Supporting Information

Synthesis and evaluation of sulfonylnitrophenylthiazoles (SNPT's) as thyroid hormone receptor-coactivator interaction inhibitors

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Table of Contents

Supplementary, Table 1. Summary of SNPT analogues.

No	Registration No.	Purity (%)	Yield (%)	TRβ vs SRC2-2 (IC_{50}, μM)	TRα vs SRC2-2 (IC_{50}, μM)	PPARγ vs DRIP-2 (IC_{50}, μM)	Transcripion inhibition at 5 μM (%)	Cytotoxicity HepG2 (EC_{50}, μM)	Permeability $x10^6$ cm/s	Solubility (μM)
2_{4,1,5}_	SJ000561913-1	100.0	30.4	0.31±0.17	0.19±0.08	>60	8.1±0.6	>27	1322±159	6.4±0.3
2_{4,1,4}_	SJ000561912-1	99.6	25.7	0.66±0.57	0.1±0.01	>60	2.3±2.7	>27	791±101	1.6±0.9
2_{1,1,4}_	SJ000561848-1	100.0	59.0	1.3±0.6	2.4±1.3	>60	11.9±6.2	>27	287±17	5.0±0.7
2_{5,1,4}_	SJ000561889-1	98.3	66.7	1.9±0.3	1.6±0.4	>60	no inhibition	17.9±0.9	971±210	2.3±0.8
2_{3,1,4}_	SJ000561686-1	99.5	66.7	1.6±0.9	2.6±2.1	>60	11.6±1.3	11.2±0.6	657±43	50.1±1.1
2_{1,1,1}_	SJ000561846-1	100.0	62.2	1.7±0.9	1.1±0.6	>60	no inhibition	6.3±0.3	379±39	0.7±0.1
2_{2,1,4}_	SJ000561632-1	99.7	70.5	1.8±0.6	2.5±1.0	>60	9.8±6.0	10.6±0.5	280±42	18.0±0.9
2_{4,1,2}_	SJ000561920-1	99.7	26.7	2.1±1.6	0.43±0.14	>60	15.4±5.2	>27	8±1	1.0±0.8
2_{3,1,2}_	SJ000561696-1	99.2	72.8	2.4±1.1	2.5±1.2	>60	42.1±5.9	11.5±5.6	949±195	2.8±0.5
2_{4,1,16}_	SJ000561923-1	100.0	25.0	2.8±1.8	1.0±0.6	>60	26.0±2.0	>27	271±79	1.2±0.9
2_{4,1,5}_	SJ000561849-1	100.0	17.5	3.3±1.3	1.7±0.7	>60	5.8±7.1	>27	702±34	38.8±1.1
2_{4,1,14}_	SJ000561921-1	100.0	26.0	3.3±1.4	0.46±0.27	>60	17.9±4.7	>27	1499±536	1.2±0.7
2_{4,1,15}_	SJ000561922-1	100.0	29.2	3.4±2.5	0.3±0.1	>60	24.7±3.3	>27	221±21	0.8±0.1
2_{4,1,11}_	SJ000561918-1	100.0	30.8	4.2±2.9	1.1±1.2	>60	33.4±1.4	14.5±0.7	84±17	0.2±0.5
2_{4,1,9}_	SJ000561917-1	100.0	35.8	5.2±2.7	1.1±1.2	>60	17.5±6.8	>27	43±6	0.4±0.4
2_{2,1,2}_	SJ000561637-1	99.6	65.8	7.1±1.9	3.5±	>60	42.1±5.6	13.9±1.5	1416±41	5.7±1.0
2_{2,1,5}_	SJ000561633-1	99.6	68.1	7.4±3.4	5.6±2.7	>60	8.1±5.2	>27	912±205	6.7±0.4
3_{6,1,13}_	SJ000561764-1	98.2	57.3	8.2±2.0	4.7±1.7	>60	14.6±2.8	13.3±0.7	1619±260	2.4±0.1
2_{1,1,16}_	SJ000561860-1	100.0	36.8	8.5±4.4	3.2±1.1	30.2±9.6	26.7±2.6	>27	1031±288	2.4±0.4
2_{4,1,3}_	SJ000561911-1	100.0	31.3	10.1±4.5	0.77±0.54	>60	no inhibition	>27	376±42	23.3±0.6
2_{1,1,14}_	SJ000561858-1	100.0	57.7	10.9±2.6	3.0±1.6	42.6±10.9	15.4±3.9	>27	1187±200	3.8±0.1
2_{3,1,5}_	SJ000561687-1	99.4	69.1	11.5±9.1	n.d.	>60	27.1±6.6	>27	1394±345	34.8±0.3
2_{2,1,1}_	SJ000561525-1	100.0	33.0	11.8±4.5	n.d.	>60	17.7±2.3	6.2±0.5	245±53	1.1±0.4
2_{1,1,2}_	SJ000561857-1	100.0	69.6	15.3±9.1	n.d.	31.7±10.2	34.9±3.3	>27	1491±203	2.7±0.4
3_{6,1,1}_	SJ000561753-1	98.3	82.6	16.3±11.8	29.4±18.8	>60	33.1±4.9	>27	599±73	1.2±0.4
2_{2,2,4}_	SJ000561645-1	99.5	52.6	16.7±4.0	21.3±4.0	>60	4.9±3.6	>27	1500±163	2.8±2.1
2_{3,3,4}_	SJ000561732-1	100.0	53.2	19.3±9.6	30.4±15.1	>60	no inhibition	>27	548±109	0.6±0.2
2_{2,3,4}_	SJ000561665-1	98.4	50.4	20.0±11.4	n.d.	n.d.	n.d.	19.9±16.4	416±1	2.2±0.6
2_{2,1,15}_	SJ000561639-1	99.4	139.1	27.1±4.8	6.8±3.9	n.d.	n.d.	>27	n.d.	n.d.
3_{6,1,17}_	SJ000561769-1	99.3	70.5	27.4±9.8	4.9±2.5	n.d.	n.d.	>27	n.d.	n.d.
2_{3,2,4}_	SJ000561709-1	100.0	75.7	20.1±6.2	25.1±13.4	n.d.	n.d.	>27	1373±48	1.4±0.1
2_{4,1,8}_	SJ000561916-1	100.0	20.8	20.6±9.5	1.9±1.2	n.d.	n.d.	12.7±0.6	n.d.	n.d.
2_{2,1,14}_	SJ000561638-1	99.4	49.5	20.8±5.7	12.0±8.3	n.d.	n.d.	>27	822±84	3.9±0.2
2_{4,1,13}_	SJ000561856-1	100.0	24.1	21.0±2.8	3.0±0.9	n.d.	n.d.	14.6±2.4	598±119	1.1±0.3
3_{6,1,2}_	SJ000561765-1	99.0	75.7	21.8±8.0	13.9±7.4	n.d.	n.d.	5.9±1.3	2884±873	1.0±1.0
3_{6,1,14}_	SJ000561766-1	98.0	53.6	21.9±6.5	10.3±5.4	n.d.	n.d.	>27	1025±105	4.2±1.4
2_{3,1,15}_	SJ000561698-1	99.5	65.4	22.1±12.8	8.7±7.1	n.d.	n.d.	>27	1448±294	1.2±0.3
2_{1,1,15}_	SJ000561859-1	100.0	58.2	22.4±6.7	n.d.	n.d.	n.d.	>27	n.d.	n.d.
2_{4,1,1}_	SJ000561910-1	100.0	38.8	31.4±16.6	n.d.	n.d.	n.d.	>27	77±42	0.9±1.9
3_{6,1,12}_	SJ000561763-1	98.1	60.5	32.4±6.5	17.7±8.4	n.d.	n.d.	11.4±0.6	730±45	32.0±0.7
2_{4,1,6}_	SJ000561914-1	99.7	17.5	34.7±6.9	8.3±3.0	n.d.	n.d.	>27	921±117	59.4±1.2
2_{4,1,9}_	SJ000561852-1	100.0	59.1	35.4±8.3	16.3±10.9	n.d.	n.d.	>27	207±41	1.6±2.3
3_{6,1,4}_	SJ000561755-1	97.1	57.5	37.6±7.6	38.8±9.5	n.d.	n.d.	>27	253±5	51.4±1.2
2_{4,1,7}_	SJ000561915-1	100.0	50.4	39.3±8.1	1.2±0.5	n.d.	n.d.	13.2±0.7	n.d.	n.d.
3_{6,1,16}_	SJ000561768-1	98.6	87.7	39.9±7.9	20.8±5.9	n.d.	n.d.	>27	1174±159	3.3±1.0
2_{1,1,3}_	SJ000561847-1	100.0	50.0	40.5±9.8	22.2±	n.d.	n.d.	>27	40±4	15.8±0.7
3_{6,1,15}_	SJ000561767-1	98.1	78.6	43.6±9.8	21.6±7.3	n.d.	n.d.	>27	1179±45	3.5±0.4
2_{2,1,13}_	SJ000561636-1	98.4	20.9	44.3±15.7	17.2±10.2	n.d.	n.d.	4.6±1.5	n.d.	n.d.
2_{4,1,19}_	SJ000561925-1	99.4	21.1	45.5±24.5	22.6±14.7	n.d.	n.d.	>27	23±5	0.8±0.6
2_{2,1,11}_	SJ000561527-1	100.0	37.0	45.9±12.0	30.8±12.1	n.d.	n.d.	>27	991±277	2.0±0.3
2_{2,2,5}_	SJ000561646-1	99.5	83.9	54.4±14.6	62.6±33.9	n.d.	n.d.	>27	1315±145	2.5±0.7
2_{5,1,5}_	SJ000561890-1	99.0	89.6	59.5±30.3	32.5±12.0	n.d.	n.d.	>27	253±129	n.d.

