# Design, synthesis and *in-vitro* anti-leukemic evaluation of ferulic acid analogues as Bcr-Abl inhibitors

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Electronic supplementary information (ESI)

## Materials and methods

### Plant collection and extraction

The aerial parts of *S. brachiata* were collected from the place called killai, near Pichavaram, Tamil Nadu, and India. A voucher specimen was matched with the authentic specimen (herbarium no 5555, regional plant resource center, Puri, India) and was deposited in the herbarium. The aerial parts (~1 kg) were shade dried and powdered. 100 g of the powder was percolated with Millipore water and after 24 h, the extract were filtered through a Whatman No. 41 filter paper. The extraction was repeated thrice and the combined extracts were concentrated in vacuo and further lyophilized to obtain a residue (35 g).

### Isolation of ferulic acid

10g of water extract of *S.brachiata* was subjected to column chromatographic separation. Initially the crude extract was separated by using Sephadex LH 20 (Sigma Aldrich, sweden). Sephadex was prepared after the swelling time of 24hrs by using chloroform-methanol (30:70) mixture. There are 18 fractions were collected by increasing polarity of the mobile phase from 30% chloroform: methanol to 100% methanol. The TLC pattern of SB 9 and SB 13 shows similar in spot nature and they were mixed up accordingly. This fraction reveals two spots in major (Rf = 0.488, 0.418) and one more with minor intensity. Further purification was done by using normal silica column (100-200 mesh). Dirty white precipitate was formed along the sides of the test tube. Further purification of the compound yielded 27mg of ferulic acid. The structures of the compound have been identified by using NMR Studies.

### Procedure for the synthesis of (*E*)-3-(4-acetoxy-3-methoxyphenyl) acrylic acid (2)

Ferulic acid (19.4g, 0.1 mol) was added to the solution of NaOH (12.7g, 0.26 mol) in 100 mL water. Then the mixture was stirred and cooled below $10^{\circ}$C. To the cold solution acetic anhydride (12.7 mL, 0.125 mol) was added in drop wise manner. The reaction mixture was stirred at $20^{0}$C for 10min and room temperature for 30min. Then dilute sulfuric acid was added in dropwise till the white precipitate form. Maintain the pH of the solution 4-5 by using dilute

sulfuric acid (5N). Filter the white precipitate and washed several times with distilled water. The product gives white precipitate (15.719 g) with yield of 81%.

**General procedure for the synthesis of amide analogues of ferulic acid (2a-2g)**

Add 1.2 equivalent Thionyl chloride (86.34 µL, 1.2mmol) to the synthesized (*E*)-3-(4-acetoxy-3-methoxyphenyl) acrylic acid (236 mg, 1mmol) and heat the reaction mixture at $80^0$C for 3 hrs. Remove the free $SOCl_2$ by using vacuum pump and dissolved in dry $CH_2Cl_2$.

Amine (1.5 mmol) was dissolved in dry $CH_2Cl_2$ followed by adding Trimethylamine (721 µL, 5 mmol) and cool the solution below $10^0$C. To this, acid chloride solution was added dropwise by using addition funnel. Maintain the temperature of reaction mixture below $10^0$C for 10min and 3hrs in room temperature. The reaction mixture was quenched with water and extracted by using $CH_2Cl_2$ (2 x 20 mL). The organic solution was dried over anhydrous sodium sulfate and solvents were evaporated using roto vacuum evaporator. The products further purified by subjected to column chromatography using chloroform/methanol (99:1) as eluent.

**Esterification and Thio-esterification of ferulic acid (2h-2k)**

Ferulic acid chlorides have been prepared as mentioned in the above procedure ($SOCl_2$ method) and dissolved this acid chloride in dry $CH_2Cl_2$. Thiol (1.5 mmol) was dissolved in dry $CH_2Cl_2$ followed by adding Trimethylamine (721 µL, 5 mmol) and cool the solution below $10^0$C. To this, acid chloride solution was added dropwise by using addition funnel. Maintain the temperature of reaction mixture below $10^0$C for 10min and 3hrs in room temperature. The reaction mixture was quenched with water and extracted by using $CH_2Cl_2$ (2 x 20 mL). The organic solution was dried over anhydrous sodium sulfate and solvents were evaporated using roto vacuum evaporator. The products further purified by subjected to column chromatography using Hexane - ethyl acetate (80:20) as eluent. The product formed as a white precipitate.

**Procedure for the synthesis of methyl- (*E*)-3-(4-hydroxy-3-methoxyphenyl) acrylate (3)**

Ferulic acid (194mg, 1mmol) was dissolved in 3mL of methanol followed by adding drops of Con. $H_2SO_4$. Then the mixture was refluxed at $80^0$C for 3hrs. After 3hrs, the mixture was quenched with water and extracted by using ethyl acetate (2 x 20mL). The organic extract was separated, washed with bicarbonate, dried over anhydrous sodium sulfate and solvents were evaporated under reduced pressure. As such of the obtained compound was used for the synthesis of its respective analogues.

**General procedure for O- alkylation of ferulic acid (3a-3l)**

Amine (2.5 mmol) was dissolved in dry $CH_2Cl_2$ and adds $K_2CO_3$ (552 mg, 4 mmol). Stir and cool the solution below $10^0$C. To this add chloroacetyl chloride (315 µL, 4 mmol) dissolved in dry $CH_2Cl_2$ dropwise by using addition funnel. Maintain the temperature below $10^0$C for 20min and 3hrs for room temperature. The reaction mixture was quenched with cold water and

extracted with ethyl acetate (2 x 20 mL). The ethyl acetate layer was dried over anhydrous sodium sulfate and solvents removed under reduced pressure. The acetamide formed as precipitate and it was subjected to O-alkylation with FA ester.

Take methyl- (*E*)-3-(4-hydroxy-3-methoxyphenyl) acrylate (208 mg, 1mmol) and dissolved acetonitrile (2mL). Add the acetamide (1.2 mmol) and $K_2CO_3$ (165.6 mg, 1.2mmol) to the reaction mixture. Reflux the reaction mixture at $120^0$C for 3hrs. After completion of the reaction, it was quenched with water and extracted with $CH_2Cl_2$ (2 x 20 mL). The organic layer then dried with anhydrous sodium sulfate and solvents were removed under reduced pressure. Product was purified by column chromatography by using methanol/chloroform (3:97) as eluent.

**General procedure for the synthesis of ferulic acid ethers (3m-3w)**

Take methyl- (*E*)-3-(4-hydroxy-3-methoxyphenyl) acrylate (208 mg, 1mmol) and dissolved Dimethyl formamide (2mL). To this add $K_2CO_3$ (414 mg, 3mmol) and alkyl bromide (1.5mmol) and heat the reaction mixture at $80^0$C for 3hrs. After the reaction completes, it was quenched with water and extracted by using ethyl acetate (3 x 20 mL). The ethyl acetate layer then dried over with anhydrous sodium sulfate and solvents were removed under reduced pressure. Product was purified by column chromatography using Hexane – ethyl acetate (95:5) as eluent.

**General procedure for the synthesis of 3H-benzo[f]chromen-3-one derivatives from Ferulic acid (4a-4c)**

Ferulic acid (194mg, 1mmol) was taken in 5mL RB flask and mixed with powdered 2-naphthol (144mg, 1mmol). Add anhydrous $AlCl_3$ (133mg, 1mmol) to the reaction mixture and mixed thoroughly. Neat reaction was performed at $120^0$C for 3hrs. After completion of the reaction, the reaction mixture was quenched with water and extracted with ethyl acetate. Then the organic layer was dried over with anhydrous sodium sulfate and solvents were removed under reduced pressure. Product was purified by column chromatography using Hexane – ethyl acetate (80:20) as eluent.

***In silico* studies**

**Ligand Preparation**

All the 39 compounds including (E)-4-(3-((4-fluorophenyl)thio)-3-oxoprop-1-en-1-yl)-2-methoxyphenyl acetate (**2i**), methyl (E)-3-(3-methoxy-4-(2-oxo-2-thiomorpholinoethoxy)phenyl)acrylate (**3j**) along with ferulic acid (**1**) were drawn by using ChemSketch and known BCR-ABL tyrosine kinase inhibitors (Imatinib) was retrieved from Pubchem database. The ligands were subjected to Energy minimization using Avagadro and subsequently the charges were added to them through Autodock 4.0.

**Protein preparation**

The crystal structure of the target protein BCR-ABL tyrosine kinase[1] (PDB ID: - 3OXZ) was retrieved from PDB database (http://www.rcsb.org/pdb) having resolution 2.2 Å. All the heteroatoms and water molecules were removed by Discovery Analyzer software. Polar hydrogens and Gasteiger charges were assigned after merging of non-polar hydrogen atoms in ADT.

**Molecular docking**

To validate drug-target association, the molecular docking stimulation was performed on ligands with BCR-ABL tyrosine kinase by Autodock software 4.0 by employing Lamarckian genetic algorithm[2]. The receptor was kept rigid, while ligands were set flexible to rotate and explore most probable binding poses. The torsional bonds of ligands were set free by Ligand module in AutoDock Tool (ADT). As per earlier reports, the Grid was set by covering active site binding pocket of the protein (chain A) with 92×92×92 points in x, y, z direction and followed by Autogrid run. The docking protocol was then implemented on the ligands in the dataset. The study was carried for 20 GA runs, which was found to be optimum to reproduce the pose in its crystal. The other GA parameters like the population size and the genetic operators were kept at their default values. The results were interpreted by observing the least binding energy (kcal/mol) and hydrogen bonds; stacking interactions involving between the active site residues of the target and ligand molecules were analyzed using PyMol molecular visualization tool and LigPlot. The RMSD was calculated to ensure that the selected ligands have conformational similarity.

**Anti-leukemic activity of FA derivatives**

**In vitro cell viability assay**

All cell lines were procured from the cell repository of the National Centre for Cell Science, Pune, India. The dose and duration dependent cytotoxicity of Ferulic acid and its derivatives on PBML, K562, U937 and HepG2 cell lines were quantitatively estimated by a non-radioactive, colorimetric assay system using tetrazolium salt, 3-[4,5- dimethylthiazol- 2-yl]-2,5-diphenil-tetrazolium bromide (MTT)**.** The percentage of proliferation was calculated by using the following equation:

% Proliferation = [$OD_{sample} - OD_{control}$] X 100/$OD_{control}$

The concentration required for a 50% inhibition of viability (IC50) was determined graphically. Multiple linear regressions were used to compare data using GraphPad prism 6 software. Among all the derivatives of FA, 2i and 3j were found as most active compounds and subjected into further biochemical studies.

**Intracellular measurement of reactive oxygen species (ROS)**

The production of intracellular ROS was measured using 2,7- dichlorofluorescein diacetate (DCFH2-DA) [43]. To the stock solution (in methanol) of 10 mM DCFH2-DAwas diluted in

culture medium without serum or other additives to yield a 100 μM working solution. At the end of exposure with Ferulic acid, 2i and 3j and the cells were washed twice with PBS. Then, cells were incubated in 1.5 mL working solution of DCFH2-DA at 37$^{o}$C for 30 min. Cells were lysed in alkaline solution and centrifuged at 3000 rpm. One milliliter of supernatant was transferred to a cuvette, and fluorescence was measured at 520 nm with a fluorescence spectrophotometer (Jasco-FP8200) using 485-nm excitation. As a positive control, those cells were incubated with $H_2O_2$ (100 mM) for 30 min prior to the analysis. The values were expressed as percent fluorescence intensity relative to control wells. Fluorescence micrographs were also taken by fluorescence microscopy (Carl Zeiss Axio Scope A1). To determine the crucial cues of ROS generation in shikonin derivatives-induced cell death, K562 cells (2×104) were seeded in a 96-well plate with 0.2 mL per well. A stock solution of *N*-acetyl-L-cysteine (NAC) was made with sterile water and added to cells at 10 mM for 1 h [42]. NAC pretreated or untreated K562 cells were cultured with 100 nM FA derivatives for 24 h and cell viability was determined by the MTT method.

**Determination of reduced glutathione (GSH)**

Reduced glutathione estimation in the cell lysate was performed by the method of Moron et al. The required amount of the cell lysate was mixed with 25% of trichloroacetic acid and centrifuged at 2,000 xg for 15 min to settle the precipitated proteins. The supernatant was aspirated and diluted to 1 mL with 0.2 M sodium phosphate buffer (pH 8.0). Later, 2 mL of 0.6 mM DTNB was added. After 10 minutes the optical density of the yellow-colored complex formed by the reaction of GSH and DTNB (Ellman's reagent) was measured at 405 nm. A standard curve was obtained with standard reduced glutathione. The levels of GSH were expressed as μg of GSH/mg protein.

**Determination of oxidized glutathione (GSSG)**

The oxidized glutathione level was measured after derivatization of GSH with 2-vinylpyidine according to the method of Griffith et al. In brief, with 0.5 mL cell lysate, 2 μl of 2-vinylpyidine was added and incubates for 1 hr at 37°C. Then the mixture was deprotenized with 4% sulfosalicylic acid and centrifuged at 1,000 xg for 10 min to settle the precipitated proteins. The supernatant was aspirated and GSSG level was estimated with the reaction of DTNB at 412 nm in spectrophotometer and calculated with standard GSSG curve.

**Redox ratio (GSH/GSSG)**

Redox ratio was determined for FA, 2i and 3j by taking the ratio of reduced glutathione/oxidized glutathione.

**Determination of lipid peroxidation (MDA)**

Lipid peroxidation was estimated by the method of Ohkawa et al. in cell lysate. The reaction mixture contains Tris-HCl buffer (50 mM, pH 7.4), tert-butyl hydroperoxide (BHP) (500 μM in

ethanol) and 1 mM FeSO4. After incubating the samples at 37°C for 90 min, the reaction was stopped by adding 0.2 mL of 8% sodium dodecyl sulfate (SDS) followed by 1.5 mL of 20% acetic acid (pH 3.5). The amount of malondialdehyde (MDA) formed during incubation was estimated by adding 1.5 mL of 0.8% thiobarbituric acid (TBA) and further heating the mixture at 95°C for 45 min. After cooling, samples were centrifuged, and the thiobarbituric acid reactive substances (TBARS) were measured in supernatants at 532 nm by using 1.53 x 105 M-1 cm-1 as extinction coefficient. The levels of lipid peroxidation were expressed in terms of n mol/mg protein.

**Quantitative estimation of DNA fragmentation by diphenylamine (DPA) assay**

After the treatment schedule, cells were lysed with hypotonic lysis buffer followed by centrifugation. Then Perchloric acid (0.5 M) was added to the pellets containing uncut DNA (resuspended with 200 mL of hypotonic lysis buffer), and to the other half of the supernatants containing DNA fragments. Then 2 volumes of a solution containing 0.088 M DPA, 98% (v/v) glacial acetic acid, 1.5% (v/v) sulfuric acid, and 0.5% (v/v) of 1.6% acetaldehyde solution were added. The samples were stored at 4 ºC for 48 h. The colorimetric reaction was quantitated spectrophotometrically at 575 nm. The percentage of fragmentation was calculated as the ratio of DNA in the supernatants to the total DNA confirm the data obtained from the spectrophotometric method, we have analyzed the DNA fragmentation by DNA laddering in 1.2% agarose gel electrophoresis.

**Apoptotic morphological changes by AO/Et-Br staining**

Two DNA-binding dyes AO and Et-Br were used for the morphological apoptotic cells. After treatment with FA derivatives for 24 h, K562 cells were collected, washed with cold PBS and then stained with a mixture of AO (100 µg/mL) and Et-Br (100 µg/mL) at room temperature for 5 min in dark. After proper washing with PBS, the stained cells were observed by a fluorescence microscope (Carl Zeiss Axio Scope A1). Untreated and FA derivatives treated K562 cells were collected and were fixed with 2.5% glutaraldehyde for 15 min, followed by permeabilized with 0.1% Triton X-100 and stained with 1 µg/mL DAPI for 5 min at 37$^{o}$C. The cells were then washed with PBS and examined by fluorescence microscopy (Carl Zeiss Axio Scope A1).

**Bcr-Abl kinase inhibitory assay - ADP-Glo™ Kinase assay kit**

The Bcr–Abl inhibitory activity assay was performed using ADP-Glo™ Kinase assay kit (Promega, USA) and Abl Kinase Enzyme System (Promega, USA) according to the manufacturer's instructions. General procedures are as the following: Kinases (4ng/µL) were incubated with substrates (0.2µg/µL), compounds ($3\times10^{-5}$ - $3\times10^{-10}$M) and ATP (25µM) in a final buffer of tris 40mM, MgCl2 10mM, BSA 0.1mg/mL, DTT 1mM in 384-well plate with the total volume of 5µL. The assay plate was incubated at 30ºC for 1h. After the plate cooled for 5min at room temperature, 5µl of ADP-Glo reagent was added into each well to stop the reaction and consume the remaining ADP within 40min. At the end, 10µL of kinase detection reagent was

added into the well and incubated for 30min to produce a luminescence signal and the luminescence was measured with the help of a plate-reading luminometer. The signal was correlated with the amount of ATP present in the reaction and was inversely correlated with the kinase activity.

**Assessment of apoptotic cell population by annexin V-FITC/PI assay**

Confluent culture of K562 cells ($2 \times 10^6$) were seeded in 6 well cell culture plates and treated with FA, 2i, 3j for 24 h. Then the K562 cells were collected, washed with PBS, and re-suspended in PBS. Apoptotic cell death was identified by double staining with annexin V-FITC and PI, using the annexin V-FITC apoptosis detection kit (BD Bioscience) according to the manufacturer's instructions. Data acquisition and analysis were performed in a Becton-Dickinson FACS verse flow cytometer using CellQuest software.

***BCR-Abl* mRNA expression study:**

Total RNA extracted from untreated and treated K562 cells after 6 hrs (TRIZOL; Invitrogen). 1 µg of total RNA were reverse transcribed using Revert Aid M-MuLV Reverse Transcriptase (Fermentas) to synthesis the cDNA. cDNA was amplified with green *Taq*DNA polymerase (Fermentas) in 25 µL reaction mixture using specific primers of *bcr-abl and gapdh* using Veriti Thermal Cycler (Applied Biosystems). Sequences of the PCR primers were as follows: *bcr-abl* product representing the BCR-ABL junction and kinase, forward: 5'-GAA GCT TCT CCC TGG CAT CCC GT-3' and reverse 5'-GCC AGG CTC TCG GGT GCA GTC C-3'; *gapdh*, forward 5'-GAG CCA AAC GGG TCA TCA TC-3' and reverse, 5'-CCT GCT TCA CCA CCT TCT TG-3'. The reaction conditions consisted of an initial activation step (5 min at 95°C) and a cycling step (denaturation for 30 s at 94°C, annealing for 30 s at 58°C and extension for 1 min at 72°C for 35 cycles). Glyceraldehyde-3-phosphate dehydrogenase (GAPDH) amplification was also done to ensure equal cDNA input. PCR-amplified product was subsequently run on 1.2% agarose gel, stained with ethidium bromide and visualized under ultraviolet light and analyzed in BioRad gel documentation system. In real time PCR, (Eppendorf RealPlex master cycler, using 2X SYBR premix Ex Taq II (TAKARA Bio), the mRNA expression levels of the target genes were normalized against those of GAPDH levels and expressed as relative fold change compared with untreated controls and quantified by the $2^{-ddCT}$ method.

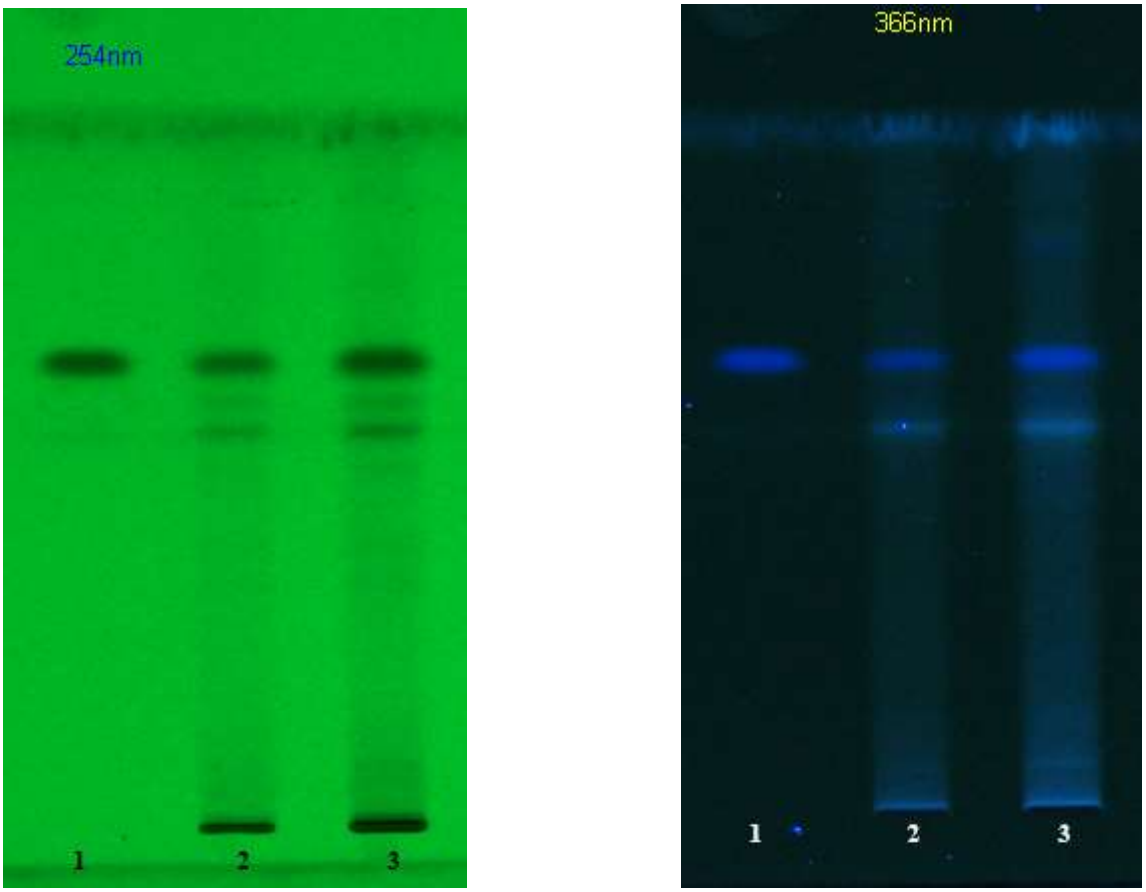



Fig. S1 High Performance Thin Layer Chromatography (HPTLC) profile of Standard Ferulic acid (Lane 1) compared with aqueous extract of *Salicornia brachiata* (Lane 2 and 3*).*

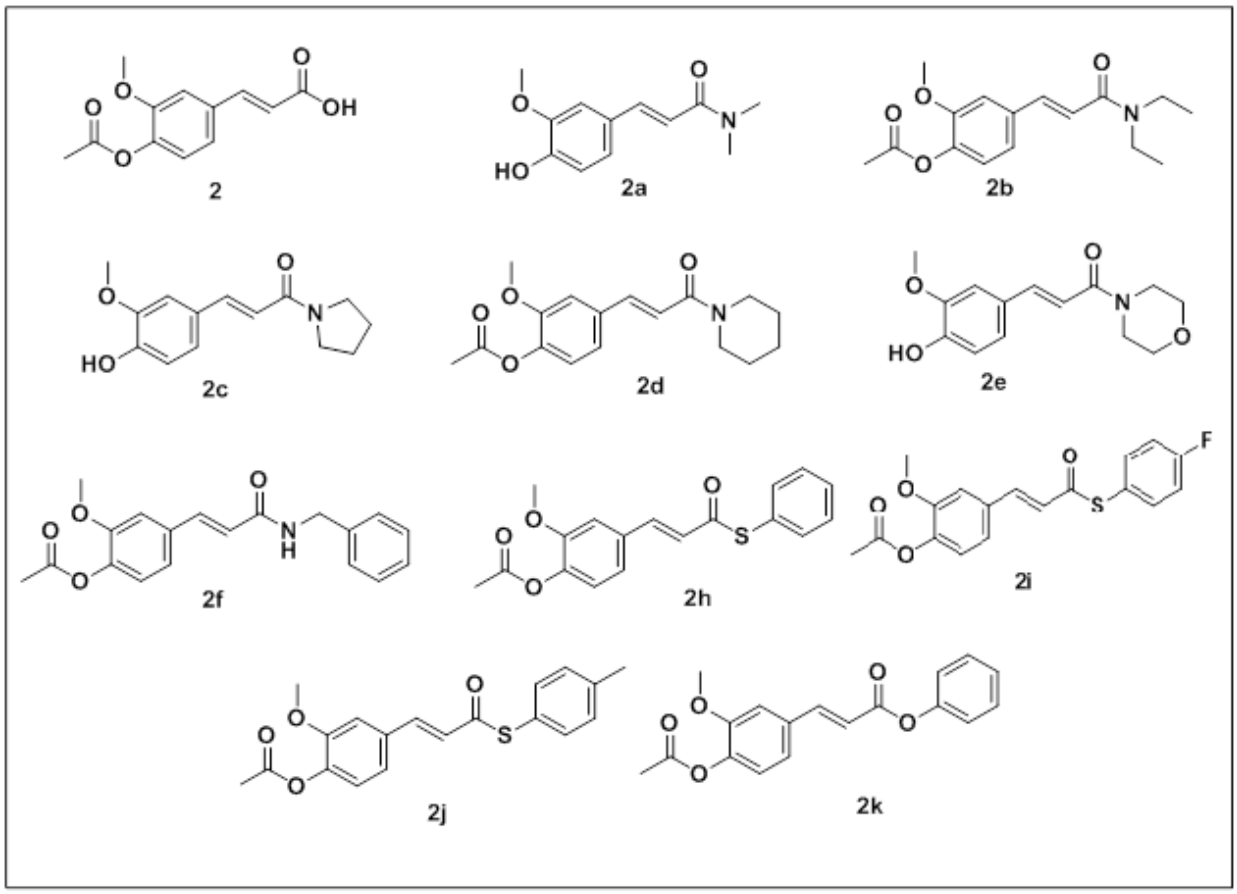



**Fig. S2 Compounds synthesized by using –OH Protected ester of ferulic acid**

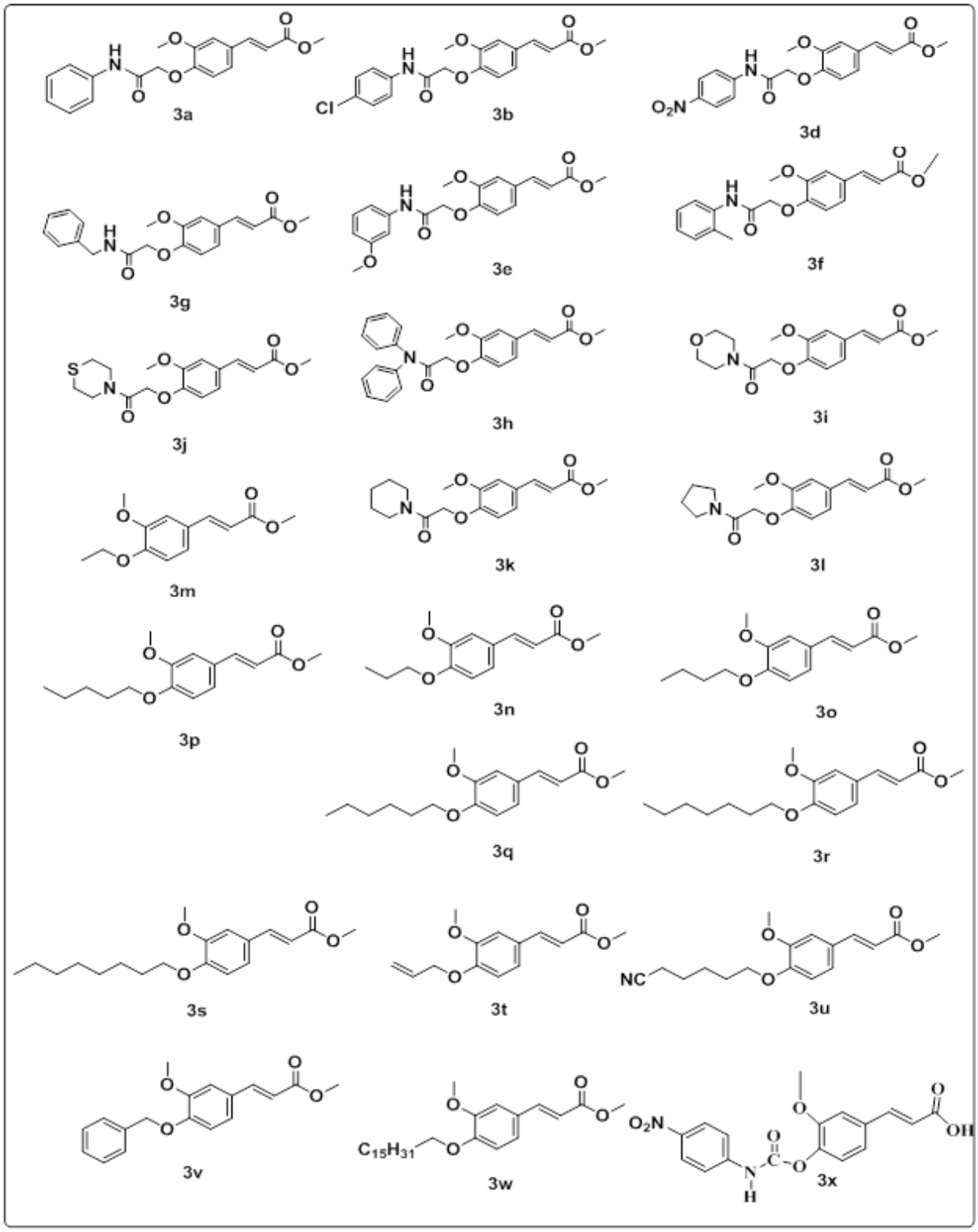



**Fig. S3 Compounds synthesized by using Methyl ferulate**

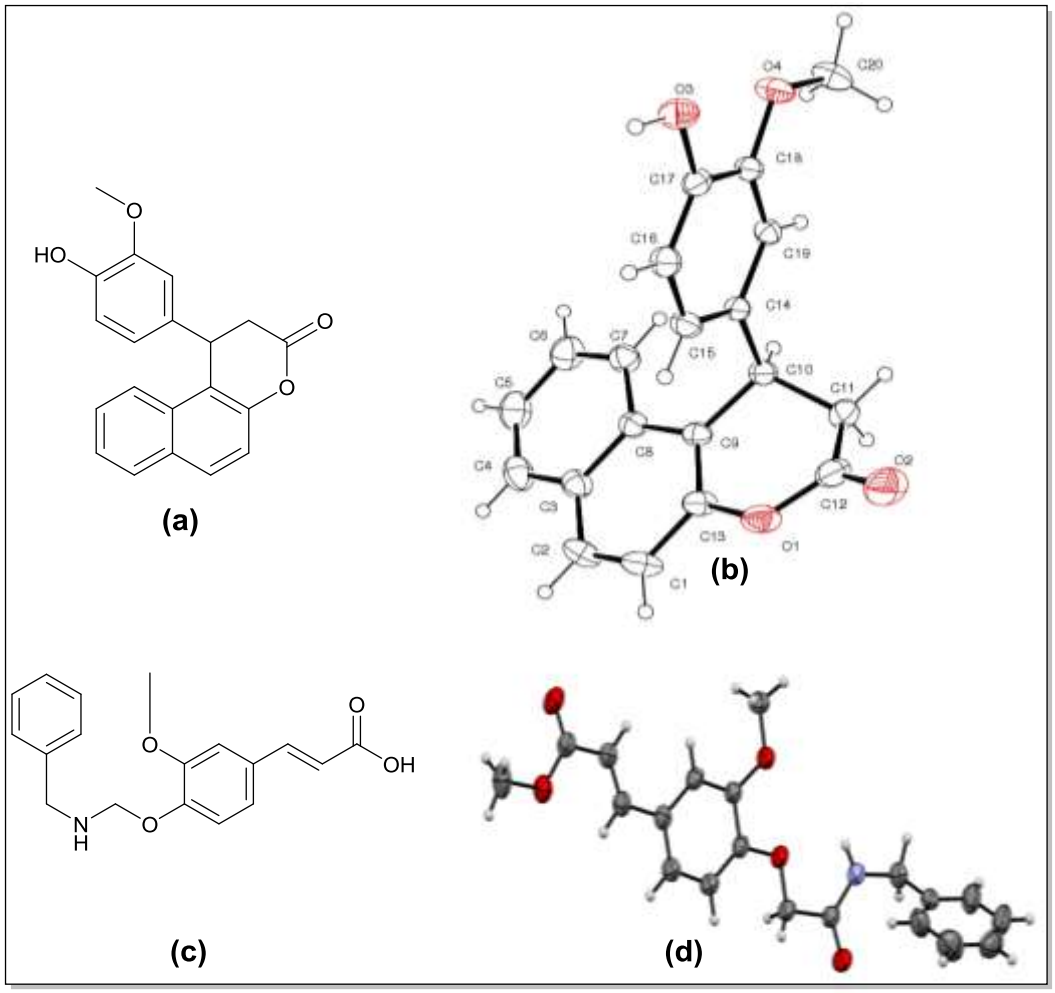
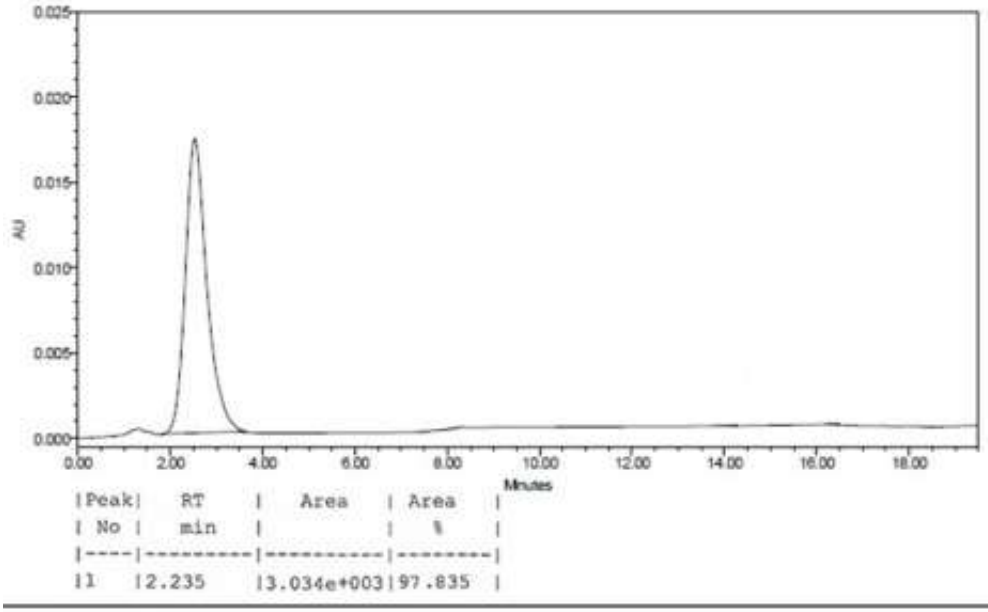



**Fig. S4 Crvstal structure of the product (a) Structure of 4a, (b) Crystal structure of 4a [CCDC 1449366], (c) Structure of 3g and (d) Crystal structure of 3g [CCDC 1454627].**



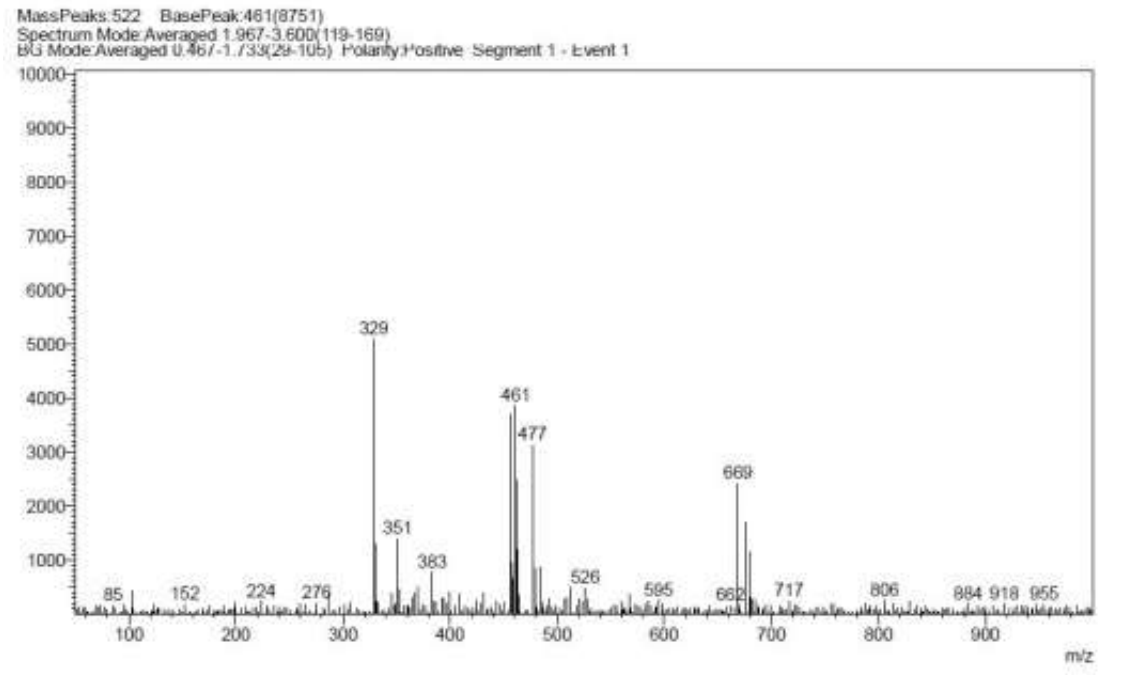
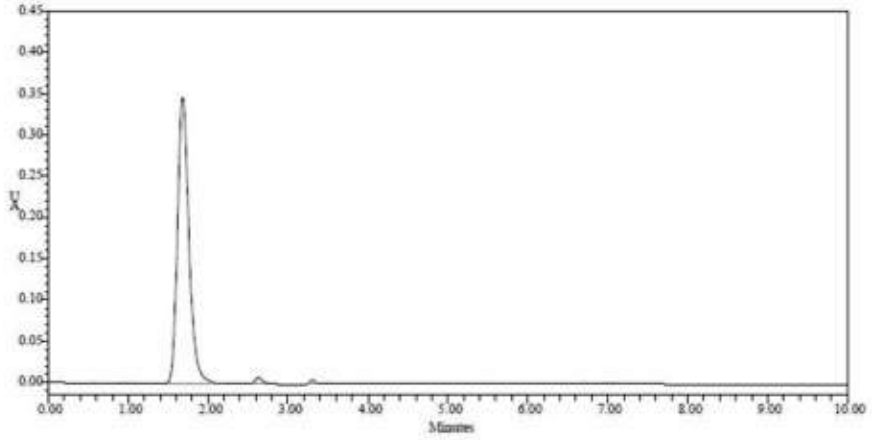




