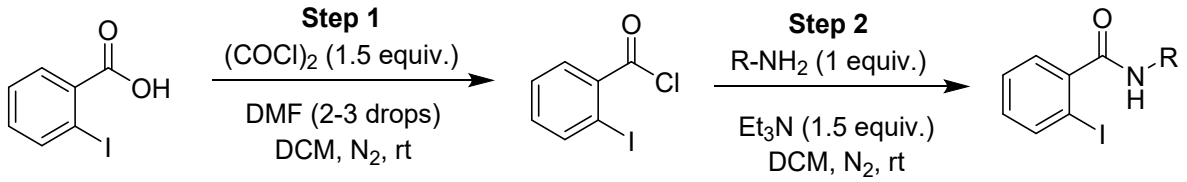


b) Reaction setup

2. General procedure for the synthesis of starting materials

2.1 General procedure A for the synthesis of 2-iodo *N*-aryl/alkylbenzamides

All the starting materials were prepared according to the literature procedure[1,2]



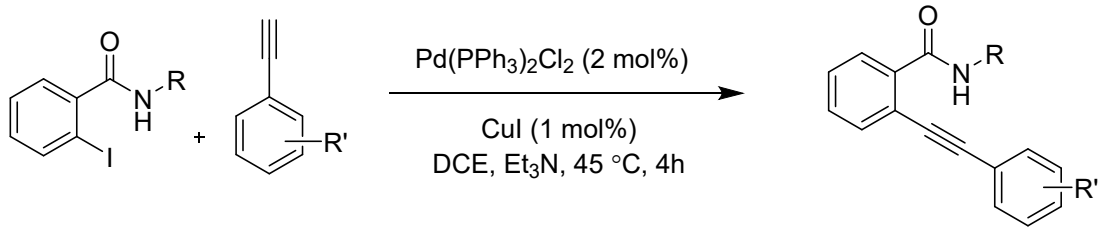
Step 1:

To a solution of 2-iodobenzoic acid (8.0 mmol, 1 equiv.) in DCM, oxalyl chloride (12 mmol, 1.5 equiv.) and 2-3 drops of DMF were added under nitrogen atmosphere. The reaction mixture was allowed to stir at room temperature for 4-5 h. Then the solvent was evaporated under reduced pressure to afford 2-iodobenzoyl chloride. The crude product was used for the next step without further purification.

Step 2:

To a solution of 2-iodobenzoylchloride (1.8 mmol, 1equiv.) in DCM, triethylamine (2.8 mmol, 1.5 equiv.) and anilines (1.8 mmol, 1equiv.) were added under nitrogen atmosphere. The resulting mixture was allowed to stir at room temperature for 6-8 h. Then, 10% HCl (20 mL) was added, extracted with DCM and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure to afford the 2-iodo-N-substituted benzamides.

2.2 General procedure B for the synthesis of *o*-alkynylbenzamides[1,2]

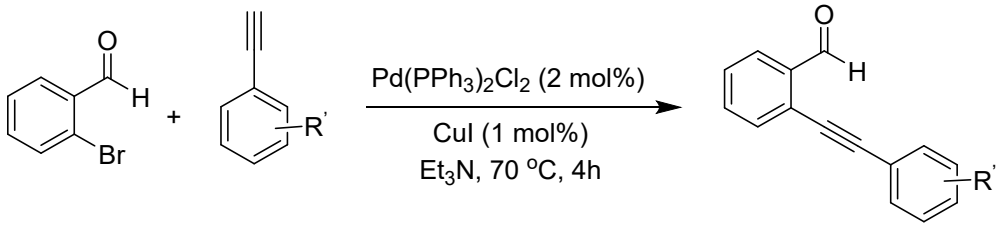


To a solution of 2-iodo-*N*-substituted benzamides (0.6 mmol, 1equiv.) in DCE (5 mL), triethylamine (2.4 mmol, 4 equiv.) were added $Pd(PPh_3)_2Cl_2$ (2 mol%) and CuI (1 mol%) under N_2 atmosphere and allowed to stir at room temperature for 20 minutes, then phenyl acetylenes (0.68 mmol, 1.1 equiv.) was added dropwise to the reaction mixture and heated at 45 ^oC on oil

bath for 4h. After completion of the reaction (monitored by TLC), the crude reaction mixture was passed through celite and washed with ethylacetate. Then the solvent was evaporated under reduced pressure. The crude product was purified by silica column chromatography using EtOAc/Hexanes (5:95) as an eluent to furnish the corresponding *o*-alkynylbenzamides.

2.3 General procedure C for the synthesis of *o*-alkynylated benzaldehydes[3]

To a solution of 2-bromobenzaldehyde (1.6 mmol, 1 equiv.) in triethylamine, $Pd(PPh_3)_2Cl_2$ (2 mol%), CuI (1 mol%) was added under nitrogen atmosphere. The mixture was stirred at room temperature for 15 minutes then, phenylacetylenes (1.7 mmol, 1.1 equiv.) was added in drops to the reaction mixture and allowed to stir at 70 ^oC in oil bath for 4 hours. After completion of reaction (monitored by TLC), the crude reaction mixture was passed through pad of celite and solvent was evaporated under reduced pressure. The crude product was purified by silica column chromatography using EtOAc/Hexanes as an eluent to furnish the corresponding *o*-alkynylated benzaldehydes.



3. General procedure D for the synthesis of isoindolin-1-ones

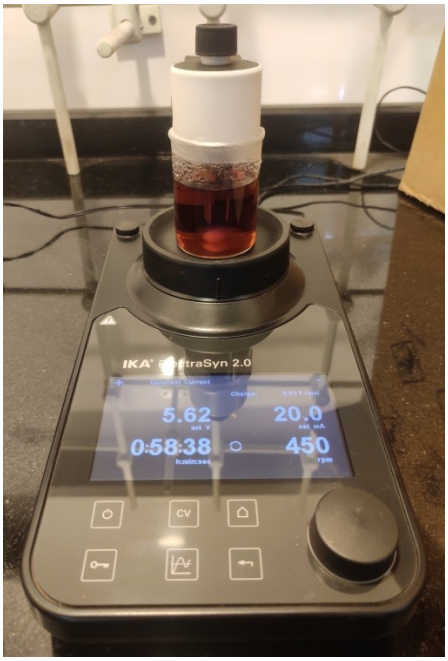
To an oven dried reaction vial was charged with **1** (0.16 mmol, 1 equiv.), DIPEA (0.25 mmol, 1.5 equiv.), $TBAPF_6$ (0.16 mmol, 1 equiv.) and ACN (8 mL). The reaction mixture was electrolyzed with Pt plate as both anode and cathode under constant current electrolysis (I = 10 mA) for 2 h. After the completion of the reaction (monitored by TLC), the solvent was evaporated under reduced pressure. The crude product was purified by silica column chromatography using EtOAc/Hexanes as eluent to furnish the corresponding 3-benzyl-2-substituted isoindolin-1-ones.

4. General procedure E for the synthesis of 11-benzylisoindolo[2,1-*a*]quinazolin-5(11H)-one

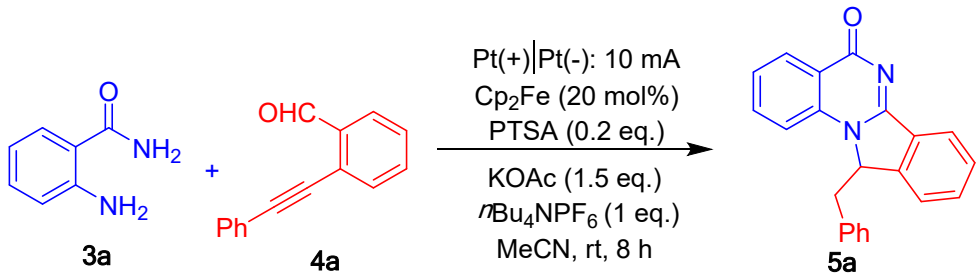
To an oven dried reaction tube was charged with 2-aminobenzamide **3** (0.22 mmol, 1equiv.), *o*-alkynylbenzaldehydes **4** (0.22 mmol, 1equiv.), PTSA (0.04 mmol, 0.2 equiv.), KOAc (0.33 mmol, 1.5 equiv), Ferrocene (20 mol%), $TBAPF_6$ (0.22 mmol, 1 equiv.) in ACN (8 mL) was electrolyzed under constant current I = 10 mA for 12 h. After the solvent was evaporated under reduced pressure. The crude products was purified by silica column chromatography using EtOAc/Hexanes as an eluent to furnish the corresponding 11-benzylisoindolo[2,1-*a*]quinazolin-5(11H)-ones.

5. General procedure for the scale up synthesis of isoindolin-1-one

To an oven dried beaker was charged with **1aa** (2.7 mmol, 1 equiv.), DIPEA (4.05 mmol, 1.5 equiv.) and $TBAPF_6$ (2.7 mmol, 1 equiv.) in ACN 40 mL was electrolyzed with Pt plate as both anode and cathode under constant current electrolysis with I = 20 mA for 12 h. After the completion of reaction (monitored by TLC), the solvent was evaporated under reduced pressure, crude product was purified by silica column chromatography using 5% Ethylacetate in *n*-hexanes as solvent gradient to furnish the isoindolin-1-one **2aa** as white solid (0.604 g) in 75% yield.



6. Optimization table for the synthesis of isoindole fused quinazolinones[a,b]

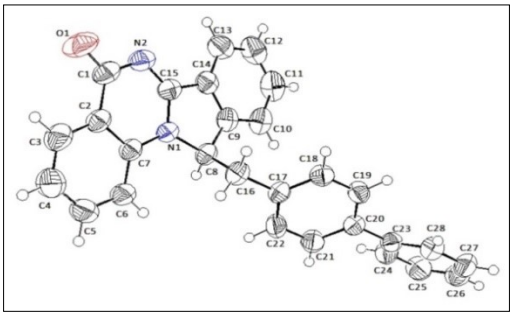


S.No	Deviation from standard conditions	Yield (%)
1	None	58
2	DIPEA instead of KOAc	10
3	K_2CO_3 instead of KOAc	0
4	Without Ferrocene	0
5	C anode Pt cathode (C|Pt)	41
6	C anode C cathode (C|C)	35

Reaction conditions: [a]All reactions were carried out with **3aa** (0.22 mmol), **4aa** (0.22 mmol), KOAc (0.33 mmol), Cp_2Fe (20 mol%) $TBAPF_6$ (0.22 mmol), PTSA (0.4 mmol) ACN (8.0 mL), Pt(+)|Pt(−), I= 10 mA, rt, 12 h. [b]Yields were determined after the purification of the compound.

7. X-ray crystallographic studies of compound 5aj (CCDC 2236020)

Single crystals of compound **5aj** for X-ray diffraction analysis were grown using mixture of DCM and Hexane (8:2) under slow evaporation method. X-ray diffraction data collection of compound **5aj** was recorded in Bruker single crystal KAPPA APEXII instrument.



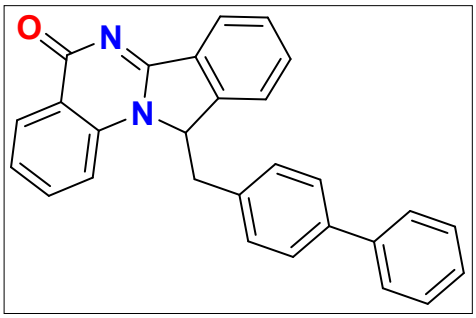


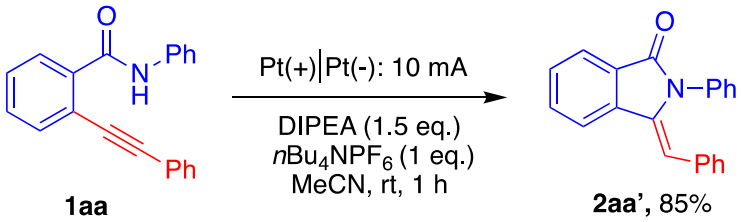
Table 1. Crystal data and structure refinement for **5aj**

Identification code	**5aj**
Empirical formula	$C_{28}\ H_{20}\ N_2O$
Formula weight	400.46
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 7.6187(6) Å α = 98.304(3) ° b = 12.5488(10) Å β = 106.817(3) ° c = 13.1109(11) Å γ = 96.575(3) °
Volume	1171.01(17) $Å^3$
Z, Calculated density	2, 1.136 Mg/m^3
Absorption coefficient	0.069 mm^{-1}
F(000)	420
Crystal size	0.282 x 0.160 x 0.081 mm
Theta range for data collection	3.327 to 26.000 °

Limiting indices	-9<=h<=9, -15<=k<=15, -16<=l<=16
Reflections collected / unique	50982 / 4580 [R(int) = 0.0876]
Completeness to theta = 25.242	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.665
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4580 / 0 / 281
Goodness-of-fit on F2	0.994
Final R indices [I>2sigma(I)]	R1 = 0.0517, wR2 = 0.1543
R indices (all data)	R1 = 0.0764, wR2 = 0.1793
Extinction coefficient	0.023(6)
Largest diff. peak and hole	0.184 and -0.175 e.$Å^{-3}$

8. Intermediates isolation

(Z)-3-benzylidene-2-phenylisoindolin-1-one 2aa'[4]



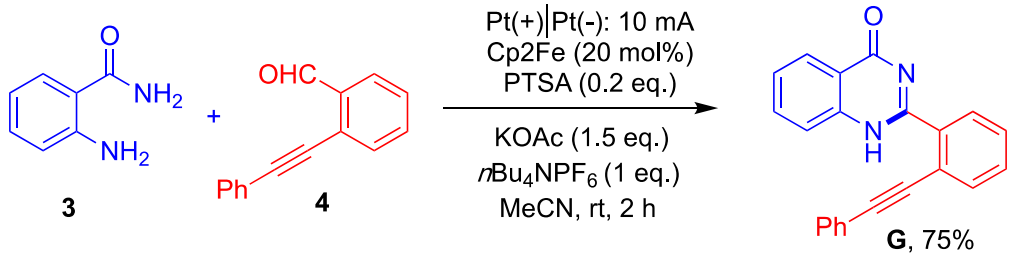
1aa **2aa'**, 85%

The title compound **2aa'** was prepared by following general procedure D and the reaction was stopped at 1 h, the solvent was evaporated under reduced pressure. The pure product was isolated using silica column chromatography. White solid, 85% yield (Solvent gradient: 3% ethylacetate in hexanes)

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.95 (d, J = 7.5 Hz, 1H), 7.86 (d, J = 7.8 Hz, 1H), 7.68 (t, J = 7.5 Hz, 1H), 7.55 (t, J = 7.5 Hz, 1H), 7.07 (s, 5H), 6.96-6.88 (m, 3H), 6.85-6.82 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 167.9, 138.6, 135.9, 134.3, 133.5, 132.4, 129.2, 129.1, 128.1, 127.8, 127.2, 126.7, 126.5, 123.8, 119.4, 107.6.

2-(2-(phenylethynyl)phenyl)quinazolin-4(3H)-one G[5]



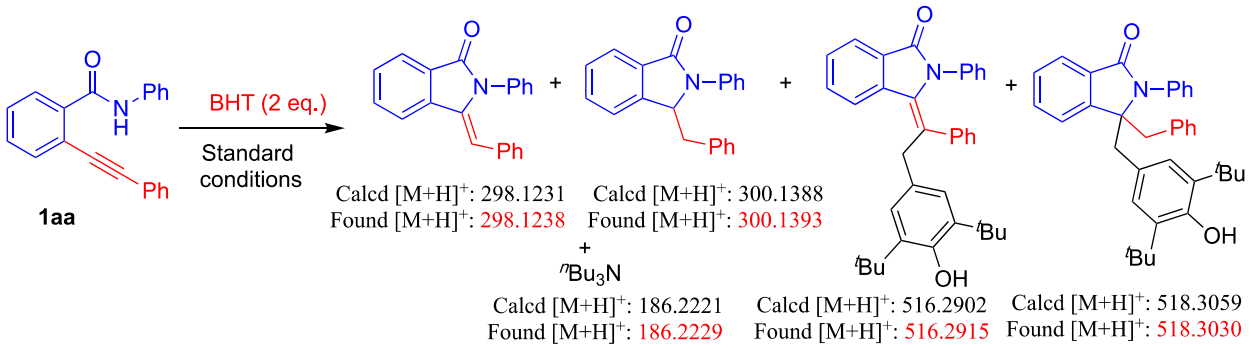
The reaction tube was charged with 2-aminobenzenesulfonamide **3aa** (0.22 mmol, 1 equiv.), 2-(phenylethynyl)benzaldehyde **4aa** (0.22 mmol, 1 equiv.), PTSA (0.04 mmol, 0.2 equiv.), KOAc (0.33 mmol, 1.5 equiv.), ferrocene (20 mol%) and $TBAPF_6$ (0.22 mmol, 1 equiv.) in ACN (8 mL) was electrolyzed with Pt plate as both anode and cathode for 2 h. after that the solvent was evaporated and pure products were isolated by silica column chromatography using 25% ethylacetate in hexanes as solvent gradient afforded intermediate **G** as white solid in 75% yield.

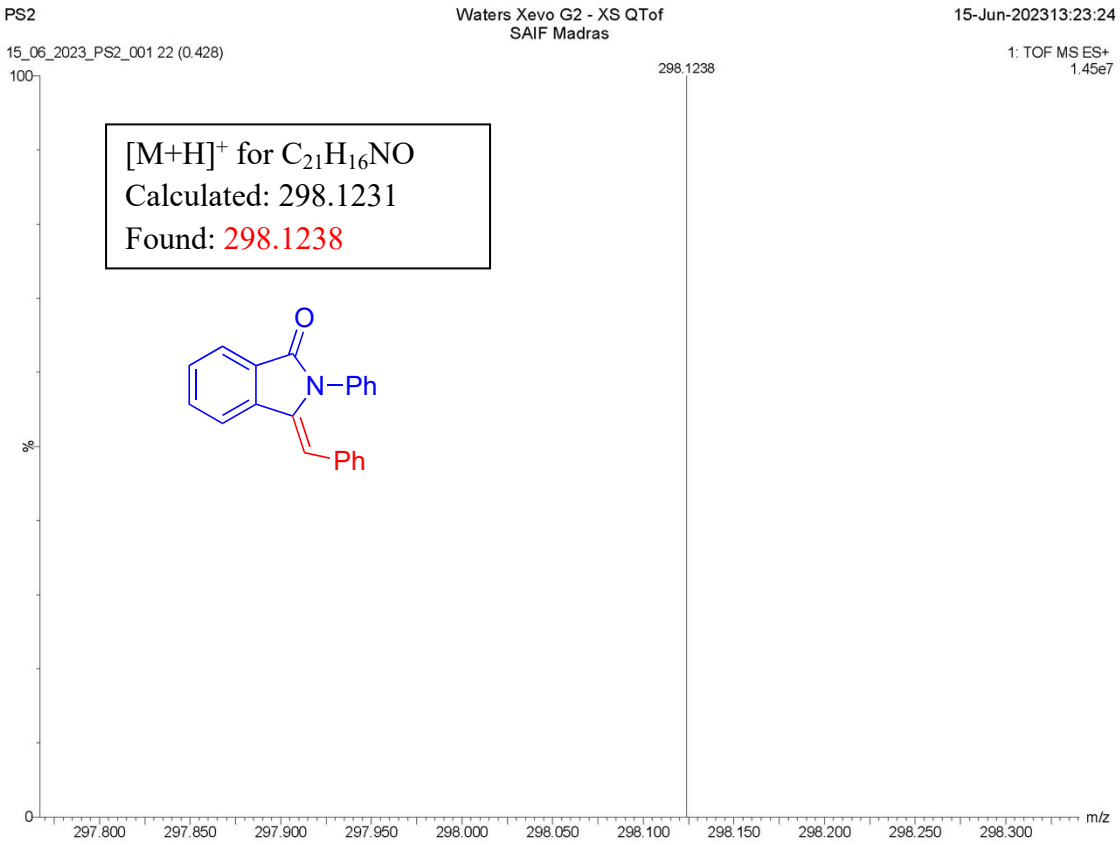
^{1}H NMR (300 MHz, $CDCl_3$): δ_H 10.85 (br s, 1H), 8.35-8.28 (m, 2H), 7.85-7.77 (m, 2H), 7.71-7.68 (m, 1H), 7.64-7.61 (m, 2H), 7.54-7.49 (m, 3H), 7.37 (t, J = 3.3 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 161.7, 151.2, 149.3, 134.7, 133.8, 133.3, 131.7, 131.0, 130.2, 129.3, 129.1, 128.6, 128.0, 127.0, 126.5, 121.7, 121.2, 120.4, 97.0, 86.6.

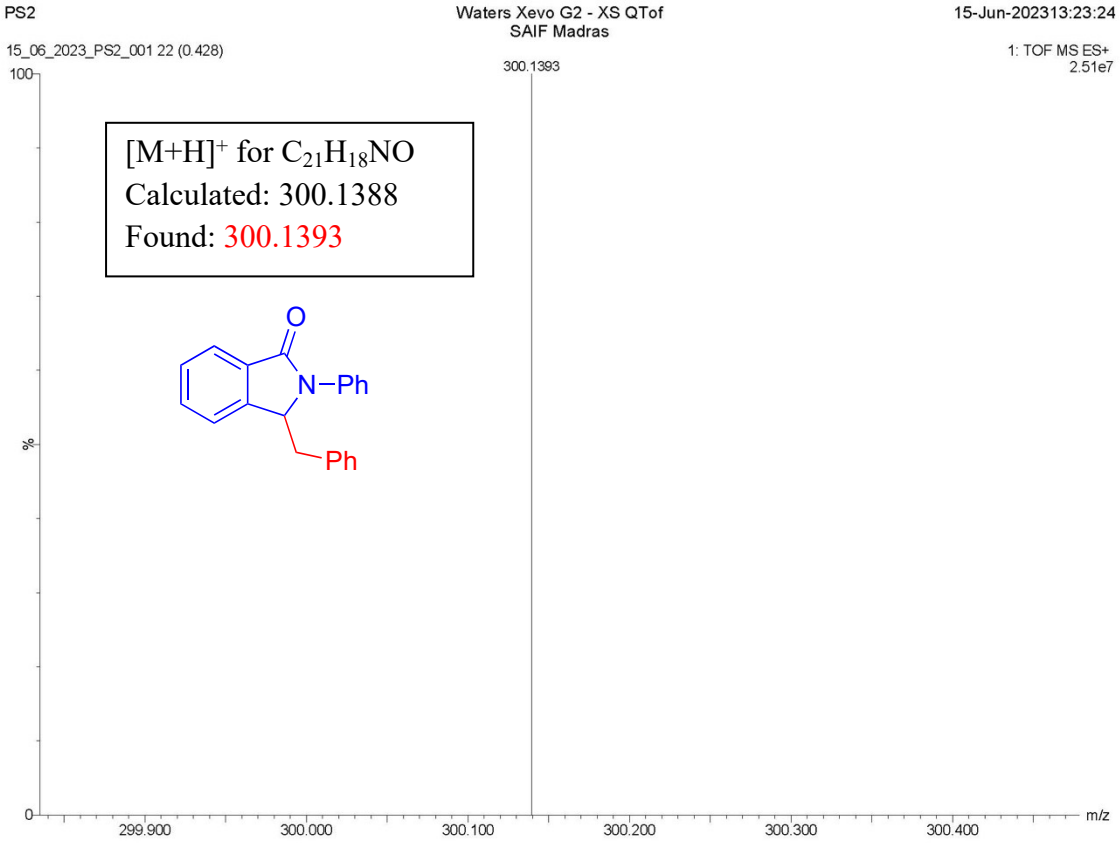
Intermediate trapping experiment by HRMS

To an oven dried reaction vial was charged with **1aa** (0.16 mmol, 1 equiv.), BHT (0.32 mmol, 2.0 equiv.) DIPEA (0.25 mmol, 1.5 equiv.) and $TBAPF_6$ (0.16 mmol, 1 equiv.). The reaction mixture was electrolyzed with Pt plate as both anode and cathode under constant current electrolysis (I = 10 mA) for 1 h and the crude reaction mixture was subjected to HRMS analysis and the results are shown below.

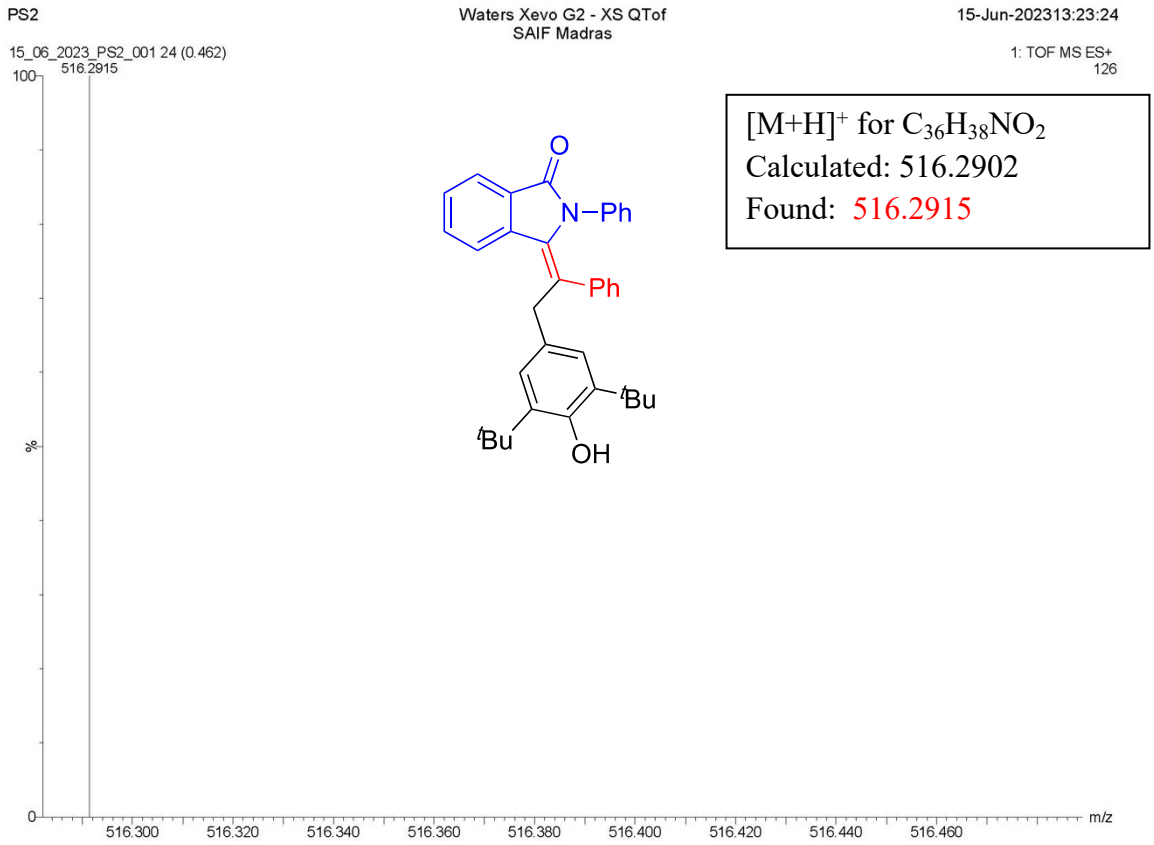




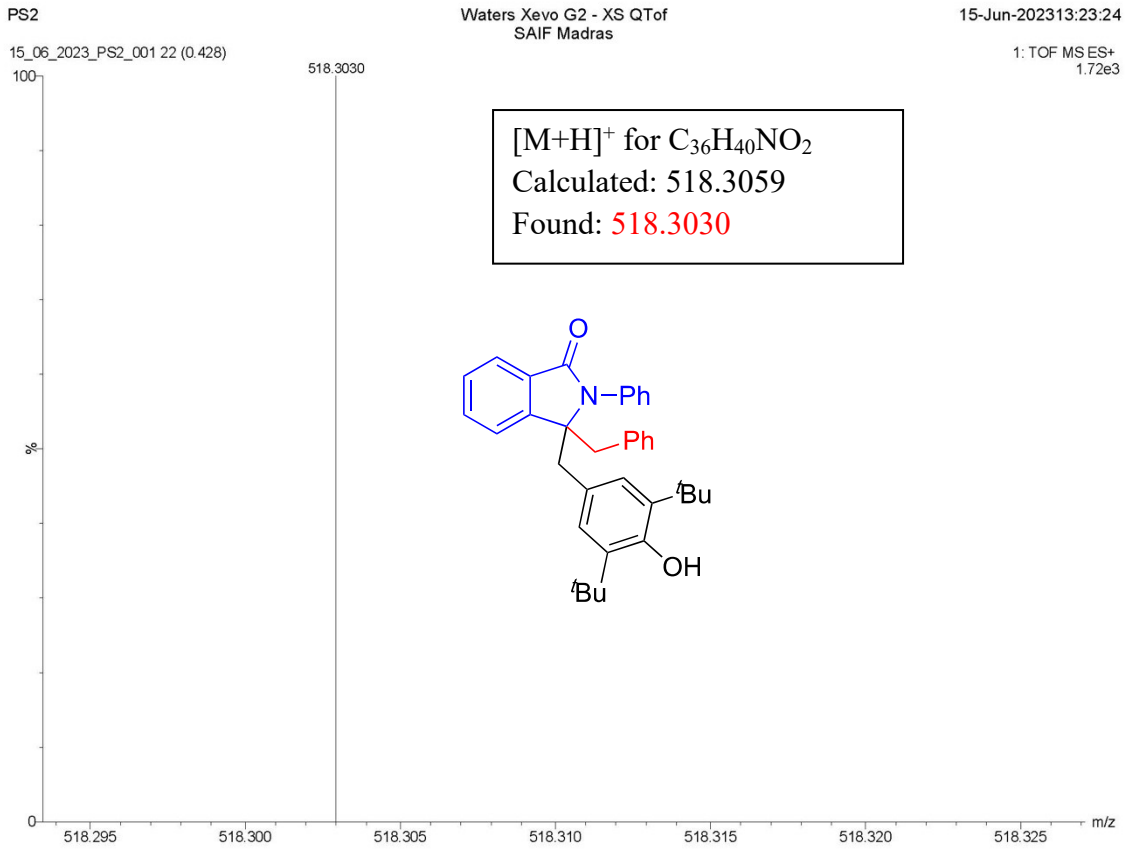
HRMS Spectrum of compound 2aa'



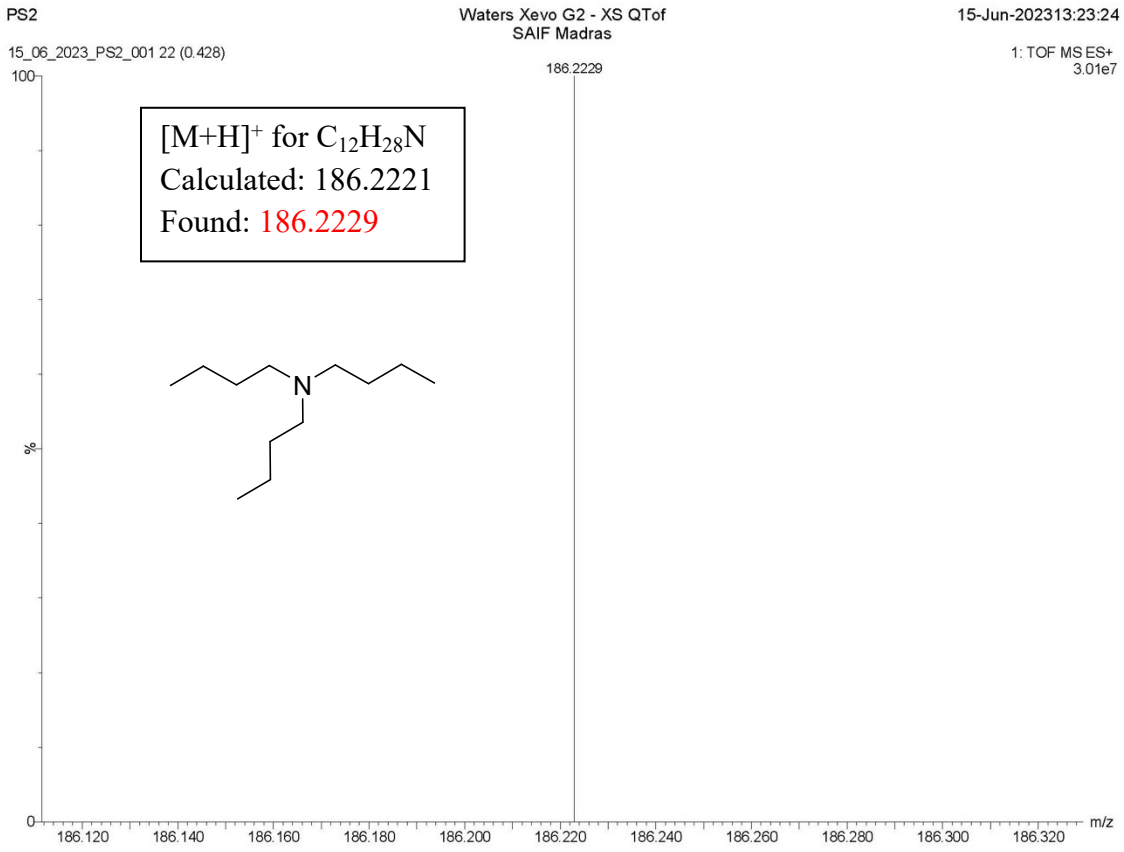
HRMS Spectrum of compound 2aa



HRMS Spectrum of intermediate C withy BHT adduct



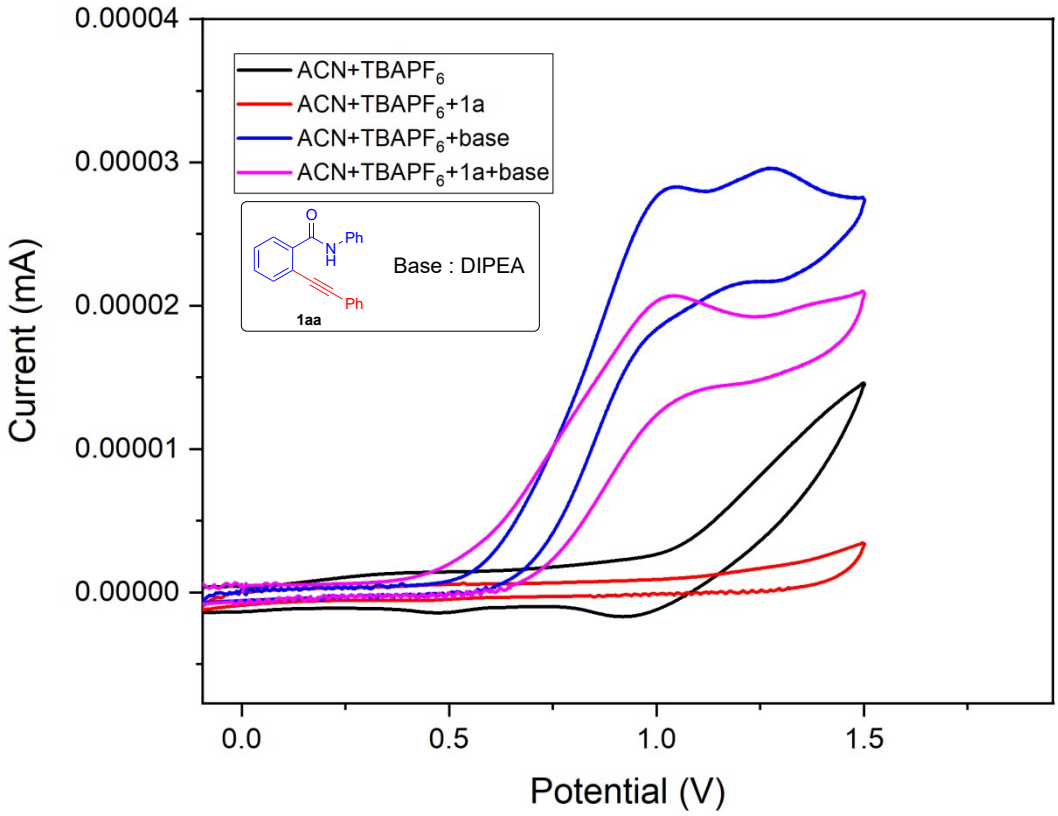
HRMS Spectrum of intermediate E withy BHT adduct



HRMS Spectrum of intermediate K

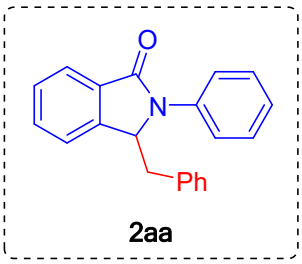
9. CV experiments

Cyclic voltammetry experiments were performed using Metrohm Autolab model AUT51540 (PGSTAT 204) in a three-electrode setup at room temperature. Working, counter and reference electrodes were glassy carbon, Platinum foil and Ag|AgCl electrode. The red curve showed no oxidation and redox peaks. The CV of base DIPEA (blue curve) had two oxidation peaks (1.03 mV and 1.27 mV) and one reduction peak. The pink curve (base+**1a)** showed similar oxidation peak slightly lower potential (1.01 mV) to the base. Therefore, the CV indicates in the presence of base substrate **1a** oxidized by electric current.



10. Spectral data

3-benzyl-2-phenylisoindolin-1-one 2aa[6]



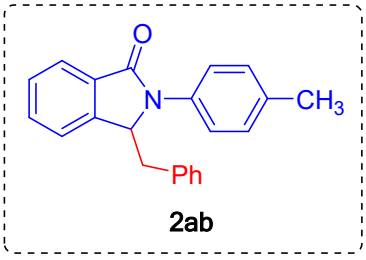
2aa

The title compound **2aa** (42 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. White solid, 83% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.86 (d, *J* = 6.6 Hz, 1H), 7.68 (d, *J*= 7.8 Hz, 2H), 7.52-7.47 (m, 4H), 7.29-7.24 (m, 1H), 7.19-7.15 (m, 3H), 7.12 (d, *J* = 6.6 Hz, 1H), 6.91-6.86 (m, 2H), 5.47 (dd, *J* = 4.5, 5.1 Hz, 1H), 3.40 (dd, *J* = 3.3, 3.6 Hz, 1H), 2.90 (dd, *J* = 8.1, 7.8 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.9, 144.4, 137.7, 135.7, 132.7, 131.4, 129.6, 129.16, 128.4, 128.2, 126.9, 125.3, 124.2, 123.4, 122.9, 61.5, 38.6.

3-benzyl-2-(p-tolyl)isoindolin-1-one 2ab



2ab

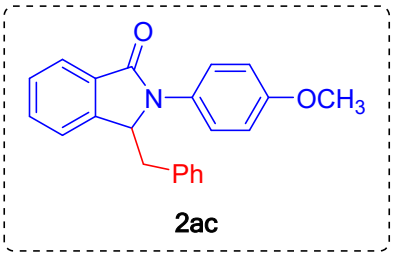
The title compound **2ab** (43 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. White solid, 81% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.84 (d, *J* = 3.9 Hz, 1H), 7.55-7.44 (m, 4H), 7.31-7.27 (m, 2H), 7.18 (d, *J* = 2.7 Hz, 3H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.91 (d, *J* = 1.8 Hz, 2H), 5.42 (dd, *J* = 3.6, 3.3 Hz, 1H), 3.39 (dd, *J* = 3.3, 3.3 Hz, 1H), 2.85 (dd, *J* = 8.4, 8.1 Hz, 1H), 2.41 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.9, 144.1, 135.5, 135.2, 134.7, 132.5, 131.3, 129.8, 129.6, 128.4, 128.2, 126.9, 124.0, 123.4, 122.9, 61.5, 38.3, 20.9.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{20}NO$: 314.1544, Found: 314.1560.

3-benzyl-2-(4-methoxyphenyl)isoindolin-1-one 2ac[7]



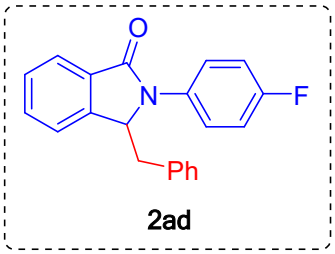
2ac

The title compound **2ac** (43 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. White solid, 78% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.86-7.83 (m, 1H), 7.54-7.44 (m, 4H), 7.27-7.15 (m, 3H), 7.06-7.01 (m, 3H), 6.92-6.85 (m, 2H), 5.36 (dd, *J* = 3.6, 2.7 Hz, 1H), 3.86 (s, 3H), 3.37 (dd, *J* = 3.3, 3.3 Hz, 1H), 2.83 (dd, *J* = 8.1, 8.1 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.8, 157.8, 144.5, 135.9, 132.8, 131.2, 130.7, 129.6, 128.4, 128.2, 126.9, 125.3, 124.1, 122.9, 114.8, 62.0, 55.6, 38.7.

3-benzyl-2-(4-fluorophenyl)isoindolin-1-one 2ad



2ad

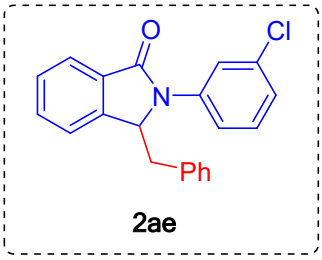
The title compound **2ad** (37 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 69% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.84-7.81 (m, 1H), 7.59-7.55 (m, 2H), 7.48-7.44 (m, 2H), 7.18-7.04-6.85 (m, 6H), 6.84 (dd, *J* = 1.8, 3.3 Hz, 2H), 5.39 (dd, *J* = 3.9, 3.9 Hz, 1H), 3.34 (dd, *J* = 3.9, 3.9 Hz, 1H), 2.87 (dd, *J* = 7.8, 7.8 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.9, 160.2 (d, *J* = 244.1 Hz), 144.0, 135.2, 133.3 (d, *J* = 2.2 Hz), 132.1, 131.5, 129.5, 128.5, 128.2, 126.9, 125.2 (d, *J* = 8.1 Hz), 124.1, 122.9, 115.9 (d, *J* = 22.4 Hz), 61.6, 38.3.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{21}H_{17}FNO$: 318.1294, Found: 318.1296.

3-benzyl-2-(3-chlorophenyl)isoindolin-1-one 2ae[8]



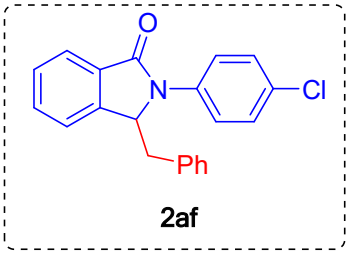
2ae

The title compound **2ae** (40 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. White solid, 71% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.82 (d, *J* = 7.2 Hz, 1H), 7.70 (d, *J* = 1.8 Hz, 1H), 7.58-7.36 (m, 4H), 7.25-7.10 (m, 5H), 6.83 (t, *J* = 1.5 Hz, 2H), 5.42 (dd, *J* = 3.3, 3.3 Hz, 1H), 3.36 (dd, *J* = 3.6, 3.3 Hz, 1H), 2.92 (dd, *J* = 7.5, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.9, 143.9, 138.8, 135.0, 134.9, 132.0, 131.8, 130.0, 129.5, 128.5, 128.2, 127.0, 125.2, 124.2, 123.0, 122.9, 120.9, 61.1, 38.2.

3-benzyl-2-(4-chlorophenyl)isoindolin-1-one 2af



2af

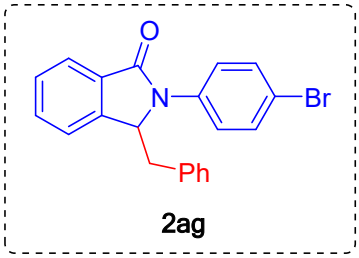
The title compound **2af** (42 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 74% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.84 (d, *J* = 6.9 Hz, 1H), 7.62 (d, 8.7 Hz, 2H), 7.54-7.44 (m, 4H), 7.17-7.12 (m, 4H), 6.84 (d, *J* = 3.9 Hz, 2H), 5.44 (dd, *J* = 3.3, 3.6 Hz, 1H), 3.37 (dd, *J* = 3.3, 3.3 Hz, 1H), 2.93 (dd, *J* = 7.5, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.9, 144.2, 136.3, 135.3, 132.4, 131.7, 130.8, 129.6, 129.3, 128.6, 128.3, 127.0, 124.4, 124.3, 122.9, 61.4, 38.6.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{21}H_{17}ClNO$: 334.0998 , Found:334.0997.

3-benzyl-2-(4-bromophenyl)isoindolin-1-one 2ag



2ag

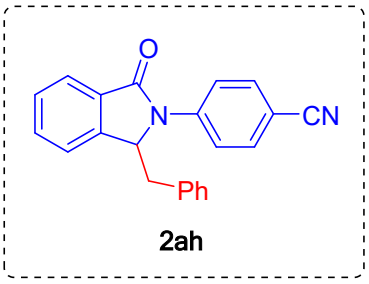
The title compound **2ag** (45 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 71% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.83-7.80 (m, 1H), 7.63-7.42 (m, 6H), 7.15-7.10 (m, 4H), 6.83-6.80 (m, 2H), 5.42 (dd, *J* = 3.6, 3.6 Hz, 1H), 3.35 (dd, *J* = 3.6, 3.6 Hz, 1H), 2.91(dd, *J* = 7.8, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.8, 143.9, 136.4, 134.9, 132.2, 132.1, 131.7, 129.5, 128.5, 128.2, 127.0, 124.5, 124.1, 122.9, 118.3, 61.1, 38.1.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{21}H_{17}BrNO$: 378.0493, Found: 378.0480.