IC_{50} values were determined using data from two independent experiments in triplicate. EC_{50}, solubility and PAMPA were determined from an triplicate experiment. *nd: not determined

Experimental Section

Compound evaluation

Protein expression and purification. hTRβ LBD (His_6; residues T209-D461) was expressed in BL21 (DE3) (Invitrogen) (10 × 1L culture) at 20 °C, 0.5 mM isopropyl-1-thio-b-D-galactopyranoside added at A_{600} = 0.6 (17). When the A_{600} reached 4, cells were harvested, resuspended in 20 ml of buffer/1 liter of culture (20 mM Tris, 300 mM NaCl, 0.025% Tween 20, 0.10 mM phenylmethylsulfonyl fluoride, 10 mg of lysozyme, pH 7.5), incubated for 30 min on ice, and then sonicated for 3 × 3 min on ice. The lysed cells were centrifuged at 100,000 × *g* for 1 h, and the supernatant was loaded onto Talon resin (20 ml, Clontech). Protein was eluted with 500 mM imidazole (3 × 5 ml) plus ligand (3,3′,5-triiodo-L-thyronine (Sigma)). Protein purity (>90%) was assessed by SDS-PAGE and high pressure size exclusion chromatography, and protein concentration was measured by the Bradford protein assay. The protein was dialyzed overnight against assay buffer (3 × 4 liters, 50 mM sodium phosphate, 150 mM NaCl, pH 7.2, 1 mM dithiothreitol, 1 mM EDTA, 0.01% Nonidet P-40, 10% glycerol). hTRα LBD (His_6; residues Glu^{148}-Val^{410}) was expressed using the same procedure as hTRβ with the exception that 0.5 mM isopropyl-1-thio-β-D-galactopyranoside was added at A_{600} = 1.2. Unliganded protein was eluted with 100 mM imidazole.

Human PPARγ (hPPARγ) was expressed and purified following the procedure above using the following modifications. Cultures were grown up and induced at 22 °C for the same amount of time as above. Induction was obtained with 500 µM of isopropyl-β-D-thiogalactoside. Buffer 1 contained 20 mM Tris (pH 7.5), 100 mM NaCl, 0.5 mM PMSF, 0.5% Triton X-100, and 10 mg/L lysozyme. Buffer 2 contained 20 mM Tris (pH 7.5), 100 mM NaCl, 1 mM imidazole, and 5 mM dithiothreitol (DTT). Buffer 3 contained 20 mM Tris (pH 7.5), 100 mM NaCl, 5 mM DTT, and 1 mM imidazole and was used to wash the beads 7 times instead of 5. Buffer 4 was not necessary in the purification of hPPARγ. Buffer 5 contained 20 mM Tris (pH 7.5), 100 mM NaCl, 5 mM DTT, and 250 mM imidazole. Buffer 6 contained 50 mM Tris (pH 8.0), 25 mM KCl, 2 mM DTT, and 10% glycerol. PPARγ does not require any ligand to remain stable in buffer 6.

Peptidesynthesis and labeling. SRC2-2 peptide was synthesized and purified by reverse phase HPLC in the Hartwell Center (St. Jude Children's Research Hospital). Texas Red- or fluorescein- maleimide (Molecular Probes) fluoroprobes were conjugated to the N-terminal cysteine of SRC2-2 peptide.

Compound transfer. Compounds were transferred to assay plates by a pin tool equipped with 100 H pins (V&P Scientific).

Fluorescence polarization assay: For the TRβ and TexasRed-SRC2-2 assay, all liquid handling was performed on a Biomek FX (Beckman Coulter). Compounds were serially diluted from 10,000 to 5 µM in DMSO into a 384-well plate (Costar). Using a pin tool, 260 nL compound was transferred to 20 µL of assay buffer (20 mM Tris (pH 7.4), 100 mM NaCl, 1 mM EDTA, 1 mM DTT, 10% glycerol, 0.01% NP-40, 1 µM T3, 0.6 µM hTR-LBD, 20 nM of Texas Red labeled SRC2-2 peptide, 4% DMSO) in a black 384-well assay plate (Corning). After a 3 h equilibration, fluorescence polarization was measured using an EnVision (PerkinElmer) plate reader. Two independent experiments, in triplicate, were carried out for each compound. The β-aminoketone SJ-1 (DHPPA, [3-dibutylamino]-1-(4-hexylphenyl)propan-1-one), a known thyroid hormone receptor antagonist, was used as a positive control.

Hormone displacement assay. Hormone displacement assay-All liquid handling was carried out using an automated liquid handling system (Biomek FX, Beckman Coulter, Fullerton, CA). To each well of a 384-well Ni-chelate-coated FlashplateR (PerkinElmer) was added 50 µL of 5 µM hTRβ-LBD in assay buffer (50 mM HEPES, 100 mM NaCl, 1 mM DTT, 0.1% bovine serum albumin (BSA), 10% glycerol, and 0.01% Triton X-100 (pH 7.2)). After two hours incubation, the protein solution was discarded, followed eventually by washes with assay buffer. Then, 25 µL of serial diluted small molecules in assay buffer containing 10% DMSO was added into each well followed by addition of 25 µL of 2 nM [125-I]-T3 solution in assay buffer. The final assay solution contained 5% DMSO. The plates were sealed with clear tape (MilliporeR tape multiscreen) and allowed to equilibrate for 3 h at room temperature. Radiocounts were measured using a TopCount Microplate Scintillation and Luminescence Counter (Packard Instrument Company, Meriden, CT). All data were analyzed using GraphPad Prism 4.03 (GraphPad Software, San Diego, CA); IC50 values were obtained by fitting data to the following equation: (sigmoidal dose response (variable slope)): y = bottom + (top – bottom)/(1 + 10^((LogIC50 – x)*Hillslope)), where x is the logarithm of concentration, and y is the response. Two independent experiments, in triplicates, were carried out for each compound.

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Transcription assay. HEK 293 (ATCC) cells were cultured in DMEM containing 10% FBS and maintained in 5% CO_2 at 37 ^oC. T3 (30 nM) was used as a positive control in all assays. HEK 293 cells were plated at 8 x 10^6 cells/dish (approximately 40-60 % confluence) in 100 mm culture dishes in 10 mL of DMEM/F 12 (1:1 mixture, Hyclone Laboratories) containing 2.5 mM L-glutamine and 10% heat inactivated charcoal stripped serum (Hyclone Laboratories). After a 6 h incubation, 460 µL of transfection mixture containing 5µg CMV-TRβ plasmid, 15 µg DR4 (AGGTCAcaggAGGTCA)-TRE-firefly luciferase reporter plasmid, 1.25 µg TK-Renilla luciferase control reporter plasmid (Promega) and 64 µL Fugene6 (Roche) was added and the cells incubated overnight. Cells were trypsinized and added to 96-well plates (Corning) at 4 x 10^4 cells/well in 75 µL DMEM/F 12 medium. Six hours after plating, serially diluted compounds in 25 µL of DMEM/F12 medium were added to the cell culture medium. After incubation for18 h, Dual-Glo (Promega) detection reagent was added and luminescence was measured using an EnVision (PerkinElmer) plate reader. TRE-mediated luciferase activity was normalized by *Renilla* luciferase activity. The inhibition data was normalized to basal expression (treated with DMSO only) and fully induced expression (treated with T3 solution in DMSO). Two experiments, in triplicate, were carried out for each compound.

Cytotoxicity assay. HepG2 (ATCC) cells were grown to 80% confluence, collected and plated at 700 cells/well in 25 µL media per well in 384-well plates (Costar 3712). Compounds were diluted and transferred to cells as described above and the plates incubated for 72 h at 37º C in 5% CO_2. CellTiter-Glo (Promega) detection reagent was added following the manufacturer's instructions and luminescence was measured using an EnVision (PerkinElmer) plate reader.