**Fig. S5 LC Chromatogram and mass spectrum of compound 2h**




| Peak No | RT min | Area | Area % |
|---|---|---|---|
| 1 | 1.740 | 1.586e+003 | 93.564 |

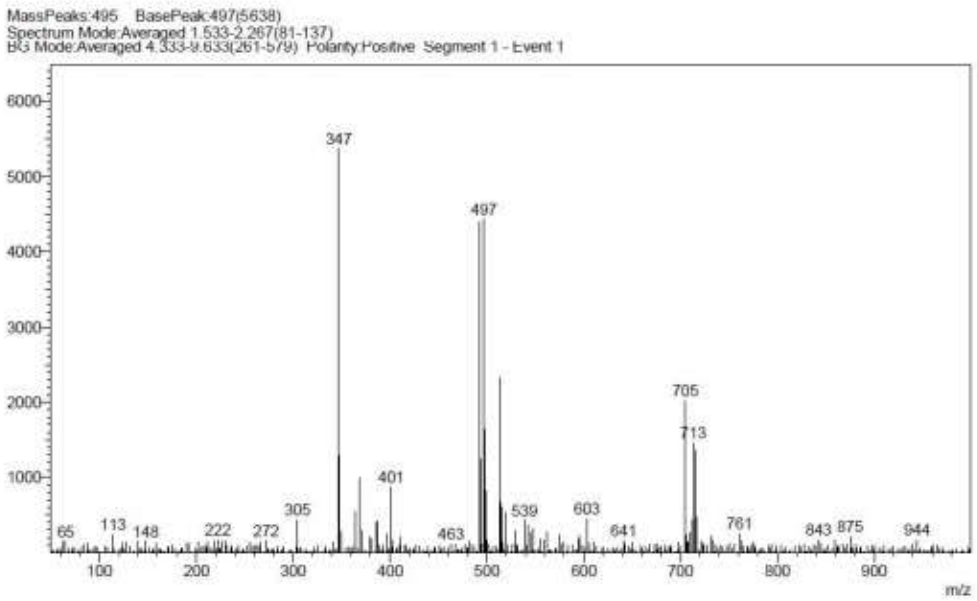
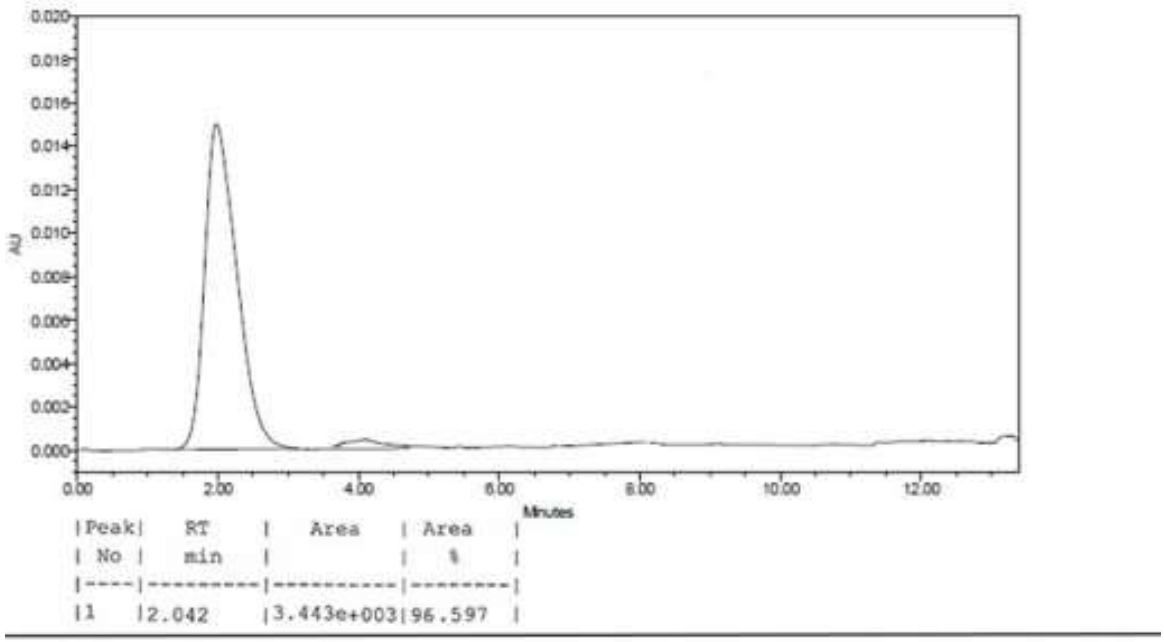



**Fig. S6 LC Chromatogram and mass spectrum of compound 2i**



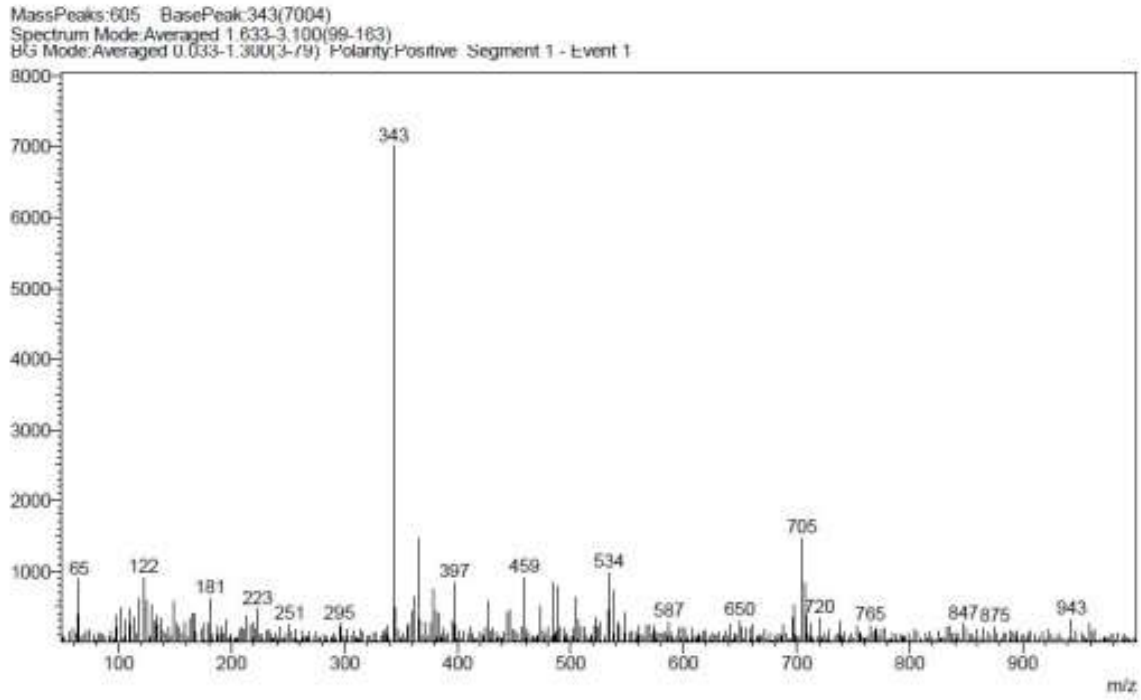




**Fig. S7 LC Chromatogram and mass spectrum of compound 2j**

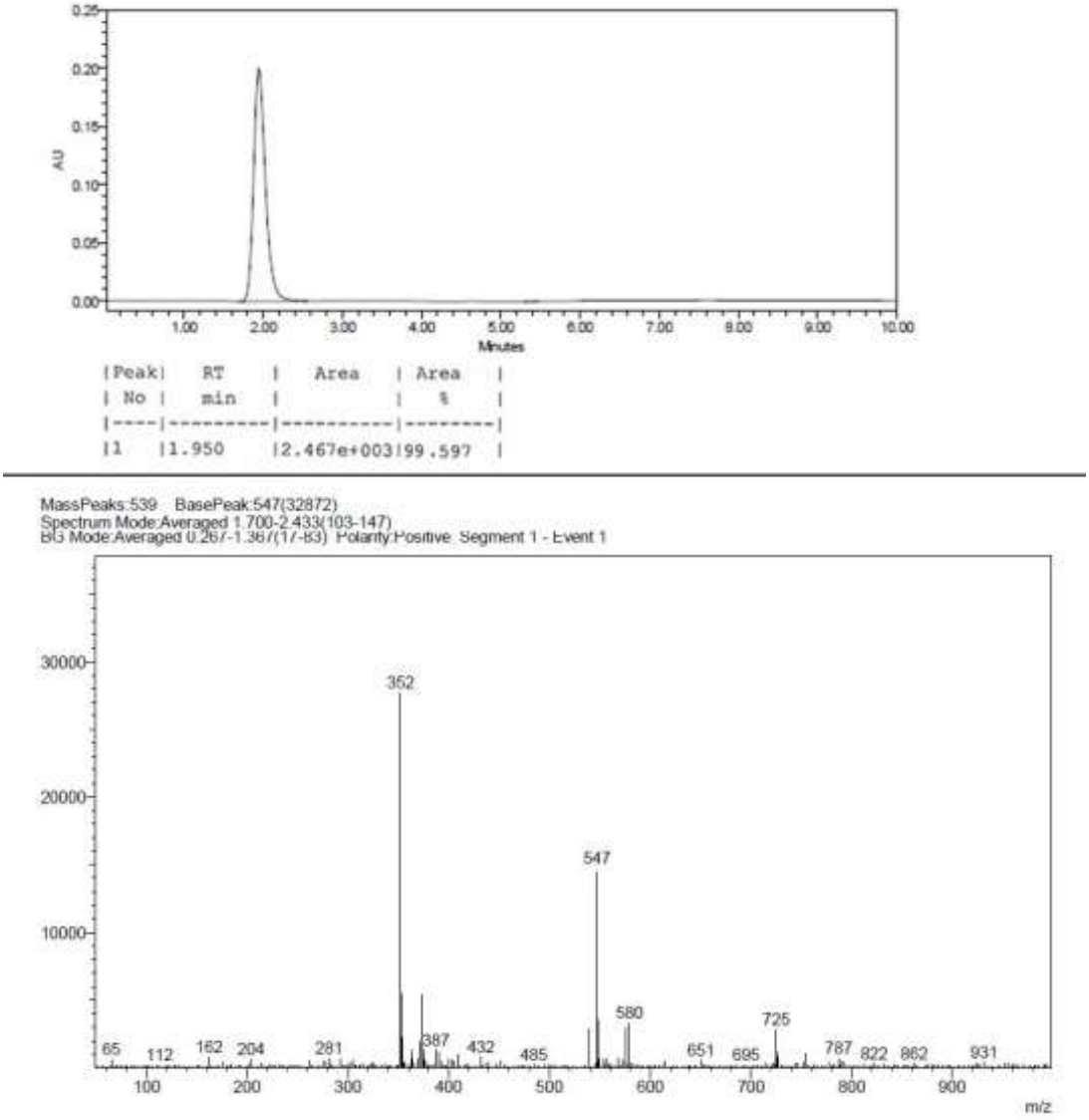



**Fig. S8 LC Chromatogram and mass spectrum of compound 3j**

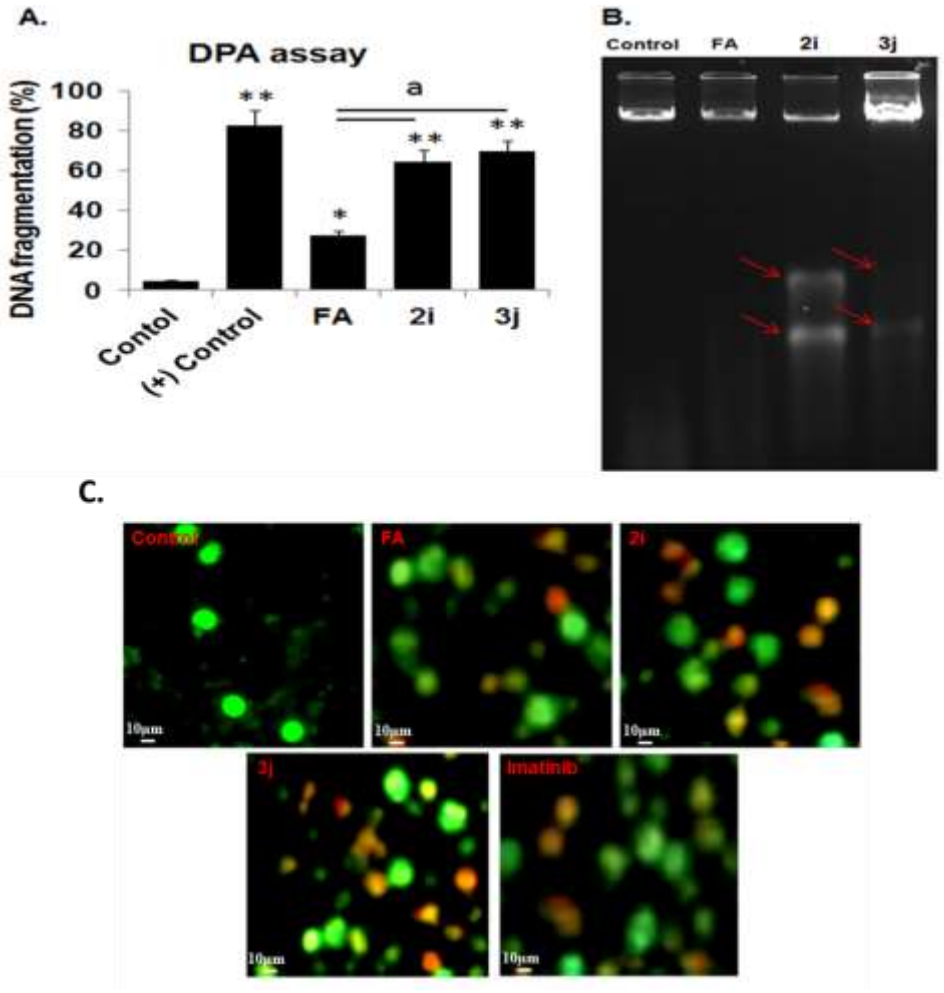



**Fig S9. DNA Fragmentation studies of FA, 2i, 3j and imatinib**

**Characterization of the compounds**

**(E)-3-(4-hydroxy-3-methoxyphenyl) acrylic acid (1)**

Mp: 169-171$^{o}$C; MF: $C_{10}H_{10}O_4$; Appearance: white solid; $^{1}$H NMR (300 MHz, $d_6$-DMSO): 12.13 (s, 1H), 9.56 (s, 1H), 7.48 (d, J=15.9Hz, 1H), 7.28 (d, J=1.8Hz, 1H), 7.08 (dd, J=1.8Hz, 6.3Hz, 1H), 6.78 (d, J=8.1Hz, 1H), 6.36 (d, J=15.9Hz, 1H), 3.81 (s, 3H); $^{13}$C NMR (300 MHz, $d_6$-DMSO): 167.98, 149.02, 147.86, 144.49, 125.73, 122.79, 115.57, 115.47, 111.06, 55.61; LC MS (m/z): [M + $H^+$ ]- 194.19

**Methyl (E)-3-(4-acetoxy-3-methoxyphenyl) acrylate (2)**

Yield : 89%; Mp: 197-199$^{o}$C (Reference 197$^{o}$C); MF: $C_{13}H_{14}O_5$; Appearance: white solid; $^{1}$H NMR (300 MHz, $d_6$-DMSO): 12.46 (s, 1H), 7.57 (d, J=15.9Hz, 1H), 7.48 (d, J=1.8Hz, 1H), 7.26 (dd, J=1.8Hz, 6.6Hz, 1H), 7.11 (d, J=8.1Hz, 1H), 6.59 (d, J=15.9Hz, 1H), 3.82 (s, 3H), 2.264 (s, 3H); ; LC MS (m/z): [M + $H^+$ ]- 250.25

**(E)-3-(4-hydroxy-3-methoxyphenyl)-N, N-dimethyl acrylamide (2a)**

Yield : 45%; Mp: 116-118$^{o}$C; MF: $C_{12}H_{15}NO_3$; Appearance: white solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.60 (d, J=15.3Hz, 1H), 7.10 (dd, J=1.8Hz, 6.3Hz, 1H), 6.99 (d, J=1.8Hz, 1H), 6.91 (d, J=8.1Hz, 1H), 6.73 (d, J=15.6Hz, 1H), 5.91 (s, 1H), 3.93(s, 3H), 3.17(s, 3H), 3.07(s, 3H); $^{13}$C NMR (300 MHz, $d_6$-DMSO): 167.04, 147.35, 146.74, 142.60, 127.87, 121.81, 114.78, 110.05, 55.98, 37.45, 35.99; ; LC MS (m/z): [M + $H^+$ ]- 221.26

**(E)-4-(3-(diethylamino)-3-oxoprop-1-en-1-yl)-2-methoxyphenyl acetate (2b)**

Yield : 53%; Mp: 110-112$^{o}$C; MF: $C_{16}H_{21}NO_4$; Appearance: white solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.66 (d, J=15.3Hz, 1H), 7.14 (d, J=8.1Hz, 1H), 7.05 (d, J=3.9Hz, 1H), 7.02 (s, 1H), 6.75 (d, J=15.3Hz, 1H), 3.8 (s, 3H), 3.53-3.44 (m, 4H), 2.32 (s, 3H), 1.28-1.17 (m, 6H); $^{13}$C NMR (300 MHz, $d_6$-DMSO): 168.88, 165.49, 151.21, 141.61, 140.64, 134.56, 123.06, 120.05,118.15, 111.79, 55.91, 42.28,41.06, 20.63, 15.05, 13.18; ; LC MS (m/z): [M + $H^+$ ]- 291.15

**(E)-3-(4-hydroxy-3-methoxyphenyl)-1-(pyrrolidin-1-yl) prop-2-en-1-one (2c)**

Yield : 45%; Mp: 174-175$^{o}$C; MF: $C_{14}H_{17}NO_3$; Appearance: white solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.66 (d, J=15.3Hz, 1H), 7.11 (dd, J=1.8Hz, 6.6Hz,1H), 7.0 (d, J=1.8Hz, 1H), 6.91 (d, J=8.1Hz, 1H), 6.57 (d, J=15.6Hz, 1H), 5.88 (s, 1H), 3.93 (s, 3H), 3.65-3.57 (m, 4H), 2.05-1.85 (m, 4H); $^{13}$C NMR (300 MHz, $CDCl_3$)165.06, 147.41, 146.74, 141.91, 127.80, 121.82, 116.19, 114.78, 110.11, 55.94, 46.58, 46.04, 26.11, 24.34; LC MS (m/z): [M + $H^+$ ]- 247.12

**(E)-2-methoxy-4-(3-oxo-3-(piperidin-1-yl) prop-1-en-1-yl) phenyl acetate (2d**)

Yield : 40%; Mp: 124-125$^{o}$C; MF: $C_{17}H_{21}NO_4$; Appearance: white solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.52 (d, J=15.6Hz, 1H), 7.05 (d, J=8.4Hz,1H), 6.97 (t, J=8.1Hz,8.4Hz, 2H), 6.76 (d, J=15.3Hz, 1H), 3.79 (s, 3H), 3.59 (s, 2H), 3.51 (s, 2H), 2.25 (s, 3H), 2.1 (s, 1H), 1.63-1.54 (m, 5H); $^{13}$C NMR (300 MHz, $CDCl_3$) 168.88, 165.16, 151.26, 141.49, 140.67, 134.56, 123.08,

120.23, 118.08, 111.53, 55.96, 47.06, 43.36, 26.78, 25.6, 24.63, 20.66;; LC MS (m/z): [M + $H^+$ ]- 303.15

**(E)-3-(4-hydroxy-3-methoxyphenyl)-1-morpholinoprop-2-en-1-one (2e)**

Yield : 30%; Mp: 116-118$^o$C; MF: $C_{14}H_{17}NO_4$; Appearance: white solid; $^1$H NMR (300 MHz, $CDCl_3$): 7.56 (d, J=15.3Hz, 1H), 7.04-7,01 (m,1H), 6.91 (d, J=1.8Hz,1H), 6.84 (d, J=8.4Hz, 1H), 6.61 (d, J=15.3Hz,1H), 5.90 (s, 1H), 3.86 (d, J=3.6Hz, 3H), 3.65 (s, 8H); $^{13}$C NMR (300 MHz, $CDCl_3$) 165.93, 147.58, 146.81, 143.52, 127.60, 121.99, 114.85, 113.79, 109.97, 66.88, 55.99, 46.26, 42.46, 29.69; ; LC MS (m/z): [M + $H^+$ ]- 263.12

**(E)-4-(3-(benzylamino)-3-oxoprop-1-en-1-yl)-2-methoxyphenyl acetate (2f)**

Yield : 35%; Mp: 126-129$^o$C; MF: $C_{19}H_{19}NO_4$; Appearance: white solid; $^1$H NMR (300 MHz, $CDCl_3$): 7.55 (d, J=15.6Hz, 1H), 7.30-7.18 (m, 6H), 7.03-6.33(m, 3H), 6.27 (d, J=15.6Hz, 1H), 5.88 (s, 1H), 4.50 (d, J=5.7Hz, 1H), 3.7 (s, 3H), 2.2 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 168.95, 165.59, 151.27, 140.89, 140.64, 138.12, 133.84, 128.76, 127.94, 127.85, 127.61, 123.15, 120.76, 120.56, 111.40, 55.87, 43.89, 20.66; ; LC MS (m/z): [M + $H^+$ ]- 325.13

**(E)-2-methoxy-4-(3-oxo-3-(phenylthio) prop-1-en-1-yl) phenyl acetate (2h)**

Yield : 65%; Mp: 119-121$^o$C; MF: $C_{18}H_{16}O_4S$; Appearance: white solid; $^1$H NMR (300 MHz, $CDCl_3$): 7.63 (d, J=15.9Hz, 1H), 7.51-7.43 (m, 5H), 7.15 (td, J=1.8Hz, 2H), 7.07 (d, J=8.1Hz, 1H), 6.73 (d, J=15.6Hz, 1H), 3.88 (s, 3H), 2.33 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 187.76, 168.70, 151.50, 141.83, 140.77, 134.62, 132.95, 129.22, 127.52, 124.30, 123.38, 121.69, 111.59, 55.97, 20.64; ; LC MS (m/z): [M + $H^+$ ]- 328.08.

**(E)-4-(3-((4-fluorophenyl) thio)-3-oxoprop-1-en-1-yl)-2-methoxyphenyl acetate (2i)**

Yield : 70%; Mp: 108-110$^o$C; MF: **$C_{18}H_{15}FO_4S$**; Appearance: white solid; $^1$H NMR (300 MHz, $CDCl_3$): 7.63 (d, J=15.6Hz, 1H), 7.48-7.43 (m, 2H), 7.19-7.11 (m, 4H), 7.08 (d, J=8.4Hz, 1H), 6.72 (d, J=15.9Hz, 1H), 3.89 (s, 3H), 2.33 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 187.76, 168.73, 151.53, 141.07, 136.78, 136.66, 132.86, 124.04, 123.43, 122.80, 122.75, 121.75, 116.68, 116.38, 111.59, 55.99, 20.66; ; LC MS (m/z): [M + $H^+$ ]- 346.07

**(E)-2-methoxy-4-(3-oxo-3-(p-tolylthio) prop-1-en-1-yl) phenyl acetate (2j)**

Yield : 40%; Mp: 153-155$^o$C; MF: $C_{19}H_{18}O_4S$; Appearance: white solid; $^1$H NMR (300 MHz, $CDCl_3$): 7.64 (d, J=15.9Hz, 1H), 7.61 (d, J=1.8Hz, 1H), 7.39-7.36 (m, 3H), 7.30 (d, J=8.4Hz ,2H), 7.21 (s, 1H), 7.16 (t, J=9.3,1H), 3.84 (s, 3H), 2.36 (s, 3H), 2.27 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 187.32, 168.32, 151.20, 141.39, 140.73, 139.40, 134.46, 132.67, 129.96, 124.48, 123.70, 123.30, 122.35, 112.27, 56.04, 20.81, 20.37; ; LC MS (m/z): [M + $H^+$ ]- 342.09

**Phenyl- (E)-3-(4-acetoxy-3-methoxyphenyl) acrylate (2k)**

Yield : 57%; Mp: 162-163$^{o}$C; MF: $C_{18}H_{16}O_5$; Appearance: white solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.83 (d, J=16.2Hz, 1H), 7.44-7.38 (m, 2H), 7.287-7.16 (m, 5H), 7.09 (d, J=8.1, 1H), 6.58 (d, J=16.2Hz, 1H), 3.84 (s, 3H), 2.54 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 168.72, 165.21, 151.45, 150.72, 145.77, 141.73, 133.08, 129.43, 125.80, 123.23, 121.57, 121.45, 117.49, 111.38, 55.90, 20.62; ; LC MS (m/z): [M + $H^+$ ]- 312.10

**Methyl (E)-3-(4-hydroxy-3-methoxyphenyl) acrylate (3)**

Yield: 88%; MF: $C_{11}H_{12}O_4$; Appearance: Brown viscus liquid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.62 (d, J=15.9Hz, 1H), 7.04 (td, J=1.8Hz, 2H), 6.91 (d, J=8.1Hz, 1H), 6.29 (d, J=15.9Hz, 1H), 3.91 (s, 3H), 3.79 (s, 3H); ; LC MS (m/z): [M + $H^+$ ]- 208.07

**Methyl (E)-3-(3-methoxy-4-(2-oxo-2-(phenylamino)ethoxy)phenyl)acrylate (3a)**

Yield: 51%; Mp: 148-150$^{o}$C; MF: $C_{19}H_{19}NO_5$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 8.76 (s, 1H), 7.66-7.57 (m, 3H), 7.38-7.33 (m, 2H), 7.18-7.10 (m, 3H), 6.96 (d, J=8.1Hz, 1H), 6.35 (d, J=15.9Hz, 1H), 4.67 (s, 2H), 3.97 (s, 3H), 3.81 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.30. 166.18, 149.84, 148.79, 144.05, 137.00, 129.76, 129.03, 124.69, 122.22, 119.86, 116.88, 115.60, 110.57, 69.68, 55.91, 51.66; ; LC MS (m/z): [M + $H^+$ ]- 341.13

**Methyl (E)-3-(4-(2-((4-chlorophenyl) amino)-2-oxoethoxy)-3-methoxyphenyl)acrylate (3b)**

Yield: 48%; Mp: 188-190$^{o}$C; MF: $C_{19}H_{18}ClNO_5$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 8.80 (s, 1H), 7.63 (d, J=15.9Hz, 1H), 7.58-7.53 (m, 2H), 7.34-7.28 (m, 2H), 7.15-7.10 (m, 2H), 6.96 (d, J=8.1Hz, 1H), 6.36 (d, J=15.9Hz, 1H), 4.66 (s, 2H), 3.97 (s, 3H), 3.81 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.33. 166.28, 149.89, 148.72, 144.02, 135.64, 130.00, 129.74, 124.12, 122.29, 121.08, 117.08, 115.84, 110.68, 69.77, 56.01, 51.74; ; LC MS (m/z): [M + $H^+$ ]- 375.09

**Methyl (E)-3-(3-methoxy-4-(2-((4-nitrophenyl)amino)-2-oxoethoxy)phenyl)acrylate (3d)**

Yield: 53%; Mp: 178-180$^{o}$C; MF: $C_{19}H_{18}N_2O_7$; Appearance: pale yellow solid; $^{1}$H NMR (300 MHz, $d_6$-DMSO): 10.66 (s, 1H), 8.65 (t, J=2.1Hz, 1H), 7.98-7.93 (m, 2H), 7.66-7.57 (m, 2H), 7.42 (d, J=1.8Hz, 1H), 7.26 (dd, J=1.8Hz, 6.6Hz, 1H), 6.96 (d, J=8.4Hz, 1H), 6.61 (d, J=15.9Hz, 1H), 4.81 (s, 2H), 3.81 (s, 3H), 3.71 (s, 3H); $^{13}$C NMR (300 MHz, $d_6$-DMSO) 167.16. 166.87, 149.37, 149.23, 147.92, 144.45, 139.49, 130.24, 127.96, 125.43, 122.48, 118.17, 115.88, 113.62, 113.57, 111.15, 67.82, 55.94, 51.30; ; LC MS (m/z): [M + $H^+$ ]- 386.11

**Methyl (E)-3-(3-methoxy-4-(2-((3-methoxyphenyl) amino)-2-oxoethoxy) phenyl)acrylate (3e)**

Yield: 40%; Mp: 168-170$^{o}$C; MF: $C_{20}H_{21}NO_6$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 8.75 (s, 1H), 7.61 (d, J=15.9Hz, 1H), 7.34 (t, J=2.1Hz, 2.4Hz, 1H), 7.27-7.22 (m, 1H), 7.14 (d, J=1.8Hz, 2H), 7.11-7.04 (m, 1H), 6.93 (d, J=8.4Hz, 1H), 6.72-6.68 (m, 1H), 6.36 (d, J=15.9Hz, 1H), 4.66 (s, 2H), 3.97 (s, 3H), 3.81 (d, J=3.6, 6H); $^{13}$C NMR (300 MHz, $CDCl_3$)

167.37. 166.26, 160.21, 149.93, 148.86, 144.11, 138.28, 129.89, 129.78, 122.29, 116.99, 115.78, 112.07, 110.43, 105.79, 69.83, 56.01, 55.34, 51.74, 29.70; ; LC MS (m/z): [M + $H^+$ ]- 371.14

**Methyl (E)-3-(3-methoxy-4-(2-oxo-2-(o-tolylamino)ethoxy) phenyl)acrylate (3f)**

Yield: 42%; Mp: 157-160$^oC$; MF: $C_{20}H_{21}NO_5$; Appearance: Grey solid; $^1H$ NMR (300 MHz, $CDCl_3$): 10.03 (s, 1H), 7.62 (d, J=15.9Hz, 1H), 7.45-7.37 (m, 3H), 7.26-7.17 (m, 2H), 6.94 (d, J=8.4Hz, 1H), 6.89 (d, J=7.8Hz, 1H) ,6.52 (d, J=15.9Hz, 1H), 4.74 (s, 2H), 3.85 (s, 3H), 3.71 (s, 3H), 2.27 (s, 3H); $^{13}C$ NMR (300 MHz, $CDCl_3$) 166.88. 166.13, 149.51, 144.48, 138.25, 137.98, 128.60, 127.82, 124.33, 122.50, 119.88, 116.55, 115.80, 113.48, 110.11, 67.93, 55.74, 51.28, 21.12; ; LC MS (m/z): [M + $H^+$ ]- 355.19

**Methyl (E)-3-(4-(2-(benzylamino)-2-oxoethoxy)-3-methoxyphenyl) acrylate (3g)**

Yield: 30%; Mp: 160-162$^oC$; MF: $C_{20}H_{21}NO_5$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 8.50 (t, J=6Hz, 5.7Hz, 1H), 7.60 (d, J=15.9Hz, 1H), 7.40 (, 1H), 7.33-7.22 (m, 6H), 6.93 (d, J=8.4Hz, 1H), 6.60 (d, J=15.9Hz, 1H), 4.613 (s, 2H), 4.33 (d, J=6Hz, 2H), 3.817 (s, 3H), 3.717 (s, 3H); ; LC MS (m/z): [M + $H^+$ ]- 355.14

**Methyl (E)-3-(4-(2-(diphenylamino)-2-oxoethoxy)-3-methoxyphenyl) acrylate (3h)**

Yield: 50%; Mp: 166-167$^oC$; MF: $C_{25}H_{23}NO_5$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.61 (d, J=15.9Hz, 1H), 7.38-7.26 (m, 10H), 7.06(t, J=1.8Hz, 8.4Hz, 2H), 6.78 (d, J=7.8Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 4.66 (s, 2H), 3.86 (s, 3H), 3.79 (s, 3H); $^3C$ NMR (300 MHz, $CDCl_3$) 167.62. 167.03, 149.64, 149.58, 144.66, 129.64, 128.42, 122.14, 115.90, 113.44, 110.56, 67.54, 55.93, 51.64; LC MS (m/z): [M + $H^+$ ]- 417.16

**Methyl (E)-3-(3-methoxy-4-(2-morpholino-2-oxoethoxy) phenyl) acrylate (3i)**

Yield: 45%; Mp: 110-120$^oC$; MF: $C_{17}H_{21}NO_6$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.62 (d, J=16.2Hz, 1H), 7.09 (t, J=1.8Hz, 8.1Hz, 2H), 6.93 (d, J=8.1Hz, 1H), 6.32 (d, J=8.1Hz, 1H), 4.79 (s, 2H), 3.90 (s, 3H), 3.80 (s, 3H); 3.64 (d, J=3.9Hz, 8H), $^{13}C$ NMR (300 MHz, $CDCl_3$) 167.47. 166.10, 149.51, 148.98, 144.39, 128.70, 122.22, 116.21, 113.53, 110.32, 68.42, 66.76, 55.83, 51.63, 45.91, 42.51; ; LC MS (m/z): [M + $H^+$ ]- 335.14

**Methyl (E)-3-(3-methoxy-4-(2-oxo-2-thiomorpholinoethoxy) phenyl) acrylate (3j)**

Yield: 52%; Mp: 110-112$^oC$; MF: $C_{17}H_{21}SNO_5$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.62 (d, J=15.9Hz, 1H), 7.09 (t, J=1.8Hz, 7.8Hz, 2H), 6.93 (d, J=8.1Hz, 1H), 6.32 (d, J=15.9Hz, 1H), 4.77 (s, 2H), 3.92-3.825 (m, 10H), 2.67-2.58 (m, 4H), $^{13}C$ NMR (300 MHz, $CDCl_3$) 167.48. 166.10, 149.44, 149.02, 144.40, 128.68, 122.23, 116.21, 113.34, 110.29, 68.59, 55.82, 51.63, 48.34, 44.78, 27.94, 27.34; ; LC MS (m/z): [M + $H^+$ ]- 351.13.