4-(1-benzyl-3-oxoisoindolin-2-yl)benzonitrile 2ah



2ah

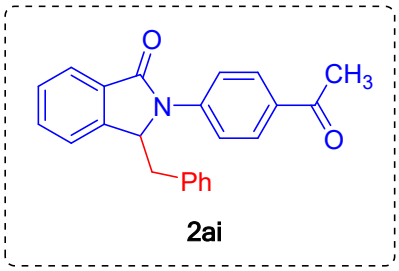
The title compound **2ah** (36 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 66% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.87-7.82 (m, 3H), 7.75 (d, *J* = 8.7 Hz, 2H), 7.59-7.46 (m, 2H), 7.27-7.13 (m, 4H), 6.77 (d, *J* = 6.6 Hz, 2H), 5.53 (dd, *J* = 3.6, 3.6 Hz, 1H), 3.38 (dd, *J* = 3.3, 3.3 Hz, 1H), 3.02 (dd, *J* = 7.5, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 167.1, 143.8, 141.6, 134.4, 133.1, 132.3, 131.6, 129.4, 128.8, 128.3, 127.2, 124.4, 122.9, 122.1, 118.6, 107.9, 60.6, 38.1.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{17}N_2O$: 325.1340, Found: 325.1349.

2-(4-acetylphenyl)-3-benzylisoindolin-1-one 2ai



2ai

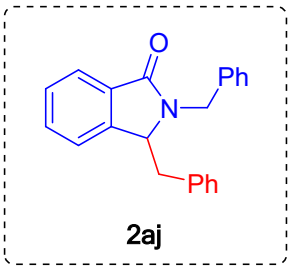
The title compound **2ai** (35 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. White solid, 61% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.10 (d, *J* = 9 Hz, 2H), 7.86-7.83 (m, 3H), 7.56-7.45 (m, 2H), 7.19-7.11 (m, 4H), 6.81-6.79 (m, 2H), 5.55 (dd, *J* =3.6, 3.6 Hz, 1H), 3.41 (dd, *J* = 3.3, 3.3 Hz, 1H), 3.00 (dd, *J* = 7.5, 7.5 Hz, 1H), 2.64 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 196.8, 167.1, 143.8, 141.8, 134.7, 133.5, 132.1, 132.0, 129.5, 128.7, 128.2, 127.1, 124.3, 122.9, 121.8, 60.8, 38.1, 26.3.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{23}H_{20}NO_2$: 342.1494, Found: 342.1490.

2,3-dibenzylisoindolin-1-one 2aj[6]



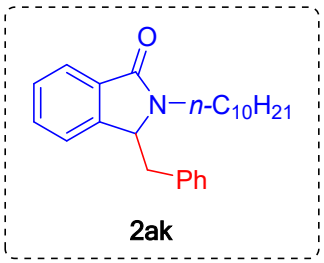
2aj

The title compound **2aj** (37 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Colorless yellow liquid, 70% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.85 (d, *J* = 6.0 Hz, 1H), 7.40-7.25 (m, 10 H), 7.04-6.96 (m, 1H), 6.89 (d, *J* = 6.0 Hz, 1H), 5.46 (d, *J* = 15 Hz, 1H), 4.61 (d, *J* = 9.6 Hz, 1H), 4.24 (d, *J* = 14.7 Hz, 1H), 3.40 (t, *J* = 12.3 Hz, 1H), 2.85 (dd, *J* = 7.8, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.4, 145.4, 137.5, 136.4, 132.4, 131.0, 129.5, 128.8, 128.5, 128.2, 128.1, 127.6, 127.0, 123.9, 122.9, 59.9, 44.6, 38.8.

3-benzyl-2-(4-decylphenyl)isoindolin-1-one 2ak



2ak

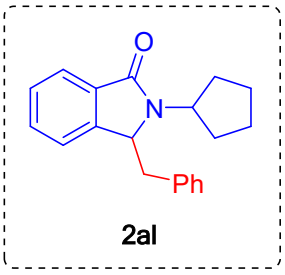
The title compound **2ak** (48 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Yellow liquid, 78% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.76-7.74 (m, 1H), 7.38-7.35 (m, 2H), 7.25-7.21 (m, 3H), 7.08-7.06 (m, 2H), 6.93-6.90 (m, 1H), 4.77 (dd, *J* = 4.8, 4.8 Hz, 1H), 4.08-3.98 (m, 1H), 3.36 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.23-3.14 (m, 1H), 2.83 (dd, *J* = 7.8, 7.8 Hz, 1H), 1.62 (t, *J* = 8.1 Hz, 2H), 1.30-1.26 (m, 14H), 0.87 (t, *J* = 6.3 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.1, 144.8, 136.1, 132.5, 130.6, 129.4, 128.4, 128.0, 126.9, 123.5, 122.7, 60.0, 40.3, 38.5, 31.8, 29.4, 29.3, 29.2, 28.3, 26.9, 22.5, 13.9.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{25}H_{34}NO$: 364.2640, Found: 364.2642.

3-benzyl-2-cyclopentylisoindolin-1-one 2al



2al

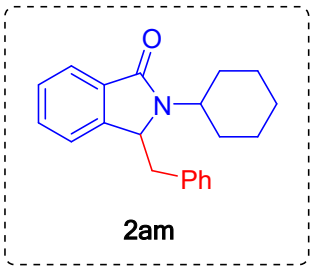
The title compound **2al** (37 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Colorless liquid, 76% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.65 (d, *J* = 7.2 Hz, 1H), 7.29-7.17 (m, 5H), 7.02 (d, *J* = 7.5 Hz, 2H), 6.62 (d, *J* = 7.2 Hz, 1H), 4.67 (dd, *J* = 4.2, 4.2 Hz, 1H), 4.06 (dd, *J* = 8.4, 8.7 Hz, 1H), 3.43 (dd, *J* = 4.2, 3.9 Hz, 1H), 2.63 (dd, *J* = 9.0, 8.7 Hz, 1H), 1.97-1.86 (m, 6H), 1.55 (d, *J* = 5.4 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.3, 145.3, 136.7, 133.5, 130.4, 129.6, 128.5, 128.0, 127.0, 123.3, 122.8, 62.2, 56.1, 40.4, 30.3, 29.9, 24.6.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{20}H_{22}NO$: 292.1701, Found: 292.1700.

3-benzyl-2-cyclohexylisoindolin-1-one 2am[6]



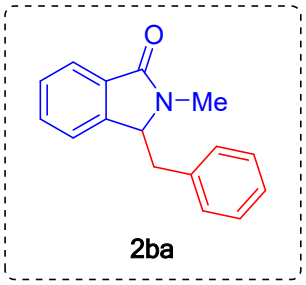
2am

The title compound **2am** (40 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Colorless liquid, 78% yield (Solvent gradient: 5% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.76 (d, *J* = 7.2 Hz, 1H), 7.38-7.26 (m, 5H), 7.15 (d, *J* = 7.5 Hz, 2H), 6.59 (d, *J* = 7.5 Hz, 1H), 4.78 (dd, *J* = 4.5, 4.5 Hz, 1H), 3.77 (d, *J* = 3.3 Hz 1H), 3.58 (dd, *J* = 4.5, 4.5 Hz, 1H), 2.64 (dd, *J* = 9.3, 9.0 Hz, 1H), 2.25-2.17 (m, 1H), 1.98-1.84 (m, 3H), 1.71 (d, *J* = 11.1 Hz, 2H), 1.42-1.26 (m, 4H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.3, 145.1, 136.8, 132.9, 130.4, 129.4, 128.5, 127.9, 126.9, 123.2, 122.8, 61.0, 54.3, 40.6, 31.3, 30.8, 26.3, 26.1, 25.5.

3-benzyl-2-methylisoindolin-1-one 2ba[6]



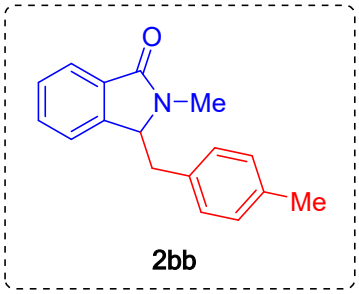
2ba

The title compound **2ba** (36 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Colorless liquid, 90% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.78-7.76 (m, 1H), 7.41-7.38 (m, 2H), 7.27-7.22 (m, 3H), 7.09-7.06 (m, 2H), 7.01-6.97 (m, 1H), 4.66 (t, *J* = 5.4 Hz, 1H), 3.35 (dd, *J* = 4.2, 4.2 Hz, 1H), 3.13 (s, 3H), 2.93 (dd, *J* = 7.5, 6.9 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.3, 145.0, 136.3, 132.7, 130.7, 129.4, 128.5, 128.1, 127.0, 123.5, 122.6, 62.8, 38.9, 27.9.

2-methyl-3-(4-methylbenzyl)isoindolin-1-one 2bb[9]



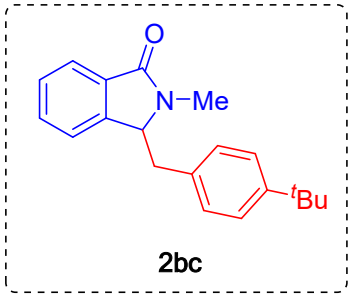
2bb

The title compound **2bb** (38 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow semisolid, 89% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.76-7.73 (m, 1H), 7.3 (t, *J* = 3.6 Hz, 2H), 7.06-6.93 (m, 5H), 4.62 (dd, *J* = 4.8, 5.1 Hz, 1H), 3.30 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.11 (s, 3H), 2.86 (dd, *J* = 7.5, 7.5 Hz, 1H), 2.30 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.4, 144.9, 136.5, 132.8, 132.4, 130.7, 129.2, 129.1, 128.0, 123.4, 122.6, 62.8, 38.1, 27.9, 20.9.

3-(4-(tert-butyl)benzyl)-2-methylisoindolin-1-one 2bc



2bc

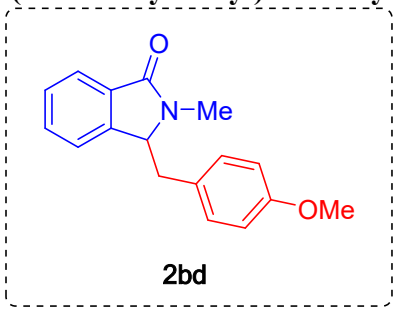
The title compound **2bc** (43 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 86% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.67 (d, *J* = 6.3 Hz, 1H), 7.31-7.28 (m, 2H), 7.20-7.12 (m, 2H), 6.89 (d, *J* = 8.4 Hz, 3H), 4.54 (s, 1H), 3.23 (dd, *J* = 8.1, 5.4 Hz, 1H), 3.05-2.98 (m, 3H), 2.79 (dd, *J* = 10.2, 7.5 Hz, 1H), 1.22-1.13 (m, 9H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.5, 149.9, 144.9, 132.8, 132.3, 130.8, 129.1, 128.1, 125.3, 123.4, 122.7, 62.7, 38.0, 34.4, 31.3, 28.0.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{20}H_{24}NO$: 294.1857, Found: 294.1860.

3-(4-methoxybenzyl)-2-methylisoindolin-1-one 2bd



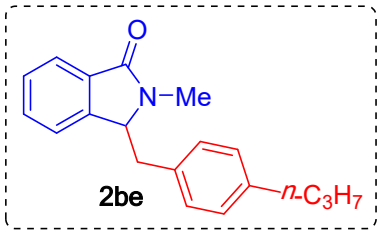
2bd

The title compound **2bd** (41 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 90% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.76-7.73 (m, 1H), 7.39 (t, *J* = 3.3 Hz, 2H), 7.01-6.93 (m, 3H), 6.76 (d, *J* = 8.4 Hz, 2H), 4.60 (dd, *J* = 4.8, 5.1 Hz, 1H), 3.75 (s, 3H), 3.30 (dd, *J* = 4.8, 4.5 Hz, 1H), 3.13 (s, 3H), 2.84 (dd, *J* = 7.5, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.5, 158.5, 144.7, 132.3, 130.8, 130.4, 128.1, 127.7, 123.3, 122.7, 113.8, 62.8, 55.1, 37.5, 28.0.

2-methyl-3-(4-propylbenzyl)isoindolin-1-one 2be



2be

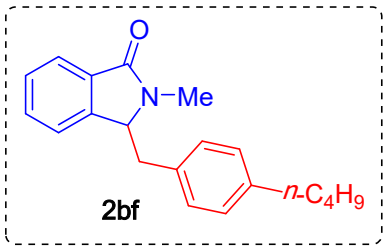
The title compound **2be** (39 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 82% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.76 (t, *J* = 4.5 Hz, 1H), 7.40-7.37 (m, 2H), 7.06 (d, *J* = 7.8 Hz, 2H), 6.98 (d, *J* = 7.8 Hz, 3H), 4.63 (dd, *J* = 5.4, 5.1 Hz, 1H), 3.33 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.13 (s, 3H), 2.85 (dd, *J* = 7.8, 8.1 Hz, 1H), 2.54 (t, *J* = 7.8 Hz, 2H), 1.67-1.55 (m, 2H), 0.94-0.89 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.4, 144.8, 141.4, 133.1, 132.3, 130.8, 129.3, 128.5, 128.1, 123.4, 122.7, 62.8, 38.2, 37.5, 28.0, 24.4, 13.7.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{19}H_{22}NO$: 280.1701, Found: 280.1705.

3-(4-butylbenzyl)-2-methylisoindolin-1-one 2bf



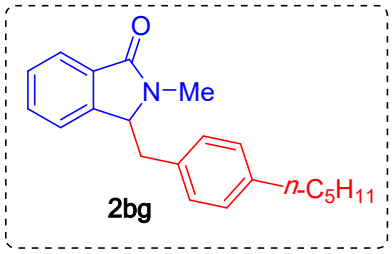
The title compound **2bf** (42 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 84% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.77-7.75 (m, 1H), 7.40-7.38 (m, 2H), 7.08-6.96 (m, 5H), 4.63 (t, *J* = 6.6 Hz, 1H), 3.33 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.13 (s, 3H), 2.85 (dd, *J* = 7.8, 7.8 Hz, 1H), 2.57 (t, *J* = 7.5 Hz, 2H), 1.59-1.52 (m, 2H), 1.37-1.25 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H)

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.5, 144.8, 141.6, 133.0, 132.3, 130.8, 129.3, 128.5, 128.1, 123.4, 122.7, 62.8, 38.2, 35.2, 33.5, 28.0, 22.3, 13.9.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{20}H_{24}NO$: 294.1857, Found: 294.1859.

2-methyl-3-(4-pentylbenzyl)isoindolin-1-one 2bg



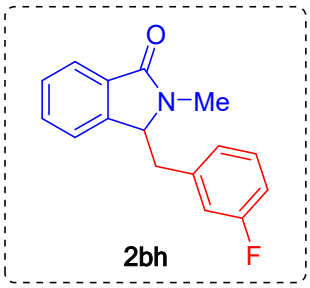
The title compound **2bg** (44 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 84% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.79-7.76 (m, 1H), 7.42-7.38 (m, 2H), 7.11-7.06 (m, 2H), 7.01-6.96 (m, 3H), 4.64 (dd, *J* = 5.1, 4.8 Hz, 1H), 3.32 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.13 (s, 3H), 2.88 (dd, *J* = 7.5, 7.5 Hz, 1H), 2.57 (t, 7.2 Hz, 2H), 1.63-1.58 (m, 2H), 1.36-1.28 (m, 4H), 0.90 (t, *J* = 6 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.3, 145.2, 141.8, 133.4, 132.7, 130.7, 129.3, 128.5, 128.0, 123.5, 122.7, 62.9, 38.6, 35.5, 31.4, 30.8, 27.9, 22.4, 13.7.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{21}H_{26}NO$: 308.2014, Found: 308.2013.

3-(3-fluorobenzyl)-2-methylisoindolin-1-one 2bh



2bh

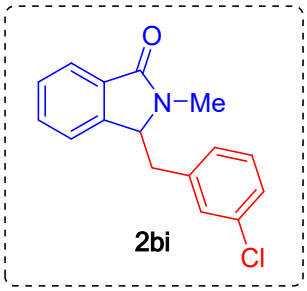
The title compound **2bh** (32 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 76% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.70-7.67 (m, 1H), 7.36-7.32 (m, 2H), 7.19-7.10 (m, 1H), 6.96-6.93 (m, 1H), 6.86-6.81 (m, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.70-6.66 (m, 1H), 4.58 (dd, *J* = 5.2, 4.8 Hz, 1H), 3.27 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.06 (s, 3H), 2.86 (dd, *J* = 7.3, 7.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ_C 168.5, 162.6 (d, *J* = 247.2 Hz), 144.3, 138.3 (d, *J* = 7.3 Hz), 132.2, 131.0, 129.9 (d, *J* = 8.3 Hz), 128.3, 125.1 (d, *J* = 2.3 Hz), 123.5, 122.5, 116.3 (d, *J* = 21.4 Hz), 114.0 (d, *J* = 21.0 Hz), 113.9, 62.4, 38.1, 28.0.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{16}H_{14}FNO$: 256.1137 , Found: 256.1132.

3-(3-chlorobenzyl)-2-methylisoindolin-1-one 2bi



2bi

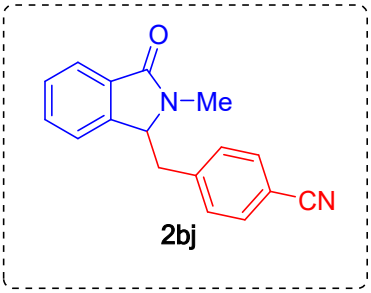
The title compound **2bi** (37 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 80% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.78-7.76 (m, 1H), 7.44-7.41 (m, 2H), 7.22-7.15 (m, 2H), 7.06 (d, *J* = 2 Hz, 1H), 7.02-7.00 (m, 1H), 6.94-6.91 (m, 1H), 4.65 (dd, *J* = 5.2, 4.8 Hz, 1H), 3.33 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.14 (s, 3H), 2.91 (dd, *J* = 7.6, 7.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ_C 168.4, 144.3, 137.9, 134.3, 132.3, 131.0, 129.7, 129.5, 128.4, 127.6, 127.3, 123.6, 122.6, 62.4, 38.1, 28.1.

HRMS (ESI) m/z: $[M]^+$ calculated for $C_{16}H_{13}ClNO$: 271.0763 , Found: 271.0736

4-((2-methyl-3-oxoisoindolin-1-yl)methyl)benzonitrile 2bj



2bj

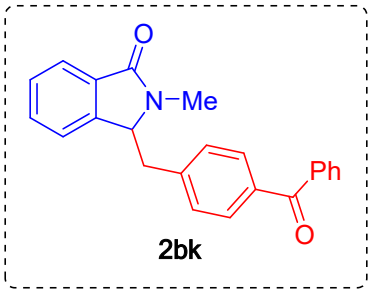
The title compound **2bj** (32 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Yellow oily liquid, 73% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.75-7.73 (m, 1H), 7.50-7.40 (m, 4H), 7.11-7.07 (m, 3H), 4.72-4.68 (m, 1H), 3.38 (dd, *J* = 4.2, 4.2 Hz, 1H), 3.15 (s, 3H), 3.12-3.07 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.3, 143.8, 141.1, 132.4, 132.0, 131.1, 130.1, 128.5, 123.7, 122.3, 118.3, 111.1, 61.9, 38.1, 27.9.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{17}H_{15}N_2O$: 263.1184, Found: 263.1195.

3-(4-benzoylbenzyl)-2-methylisoindolin-1-one 2bk



2bk

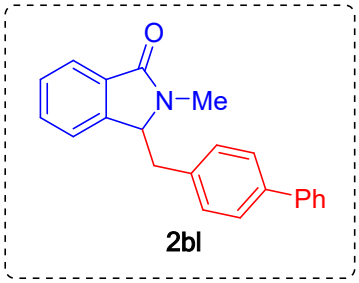
The title compound **2bk** (41 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 71% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.79-7.69 (m, 5H), 7.59-7.57 (m, 1H), 7.51-7.42 (m, 4H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.10-7.07 (m, 1H), 4.74 (dd, *J* = 5.1, 4.8 Hz, 1H), 3.45 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.18 (s, 3H), 3.10 (dd, *J* = 6.0, 2.4 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 196.1, 168.4, 144.4, 140.8, 137.7, 136.4, 132.4, 132.3, 131.1, 130.3, 129.9, 129.4, 128.4, 128.3, 123.7, 122.5, 62.4, 38.4, 28.1.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{23}H_{20}NO_2$: 342.1494, Found: 342.1493.

3-([1,1'-biphenyl]-4-ylmethyl)-2-methylisoindolin-1-one 2bl



2bl

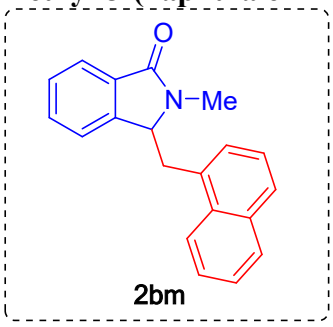
The title compound **2bl** (43 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. White solid, 82% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.79 (d, *J* = 4.8 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 2H), 7.51-7.34 (m, 7H), 7.15 (d, *J* = 7.5 Hz, 2H), 7.07 (d, *J* = 6.9 Hz, 1H), 4.70 (t, *J* = 5.1Hz, 1H), 3.41 (dd, *J* = 4.8, 4.8 Hz, 1H), 3.18 (s, 3H), 2.97 (dd, *J* = 7.5, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.3, 144.7, 140.5, 139.8, 134.9, 132.3, 130.8, 129.7, 128.6, 128.1, 127.2, 127.0, 126.8, 123.4, 122.6, 62.6, 38.1, 27.9.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{20}NO$: 314.1544, Found: 314.1547.

2-methyl-3-(naphthalen-1-ylmethyl)isoindolin-1-one 2bm



2bm

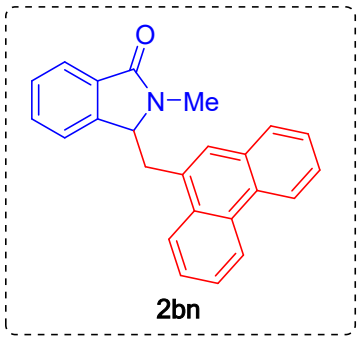
The title compound **2bm** (35 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Yellow liquid, 71% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.05 (d, *J* = 7.5 Hz, 1H), 7.93 (t, *J* = 6.9 Hz, 1H), 7.87-7.84 (m, 2H), 7.59-7.52 (m, 2H), 7.48-7.38 (m, 2H), 7.29 (t, *J* = 6.0 Hz, 2H), 6.61 (d, *J* = 7.5 Hz, 1H), 4.83 (t, *J* = 7.8Hz, 1H), 3.8 (dd, *J* = 5.7, 5.7 Hz, 1H), 3.16 (s, 3H), 3.12-3.01 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.4, 145.0, 133.9, 132.6, 132.0, 131.8, 130.6, 129.1, 128.5, 128.1, 128.0, 126.3, 125.8, 125.3, 123.4, 123.1, 61.9, 36.9, 28.25.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{20}H_{18}NO$: 288.1388, Found: 288.1392.

2-methyl-3-(phenanthren-9-ylmethyl)isoindolin-1-one 2bn



2bn

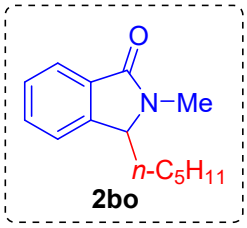
The title compound **2bn** (37 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 64% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.83 (d, J = 7.8 Hz, 1H), 8.74 (d, J = 8.1 Hz, 1H), 8.15 (d, J = 7.5 Hz, 1H), 7.89-7.82 (m, 2H), 7.76-7.59 (m, 5H), 7.42 (t, J = 7.2 Hz, 1H), 7.27 (s, 1H), 6.79 (d, J = 7.5 Hz, 1H), 4.94 (dd, J = 6.6, 6.0 Hz, 1H), 3.92 (dd, J = 5.7, 5.7 Hz, 1H), 3.19 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.5, 145.3, 132.2, 131.4, 131.1, 130.9, 130.8, 130.2, 129.3, 128.3, 128.2, 127.1, 127.0, 126.9, 126.7, 123.9, 123.7, 123.6, 123.2, 122.6, 61.7, 37.7, 28.4.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{24}H_{20}NO$: 338.1544, Found: 338.1554.

2-methyl-3-pentylisoindolin-1-one 2bo



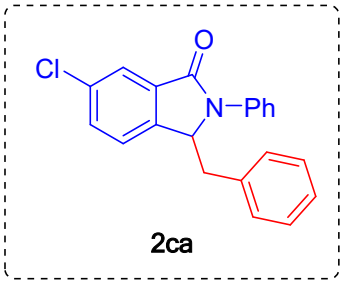
2bo

The title compound **2bo** (11 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Yellow liquid, 32% yield (Solvent gradient: 15% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.82 (d, J = 7.5 Hz, 1H), 7.54-7.49 (m, 1H), 7.46-7.39 (m, 2H), 4.48 (t, J = 4.2 Hz, 1H), 3.10 (s, 3H), 2.01-1.92 (m, 2H), 1.25-1.19 (m, 6H), 0.81 (t, J = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 168.6, 145.1, 132.8, 131.1, 127.9, 123.4, 121.8, 61.5, 31.7, 30.5, 27.2, 22.4, 22.0, 13.9.

3-benzyl-6-chloro-2-phenylisoindolin-1-one 2ca



2ca

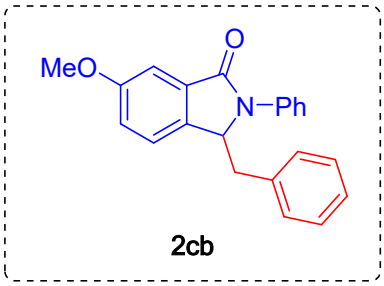
The title compound **2ca** (35 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 63% yield (Solvent gradient: 2% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.85-7.83 (m, 1H), 7.66 (d, *J* = 7.8 Hz, 2H), 7.52-7.45 (m, 4H), 7.17-7.16 (m, 3H), 7.07 (d, *J* = 6.9 Hz, 1H), 6.88-6.85 (m, 2H), 5.47 (dd, *J* = 3.6, 3.6 Hz, 1H), 3.39 (dd, *J* = 3.3, 3.6 Hz, 1H), 2.87 (dd, *J* = 8.1, 8.1 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 167.0, 144.0, 137.1, 135.2, 132.3, 131.5, 129.6, 129.2, 128.4, 128.2, 126.9, 125.4, 124.1, 123.3, 122.9, 61.3, 38.1.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{21}H_{17}ClNO$: 334.0998, Found: 334.0993.

3-benzyl-6-methoxy-2-phenylisoindolin-1-one 2cb



2cb

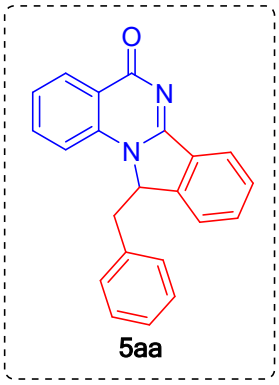
The title compound **2cb** (42 mg) was prepared by following general procedure D. Pure product was isolated using silica column chromatography. Pale yellow liquid, 75% yield (Solvent gradient: 2% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.57-7.54 (m, 2H), 7.43-7.38 (m, 2H), 7.23-7.15 (m, 2H), 7.09-7.07 (m, 3H), 6.95 (dd, *J* = 2.4, 2.4 Hz, 1H), 6.79-6.77 (m, 3H), 5.30 (dd, *J* = 3.6, 3.3 Hz, 1H), 3.75 (s, 3H), 3.26 (dd, *J* = 3.6, 3.3 Hz, 1H), 2.72 (dd, *J* = 8.1, 8.1 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 166.9, 160.2, 137.2, 136.3, 135.4, 133.6, 129.6, 129.2, 128.2, 126.9, 125.4, 123.3, 120.1, 106.4, 60.9, 55.6, 38.2.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{20}NO_2$: 330.1494, Found: 330.1496.

11-benzylisoindolo[2,1-a]quinazolin-5(11H)-one 5aa



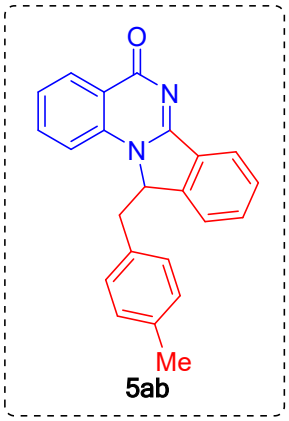
The title compound **5aa** (41 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 58% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.41 (d, J = 7.5 Hz, 1H), 8.02 (d, J = 7.5 Hz, 1H), 7.81 (t, J = 7.2 Hz, 1H), 7.58-7.45 (m, 4H), 7.22-7.05 (m, 4H), 6.70 (d, J = 7.2 Hz, 2H), 5.72 (dd, J = 3.0, 2.7 Hz, 1H), 3.69 (dd, J = 2.7, 3.0 Hz, 1H), 3.25 (dd, J = 7.5, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 170.3, 160.4, 143.6, 138.3, 133.6, 133.3, 132.5, 132.3, 129.8, 129.3, 129.2, 128.4, 127.5, 125.6, 124.5, 122.8, 119.6, 114.4, 63.5, 39.0.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{17}N_2O$: 325.1340, Found: 325.1350.

11-(4-methylbenzyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5ab



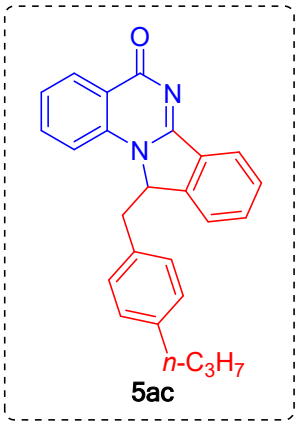
The title compound **5ab** (38 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 51% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.44 (d, *J* = 8.1 Hz, 1H), 8.07 (d, *J* = 7.2 Hz, 1H), 7.86-7.80 (m, 1H), 7.59-7.48 (m, 5H), 6.89 (d, *J* = 7.8 Hz, 2H), 6.58 (d, *J* = 8.1 Hz, 2H), 5.71 (dd, *J* = 2.7, 2.7 Hz, 1H), 3.66 (dd, *J* = 2.7, 3 Hz, 1H), 3.24 (dd, *J* = 7.5, 7.5 Hz, 1H), 2.23 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 170.7, 160.5, 143.7, 138.3, 137.3, 133.9, 132.5, 132.2, 129.9, 129.7, 129.4, 129.2, 129.1, 125.8, 124.5, 122.9, 119.4, 114.6, 63.7, 38.5, 21.0.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{23}H_{19}N_2O$: 339.1497, Found: 339.1495

11-(4-propylbenzyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5ac



5ac

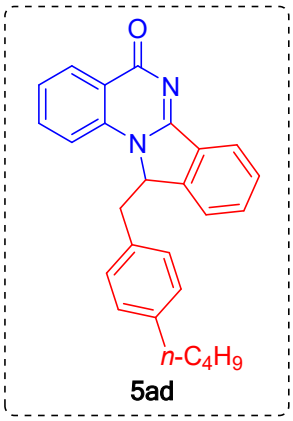
The title compound **5ac** (43 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 53% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.44 (dd, *J* = 1.2, 1.2 Hz, 1H), 8.06 (d, *J* = 7.2 Hz, 1H), 7.81-7.79 (m, 1H), 7.57-7.54 (m, 2H), 7.52-7.48 (m, 2H), 7.20 (d, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.64 (d, *J* = 8.0 Hz, 2H), 5.70 (dd, *J* = 3.2, 3.2 Hz, 1H), 3.68 (dd, *J* = 3.2, 3.2 Hz, 1H), 3.20 (dd, *J* = 8.0, 8.0 Hz, 1H), 2.47 (t, *J* = 7.6 Hz, 2H), 1.57-1.52 (m, 2H), 0.86 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ_C 170.6, 160.4, 143.8, 142.1, 138.3, 133.8, 132.4, 130.4, 129.8, 129.3, 129.1, 128.6, 125.7, 124.5, 122.9, 119.5, 114.5, 63.6, 38.6, 37.5, 24.3, 13.7.

HRMS (ESI) m/z: $[M+H]^+$ calculated for m/z $C_{25}H_{23}N_2O$: 367.1810 , Found: 367.1802.

11-(4-butylbenzyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5ad



5ad

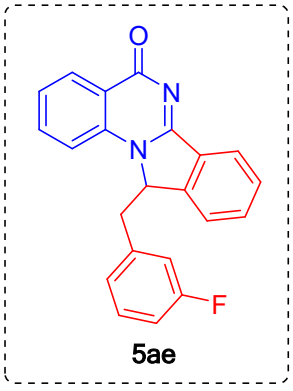
The title compound **5ad** (49 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 58% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ_H 8.39 (d, *J* = 8 Hz, 1H), 8.01 (d, *J* = 7.5 Hz, 1H), 7.79 (t, *J* = 7.5 Hz, 1H), 7.56-7.52 (m, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.19 (d, *J* = 7.5 Hz, 1H), 6.89 (d, *J* = 7.5 Hz, 2H), 6.61 (d, *J* = 7.5 Hz, 2H), 5.69 (d, *J* = 5 Hz, 1H), 3.65 (dd, *J* = 2.5, 1.5 Hz, 1H), 3.18 (dd, *J* = 8, 7.5 Hz, 1H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.52-1.46 (m, 2H), 1.29-1.25 (m, 2H), 0.88 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ_C 170.5, 160.3, 143.8, 142.2, 138.2, 133.8, 132.4, 132.2, 130.3, 129.6, 129.2, 129.1, 128.5, 125.7, 124.4, 122.9, 119.4, 114.7, 63.6, 38.5, 35.1, 33.3, 22.2, 13.9.

HRMS (ESI) m/z: $[M+H]^+$ m/z calculated for $C_{26}H_{25}N_2O$: 381.1966, Found: 381.1960.

11-(3-fluorobenzyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5ae



5ae

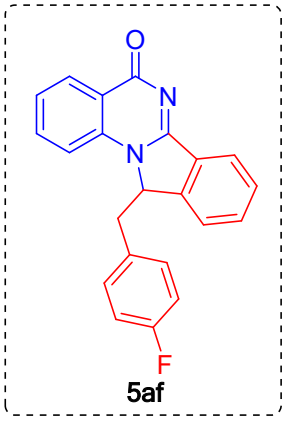
The title compound **5ae** (42 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 56% yield (Solvent gradient: 60% ethylacetate in hexanes)

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.34 (d, *J* = 7.8 Hz, 1H), 7.95 (d, *J* = 7.5 Hz, 1H), 7.78 (t, *J* = 7.8 Hz, 1H), 7.58-7.53 (m, 2H), 7.47-7.40 (m, 2H), 7.26 (d, *J* = 7.5 Hz, 1H), 7.04-6.97 (m, 1H), 6.80 (t, *J* = 8.1 Hz, 1H), 6.42-6.33 (m, 2H), 5.73 (dd, *J* = 2.4, 2.4 Hz, 1H), 3.64 (dd, *J* = 1.5, 1.5 Hz, 1H), 3.30 (dd, *J* = 7.2, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 170.3, 162.3 (d, *J* = 245.4 Hz), 160.2, 143.3, 138.1, 135.5 (d, *J* = 7.3 Hz), 133.9, 132.6, 132.2, 129.9 (d, *J* = 8.2 Hz), 129.5 (d, *J* = 11.8 Hz), 125.7, 124.94 (d, *J* = 2.7 Hz), 124.3, 122.8, 119.2, 116.2 (d, *J* = 21.4 Hz), 114.6, 114.5, 114.3, 63.1, 38.3.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{16}FN_2O$: 343.1246, Found: 343.1246.

11-(4-fluorobenzyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5af



5af

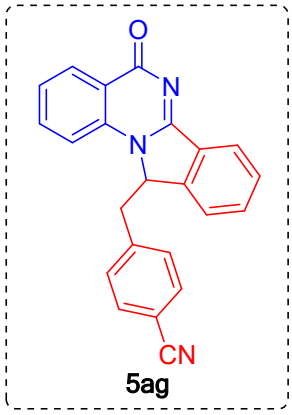
The title compound **5af** (41 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 54% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.44 (d, *J* = 7.8 Hz, 1H), 8.04 (d, *J* = 6.0 Hz, 1H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.62-7.49 (m, 4H), 7.29 (t, *J* = 7.2 Hz, 1H), 6.74 (t, *J* = 8.7 Hz, 2H), 6.60-6.56 (m, 2H), 5.74 (d, *J* = 4.2 Hz, 1H), 3.63 (d, *J* = 14.1 Hz, 1H), 3.37 (dd, *J* = 6.9, 6.9 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 170.4, 162.0 (d, *J* = 245.4 Hz), 160.4, 143.3, 138.2, 133.9, 132.6, 132.4, 130.8 (d, *J* = 8.0 Hz), 129.9, 129.5, 128.6 (d, *J* = 3.2 Hz), 125.9, 124.6, 122.7, 119.4, 115.4 (d, *J* = 21.3 Hz), 114.4, 63.3, 37.9.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{16}FN_2O$: 343.1246, Found: 343.1246.

4-((5-oxo-5,11-dihydroisoindolo[2,1-a]quinazolin-11-yl)methyl)benzonitrile 5ag



5ag

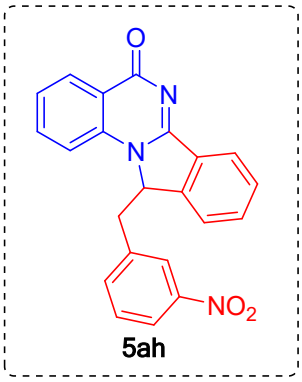
The title compound **5ag** (42 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 55% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.41 (dd, *J* = 1.2, 1.2 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.85-7.80 (m, 1H), 7.64-7.60 (m, 1H), 7.55-7.48 (m, 3H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 8.0 Hz, 2H), 5.80 (dd, *J* = 2.8, 2.8 Hz, 1H), 3.67 (dd, *J* = 2.8, 2.8 Hz, 1H), 3.53 (dd, *J* = 6.8, 6.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ_C 170.1, 160.2, 142.7, 138.4, 138.0, 134.0, 132.8, 132.4, 132.0, 130.1, 130.0, 129.7, 126.0, 124.7, 122.5, 119.3, 118.1, 114.2, 111.6, 62.6, 38.5.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{23}H_{16}N_3O$: 350.1293, Found: 350.1289.

11-(3-nitrobenzyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5ah



5ah

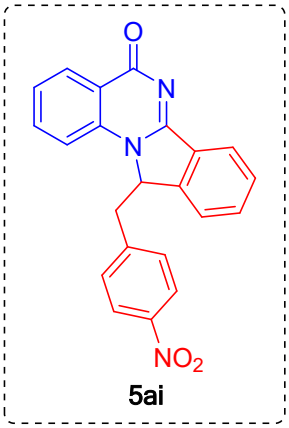
The title compound **5ah** (39 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Yellow solid, 48% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.35 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 7.2 Hz, 2H), 7.83 (s, 1H), 7.64-7.58 (m, 2H), 7.47 (d, *J* = 6.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.15 (t, *J* = 7.2 Hz, 1H), 6.80 (d, *J* = 6.0 Hz, 1H), 5.85 (s, 1H), 3.73-3.69 (m, 1H), 3.62 (dd, *J* = 5.2, 5.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ_C 170.1, 160.2, 147.7, 142.6, 138.0, 135.1, 134.7, 134.2, 133.0, 132.2, 129.8, 129.7, 129.3, 126.0, 124.5, 124.1, 122.6, 122.5, 119.2, 114.4, 62.7, 38.0.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{16}N_3O_3$: 370.1191, Found: 370.1191.

11-(4-nitrobenzyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5ai



5ai

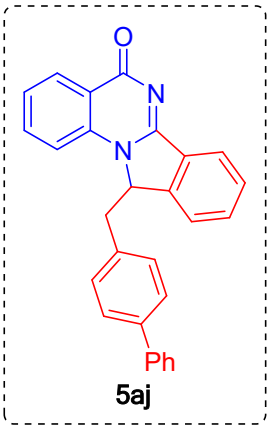
The title compound **5ai** (42 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Yellow solid, 51% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.35 (d, *J* = 6.4 Hz, 1H), 7.92-7.82 (m, 4H), 7.60 (s, 2H), 7.47-7.41 (m, 3H), 6.71 (d, *J* = 6.4 Hz, 2H), 5.86 (s, 1H), 3.71 (d, *J* = 13.2 Hz, 1H), 3.63 (d, *J* = 4.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ_C 170.1, 160.2, 147.2, 142.7, 140.4, 138.0, 134.2, 132.9, 132.2, 130.1, 129.8, 129.7, 126.0, 124.5, 123.3, 122.6, 119.2, 114.4, 62.7, 38.1.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{22}H_{16}N_3O_3$: 370.1191, Found: 370.1189.

11-([1,1'-biphenyl]-4-ylmethyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5aj



5aj

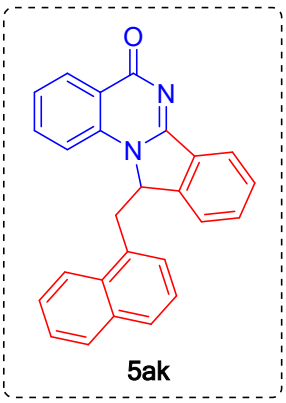
The title compound **5aj** (51 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 58% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.41 (d, *J* = 7.8 Hz, 1H), 8.03 (d, *J* = 7.2 Hz, 1H), 7.81(t, *J* = 7.5 Hz, 1H), 7.59-7.53 (m, 2H), 7.50-7.45 (m, 4H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 3H), 7.25 (d, *J* = 6.0 Hz, 1H), 6.77 (d, *J* = 7.8 Hz, 2H), 5.73 (dd, *J* = 3.0, 2.4 Hz, 1H), 3.72 (dd, *J* = 3.0 Hz, 2.4 Hz, 1H), 3.28 (dd, *J* = 7.5 Hz, 7.5 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ_C 170.5, 160.3, 143.6, 140.3, 140.1, 138.2, 133.8, 132.5, 132.3, 132.2, 129.7,129.3, 128.7, 127.4, 127.0, 126.9, 125.7, 124.5, 122.9, 119.4, 114.6, 63.5, 38.5.

HRMS (ESI) m/z: $[M+H]^+$ m/z calculated for $C_{28}H_{21}N_2O$: 401.1653, Found: 401.1652.

11-(naphthalen-1-ylmethyl)isoindolo[2,1-a]quinazolin-5(11H)-one 5ak



5ak

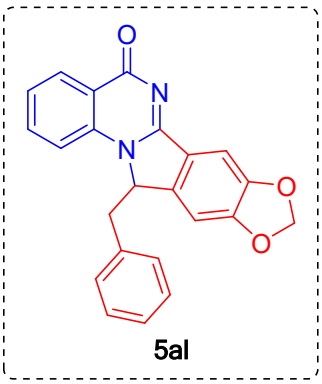
The title compound **5ak** (32 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 39% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.44 (dd, *J* = 1.2, 1.2 Hz, 1H), 8.15 (d, *J* = 7.6 Hz, 1H), 7.91-7.86 (m, 2H), 7.83 (d, *J* = 8 Hz, 1H), 7.76-7.72 (m, 1H), 7.53-7.44 (m, 5H), 7.38-7.35 (m, 1H), 7.32-7.28 (m, 1H), 7.15 (d, *J* = 7.2 Hz, 1H), 6.54 (d, *J* = 8.0 Hz,1H), 5.90 (dd, *J* = 5.2, 4.8 Hz, 1H), 4.25 (dd, *J* = 5.2, 4.8 Hz, 1H), 3.27 (dd, *J* = 9.2, 9.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ_C 170.5, 160.3, 143.6, 138.3, 133.8, 133.6, 132.0, 131.9, 130.9, 129.7, 129.3, 129.2, 128.7, 128.6, 126.5, 126.0, 125.7, 125.2, 124.6, 123.6, 122.9, 119.6, 114.6, 63.1, 37.3.

HRMS (ESI) m/z: $[M+H]^+$ calculated for $C_{26}H_{19}N_2O$: 375.1497, Found: 375.1497.

12-benzyl-[1,3]dioxolo[4',5':5,6]isoindolo[2,1-a]quinazolin-5(12H)-one 5al



5al

The title compound **5al** (42 mg) was prepared by following general procedure E. Pure product was isolated using silica column chromatography. Pale yellow solid, 52% yield (Solvent gradient: 60% ethylacetate in hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.23 (d, *J* = 8 Hz, 1H), 7.68 (t, *J* = 7.2 Hz, 1H), 7.42 (d, *J* = 8 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.22 (s, 1H), 7.07-6.99 (m, 3H), 6.63 (d, *J* = 7.2 Hz, 2H), 6.49 (s, 1H), 5.98 (d, *J* = 8.8 Hz, 2H), 5.52 (d, *J* = 4.8 Hz, 1H), 3.56-3.50 (m, 1H), 3.11 (dd, *J* = 7.2, 7.2 Hz, 1H).