RNA extraction and real time. HepG2 cells were split into 6 well plates at a density of 1 X 10^6 cells $well^{-1}$ in DMEM/F-12 media with 10% CSS. Twenty four hours later, the cells were treated with T3 or a combination of T3 with **compound**. 24 hours after treatment, cells were harvested for RNA using RNA Stat-60, following the manufacturer's instructions. The resulting RNA was treated with DNase I (Invitrogen, Cat. No. 18068-015) to remove contaminating genomic DNA. Then RNA was cleaned up using Qiagen RNeasy Mini (Qiagen), following the manufacturer's instructions. Equal quantities of RNA were then reserve transcribed using Superscript III (Invitrogen), following the manufacturer's instructions. The resulting cDNA was diluted 1:50 in nuclease free water and used in real time PCR reactions with the Quantifast master mix (Qiagen) in an ABI 7900 HT. The following primers were used: 18S primer mix from Qiagen (cat# QT00199367), PEPCK, forward: ACGGATTCACCCTACGTGGT, reverse: CCCCACAGAATGGAGGCATTT. MMP11 real time PCR assay was ordered from Qiagen (cat. No. QT00024031). The expression of target genes was normalized to the expression of the 18S subunit of the ribosome. The PCR quantization was carried out using ΔΔCt method and data was expressed as fold change over DMSO treated controls.

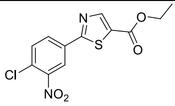
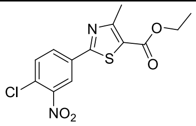
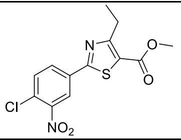
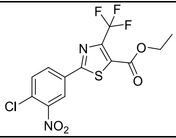
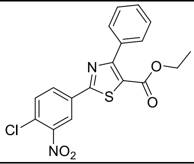
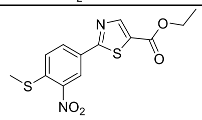
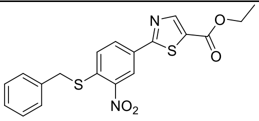
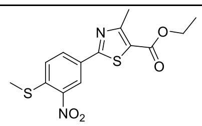
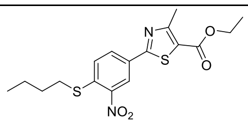
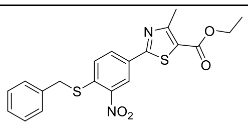
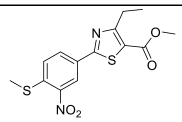
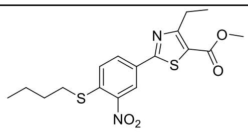
Solubility. The solubility assay was carried out on Biomek FX lab automation workstation (Beckman Coulter, Inc.). Ten µL of compound stock was added to 190 µL 1-propanol to make a reference stock plate. Five µL from this reference stock plate was mixed with 70 µL 1-propanol and 75 µL phosphate buffered saline (PBS, pH 7.4) to make the reference plate and the UV spectrum (250 – 500 nm) of the reference plate was measured using a SPECTRAmax PLUS plate reader (Molecular Devices). Six µL of 10 mM test compound stock was added to 600 µL PBS in a 96-well storage plate and mixed. The storage plate was sealed and incubated at room temperature for 18 h. The suspension was then filtered through a 96-well filter plate (pION Inc.). Seventy five µL of filtrate was mixed with 75 µL 1-propanol to make the sample plate for UV spectroscopic analysis. A single experiment was performed in triplicate for each compound. Solubility was calculated using uSOL Evolution software based on the AUC (area under the curve) of the UV spectrum of the sample plate and the reference plate.

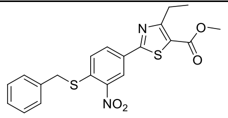
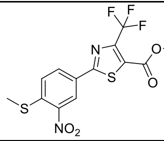
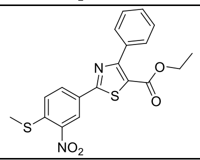
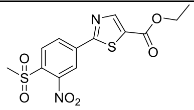
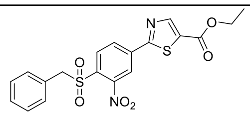
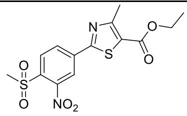
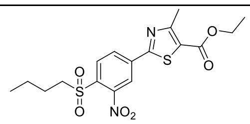
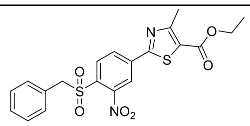
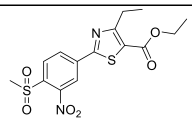
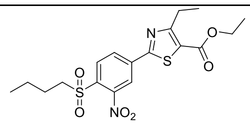
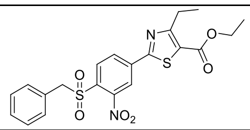
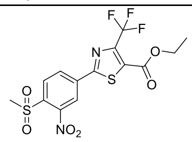
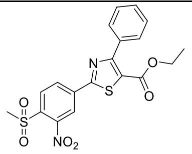
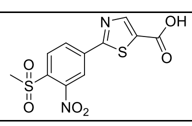
Permeability assay. The Parallel Artificial Membrane Permeability Assay (PAMPA) was carried out on a Biomek FX lab automation workstation (Beckman Coulter, Inc.). Three µL of test compound stock (10 mM in DMSO) was mixed with 600 µL of SSB (system solution buffer, pH 7.4 or 4, pION Inc.) to dilute the test compound. One hundred fifty µL of diluted test compound in SSB was transferred to a UV plate (pION Inc.) and the UV spectrum was measured on a SPECTRAmax PLUS plate reader (Molecular Devices) to establish a reference plate. The membrane on a pre-loaded PAMPA sandwich (pION Inc.) was painted with 4 µL GIT lipid (pION Inc.). The acceptor chamber was then filled with 200 µL ASB (acceptor solution buffer, pION Inc.) and the donor chamber was filled with 180 µL test compound diluted in SSB. The PAMPA sandwich (donor and acceptor chamber) was assembled, placed on the Gut-box (pION Inc.) and stirred for 30 minutes. The Aqueous Boundary Layer was set to 40 µM for stirring and the UV spectrum (250-500 nm) of the donor and the acceptor chambers were read. A single experiment was performed in triplicate for each compound. The permeability coefficient was calculated using PAMPA Evolution 96 Command software (pION Inc.) based on the AUC of the reference, donor, and acceptor plates.

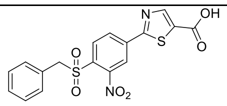
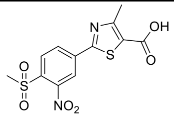
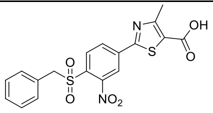
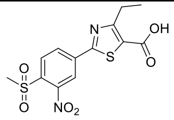
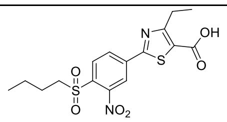
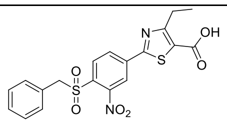
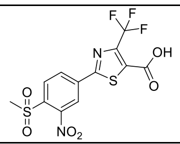
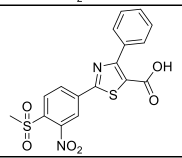
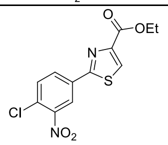
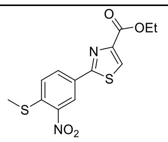
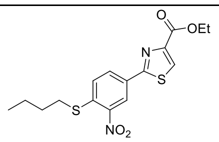
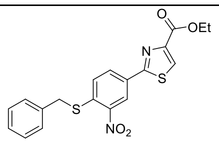
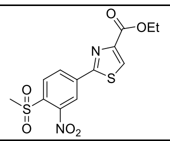
Data Analysis. Curves were fit to Titration-response data using GraphPad Prism 4.03 (GraphPad Software). IC_{50} values were obtained by fitting data to the following equation: (sigmoidal dose response (variable slope)): y = bottom + (top –bottom)/(1 + 10^((LogIC_{50} – x)*Hill slope)), where x is the logarithm of concentration and y is the response.

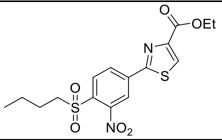
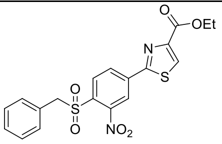
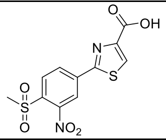
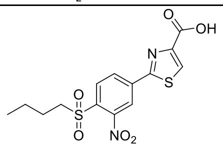
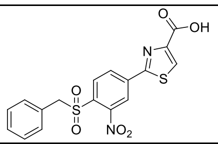
NMR data

Intermediates.