**Methyl (E)-3-(3-methoxy-4-(2-oxo-2-(piperidin-1-yl) ethoxy) phenyl) acrylate (3k)**

Yield: 38%; Mp: 170-172$^{o}$C; MF: $C_{18}H_{23}NO_5$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.62 (d, J=15.9Hz, 1H), 7.08 (t, J=1.8Hz, 7.5Hz, 2H), 6.93 (d, J=8.4Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 4.78 (s, 2H), 3.92 (s, 3H), 3.80 (s, 3H), 3.54-3.49 (m, 4H), 1.66-1.60 (m, 5H), 1.25 (s, 1H), $^{13}$C NMR (300 MHz, $CDCl_3$) 167.56. 165.65, 149.53, 144.60, 128.31, 122.33, 115.91, 113.37, 110.34, 68.29, 55.90, 51.60, 46.33, 43.26, 29.66, 26.41, 25.52, 24.41; ; LC MS (m/z): [M + $H^+$ ]- 333.16

**Methyl (E)-3-(3-methoxy-4-(2-oxo-2-(pyrrolidin-1-yl) ethoxy)phenyl)acrylate (3l)**

Yield: 40%; Mp: 123-127$^{o}$C; MF: $C_{17}H_{21}NO_5$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.63 (d, J=15.9Hz, 1H), 7.08 (t, J=2.1Hz, 7.2Hz, 2H), 6.91 (t, J=1.2Hz, 7.5Hz, 1H), 6.30 (d, J=15.9Hz, 1H), 4.72 (s, 2H), 3.90 (s, 3H), 3.80 (s, 3H), 3.56-3.49 (m, 4H), 2.01-1.80 (m, 4H); LC MS (m/z): [M + $H^+$ ]- 319.20

**Methyl (E)-3-(4-ethoxy-3-methoxyphenyl) acrylate (3m)**

Yield: 61%; Mp: 94-96$^{o}$C; MF: $C_{13}H_{16}O_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.64 (d, J=15.9Hz, 1H), 7.10-7.04 (m, 2H), 6.85 (d, J=8.1Hz, 1H), 6.32 (d, J=15.9Hz, 1H), 4.13 (q, J=7.4Hz,6.9Hz, 2H), 3.90 (s, 3H), 3.80 (s, 3H), 1.48 (t, J=6.9Hz, 7.2Hz, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.70, 150.52, 149.39, 144.85, 127.18, 122.57, 115.33, 112.13, 109.92, 64.35, 55.92, 51.59, 14.68; ; LC MS (m/z): [M + $H^+$ ]- 236.10

**Methyl (E)-3-(3-methoxy-4-propoxyphenyl) acrylate (3n)**

Yield: 70%; Mp: 116-118$^{o}$C; MF: $C_{14}H_{18}O_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.63 (d, J=16.2Hz, 1H), 7.101-7.047 (m, 2H), 6.81 (d, J=8.1Hz, 1H), 6.30 (d, J=15.9Hz, 1H), 4.01 (t, J=5.4Hz, 6.9Hz, 2H), 3.89 (s, 3H), 3.80 (s, 3H), 1.94-1.82 (m, 2H),1.045 (t, J=7.5Hz, 7.2Hz, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.67, 150.76, 149.48, 144.84, 127.12, 122.54, 115.26, 112.32, 110.11, 70.41, 55.96, 51.55, 22.33, 10.35; ; LC MS (m/z): [M + $H^+$ ]- 250.12

**Methyl (E)-3-(4-butoxy-3-methoxyphenyl) acrylate (3o)**

Yield: 52%; Mp: 104-106$^{o}$C; MF: $C_{15}H_{20}O_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.62 (d, J=15.9Hz, 1H), 7.101-7.045 (m, 2H), 6.81 (d, J=8.1Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 4.05 (t, J=6.9Hz, 2H), 3.89 (s, 3H), 3.80 (s, 3H), 1.89-1.79 (m, 2H), 1.56-1.43 (m, 2H), 1.045 (t, J=7.5Hz, 7.2Hz, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.66, 150.79, 149.47, 144.83, 127.09, 122.53, 115.23, 112.28, 110.09, 68.64, 55.95, 51.53, 31.04,19.13,13.91; ; LC MS (m/z): [M + $H^+$ ]- 264.14

**Methyl (E)-3-(3-methoxy-4-(pentyloxy) phenyl) acrylate (3p)**

Yield: 55%; Mp: 82-84$^{o}$C; MF: $C_{16}H_{22}O_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.63 (d, J=15.9Hz, 1H), 7.101-7.045 (m, 2H), 6.81 (d, J=8.1Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 4.04 (t, J=6.9Hz, 2H), 3.89 (s, 3H), 3.79 (s, 3H), 1.90-1.816 (m, 2H), 1.49-1.32 (m, 4H), 0.98 (t, J=7.2Hz, 7.5Hz, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.62, 150.75, 149.43, 144.80,

127.06, 122.50, 115.20, 112.24, 110.05, 68.91, 55.91, 51.49, 28.17, 27.99, 22.37, 13.91; ; LC MS (m/z): [M + $H^+$ ]- 278.15

**Methyl (E)-3-(4-(hexyloxy)-3-methoxyphenyl) acrylate (3q)**

Yield: 41%; Mp: 74-76$^oC$; MF: $C_{17}H_{24}O_4$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.62 (d, J=15.9Hz, 1H), 7.10-7.04 (m, 2H), 6.80 (d, J=8.1Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 4.04 (t, J=6.9Hz, 2H), 3.89 (s, 3H), 3.79 (s, 3H), 1.90-1.80 (m, 2H), 1.50-1.41 (m, 2H), 1.36-1.28 (m, 4H), 0.90 (t, J=7.5Hz, 7.2Hz, 3H); $^{13}C$ NMR (300 MHz, $CDCl_3$) 167.68, 150.78, 149.46, 144.85, 127.09, 122.55, 115.23, 112.28, 110.07, 68.98, 55.95, 51.55, 31.52, 28.96, 25.56, 22.53, 13.97; ; LC MS (m/z): [M + $H^+$ ]- 292.17

**Methyl (E)-3-(4-(heptyloxy)-3-methoxyphenyl) acrylate (3r)**

Yield: 52%; Mp: 66-68$^oC$; MF: $C_{18}H_{26}O_4$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.63 (d, J=15.9Hz, 1H), 7.07 (dd, J=1.8Hz, 2H), 6.85 (d, J=8.1Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 4.04 (t, J=6.9Hz, 6.6Hz, 2H), 3.89 (s, 3H), 3.79 (s, 3H), 1.90-1.80 (m, 2H), 1.49-1.25 (m, 8H), 0.88 (q, J=2.1Hz, 4.5Hz, 3H); $^{13}C$ NMR (300 MHz, $CDCl_3$) 167.72, 150.82, 149.50, 144.89, 127.13, 122.58, 115.26, 112.58, 110.10, 69.02, 55.98, 51.59, 31.74, 29.03, 25.89, 22.59, 14.09; ; LC MS (m/z): [M + $H^+$ ]- 306.18

**Methyl (E)-3-(3-methoxy-4-(octyloxy)phenyl)acrylate (3s)**

Yield: 55%; Mp: 68-70$^oC$; MF: $C_{19}H_{28}O_4$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.63 (d, J=15.9Hz, 1H), 7.09 (d, J=1.8Hz, 1H), 7.07-7.043 (m, 1H), 6.85 (d, J=8.4Hz, 1H), 6.30 (d, J=15.9Hz, 1H), 4.04 (t, J=6.9Hz, 2H), 3.89 (s, 3H), 3.79 (s, 3H), 1.90-1.80 (m, 2H), 1.47-1.28 (m, 10H), 0.90-0.86 (m, 3H); $^{13}C$ NMR (300 MHz, $CDCl_3$) 167.71, 150.82, 149.50, 144.88, 127.12, 122.58, 115.26, 112.31, 110.10, 69.01, 55.97, 51.58, 31.79, 29.33, 29.20, 29.03, 25.92, 22.64, 14.09; ; LC MS (m/z): [M + $H^+$ ]- 320.30

**Methyl (E)-3-(4-(allyloxy)-3-methoxyphenyl) acrylate (3t)**

Yield: 46%; Mp: 84-86$^oC$; MF: $C_{14}H_{16}O_4$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.62 (d, J=15.9Hz, 1H), 7.10-7.04 (m, 2H), 6.80 (d, J=8.1Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 5.45-5.44(m, 1H), 5.38-5.29 (m, 1H), 4.66-4.64 (m, 2H), 3.90 (s, 3H), 3.80 (s, 3H); $^{13}C$ NMR (300 MHz, $CDCl_3$) 167.61, 150.06, 149.49, 144.72, 132.70, 127.50, 122.31, 118.34, 115.49, 112.80, 110.01, 69.68, 55.87, 51.56; ; LC MS (m/z): [M + $H^+$ ]- 248.10

**Methyl (E)-3-(4-((5-cyanopentyl) oxy)-3-methoxyphenyl) acrylate (3u)**

Yield: 78%; Mp: 92-94$^oC$; MF: $C_{17}H_{21}NO_4$; Appearance: White solid; $^1H$ NMR (300 MHz, $CDCl_3$): 7.62 (d, J=15.9Hz, 1H), 7.10-7.04 (m, 2H), 6.80 (d, J=8.1Hz, 1H), 6.31 (d, J=15.9Hz, 1H), 4.06 (t, J=5.4Hz, 6.9Hz, 2H), 3.90 (s, 3H), 3.80 (s, 3H), 2.42-2.37 (m, 2H), 1.92-1.59 (m, 6H); $^{13}C$ NMR (300 MHz, $CDCl_3$) 167.64, 150.48, 149.55, 144.75, 127.48, 122.48, 119.60, 115.52, 112.48, 110.16, 68.43, 55.95, 51.60, 31.79, 28.24, 25.36, 25.16, 17.07; ; LC MS (m/z): [M + $H^+$ ]- 303.15

**Methyl (E)-3-(4-(benzyloxy)-3-methoxyphenyl) acrylate (3v)**

Yield: 42%; Mp: 76-78$^{o}$C; MF: $C_{18}H_{18}O_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.61 (d, J=15.9Hz, 1H), 7.44-7.30 (m, 5H), 7.06-7.01 (m, 2H), 6.81 (d, J=8.1Hz, 1H), 6.30 (d, J=15.9Hz, 1H), 5.19 (s, 2H), 3.91 (s, 3H), 3.79 (s, 3H); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.66, 150.27, 149.76, 144.76, 136.58, 128.65, 128.28, 128.03, 127.73, 127.21,122.37, 115.62, 113.43, 110.26, 70.86, 66.27, 56.00, 51.52; ; LC MS (m/z): [M + $H^+$ ]- 298.12

**Methyl (E)-3-(4-(hexadecyloxy)-3-methoxyphenyl) acrylate (3w)**

Yield: 57%; Mp: 68-70$^{o}$C; MF: $C_{27}H_{44}O_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.61 (d, J=15.9Hz, 1H), 7.06-7.04 (m, 2H), 6.81 (d, J=8.1Hz, 1H), 6.30 (d, J=15.9Hz, 1H), 4.04 (t,J= 6.9, 2H), 3.89 (s, 3H), 3.80 (s, 3H), 1.90-1.80 (m, 2H), 1.30 (d, J=13.5Hz, 26H), 0.89 (t, J=6.6Hz, 6.3Hz, 3H); ); $^{13}$C NMR (300 MHz, $CDCl_3$) 167.69, 150.81, 149.49, 144.86, 127.11, 122.55, 115.24, 112.30, 110.10, 69.01, 63.06, 55.96, 51.55, 32.80, 31.90, 29.67, 29.63, 29.56, 29.51, 29.42, 29.34, 29.01, 25.89, 25.72, 22.67, 14.09; ; LC MS (m/z): [M + $H^+$ ]- 432.32

**(E)-3-(3-methoxy-4-(((4-nitrophenyl) carbamoyl) oxy) phenyl) acrylic acid (3x)**

Yield: 40%; Mp: 172-174$^{o}$C; MF: $C_{17}H_{14}N_2O_7$; Appearance: pale yellow solid; $^{1}$H NMR (300 MHz, d6-DMSO): 12.4 (s, 1H), 11.03 (s, 1H), 8.25 (d, J=9.3Hz, 2H), 7.73 (d, J=9Hz, 2H), 7.63-7.53 (m, 3H), 7.29 (s, 2H), 6.62 (d, J=16.2Hz, 1H), 3.85 (s, 3H); $^{13}$C NMR (300 MHz, d6-DMSO) 167.98, 155.65, 149.01, 147.86, 144.46, 135.59, 126.36, 125.72, 125.10, 122.76, 118, 117.97, 115.58, 115.47, 112.35, 111.08, 55.63, ; LC MS (m/z): [M + $H^+$ ]- 358.08

**1-(4-hydroxy-3-methoxyphenyl)-1,2-dihydro-3H-benzo[f]chromen-3-one (4a)**

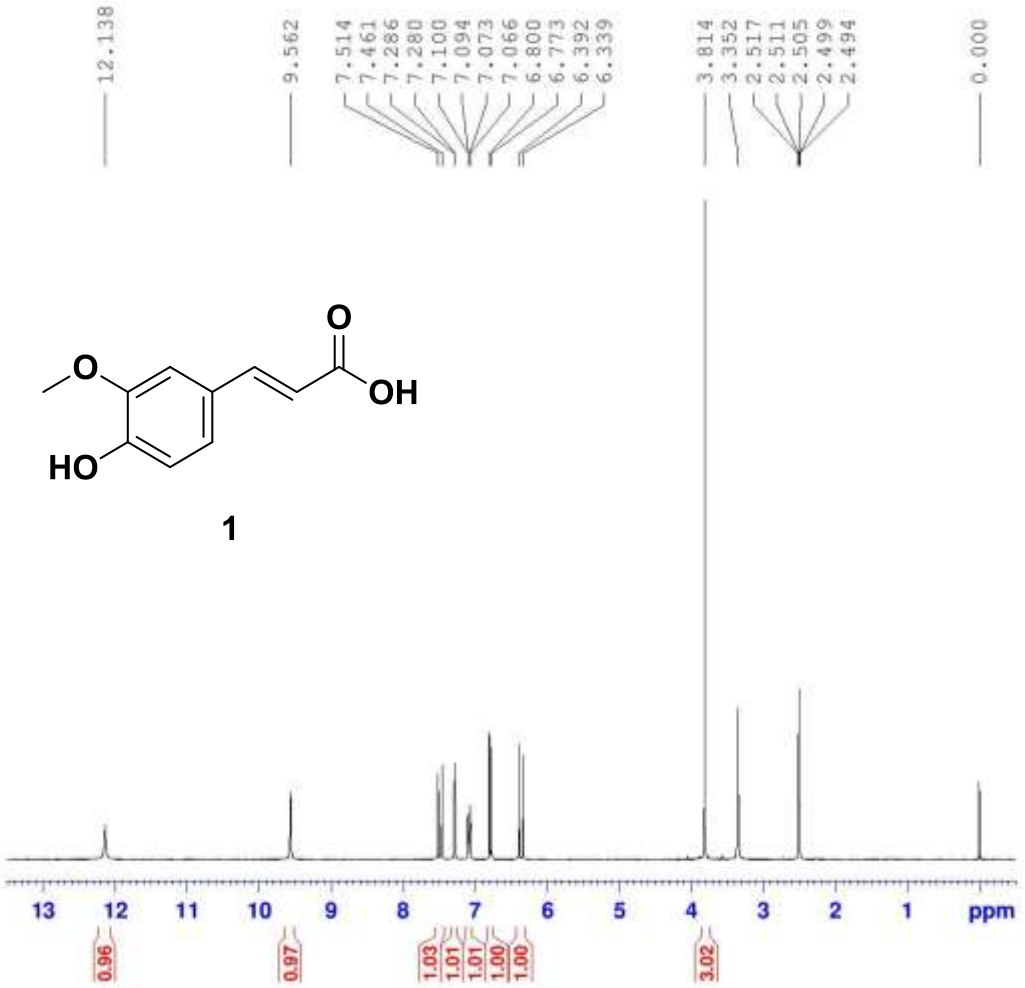
Yield : 35%; Mp: 160-162; MF: $C_{20}H_{16}O_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.83 (q, J=8.7Hz,7.2Hz, 3H), 7.46 (pd, J=1.5Hz, 2H), 7.34 (d, J=8.7Hz, 1H), 6.78 (d, J=8.4Hz, 1H), 6.61 (q, J=1.8Hz, 3.9Hz, 2H), 5.53(s, 1H), 4.88(q, J=2.4Hz, 3.6Hz, 1H) 3.75 (s, 3H), 3.15 (t, J=6.6Hz, 3.3Hz, 2H); C=74.11%, H=4.99%, O=19.79%; ; LC MS (m/z): [M + $H^+$ ]- 320.10

**8-bromo-1-(4-hydroxy-3-methoxyphenyl)-1,2-dihydro-3H-benzo[f]chromen-3-one (4b)**

Yield : 61%; Mp: 174-176; MF: $C_{20}H_{15}BrO_4$; Appearance: White solid; $^{1}$H NMR (300 MHz, $CDCl_3$): 7.94 (d, J=1.8Hz, 1H), 7.70 (d, J=8.7Hz, 1H), 7.60 (d, J=9Hz, 1H), 7.47 (dd, J=2.1Hz, 1H), 7.29 (d, J=9Hz, 1H), 6.718 (t, J=4.2Hz,4.5Hz,1H), 6.51-6.47(m, 2H), 5.47(s, 1H), 4.71(q, J=2.7Hz,3.6Hz, 1H), 3.69 (s, 3H), 3.16-3.02 (m, 2H); $^{13}$C NMR (300 MHz, $CDCl_3$):166.89, 149.87, 147.08, 145.17, 132.23, 132.11, 130.78, 130.71, 129.59, 129.0, 124.87, 119.8, 119.26, 118.73, 118.21, 114.95, 108.99, 55.86, 37.64, 37.43; C=60.1%, H=3.699%, O=15.99%; ; LC MS (m/z): [M + $H^+$ ]- 398.02

**7-hydroxy-4-(4-hydroxy-3-methoxyphenyl) chroman-2-one (4c)**

Yield : 30%; Mp: 168-170; MF: $C_{16}H_{14}O_5$; Appearance: White solid; $^{1}H$ NMR (300 MHz, d6-DMSO): 9.72 (s, 1H), 8.93 (s, 1H), 6.83 (d, J=8.1Hz, 1H), 6.78(d, J=1.8Hz, 1H), 6.69 (d, J=8.1Hz, 1H), 6.55-6.50 (m, 2H), 6.43 (dd, J=1.8Hz, 1H), 4.24 (t, J=6Hz, 6.3Hz, 1H), 3.71 (s, 3H), 3.02 (d, J=6.3Hz, 2H); $^{13}C$ NMR (300 MHz, d6-DMSO): 167.86, 157.37, 151.79, 147.63, 145.45, 132.37, 128.83, 119.27, 116.65, 115.37, 111.55, 111.48, 103.12, 55.50, 36.77, 30.59; C=67.15%, H=5.01%, O=28.02%; ; LC MS (m/z): [M + $H^+$ ]- 286.08




1

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EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
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Time                  15.32
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES             0.094423 Hz
AQ                 5.2953567 sec
RG                      322
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.00 usec
PL1                   -2.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF             300.1299995 MHz
WDW                        EM
SSB                        0
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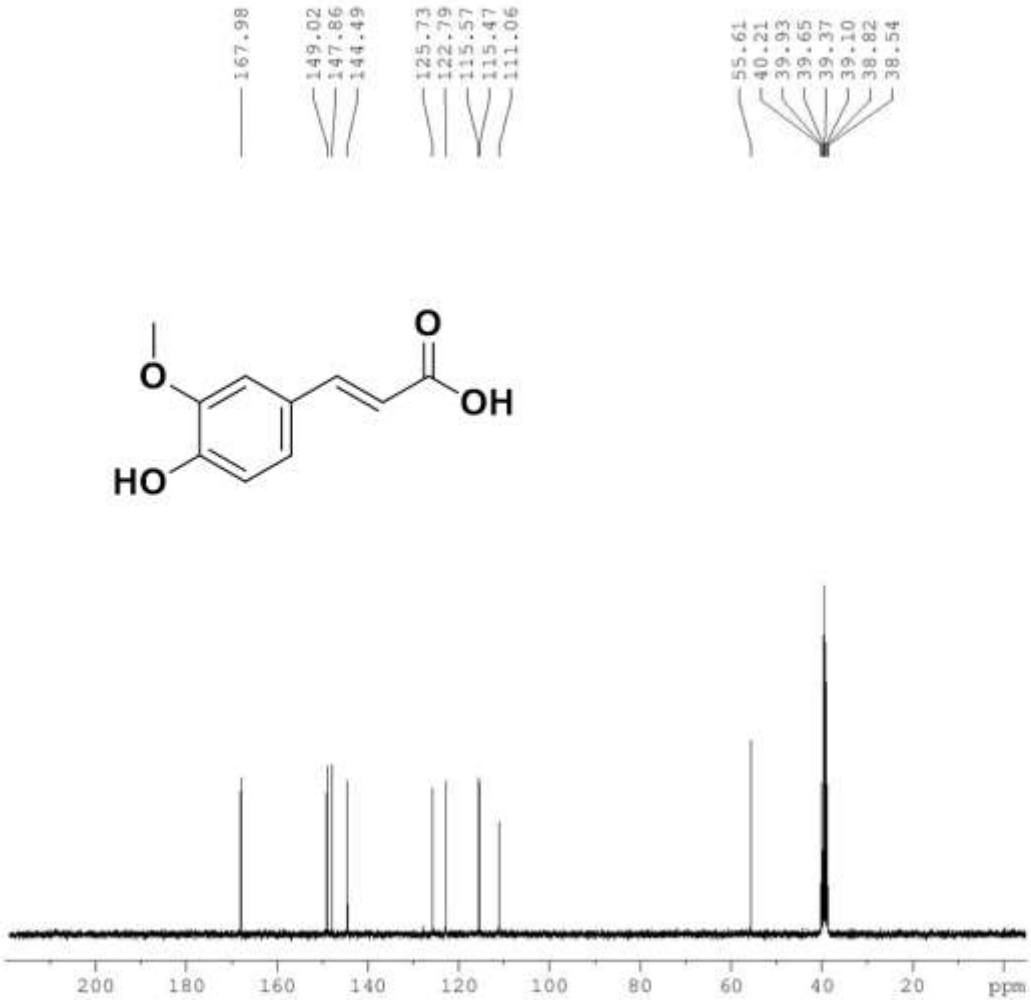


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NAME                  1388F_C13
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20160222
Time                      15.10
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                         128
DS                           4
SWH                  18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175818 sec
RG                         228
DW                      27.733 usec
DE                        6.00 usec
TE                       300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                        10.00 usec
PL1                        0.00 dB
SFO1                75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                       -2.00 dB
PL12                      16.98 dB
PL13                      20.00 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                  75.4677867 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                          1.40
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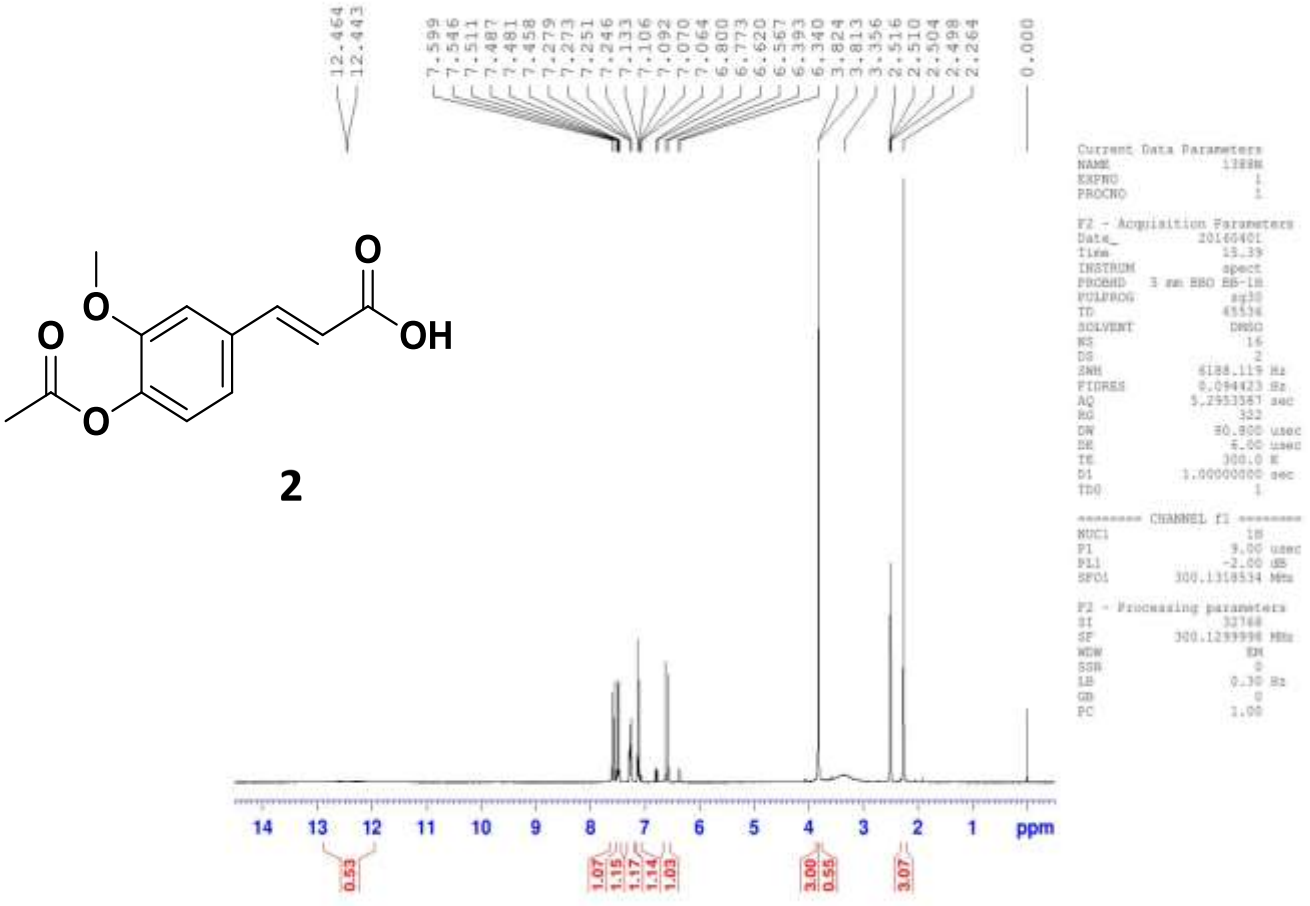


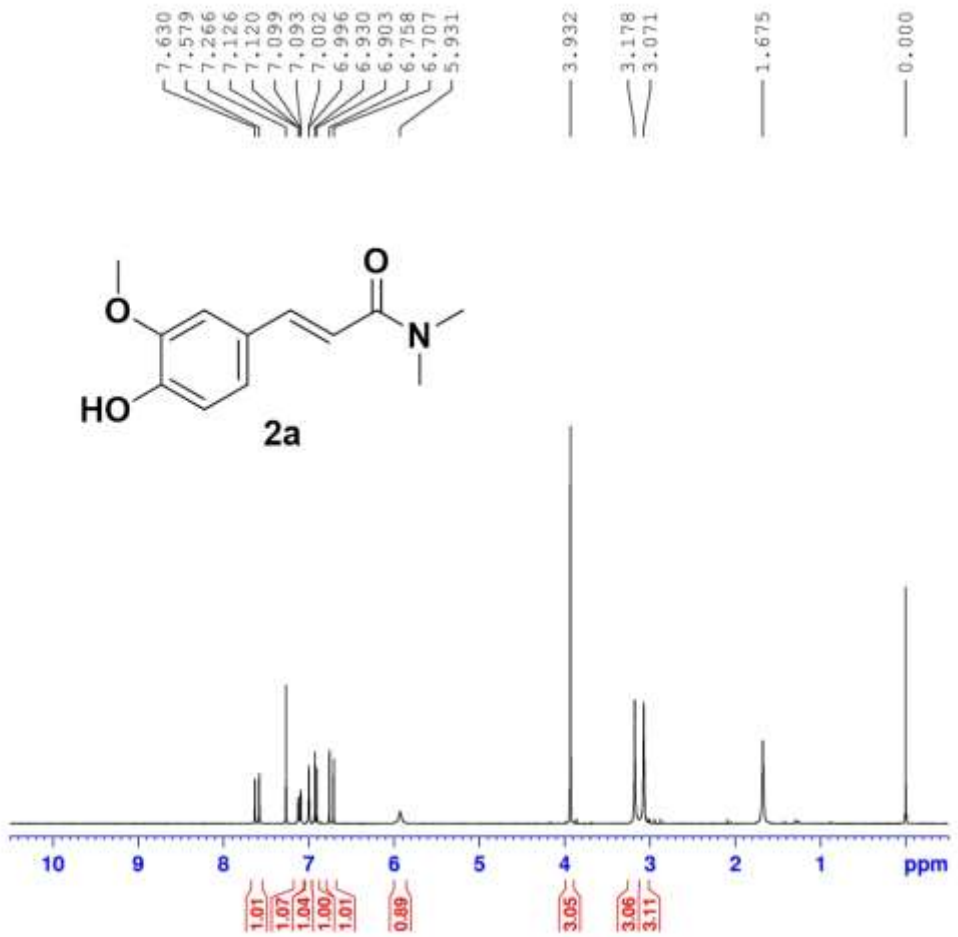

**2**

Current Data Parameters
NAME 13888
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160401
Time 15.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953367 sec
RG 322
DW 80.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299996 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Current Data Parameters
NAME                 11810
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20151228
Time                 14.12
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                     362
DW                  80.800 usec
DE                   6.00 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300044 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
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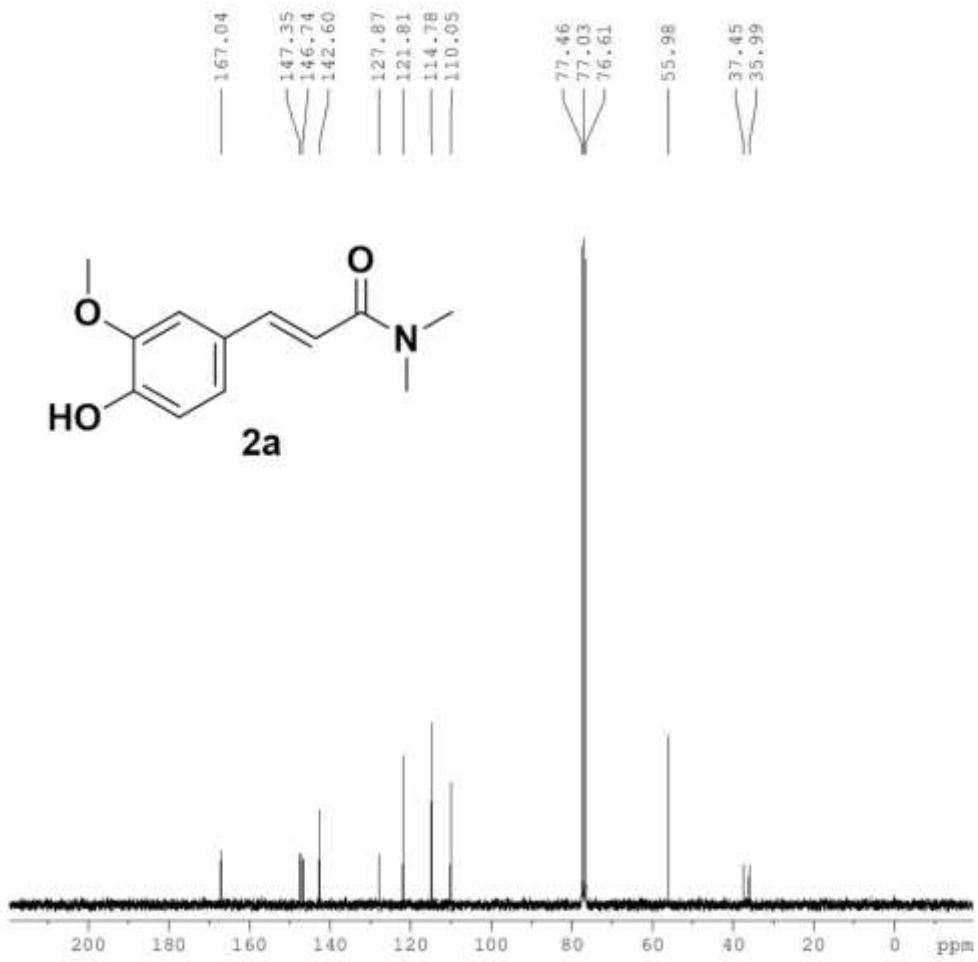


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Current Data Parameters
NAME         1827E-FA+DMA
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160606
Time               18.08
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  820
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  228
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               16.98 dB
PL13               20.00 dB
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
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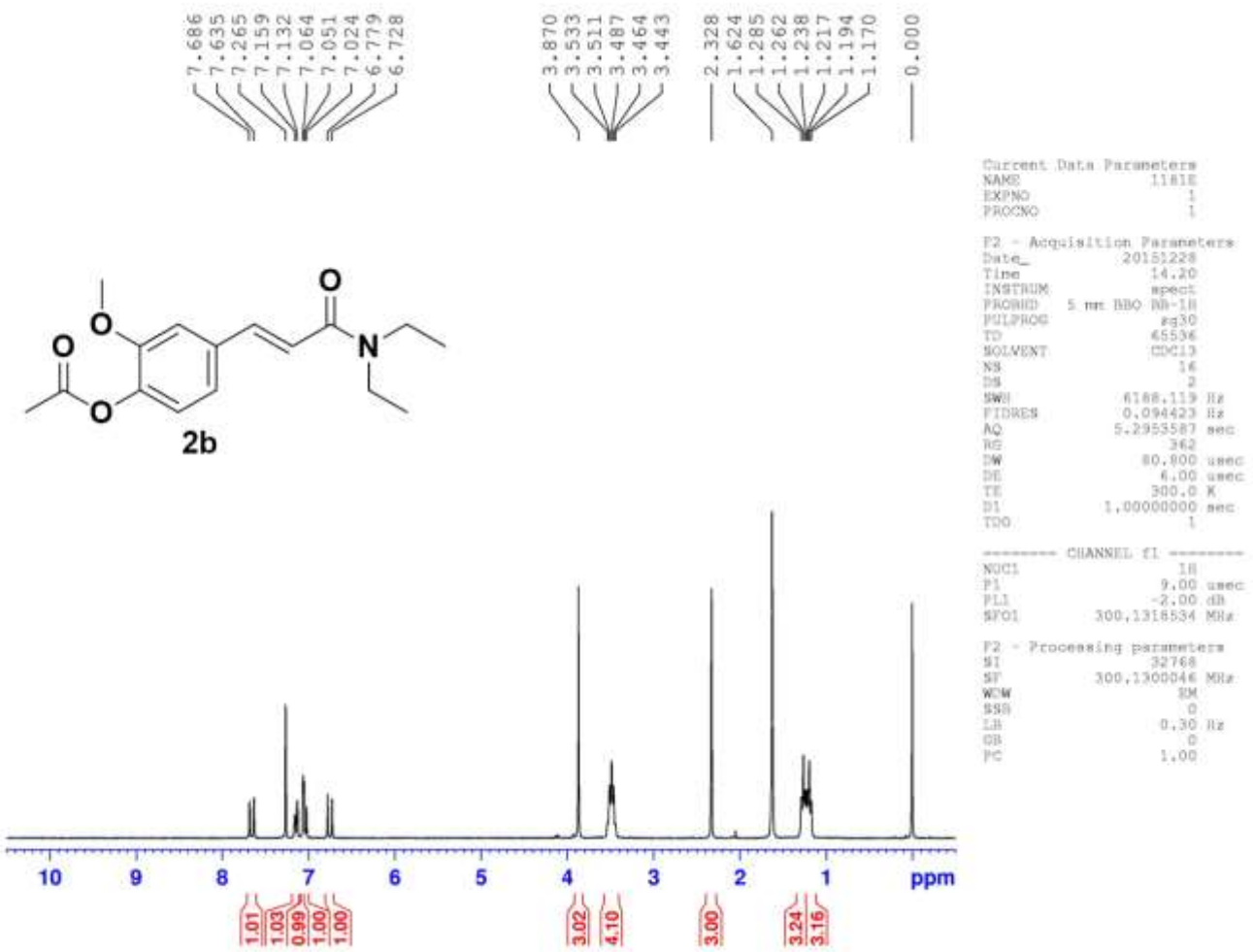


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Current Data Parameters
NAME                  1181E
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20151228
Time                  14.20
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES             0.094423 Hz
AQ                 5.2955587 sec
RG                      362
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1            1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    1H
P1                   9.00 usec
PL1                 -2.00 dB
SFO1          300.1316534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300046 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
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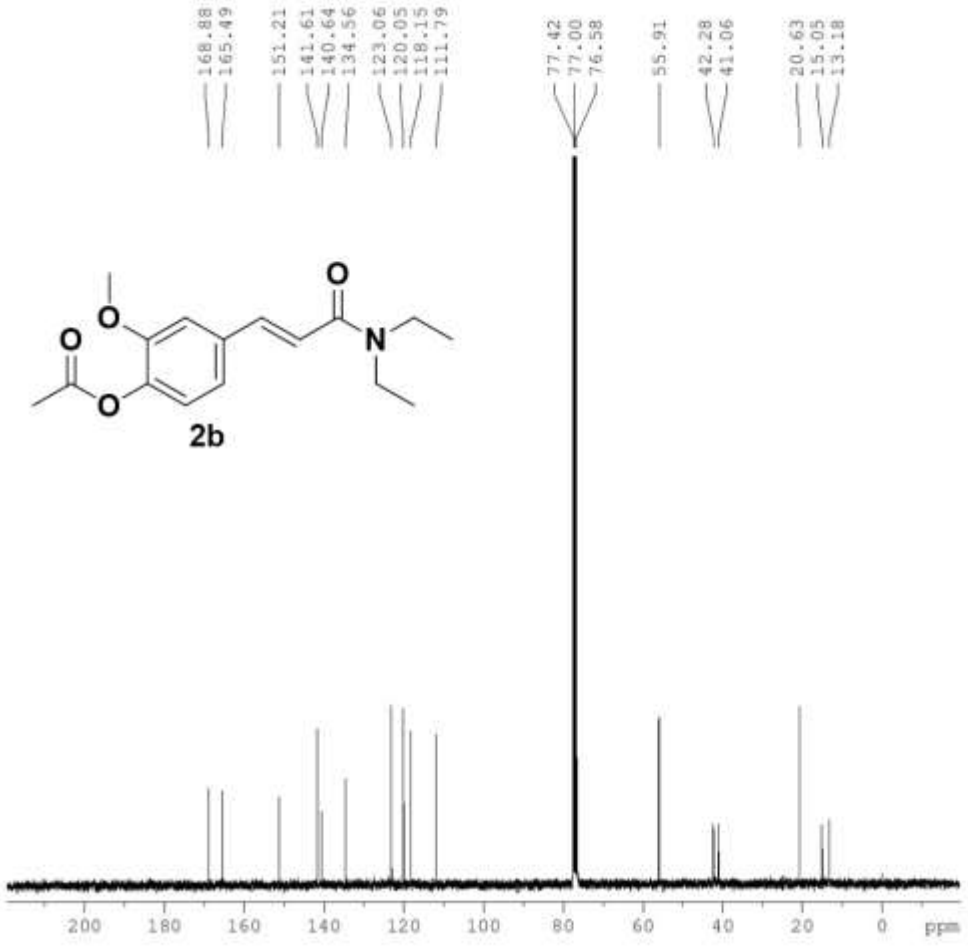


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Current Data Parameters
NAME          1827D-FA+DEA
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160606
Time                  16.47
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1430
DS                       4
SWH             18028.846 Hz
FIDRES              0.275098 Hz
AQ                1.8175818 sec
RG                     161
DW                  27.733 usec
DE                    6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 16.98 dB
PL13                 20.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                   32768
SF             75.4677516 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
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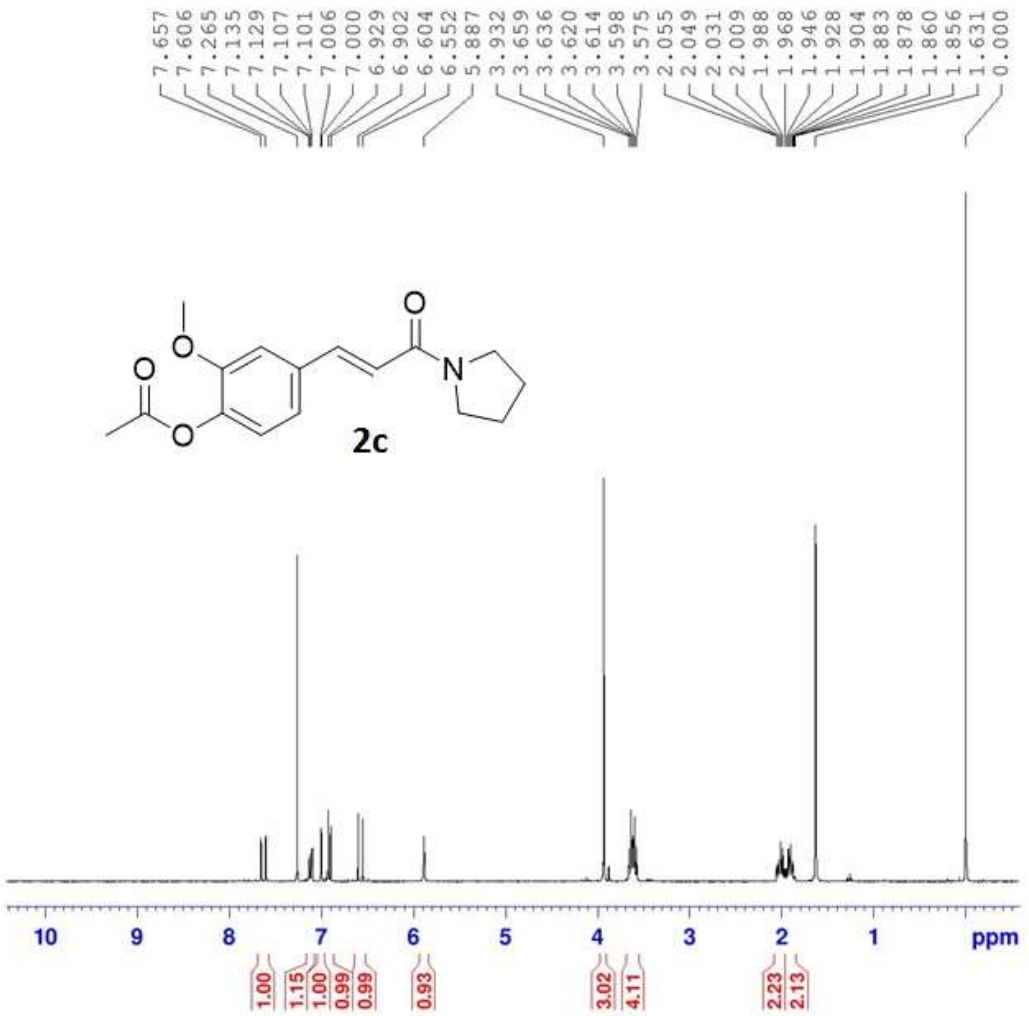