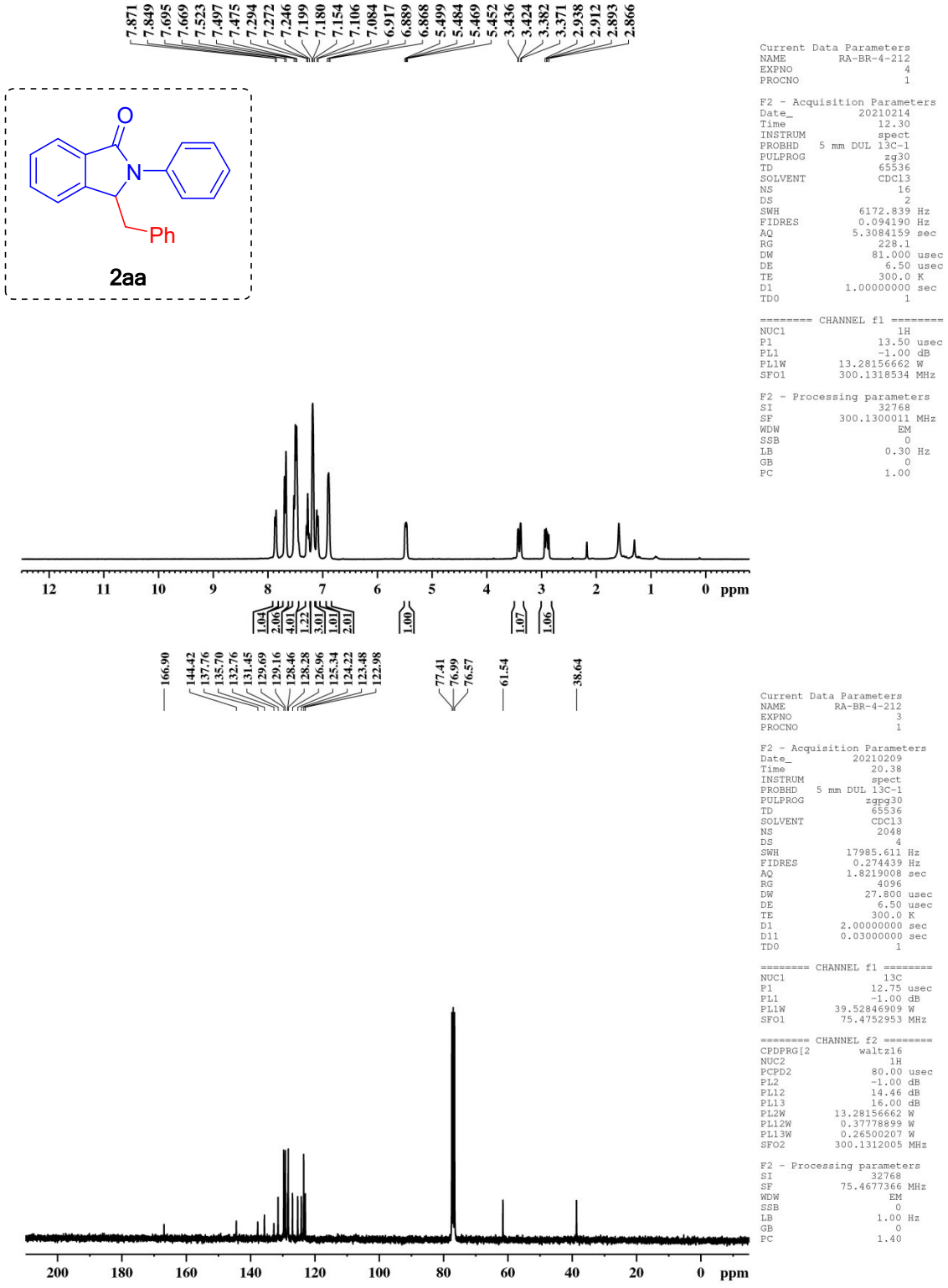
^{13}C NMR (101 MHz, $CDCl_3$): δ_C 169.9, 159.9, 152.3, 148.9, 140.0, 138.2, 133.9, 133.1, 129.4, 129.2, 128.5, 127.5, 125.5, 125.4, 118.8, 114.5, 103.4, 103.3, 102.4, 63.2, 38.8.

HRMS (ESI) m/z: $[M+H]^+$ m/z calculated for $C_{23}H_{17}N_2O_3$: 369.1239, Found: 369.1231.

11. References:

1. B. Yao, C. Jaccoud, Q. Wang and J. Zhu, *Chem. Eur. J.,* 2012, **18**, 5864-5868.
2. B. Tang and R. Hua, *Molecules,* 2022, **27**, 3393.
3. A. D. Sonawane, R. A. Sonawane, K. M. N. Win, M. Ninomiya and M. Koketsu, *Org. Biomol. Chem.,* 2020, **18**, 2129– 2138.
4. C. Kanazawa and M. Terada, *Chem. Asian J.,* 2009, **4**, 1668– 1672.
5. A. D. Sonawane, R. A. Sonawane, K. M. N. Win, M. Ninomiya and M. Koketsu, *Org. Biomol. Chem.,* 2020, **18**, 2129– 2138.
6. Z. Y. Chen, L. Y. Wu, H. S. Fang, T. Zhang, Z. F. Mao, Y. Zou, X. J. Zhang and M. Yan, *Adv. Synth. Catal*., 2017, **359**, 3894–3899.
7. M. Hari Balakrishnan and S. Mannathan, *Org.Lett*., 2020, **22**, 542–546.
8. N. G. Kundu and M. W. Khan, *Tetrahedron*, 2000, **56**, 4777-4792.
9. N. Muniraj and K. R. Prabhu, *Adv. Synth. Catal*., 2018, **360**, 3579-3584.

12. Copies of NMR and HRMS data



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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084159 sec
RG 228.1
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
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PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz

F2 - Processing parameters
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SF 300.1300011 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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PROCNO 1

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Time 20.38
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219008 sec
RG 4096
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
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P1 12.75 usec
PL1 -1.00 dB
PL1W 39.52846909 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
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PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.46 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.37778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz

F2 - Processing parameters
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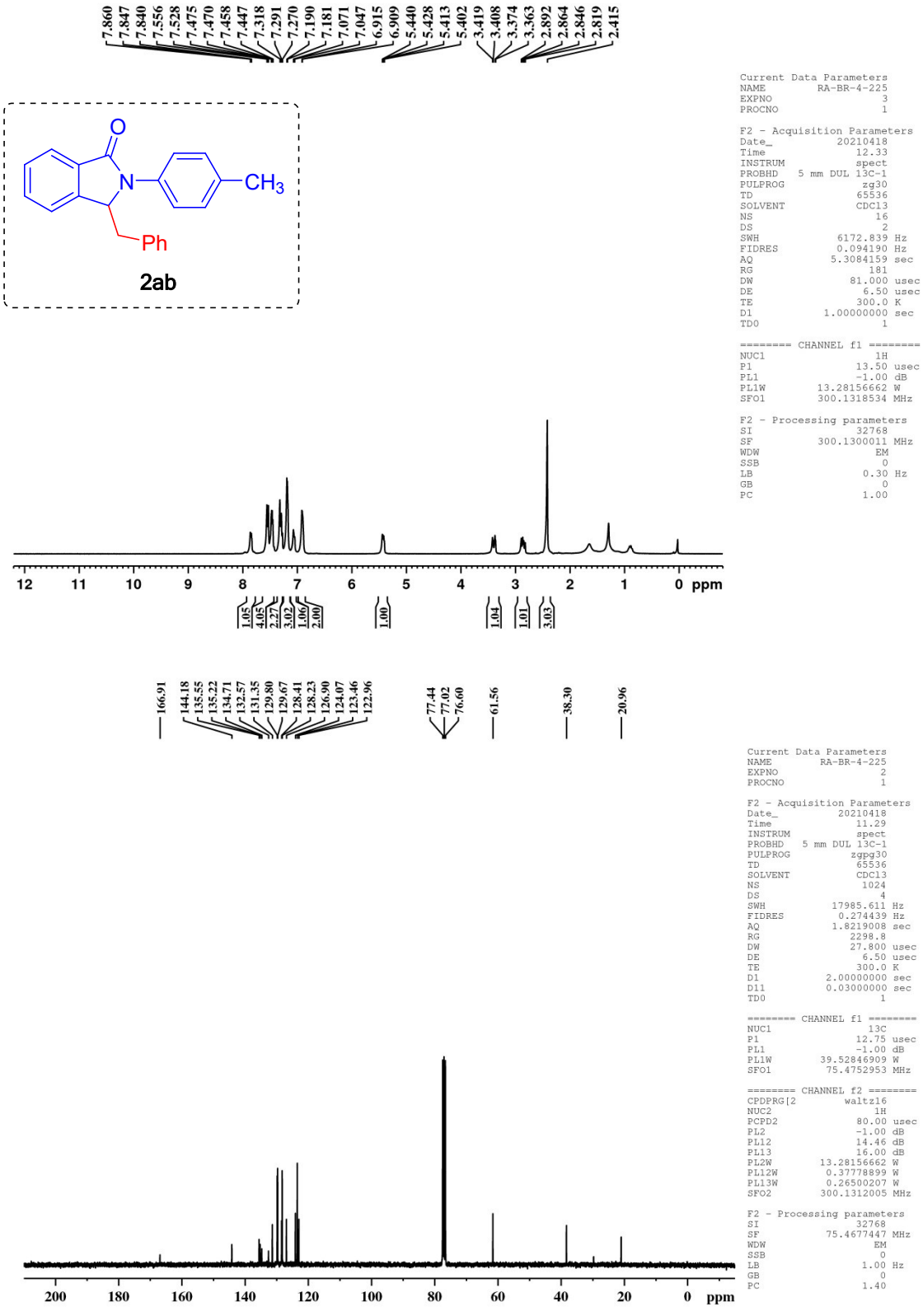
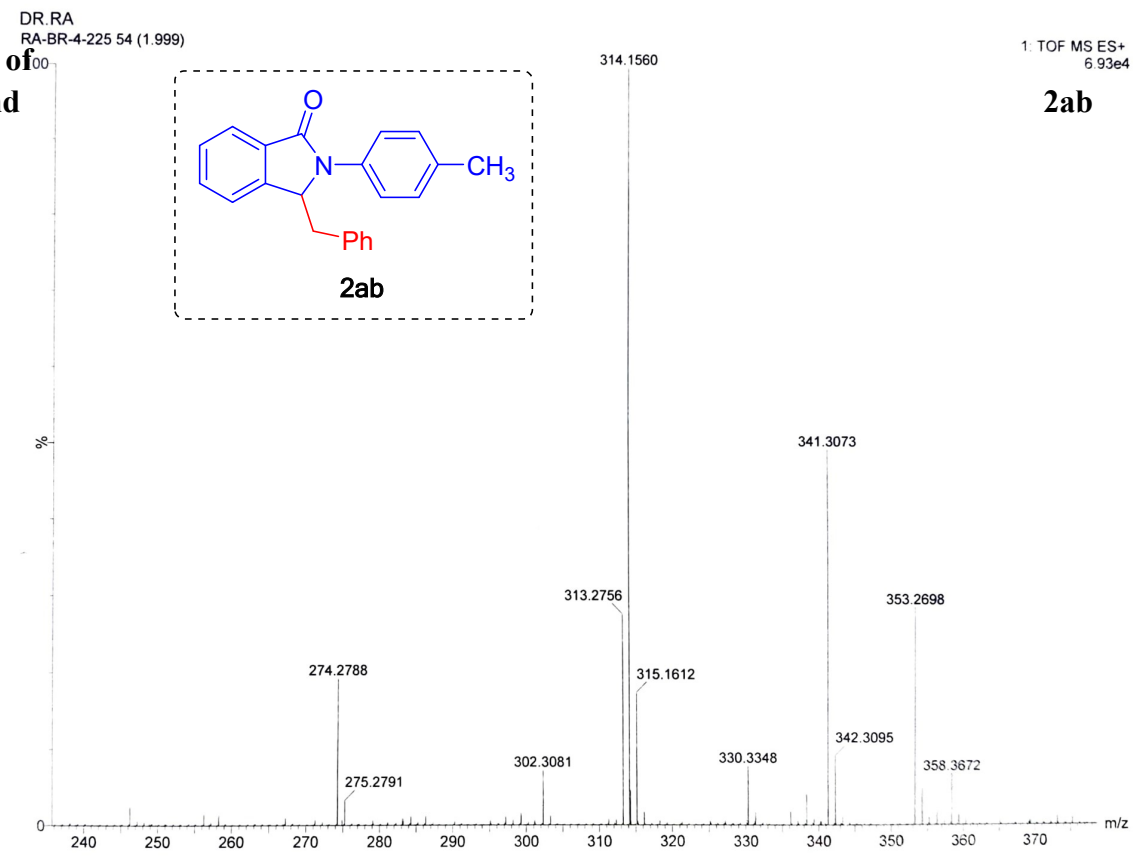
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

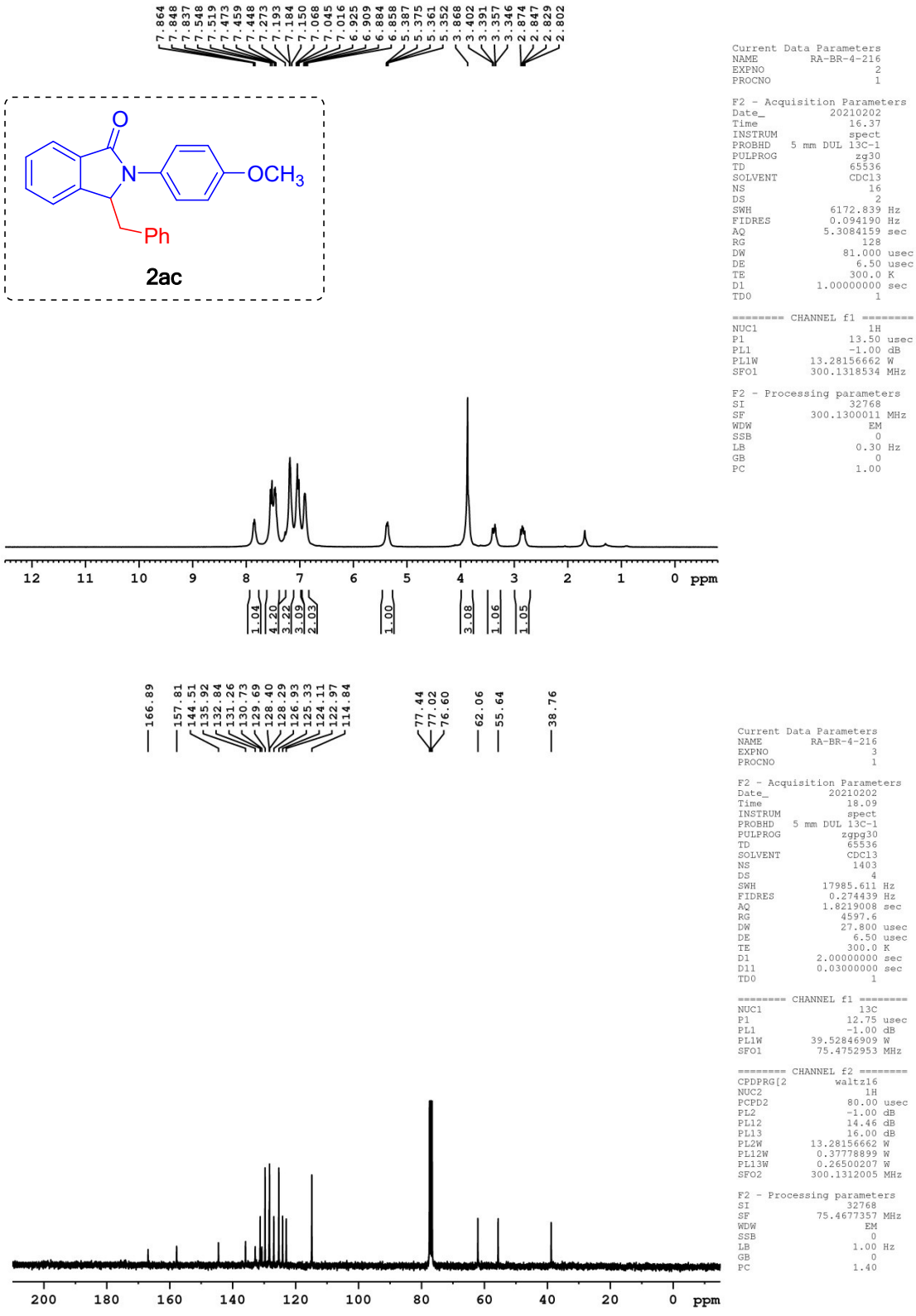
^{1}H and ^{13}C NMR Spectra of compound 2aa



^{1}H and ^{13}C NMR Spectra of compound 2ab

HRMS Spectrum of compound 2ab



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PROCNO                 1

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PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ             5.3084159 sec
RG                  128
DW                81.000 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

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PL1                -1.00 dB
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F2 - Processing parameters
SI                 32768
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SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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EXPNO                  3
PROCNO                 1

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TD                65536
SOLVENT           CDCl3
NS                 1403
DS                    4
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219008 sec
RG                4597.6
DW                27.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

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P1                 12.75 usec
PL1                -1.00 dB
PL1W         39.52846909 W
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
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PCPD2              80.00 usec
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PL12               14.46 dB
PL13               16.00 dB
PL2W         13.28156662 W
PL12W         0.37778899 W
PL13W         0.26500207 W
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
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GB                     0
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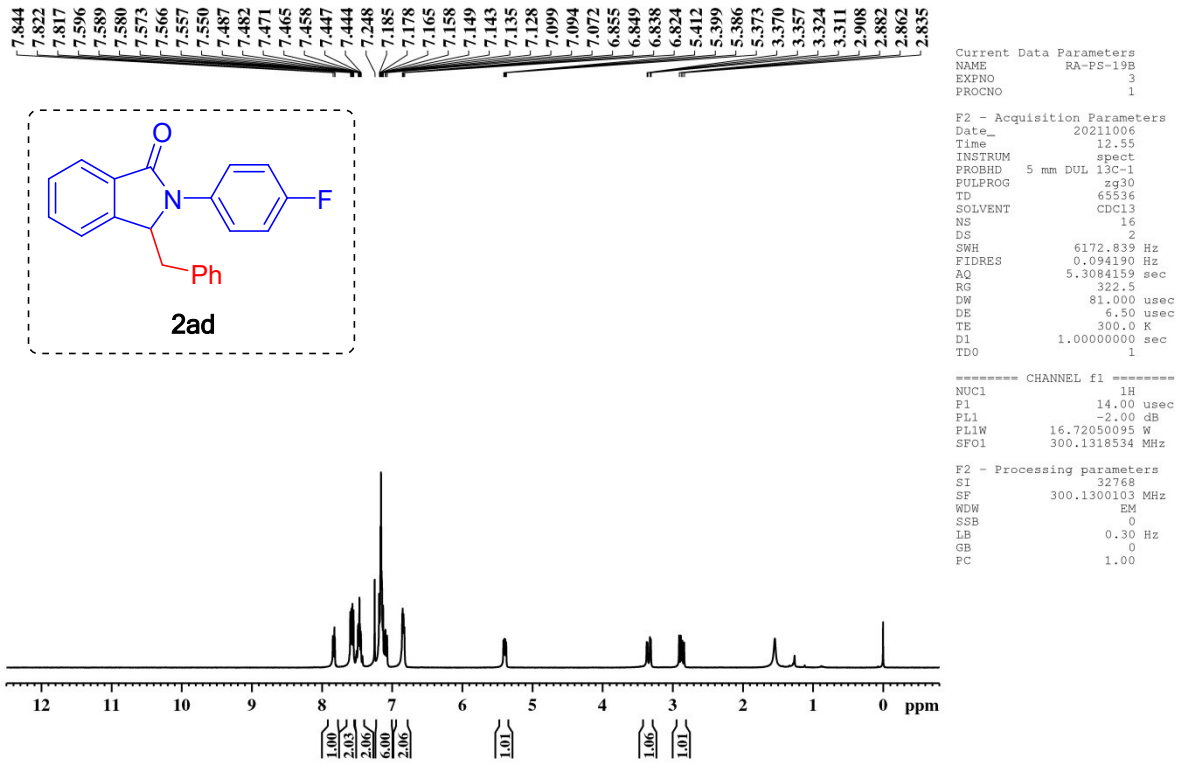
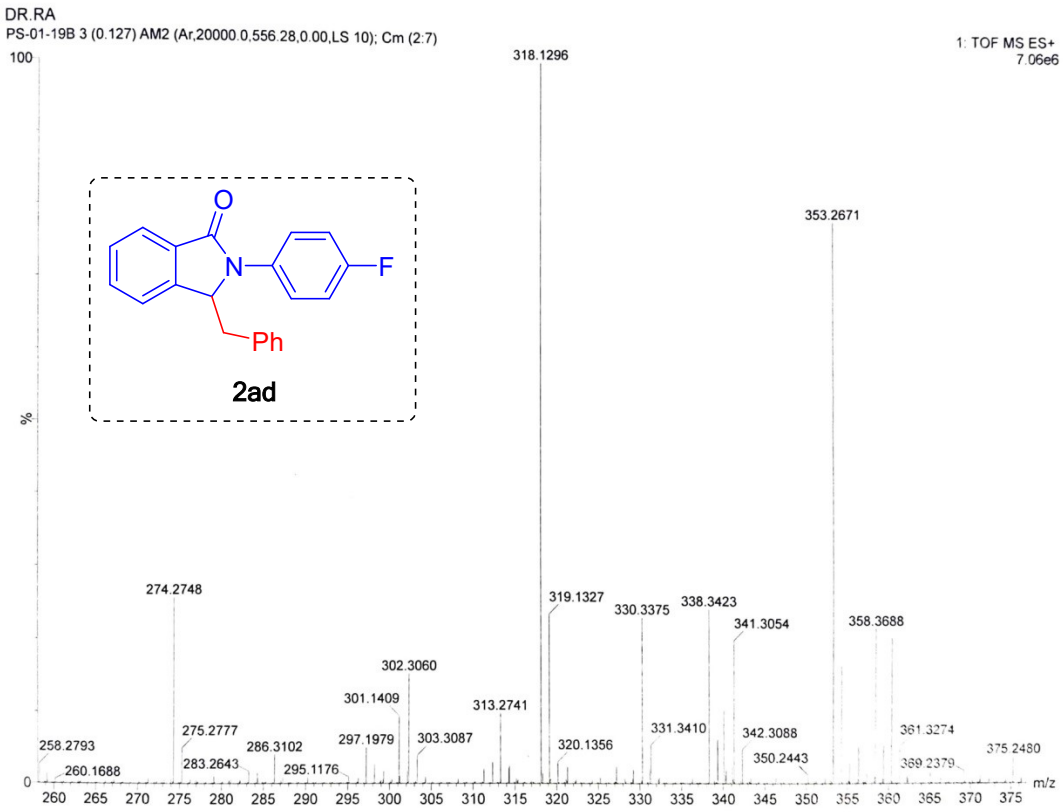
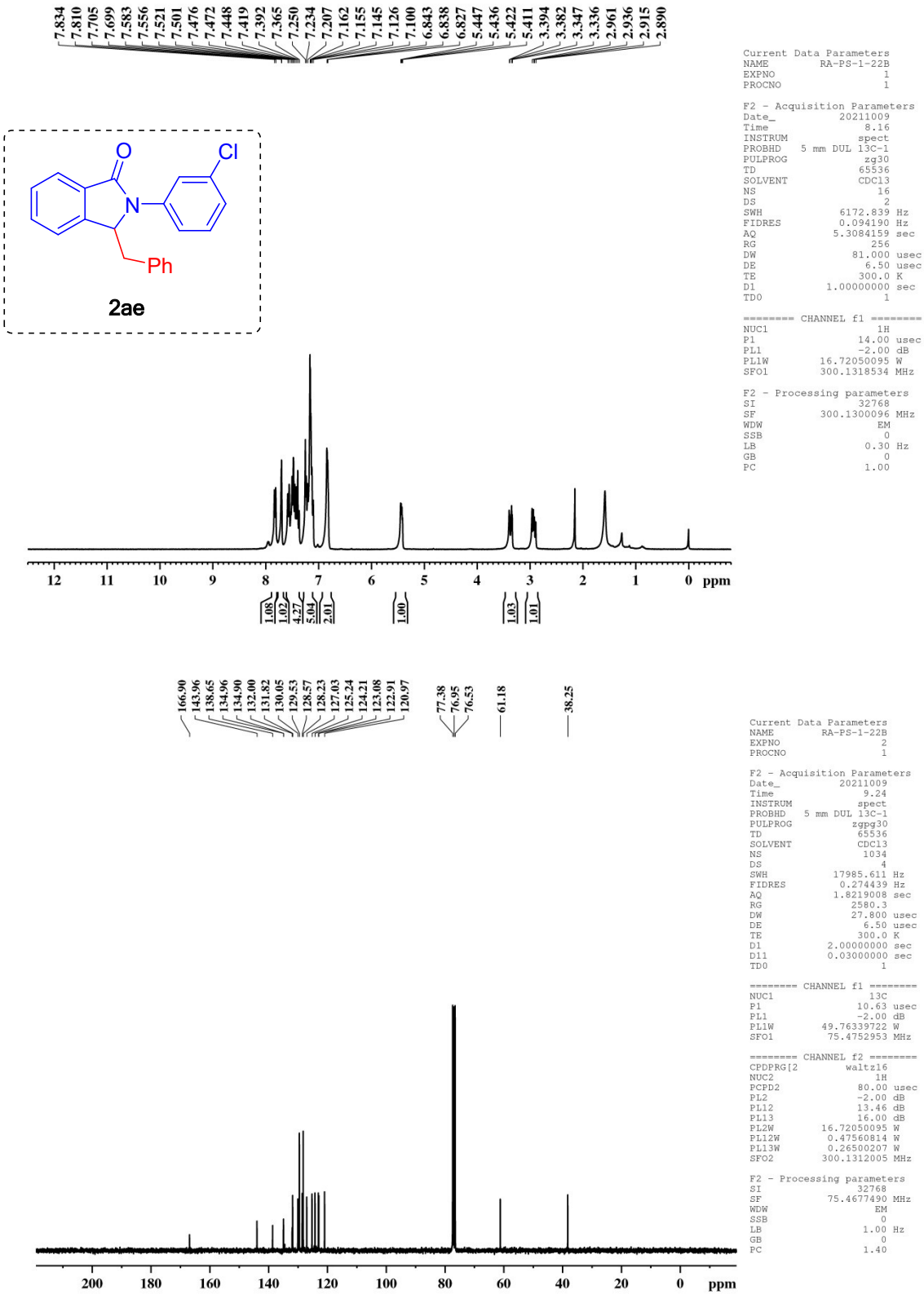
^{1}H and ^{13}C NMR Spectra of compound 2ac



^{1}H and ^{13}C NMR Spectra of compound 2ad



HRMS Spectrum of compound 2ad

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Current Data Parameters
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PROCNO                 1

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INSTRUM            spect
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TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084159 sec
RG                   256
DW                81.000 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
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P1                14.00 usec
PL1               -2.00 dB
PL1W         16.72050095 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300096 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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Current Data Parameters
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EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
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PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1034
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219008 sec
RG                2580.3
DW                27.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
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P1                10.63 usec
PL1               -2.00 dB
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======== CHANNEL f2 ========
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PL12              13.46 dB
PL13              16.00 dB
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F2 - Processing parameters
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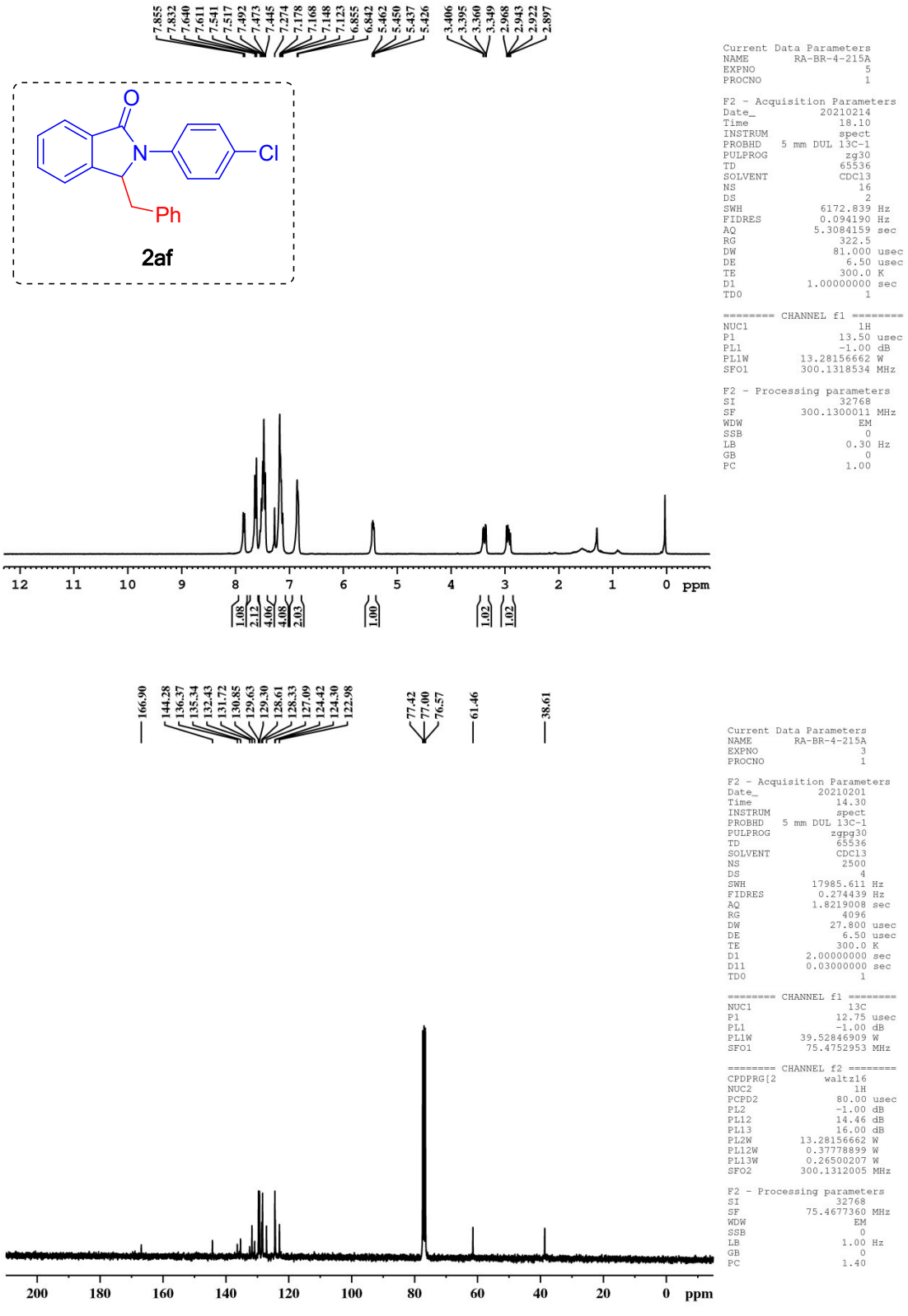
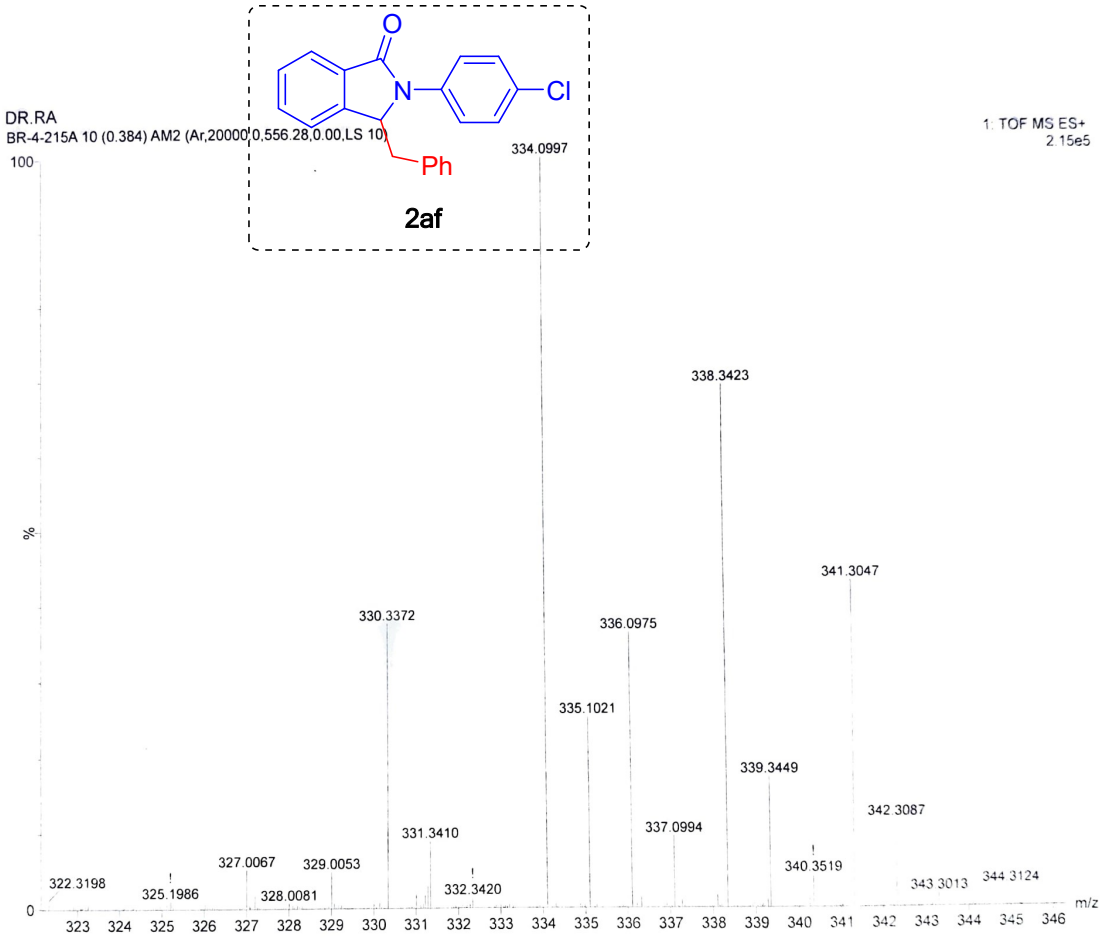
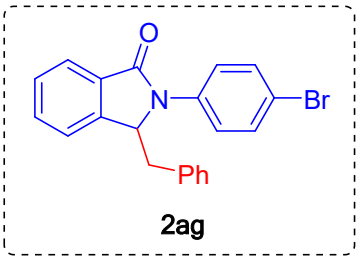
^{1}H and ^{13}C NMR Spectra of compound 2ae



^{1}H and ^{13}C NMR Spectra of compound 2af



HRMS Spectrum of compound 2af

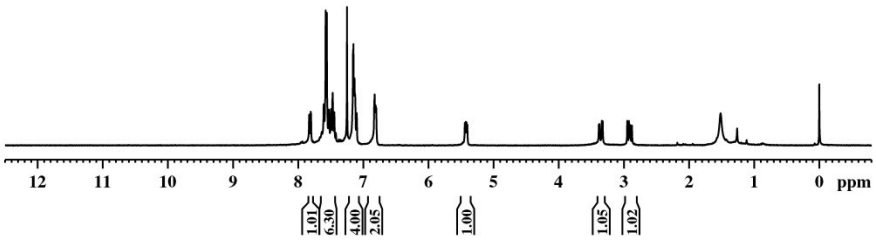



```
Current Data Parameters
NAME         RA-PS-1-21B
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211010
Time               10.38
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084159 sec
RG                   362
DW                81.000 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1               -2.00 dB
PL1W         16.72050095 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300098 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME         RA-PS-1-21B
EXPNO                  1
PROCNO                 1

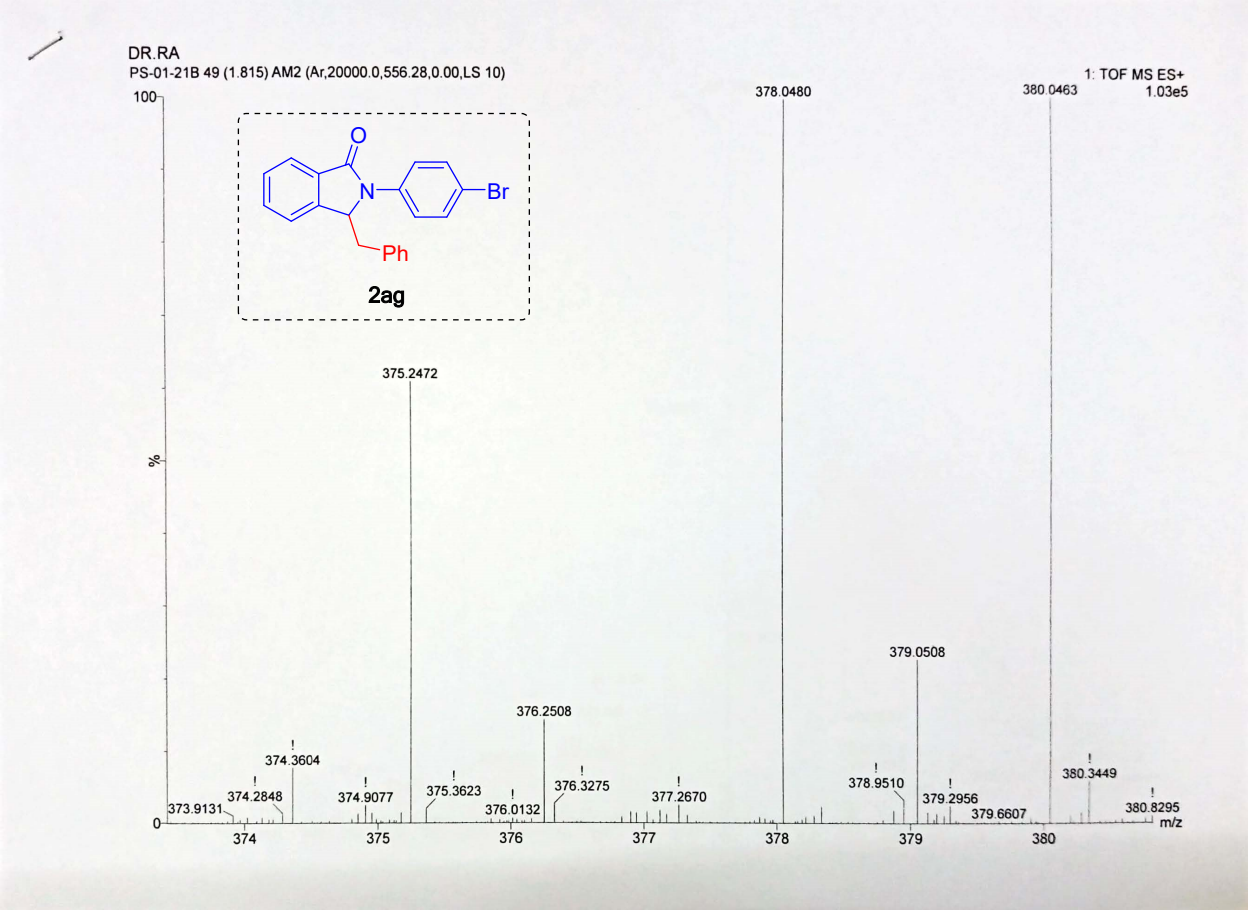
F2 - Acquisition Parameters
Date_           20211010
Time               10.05
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2500
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219008 sec
RG                1290.2
DW                27.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.63 usec
PL1               -2.00 dB
PL1W         49.76339722 W
SFO1         75.4752953 MHz

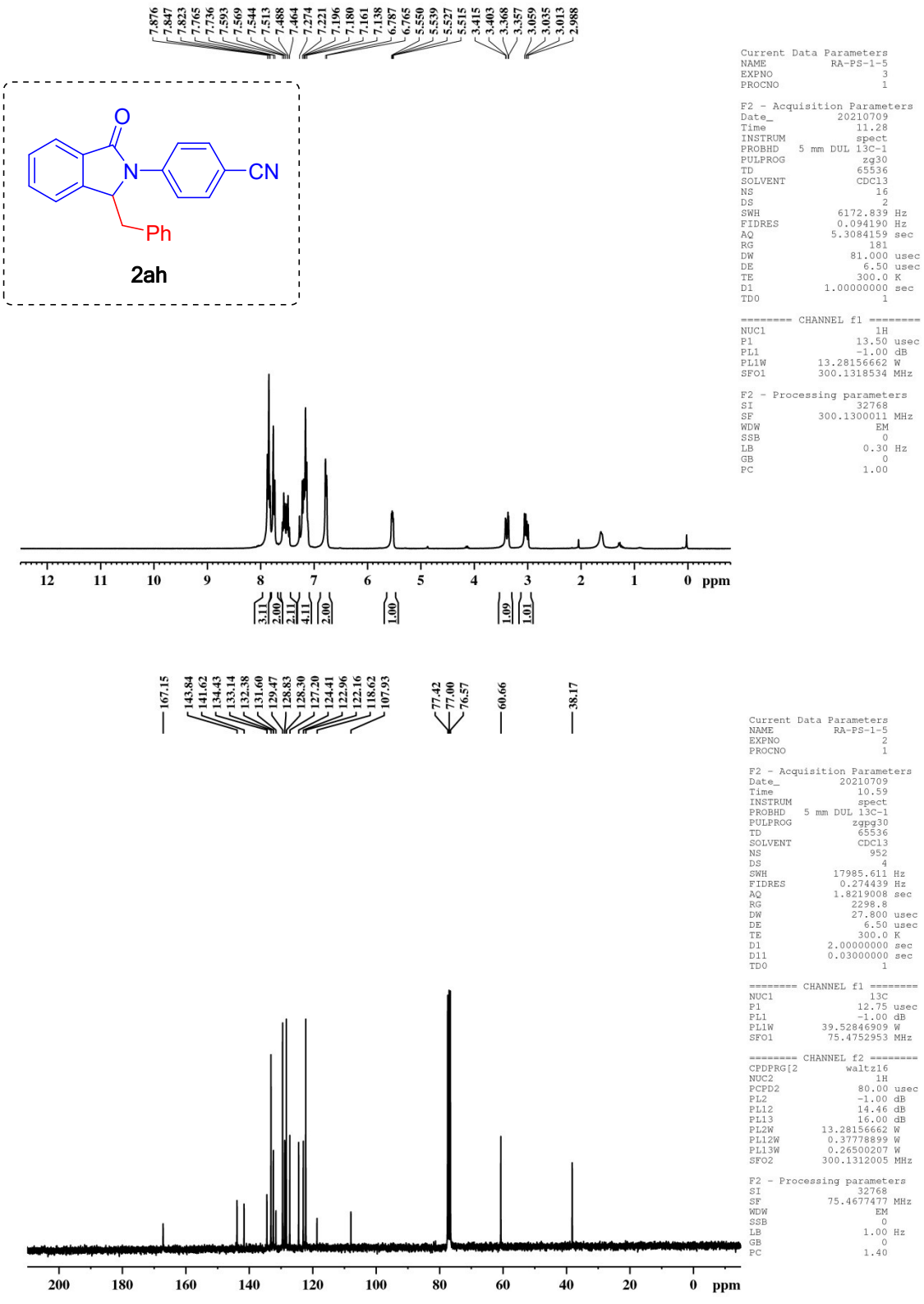
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              13.46 dB
PL13              16.00 dB
PL2W         16.72050095 W
PL12W         0.47560814 W
PL13W         0.26500207 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

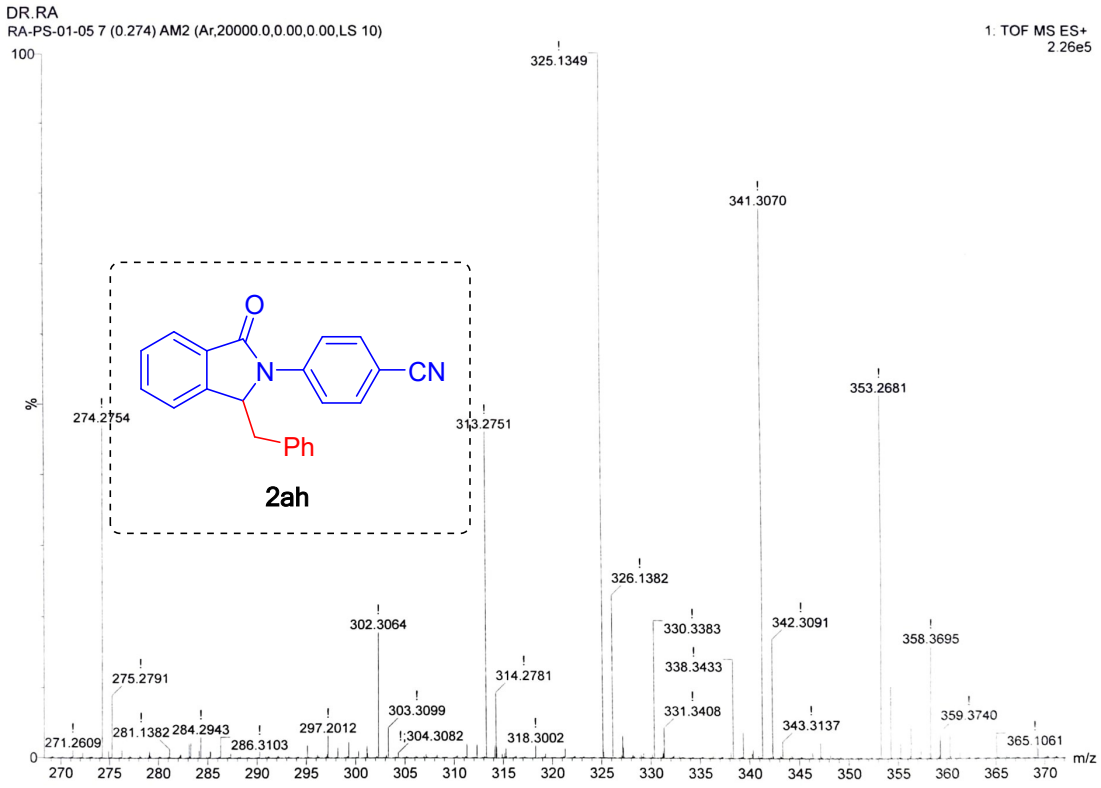

^{1}H and ^{13}C NMR Spectra of compound 2ag



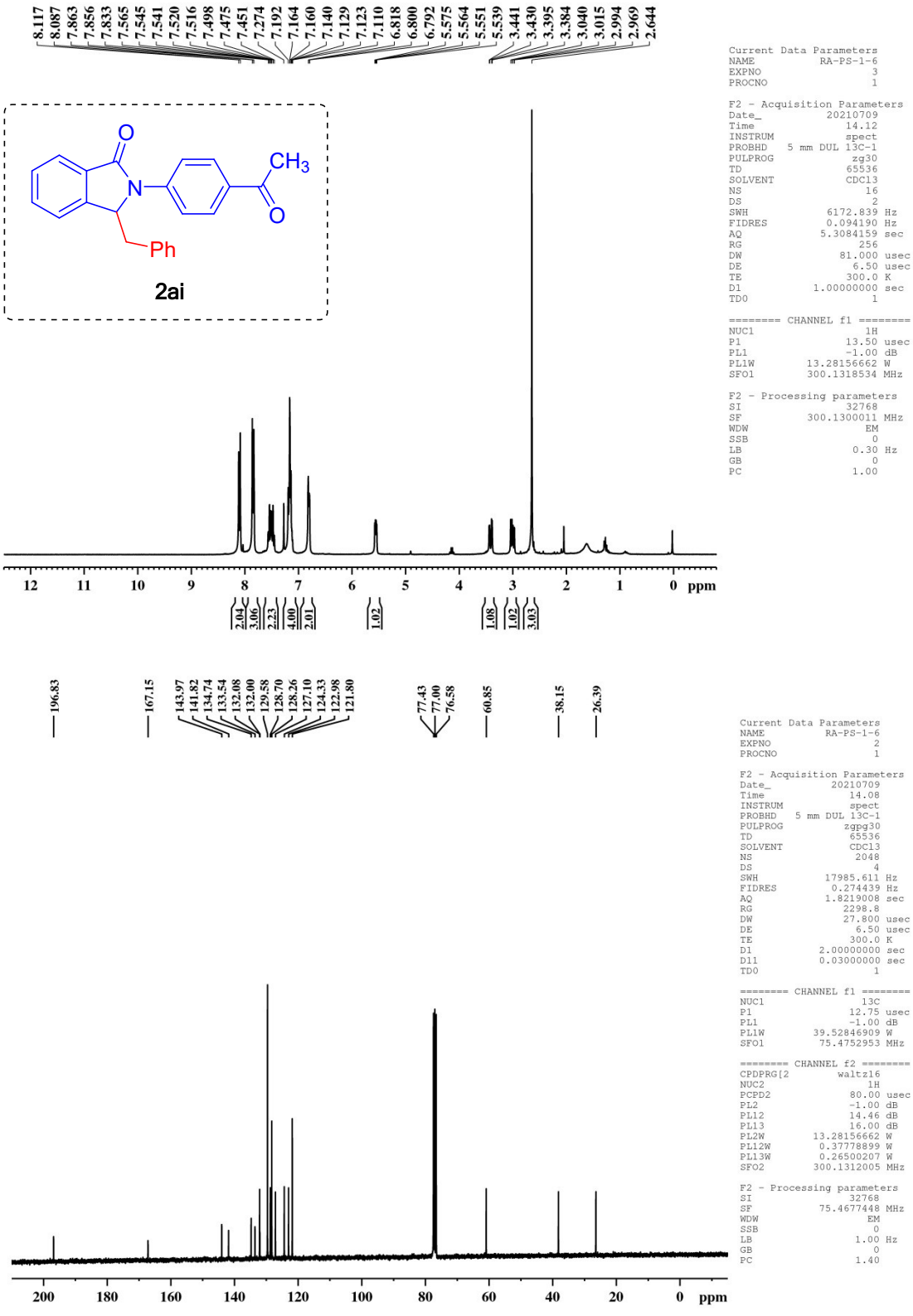
HRMS Spectrum of compound 2ag



^{1}H and ^{13}C NMR Spectra of compound 2ah



HRMS Spectrum of compound 2ah