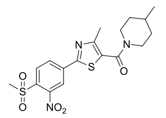
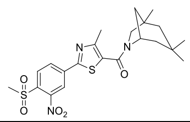
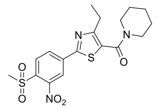
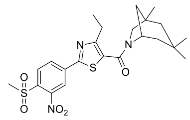
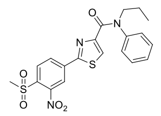
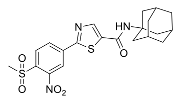
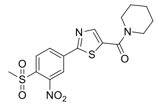
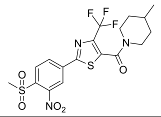
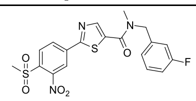
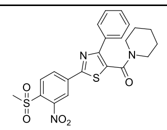
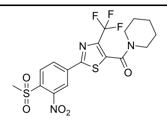
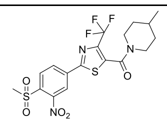
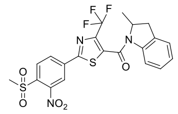
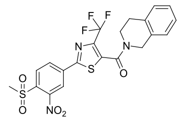
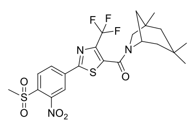
8{*1*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.51 (d, *J* = 2.1 Hz, 1H), 8.45 (s, 1H), 8.10 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, CDCl$_3$) δ 168.67, 160.86, 149.35, 132.83, 132.76, 130.82, 130.62, 129.30, 123.58, 62.08, 14.31.
8{*2*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.48 (d, *J* = 2.1 Hz, 1H), 8.07 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.66 – 7.56 (m, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.79 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, CDCl$_3$) δ 165.26, 161.77, 161.40, 148.40, 132.88, 132.63, 130.53, 129.00, 123.54, 123.44, 61.65, 17.48, 14.33.
8{*3*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.49 (d, *J* = 2.1 Hz, 1H), 8.08 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 3.91 (s, 3H), 3.21 (q, *J* = 7.5 Hz, 2H), 1.35 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 167.31, 165.62, 162.01, 148.40, 132.98, 132.59, 130.60, 128.96, 123.47, 122.44, 77.36, 77.05, 76.73, 52.43, 24.39, 13.58.
8{*4*}		^{1}H NMR (400 MHz, DMSO) δ 8.69 (d, *J* = 2.2 Hz, 1H), 8.34 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.98 – 7.94 (m, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 166.58, 157.96, 148.12, 144.93 (q, $^{2}J_{CF}$= 37.4 Hz), 132.82, 131.55, 131.30, 131.04, 128.10, 123.50, 119.60 (q, $^{1}J_{CF}$= 273.7 Hz),, 62.83, 13.78.
8{*5*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.54 (d, *J* = 2.1 Hz, 1H), 8.14 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.85 – 7.76 (m, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.52 – 7.42 (m, 3H), 4.32 (q, *J* = 7.1 Hz, 2H), 1.32 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, CDCl$_3$) δ 165.29, 161.08, 161.04, 148.43, 133.48, 132.77, 132.66, 130.65, 129.93, 129.60, 129.21, 127.92, 124.02, 123.53, 61.93, 14.13.
9{*1,1*}		JYD82^{1}H NMR (400 MHz, CDCl$_3$) δ 8.75 (d, *J* = 2.0 Hz, 1H), 8.21 (dd, *J* = 8.6, 2.0 Hz, 1H), 8.15 (s, 1H), 7.39 (d, *J* = 8.6 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.50 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 169.38, 160.42, 149.21, 145.09, 141.92, 131.42, 129.31, 128.44, 127.63, 123.27, 15.38, 14.11.
9{1,*3*}		^{1}H NMR (400 MHz, DMSO) δ 8.74 (d, *J* = 2.0 Hz, 1H), 8.55 (s, 1H), 8.28 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.41 – 7.35 (m, 2H), 7.35 – 7.28 (m, 1H), 4.47 (s, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 169.25, 160.41, 149.20, 145.24, 140.20, 135.17, 131.30, 129.43, 129.28, 128.88, 128.71, 128.47, 127.65, 123.27, 61.72, 36.09, 14.10.
9{*2,1*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.86 (d, *J* = 2.0 Hz, 1H), 8.18 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.47 (d, *J* = 8.6 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.82 (s, 3H), 2.59 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, CDCl$_3$) δ 166.45, 161.97, 161.33, 145.54, 142.27, 130.91, 129.48, 126.22, 124.11, 122.61, 61.51, 17.53, 16.16, 14.36.
9{*2,2*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.78 (d, *J* = 2.0 Hz, 1H), 8.11 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.47 (d, *J* = 8.5 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.06 – 2.97 (m, 2H), 2.79 (s, 3H), 1.85 – 1.69 (m, 2H), 1.54 (dt, *J* = 14.5, 7.4 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H), 0.99 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.49, 161.97, 161.30, 145.95, 141.50, 130.64, 129.40, 126.94, 124.09, 122.56, 61.50, 32.16, 29.78, 22.26, 17.52, 14.36, 13.68.
9{*2,3*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.79 (d, *J* = 2.0 Hz, 1H), 8.10 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.53 (d, *J* = 8.6 Hz, 1H), 7.44 (d, *J* = 7.0 Hz, 2H), 7.42 – 7.30 (m, 3H), 4.37 (q, *J* = 7.2 Hz, 2H), 4.26 (s, 2H), 2.78 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, CDCl$_3$) δ 166.34, 161.94, 161.30, 145.74, 140.87, 134.46, 130.81, 129.84, 129.07, 128.98, 128.01, 127.28, 124.02, 122.68, 61.51, 37.63, 17.51, 14.35.
9{*3,1*}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.84 (d, *J* = 2.0 Hz, 1H), 8.17 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.45 (d, *J* = 8.6 Hz, 1H), 3.91 (s, 3H), 3.21 (q, *J* = 7.5 Hz, 2H), 2.56 (s, 3H), 1.38 – 1.31 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 167.26, 166.79, 162.21, 145.55, 142.22, 131.02, 129.58, 126.21, 124.14, 121.50, 52.34, 24.42, 16.16, 13.62.
9{*3*,2}		^{1}H NMR (400 MHz, CDCl$_3$) δ 8.79 (d, *J* = 2.0 Hz, 1H), 8.12 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.48 (d, *J* = 8.6 Hz, 1H), 3.91 (s, 3H), 3.21 (q, *J* = 7.5 Hz, 2H), 3.05 – 2.96 (m, 2H), 1.76 (dt, *J* = 15.0, 7.4 Hz, 2H), 1.54 (dt, *J* = 14.6, 7.4 Hz, 2H), 1.35 (t, *J* = 7.5 Hz, 3H), 0.99 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 167.24, 166.84, 162.21, 145.98, 141.43, 130.75, 129.52, 126.93, 124.12, 121.46, 32.17, 30.96, 29.80, 24.42, 22.26, 13.68, 13.61.