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Current Data Parameters
NAME                  0852N2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20151208
Time                  12.09
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                       456
DW                  80.800 usec
DE                   6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF            300.1300049 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
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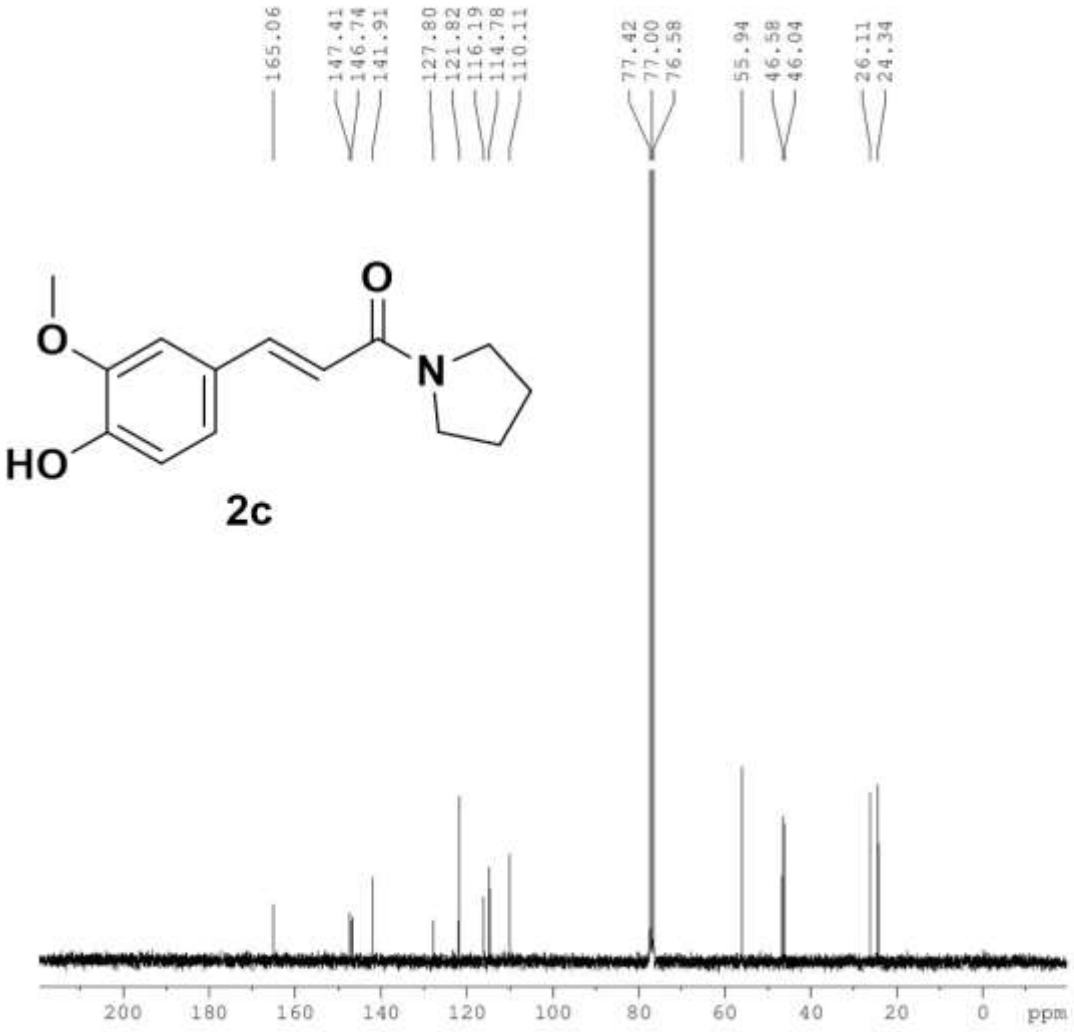


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Current Data Parameters
NAME      1854C-Pyrrolidine-AAC
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20160701
Time                   13.42
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH              18028.846 Hz
FIDRES               0.275098 Hz
AQ                1.8175818 sec
RG                       181
DW                    27.733 usec
DE                     6.00 usec
TE                    300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.00 usec
PL1                     0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   16.98 dB
PL13                   20.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                      32768
SF             75.4677515 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
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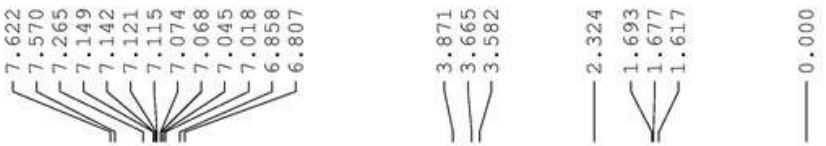


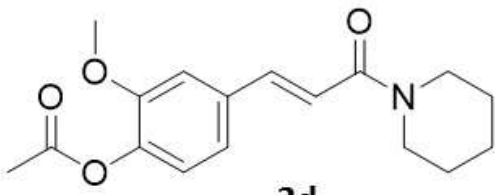

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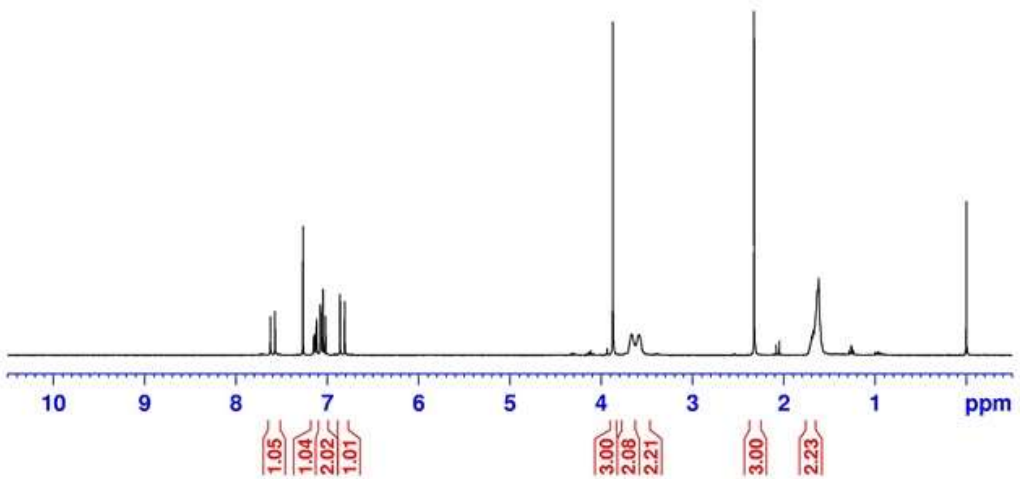


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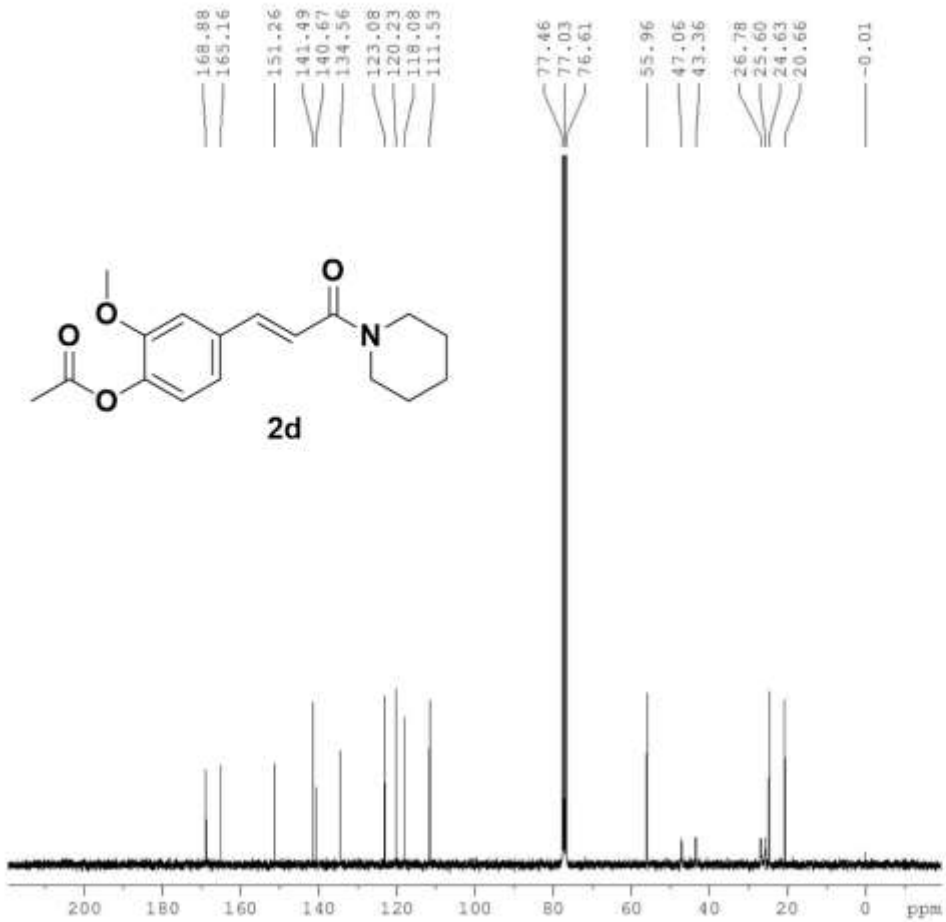
Current Data Parameters
NAME      1535G-AAC-Piper
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160418
Time               12.22
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   406
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.00 usec
PL1               -2.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300048 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



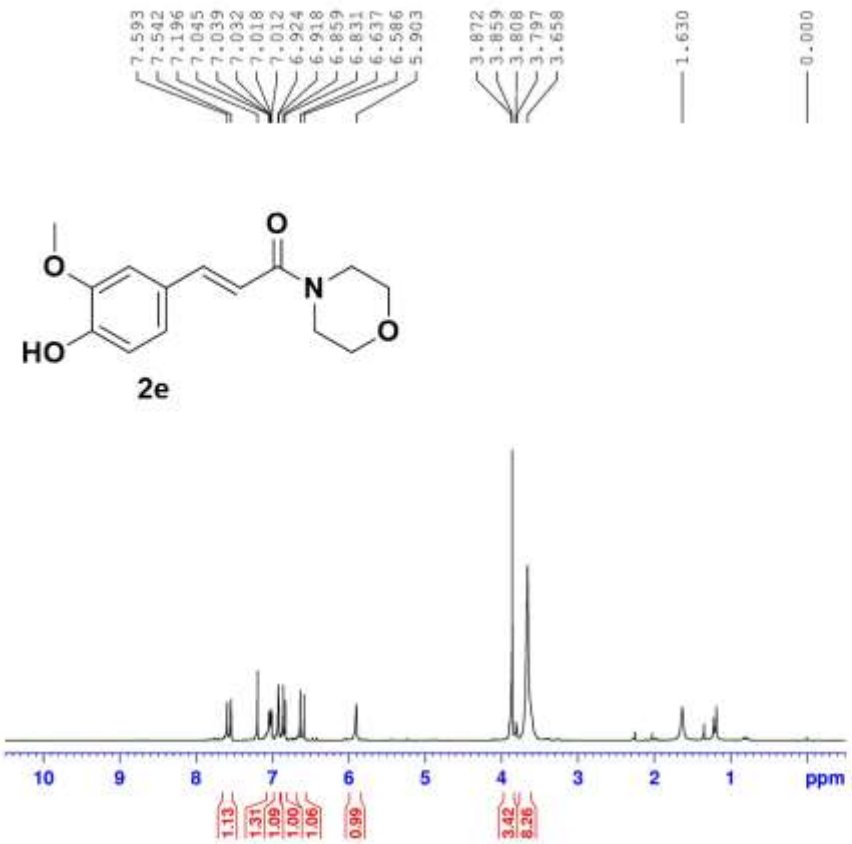

```
Current Data Parameters
NAME      1854D-Piperidine
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160701
Time                  15.27
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1572
DS                       4
SWH               18028.846 Hz
FIDRES            0.275098 Hz
AQ                1.8175618 sec
RG                     228
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PL1                  0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                 -2.00 dB
PL12                16.98 dB
PL13                20.00 dB
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
```

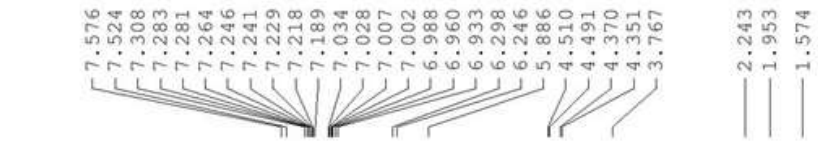


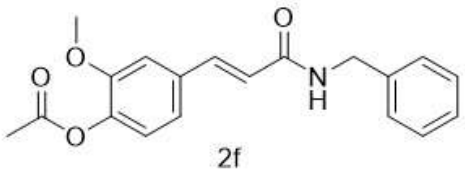

```
Current Data Parameters
NAME                 0052f1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_             20151017
Time                 11.56
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                     322
DW                  80.800 usec
DE                   6.00 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                      1

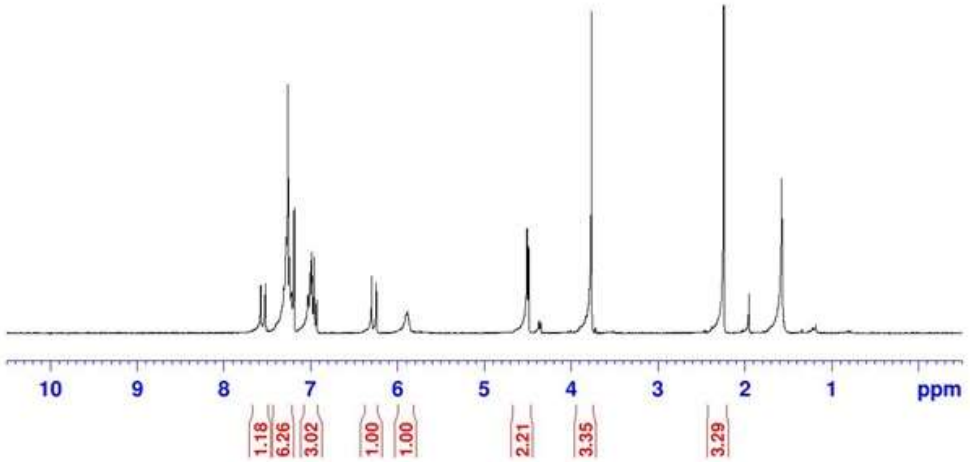
======== CHANNEL f1 ========
NUC1                    1H
P1                   9.00 usec
PL1                 -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300200 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




2f

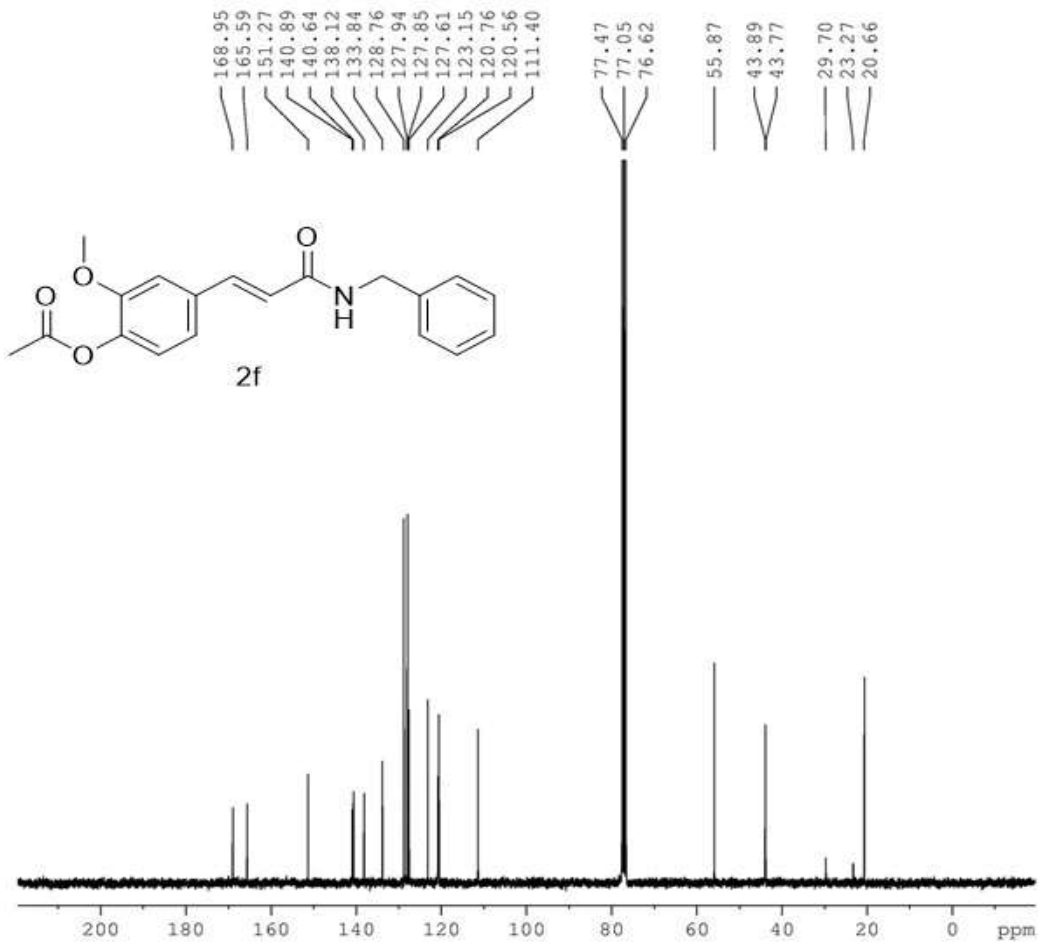



```
Current Data Parameters
NAME                  0852J1
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20151027
Time                  15.24
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                       362
DW                  80.800 usec
DE                   6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.00 usec
PL1                   -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF            300.1300267 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



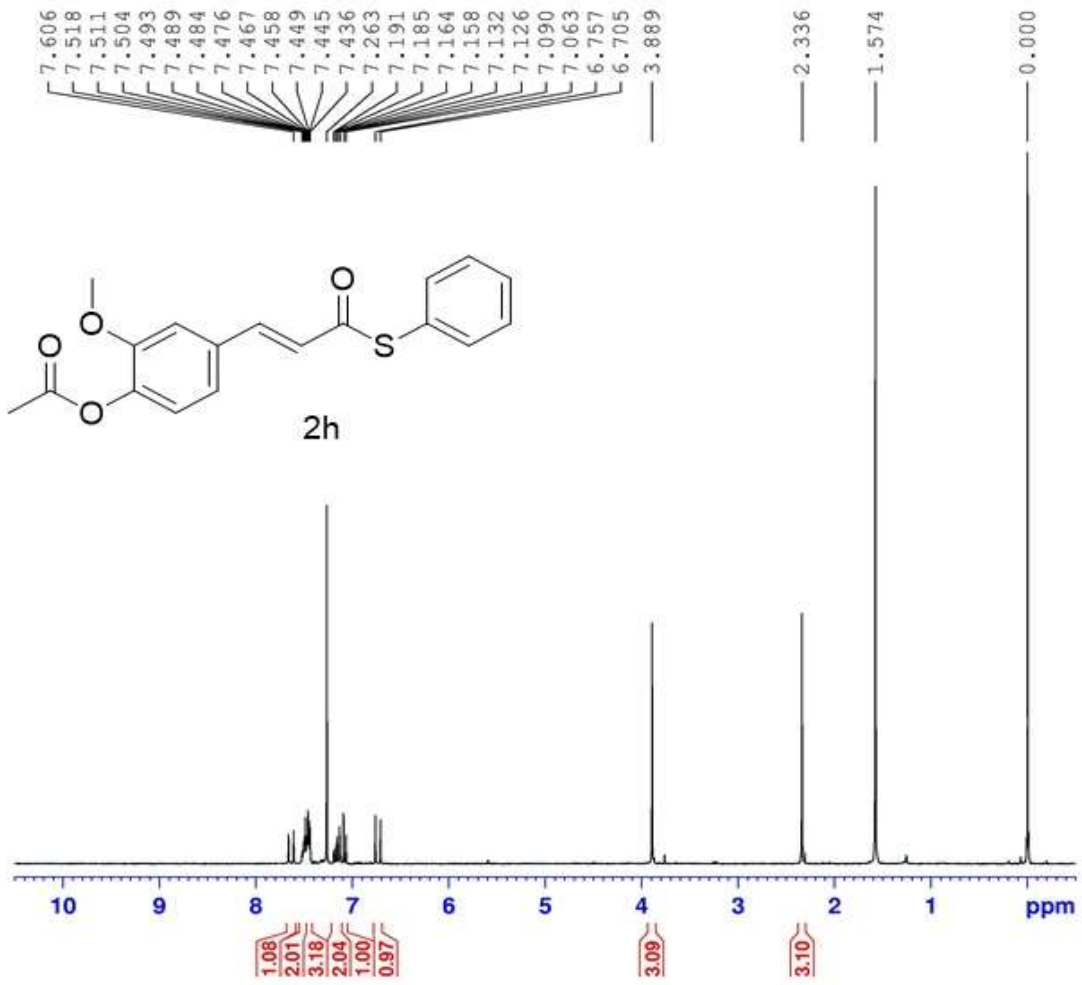

```
Current Data Parameters
NAME                  0852K
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20151028
Time                  11.40
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1905
DS                       4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 sec
RG                     228
DW                27.733 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 0.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               16.98 dB
PL13               20.00 dB
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
```




```
Current Data Parameters
NAME                  1117L
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20151212
Time                  13.46
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      512
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300054 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

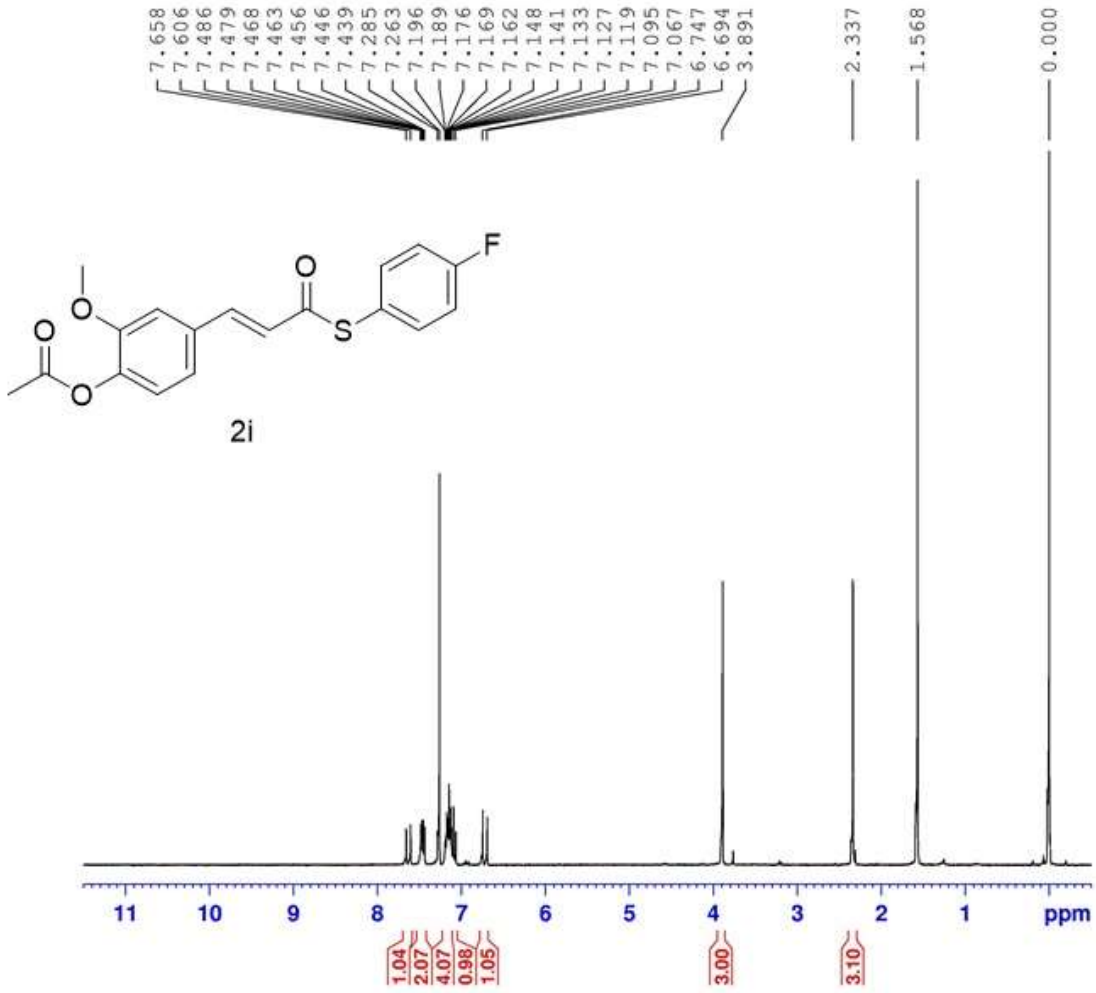

```
Current Data Parameters
NAME      1854A-Thiophenol
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160630
Time               16.39
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1255
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  181
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677504 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

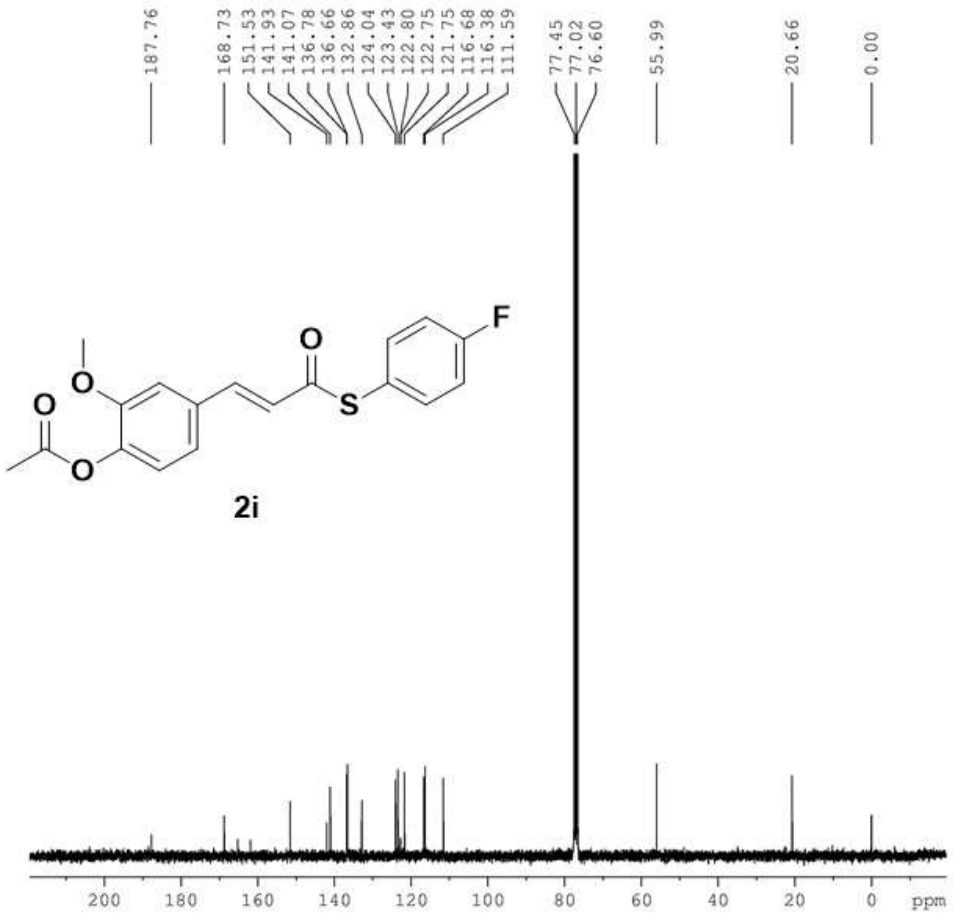



Current Data Parameters
NAME 1128D
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151207
Time 15.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 512
DW 80.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



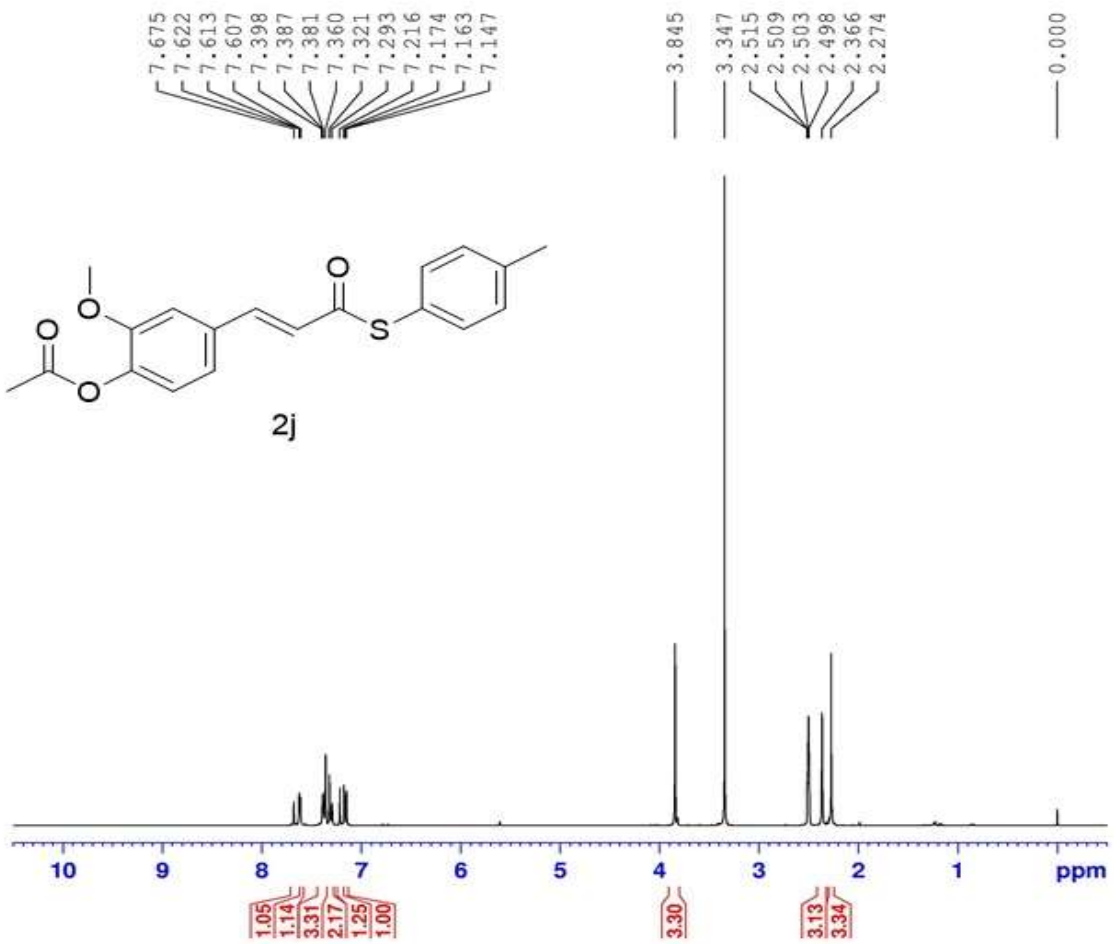

```
Current Data Parameters
NAME                  1128E-F
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20151208
Time                    17.42
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1820
DS                          4
SWH                 18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175818 sec
RG                        228
DW                     27.733 usec
DE                      6.00 usec
TE                      300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                     10.00 usec
PL1                     0.00 dB
SFO1               75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   16.98 dB
PL13                   20.00 dB
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
```

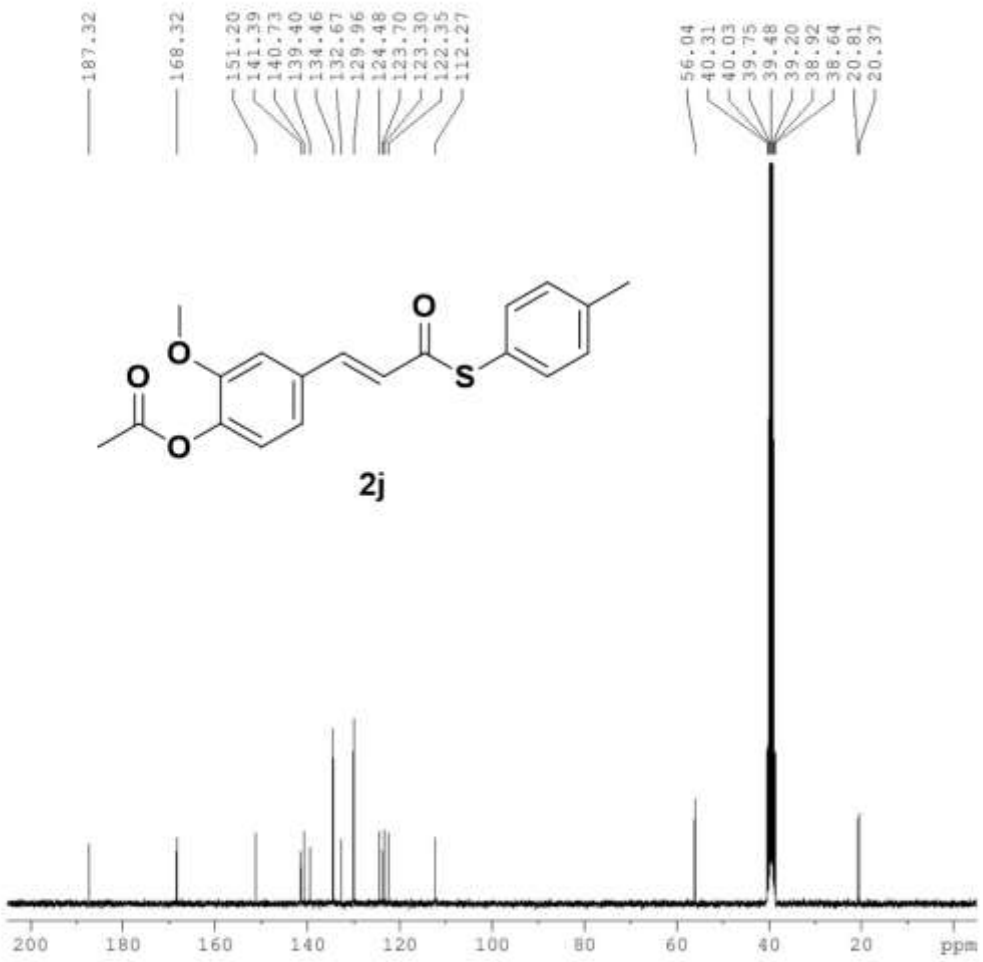



```
Current Data Parameters
NAME                  0852L2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20151120
Time                  14.31
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                       322
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1             1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.00 usec
PL1                   -2.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF             300.1299999 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



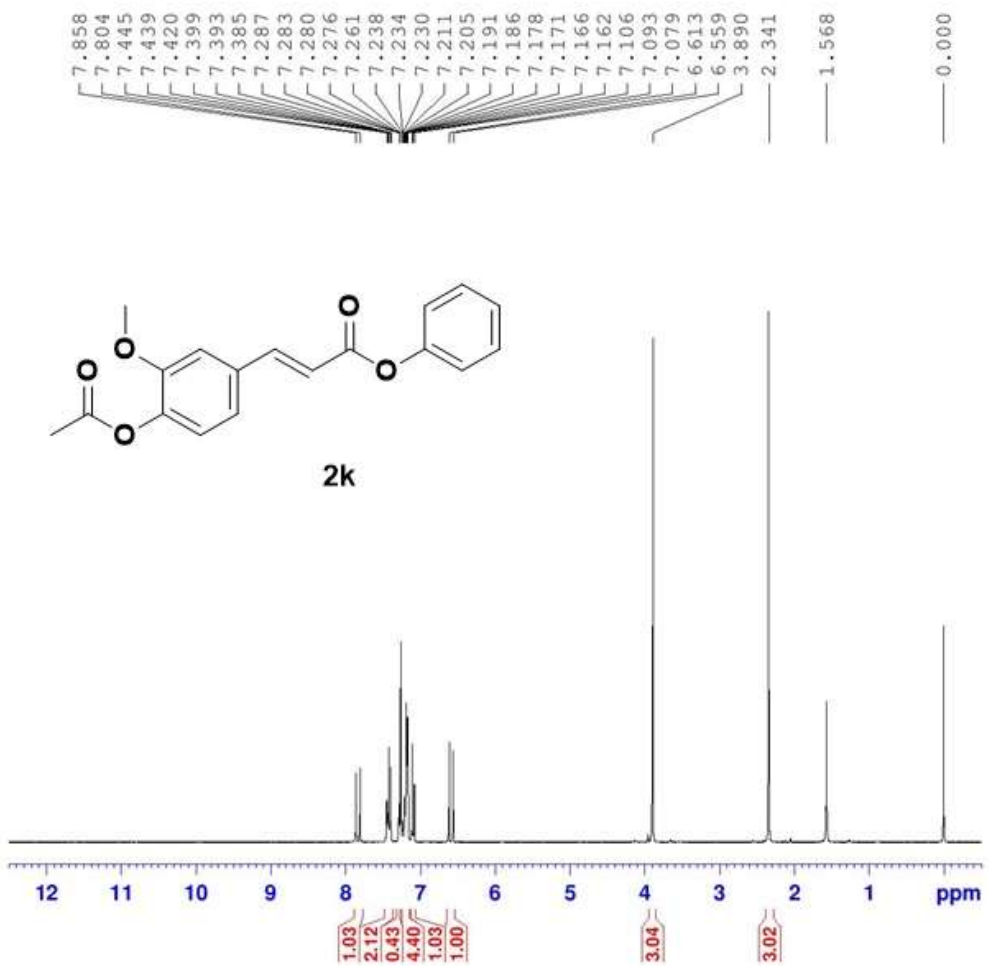