```
Current Data Parameters
NAME                  RA-PS-1-6
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210709
Time                      14.12
INSTRUM                   spect
PROBHD    5 mm DUL 13C-1
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   6172.839 Hz
FIDRES                0.094190 Hz
AQ                    5.3084159 sec
RG                          256
DW                       81.000 usec
DE                        6.50 usec
TE                       300.0 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        1H
P1                       13.50 usec
PL1                      -1.00 dB
PL1W                13.28156662 W
SFO1                300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF                  300.1300011 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

```
Current Data Parameters
NAME                  RA-PS-1-6
EXPNO                         2
PROCNO                        1

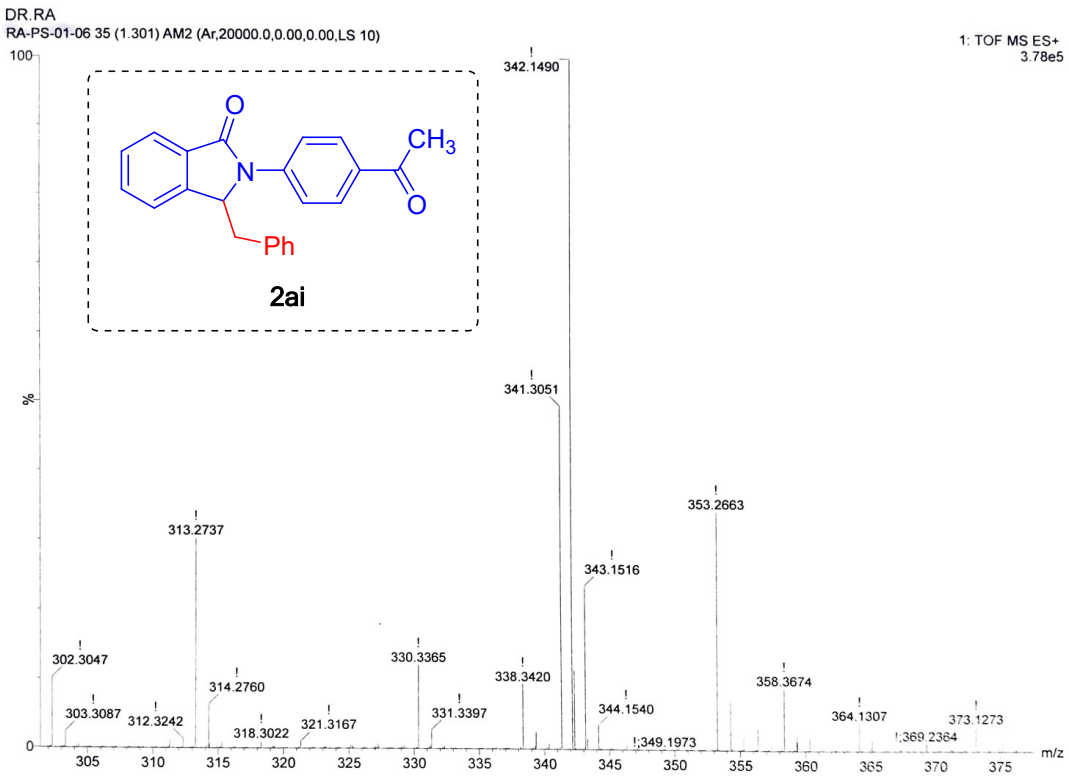
F2 - Acquisition Parameters
Date_                  20210709
Time                      14.08
INSTRUM                   spect
PROBHD    5 mm DUL 13C-1
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        2048
DS                           4
SWH                  17985.611 Hz
FIDRES                0.274439 Hz
AQ                    1.8219008 sec
RG                       2298.8
DW                       27.800 usec
DE                        6.50 usec
TE                       300.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                       13C
P1                       12.75 usec
PL1                      -1.00 dB
PL1W               39.52846909 W
SFO1                75.4752953 MHz

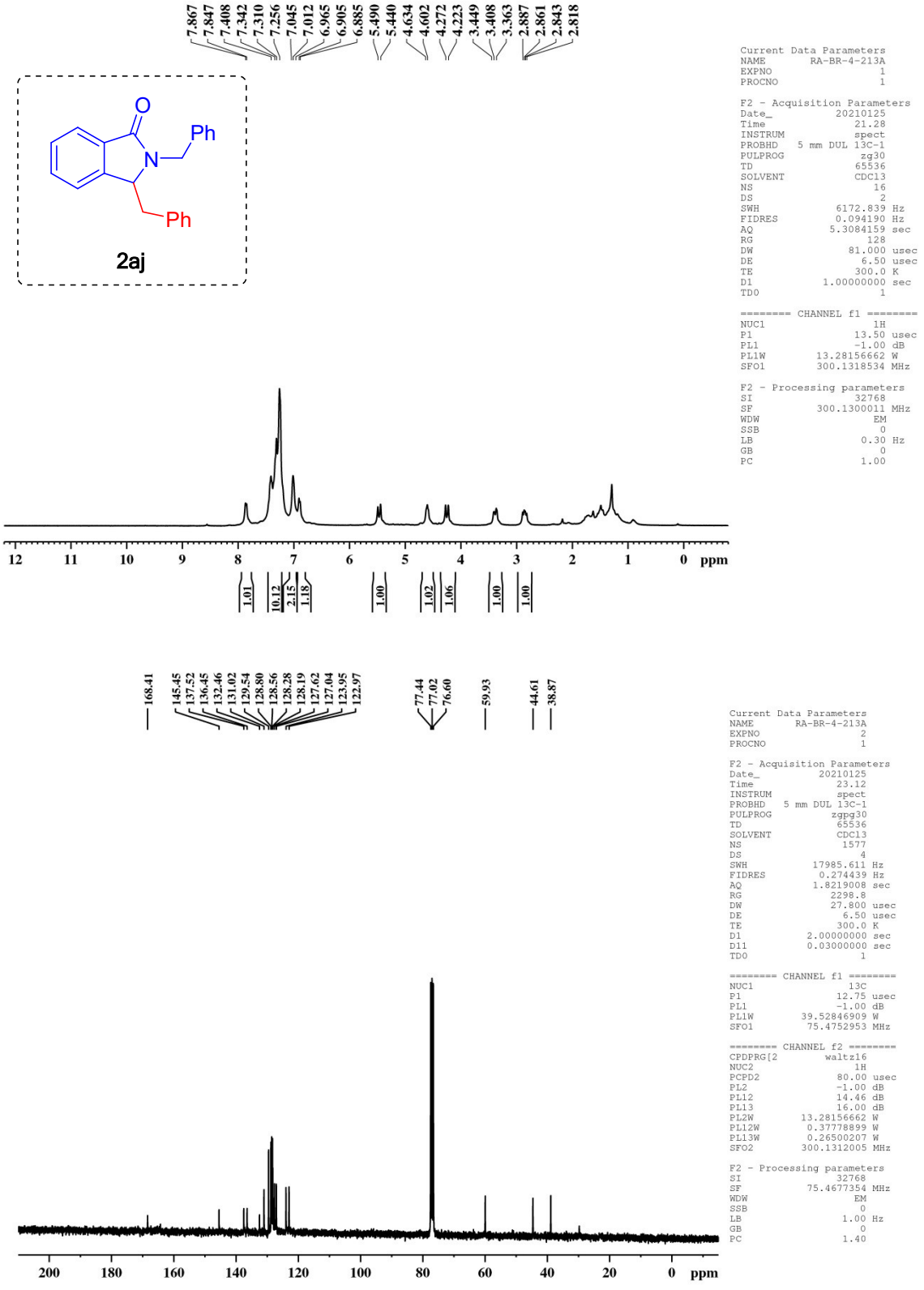
======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     14.46 dB
PL13                     16.00 dB
PL2W                13.28156662 W
PL12W                0.37778899 W
PL13W                0.26500207 W
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                  75.4677448 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

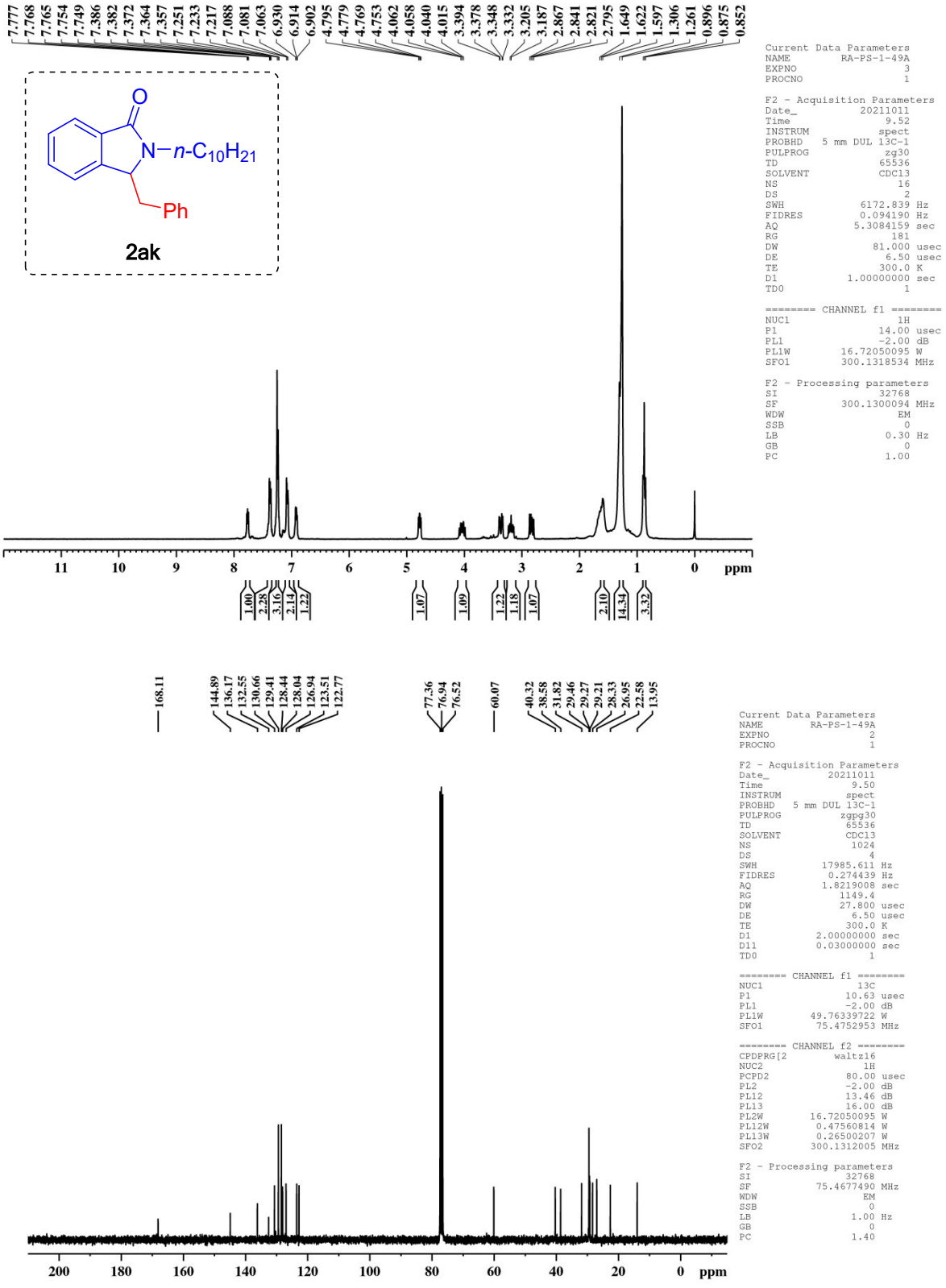
^{1}H and ^{13}C NMR Spectra of compound 2ai



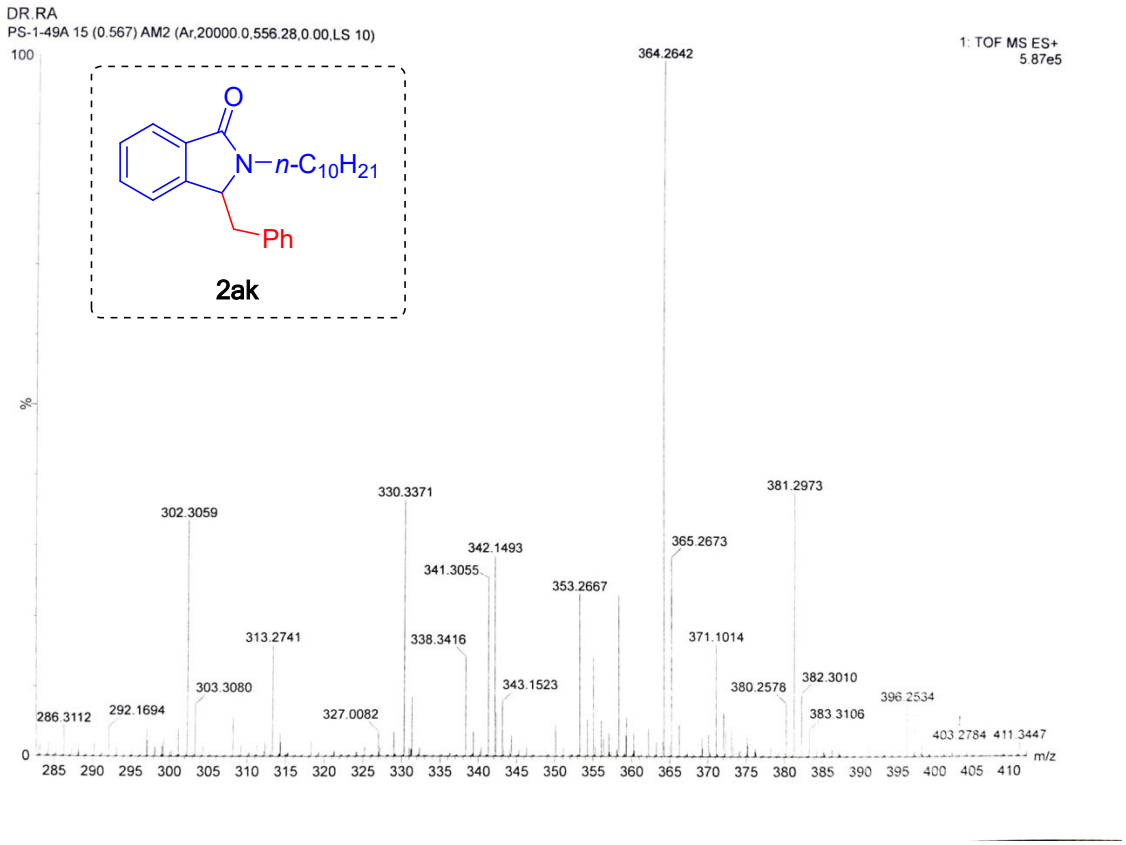
HRMS Spectrum of compound 2ai



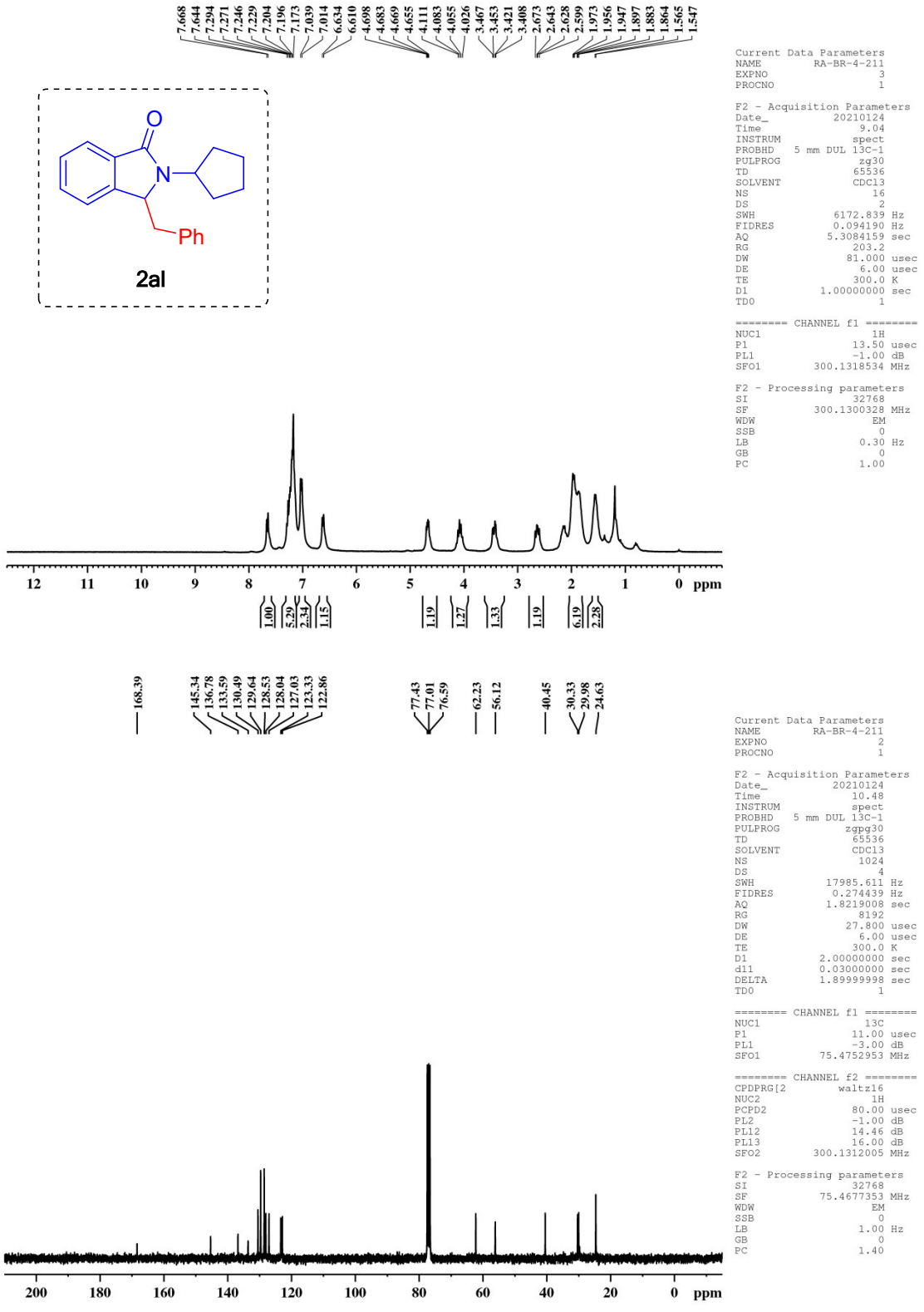
^{1}H and ^{13}C NMR Spectra of compound 2aj



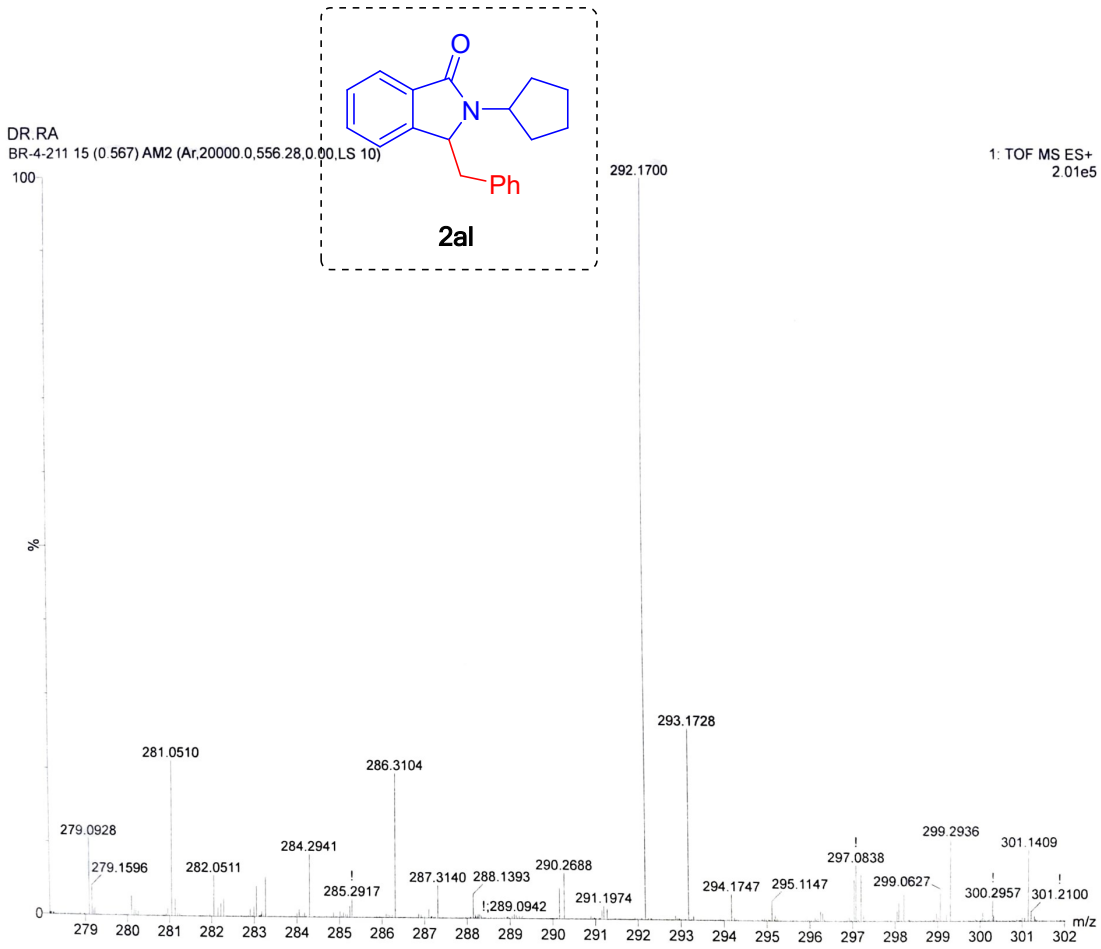
^{1}H and ^{13}C NMR Spectra of compound 2ak



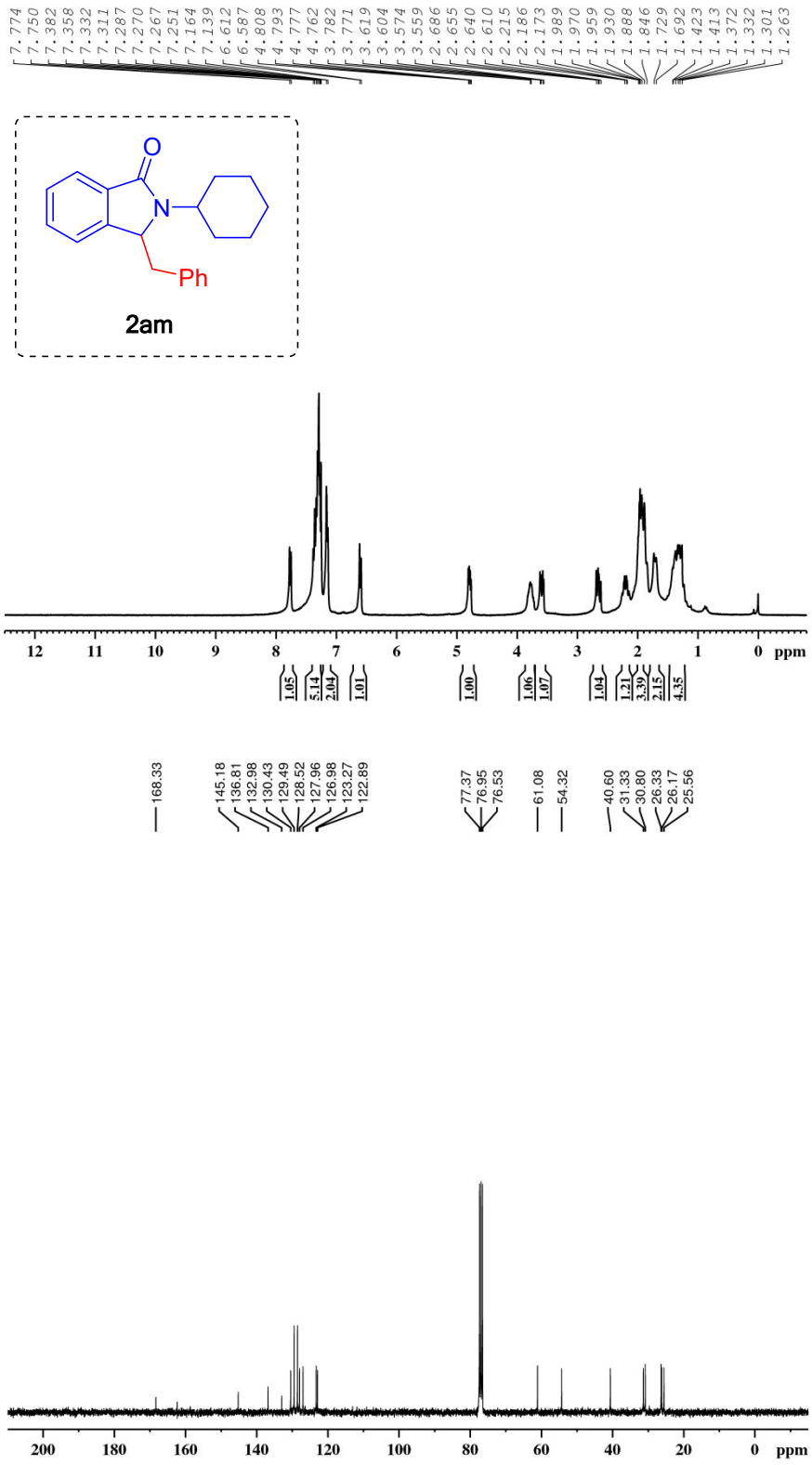
HRMS Spectrum of compound 2ak



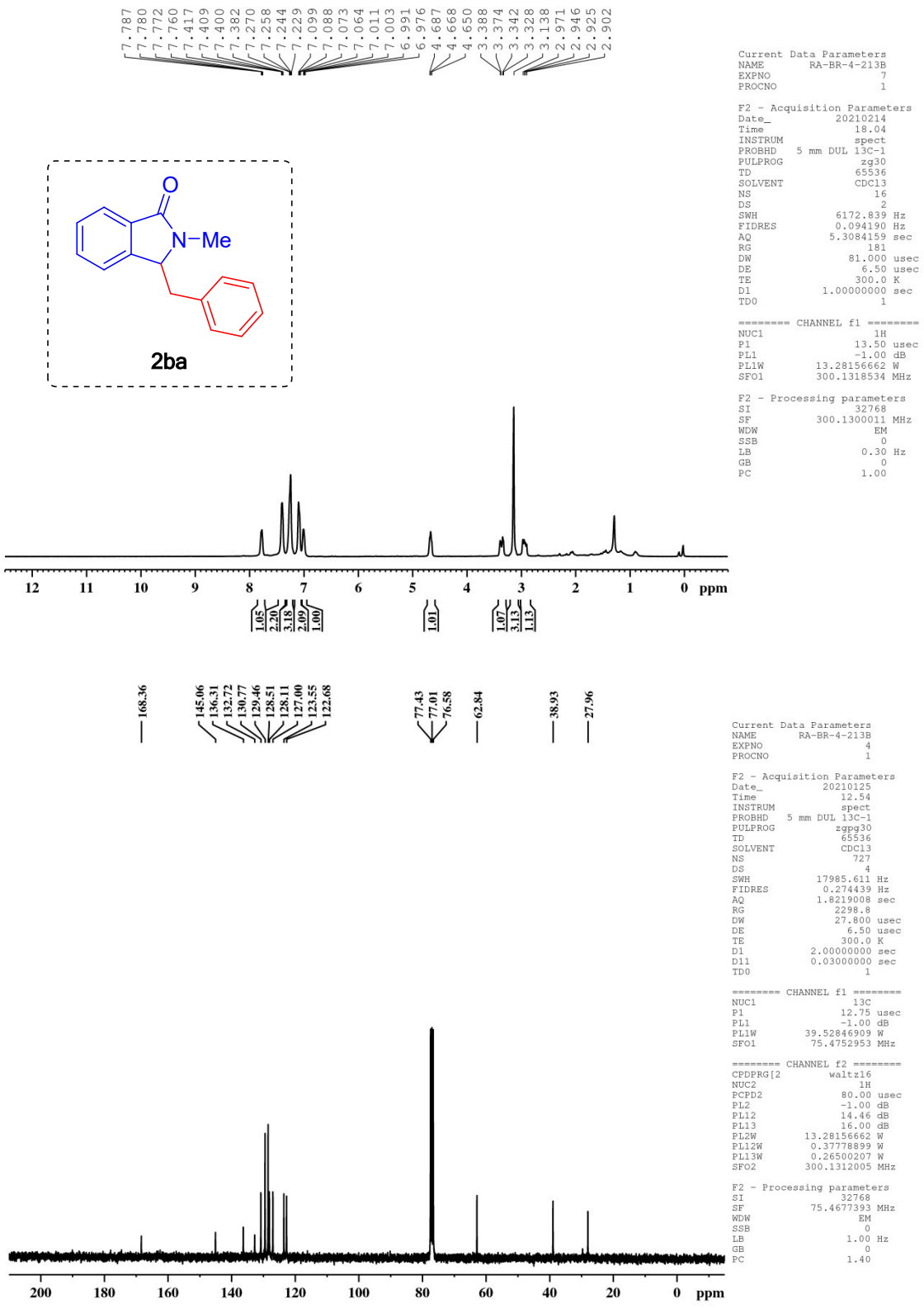
^{1}H and ^{13}C NMR Spectra of compound 2al



HRMS Spectrum of compound 2al



^{1}H and ^{13}C NMR Spectra of compound 2am



Current Data Parameters
NAME RA-BR-4-213B
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210214
Time 18.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084159 sec
RG 181
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300011 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME RA-BR-4-213B
EXPNO 4
PROCNO 1

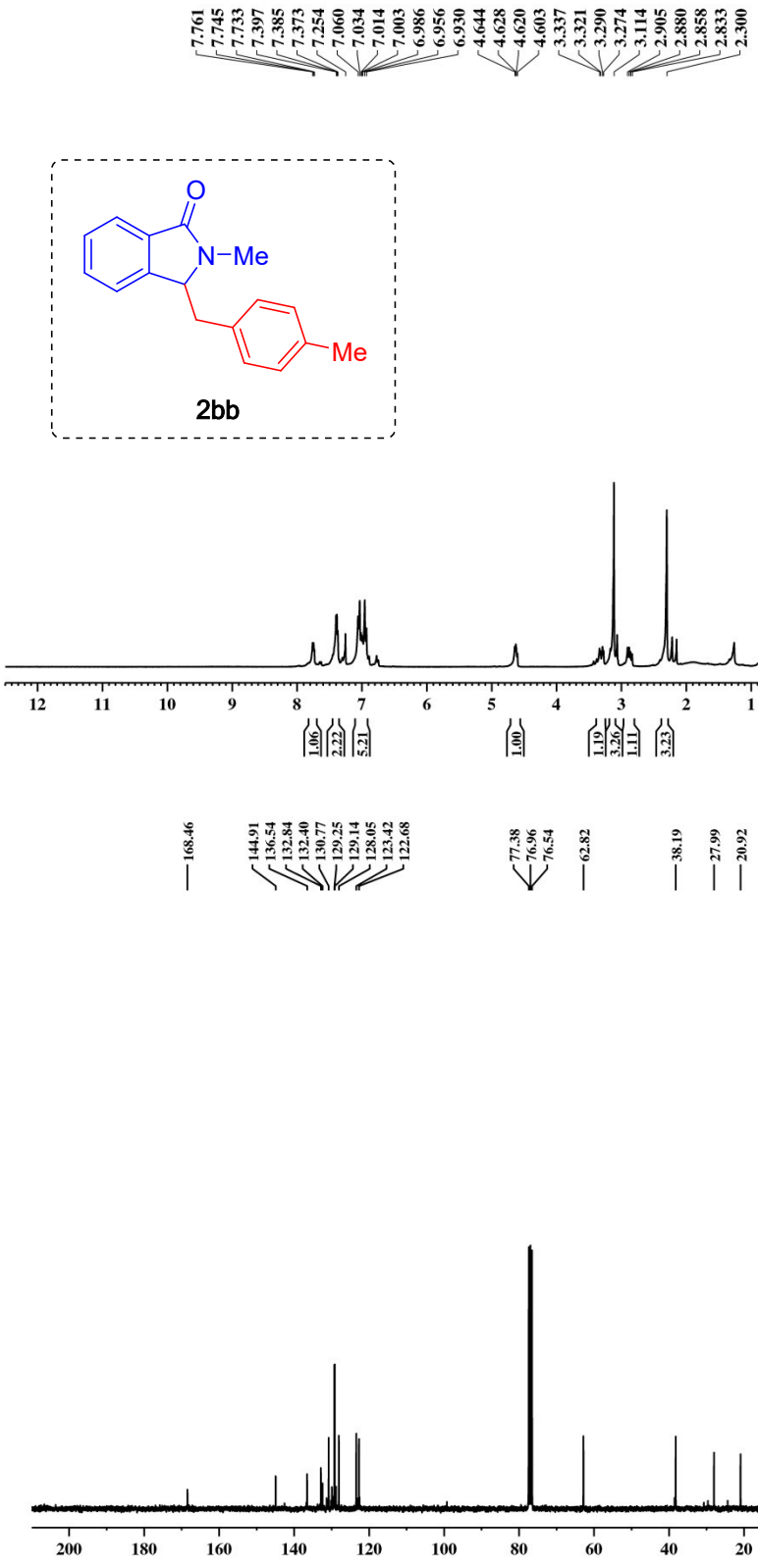
F2 - Acquisition Parameters
Date_ 20210125
Time 12.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 727
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219008 sec
RG 2298.8
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.75 usec
PL1 -1.00 dB
PL1W 39.52846909 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.46 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.37778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H and ^{13}C NMR Spectra of compound 2ba