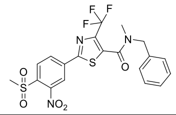
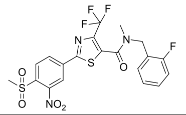
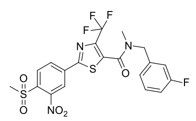
9{*3,3*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 2.0 Hz, 1H), 8.09 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.53 (d, *J* = 8.6 Hz, 1H), 7.46 – 7.42 (m, 2H), 7.39 – 7.28 (m, 3H), 4.26 (s, 2H), 3.91 (s, 3H), 3.20 (q, *J* = 7.5 Hz, 2H), 1.35 (t, *J* = 7.5 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 167.23, 166.69, 162.18, 145.73, 140.82, 134.47, 130.90, 129.94, 129.05, 128.97, 128.00, 127.26, 124.05, 121.57, 37.62, 30.96, 24.41, 13.61.
9{*4,1*}		[1]H NMR (400 MHz, DMSO) δ 8.77 (d, *J* = 2.1 Hz, 1H), 8.33 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.63 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 4H).
9{*5,1*}		[1]H NMR (400 MHz, DMSO) δ 8.79 (s, 1H), 8.33 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 3.6 Hz, 2H), 7.74 (d, *J* = 8.6 Hz, 1H), 7.50 (s, 3H), 4.26 (q, *J* = 6.9 Hz, 2H), 2.62 (s, 3H), 1.24 (t, *J* = 7.0 Hz, 3H).
10{*1,1*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 8.48 (t, *J* = 3.6 Hz, 1H), 8.34 – 8.26 (m, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 3.47 (s, 3H), 1.42 (dd, *J* = 9.0, 5.2 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 167.33, 160.59, 149.73, 149.61, 139.11, 135.25, 132.47, 132.13, 130.04, 122.83, 62.30, 45.17, 14.29.
10{*1,3*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.43 (d, *J* = 1.7 Hz, 1H), 8.00 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.38 – 7.28 (m, 5H), 4.84 (s, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 167.42, 160.59, 149.98, 149.54, 138.80, 133.90, 132.96, 132.06, 131.05, 129.34, 129.08, 128.96, 127.19, 122.47, 62.85, 62.28, 14.28.
10{*2,1*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.24 – 8.18 (m, 2H), 4.32 (q, *J* = 7.1 Hz, 2H), 3.40 (s, 3H), 2.74 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 163.91, 161.77, 161.53, 149.71, 139.21, 134.99, 132.37, 129.87, 124.90, 122.70, 61.87, 45.18, 17.50, 14.32.
10{*2,2*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 1.6 Hz, 1H), 8.26 (dd, *J* = 8.2, 1.6 Hz, 1H), 8.20 (d, *J* = 8.2 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.62 – 3.53 (m, 2H), 2.81 (s, 3H), 1.81 (m, 2H), 1.55 – 1.44 (m, 2H), 1.41 (t, *J* = 7.1 Hz, 3H), 0.96 (t, *J* = 7.3 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 164.02, 161.73, 161.54, 149.94, 139.05, 133.88, 133.14, 129.57, 124.84, 122.67, 61.85, 56.56, 24. 58, 21.59, 17.49, 14.32, 13.53.
10{*2,3*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 1.7 Hz, 1H), 7.97 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.63 – 7.57 (m, 1H), 7.35 – 7.27 (m, 5H), 4.83 (s, 2H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.79 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H).[13]C NMR (101 MHz, $CDCl_3$) δ 164.01, 161.66, 161.50, 149.95, 138.89, 133.80, 132.65, 131.04, 129.31, 128.94, 127.23, 124.84, 122.32, 62.85, 61.84, 17.46, 14.31.
10{*3,1*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 2.1 Hz, 1H), 8.08 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 3.91 (s, 3H), 3.21 (q, *J* = 7.5 Hz, 2H), 1.35 (t, *J* = 7.5 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 167.63, 164.30, 161.78, 149.70, 139.30, 134.96, 132.34, 129.94, 123.80, 122.75, 52.61, 45.18, 24.40, 13.56.
10{*3,2*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 1.6 Hz, 1H), 8.27 (dd, *J* = 8.2, 1.7 Hz, 1H), 8.20 (d, *J* = 8.2 Hz, 1H), 3.93 (s, 3H), 3.63 – 3.53 (m, 2H), 3.23 (q, *J* = 7.5 Hz, 2H), 1.81 (m, 2H), 1.55 – 1.43 (m, 2H), 1.36 (t, *J* = 7.5 Hz, 3H), 0.96 (t, *J* = 7.3 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 167.60, 164.41, 161.79, 149.93, 139.14, 133.83, 133.13, 129.64, 123.74, 122.71, 56.56, 52.59, 24.62, 24.40, 21.58, 13.55, 13.54.
10{*3,3*}		[1]H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 2.1 Hz, 1H), 8.08 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 3.91 (s, 3H), 3.21 (q, *J* = 7.5 Hz, 2H), 1.35 (t, *J* = 7.5 Hz, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 167.54, 164.39, 161.76, 149.95, 138.97, 133.80, 132.65, 131.04, 129.31, 128.99, 128.94, 127.24, 123.74, 122.37, 62.84, 52.58, 24.38, 13.55.
10{*4,1*}		[1]H NMR (400 MHz, $CDCl_3$) δ [1]H NMR (400 MHz, $CDCl_3$) δ 8.50 – 8.44 (m, 1H), 8.33 (d, *J* = 1.0 Hz, 2H), 4.49 – 4.42 (m, 2H), 3.48 (s, 3H), 1.43 (t, *J* = 7.1 Hz, 3H).[13]C NMR (101 MHz, $CDCl_3$) δ 164.81, 158.28, 149.80, 147.55 (q, $^{2}J_{CF}$= 39.4 Hz), 137.85, 136.03, 132.65, 130.22, 122.90, 119.45 (q, $^{1}J_{CF}$= 274.7 Hz), 63.33, 45.17, 13.99.
10{*5,1*}		[1]H NMR (400 MHz, $CDCl_3$) [1]H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 1.6 Hz, 1H), 8.35 (dd, *J* = 8.2, 1.7 Hz, 1H), 8.32 – 8.27 (m, 1H), 7.85 – 7.77 (m, 2H), 7.52 – 7.46 (m, 3H), 4.34 (q, *J* = 7.1 Hz, 2H), 3.47 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H).[13]C NMR (101 MHz, $CDCl_3$) δ 164.00, 161.41, 160.82, 149.73, 139.07, 135.19, 133.19, 132.40, 130.02, 129.93, 129.79, 128.00, 125.32, 122.79, 62.16, 45.18, 14.12.
11{*1,1*}		[1]H NMR (400 MHz, DMSO) δ 8.67 (d, *J* = 1.8 Hz, 1H), 8.58 (s, 1H), 8.55 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.28 – 8.25 (m, 1H), 3.54 (s, 3H); [13]C NMR (101 MHz, DMSO) δ 167.26, 161.67, 149.08, 148.86, 138.18, 133.88, 133.17, 132.34, 130.46, 122.44, 44.43

11{*1*,*3*}		^{1}H NMR (400 MHz, DMSO) δ 8.69 (d, *J* = 1.8 Hz, 1H), 8.57 (s, 1H), 8.40 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.82 – 7.77 (m, 1H), 7.42 – 7.33 (m, 3H), 7.30 (m, 2H), 4.99 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 167.15, 161.66, 149.24, 149.08, 138.33, 133.21, 131.73, 131.19, 129.82, 129.00, 128.67, 127.23, 122.52, 61.68.
11{*2*,*2*}		^{1}H NMR (400 MHz, DMSO) δ 8.63 (d, *J* = 1.8 Hz, 1H), 8.50 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.20 (d, *J* = 8.3, 1H), 3.62 (dd, *J* = 14.8, 7.0 Hz, 3H), 2.72 (s, 3H), 1.73 – 1.61 (m, 2H), 1.48 – 1.34 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 163.78, 162.51, 159.93, 149.14, 138.20, 132.93, 132.27, 130.14, 125.85, 122.38, 55.35, 23.96, 20.77, 16.99, 13.33.
11{*2*,*3*}		^{1}H NMR (400 MHz, DMSO) δ 8.64 (d, *J* = 1.8 Hz, 1H), 8.35 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.77 (d, *J* = 8.3 Hz, 1H), 7.41 – 7.33 (m, 3H), 7.33 – 7.27 (m, 2H), 4.98 (s, 2H), 2.71 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 163.68, 162.50, 159.93, 149.23, 138.24, 133.19, 131.60, 131.18, 129.63, 128.99, 128.66, 127.24, 125.89, 122.34, 61.68, 16.98.
11{*3*,*1*}		^{1}H NMR (400 MHz, DMSO) δ 8.69 (d, *J* = 1.8 Hz, 1H), 8.58 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.31 (d, *J* = 8.3 Hz, 1H), 3.60 (s, 3H), 3.22 (q, *J* = 7.5 Hz, 3H), 1.35 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 165.33, 164.07, 162.35, 148.86, 138.18, 133.76, 132.31, 130.31, 125.37, 122.25, 44.45, 23.51, 13.55.
11{3,2}		^{1}H NMR (400 MHz, DMSO) δ 8.64 (d, *J* = 1.7 Hz, 1H), 8.50 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.21 (d, *J* = 8.3 Hz, 1H), 3.66 – 3.58 (m, 3H), 3.15 (q, *J* = 7.5 Hz, 3H), 1.72 – 1.62 (m, 2H), 1.48 – 1.34 (m, 2H), 1.28 (t, *J* = 7.5 Hz, 3H), 0.88 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 165.33, 164.06, 162.35, 149.14, 138.30, 132.93, 132.21, 130.16, 125.39, 122.38, 55.37, 23.99, 23.51, 20.77, 13.55, 13.32.
11{*3*,*3*}		^{1}H NMR (400 MHz, DMSO) δ 8.65 (d, *J* = 1.8 Hz, 1H), 8.36 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.81 – 7.72 (m, 1H), 7.41 – 7.31 (m, 3H), 7.31 – 7.26 (m, 2H), 4.98 (s, 2H), 3.18 – 3.09 (m, 3H), 1.28 (m, 3H). ^{13}C NMR (101 MHz, DMSO) δ 165.34, 163.96, 162.34, 149.23, 138.32, 133.19, 131.57, 131.17, 129.65, 128.99, 128.66, 127.27, 125.43, 122.33, 61.69, 23.50, 13.55.
11{*4*,*1*}		^{1}H NMR (400 MHz, DMSO) δ 8.69 (d, *J* = 1.8 Hz, 1H), 8.57 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.29 (d, *J* = 8.3 Hz, 1H), 3.55 (s, 3H).
11{*5*,*1*}		^{1}H NMR (400 MHz, DMSO) δ 8.70 (d, *J* = 1.8 Hz, 1H), 8.57 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.29 – 8.24 (m, 1H), 7.86 – 7.80 (m, 2H), 7.53 – 7.45 (m, 3H), 3.54 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 163.80, 161.77, 159.24, 148.87, 138.09, 133.87, 133.33, 132.31, 130.48, 129.90, 129.26, 127.78, 126.69, 122.41, 44.45.
13{*6*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 1.7 Hz, 1H), 8.25 (s, 1H), 8.16 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 4.47 (q, *J* = 7.1 Hz, 2H), 2.24 – 2.11 (m, 2H), 1.44 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 164.64, 160.99, 148.79, 148.36, 132.64, 132.61, 130.77, 128.91, 128.19, 123.60, 61.86, 14.37.
14{*6*,*1*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 2.0 Hz, 1H), 8.27 (dt, *J* = 6.4, 3.2 Hz, 1H), 8.21 (s, 1H), 7.46 (d, *J* = 8.6 Hz, 1H), 4.47 (q, *J* = 7.1 Hz, 2H), 2.57 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.72, 161.16, 148.49, 145.43, 142.14, 131.21, 129.26, 127.56, 126.22, 124.25, 61.76, 16.14, 14.38.
14{*6*,*2*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 2.0 Hz, 1H), 8.25 – 8.21 (m, 1H), 8.21 (s, 1H), 7.51 – 7.46 (m, 1H), 4.46 (q, *J* = 7.1 Hz, 2H), 3.06 – 2.98 (m, 2H), 1.76 (dt, *J* = 14.9, 7.3 Hz, 2H), 1.60 – 1.49 (m, 2H), 1.45 (t, *J* = 7.1 Hz, 3H), 0.99 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.76, 161.17, 148.47, 145.85, 141.34, 130.95, 129.22, 127.53, 126.96, 124.24, 32.15, 30.96, 29.78, 22.25, 14.38, 13.69.
14{*6*,*3*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 2.0 Hz, 1H), 8.23 – 8.16 (m, 2H), 7.58 – 7.50 (m, 1H), 7.46 – 7.41 (m, 2H), 7.38 – 7.28 (m, 3H), 4.46 (q, *J* = 7.1 Hz, 2H), 4.26 (s, 2H), 1.44 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.60, 161.13, 148.49, 145.64, 140.68, 134.46, 131.09, 129.63, 129.08, 128.96, 127.99, 127.61, 127.32, 124.13, 37.61, 30.96, 14.38.
15{*6*,*1*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 1.7 Hz, 1H), 8.38 – 8.31 (m, 2H), 8.31 – 8.19 (m, 1H), 4.48 (q, *J* = 7.1 Hz, 2H), 3.47 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.51, 160.78, 149.71, 149.33, 138.93, 134.96, 132.34, 130.08, 129.27, 122.86, 45.18, 30.96, 14.36.