```
Current Data Parameters
NAME                  0852M
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20151120
Time                  17.12
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    1750
DS                       4
SWH              18028.846 Hz
FIDRES           0.275099 Hz
AQ               1.8175818 sec
RG                     287
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 16.98 dB
PL13                 20.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677867 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.40
```

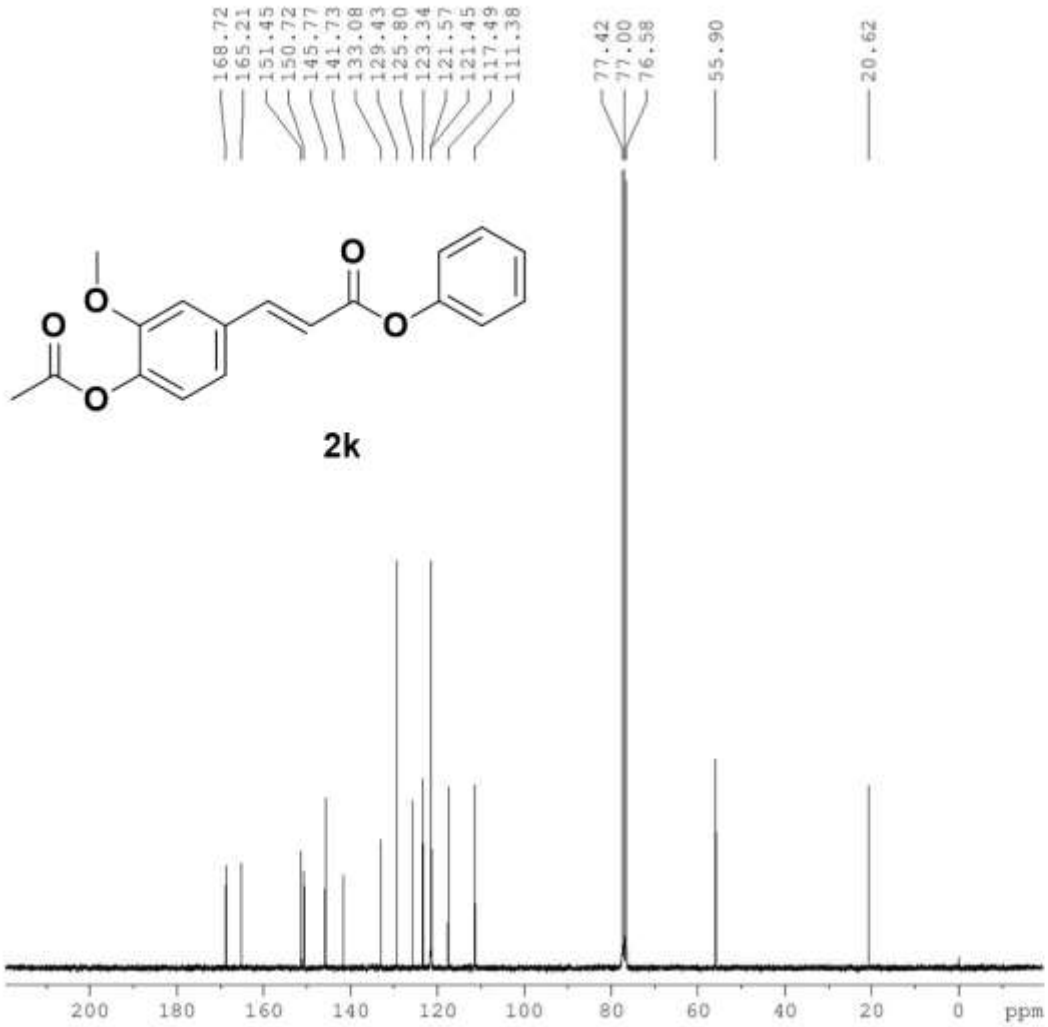



```
Current Data Parameters
NAME      1535E-FA-Phenol
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160413
Time               17.53
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   406
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.00 usec
PL1                -2.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300058 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



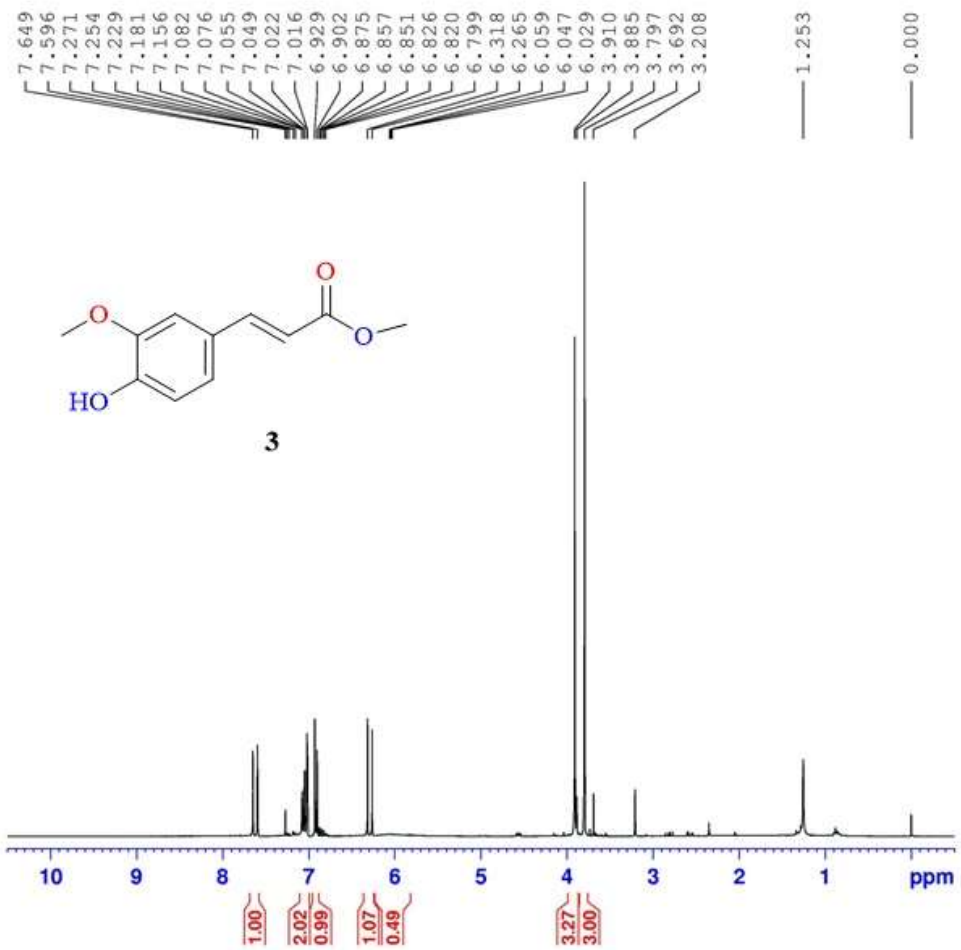

```
Current Data Parameters
NAME      1854B-FA+Phenol
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160630
Time               20.40
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  161
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677527 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```



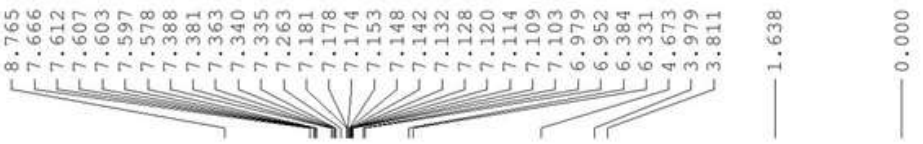

**3**

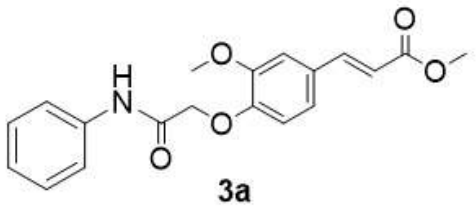
```
Current Data Parameters
NAME                  0222
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150228
Time                 14.45
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      64
DW                 80.800 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                      1

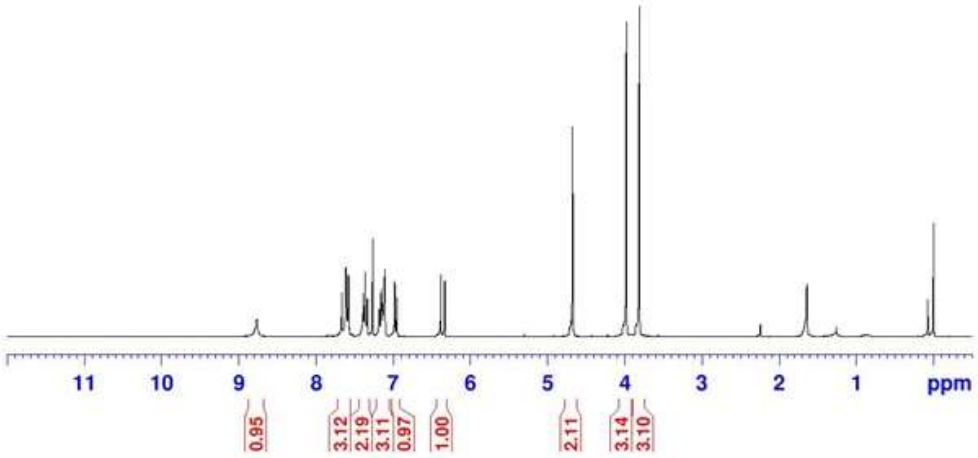
======== CHANNEL f1 ========
NUC1                    1H
P1                   8.60 usec
PL1                 -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300027 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




3a

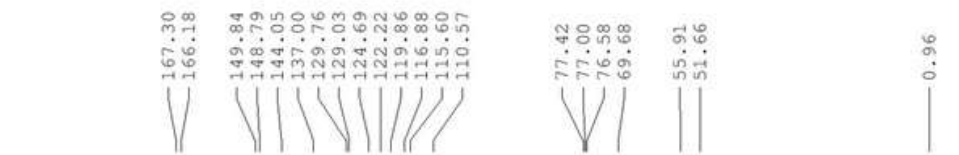


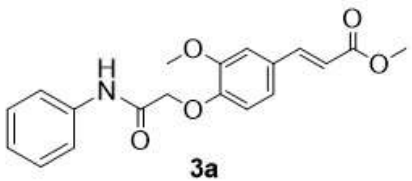

```
Current Data Parameters
NAME                  0852H
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150805
Time                  11.31
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953567 sec
RG                      322
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1             1.00000000 sec
TD0                       1

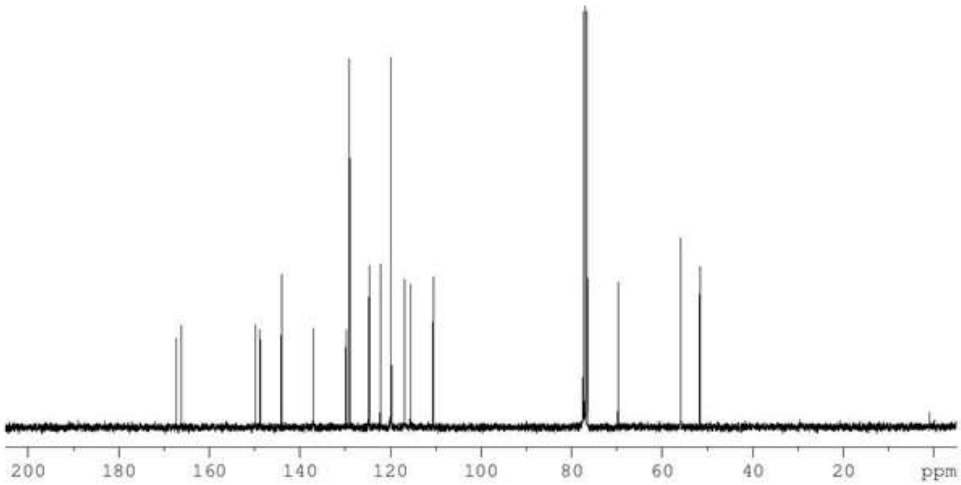
======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300048 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```



3a



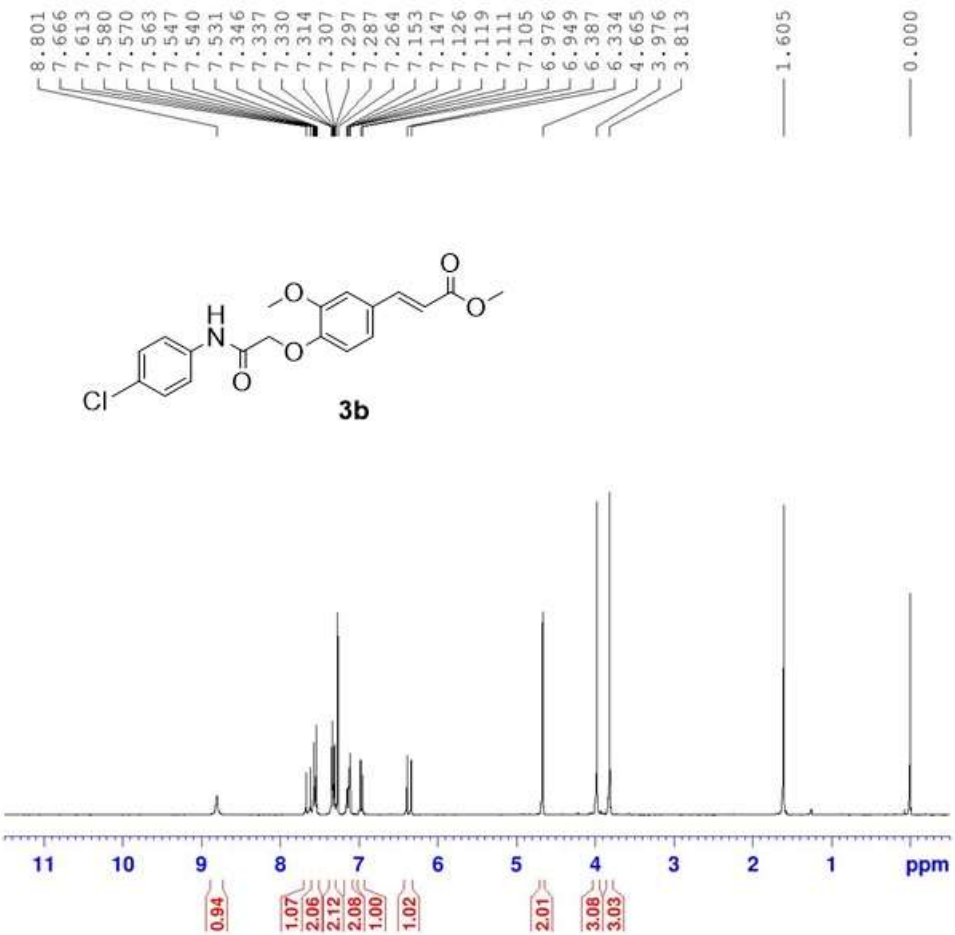

```
Current Data Parameters
NAME                  0852B
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150805
Time                  17.20
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG               zgpg30
TD                     65536
SOLVENT                CDC13
NS                       600
DS                         4
SWH               18028.846 Hz
FIDRES             0.275098 Hz
AQ                 1.8175818 sec
RG                       203
DW                  27.733 usec
DE                   6.00 usec
TE                   300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                   10.00 usec
PL1                   0.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 16.98 dB
PL13                 20.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                       32768
SF              75.4677547 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                        1.40
```

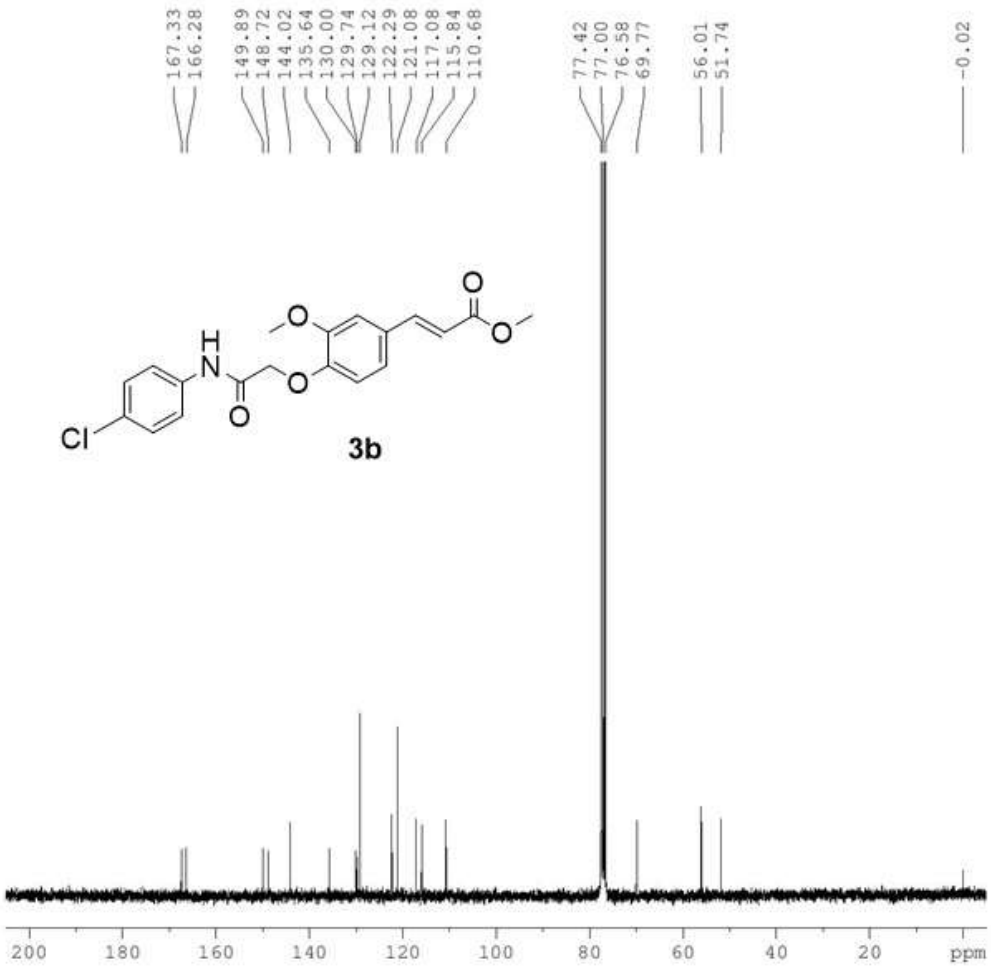



```
Current Data Parameters
NAME                  0852I
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150808
Time                  10.35
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      406
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300047 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```



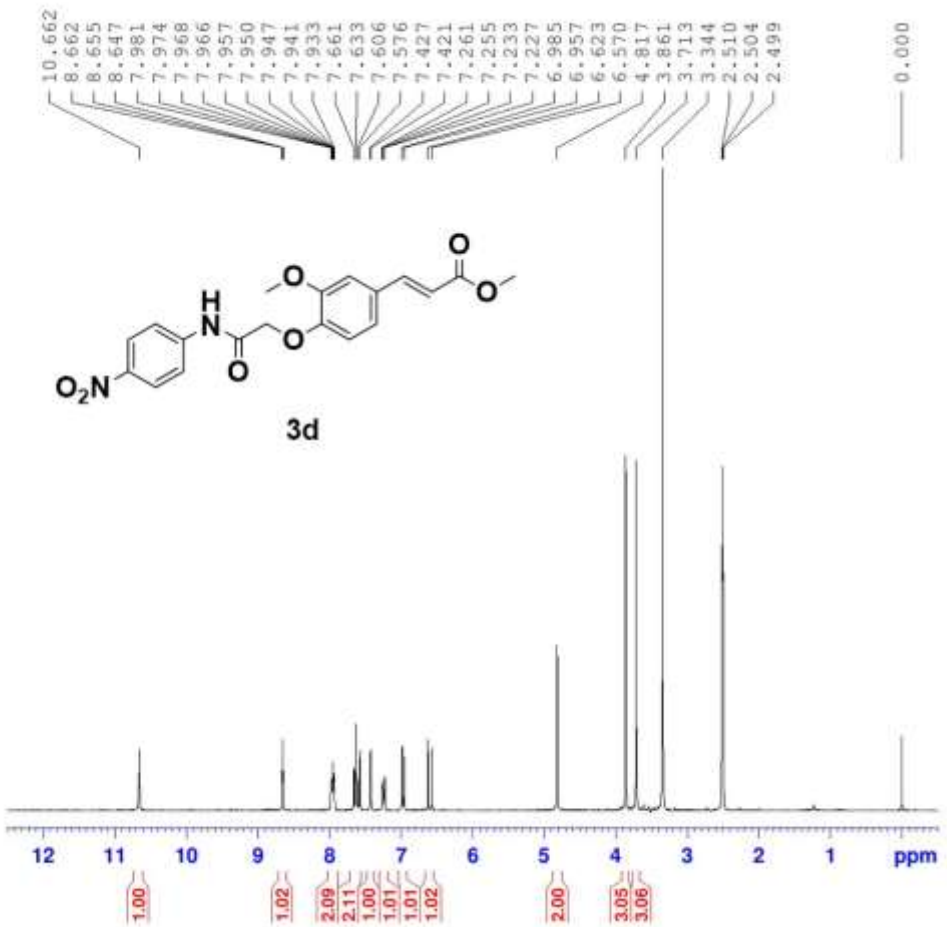

```
Current Data Parameters
NAME                  0778E
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150808
Time                 14.07
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1897
DS                      4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175818 sec
RG                    181
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 0.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               16.98 dB
PL13               20.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677508 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME       1855A-4-Nitro
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20160628
Time               10.02
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   287
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.00 usec
PL1               -2.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299996 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

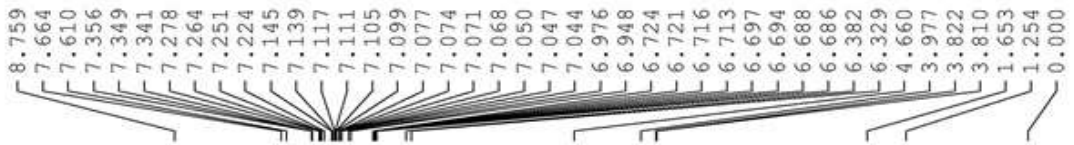

```
Current Data Parameters
NAME                  1388O_C13
EXPNO                         1
PROCNO                        1

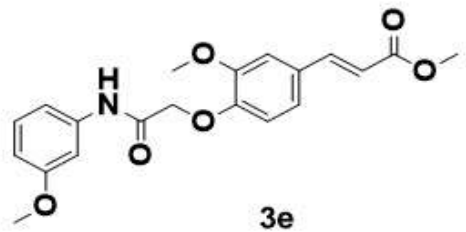
F2 - Acquisition Parameters
Date_                  20160628
Time                      20.31
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                        2500
DS                           4
SWH                  18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175818 sec
RG                          228
DW                       27.733 usec
DE                        6.00 usec
TE                       300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                        10.00 usec
PL1                        0.00 dB
SFO1                75.4752953 MHz

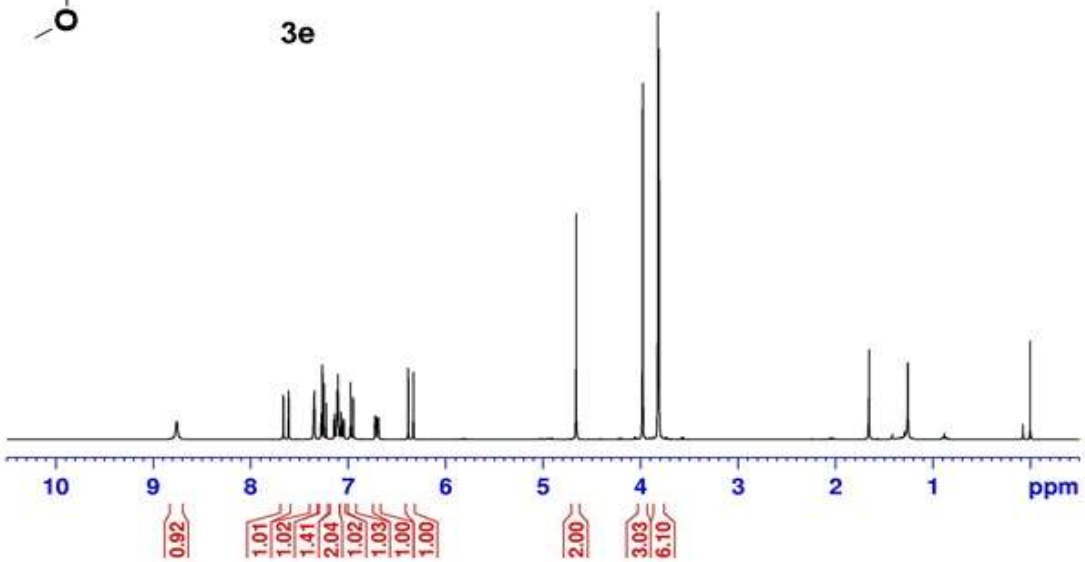
======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                       -2.00 dB
PL12                      16.98 dB
PL13                      20.00 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                 75.4677867 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```



3e

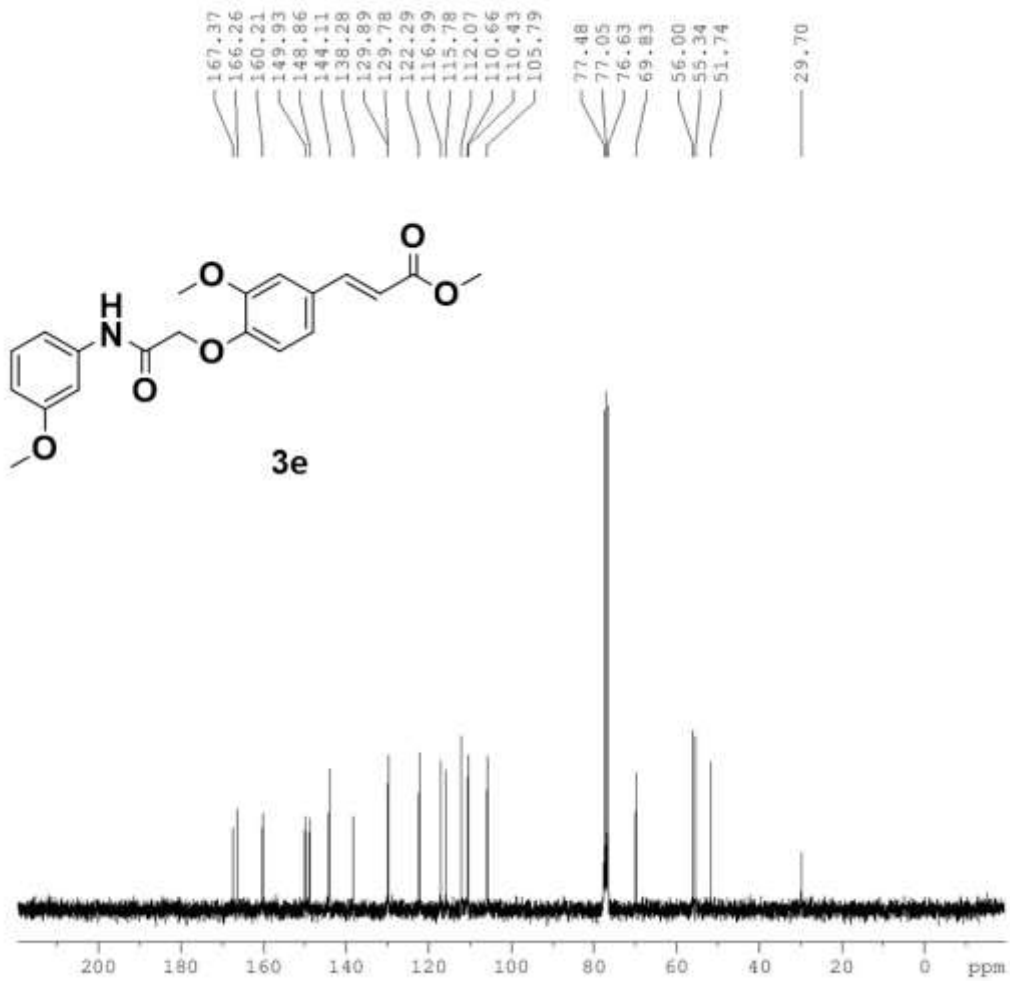



```
Current Data Parameters
NAME      1535I-FAE+Anisi
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160418
Time                12.35
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   287
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.00 usec
PL1                -2.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300048 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



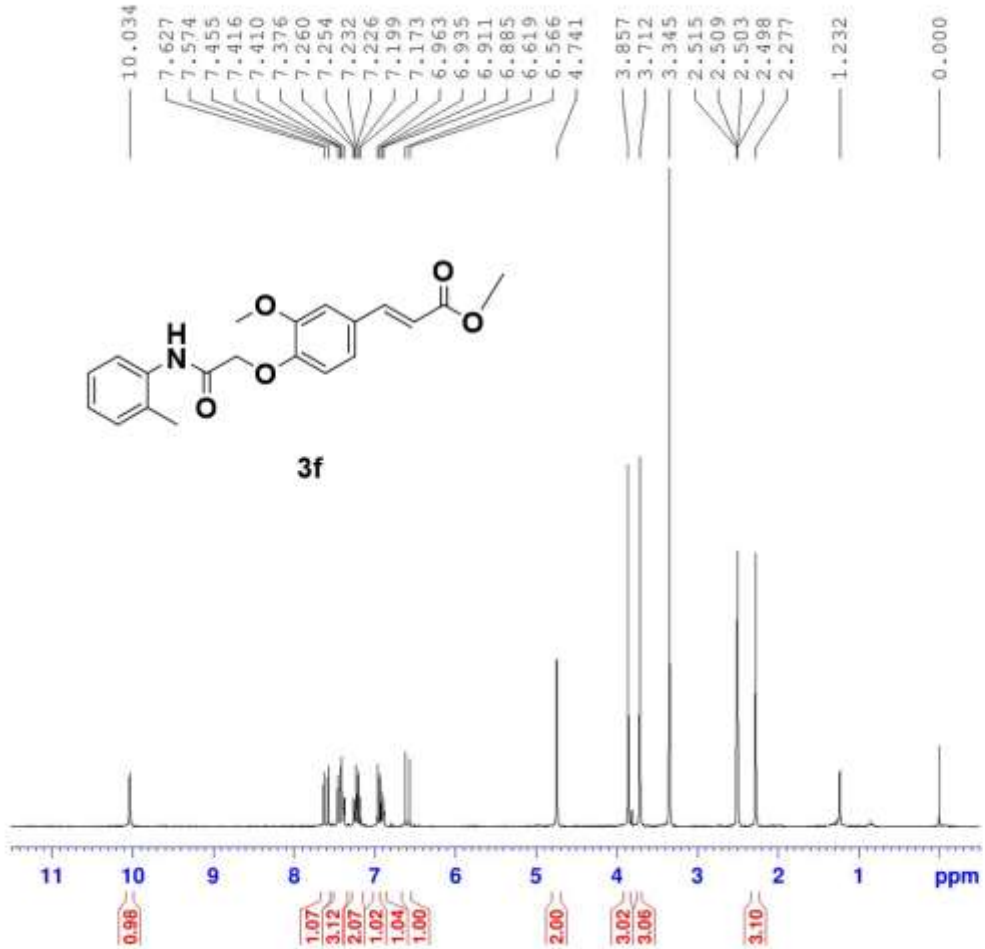

```
Current Data Parameters
NAME      1535F_C13-FAE+Anis
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_           20160425
Time              15.47
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  370
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 sec
RG                  161
DW                27.733 use
DE                 6.00 use
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 use
PL1                 0.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 use
PL2                -2.00 dB
PL12               16.98 dB
PL13               20.00 dB
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
```

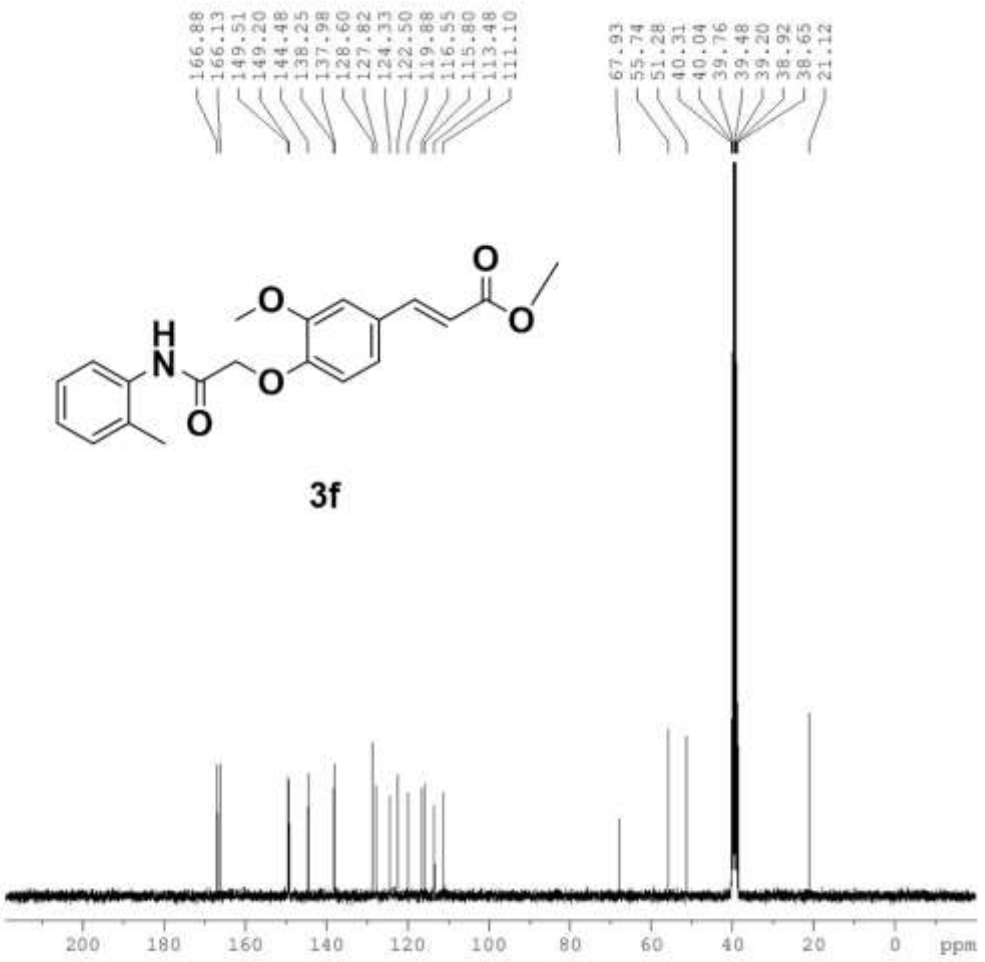



```
Current Data Parameters
NAME      1855B-Toluidine
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160628
Time               10.08
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   256
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.00 usec
PL1               -2.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