```
Current Data Parameters
NAME          RA-PS-1-45
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211008
Time               19.38
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES             0.094190 Hz
AQ              5.3084159 sec
RG                 161.3
DW                81.000 usec
DE                 6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                -2.00 dB
PL1W         16.72050095 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300083 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

```
Current Data Parameters
NAME          RA-PS-1-45
EXPNO                 10
PROCNO                 1

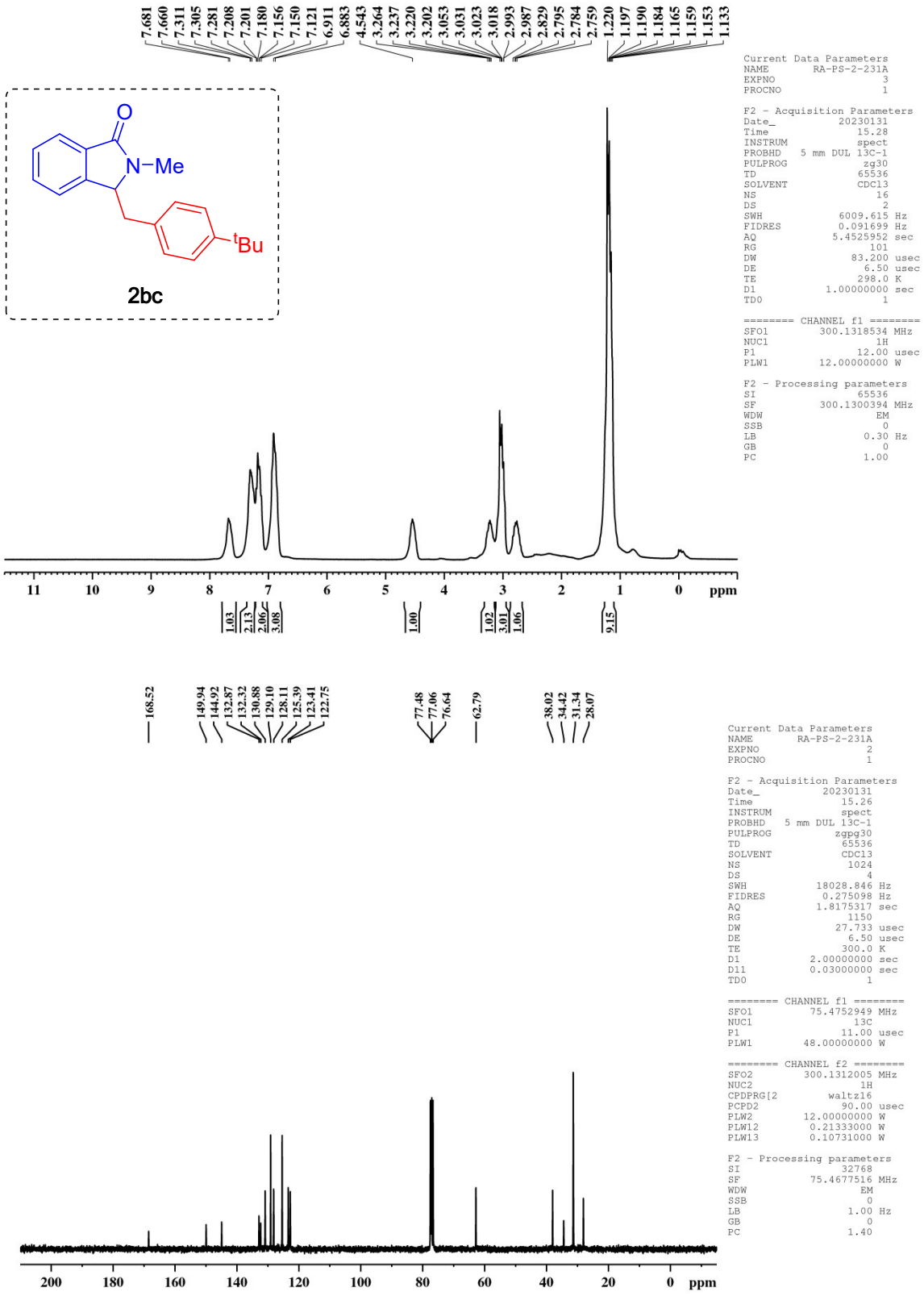
F2 - Acquisition Parameters
Date_           20211008
Time               20.45
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            17985.611 Hz
FIDRES             0.274439 Hz
AQ              1.8219008 sec
RG                 2048
DW                27.800 usec
DE                 6.50 usec
TE                 300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.63 usec
PL1                -2.00 dB
PL1W         49.76339722 W
SFO1         75.4752953 MHz

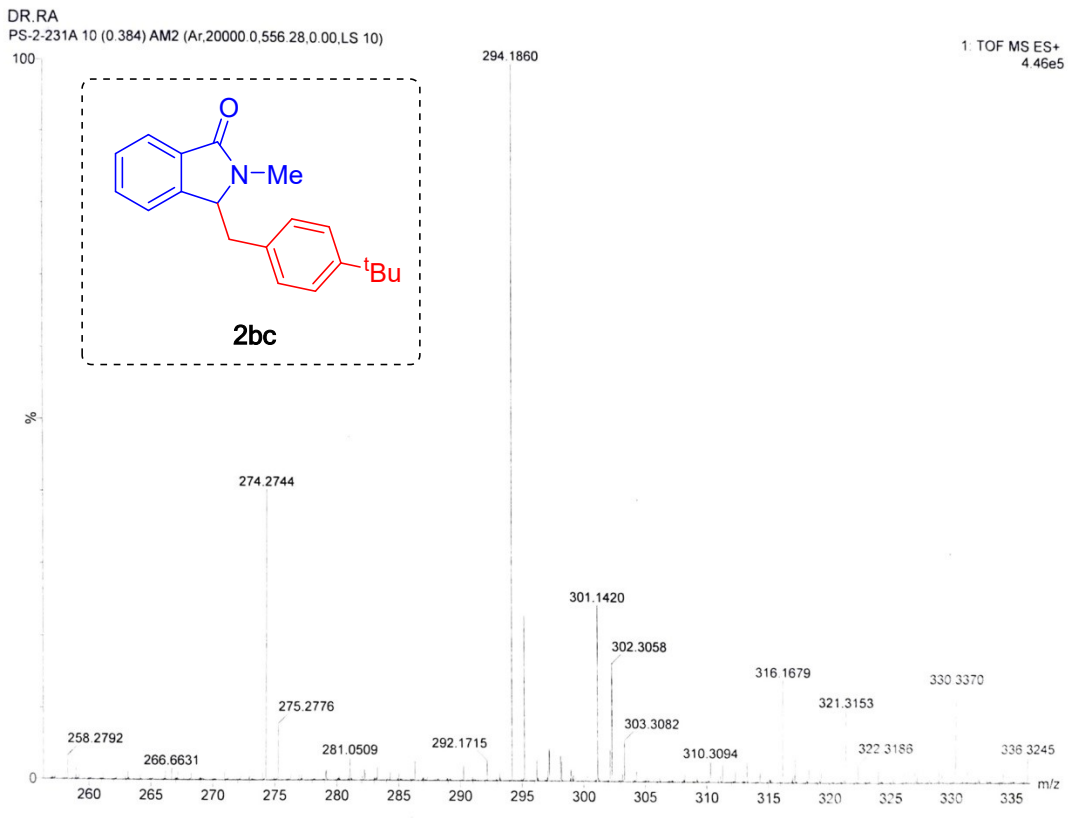
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               13.46 dB
PL13               16.00 dB
PL2W         16.72050095 W
PL12W         0.47560814 W
PL13W         0.26500207 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

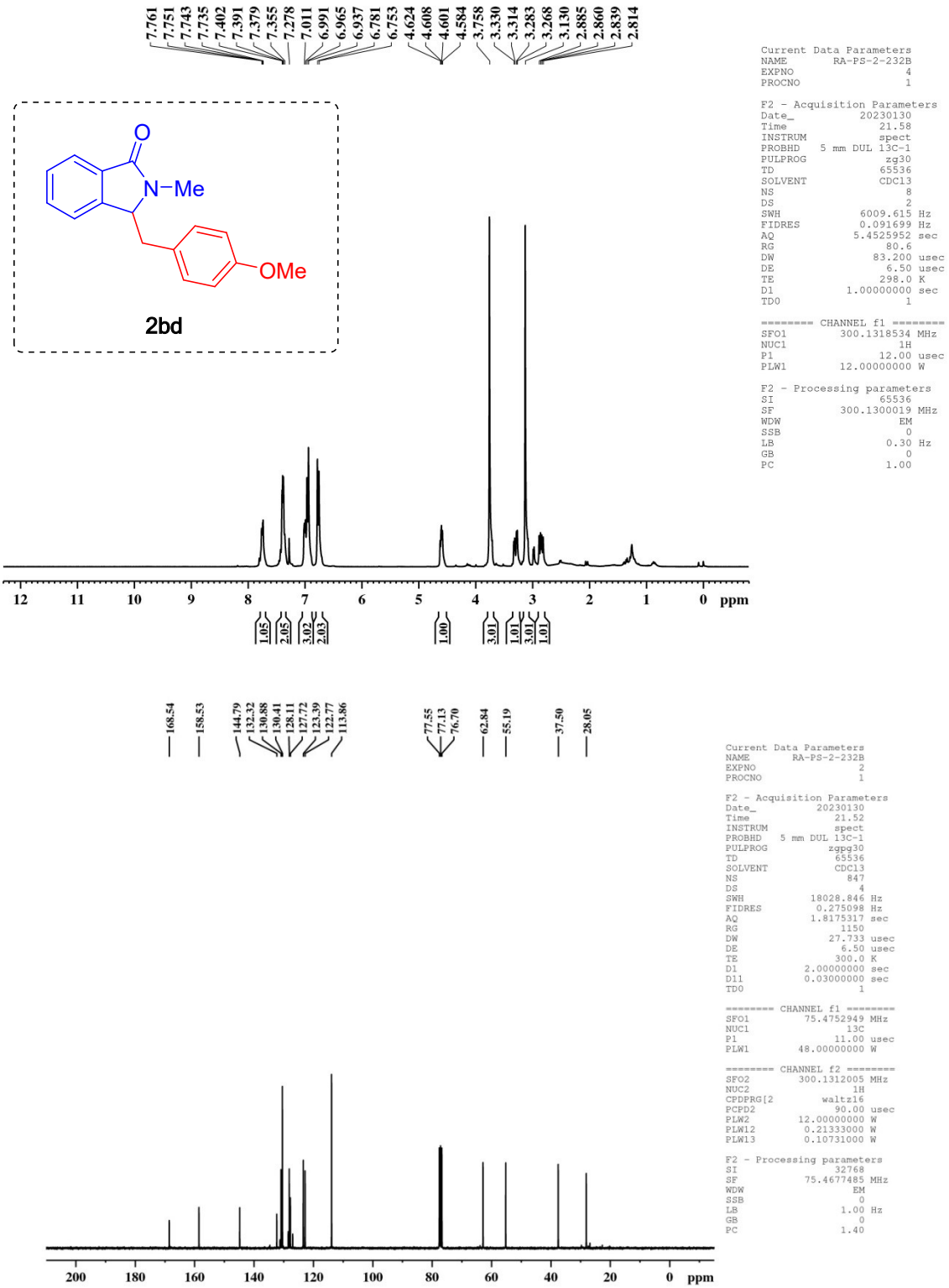
^{1}H and ^{13}C NMR Spectra of compound 2bb



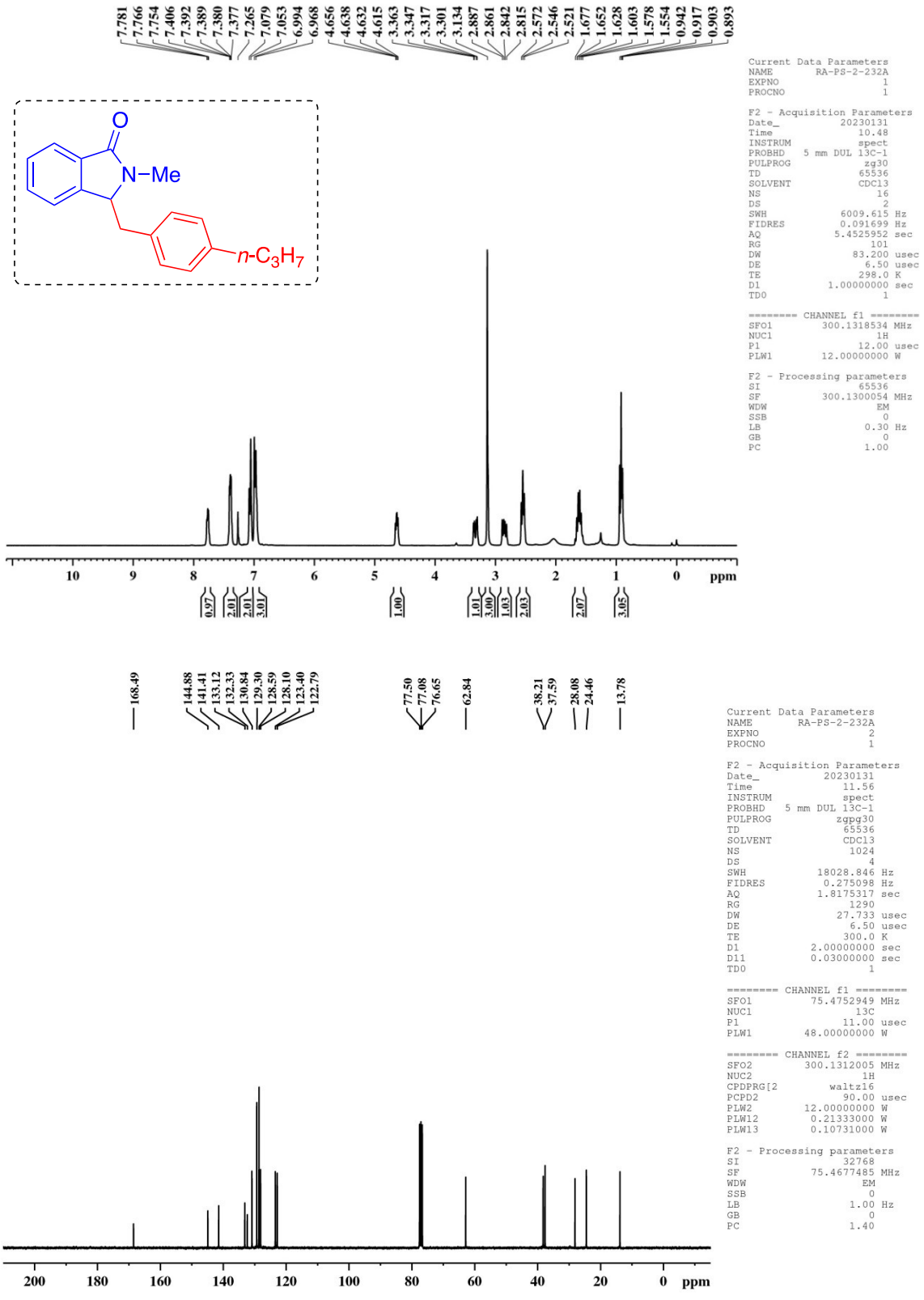
^{1}H and ^{13}C NMR Spectra of compound 2bc



HRMS Spectrum of compound 2bc



^{1}H and ^{13}C NMR Spectra of compound 2bd



Current Data Parameters
NAME RA-PS-2-232A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230131
Time 10.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 101
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 12.00 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME RA-PS-2-232A
EXPNO 2
PROCNO 1

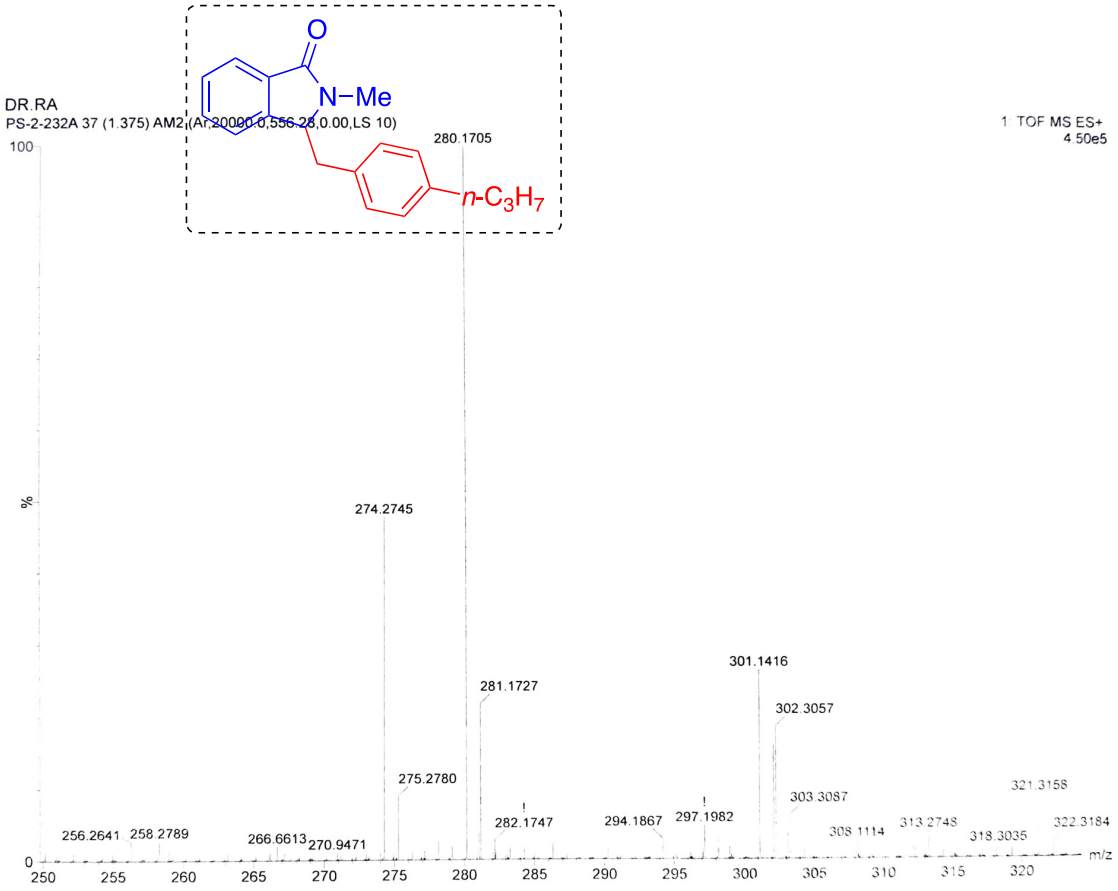
F2 - Acquisition Parameters
Date_ 20230131
Time 11.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 1290
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 11.00 usec
PLW1 48.00000000 W

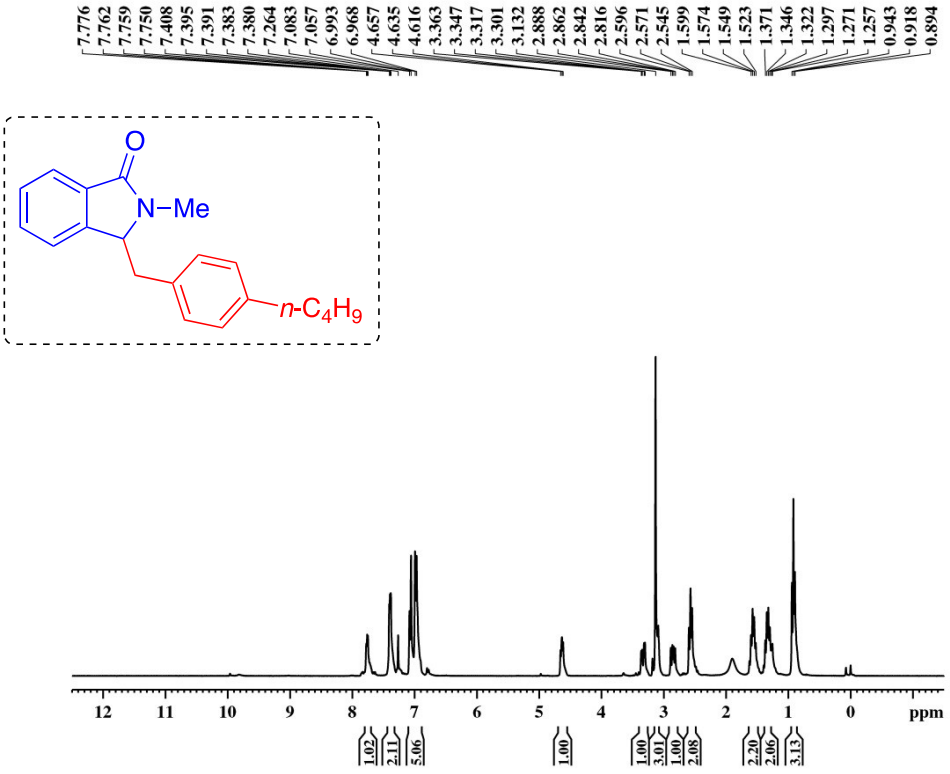
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.10731000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H and ^{13}C NMR Spectra of compound 2be



HRMS Spectrum of compound 2be

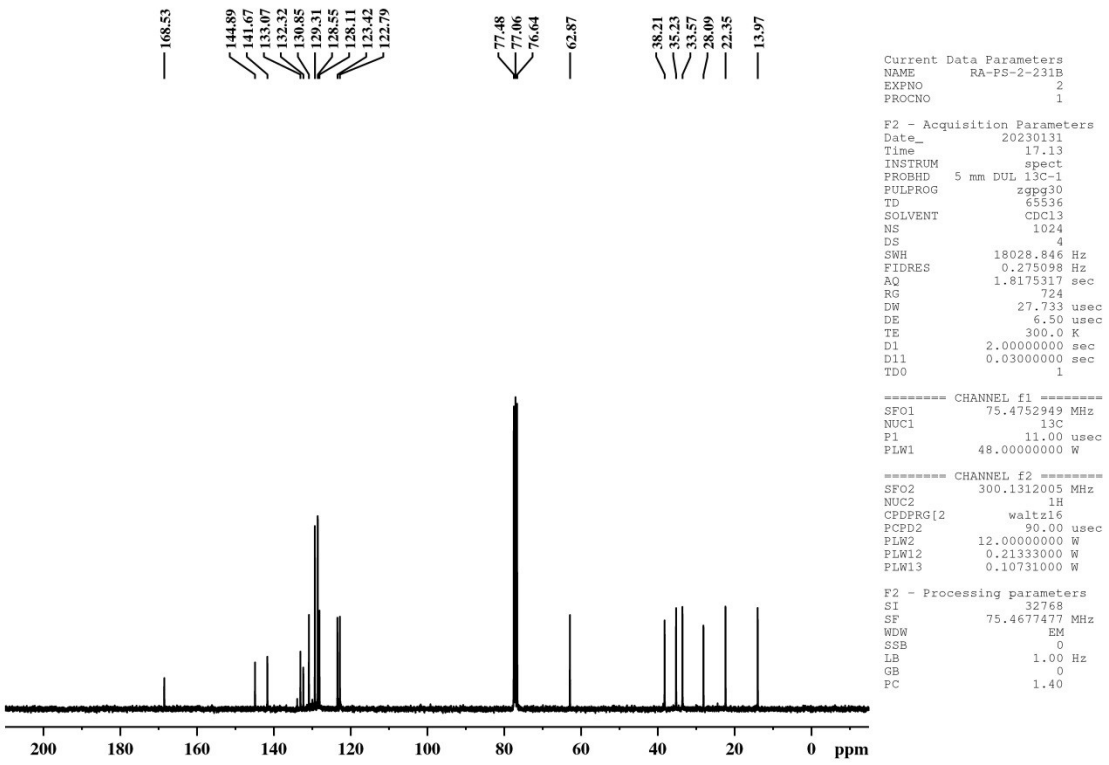



```
Current Data Parameters
NAME        RA-PS-2-231B
EXPNO                  1
PROCNO                 1

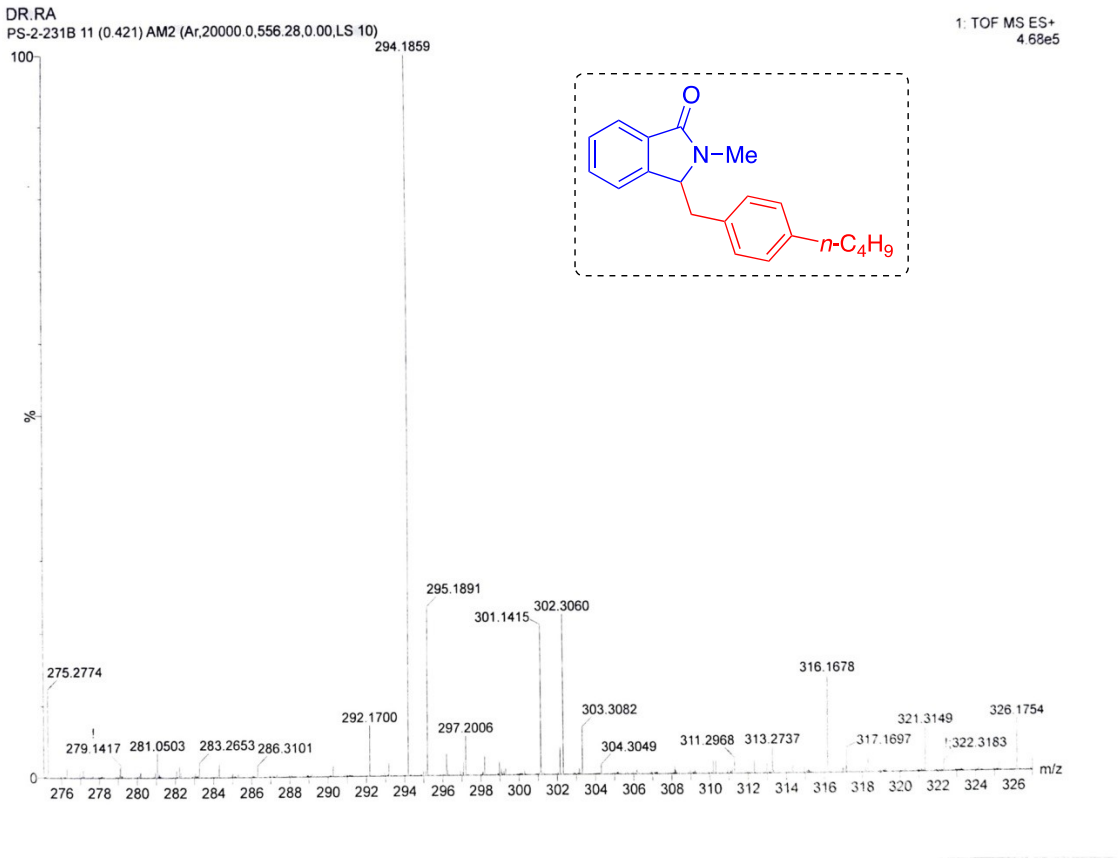
F2 - Acquisition Parameters
Date_           20230131
Time              16.05
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES         0.091699 Hz
AQ             5.4525952 sec
RG                  144
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                 1H
P1                12.00 usec
PLW1         12.00000000 W

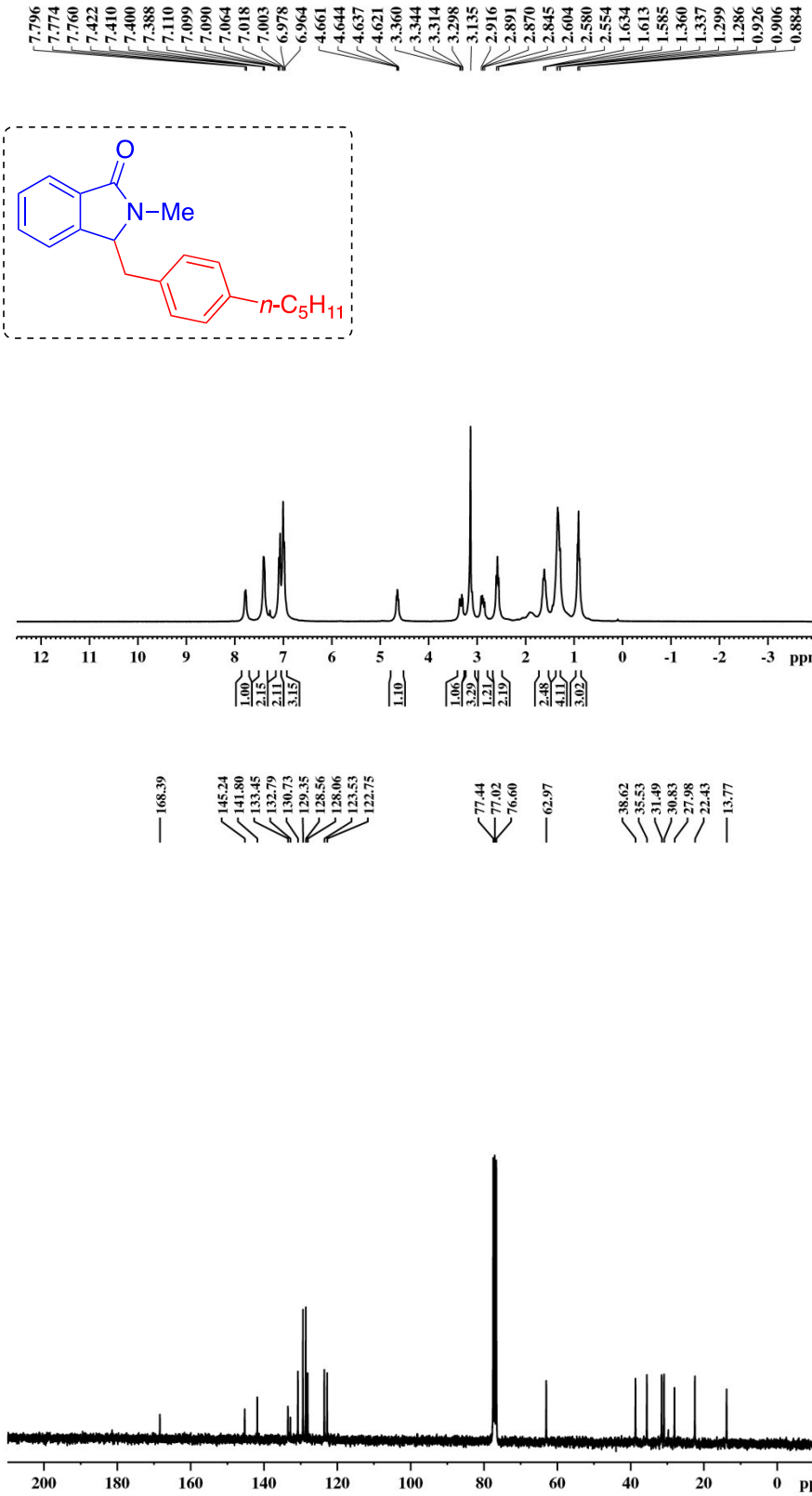
F2 - Processing parameters
SI                65536
SF           300.1300056 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



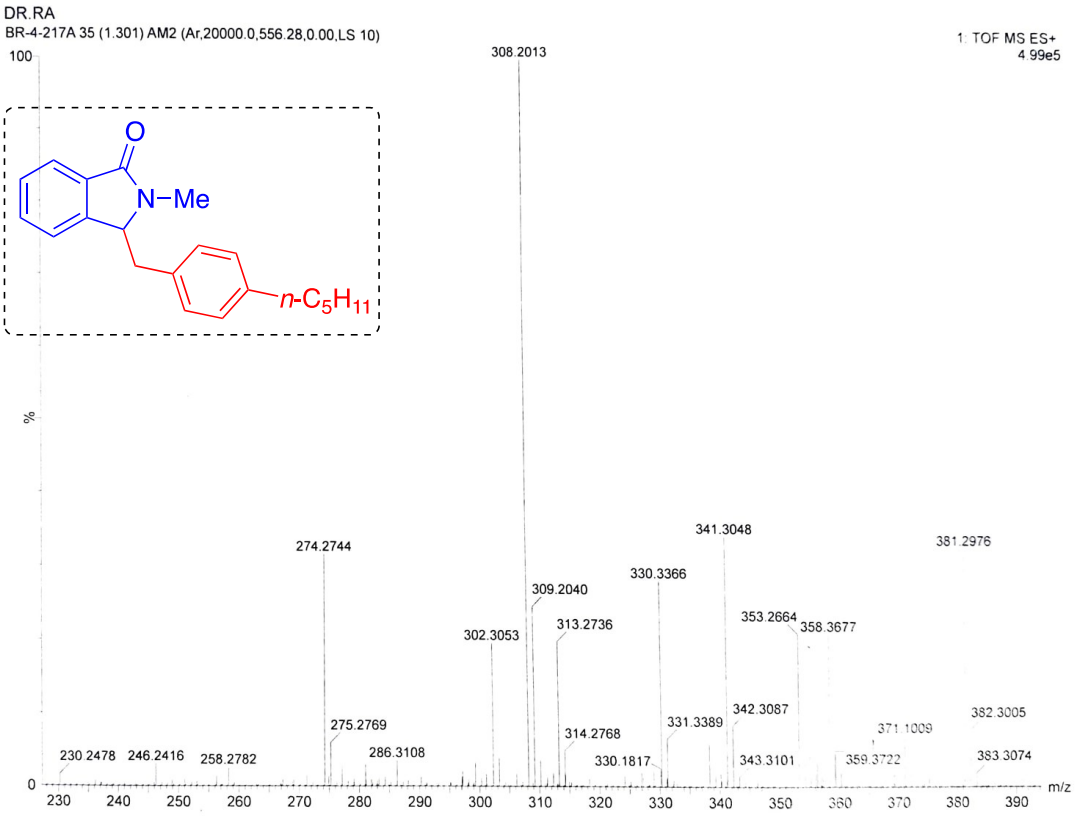
^{1}H and ^{13}C NMR Spectra of compound 2bf



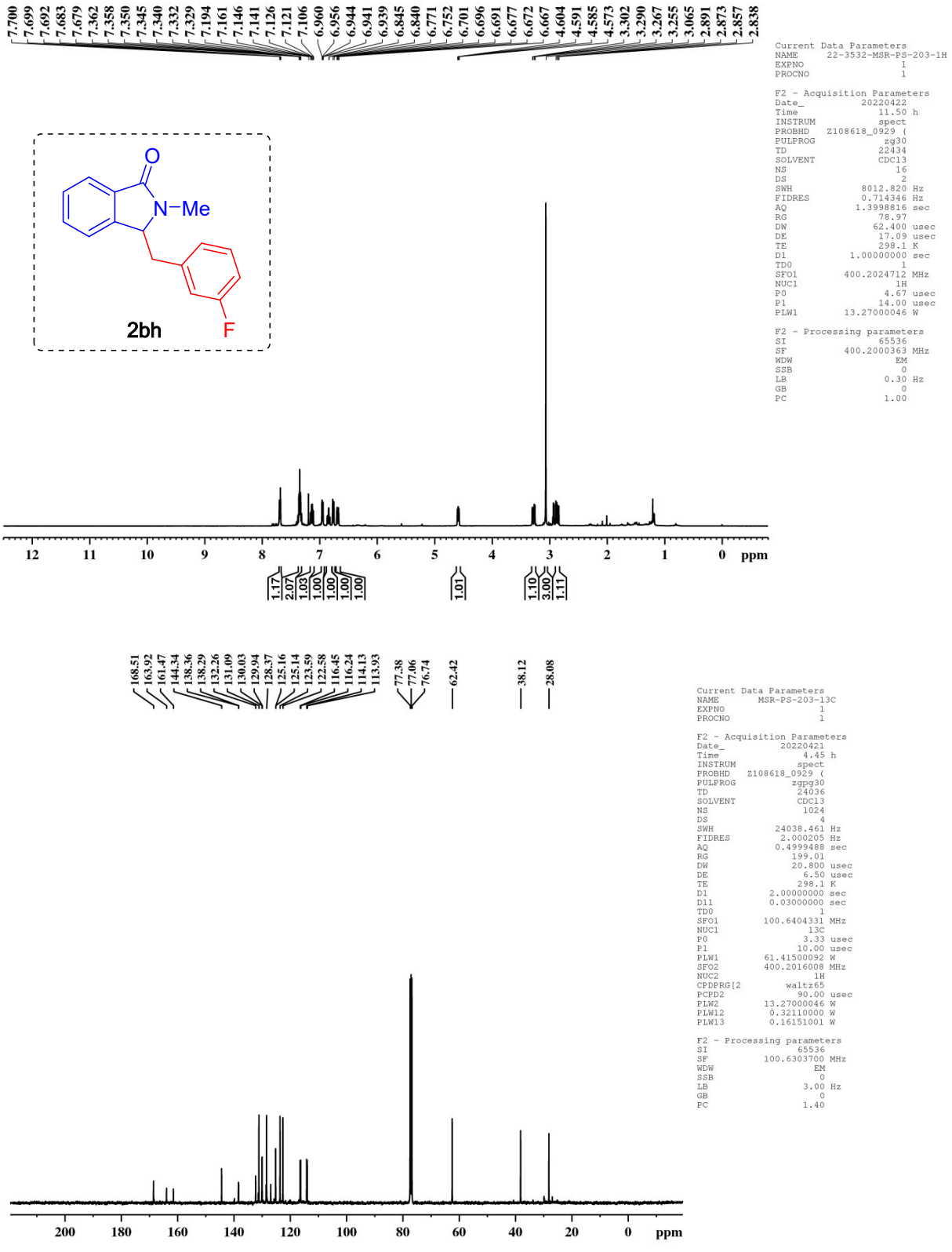
HRMS Spectrum of compound 2bf



^{1}H and ^{13}C NMR Spectra of compound 2bg



HRMS Spectrum of compound 2bg



Current Data Parameters
NAME 22-3532-MSR-PS-203-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220422
Time 11.50 h
INSTRUM spect
PROBHD Z108618_0929 (
PULPROG zg30
TD 22434
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.714346 Hz
AQ 1.3998816 sec
RG 78.97
DW 62.400 usec
DE 17.09 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.2024712 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 13.27000046 W

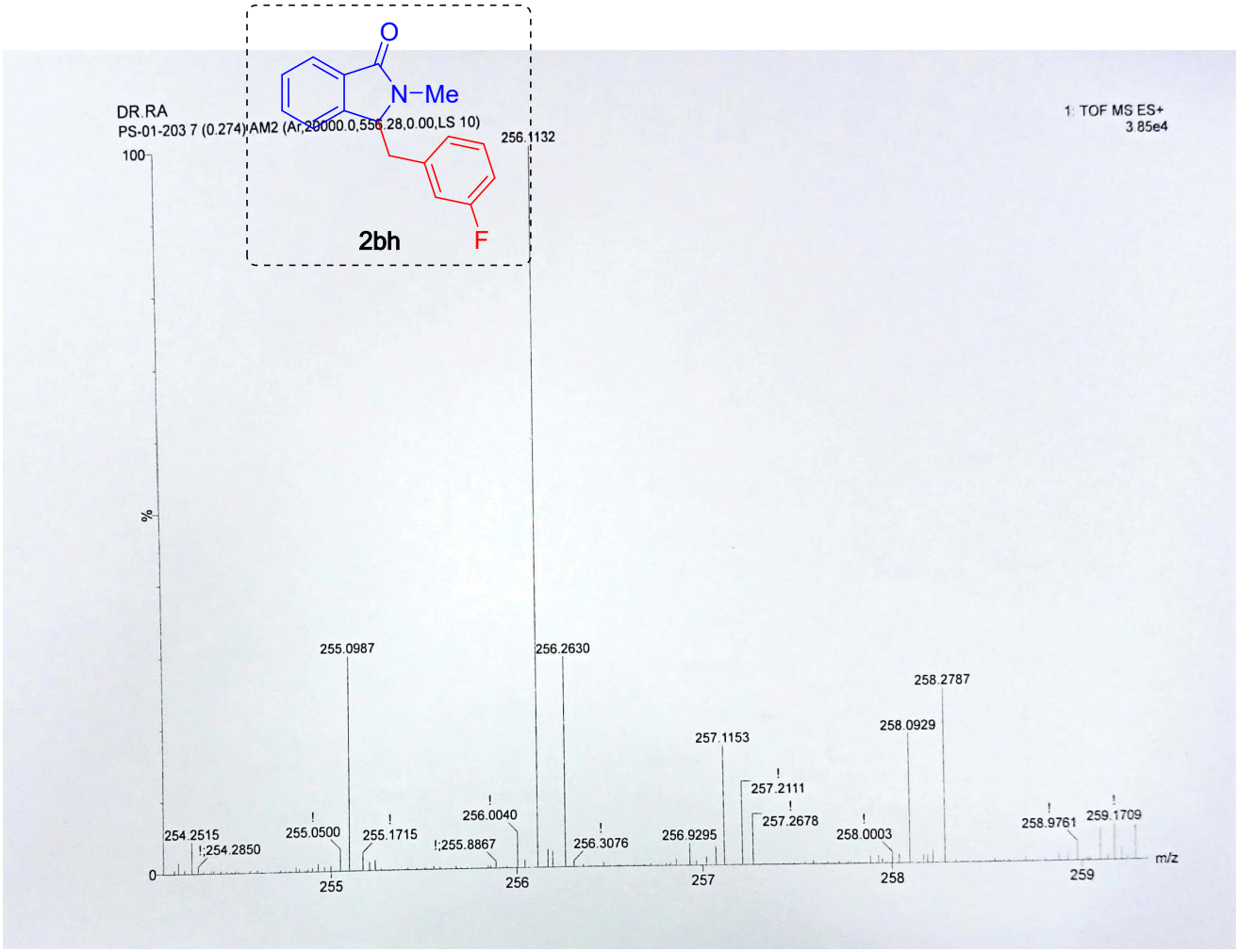
F2 - Processing parameters
SI 65536
SF 400.2000363 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME MSR-PS-203-13C
EXPNO 1
PROCNO 1

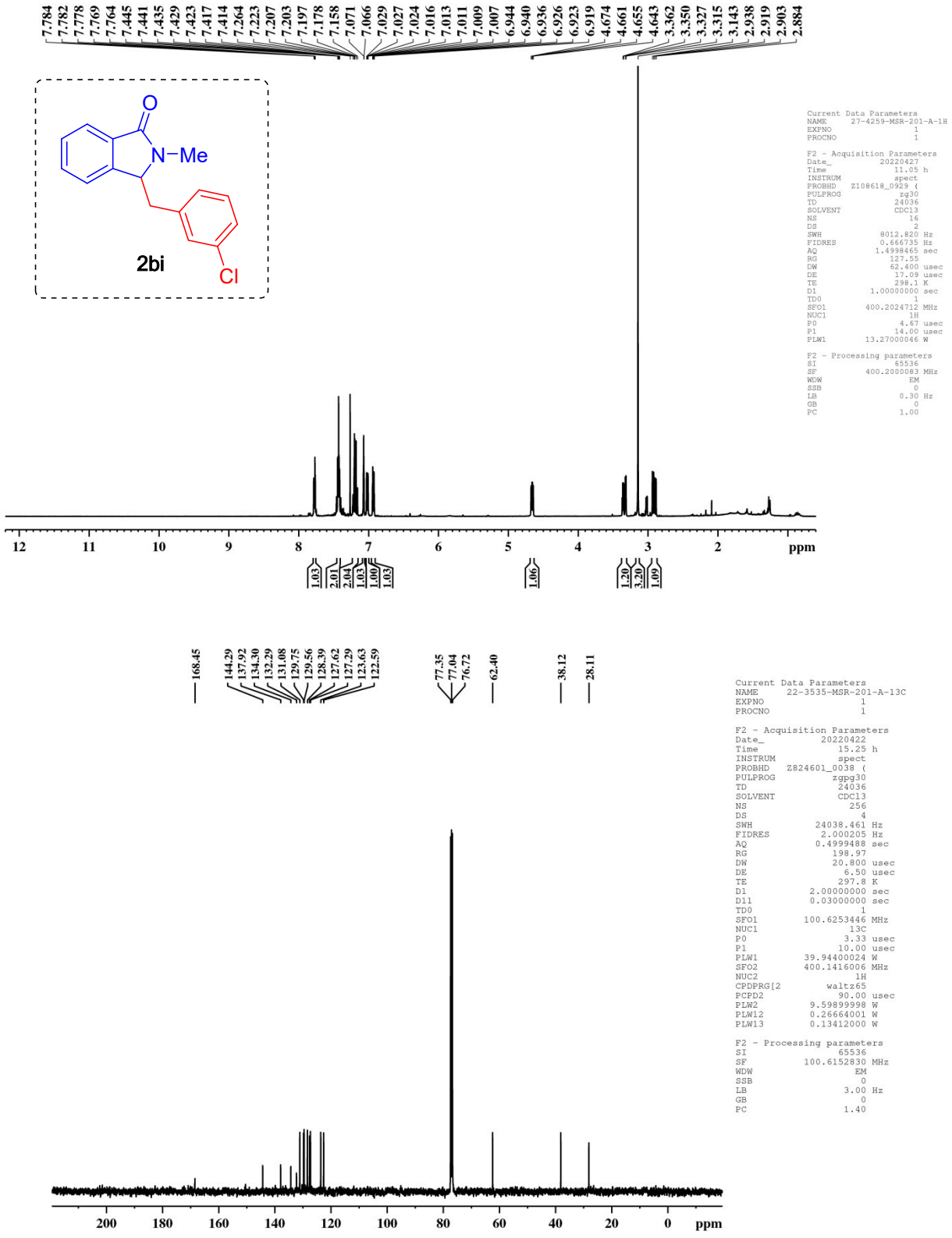
F2 - Acquisition Parameters
Date_ 20220421
Time 4.45 h
INSTRUM spect
PROBHD Z108618_0929 (
PULPROG zgpg30
TD 24036
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 2.000205 Hz
AQ 0.4999488 sec
RG 199.01
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6404331 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 61.41500092 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 13.27000046 W
PLW12 0.32110000 W
PLW13 0.16151001 W

F2 - Processing parameters
SI 65536
SF 100.6303700 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

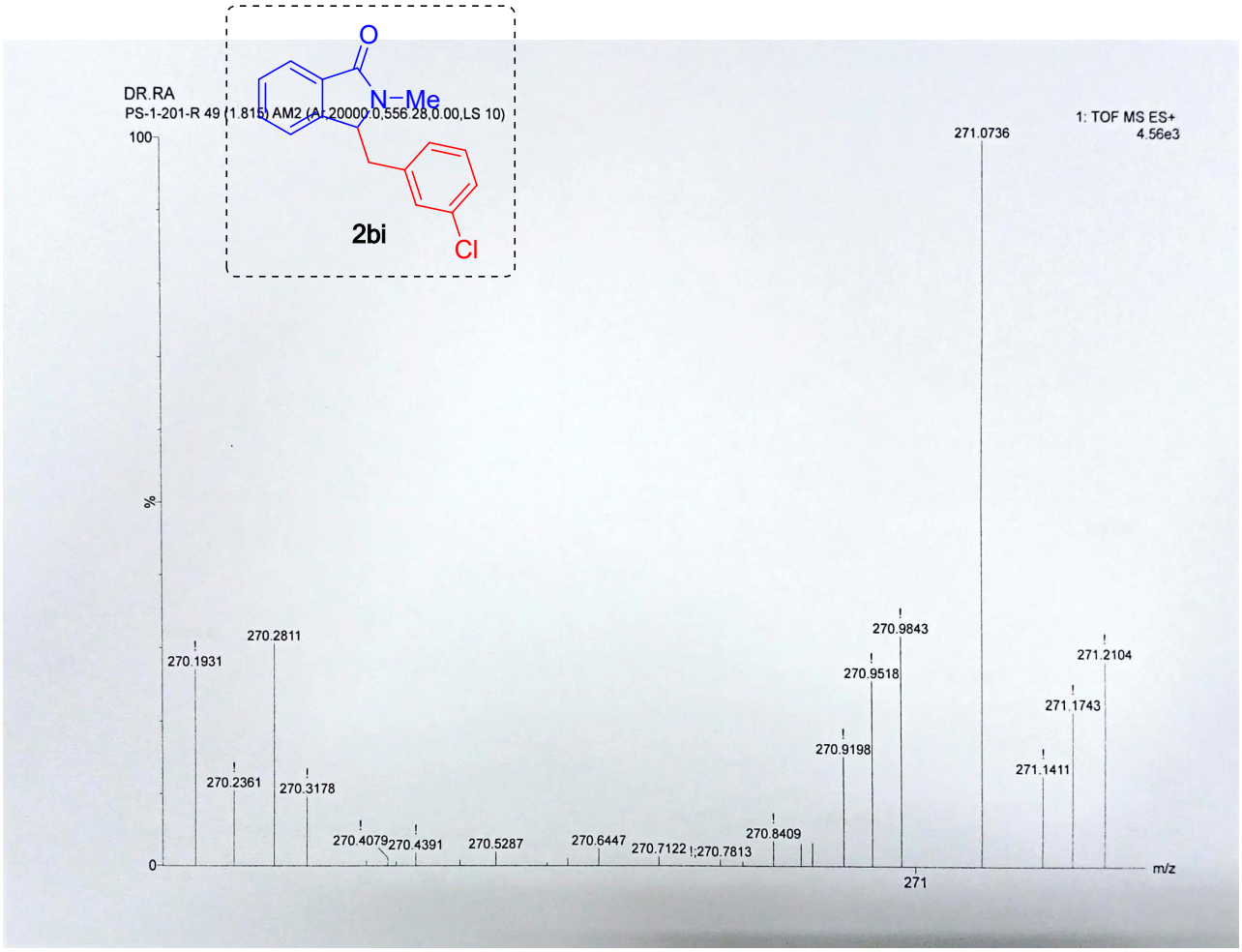
^{1}H and ^{13}C NMR Spectra of compound 2bh



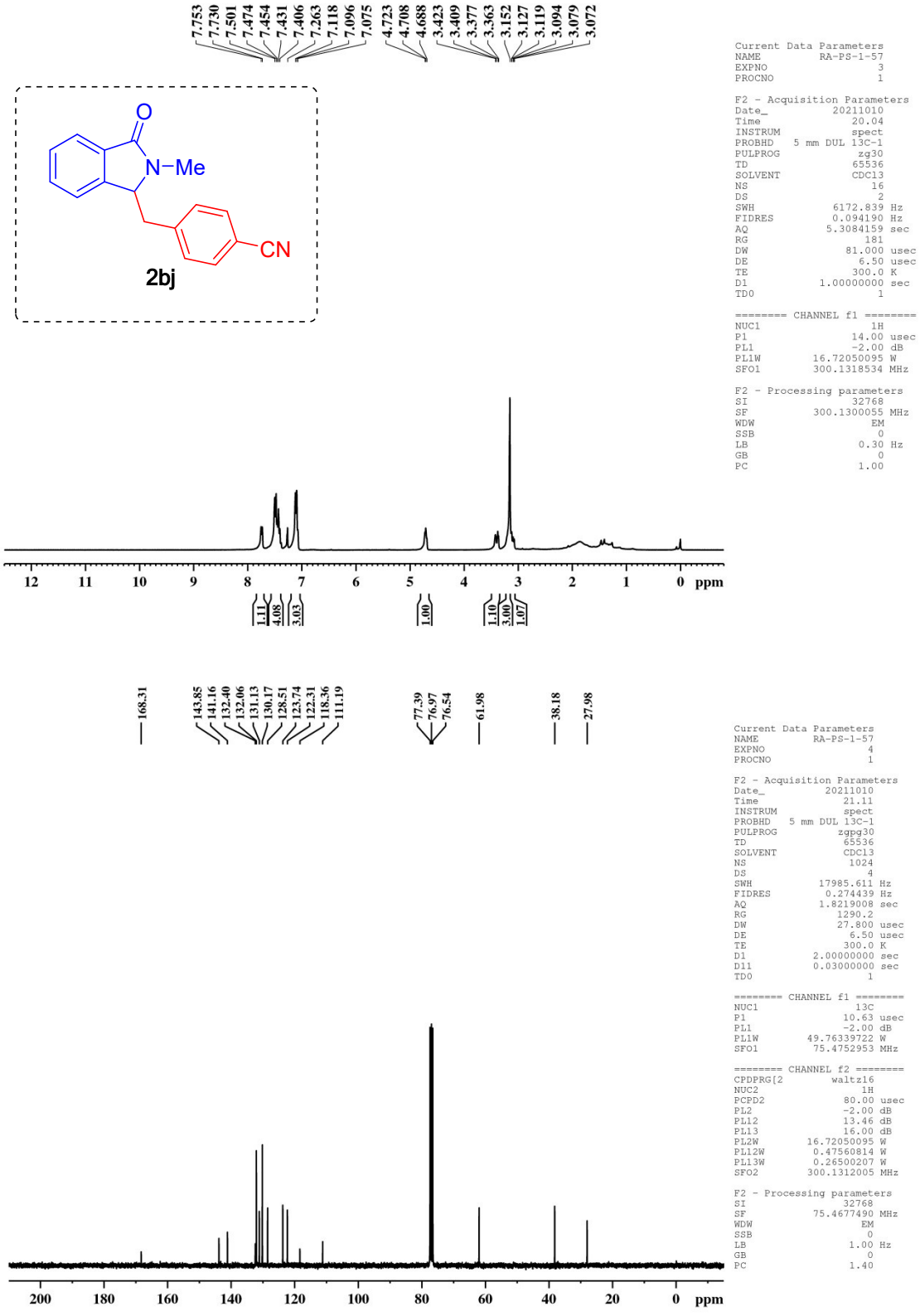
HRMS Spectrum of compound 2bh



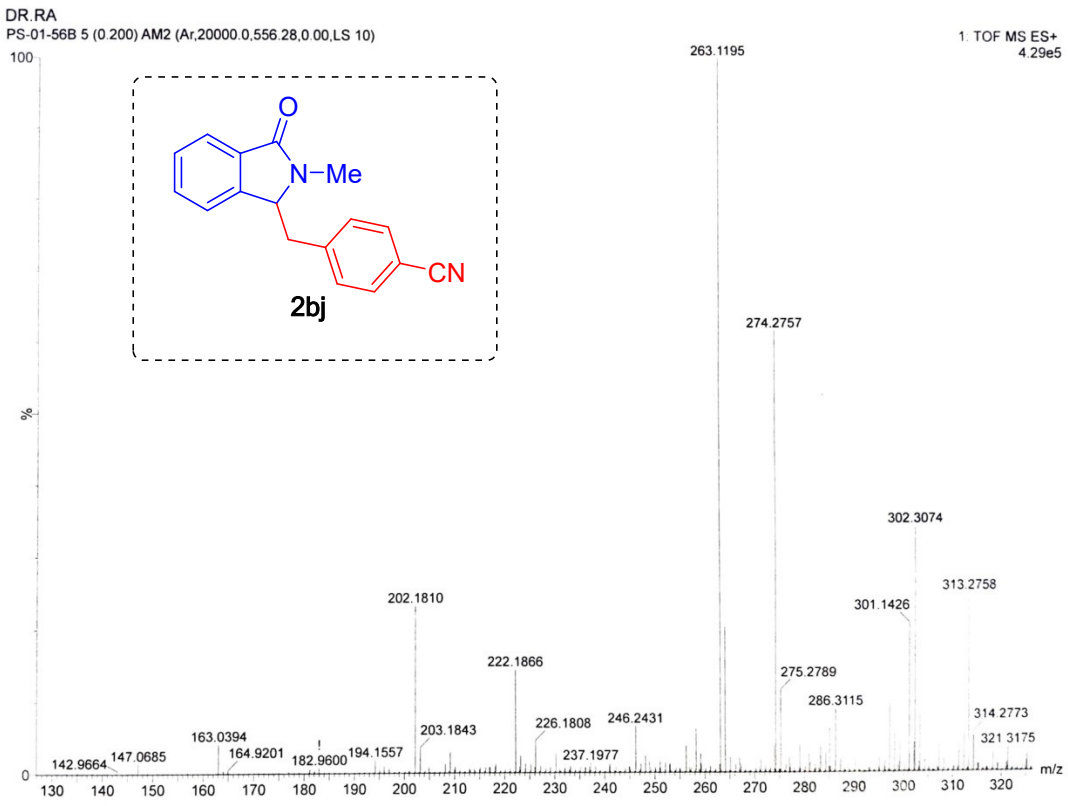
^{1}H and ^{13}C NMR Spectra of compound 2bi