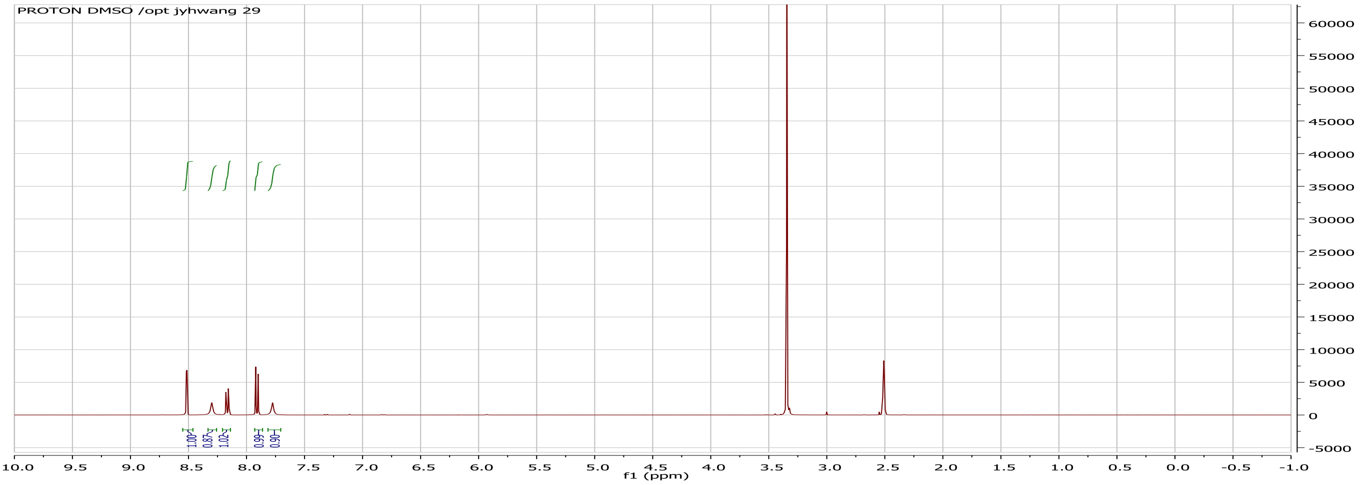
15{*6,2*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 1.7 Hz, 1H), 8.33 (m, 2H), 8.23 – 8.20 (m, 1H), 4.48 (q, *J* = 7.1 Hz, 2H), 3.64 – 3.50 (m, 2H), 1.87 – 1.73 (m, 2H), 1.48 (m, 5H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.60, 160.79, 149.91, 149.27, 138.80, 133.78, 133.10, 129.81, 129.29, 122.81, 61.99, 56.55, 24.55, 21.57, 14.36, 13.53.
15{*6,3*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 1.7 Hz, 1H), 8.32 (s, 1H), 8.04 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.62 – 7.58 (m, 1H), 7.32 – 7.23 (m, 6H), 4.83 (s, 2H), 4.52 – 4.40 (m, 3H), 1.49 – 1.40 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.60, 160.76, 149.89, 149.22, 138.60, 133.77, 132.51, 130.99, 129.32, 129.22, 129.17, 128.93, 127.23, 122.51, 62.83, 62.00, 14.33.
16{*6,1*}		^{1}H NMR (400 MHz, DMSO) δ 13.37 (s, 1H), 8.72 (s, 1H), 8.63 (d, *J* = 1.8 Hz, 1H), 8.52 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.26 (d, *J* = 8.3 Hz, 1H), 3.54 (s, 3H).^{13}C NMR (101 MHz, DMSO) δ 163.23, 161.68, 148.86, 148.68, 138.33, 133.50, 132.33, 131.56, 130.20, 122.26, 44.47.
16{*6,2*}		^{1}H NMR (400 MHz, DMSO) δ 13.36 (s, 1H), 8.72 (s, 1H), 8.64 (d, *J* = 1.6 Hz, 1H), 8.51 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.23 (d, *J* = 8.3 Hz, 1H), 3.68 – 3.57 (m, 2H), 1.75 – 1.61 (m, 2H), 1.49 – 1.36 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 4H).^{13}C NMR (101 MHz, DMSO) δ 163.23, 161.68, 149.14, 148.67, 138.45, 132.95, 131.96, 131.60, 130.07, 122.39, 55.37, 23.98, 20.78, 13.33.
16{*6,3*}		^{1}H NMR (400 MHz, DMSO) δ 13.26 (s, 1H), 8.63 (s, 1H), 8.56 (d, *J* = 1.8 Hz, 1H), 8.27 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.72 – 7.67 (m, 1H), 7.31 – 7.25 (m, 3H), 7.24 – 7.18 (m, 2H), 4.90 (s, 2H).^{13}C NMR (101 MHz, DMSO) δ 163.15, 161.66, 149.23, 148.65, 138.48, 133.22, 131.66, 131.27, 131.18, 129.56, 128.98, 128.65, 127.30, 126.46, 122.35, 61.69.

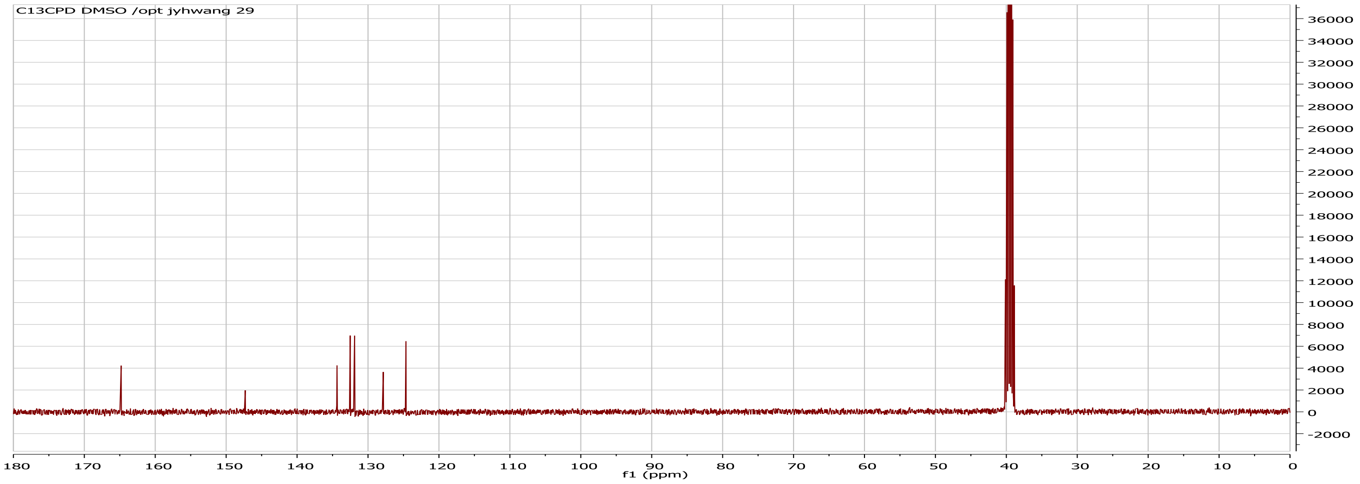
Final products.