**3f**

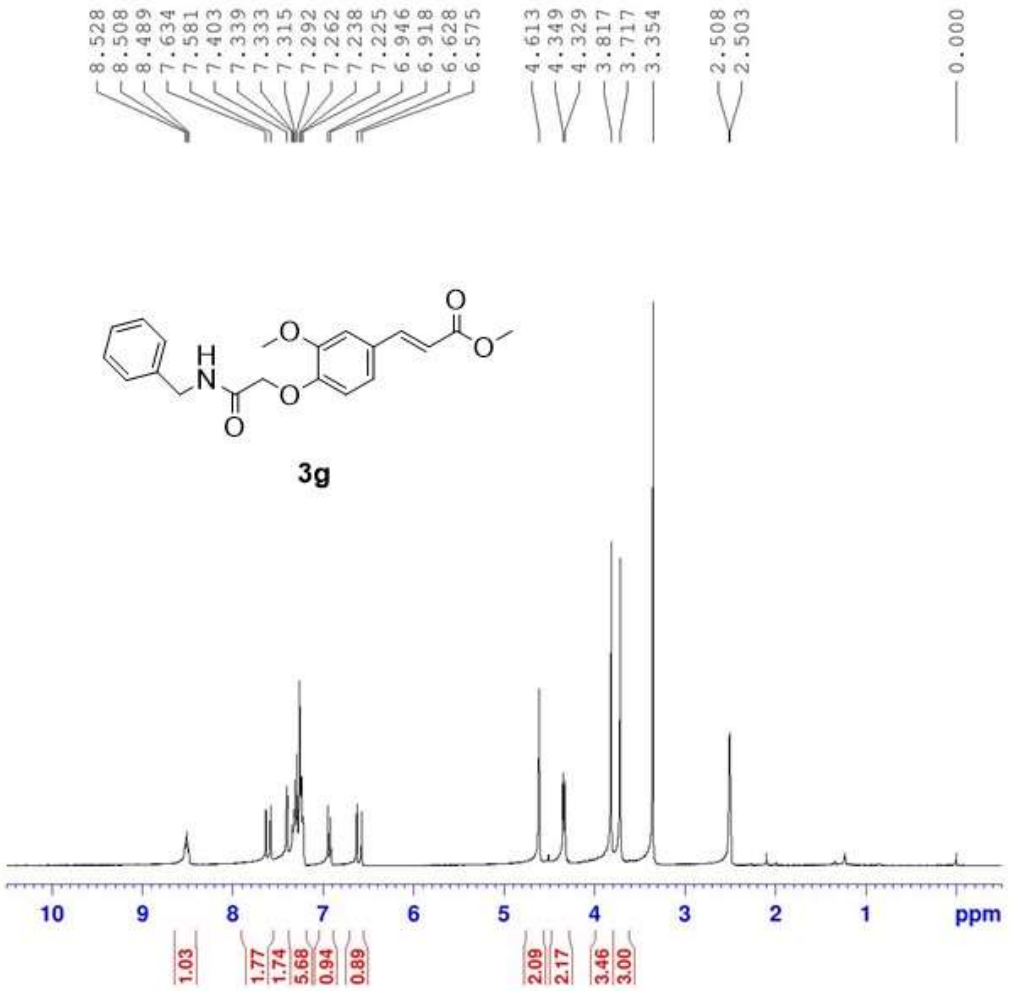
```
Current Data Parameters
NAME      1754E_C13-Toluidine
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20160628
Time                  17.46
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                     651
DS                       4
SWH              18028.846 Hz
FIDRES               0.275098 Hz
AQ                1.8175818 sec
RG                     203
DW                  27.733 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.00 usec
PL1                     0.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   16.98 dB
PL13                   20.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF              75.4677867 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

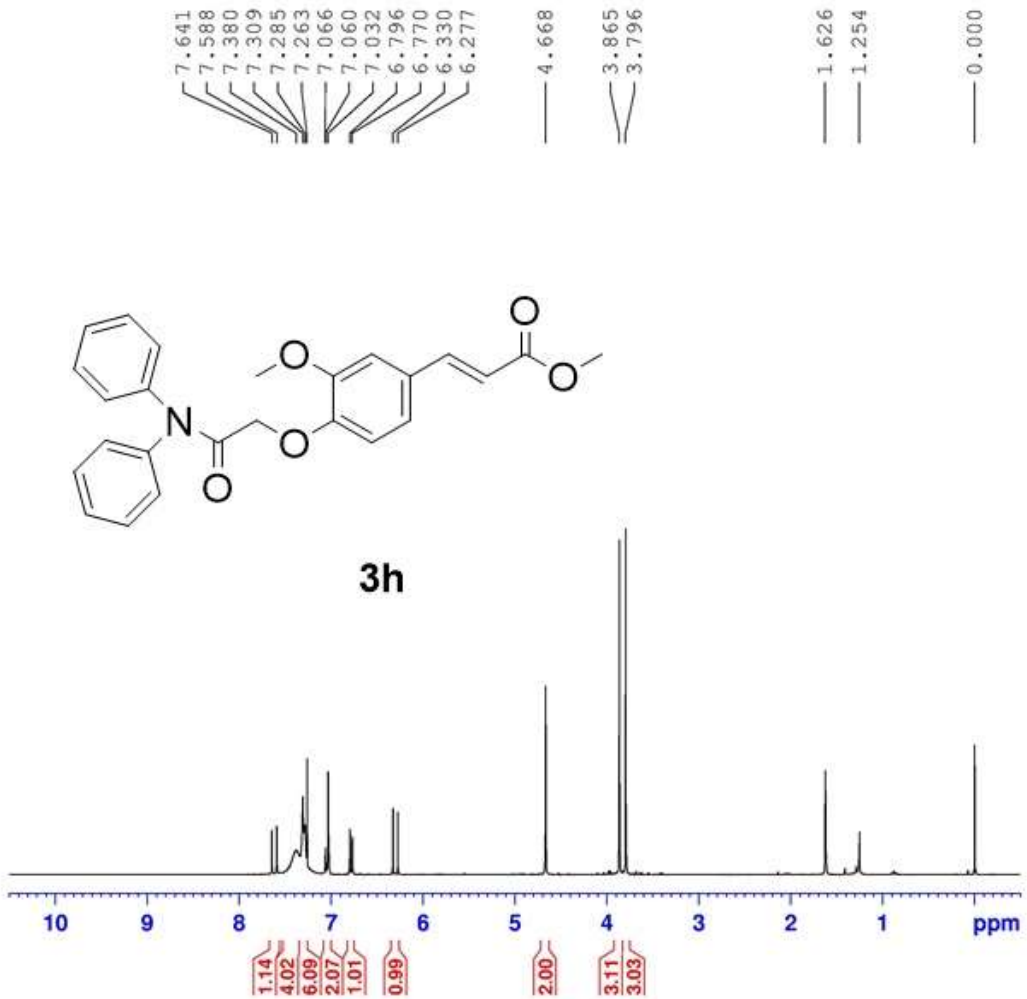



```
Current Data Parameters
NAME                  0852-D1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20151009
Time                  14.41
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      256
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1             1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1299990 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

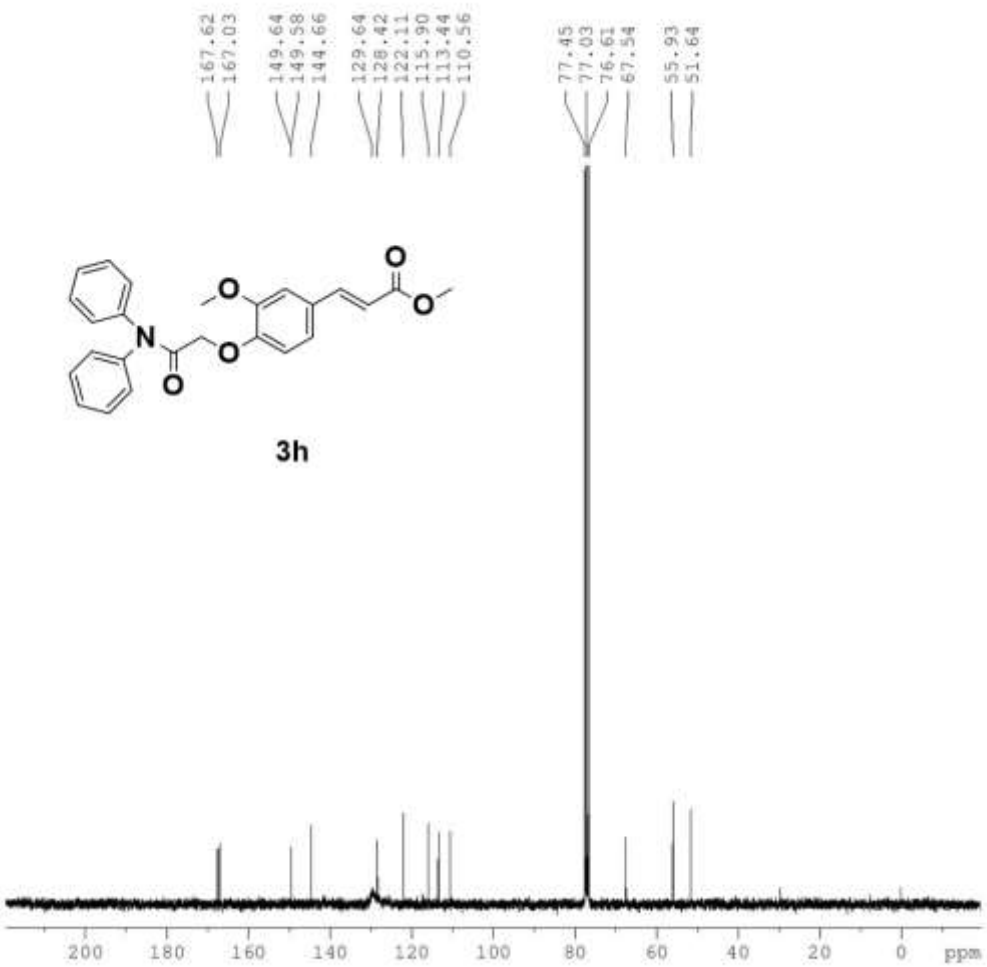



```
Current Data Parameters
NAME      1535A1-Ester+DPA
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160418
Time                 12.41
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                    362
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  9.00 usec
PL1                -2.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300055 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



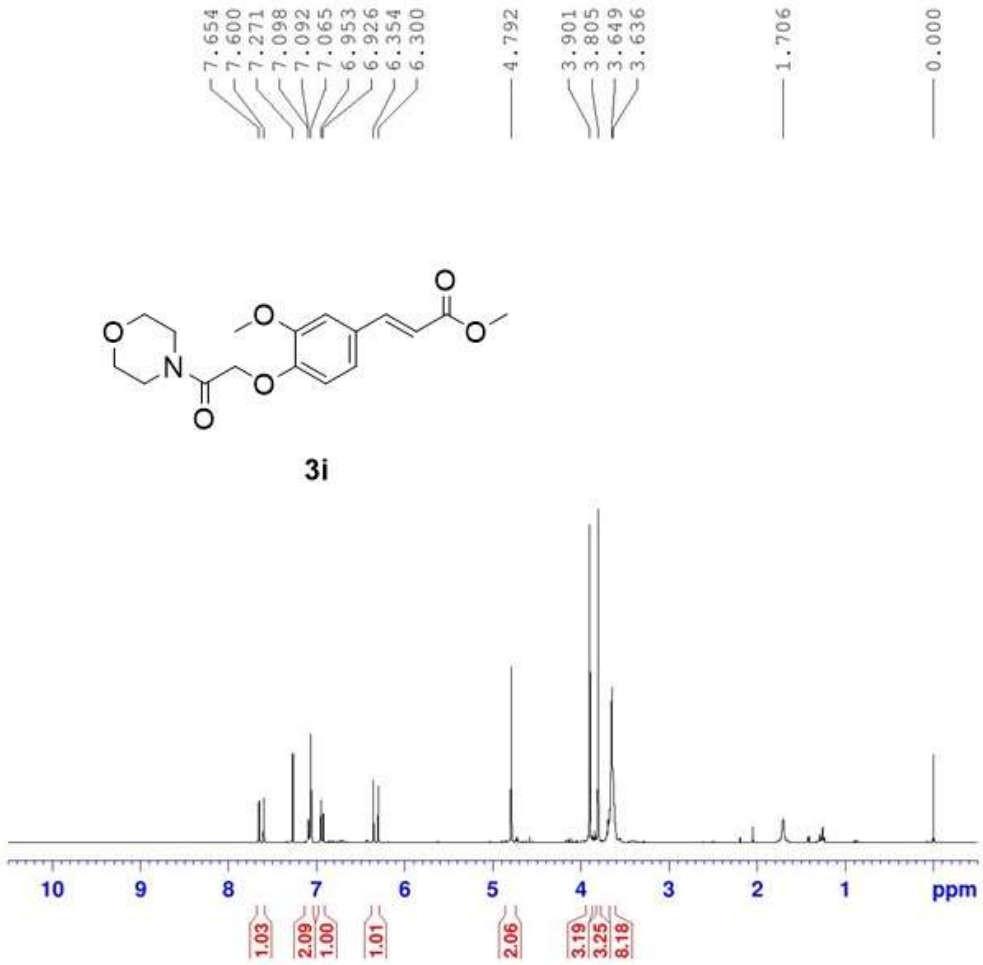

```
Current Data Parameters
NAME      1535D_C13-ESTER+DPA
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20160425
Time                  14.33
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175818 sec
RG                     256
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PL1                   0.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 16.98 dB
PL13                 20.00 dB
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
```

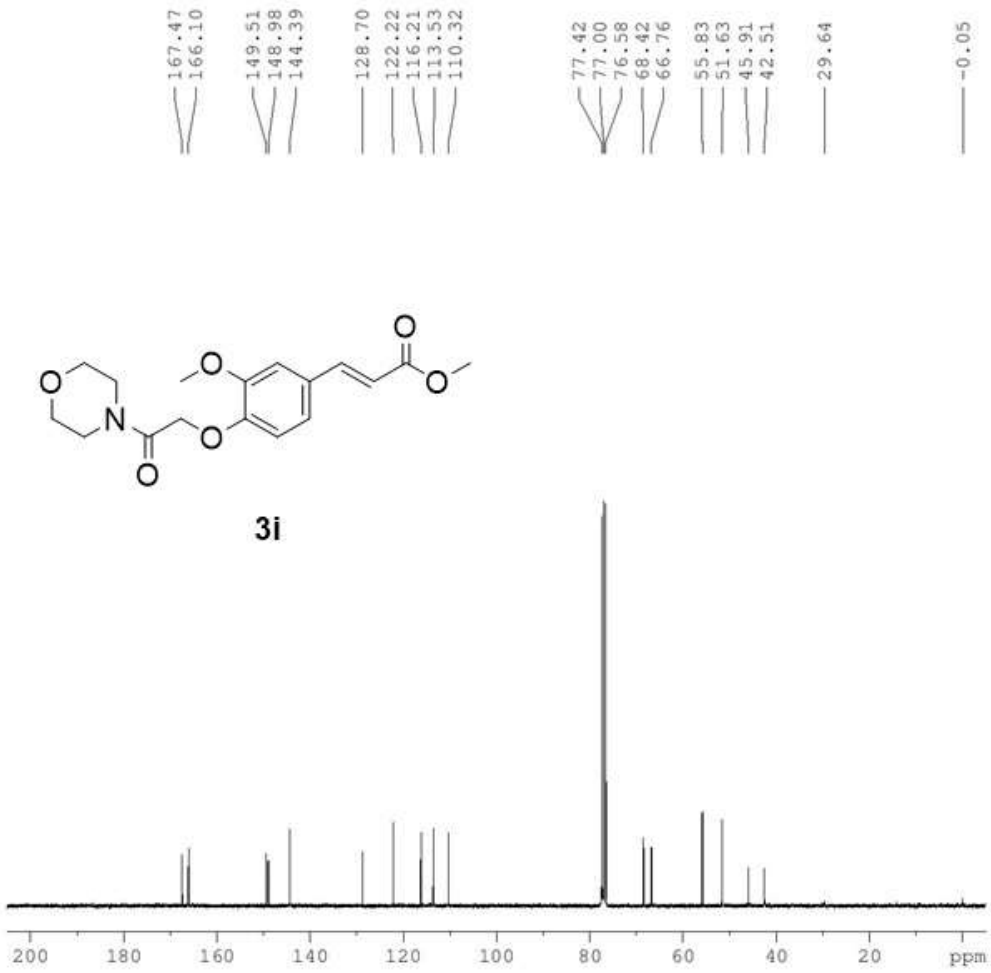



```
Current Data Parameters
NAME                  0852K
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150811
Time                  15.14
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      228
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF              300.1300028 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```




**3i**

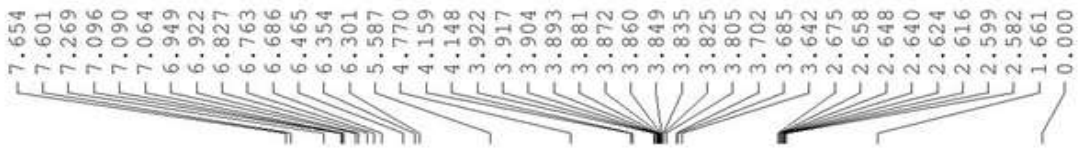
```
Current Data Parameters
NAME                  0852C-C13
EXPNO                         1
PROCNO                        1

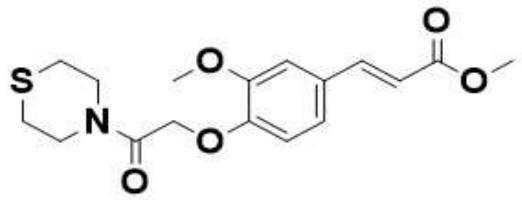
F2 - Acquisition Parameters
Date_                  20150812
Time                      13.51
INSTRUM                   spect
PROBHD   5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        2048
DS                           4
SWH                  18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175818 sec
RG                          203
DW                       27.733 usec
DE                        6.00 usec
TE                       300.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                        10.00 usec
PL1                        0.00 dB
SFO1                75.4752953 MHz

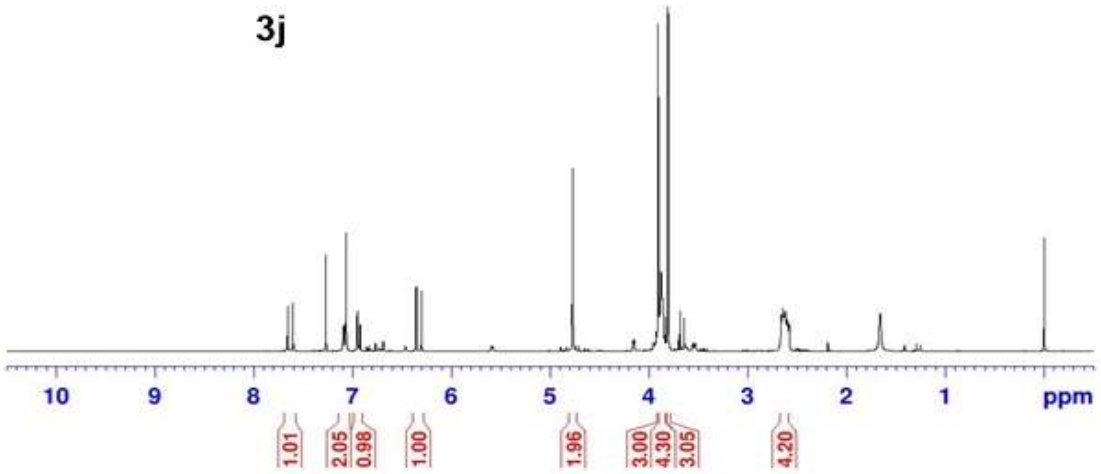
======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                       -2.00 dB
PL12                      16.98 dB
PL13                      20.00 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                 75.4677525 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```




3j

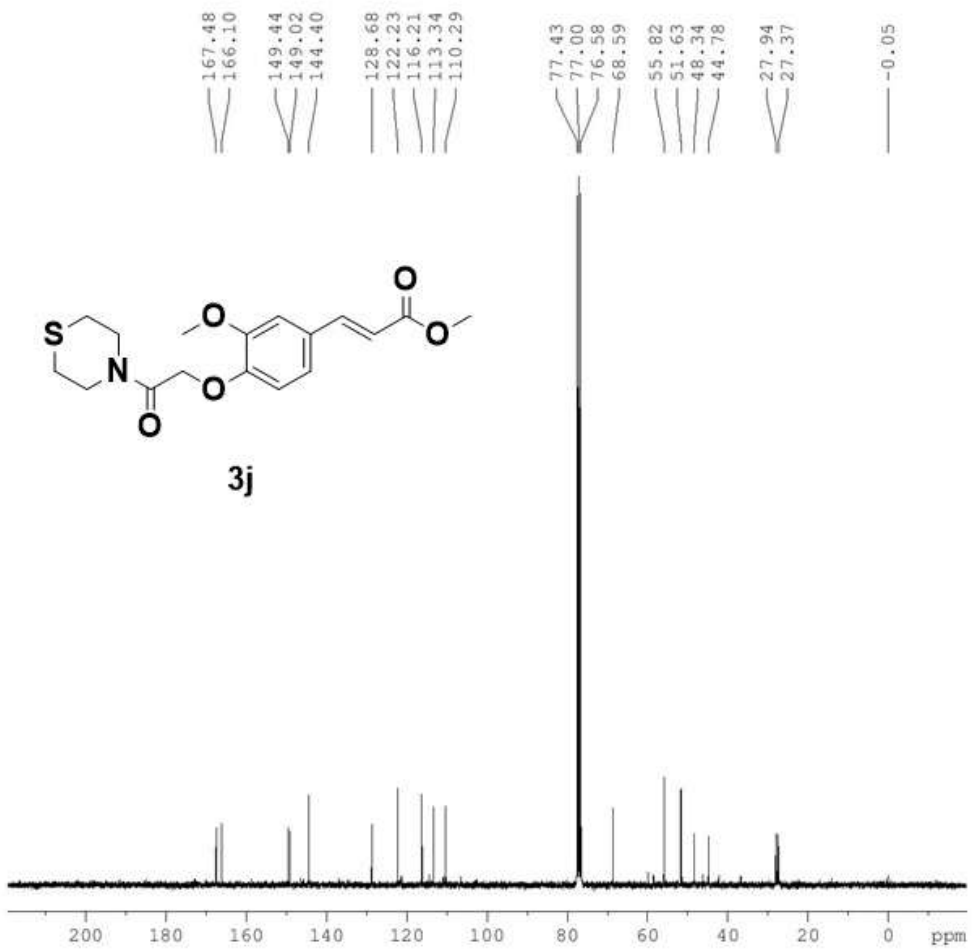



```
Current Data Parameters
NAME                  1332G
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160314
Time                  12.24
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      287
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300036 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```



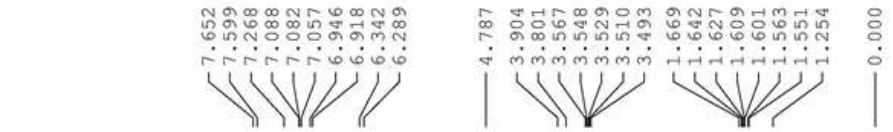

```
Current Data Parameters
NAME                  1525
EXPNO                    1
PROCNO                   1

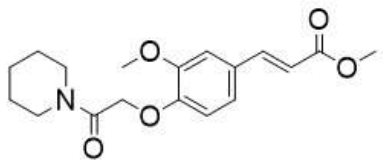
F2 - Acquisition Parameters
Date_              20160317
Time                 18.02
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                    1375
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175818 sec
RG                     256
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                 10.00 usec
PL1                 0.00 dB
SFO1           75.4752953 MHz

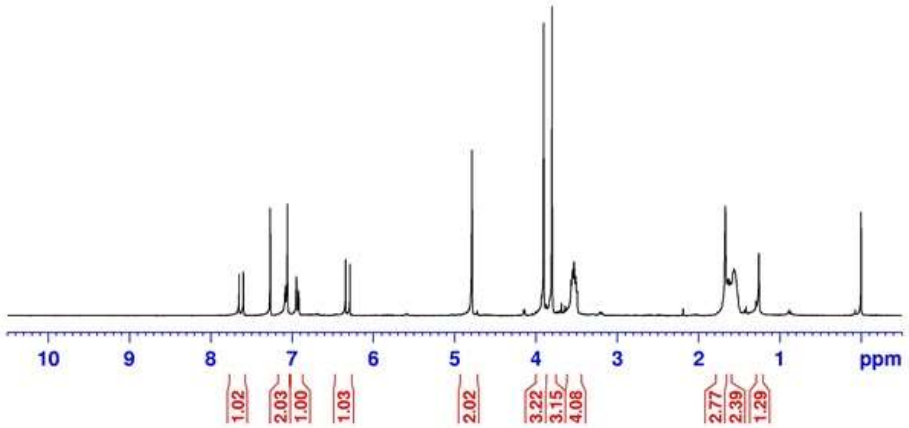
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               16.98 dB
PL13               20.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                   32768
SF             75.4677521 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```



3k

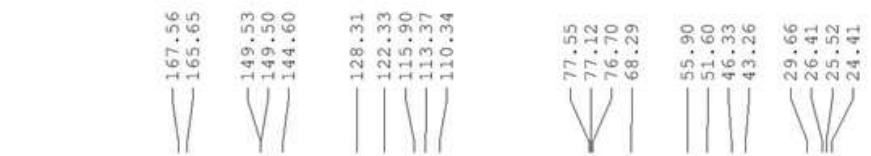


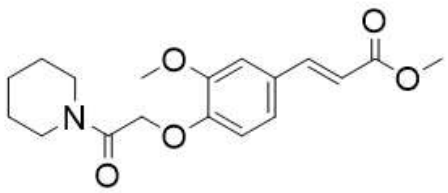

```
Current Data Parameters
NAME                  0852L-R
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150814
Time                  12.33
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                     322
DW                  80.800 usec
DE                   6.00 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                      1

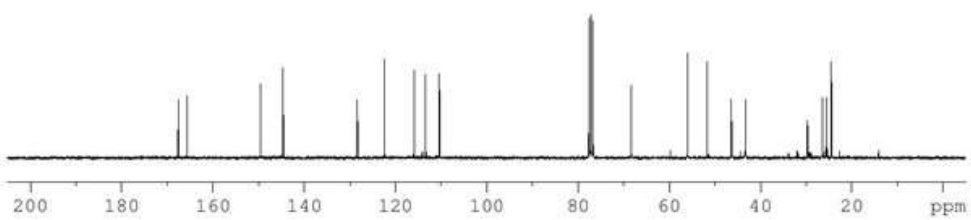
======== CHANNEL f1 ========
NUC1                    1H
P1                   9.00 usec
PL1                 -2.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF             300.1300036 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



**3k**



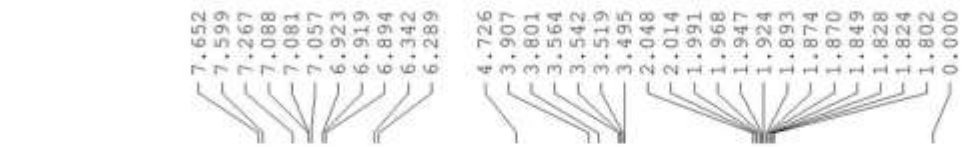

```
Current Data Parameters
NAME                  0852D
EXPNO                     1
PROCNO                    1

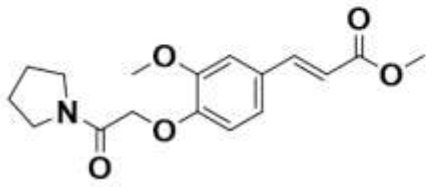
F2 - Acquisition Parameters
Date_              20150814
Time                  14.12
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                     745
DS                       4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 sec
RG                     203
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 0.00 dB
SFO1          75.4752953 MHz

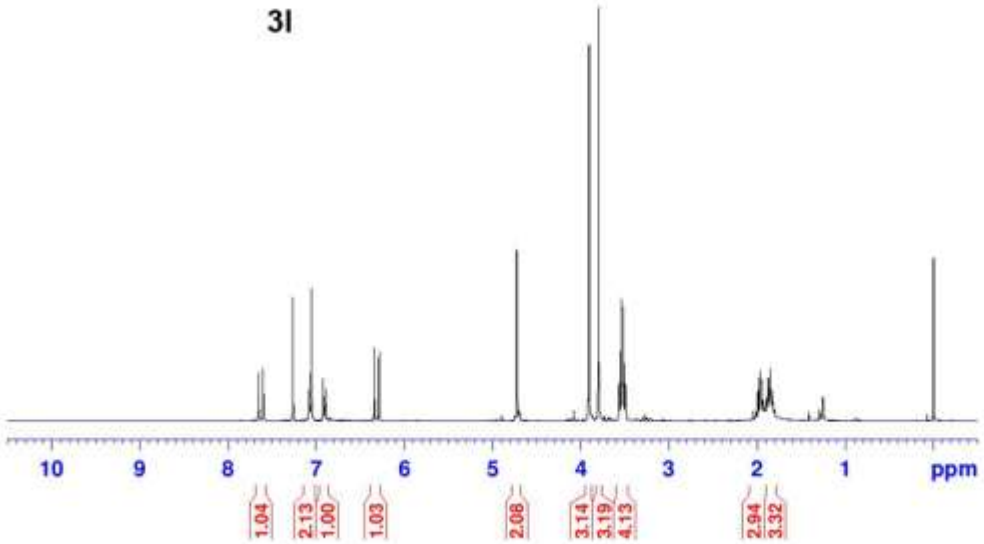
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               16.98 dB
PL13               20.00 dB
SFO2         300.1312005 MHz

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




**3l**

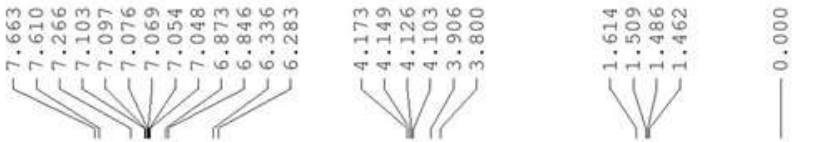


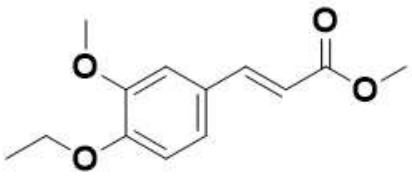

```
Current Data Parameters
NAME      1854F2-Pyrrolidine ester
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20160630
Time             18.08
INSTRUM          spect
PROBHD   5 mm BBO BB-1H
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                 16
DS                  2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                362
DW               80.800 usec
DE                6.00 usec
TE              300.0 K
D1            1.00000000 sec
TD0                 1

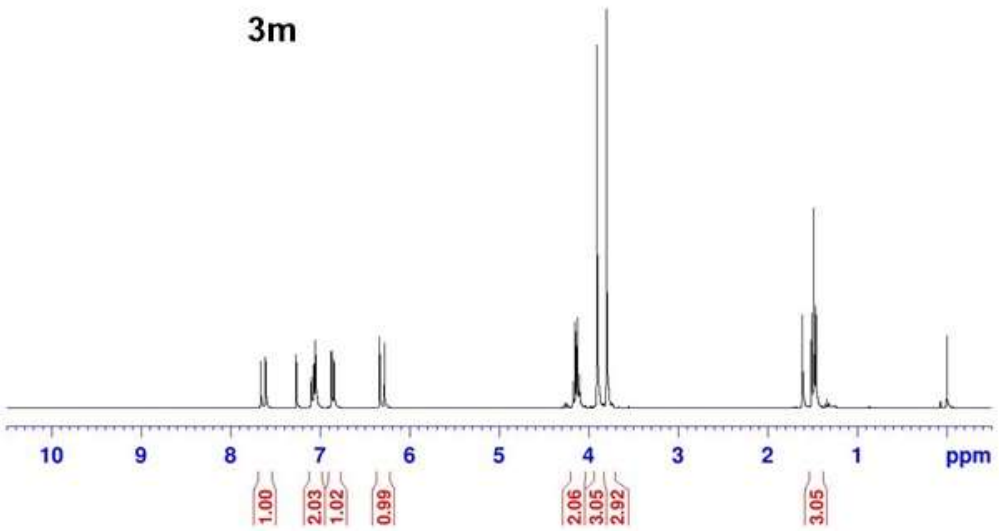
======== CHANNEL f1 ========
NUC1                1H
P1                9.00 usec
PL1              -2.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI              32768
SF          300.1300042 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



3m

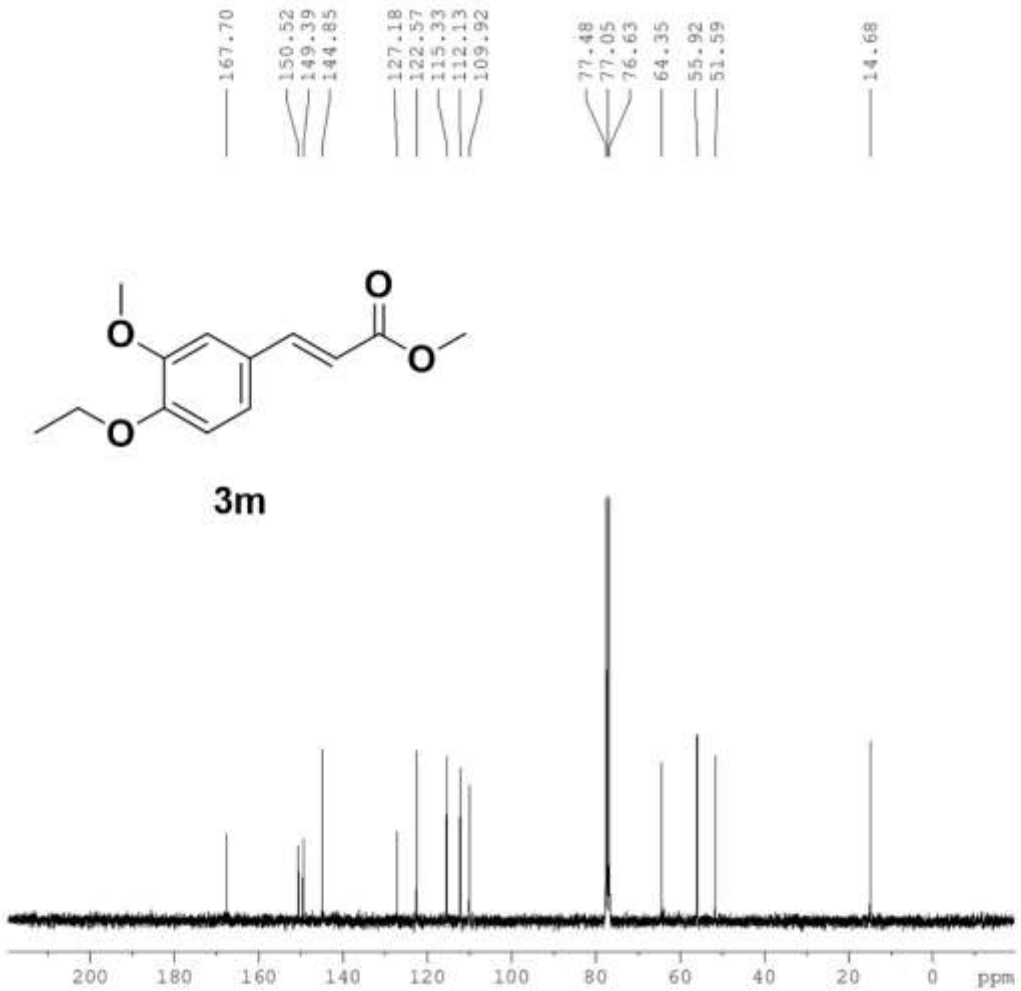



```
Current Data Parameters
NAME      1535B1-Ether-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160418
Time               16.24
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   287
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.00 usec
PL1                -2.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300046 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



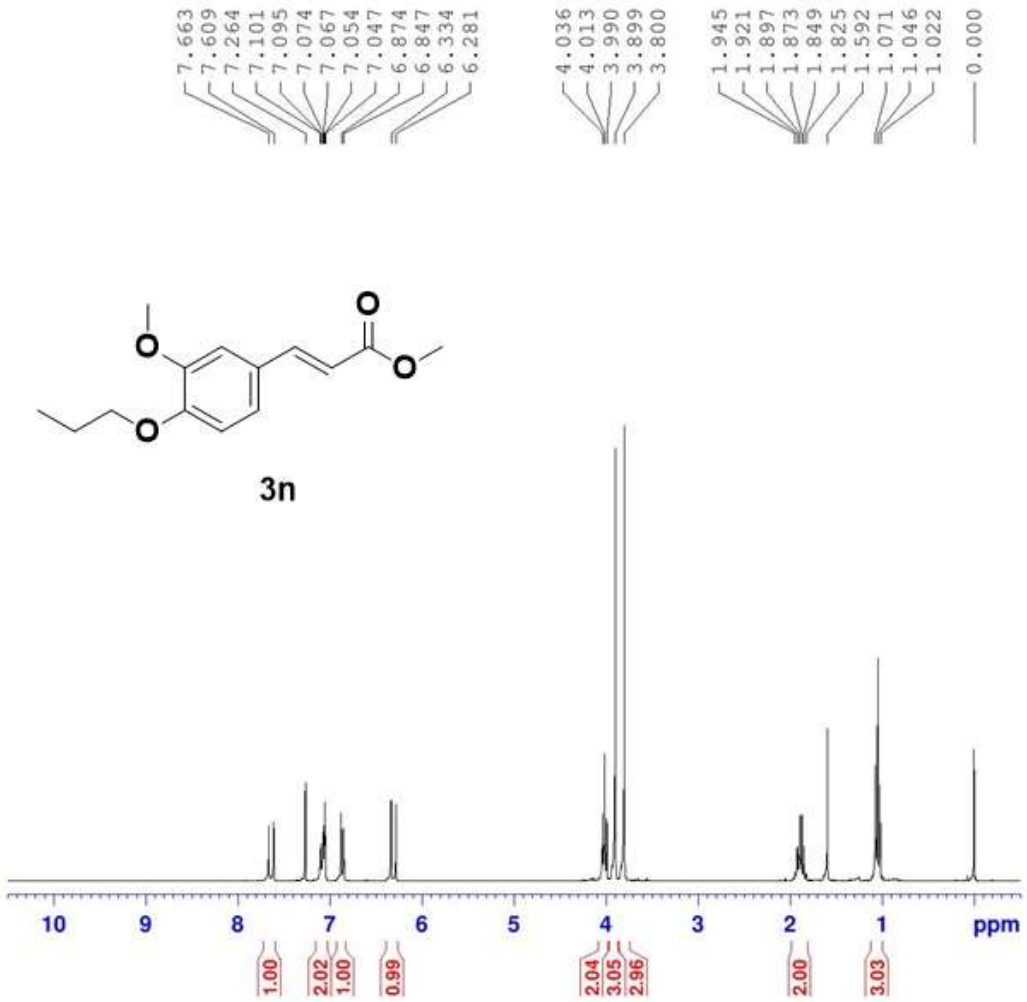