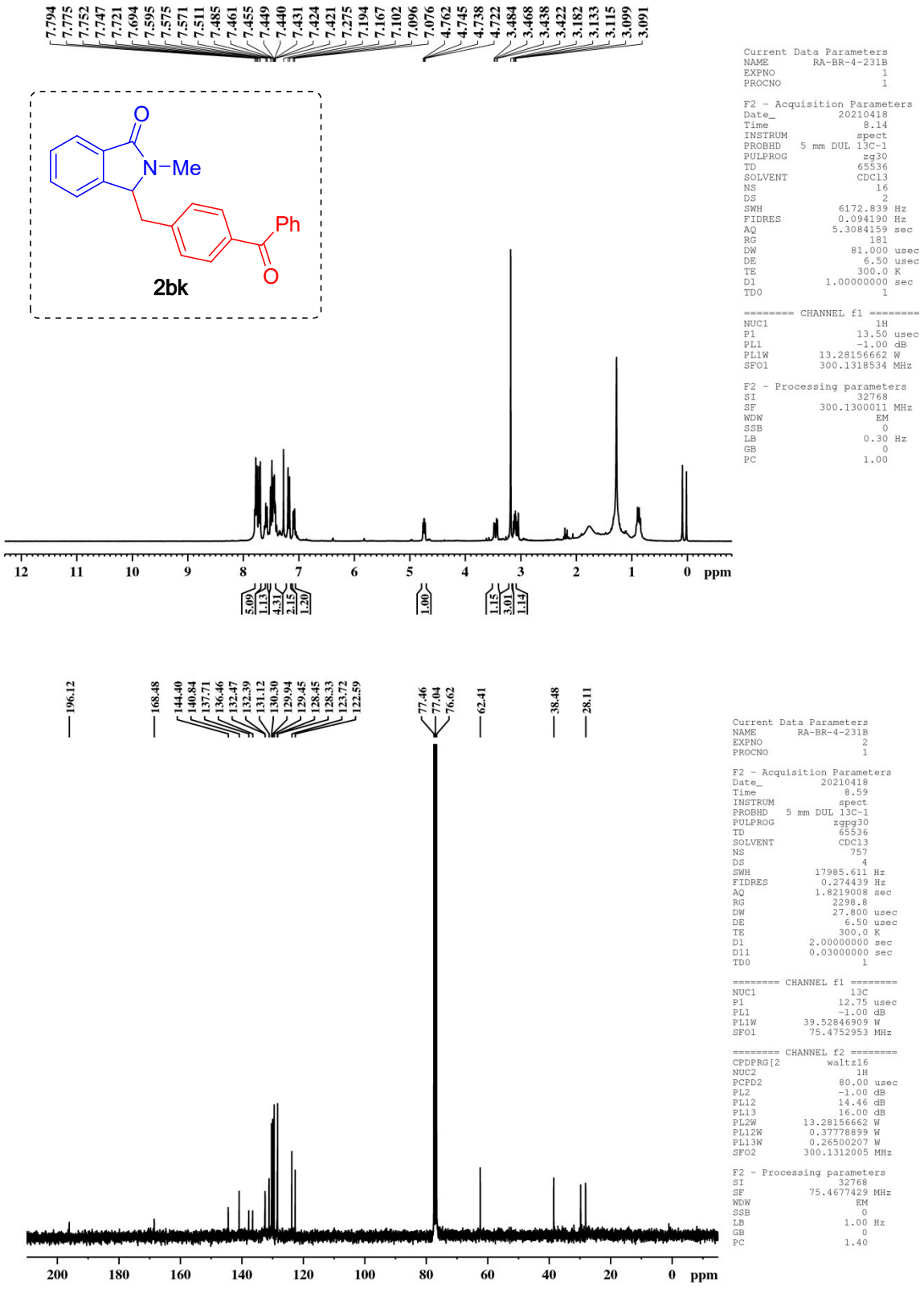
HRMS Spectrum of compound 2bi



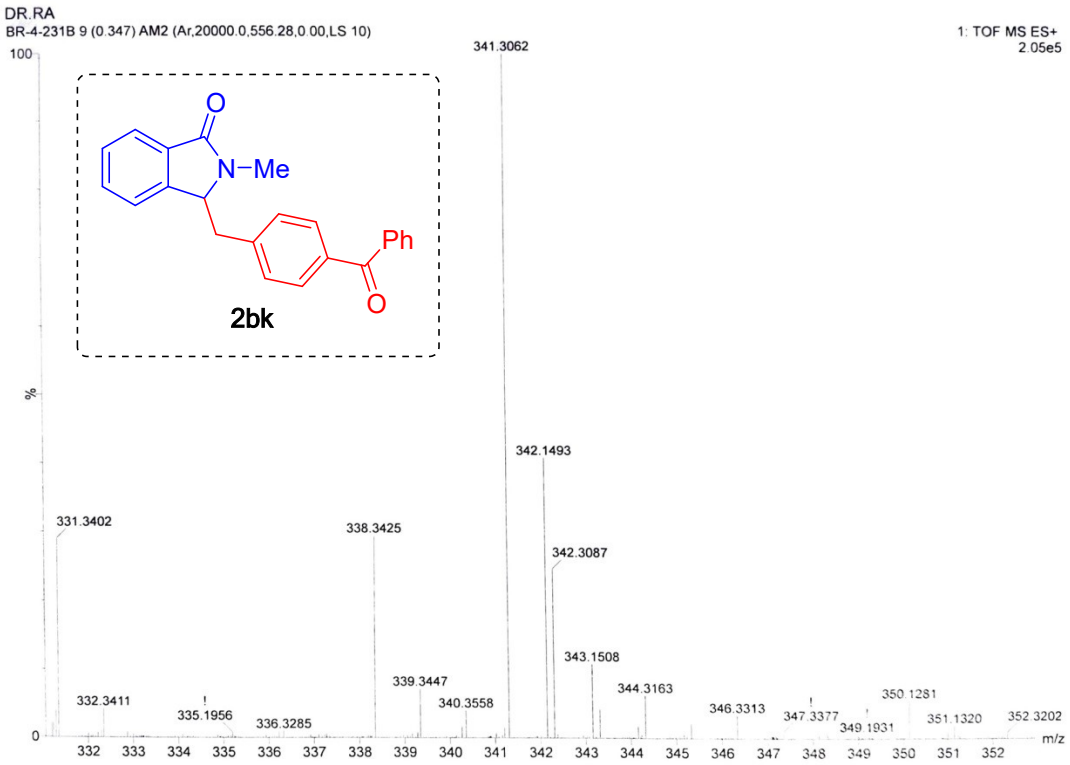
^{1}H and ^{13}C NMR Spectra of compound 2bj



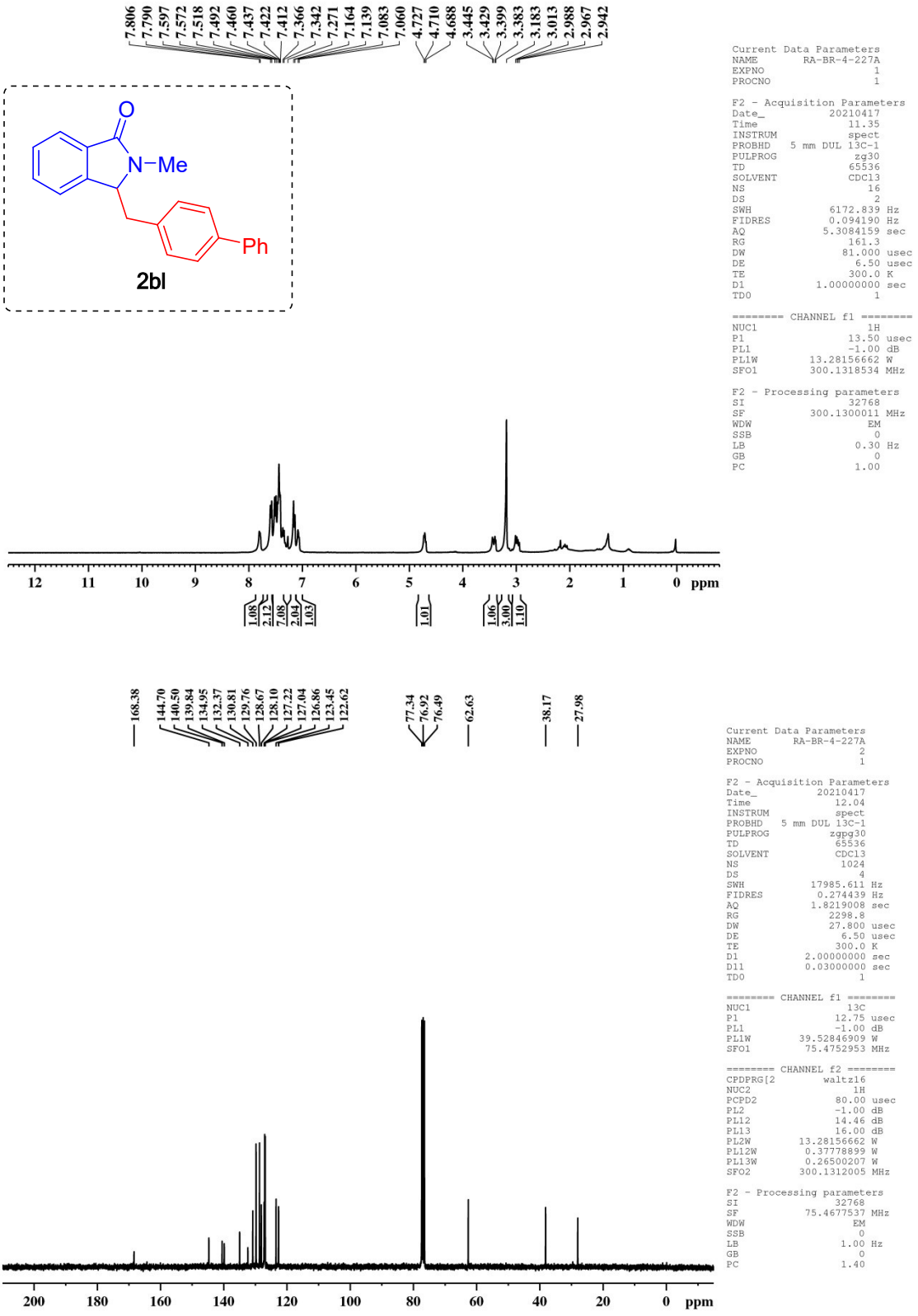
^{1}H and ^{13}C NMR Spectra of compound 2bj



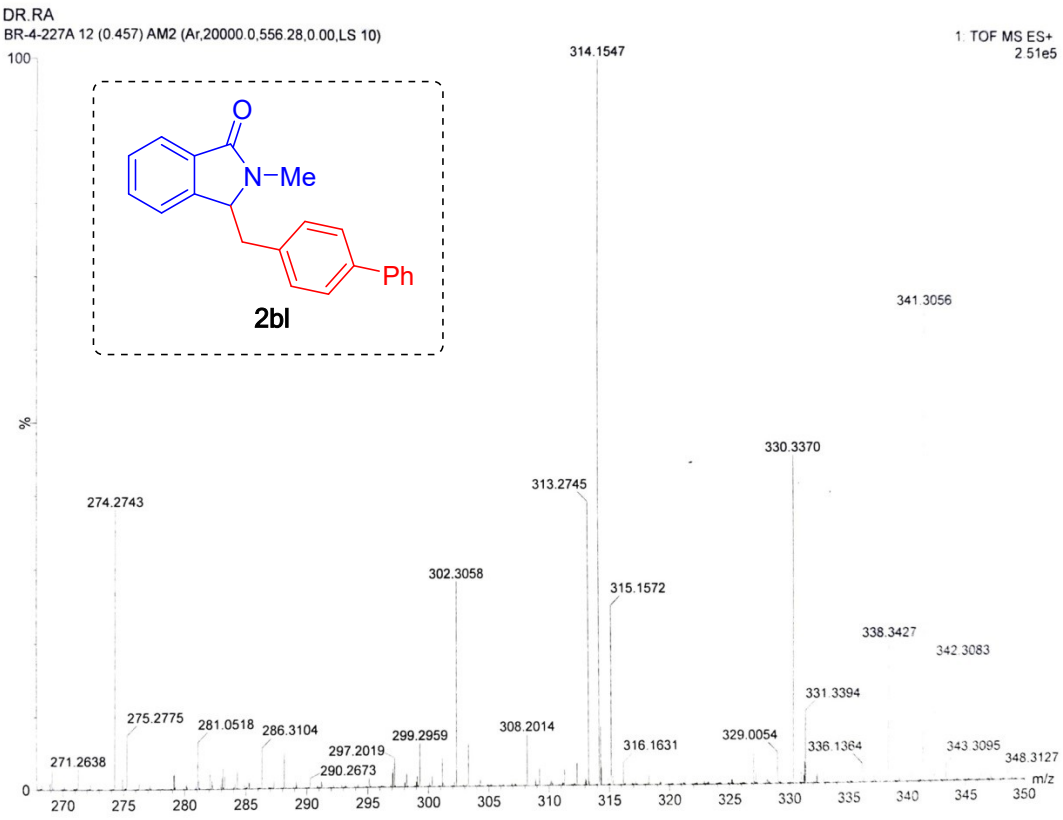
^{1}H and ^{13}C NMR Spectra of compound 2bk



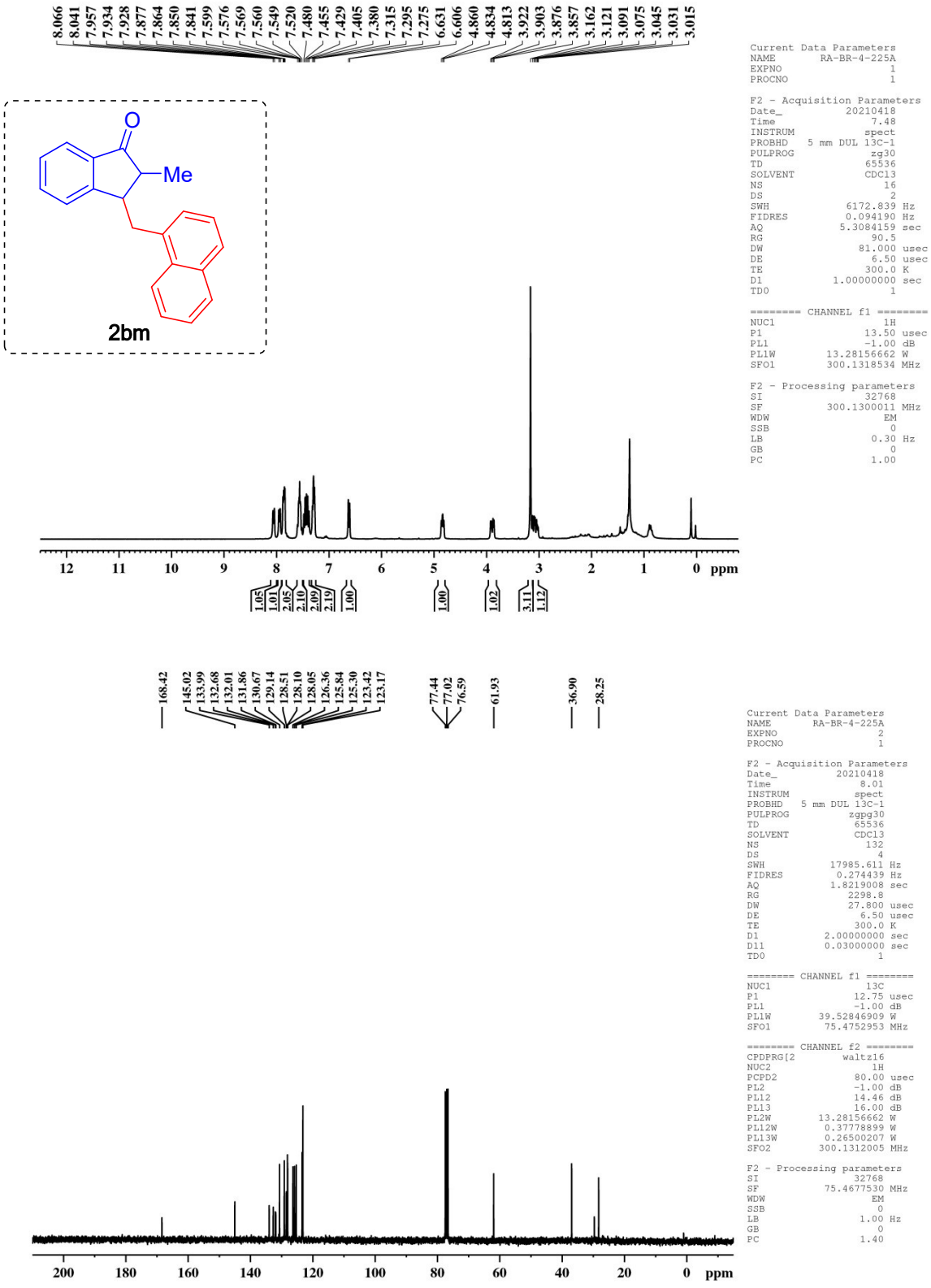
HRMS Spectrum of compound 2bk



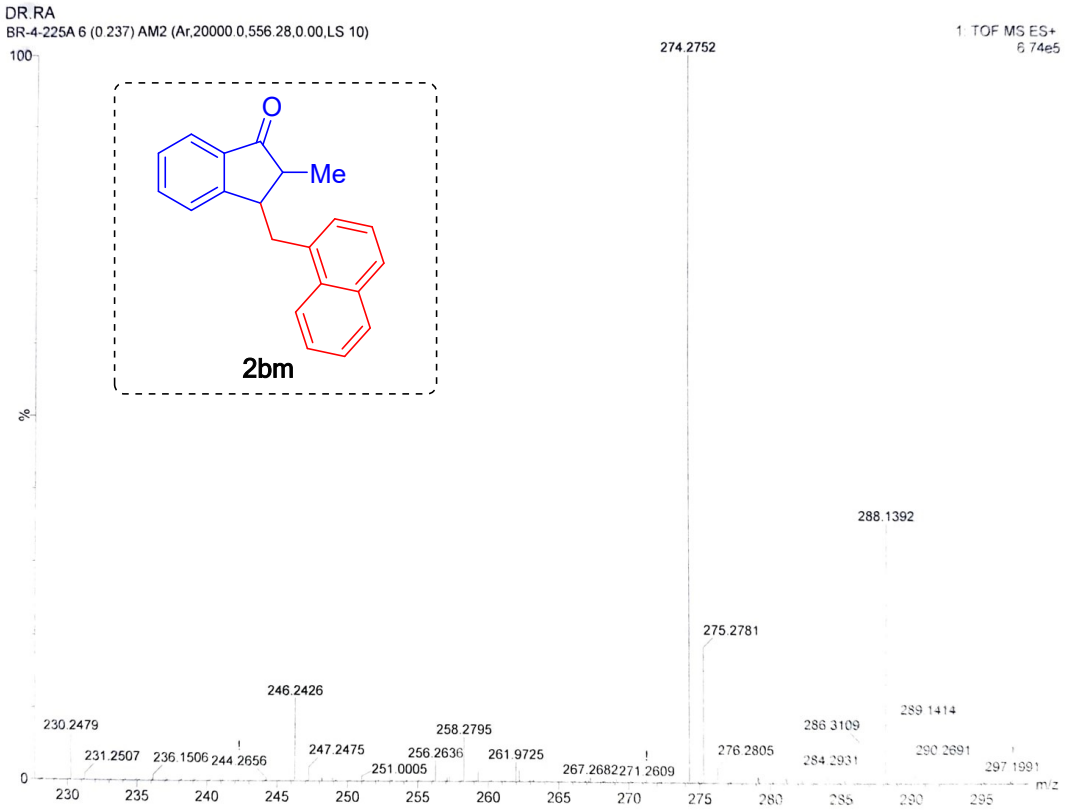
^{1}H and ^{13}C NMR Spectra of compound 2bl



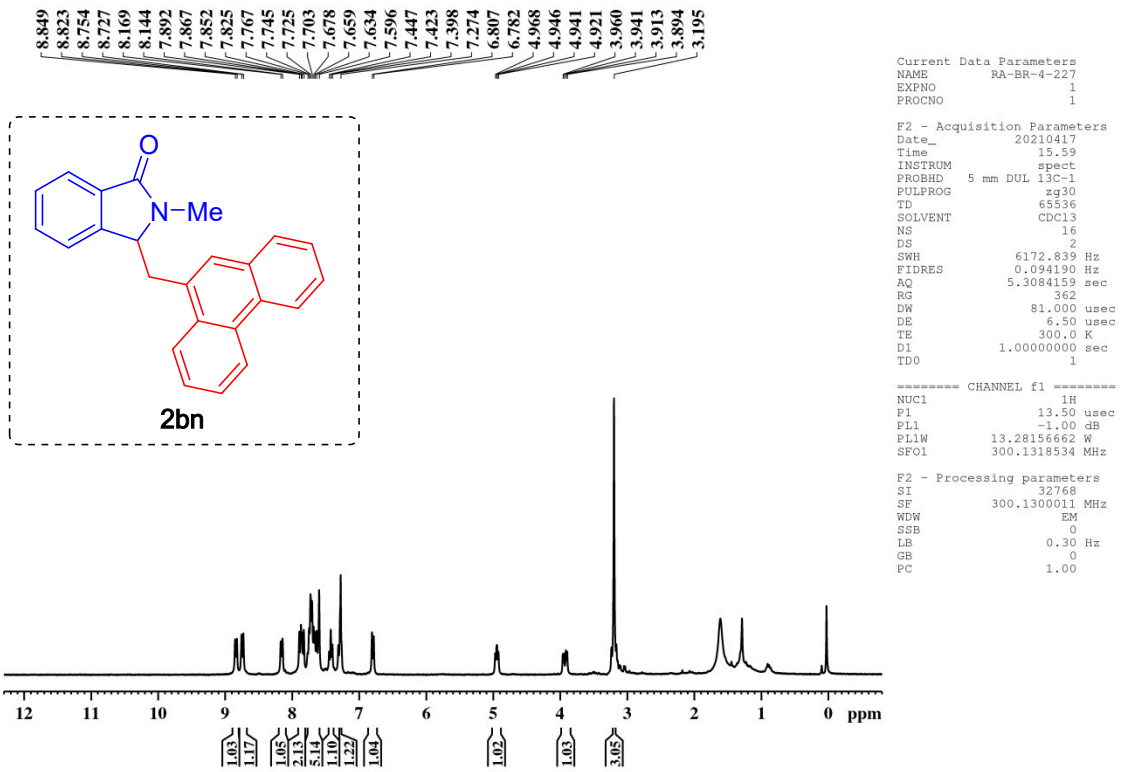
HRMS Spectrum of compound 2bl



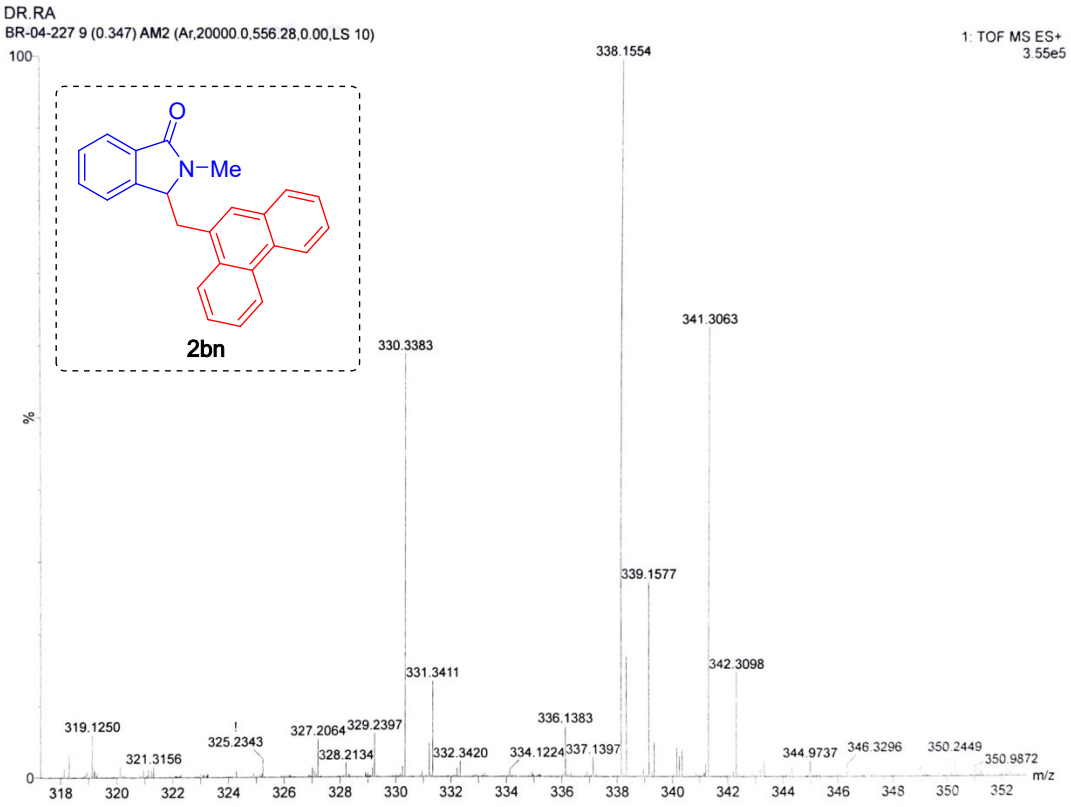
^{1}H and ^{13}C NMR Spectra of compound 2bm



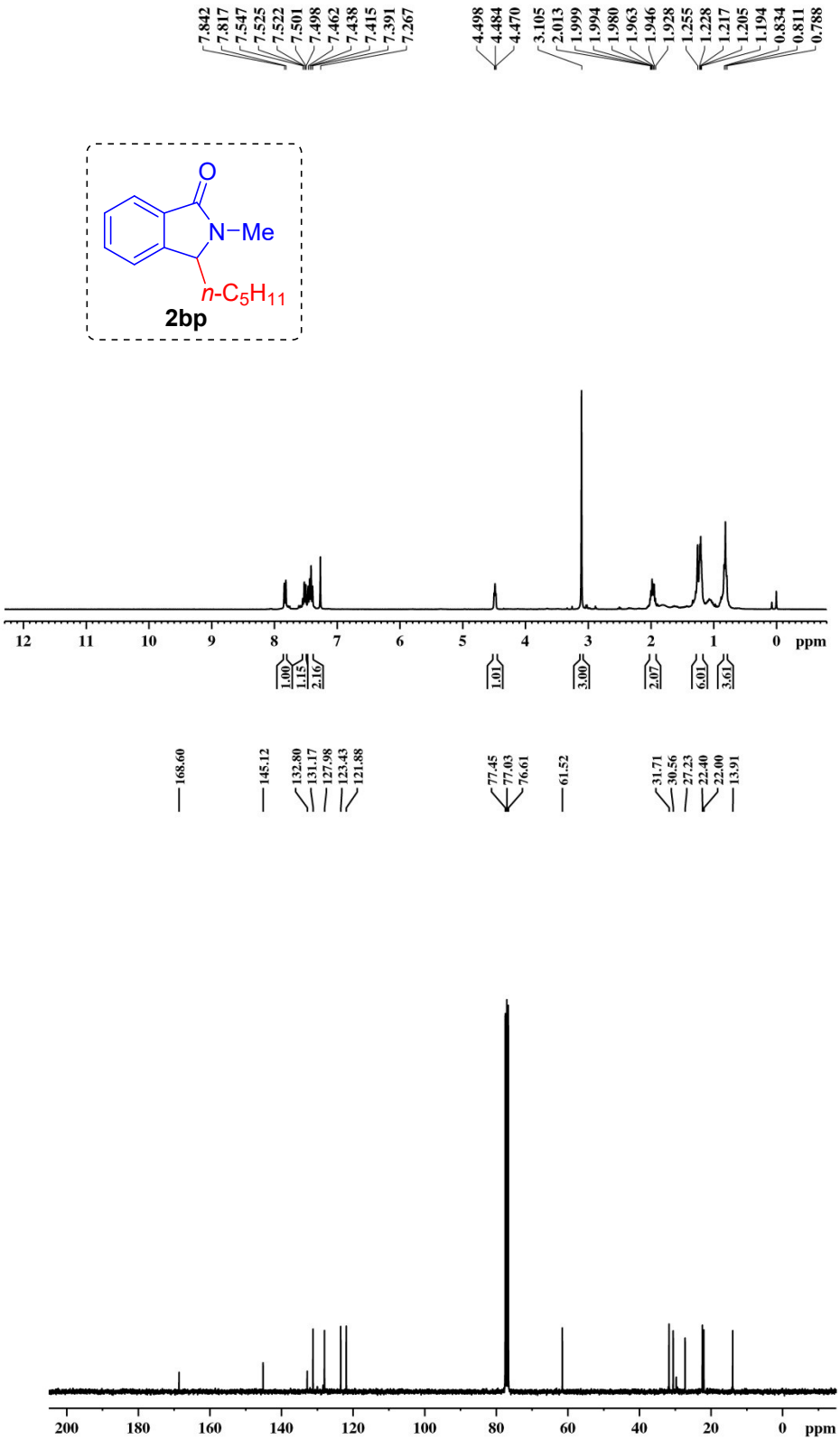
HRMS Spectrum of compound 2bm



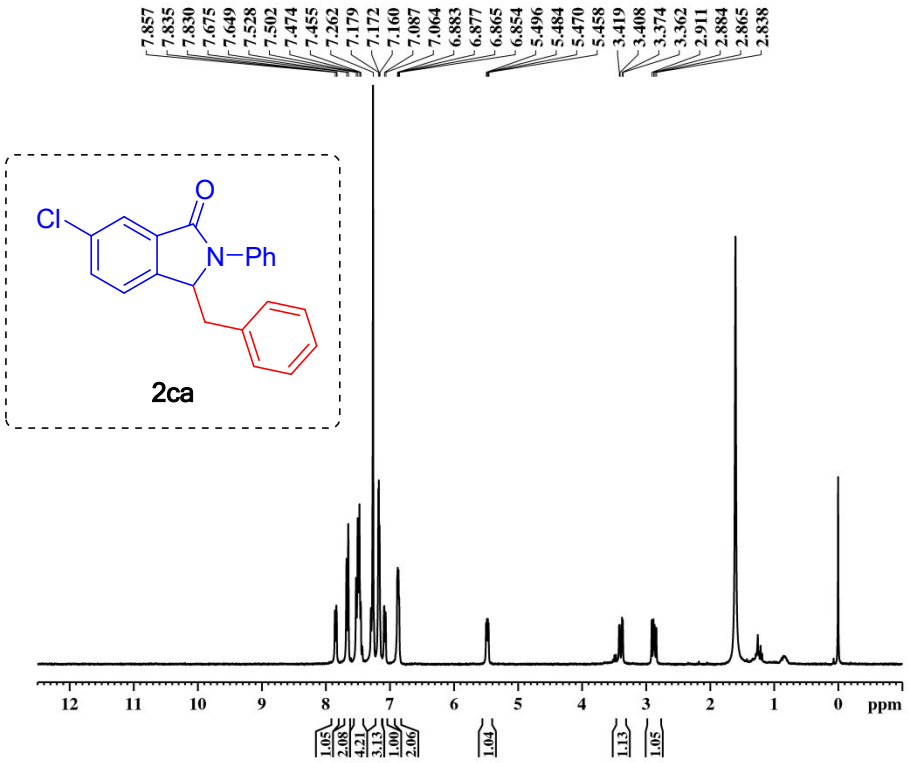
^{1}H and ^{13}C NMR Spectra of compound 2bn



HRMS Spectrum of compound 2bn



^{1}H and ^{13}C NMR Spectra of compound 2bo

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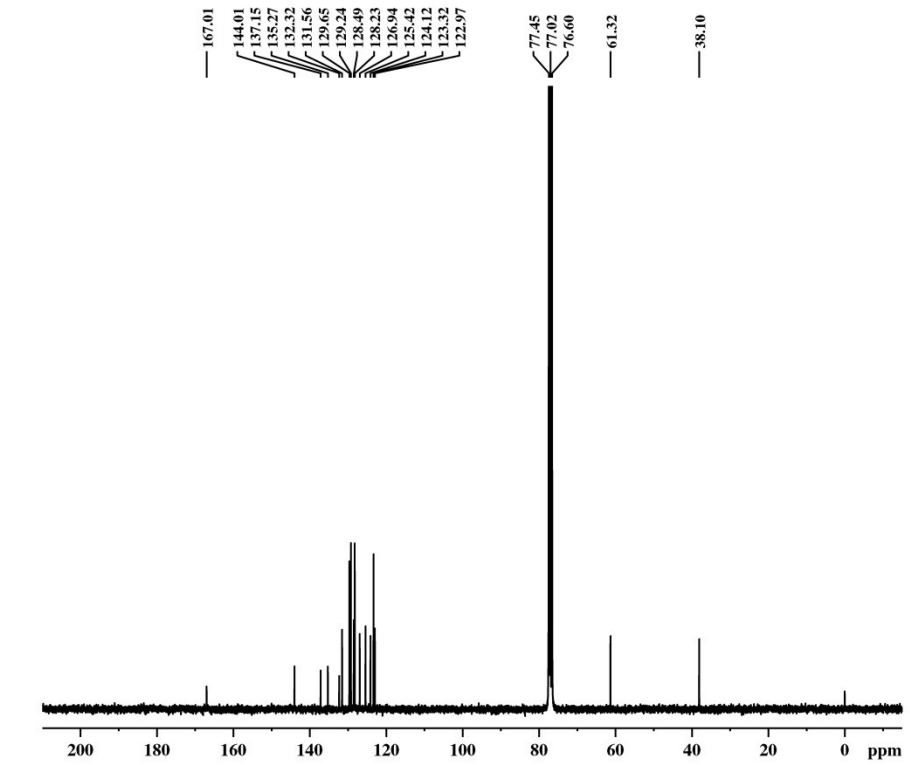
Current Data Parameters
NAME        RA-PS-2-242A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230203
Time               18.59
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   406
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1300061 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME        RA-PS-2-242A
EXPNO                  4
PROCNO                 1

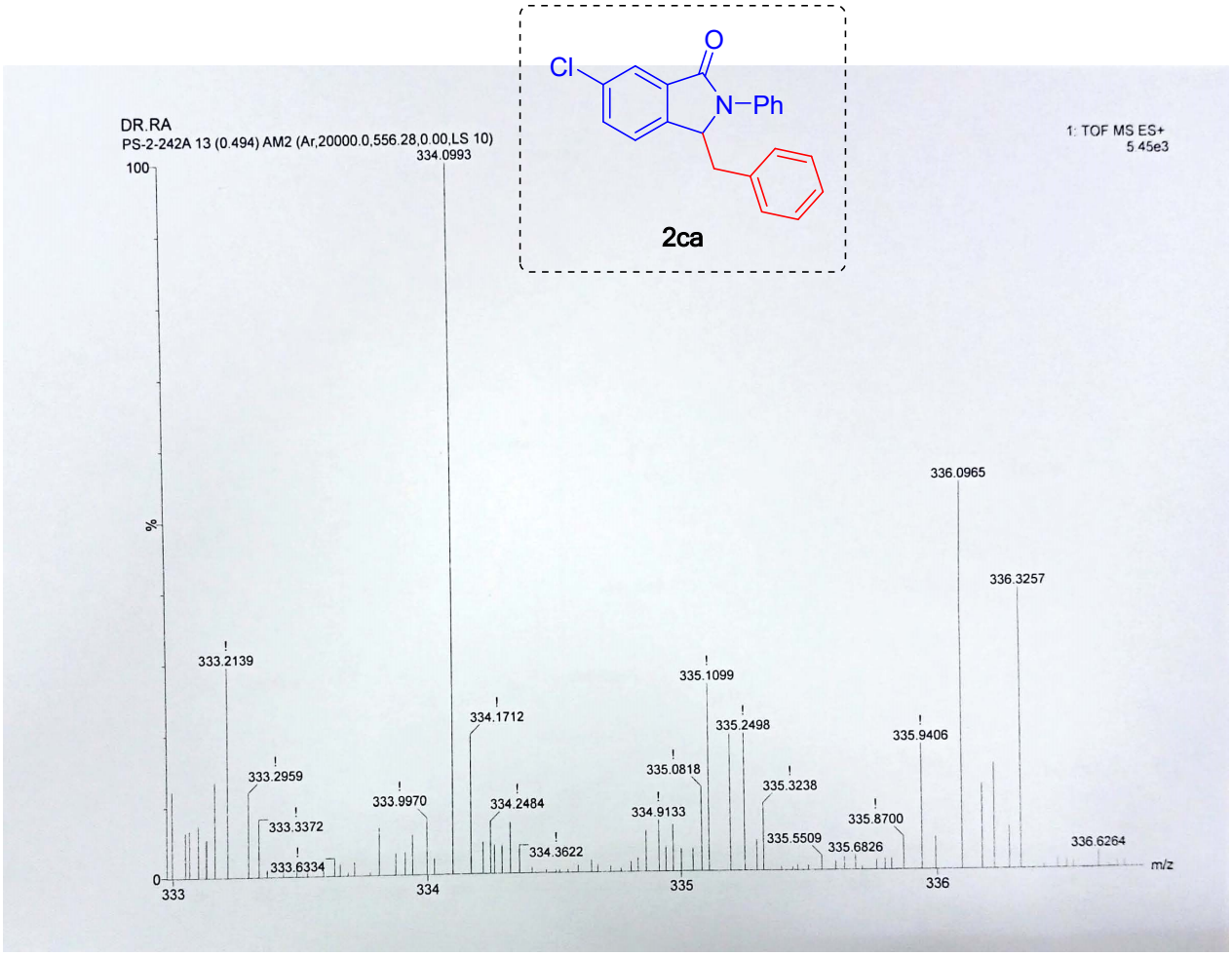
F2 - Acquisition Parameters
Date_           20230204
Time               9.40
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  9000
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175317 sec
RG                   645
DW                27.733 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                  13C
P1                 11.00 usec
PLW1          48.00000000 W

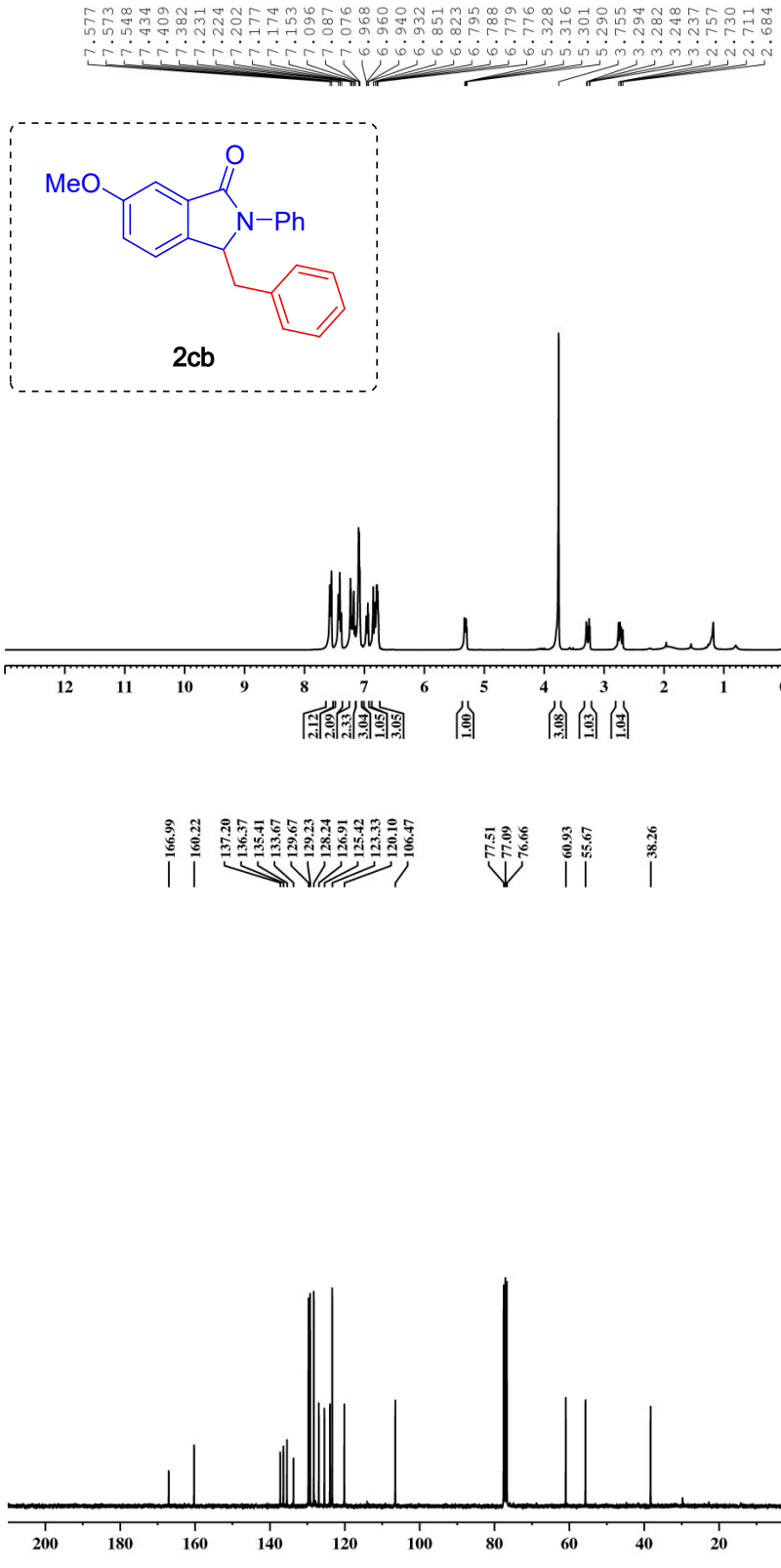
======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.21333000 W
PLW13          0.10731000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

^{1}H and ^{13}C NMR Spectra of compound 2ca



HRMS Spectrum of compound 2ca




```
Current Data Parameters
NAME        RA-PS2-242-B
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230202
Time              23.12
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4525952 sec
RG                  114
DW               83.200 usec
DE                6.50 usec
TE               298.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 12.00 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300321 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

```
Current Data Parameters
NAME        RA-PS2-242-B
EXPNO                  2
PROCNO                 1