2{*2,1,5*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 1.6 Hz, 1H), 8.31 – 8.18 (m, 2H), 4.23 (br, 2H), 3.46 (s, 3H), 2.92 (brs, 2H), 2.52 (s, 3H), 1.84 – 1.69 (m, 3H), 1.16 (t, *J* = 23.1 Hz, 2H), 1.00 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.62, 161.23, 153.55, 149.70, 139.35, 134.42, 132.32, 129.57, 128.23, 122.37, 45.18, 34.28, 31.05, 21.62, 16.39. LC/MS (ESI) *m/z* 424.28 $[M+H]^+$
2{*2,1,2*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.26 (m, 2H), 4.61 (s, 0.5H), 4.14 (t, *J* = 4.1 Hz, 0.5H), 3.67 (d, *J* = 12.5 Hz, 0.5), 3.46 (s, 3H), 3.43 (d, *J* = 10.2 Hz, 0.5H), 3.27 (dd, *J* = 15.5, 5.1 Hz, 1H), 2.60 (d, *J* = 7.8 Hz, 1.5H), 2.57 (s, 1.5H), 2.28 – 2.18 (m, 0.5H), 1.89 – 1.75 (m, 1H), 1.74 – 1.55 (m, 2H), 1.55 – 1.29 (m, 3.5H), 1.10 (m, 6H), 0.98 (d, *J* = 7.6 Hz, 3H). LC/MS (ESI) *m/z* 478.32 $[M+H]^+$
2{*3,1,4*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 1.5 Hz, 1H), 8.28 – 8.13 (m, 2H), 3.76 – 3.48 (m, 4H), 3.46 (s, 3H), 2.81 (t, *J* = 7.5 Hz, 2H), 1.81 – 1.57 (m, 7H), 1.36 (t, *J* = 7.5 Hz, 3H). LC/MS (ESI) *m/z* 424.28 $[M+H]^+$
2{*3,1,2*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 0.9 Hz, 1H), 8.28 – 8.21 (m, 2H), 4.61 (s, 0.5H), 4.11 (m, 0.5H), 3.66 (d, *J* = 12.5 Hz, 0.5H), 3.46 (s, 3H), 3.42 (d, *J* = 10.0 Hz, 0.5H), 3.30 – 3.19 (m, 1H), 2.97 – 2.82 (m, 2H), 2.22 (d, *J* = 10.7 Hz, 0.5H), 1.88 – 1.74 (m, 1H), 1.70 – 1.27 (m, 8H), 1.10 (m, 6H), 0.98 (d, *J* = 6.8 Hz, 3H). LC/MS (ESI) *m/z* 492.37 $[M+H]^+$
3{*6,1,13*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.2 Hz, 1H), 7.99 (s, 1H), 7.85 (t, *J* = 11.9 Hz, 1H), 7.78 (s, 1H), 7.40 – 7.28 (m, 3H), 7.16 (d, *J* = 7.0 Hz, 2H), 3.96 – 3.87 (m, 2H), 3.42 (s, 3H), 2.17 (s, 2H), 1.77 – 1.66 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). LC/MS (ESI) *m/z* 446.24 $[M+H]^+$
2{*1,1,1*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 0.7 Hz, 1H), 8.30 – 8.18 (m, 2H), 8.14 (s, 1H), 5.78 (s, 1H), 3.46 (s, 3H), 2.18 – 2.10 (m, 9H), 1.73 (s, 5H). LC/MS (ESI) *m/z* 462.1 $[M+H]^+$
2{*1,1,4*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 0.6 Hz, 1H), 8.33 – 8.22 (m, 2H), 8.05 (s, 1H), 3.70 (s, 4H), 3.47 (s, 3H), 1.80 – 1.72 (m, 2H), 1.72 – 1.64 (m, 4H). LC/MS (ESI) *m/z* 396.25 $[M+H]^+$
2{*4,1,5*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (dd, *J* = 4.7, 4.2 Hz, 1H), 8.31 – 8.21 (m, 2H), 8.05 (s, 1H), 4.40 (br, 2H), 3.47 (s, 3H), 3.13 (br, 2H), 1.83 – 1.65 (m, 3H), 1.33 – 1.16 (m, 2H), 1.02 (d, *J* = 6.4 Hz, 3H). LC/MS (ESI) *m/z* 478.26 $[M+H]^+$
2{*1,1,16*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 8.33 – 8.22 (m, 2H), 8.18 (s, 1H), 7.37 (s, 1H), 7.15 – 6.96 (m, 3H), 4.78 (s, 2H), 3.47 (s, 3H), 3.21 (s, 3H), 2.17 (s, 3H). LC/MS (ESI) *m/z* 450.22 $[M+H]^+$
2{*5,1,4*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.46 (m, 1H), 8.32 – 8.24 (m, 2H), 7.80 (dt, *J* = 8.5, 2.3 Hz, 2H), 7.50 – 7.41 (m, 3H), 3.70 (s, 2H), 3.47 (s, 3H), 3.08 (s, 2H), 1.66 – 1.46 (m, 2H), 1.05 (s, 2H). LC/MS (ESI) *m/z* 472.31 $[M+H]^+$
2{*4,1,4*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 1.6 Hz, 1H), 8.33 – 8.29 (m, 1H), 8.28 – 8.25 (m, 1H), 3.79 – 3.70 (m, 2H), 3.47 (s, 3H), 3.35 – 3.30 (m, 2H), 1.71 (s, 4H), 1.59 (s, 2H). LC/MS (ESI) *m/z* 464.21 $[M+H]^+$
2{*4,1,5*}	 -	^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 1.6 Hz, 1H), 8.31 (d, *J* = 8.2 Hz, 1H), 8.27 (dd, *J* = 8.2, 1.7 Hz, 1H), 4.68 (d, *J* = 13.2 Hz, 1H), 3.54 (d, *J* = 13.1 Hz, 1H), 3.47 (s, 3H), 3.19 – 3.07 (m, 1H), 2.92 – 2.76 (m, 1H), 1.81 (d, *J* = 13.5 Hz, 1H), 1.77 – 1.63 (m, 2H), 1.34 – 1.10 (m, 2H), 1.00 (d, *J* = 6.3 Hz, 3H). LC/MS (ESI) *m/z* 478.26 $[M+H]^+$
2{*4,1,9*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 1.0 Hz, 1H), 8.35 – 8.28 (m, 2H), 8.23 (br, 0.3H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.08 (br, 1.7H), 6.04 (s, 0.5H), 5.06 (s, 0.5H), 4.41 (s, 0.7H), 3.48 (s, 4.3H), 2.71 (d, *J* = 15.9 Hz, 1H), 1.32 (m, 3H). LC/MS (ESI) *m/z* 512.23 $[M+H]^+$
2{*4,1,11*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 1.5 Hz, 1H), 8.30 (m, 2H), 7.29 – 7.12 (m, 3.6H), 6.96 (d, *J* = 7.2 Hz, 0.41H), 4.94 (s, 1.2H), 4.52 (s, 0.8H), 4.03 (t, *J* = 6.0 Hz, 0.8H), 3.64 (t, *J* = 5.8 Hz, 1.2H), 3.48 (s, 3H), 3.01 (t, *J* = 5.8 Hz, 0.8H), 2.91 (t, *J* = 5.6 Hz, 1.2H). LC/MS (ESI) *m/z* 512.23 $[M+H]^+$
2{*4,1,2*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 – 8.40 (m, 1H), 8.36 – 8.25 (m, 2H), 4.71 – 4.61 (m, 0.4H), 3.96 (t, *J* = 4.1 Hz, 0.6H), 3.78 – 3.73 (m, 0.5H), 3.70 – 3.61 (m, 0.5H), 3.48 (s, 3H), 3.31 – 3.18 (m, 0.6H), 3.08 (d, *J* = 9.1 Hz, 0.4H), 1.87 – 1.73 (m, 1H), 1.66 – 1.35 (m, 4H), 1.35 – 1.24 (m, 1H), 1.16 (s, 2H), 1.10 (m, 4H), 0.99 (d, *J* = 12.3 Hz, 3H). LC/MS (ESI) *m/z* 532.29 $[M+H]^+$