```
Current Data Parameters
NAME      1535E_C13-Ether-2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160425
Time                  15.18
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     440
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175818 sec
RG                     161
DW                27.733 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PL1                  0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -2.00 dB
PL12                16.98 dB
PL13                20.00 dB
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
```

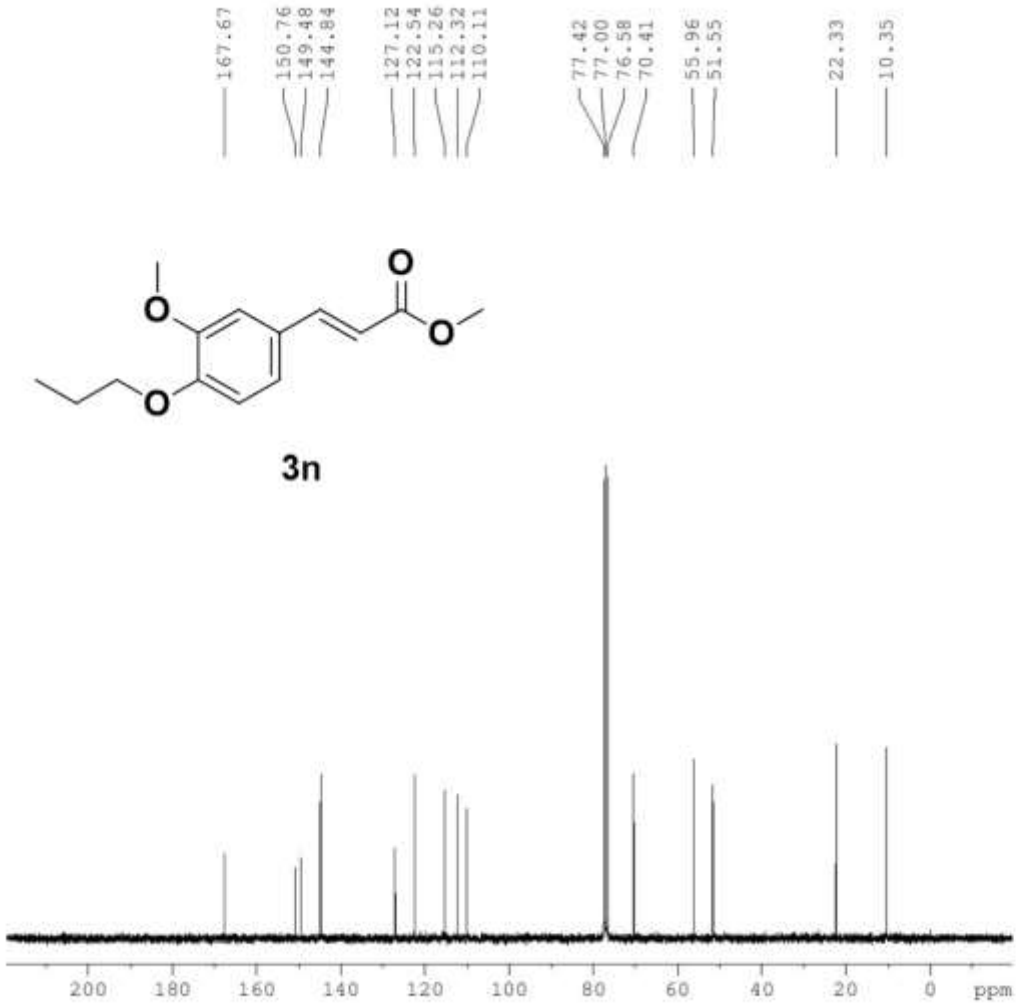



```
Current Data Parameters
NAME      1535D-FA-Propane
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20160413
Time                 17.47
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    362
DW                 80.800 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  9.00 usec
PL1                -2.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1300046 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



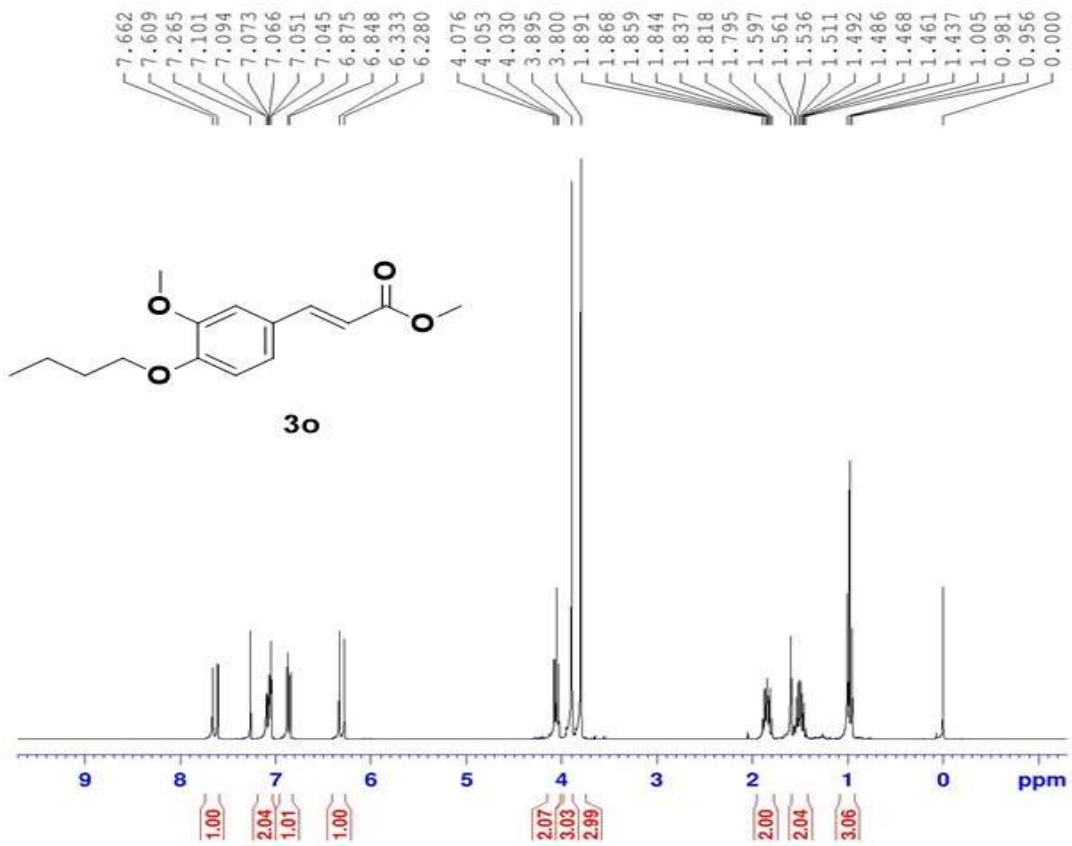

```
Current Data Parameters
NAME       1814A-Br-Prop
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20160527
Time              12.14
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH          18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 sec
RG                 228
DW              27.733 usec
DE               6.00 usec
TE              300.0 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677518 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

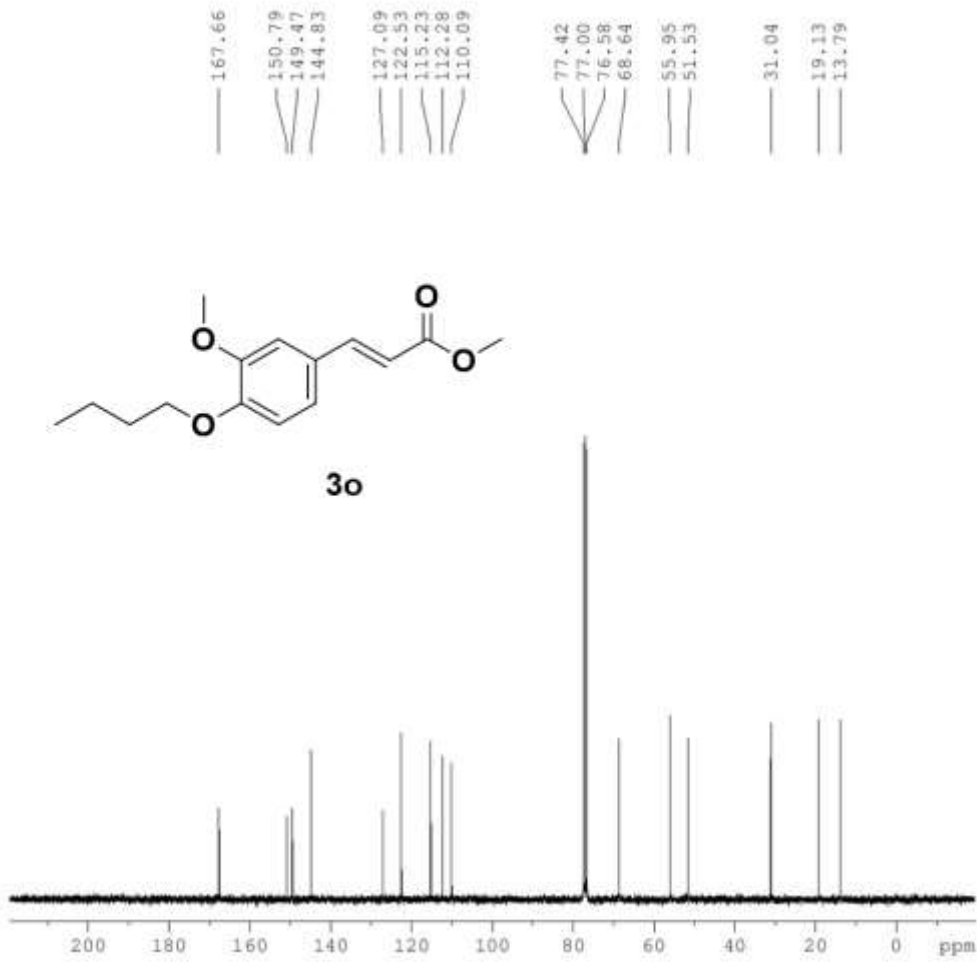



```
Current Data Parameters
NAME      1535F-FA-Butane
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160413
Time                17.59
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                    322
DW                 80.800 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.00 usec
PL1                 -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF            300.1300046 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



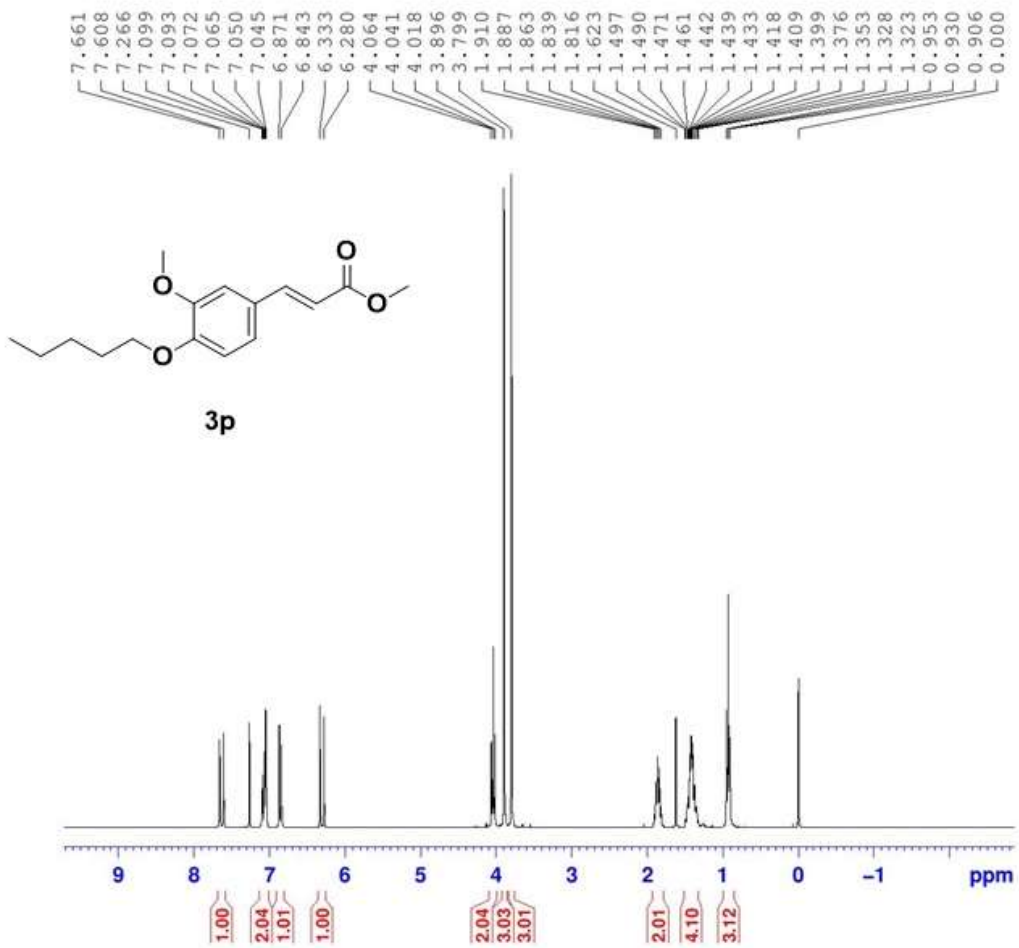

```
Current Data Parameters
NAME       1814B-Br-Buta
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20160527
Time              12.52
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                 228
DW              27.733 usec
DE                6.00 usec
TE               300.0 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF         75.4677525 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```



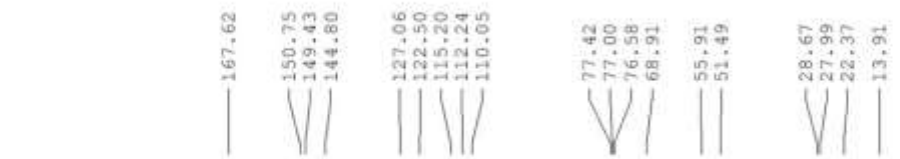

3p

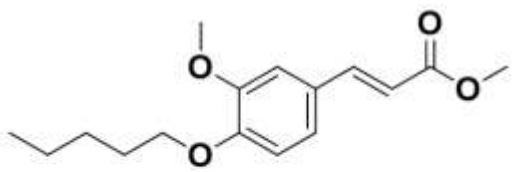
```
Current Data Parameters
NAME                  1332D
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160128
Time                  14.46
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      228
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

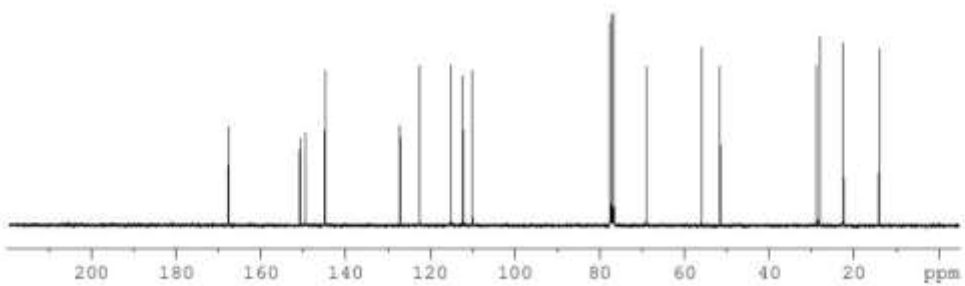
======== CHANNEL f1 ========
NUC1                    1H
P1                   9.00 usec
PL1                 -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300046 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```




**3p**



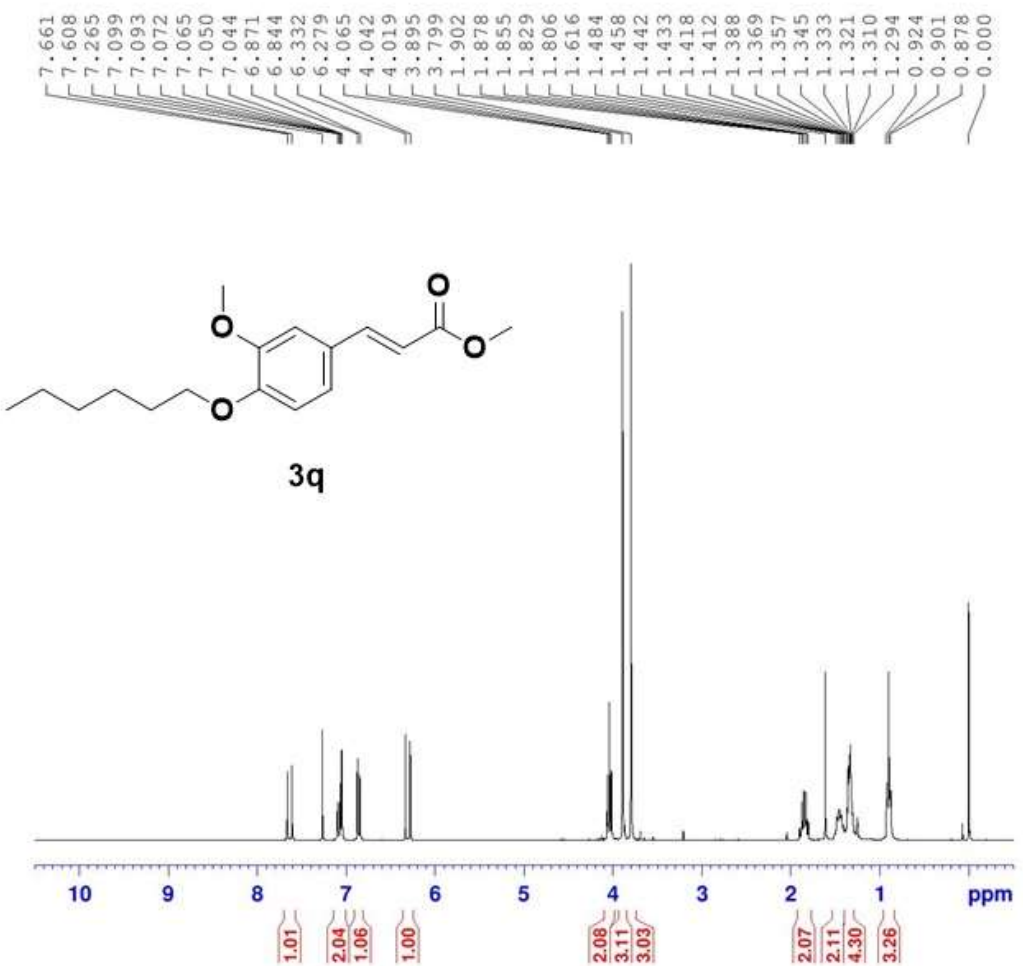

```
Current Data Parameters
NAME       1814C-Br-Pent
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20160527
Time              13.53
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 865
DS                   4
SWH          18028.846 Hz
FIDRES        0.275099 Hz
AQ            1.8175818 sec
RG                 228
DW              27.733 usec
DE                6.00 usec
TE               300.0 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF         75.4677541 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

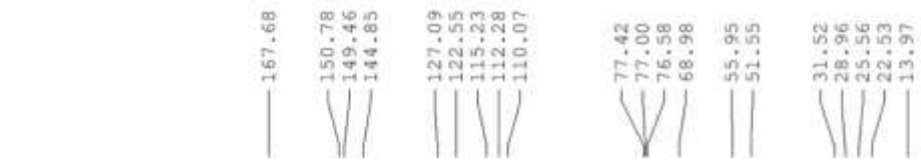


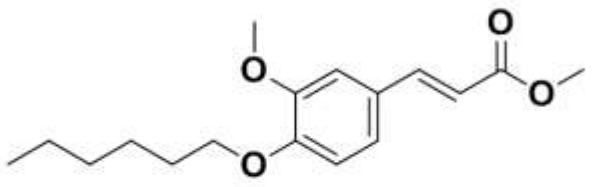

```
Current Data Parameters
NAME                  1283G
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160112
Time                  16.21
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      256
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

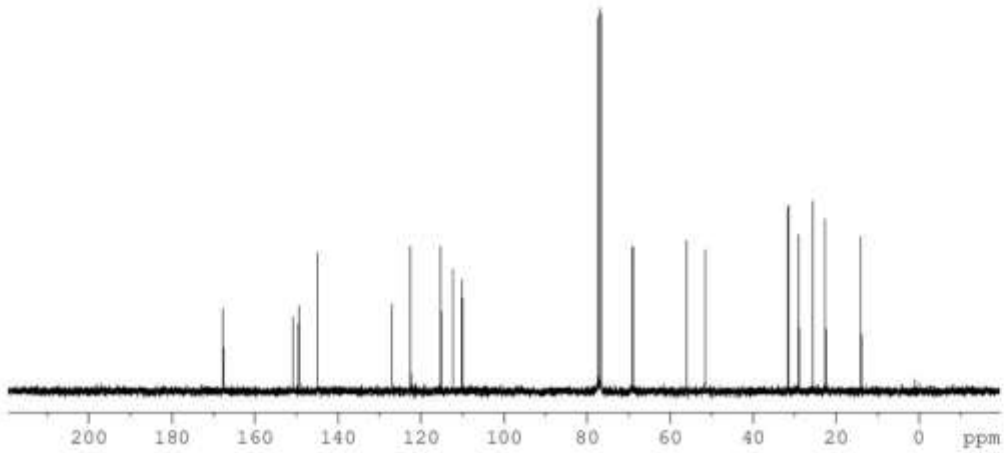
======== CHANNEL f1 ========
NUC1                      1H
P1                     9.00 usec
PL1                   -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300048 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```




**3q**



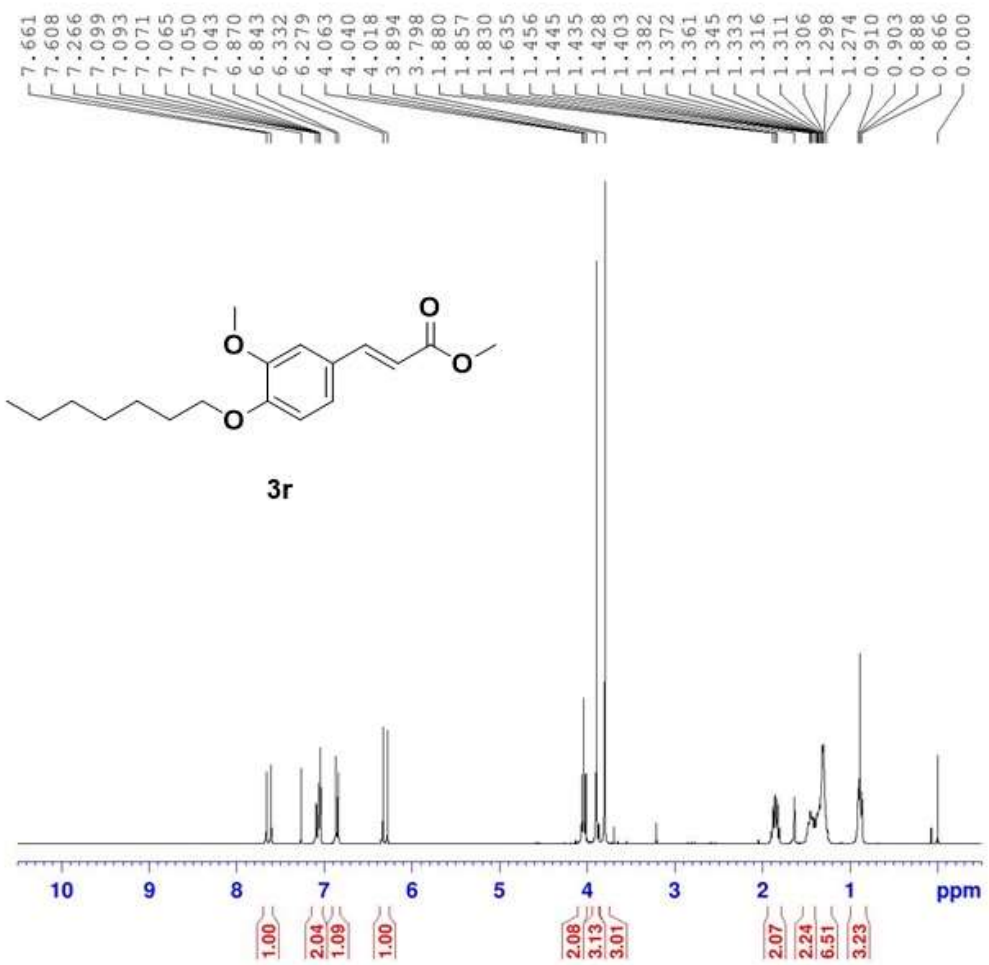

```
Current Data Parameters
NAME      1814D-FA+Hexane
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160528
Time               16.25
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  450
DS                    4
SWH           18028.846 Hz
FIDRES            0.275098 Hz
AQ            1.8175818 sec
RG                  181
DW                27.733 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                  32768
SF           75.4677520 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

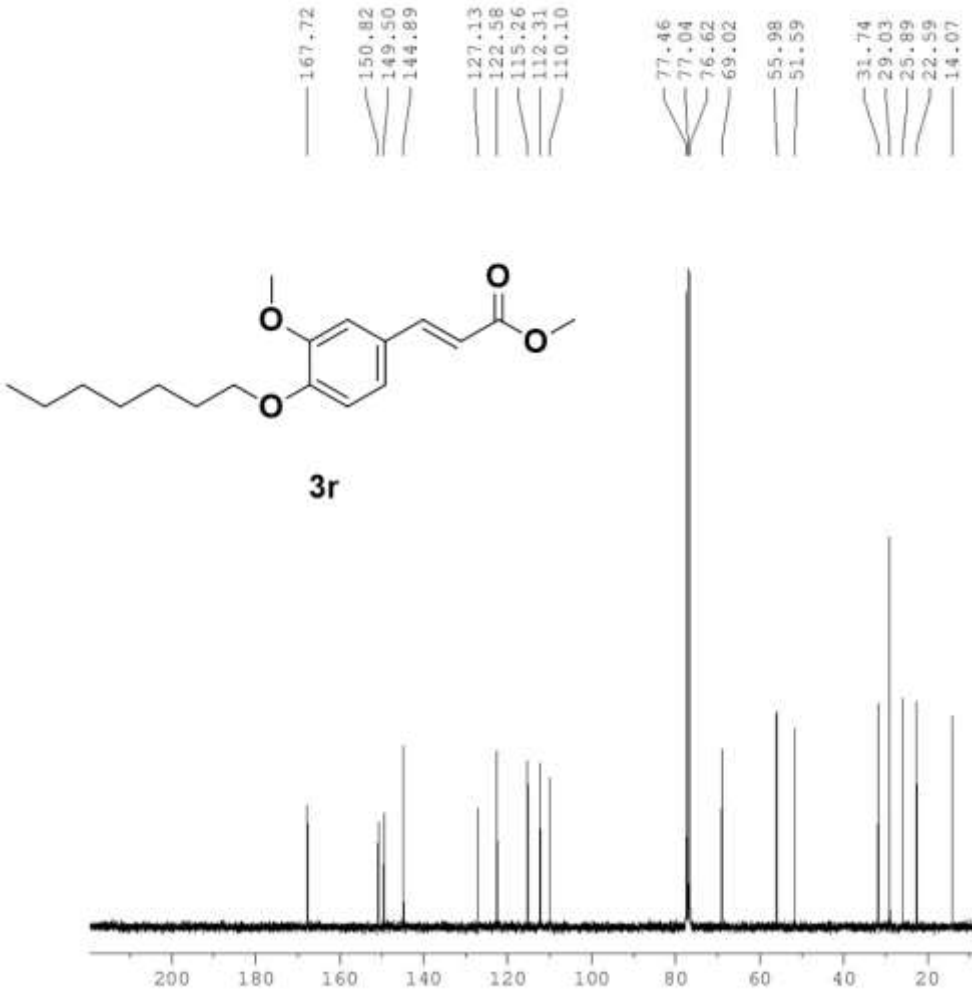



```
Current Data Parameters
NAME      1535A2-Ether-7
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160418
Time               16.03
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   161
DW                80.800 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.00 usec
PL1               -2.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300042 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



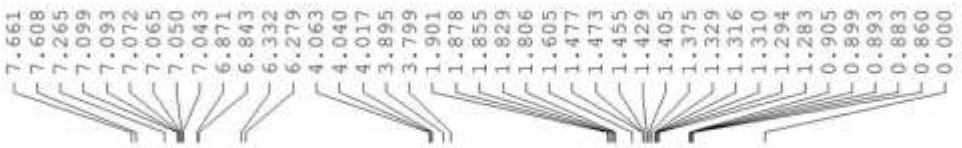

```
Current Data Parameters
NAME      1814E-FA+Hepta
EXPNO                  1
PROCNO                 1

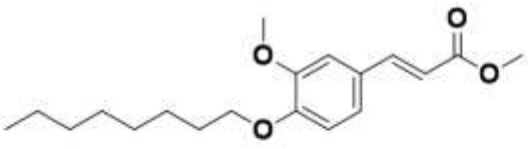
F2 - Acquisition Parameters
Date_           20160526
Time               17.04
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  516
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  228
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

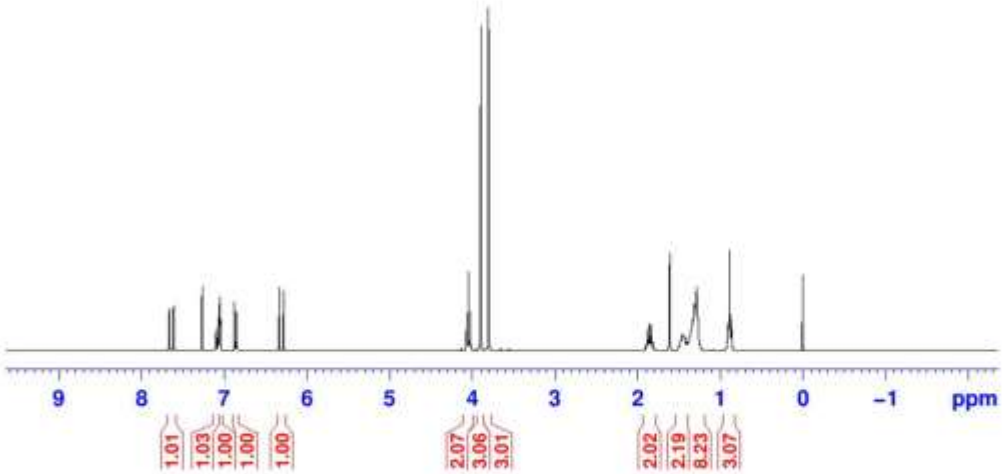
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

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



3s

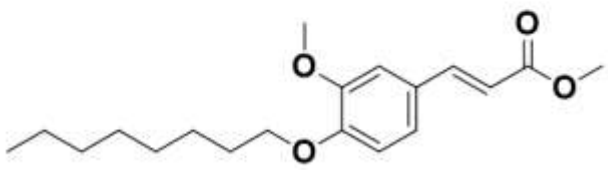



```
Current Data Parameters
NAME      1854F1-FA+Octane
EXPNO                    1
PROCNO                   1

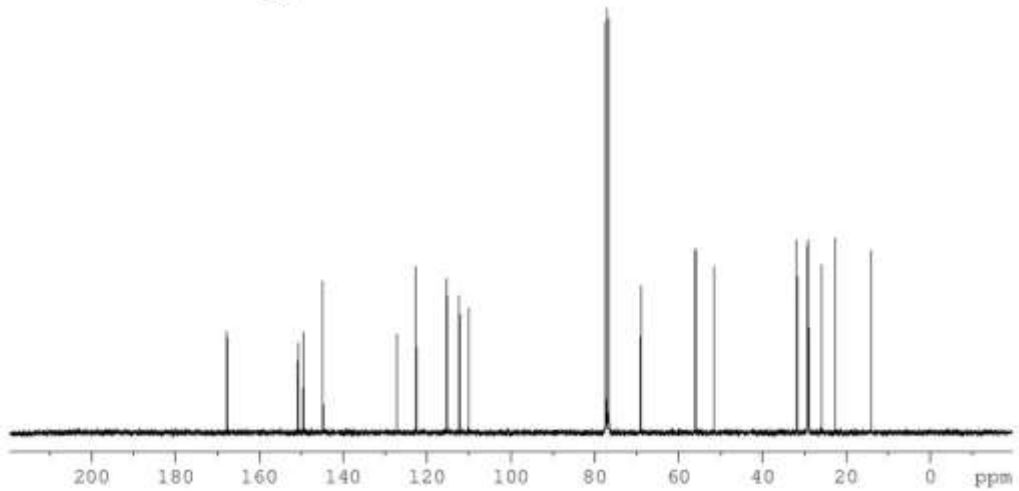
F2 - Acquisition Parameters
Date_             20160630
Time                 17.23
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    228
DW                 80.800 usec
DE                  6.00 usec
TE                 300.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  9.00 usec
PL1                -2.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1300048 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```


**3s**



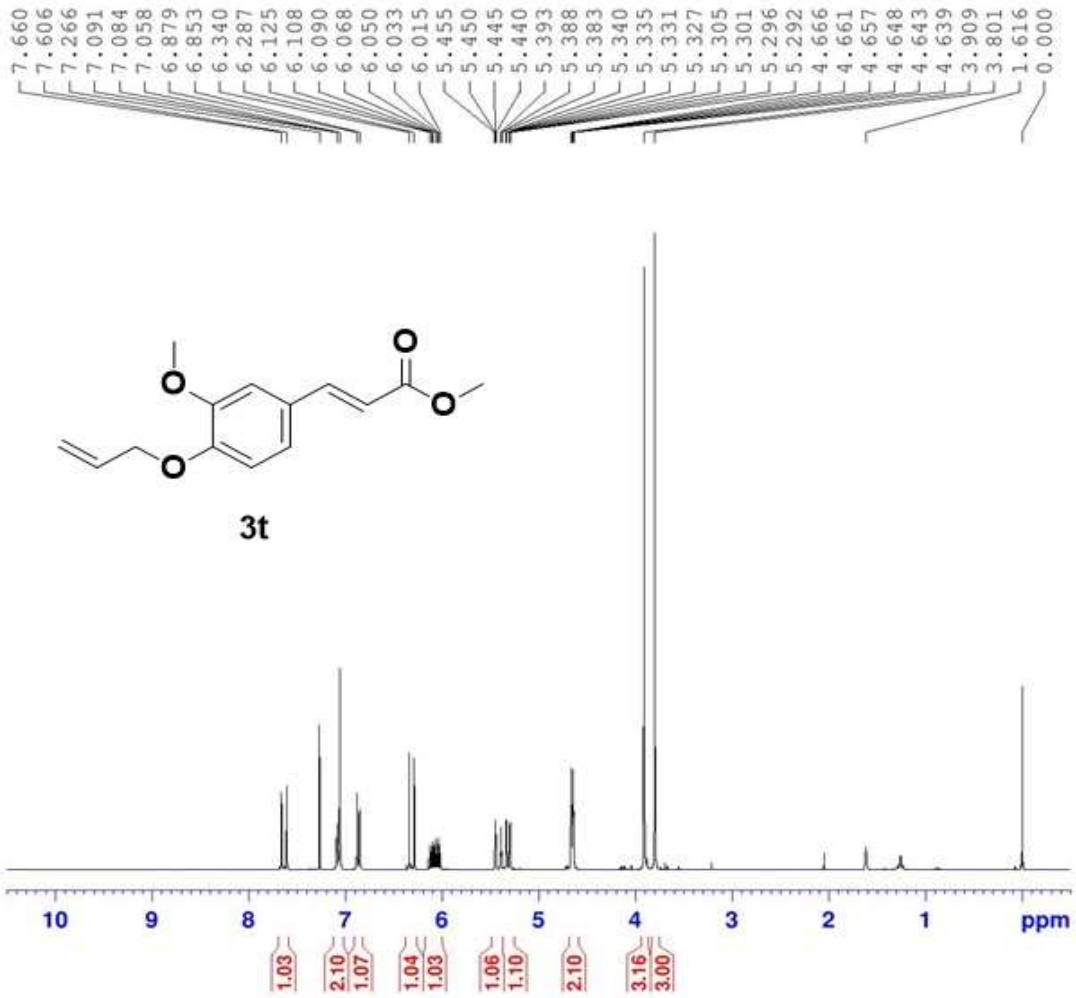

```
Current Data Parameters
NAME      1814F-FA+Octa
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20160528
Time              17.54
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 700
DS                   4
SWH          18028.846 Hz
FIDRES         0.275098 Hz
AQ           1.8175818 sec
RG                 203
DW              27.733 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PL1               0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -2.00 dB
PL12             16.98 dB
PL13             20.00 dB
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
```

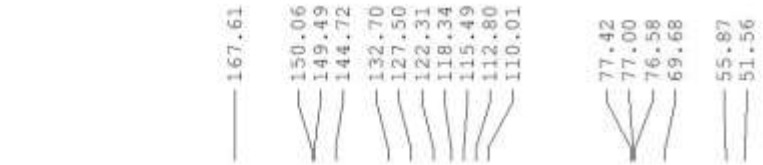


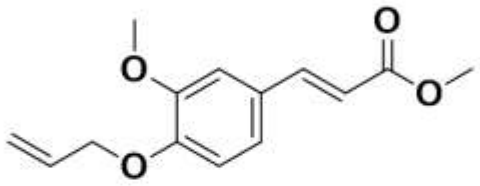

```
Current Data Parameters
NAME                  1332C
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160128
Time                  14.40
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      287
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1             1.00000000 sec
TD0                       1

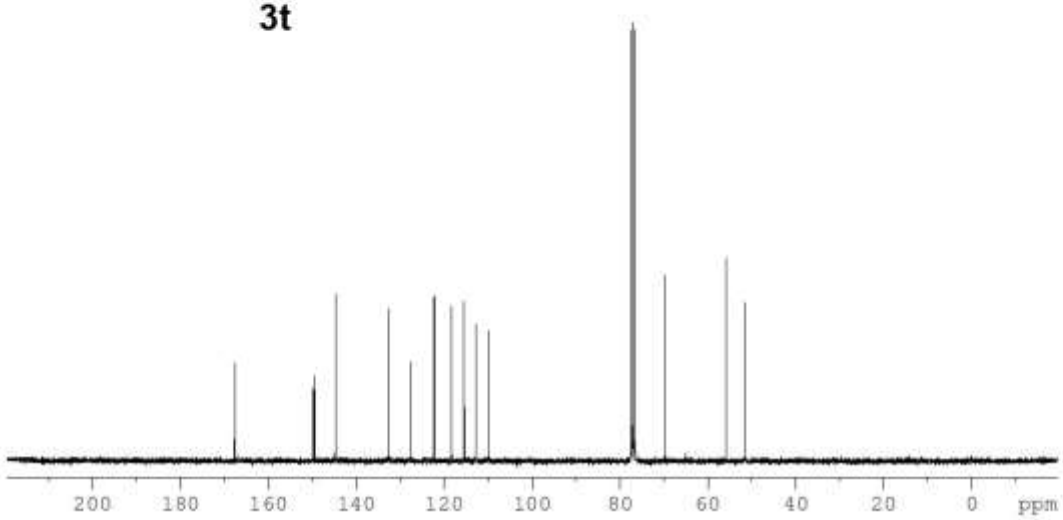
======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300044 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```



**3t**



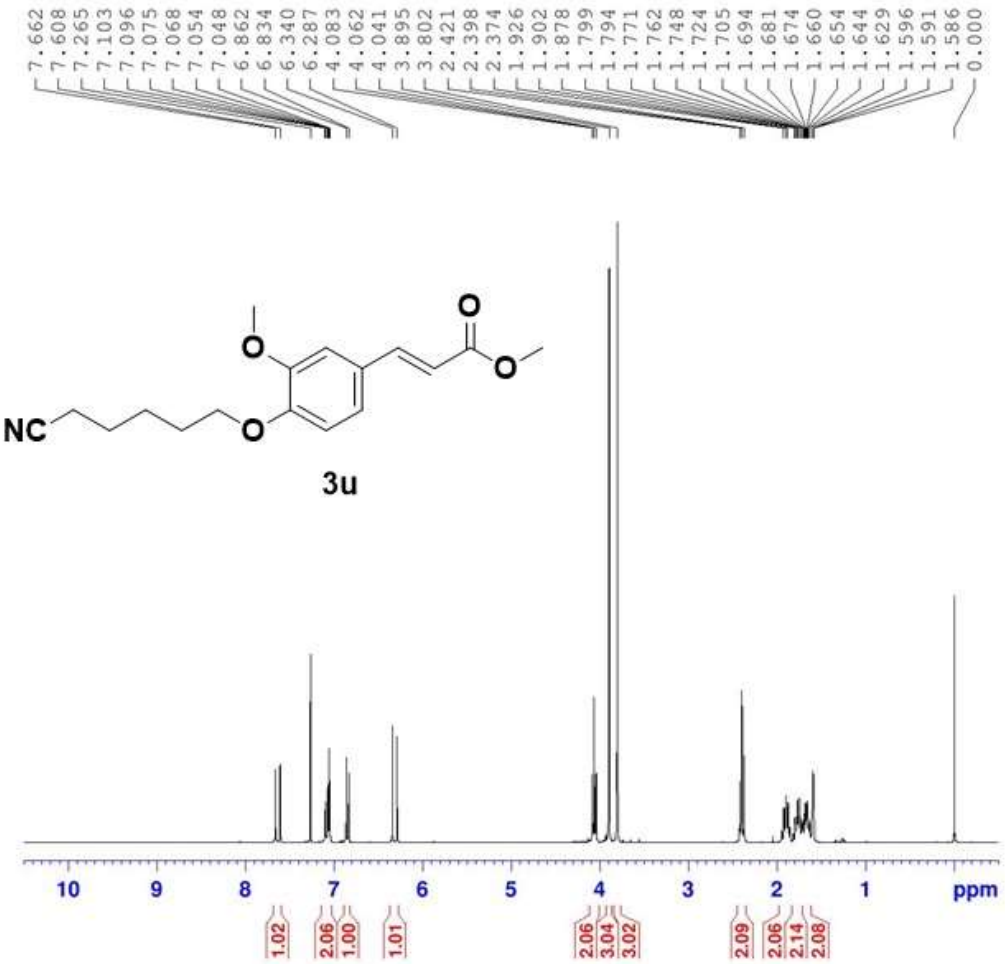