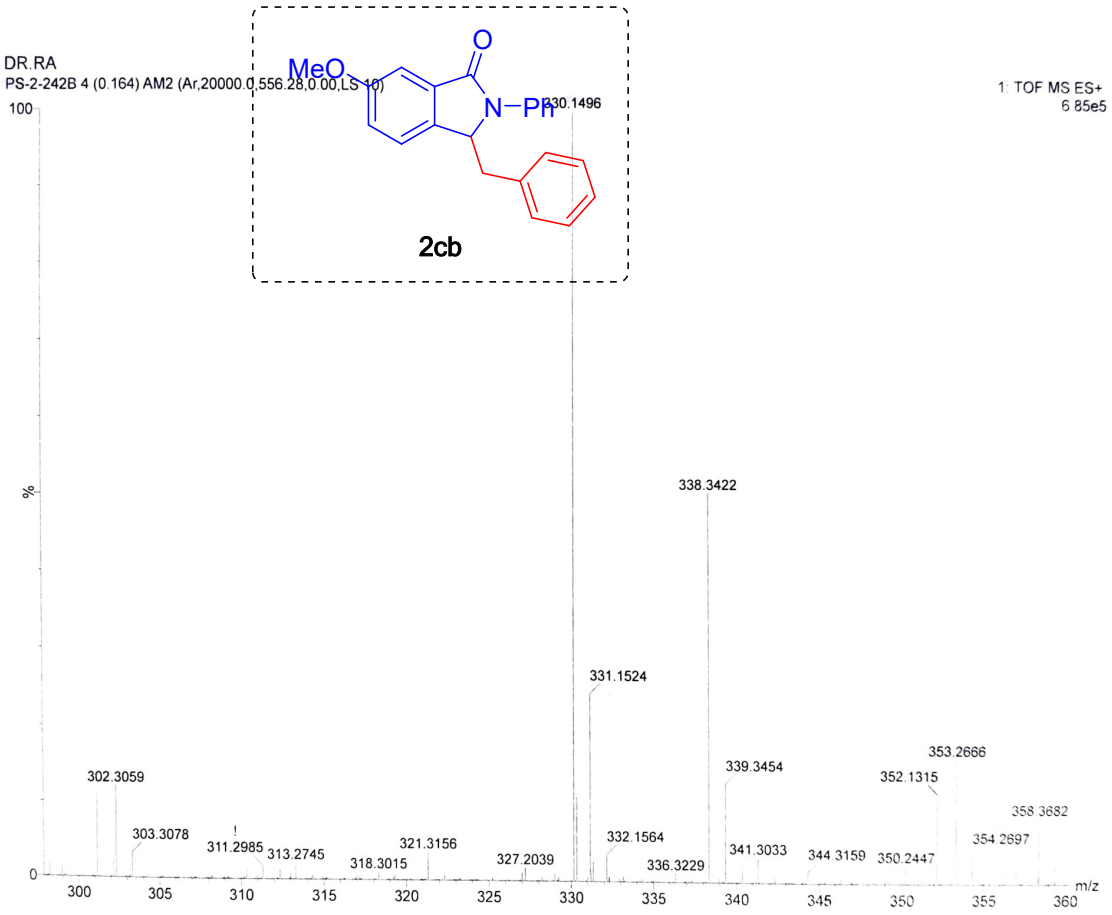
F2 - Acquisition Parameters
Date_           20230203
Time              0.20
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175317 sec
RG                 1150
DW               27.733 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                  13C
P1                 11.00 usec
PLW1         48.00000000 W

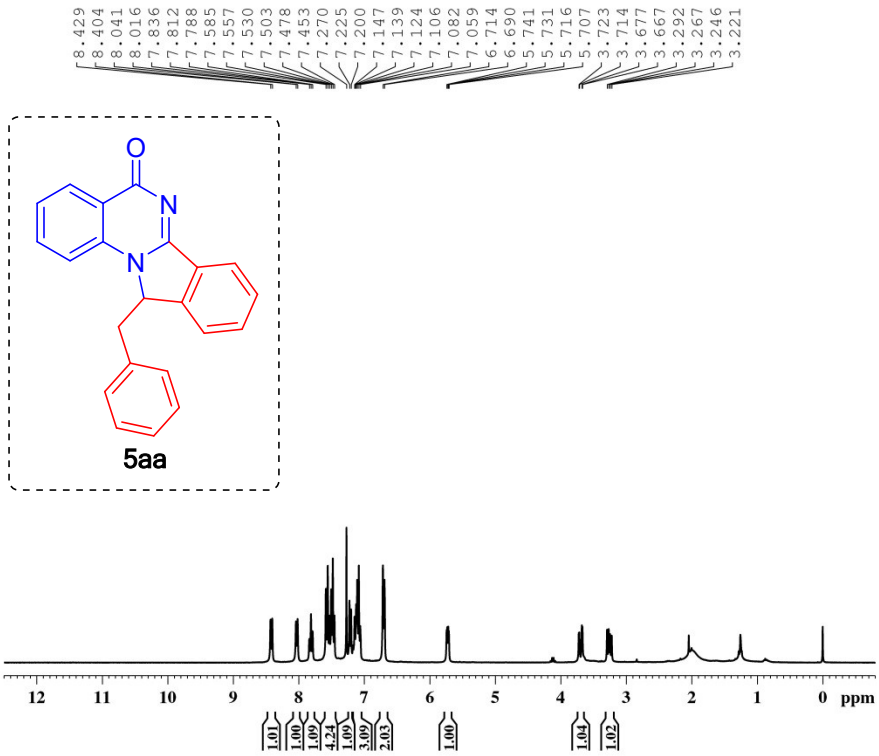
======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         12.00000000 W
PLW12         0.21333000 W
PLW13         0.10731000 W

F2 - Processing parameters
SI                 32768
SF           75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

^{1}H and ^{13}C NMR Spectra of compound 2cb



HRMS Spectrum of compound 2cb

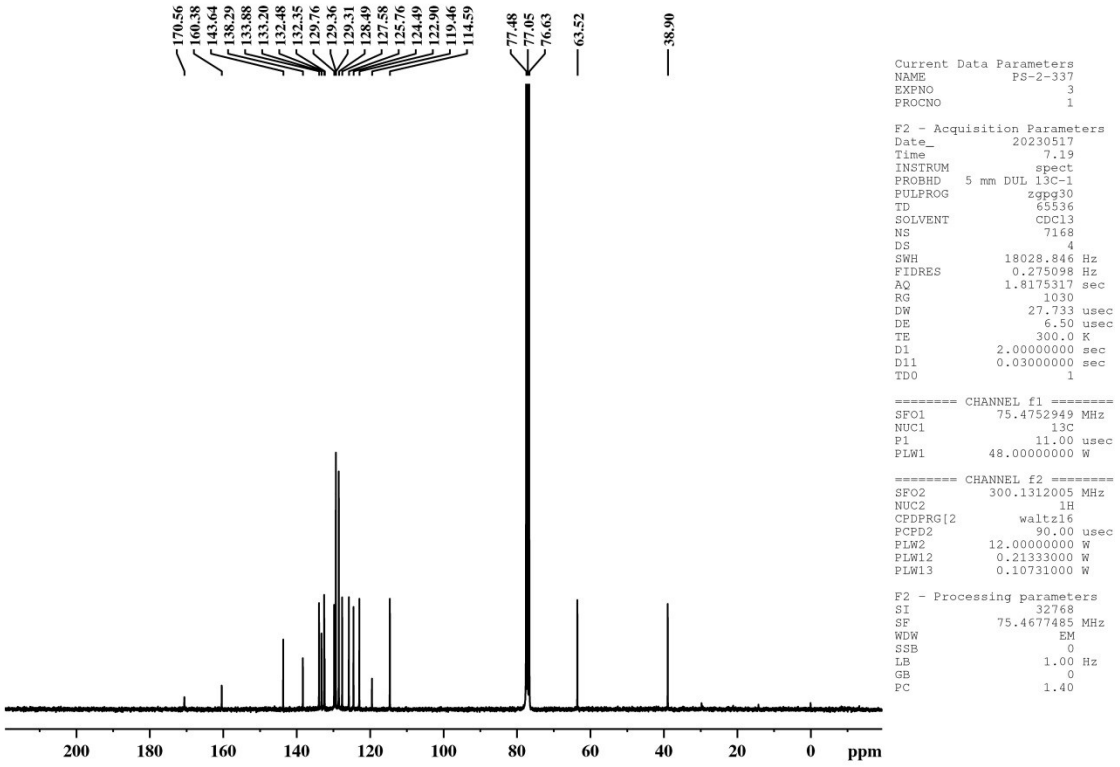



```
Current Data Parameters
NAME                  PS-2-337
EXPNO                        4
PROCNO                       1

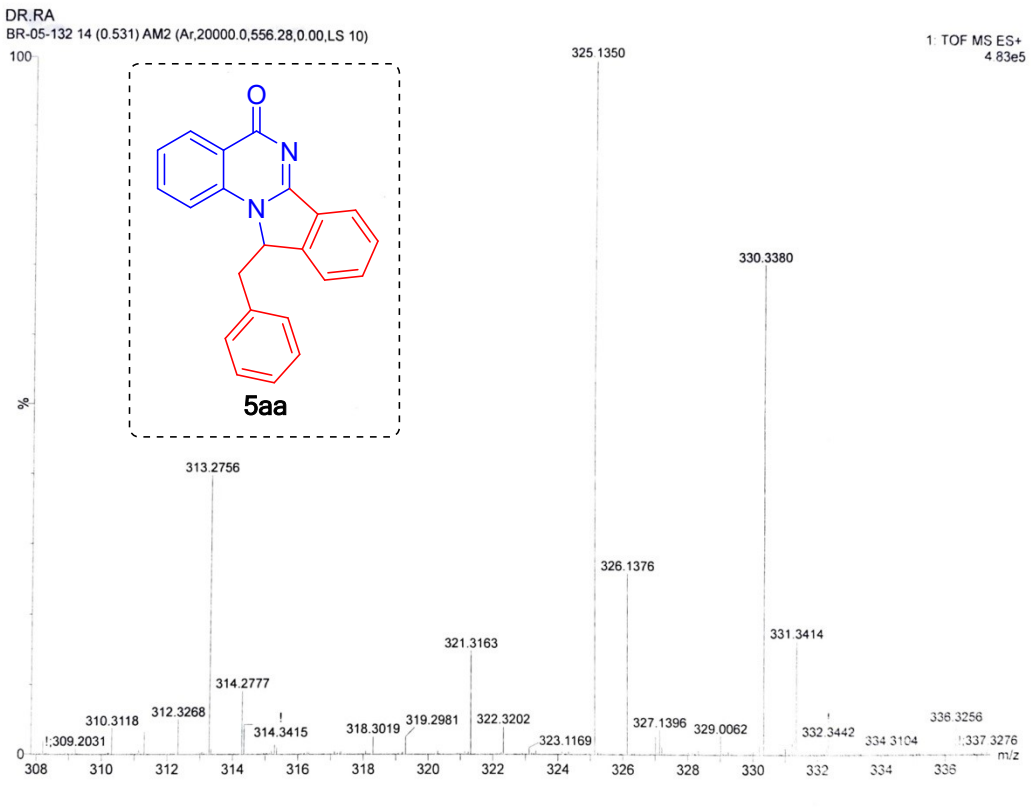
F2 - Acquisition Parameters
Date_                 20230517
Time                      7.23
INSTRUM                  spect
PROBHD    5 mm DUL 13C-1
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         32
DS                          2
SWH                  6009.615 Hz
FIDRES               0.091699 Hz
AQ                   5.4525952 sec
RG                        228
DW                     83.200 usec
DE                      6.50 usec
TE                      298.0 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               300.1318534 MHz
NUC1                       1H
P1                      12.00 usec
PLW1               12.00000000 W

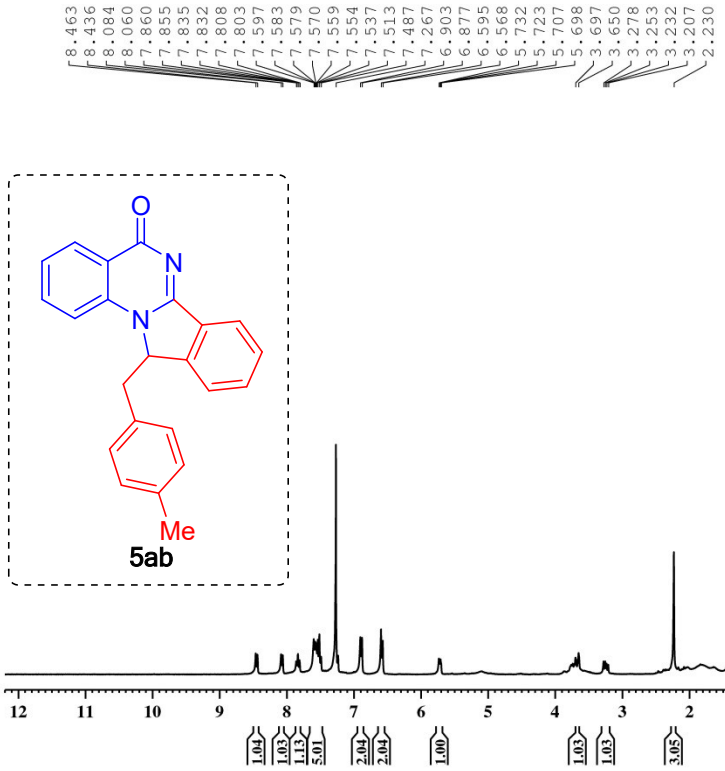
F2 - Processing parameters
SI                       65536
SF                 300.1300035 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```



^{1}H and ^{13}C NMR Spectra of compound 5aa



HRMS Spectrum of compound 5aa

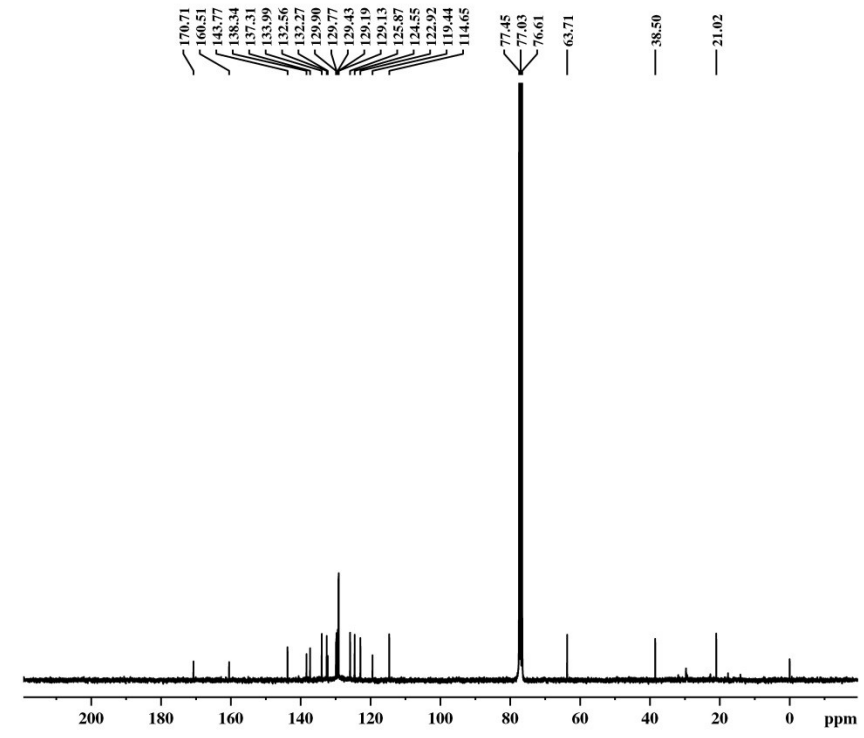



```
Current Data Parameters
NAME          PS-2-344AR
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230603
Time               14.36
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    48
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   287
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1300044 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME         RA-PS-2-252
EXPNO                  8
PROCNO                 1

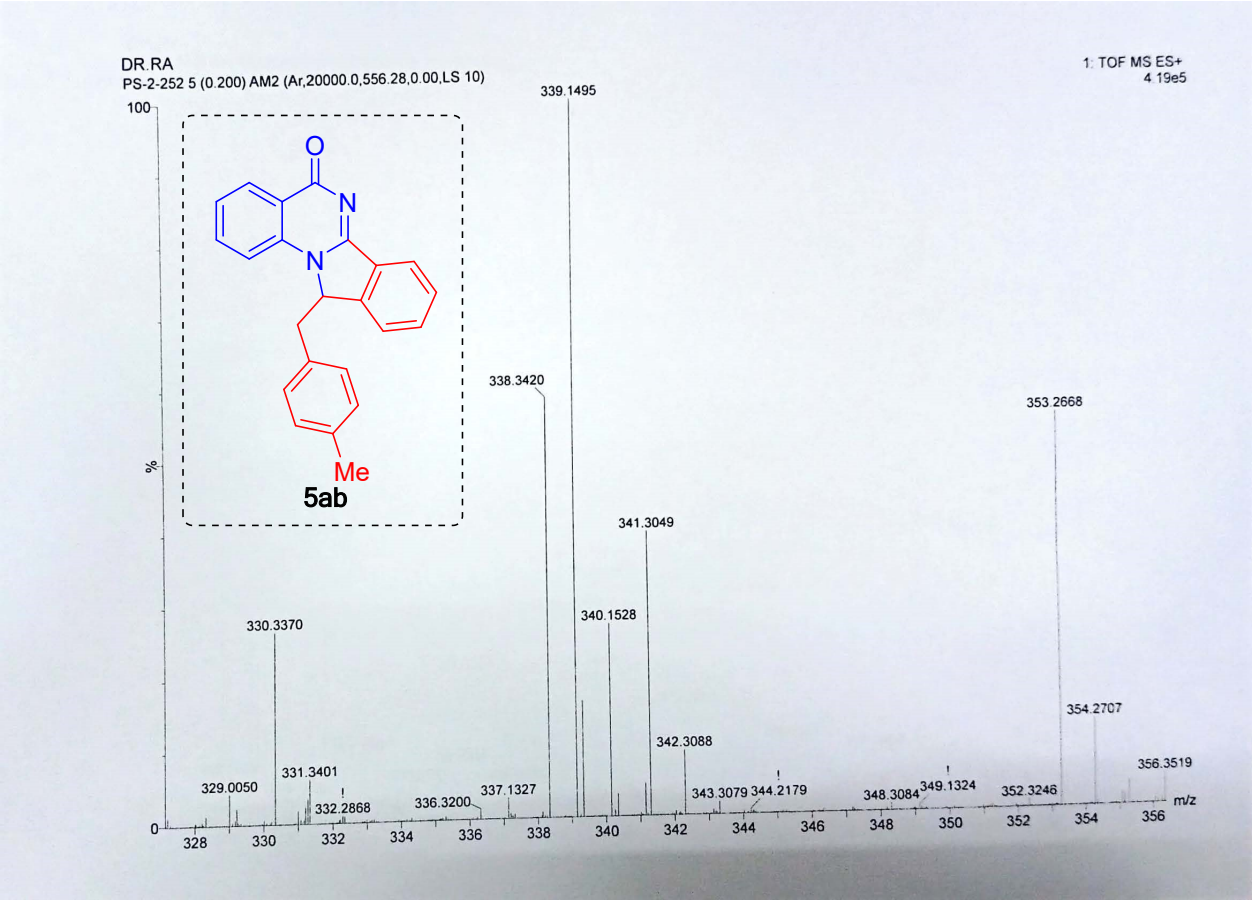
F2 - Acquisition Parameters
Date_           20230317
Time               9.36
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  8000
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175317 sec
RG                  1290
DW                27.733 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                  13C
P1                 11.00 usec
PLW1          48.00000000 W

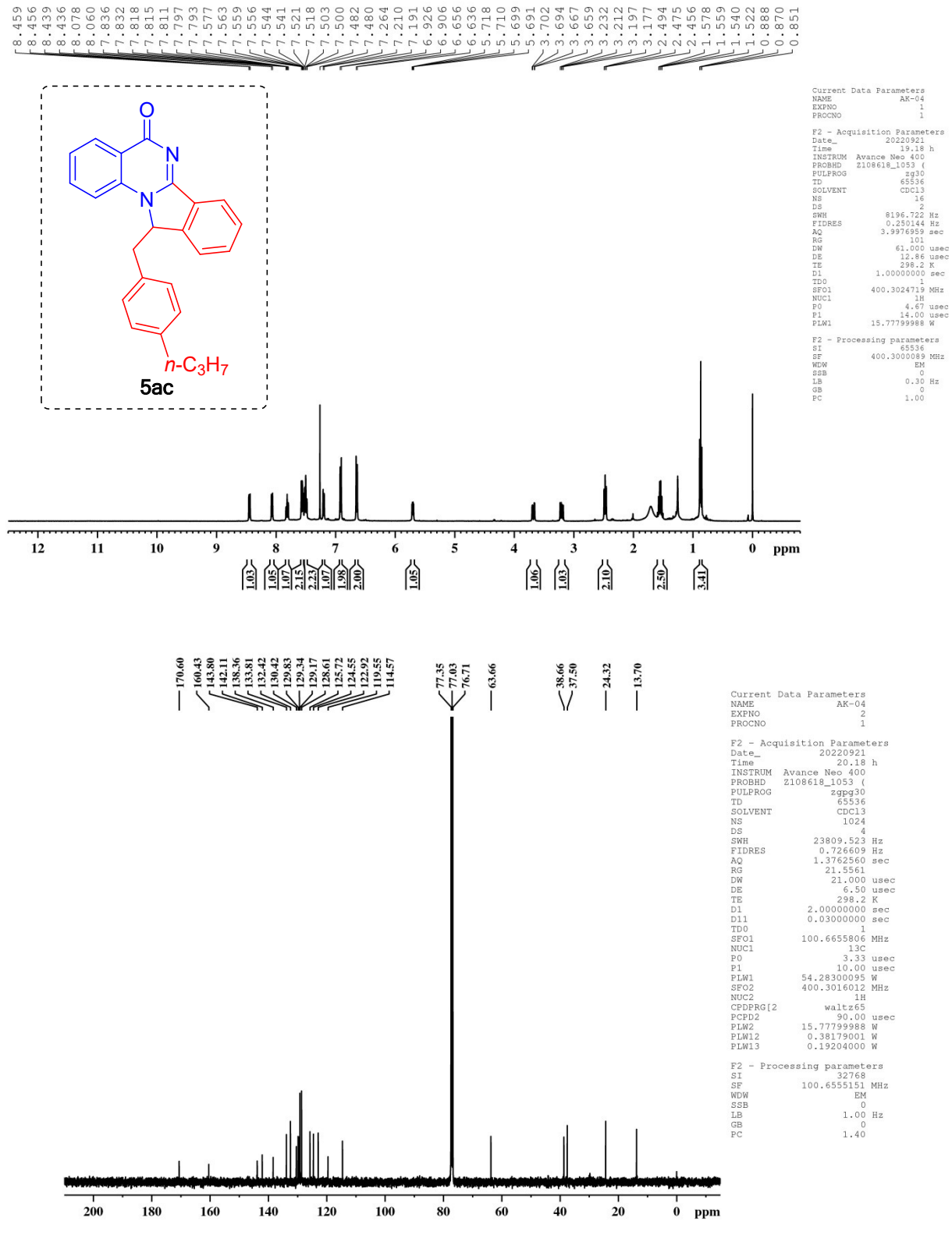
======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.21333000 W
PLW13          0.10731000 W

F2 - Processing parameters
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

^{1}H and ^{13}C NMR Spectra of compound 5ab

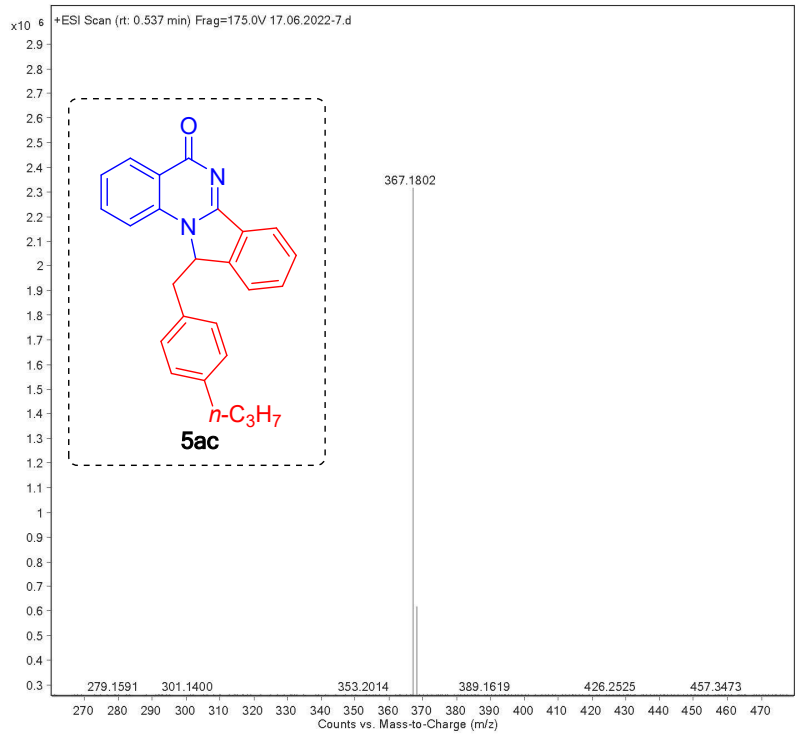


HRMS Spectrum of compound 5ab

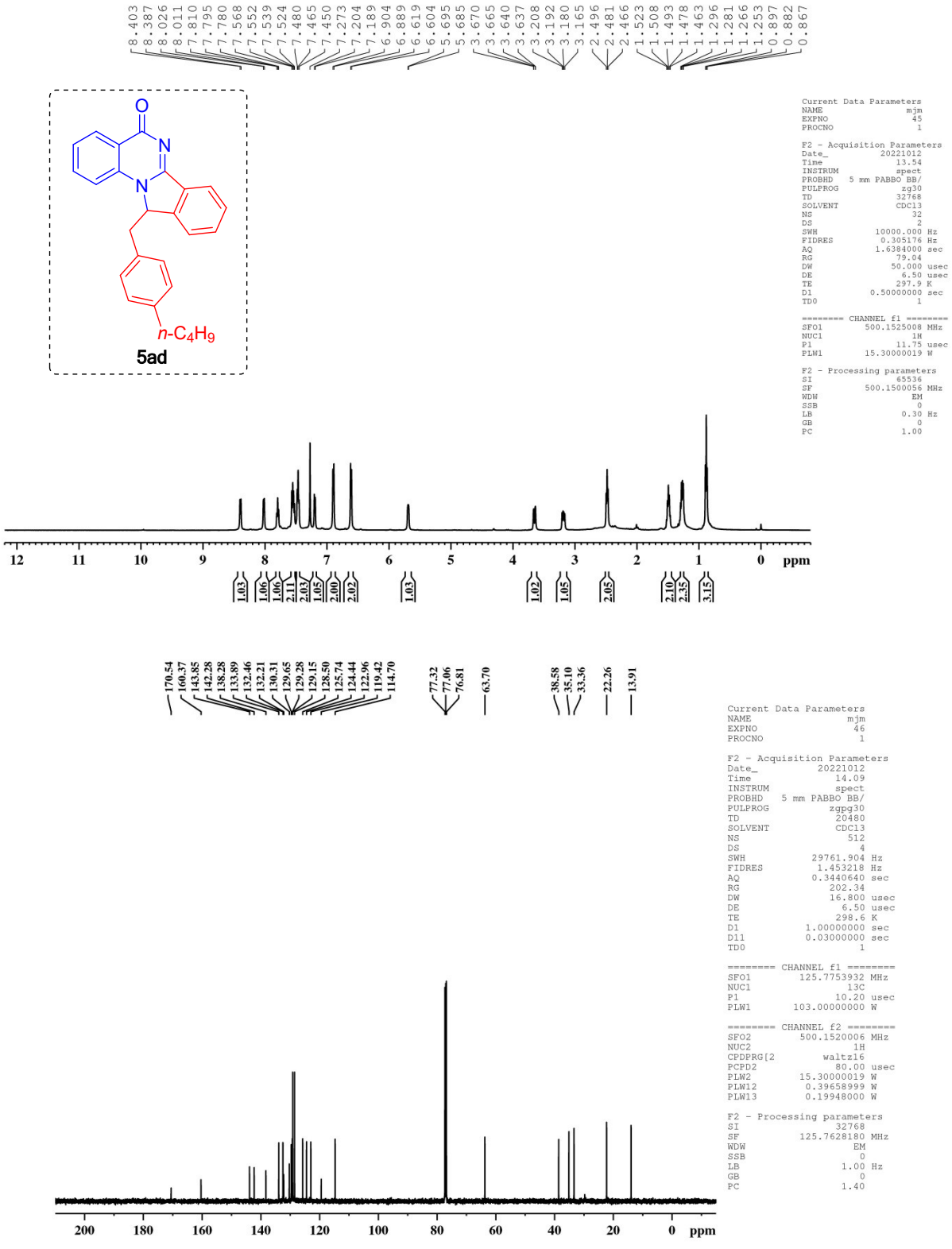


^{1}H and ^{13}C NMR Spectra of compound 5ac

Sample Name	ps-1-275	**Position**	P1-A7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	17.06.2022-7.d
ACQ Method	NITW-W.m	**Comment**		**Acquired Time**	17-Jun-22 3:28:55 PM

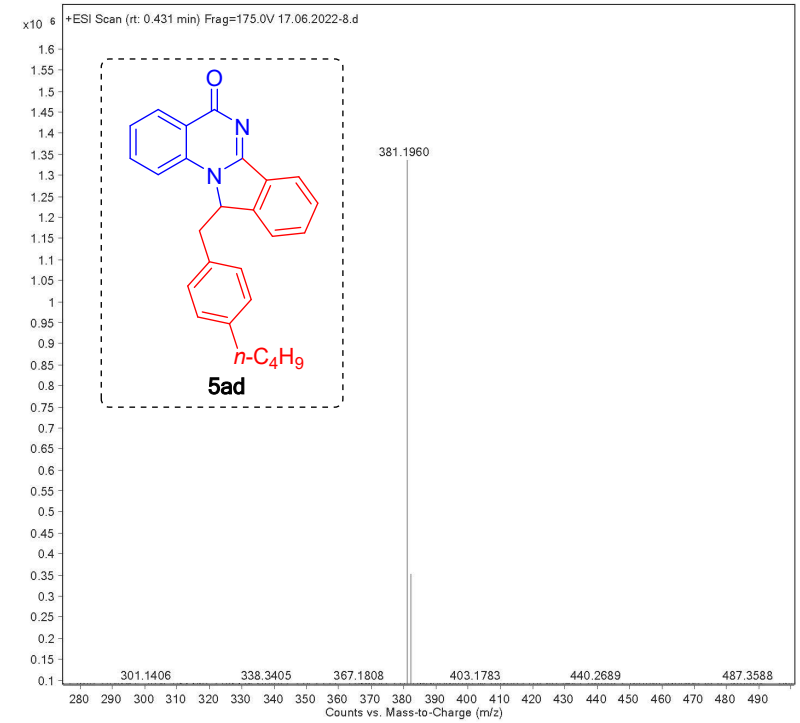


HRMS Spectrum of compound 5ac

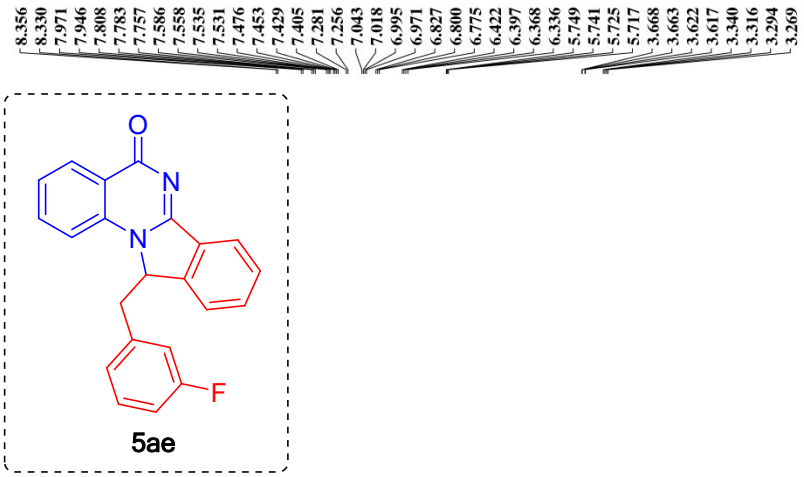


^{1}H and ^{13}C NMR Spectra of compound 5ad

Sample Name	ps-1-276	**Position**	P1-A8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	17.06.2022-8.d
ACQ Method	NITW-W.m	**Comment**		**Acquired Time**	17-Jun-22 3:32:54 PM



HRMS Spectrum of compound 5ad

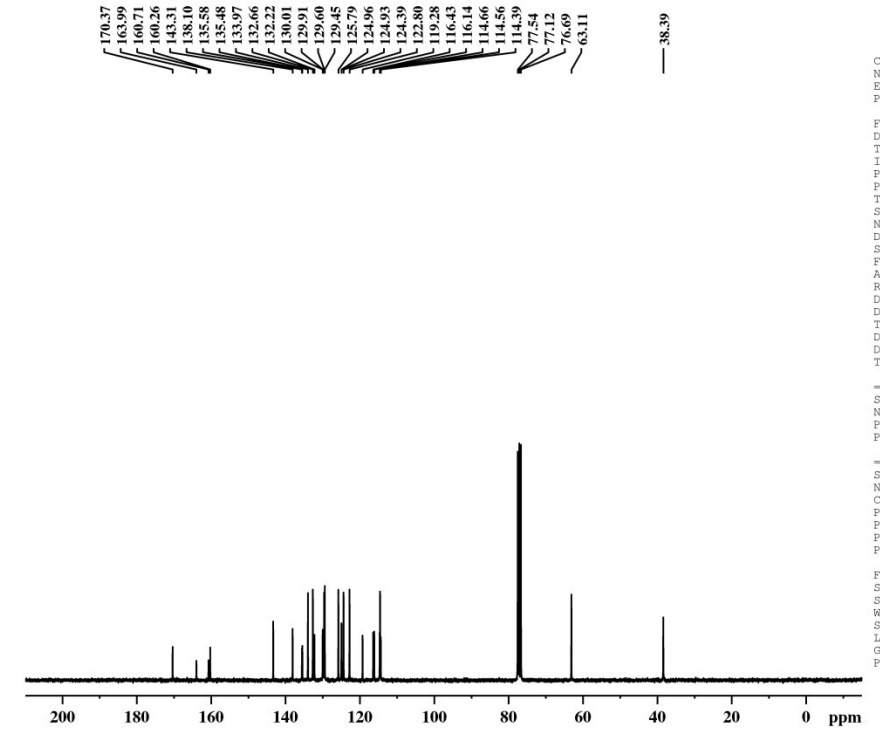



```
Current Data Parameters
NAME                  PS-2-31
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_              20230425
Time                  11.46
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4525952 sec
RG                      128
DW                   83.200 usec
DE                    6.50 usec
TE                  298.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             300.1318534 MHz
NUC1                       1H
P1                      12.00 usec
PLW1            12.00000000 W

F2 - Processing parameters
SI                        65536
SF               300.1299967 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```




```
Current Data Parameters
NAME                  PS-2-31
EXPNO                       2
PROCNO                      1

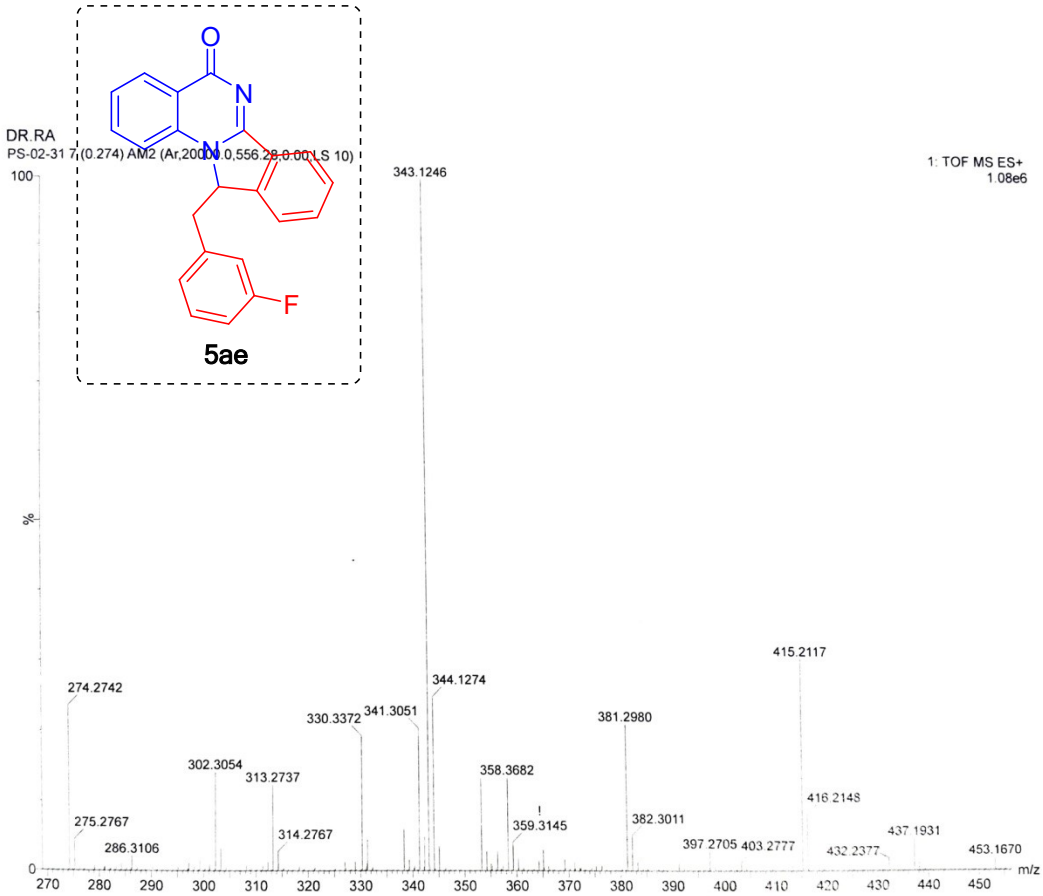
F2 - Acquisition Parameters
Date_              20230425
Time                  11.43
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               18028.846 Hz
FIDRES            0.275098 Hz
AQ                1.8175317 sec
RG                      1030
DW                   27.733 usec
DE                    6.50 usec
TE                  300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             75.4752949 MHz
NUC1                      13C
P1                      11.00 usec
PLW1            48.00000000 W

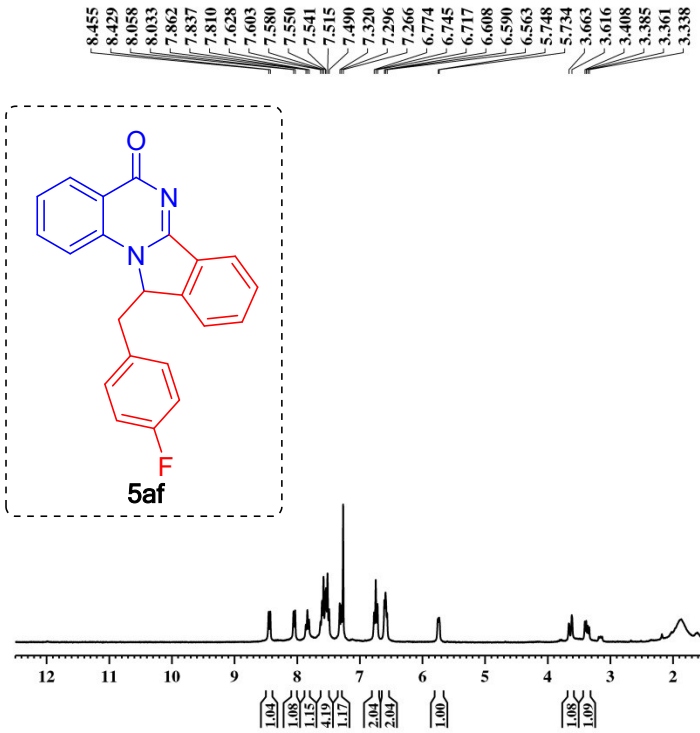
======== CHANNEL f2 ========
SFO2            300.1312005 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                   90.00 usec
PLW2            12.00000000 W
PLW12            0.21333000 W
PLW13            0.10731000 W

F2 - Processing parameters
SI                        32768
SF               75.4677485 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

^{1}H and ^{13}C NMR Spectra of compound 5ae



HRMS Spectrum of compound 5ae

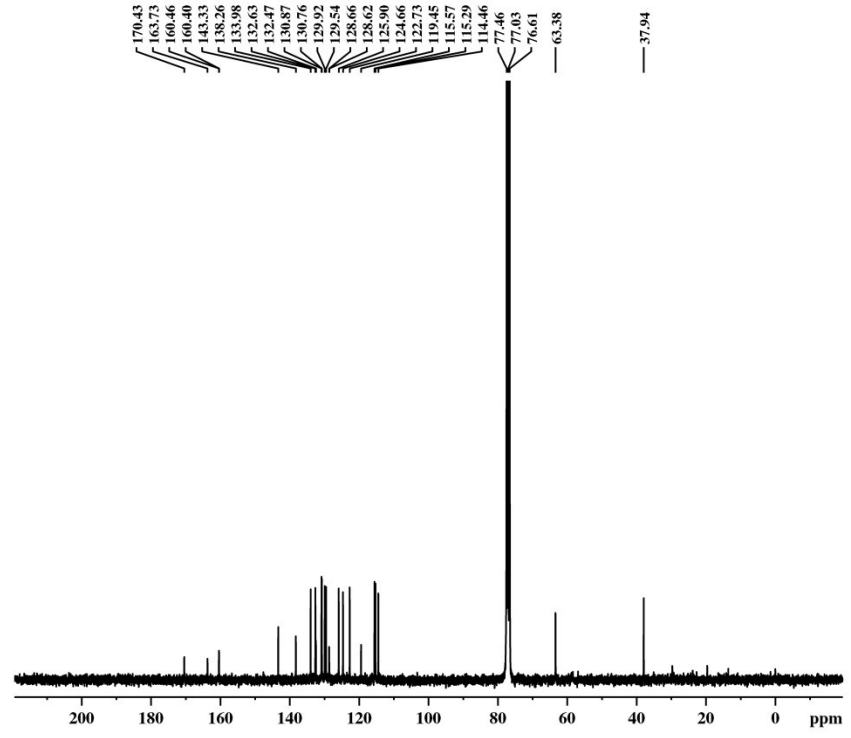



```
Current Data Parameters
NAME          PS-1-197-B
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230426
Time               10.07
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   362
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1300051 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME          PS-1-197-B
EXPNO                  1
PROCNO                 1

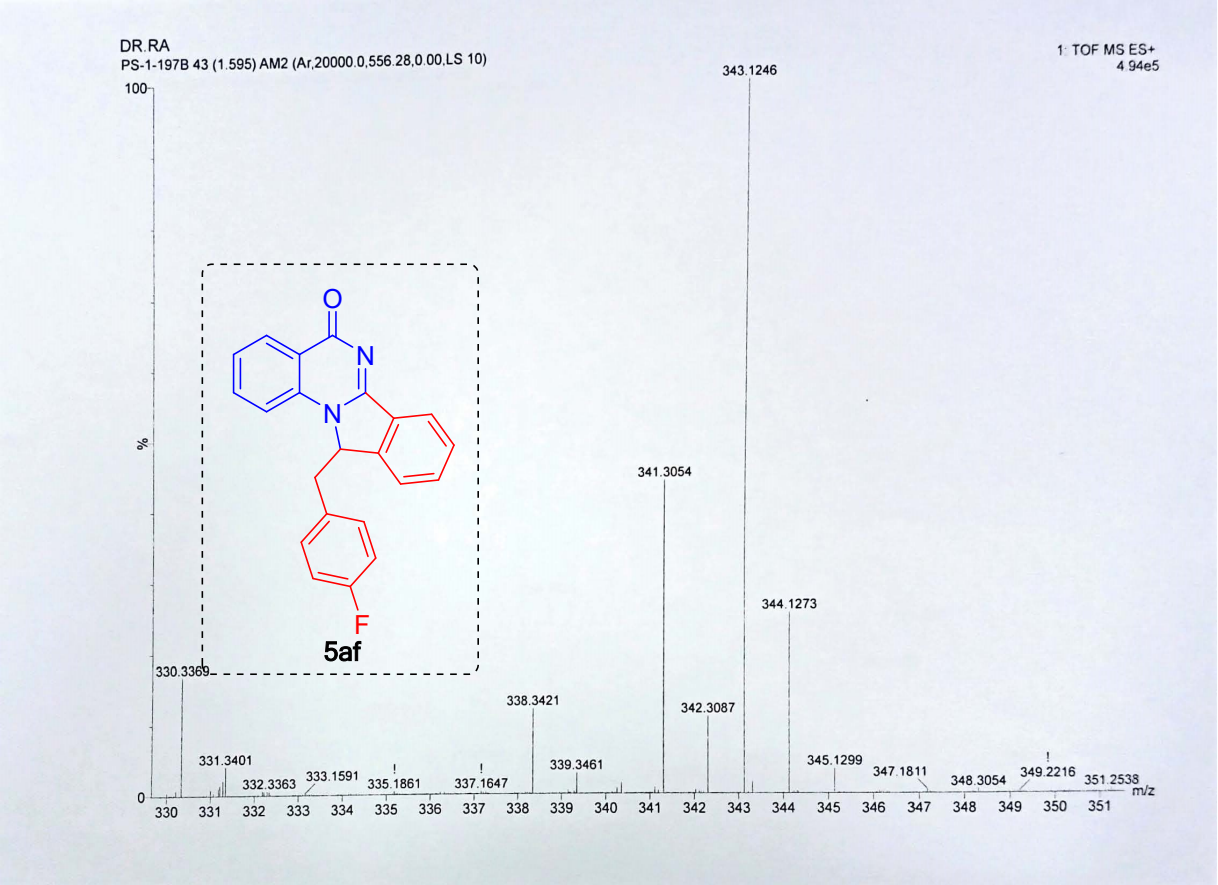
F2 - Acquisition Parameters
Date_           20230426
Time               10.03
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDC13
NS                  8642
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175317 sec
RG                  1150
DW                27.733 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                  13C
P1                 11.00 usec
PLW1          48.00000000 W

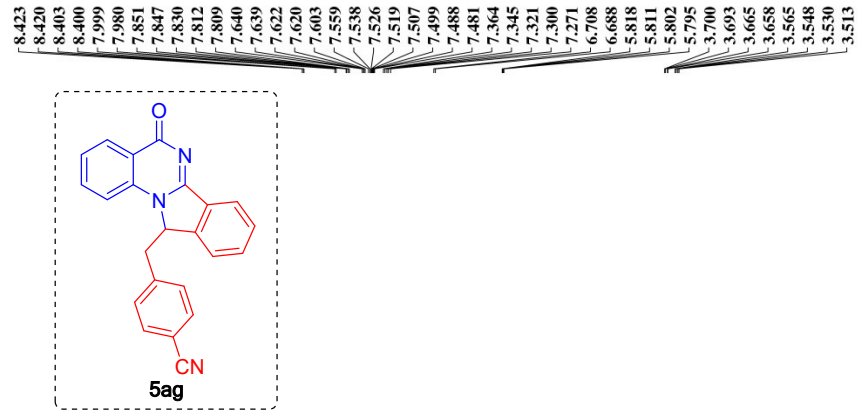
======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.21333000 W
PLW13          0.10731000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

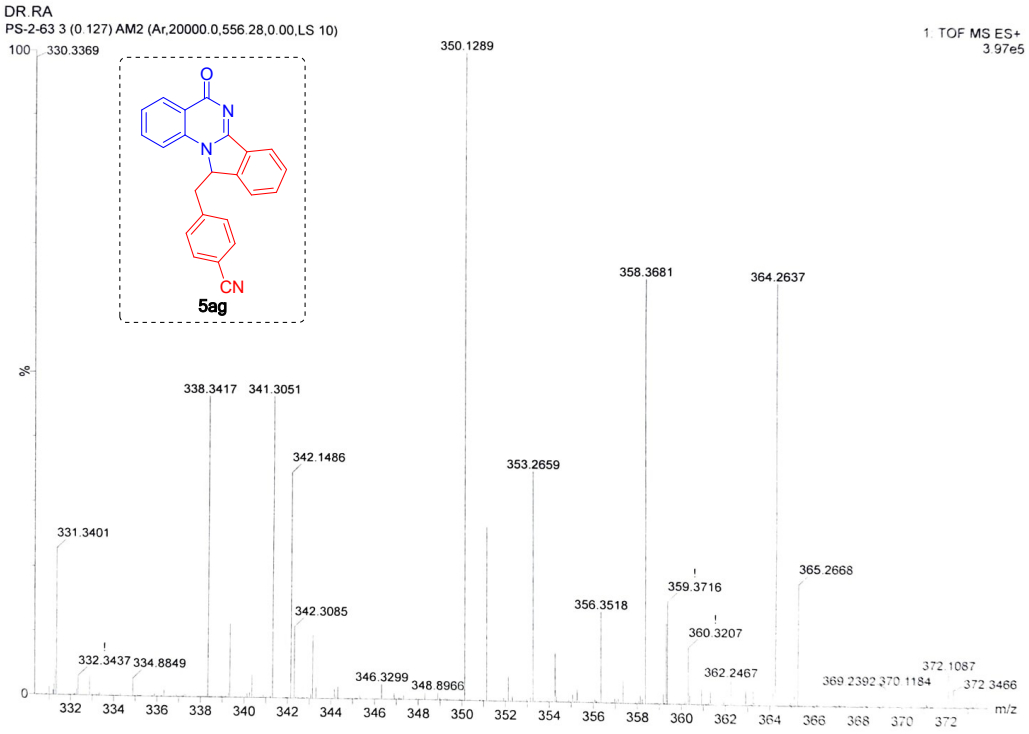
^{1}H and ^{13}C NMR Spectra of compound 5af



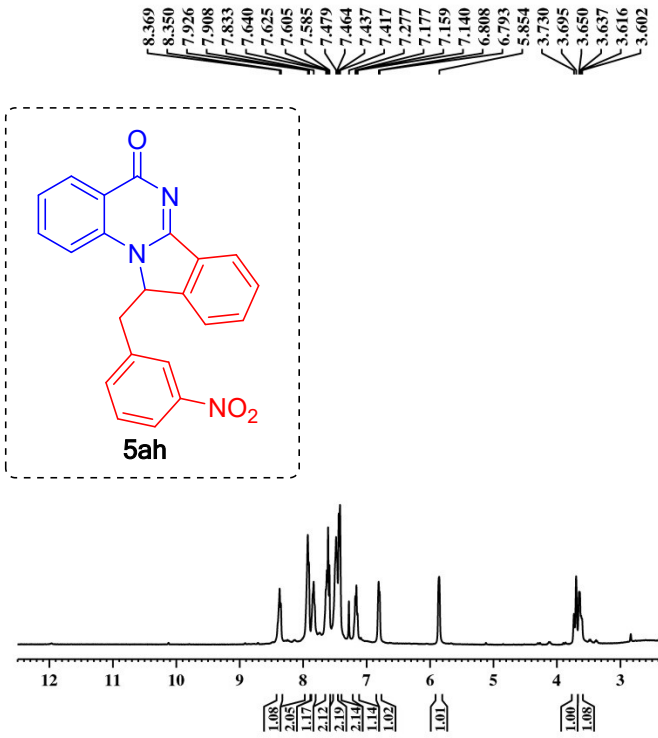
HRMS Spectrum of compound 5af



^{1}H and ^{13}C NMR Spectra of compound 5ag



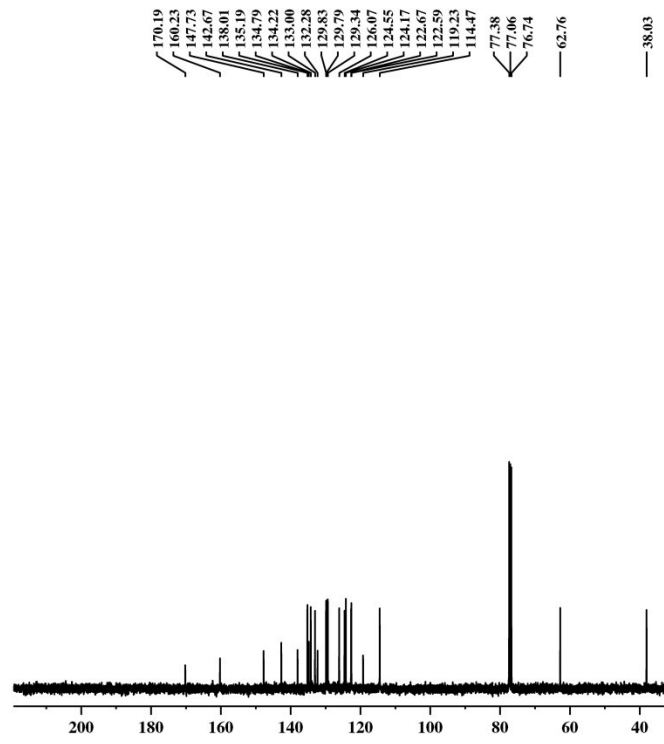
HRMS Spectrum of compound 5ag