```
Current Data Parameters
NAME      1827A-FA+Allyl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160602
Time               11.47
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  885
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  228
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677527 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                 1.40
```

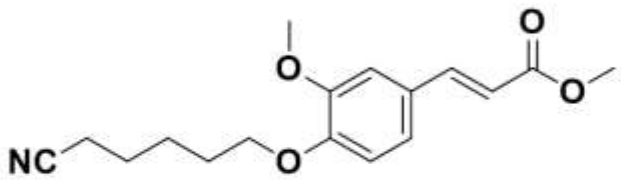



```
Current Data Parameters
NAME         1535B-CN-Br
EXPNO                  1
PROCNO                 1

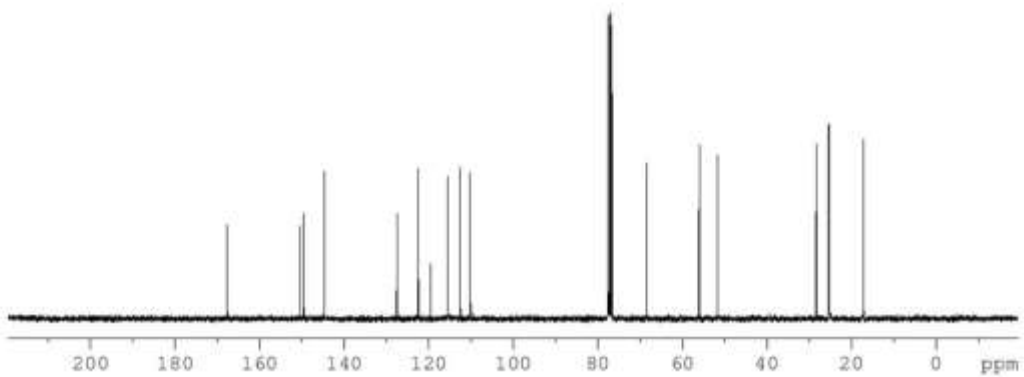
F2 - Acquisition Parameters
Date_           20160413
Time               17.18
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                   362
DW              80.800 usec
DE               6.00 usec
TE               300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.00 usec
PL1               -2.00 dB
SFO1       300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF         300.1300047 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```


**3u**



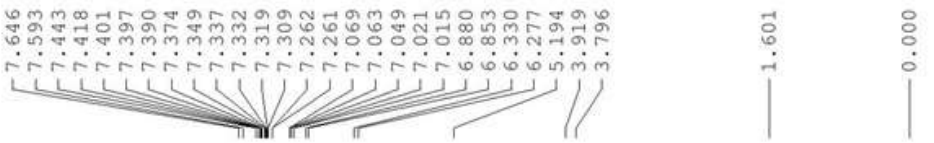

```
Current Data Parameters
NAME      1535C_C13-CNBr
EXPNO                  1
PROCNO                 1

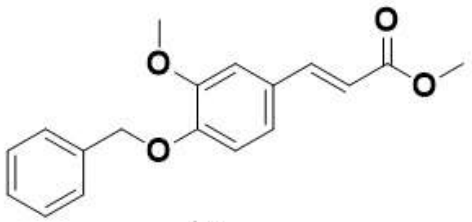
F2 - Acquisition Parameters
Date_           20160425
Time               13.02
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  566
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  256
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

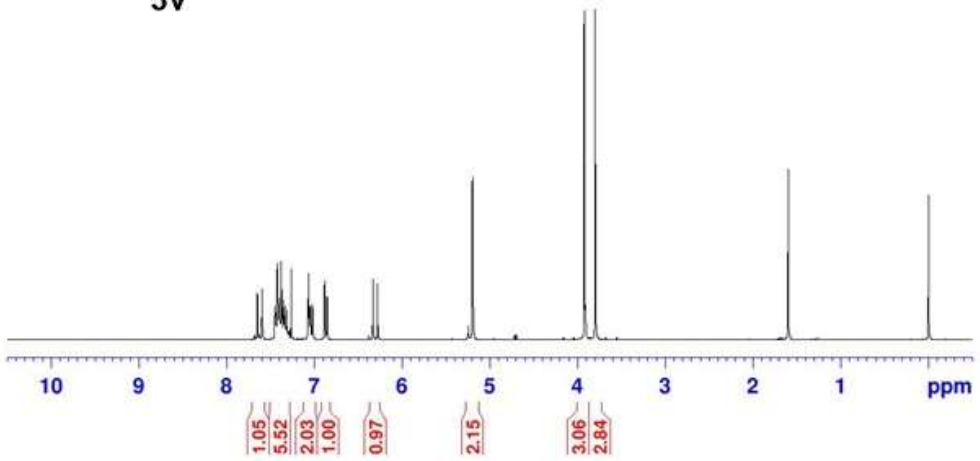
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

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



3v

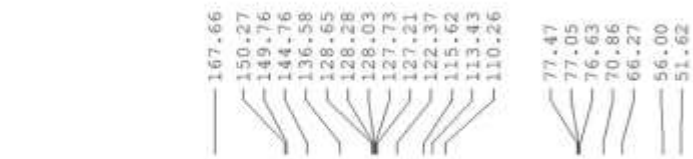


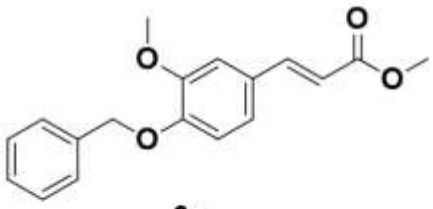

```
Current Data Parameters
NAME                  1283H
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160113
Time                  15.28
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                      322
DW                   80.800 usec
DE                    6.00 usec
TE                   300.0 K
D1             1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.00 usec
PL1                   -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300058 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



3v



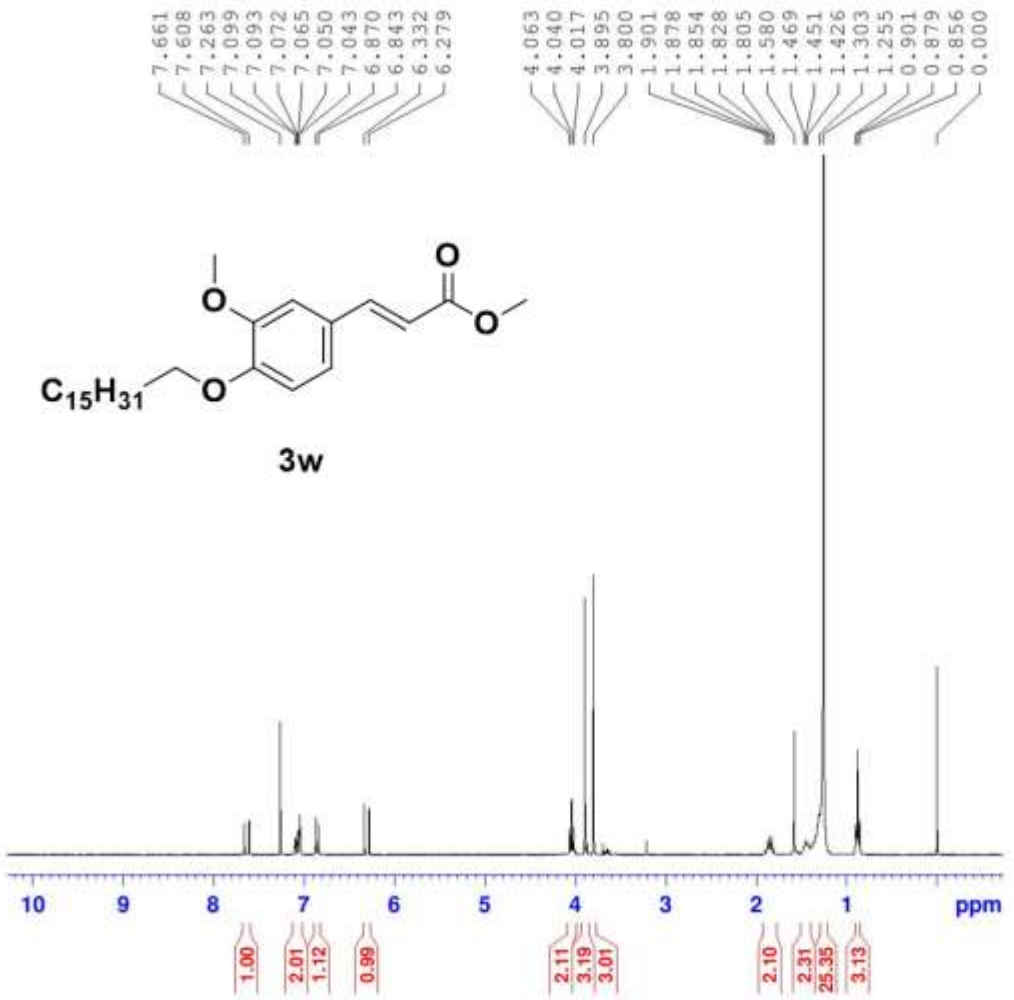

```
Current Data Parameters
NAME      1827B-FA+Benzyl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160602
Time               13.23
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1412
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  181
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
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
```

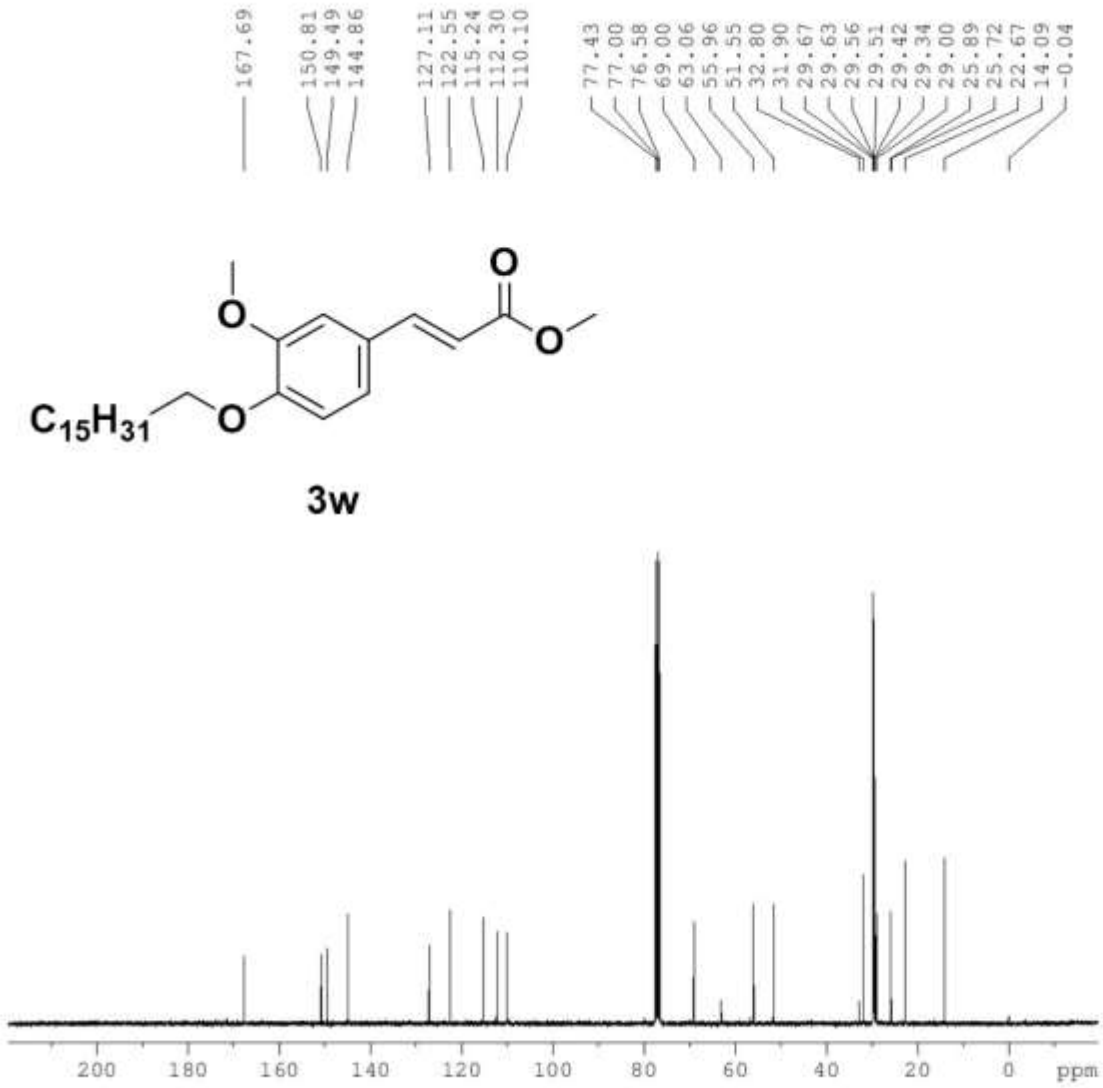



```
Current Data Parameters
NAME      1535C-FA-Cetane
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160413
Time                17.41
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                   287
DW              80.900 usec
DE               6.00 usec
TE               300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.00 usec
PL1               -2.00 dB
SFO1        300.1316534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300052 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



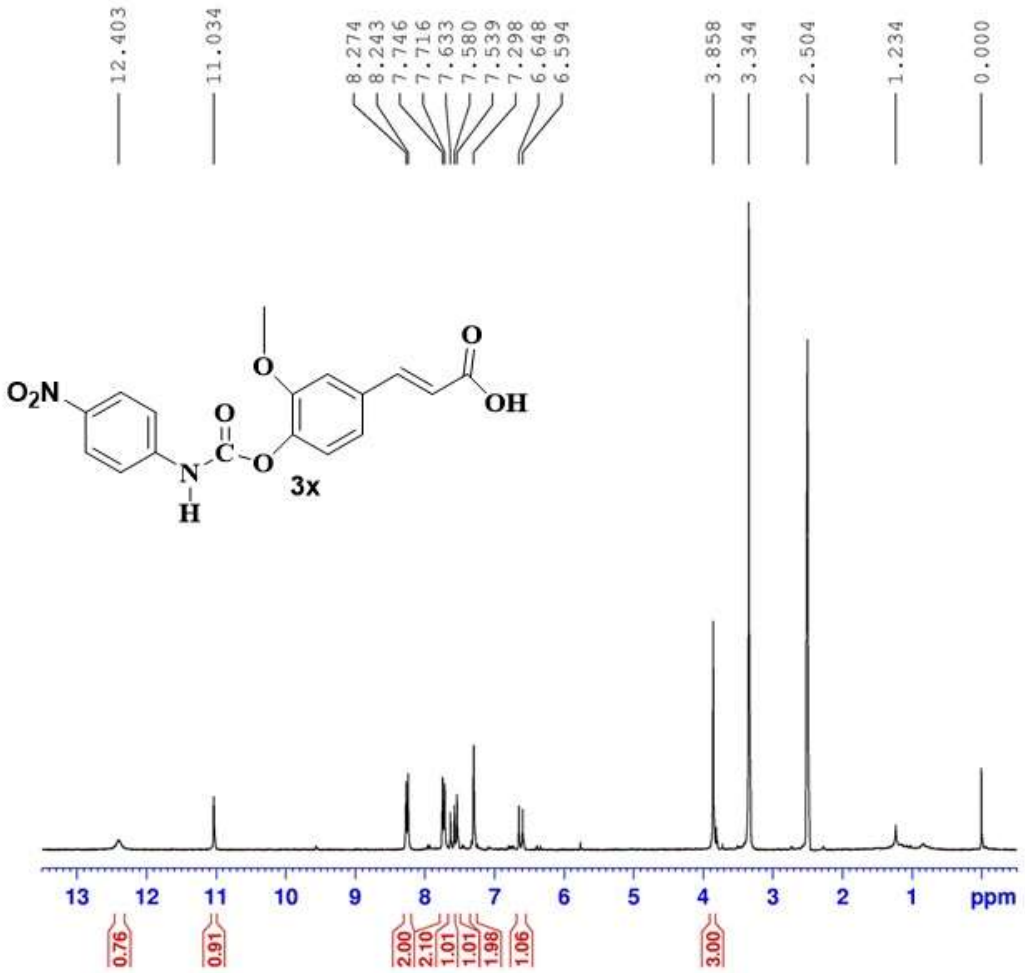

```
Current Data Parameters
NAME      1827C-FA+Cetane
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160602
Time               15.17
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1690
DS                    4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG                  228
DW               27.733 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              16.98 dB
PL13              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677509 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

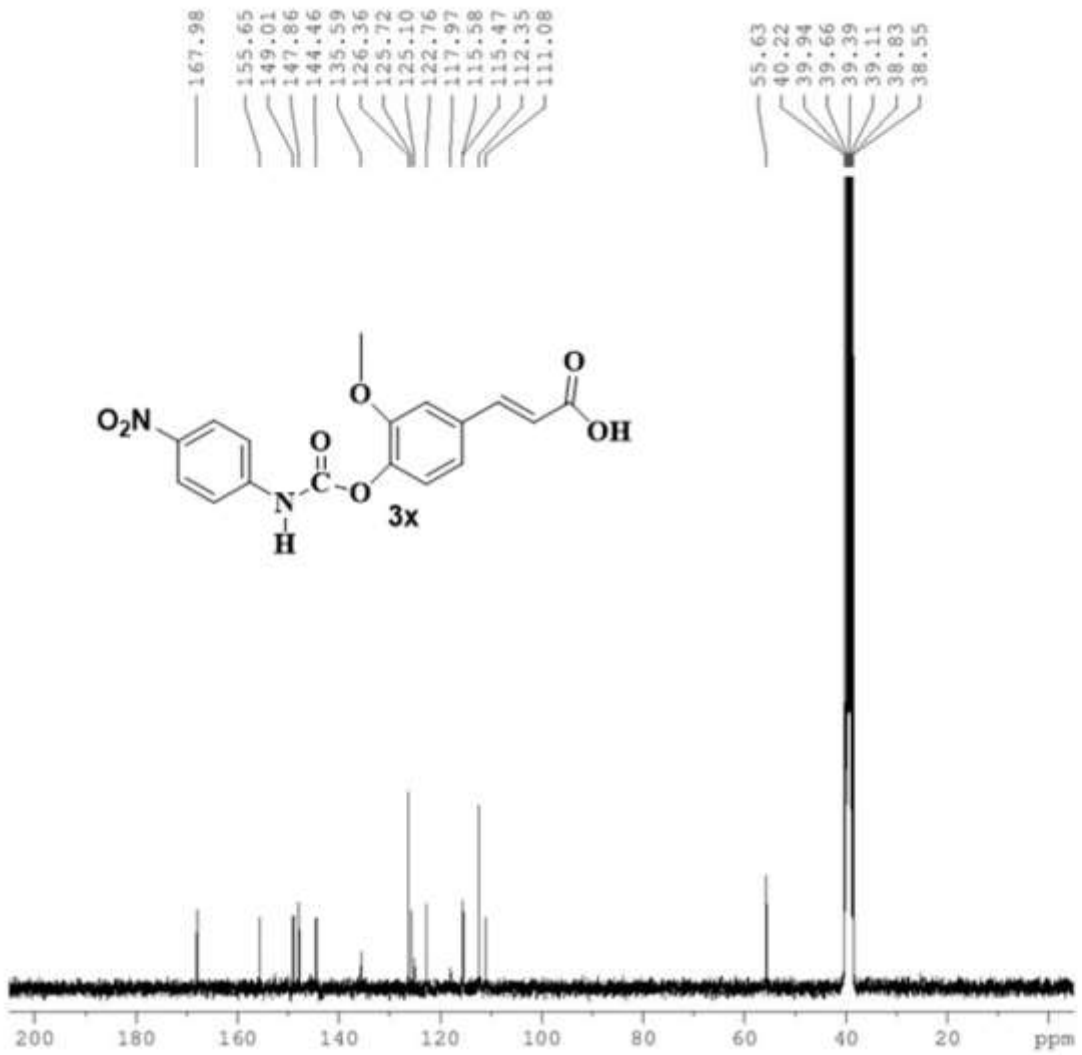



```
Current Data Parameters
NAME                  0717T
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150617
Time                  14.57
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                       362
DW                  80.800 usec
DE                   6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    8.60 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF            300.1299997 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```



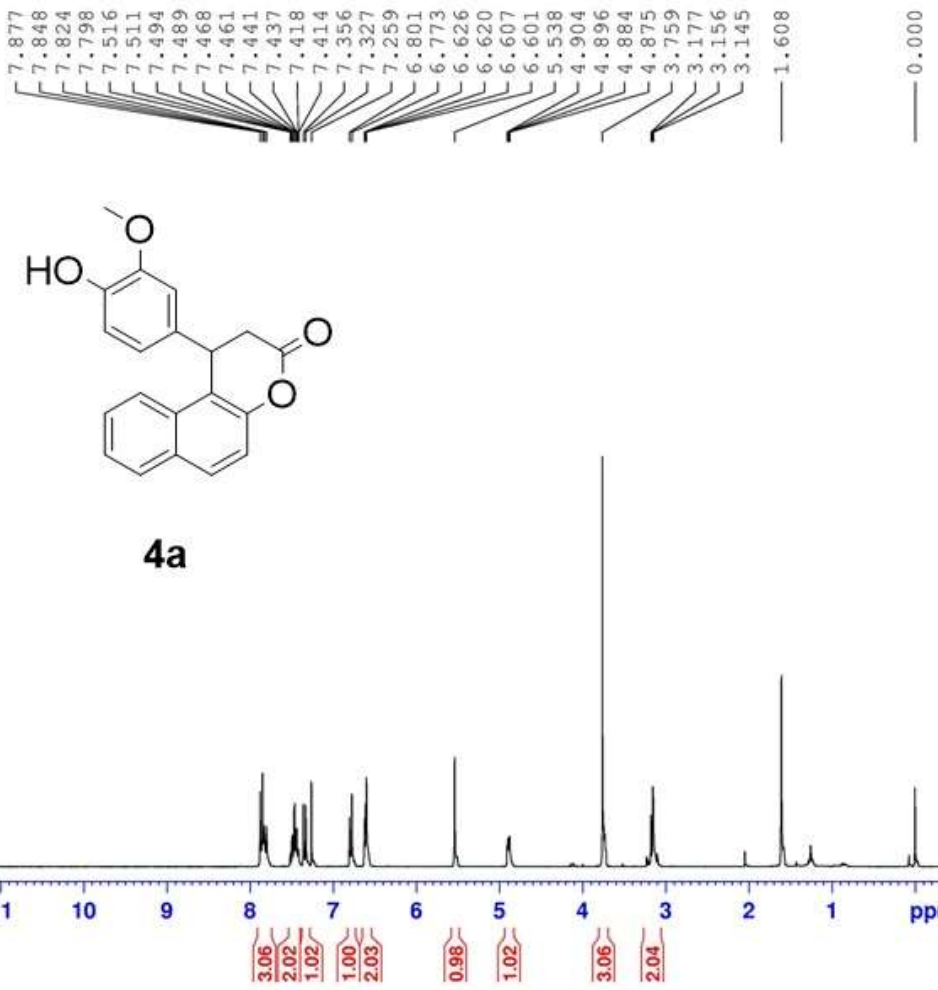

```
Current Data Parameters
NAME                  0778B
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150626
Time                   3.54
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                   10000
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175818 sec
RG                     256
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.50 usec
PL1                 0.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               17.37 dB
PL13               20.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF            75.4677867 MHz
WDW                      EM
SSB                       0
LB                  1.00 Hz
GB                        0
PC                     1.40
```

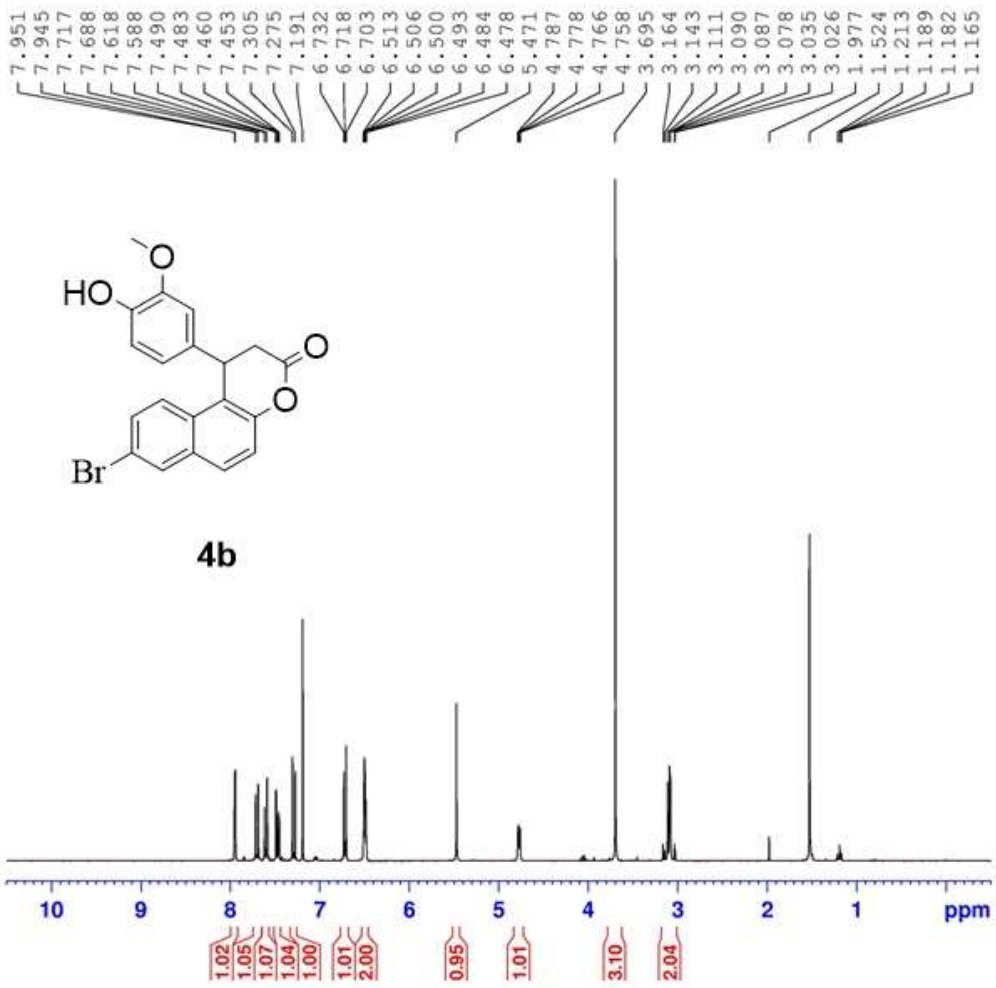



```
Current Data Parameters
NAME                  0667A
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150513
Time                 10.56
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                     256
DW                  80.800 usec
DE                   6.00 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                   1H
P1                   8.60 usec
PL1                 -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300066 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

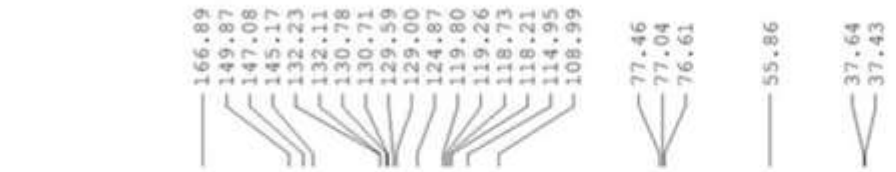


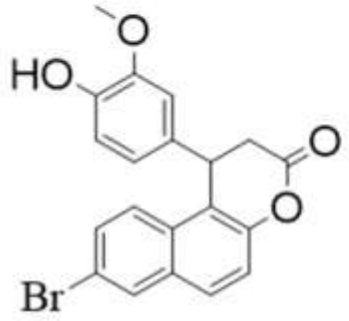

```
Current Data Parameters
NAME                  0852E2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20151016
Time                  10.32
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                       362
DW                  80.800 usec
DE                   6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    9.00 usec
PL1                  -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF            300.1300270 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```




**4b**



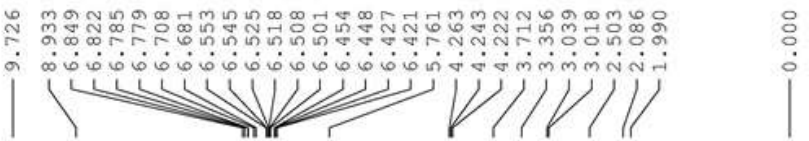

```
Current Data Parameters
NAME                  0852G-C13
EXPNO                         1
PROCNO                        1

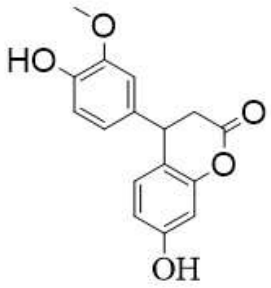
F2 - Acquisition Parameters
Date_              20151022
Time                  10.51
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       600
DS                         4
SWH               18028.846 Hz
FIDRES             0.275098 Hz
AQ                 1.8175818 sec
RG                       228
DW                    27.733 usec
DE                     6.00 usec
TE                    300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.00 usec
PL1                      0.00 dB
SFO1             75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   16.98 dB
PL13                   20.00 dB
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
```




**4c**

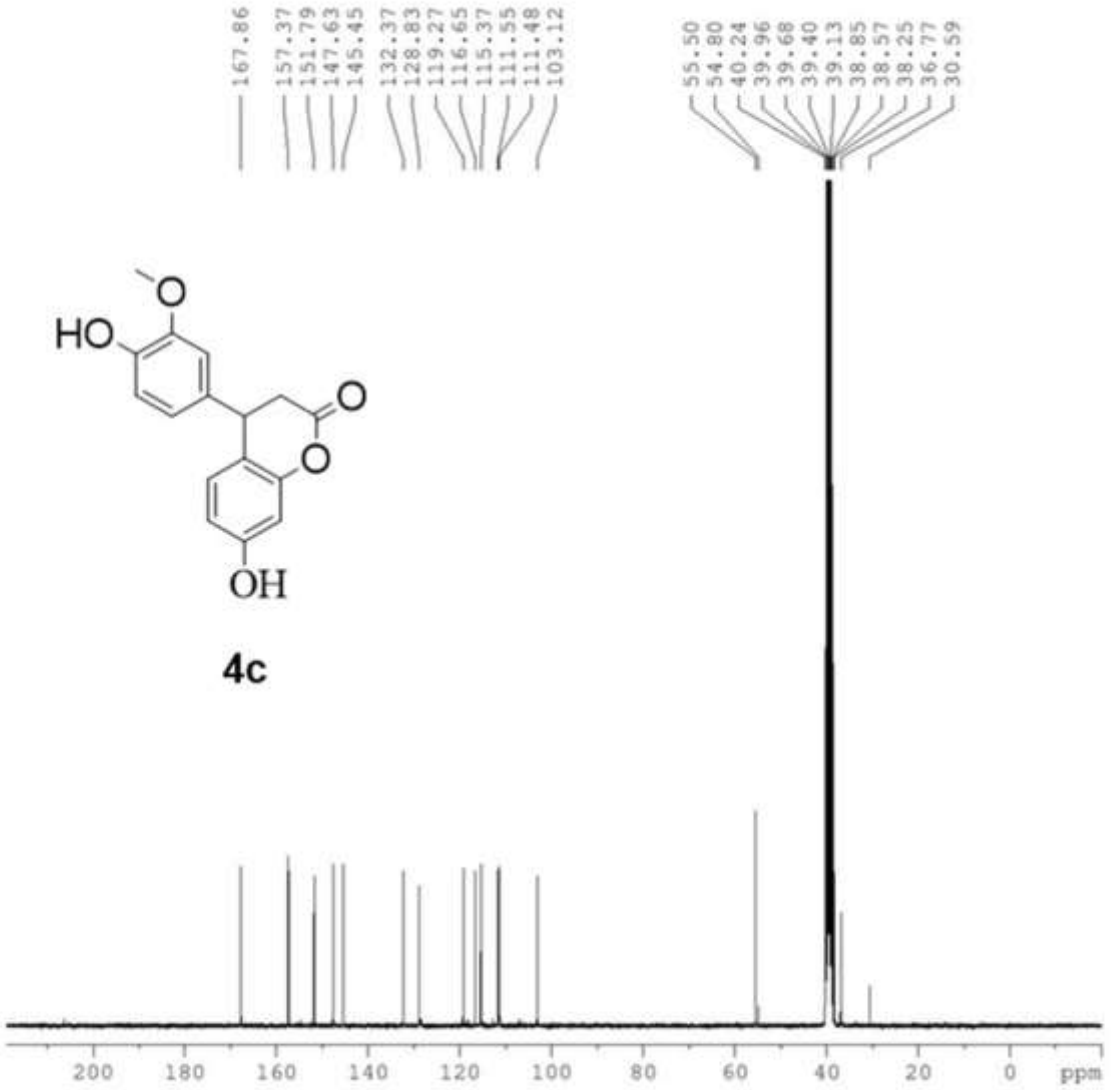



```
Current Data Parameters
NAME                  0667C-R
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150604
Time                  13.32
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                6188.119 Hz
FIDRES            0.094423 Hz
AQ                5.2953587 sec
RG                       256
DW                  80.800 usec
DE                   6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     8.60 usec
PL1                   -2.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF            300.1299997 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```




**4c**

```
Current Data Parameters
NAME                  0745BC
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150609
Time                  10.15
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                   18000
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175818 sec
RG                     256
DW                27.733 usec
DE                 6.00 usec
TE                 300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.50 usec
PL1                  0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -2.00 dB
PL12                17.37 dB
PL13                20.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF             75.4677916 MHz
WDW                    EM
SSB                    0
LB                   1.00 Hz
GB                     0
PC                   1.40
```

| Compound code | $IC_{50}$ value against K562 cells ( µg/mL) | $IC_{50}$ value against U937 cells ( µg/mL) | $IC_{50}$ value against HepG-2 cells ( µg/mL) | $IC_{50}$ value against Normal PBMC cells ( µg/mL) |
|---|---|---|---|---|
| 1 | >100 | 54.68 | 35.07 | 76.54 |
| 2 | >100 | 32.21 | >100 | >100 |
| 2a | >100 | >100 | >100 | >100 |
| 2b | >100 | >100 | >100 | >100 |
| 2c | >100 | >100 | >100 | >100 |
| 2d | >100 | >100 | >100 | >100 |
| 2e | >100 | >100 | >100 | >100 |
| 2f | >100 | 16.89 | >100 | >100 |
| 2h | **35** | 21.11 | 42.18 | 68.14 |
| 2i | **4.02** | **33.14** | **32.94** | 51.32 |
| 2j | **60** | >100 | 51.01 | 74.18 |
| 2k | >100 | >100 | >100 | >100 |
| 3 | >100 | >100 | >100 | >100 |
| 3a | >100 | >100 | >100 | >100 |
| 3b | >100 | >100 | >100 | >100 |
| 3d | >100 | >100 | >100 | >100 |
| 3e | >100 | 10.12 | 22.64 | >100 |
| 3f | >100 | >100 | >100 | >100 |
| 3g | >100 | >100 | >100 | >100 |
| 3h | >100 | >100 | >100 | >100 |
| 3i | >100 | >100 | >100 | >100 |
| 3j | **6.30** | **40.21** | **38.54** | 56.98 |
| 3k | >100 | >100 | >100 | >100 |
| 3l | >100 | >100 | >100 | >100 |
| 3m | >100 | >100 | >100 | >100 |
| 3n | >100 | >100 | >100 | >100 |
| 3o | >100 | >100 | >100 | >100 |
| 3p | >100 | >100 | >100 | >100 |
| 3q | >100 | >100 | >100 | >100 |
| 3r | >100 | >100 | >100 | >100 |
| 3s | >100 | >100 | >100 | >100 |
| 3t | >100 | >100 | >100 | >100 |
| 3u | >100 | 19.23 | 34.56 | 79.34 |
| 3v | >100 | >100 | >100 | >100 |
| 3w | >100 | >100 | >100 | >100 |
| 3x | >100 | >100 | >100 | >100 |
| 4a | >100 | >100 | >100 | >100 |
| 4b | >100 | >100 | >100 | >100 |
| 4c | >100 | >100 | >100 | >100 |
| Imatinib | 0.1 | | n.d | - |

**Table S1. *In vitro* anti-proliferative activity of Ferulic acid derivatives**