```
Current Data Parameters
NAME                  prabu
EXPNO                   323
PROCNO                    1

F2 - Acquisition Parameters
Date_              20220730
Time                   5.26 h
INSTRUM               spect
PROBHD    Z129392_0001 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                   153.13
DW                   62.400 usec
DE                    6.50 usec
TE                   300.5 K
D1                0.50000000 sec
TD0                       1
SFO1           400.1320007 MHz
NUC1                     1H
P1                   15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                    65536
SF               400.1300024 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

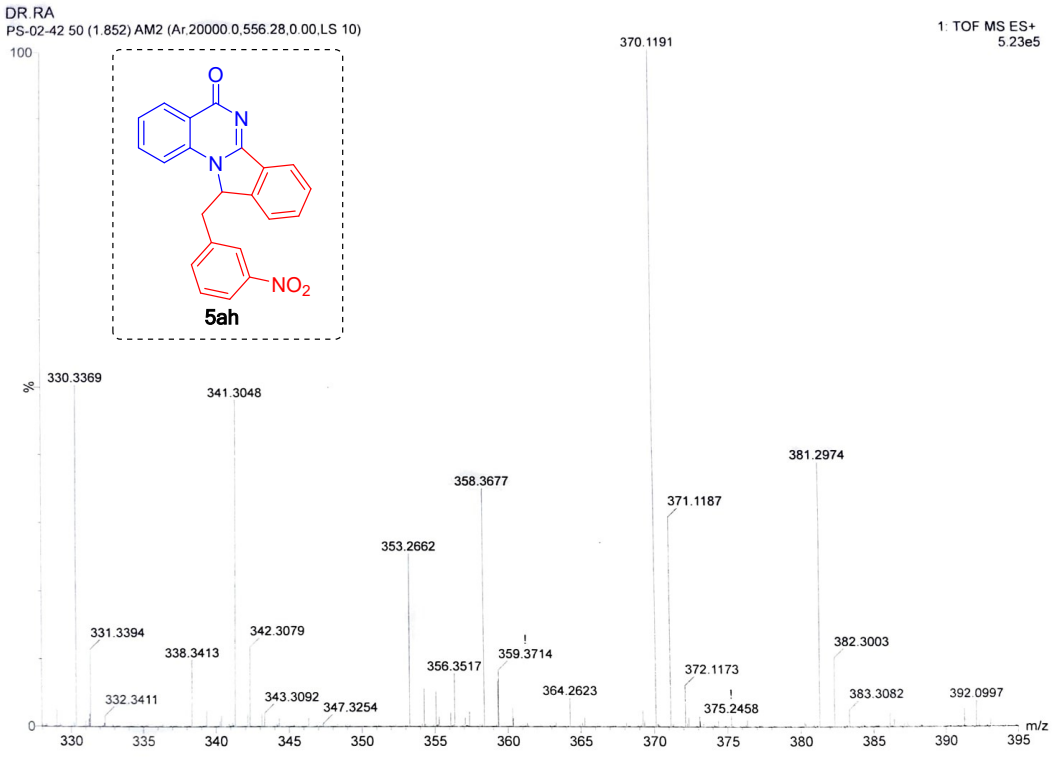



```
Current Data Parameters
NAME                  prabu
EXPNO                   286
PROCNO                    1

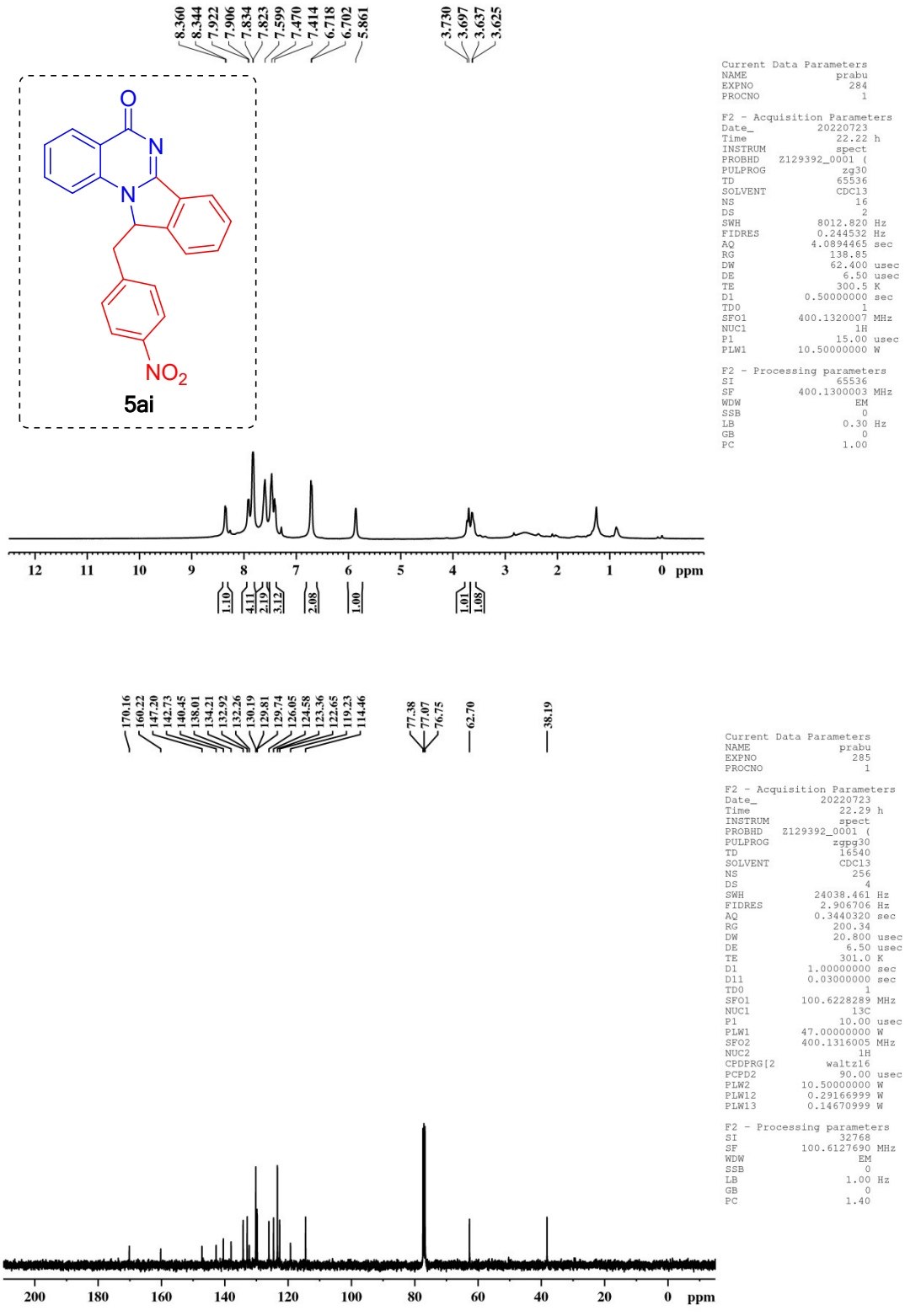
F2 - Acquisition Parameters
Date_              20220723
Time                  22.38 h
INSTRUM               spect
PROBHD    Z129392_0001 (
PULPROG              zgpg30
TD                    16540
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 Hz
FIDRES            2.906706 Hz
AQ                0.3440320 sec
RG                   200.34
DW                   20.800 usec
DE                    6.50 usec
TE                   301.1 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1           100.6228289 MHz
NUC1                     13C
P1                   10.00 usec
PLW1          47.00000000 W
SFO2           400.1316005 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

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

^{1}H and ^{13}C NMR Spectra of compound 5ah



HRMS Spectrum of compound 5ah




```
Current Data Parameters
NAME                  prabu
EXPNO                   284
PROCNO                    1

F2 - Acquisition Parameters
Date_              20220723
Time                 22.22 h
INSTRUM              spect
PROBHD    Z129392_0001 (
PULPROG              zg30
TD                  65536
SOLVENT             CDC13
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES               0.244532 Hz
AQ                4.0894465 sec
RG                   138.85
DW                   62.400 usec
DE                    6.50 usec
TE                   300.5 K
D1                0.50000000 sec
TD0                       1
SFO1            400.1320007 MHz
NUC1                     1H
P1                    15.00 usec
PLW1           10.50000000 W

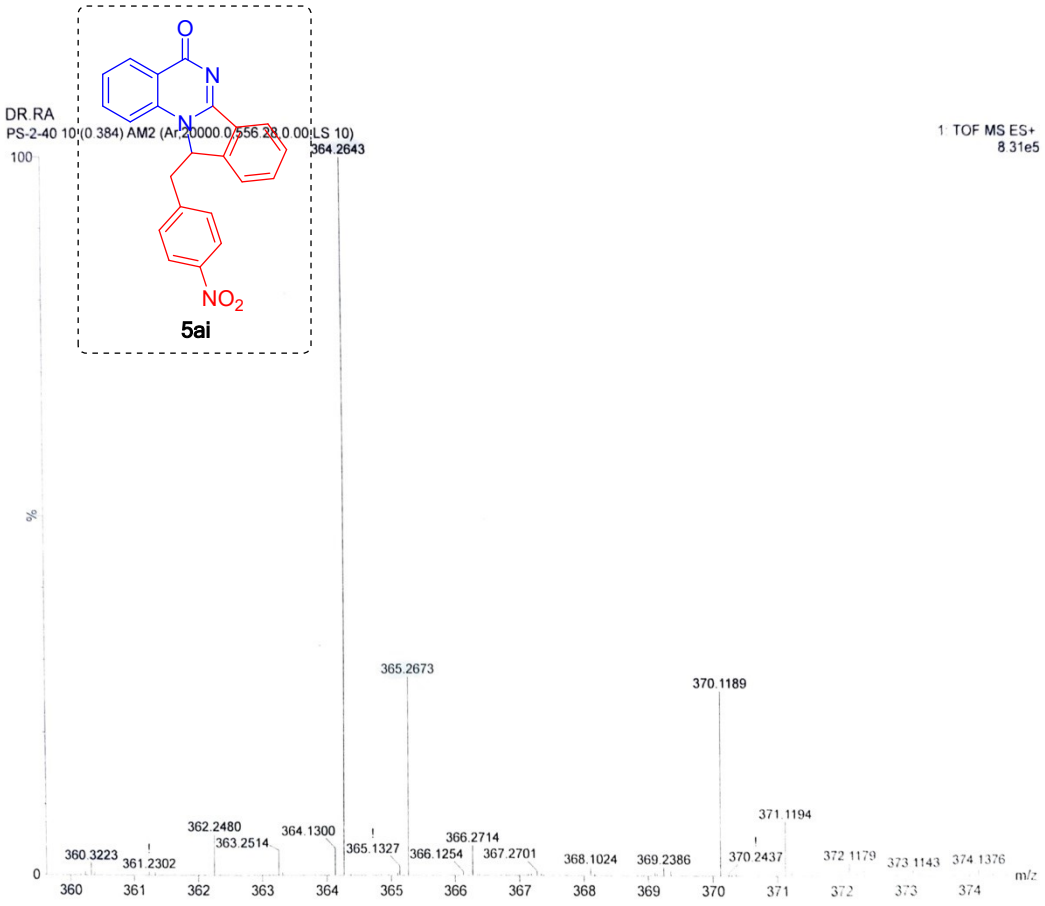
F2 - Processing parameters
SI                    65536
SF              400.1300003 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

```
Current Data Parameters
NAME                  prabu
EXPNO                   285
PROCNO                    1

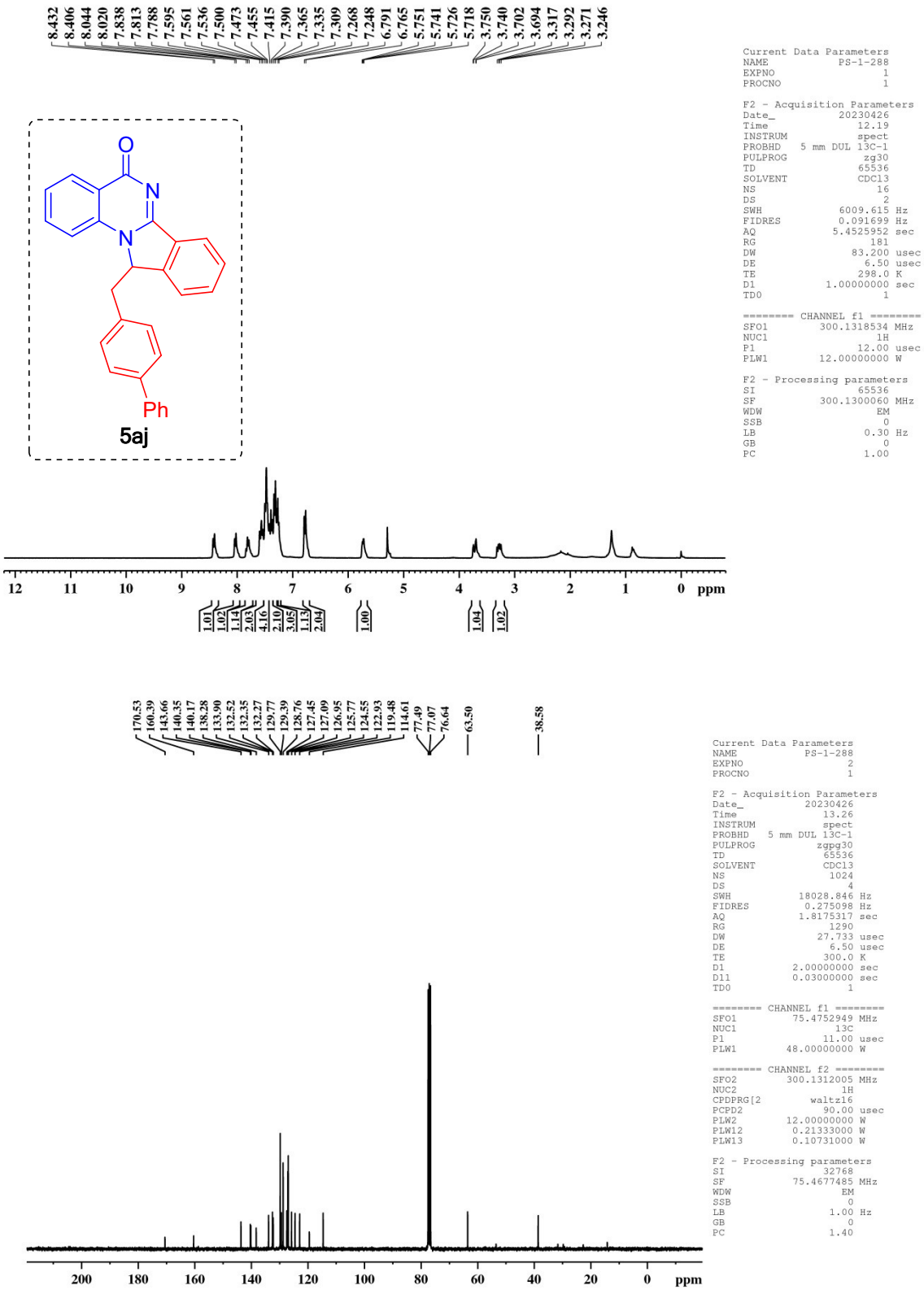
F2 - Acquisition Parameters
Date_              20220723
Time                 22.29 h
INSTRUM              spect
PROBHD    Z129392_0001 (
PULPROG            zgpg30
TD                  16540
SOLVENT             CDC13
NS                     256
DS                       4
SWH              24038.461 Hz
FIDRES               2.906706 Hz
AQ                0.3440320 sec
RG                   200.34
DW                   20.800 usec
DE                    6.50 usec
TE                   301.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1            100.6228289 MHz
NUC1                     13C
P1                    10.00 usec
PLW1           47.00000000 W
SFO2            400.1316005 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                 90.00 usec
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

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

^{1}H and ^{13}C NMR Spectra of compound 5ai



HRMS Spectrum of compound 5ai




```
Current Data Parameters
NAME                  PS-1-288
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20230426
Time                   12.19
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4525952 sec
RG                      181
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                     1H
P1                    12.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                    65536
SF            300.1300060 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

```
Current Data Parameters
NAME                  PS-1-288
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20230426
Time                   13.26
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               18028.846 Hz
FIDRES            0.275098 Hz
AQ                1.8175317 sec
RG                     1290
DW                   27.733 usec
DE                    6.50 usec
TE                   300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

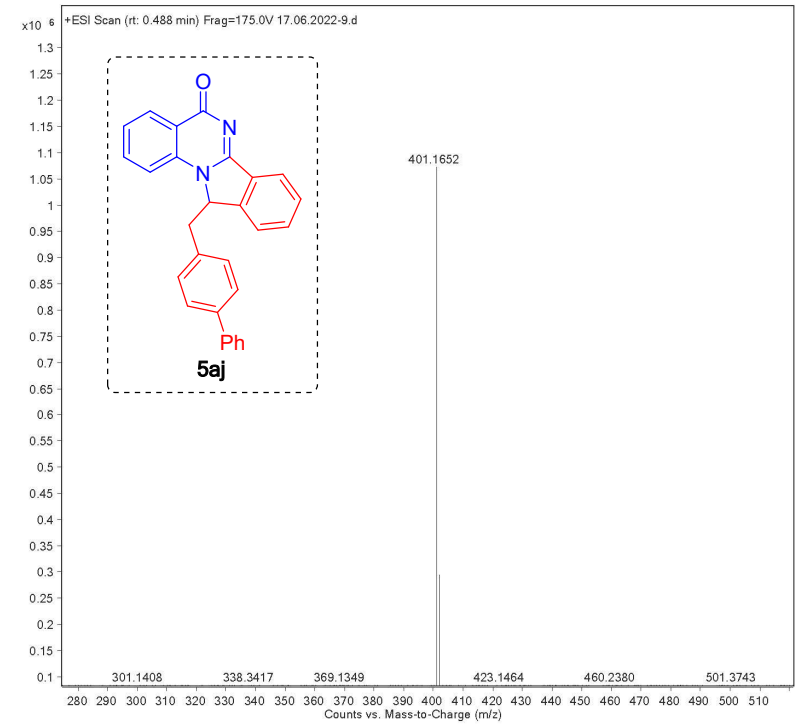
======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                     13C
P1                    11.00 usec
PLW1          48.00000000 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                     1H
CPDPRG[2           waltz16
PCPD2                 90.00 usec
PLW2          12.00000000 W
PLW12          0.21333000 W
PLW13          0.10731000 W

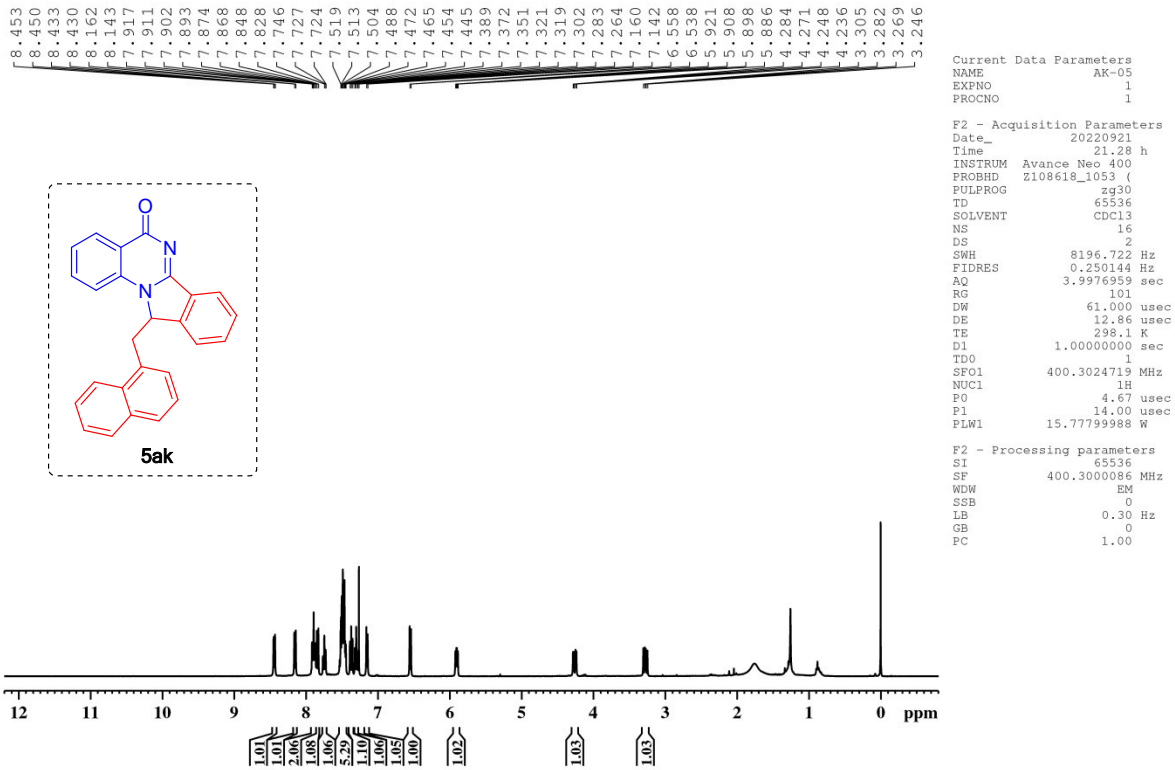
F2 - Processing parameters
SI                    32768
SF            75.4677485 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

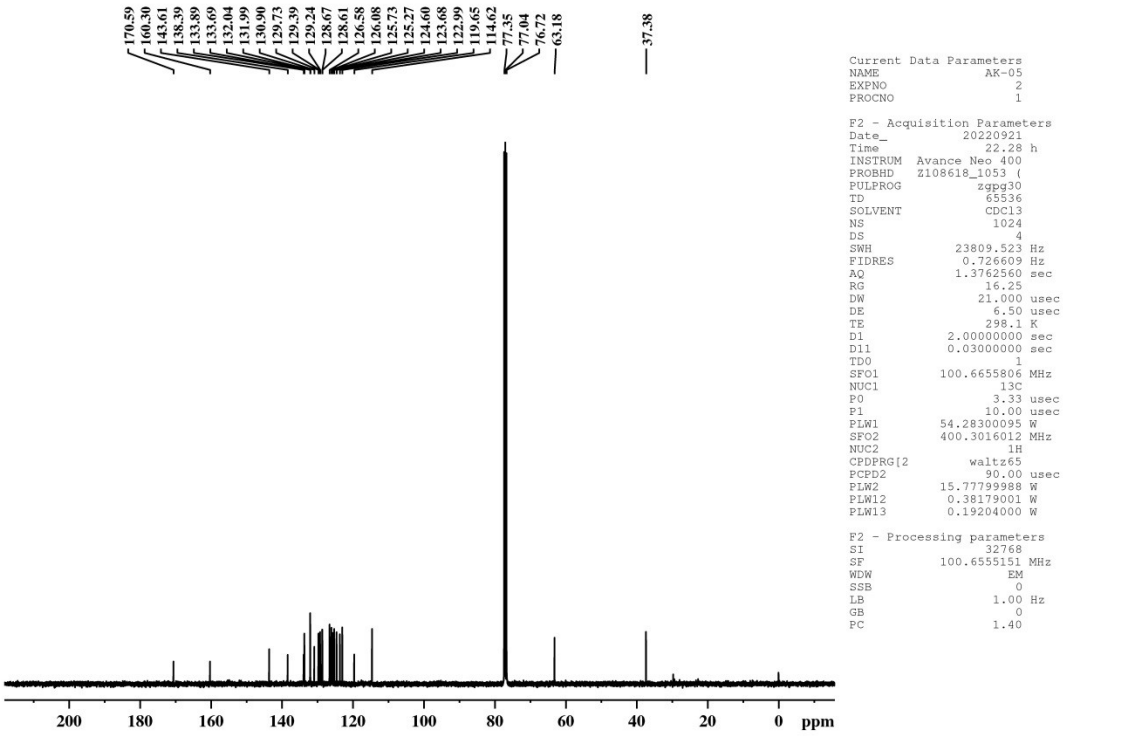
^{1}H and ^{13}C NMR Spectra of compound 5aj

Sample Name	ps-1-288	**Position**	P1-A9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	17.06.2022-9.d
ACQ Method	NITW-W.m	**Comment**		**Acquired Time**	17-Jun-22 3:36:51 PM

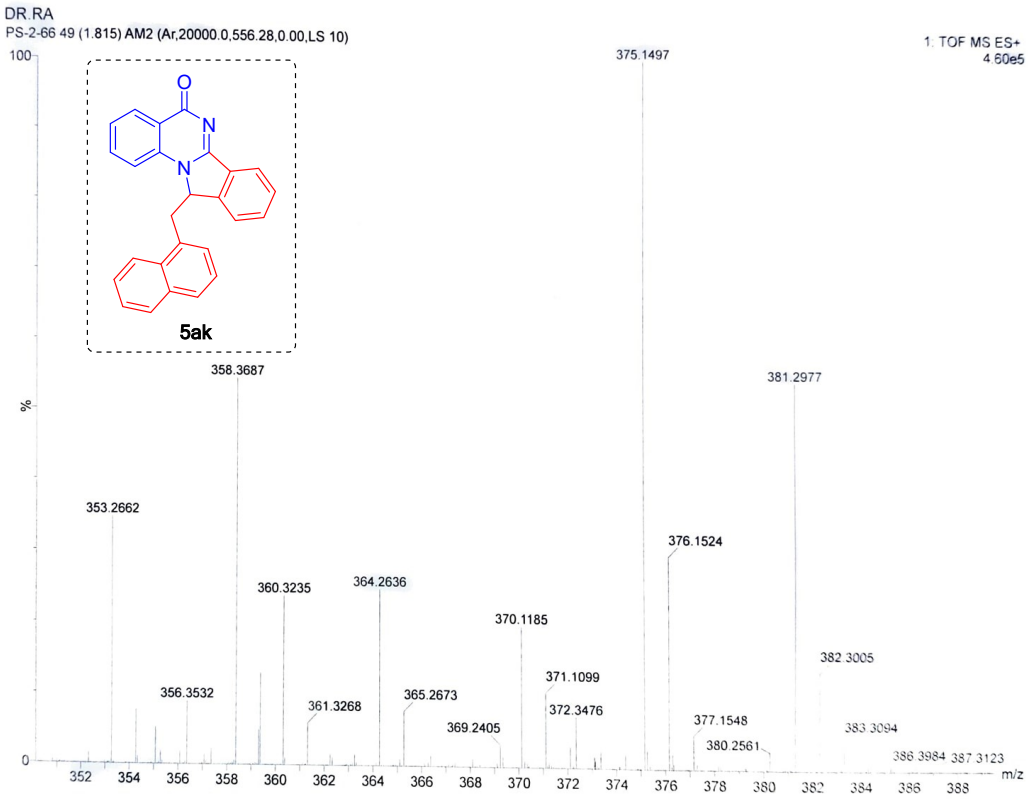


HRMS Spectrum of compound 5aj



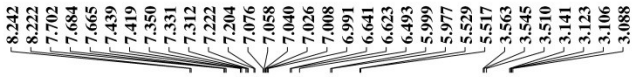


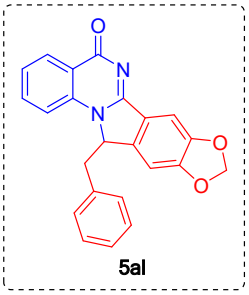
^{1}H and ^{13}C NMR Spectra of compound 5ak



H

RMS Spectrum of compound 5ak

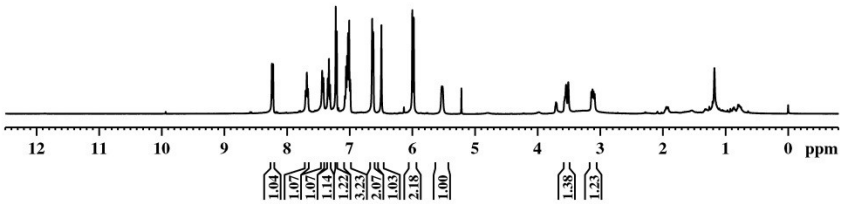





```
Current Data Parameters
NAME      PS-1-231-H-NMR
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220705
Time               9.55 h
INSTRUM           spect
PROBHD    Z108618_0738 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES            0.244532 Hz
AQ             4.0894465 sec
RG                31.07
DW                62.400 usec
DE                 6.50 usec
TE                300.1 K
D1             1.00000000 sec
TD0                   1
SFO1          400.1324708 MHz
NUC1                 1H
P1                15.00 usec
PLW1          13.03199959 W

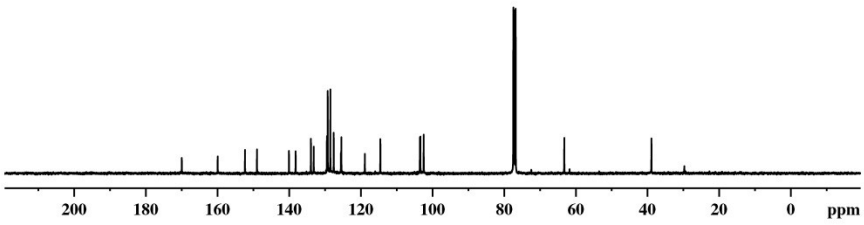
F2 - Processing parameters
SI                65536
SF          400.1300321 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME      PS-1-231-C13-NMR
EXPNO                   2
PROCNO                  1

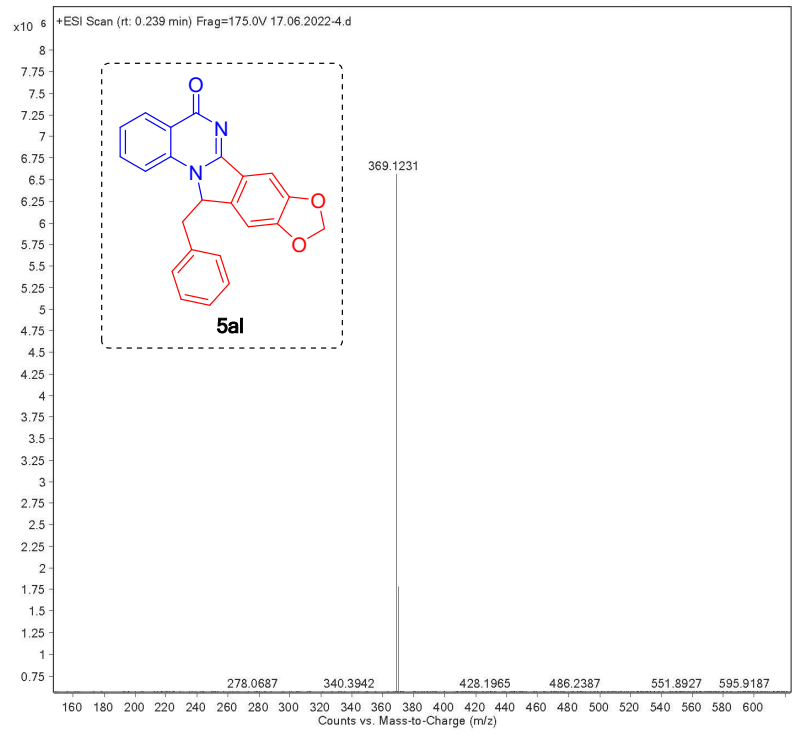
F2 - Acquisition Parameters
Date_           20220707
Time              18.11 h
INSTRUM           spect
PROBHD    Z108618_0738 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  685
DS                    4
SWH           24038.461 Hz
FIDRES            0.733596 Hz
AQ             1.3631488 sec
RG                200.47
DW                20.800 usec
DE                 6.50 usec
TE                300.3 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1          100.6228298 MHz
NUC1                 13C
P1                10.00 usec
PLW1          51.31299973 W
SFO2          400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          13.03199959 W
PLW12          0.36199999 W
PLW13          0.18208000 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.40
```

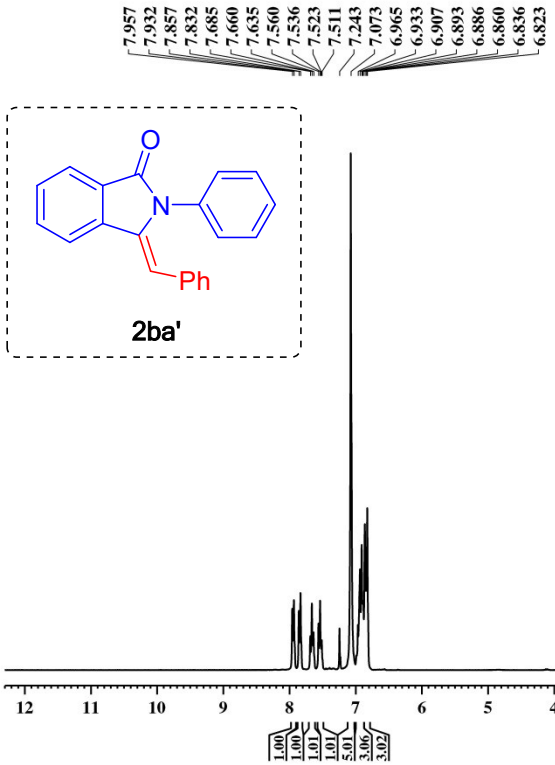


^{1}H and ^{13}C NMR Spectra of compound 5al

Sample Name	ps-1-231	**Position**	P1-A4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	2	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	17.06.2022-4.d
ACQ Method	NITW-W.m	**Comment**		**Acquired Time**	17-Jun-22 3:16:59 PM



HRMS Spectrum of compound 5al

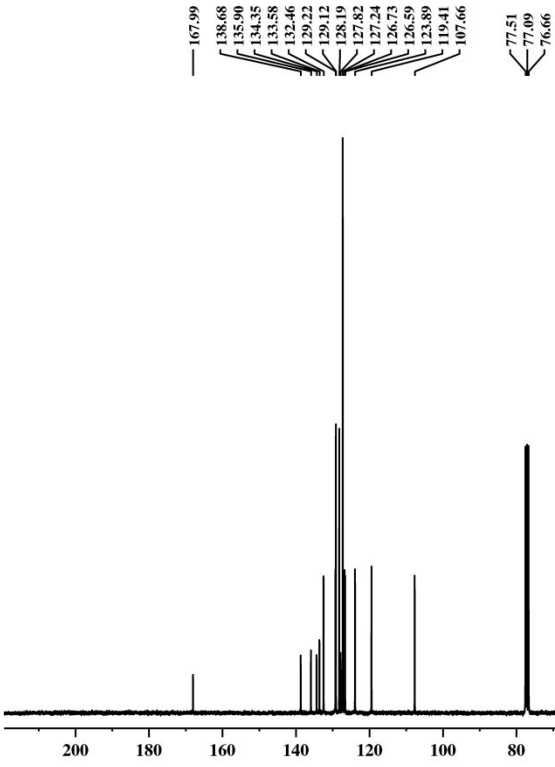



```
Current Data Parameters
NAME        RA-PS-2-219B
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230106
Time               13.26
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   128
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1300124 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME        RA-PS-2-219B
EXPNO                  2
PROCNO                 1

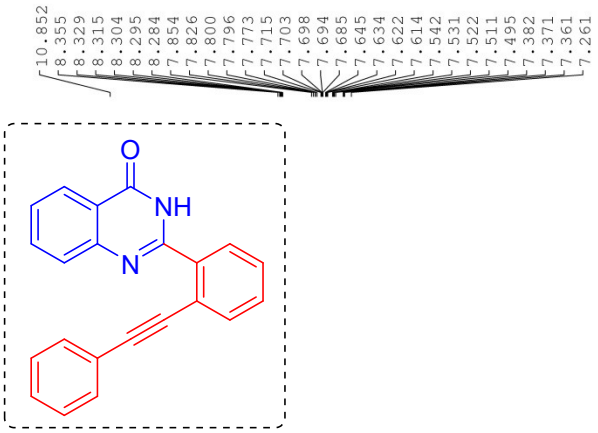
F2 - Acquisition Parameters
Date_           20230106
Time               14.34
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175317 sec
RG                   912
DW                27.733 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

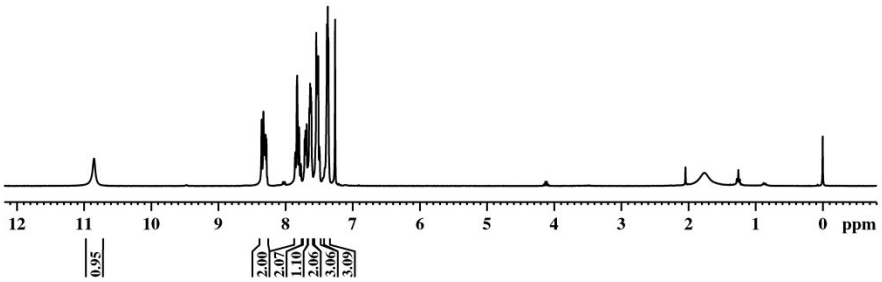
======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                  13C
P1                 11.00 usec
PLW1          48.00000000 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.21333000 W
PLW13          0.10731000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

^{1}H and ^{13}C NMR Spectra of compound 2aa'



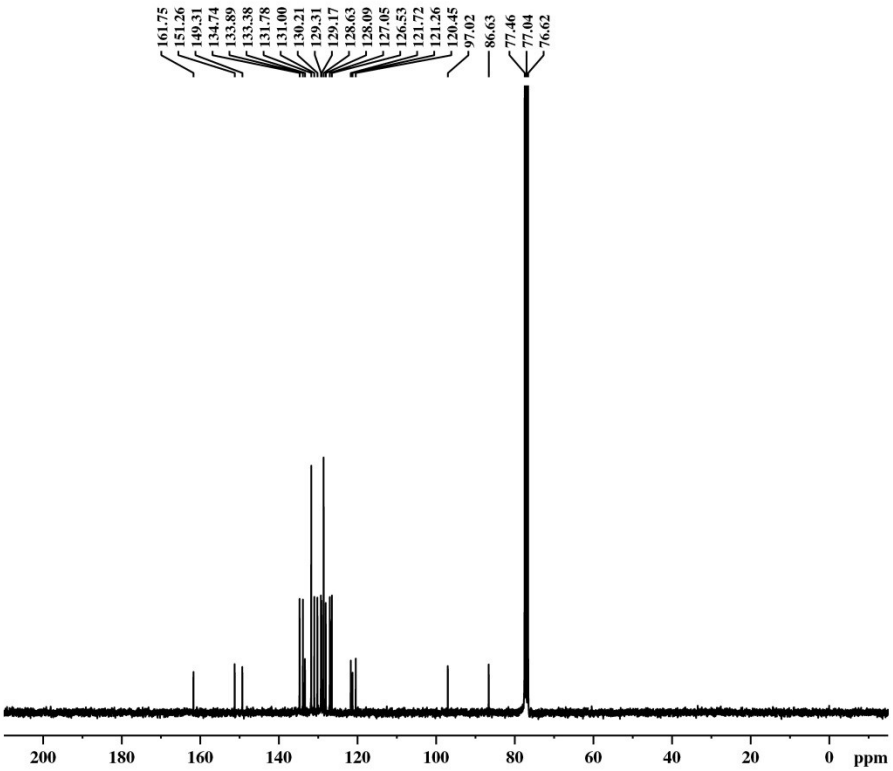



```
Current Data Parameters
NAME        RA-PS-2-209A
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221227
Time                1.28
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   256
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318534 MHz
NUC1                    1H
P1                  12.00 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF          300.1300062 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME        RA-PS-2-209A
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221227
Time                2.37
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175317 sec
RG                  1030
DW                27.733 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                   13C
P1                  11.00 usec
PLW1          48.00000000 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.00000000 W
PLW12          0.21333000 W
PLW13          0.10731000 W

F2 - Processing parameters
SI                 32768
SF          75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

^{1}H and ^{13}C NMR Spectra of compound G