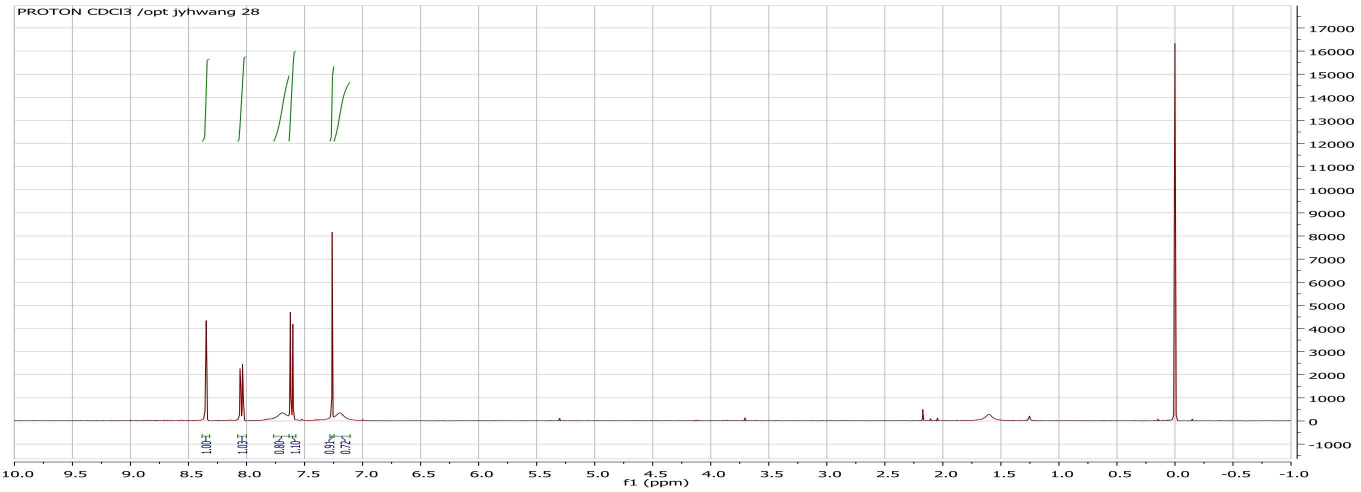
2{*4,1,14*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (dd, *J* = 19.5, 1.3 Hz, 1H), 8.35 – 8.19 (m, 2H), 7.43 – 7.28 (m, 4H), 7.14 (d, *J* = 7.1 Hz, 1H), 4.78 (s, 1.2H), 4.50 (s, 0.8H), 3.50 – 3.44 (m, 3H), 3.07 (s, 1H), 2.88 (s, 2H). LC/MS (ESI) *m/z* 500.28 $[M+H]^+$
2{*4,1,15*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 – 8.38 (m, 1H), 8.33 – 8.22 (m, 2H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.39 – 7.29 (m, 1H), 7.23 – 7.15 (m, 1H), 7.15 – 7.04 (m, 1H), 4.85 (s, 1.2H), 4.54 (s, 0.8H), 3.48 (s, 3H), 3.07 (s, 1H), 2.94 (s, 2H). LC/MS (ESI) *m/z* 518.24 $[M+H]^+$
2{*4,1,16*}		^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 1.4 Hz, 0.6H), 8.39 (s, 0.4H), 8.28 (m, 2H), 7.40 – 7.30 (m, 1H), 7.12 (d, *J* = 7.7 Hz, 0.7H), 7.09 – 7.02 (m, 1.6H), 6.90 (m, 0.7H), 4.77 (s, 1.3H), 4.50 (s, 0.7H), 3.47 (s, 3H), 3.10 (s, 1H), 2.91 (s, 2H). LC/MS (ESI) *m/z* 518.24 $[M+H]^+$

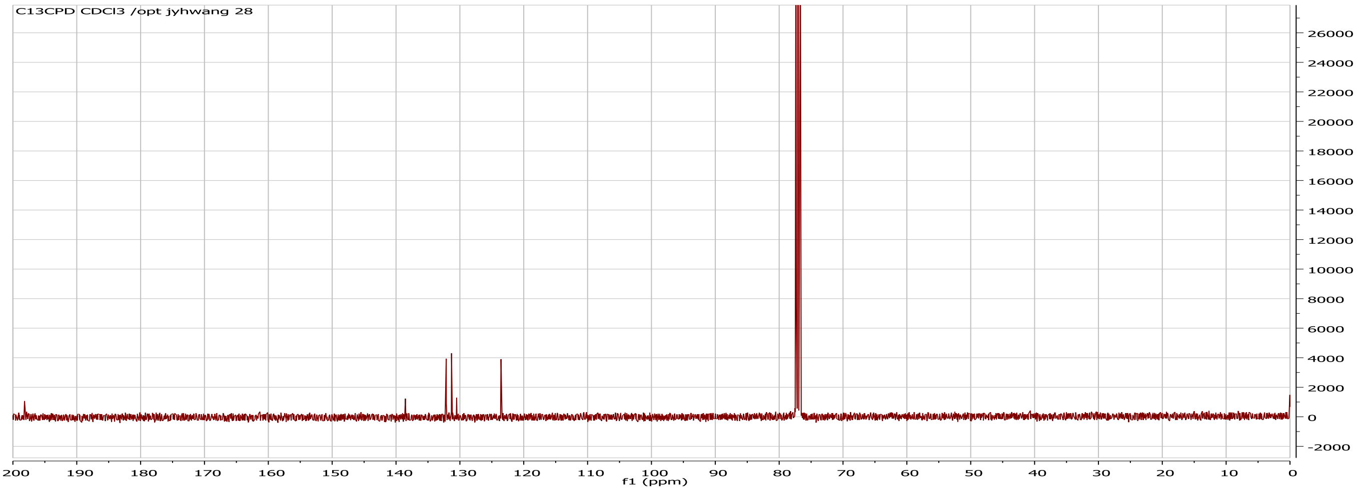
Compound 5



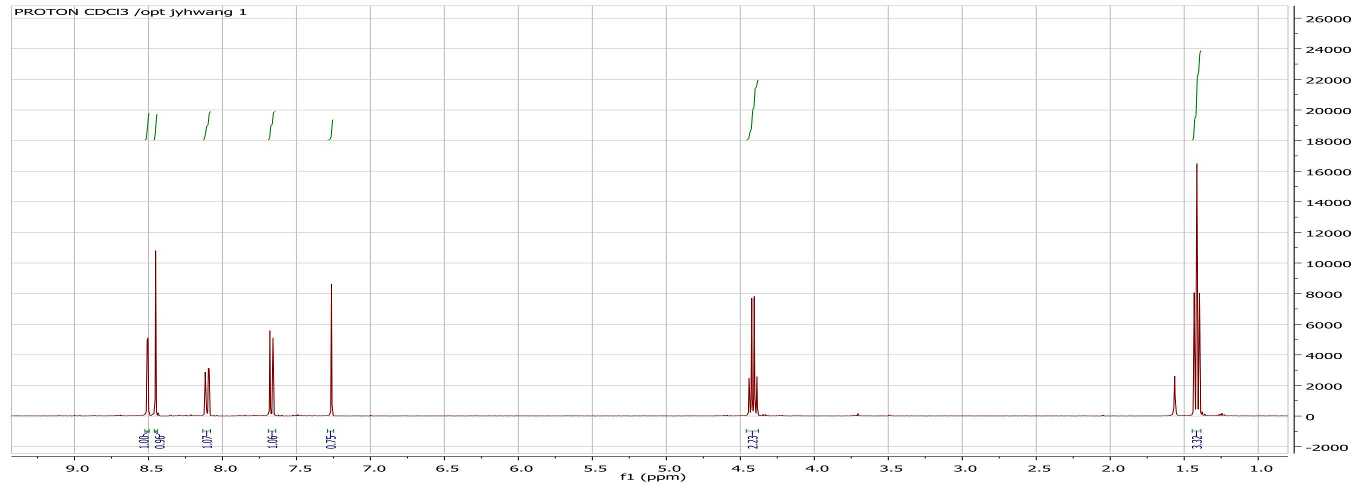


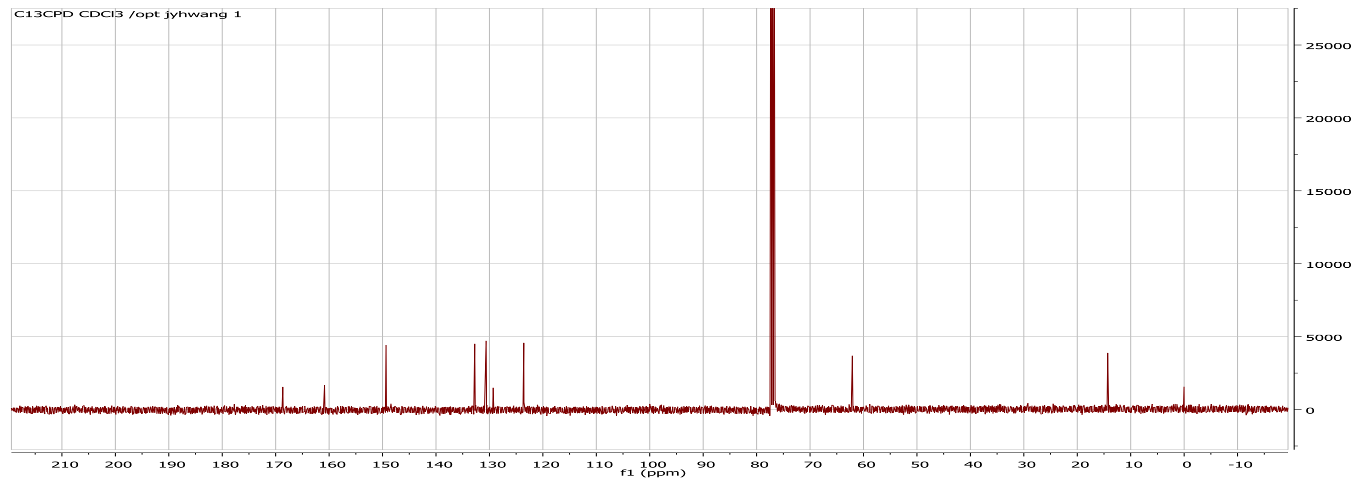
Comound 6



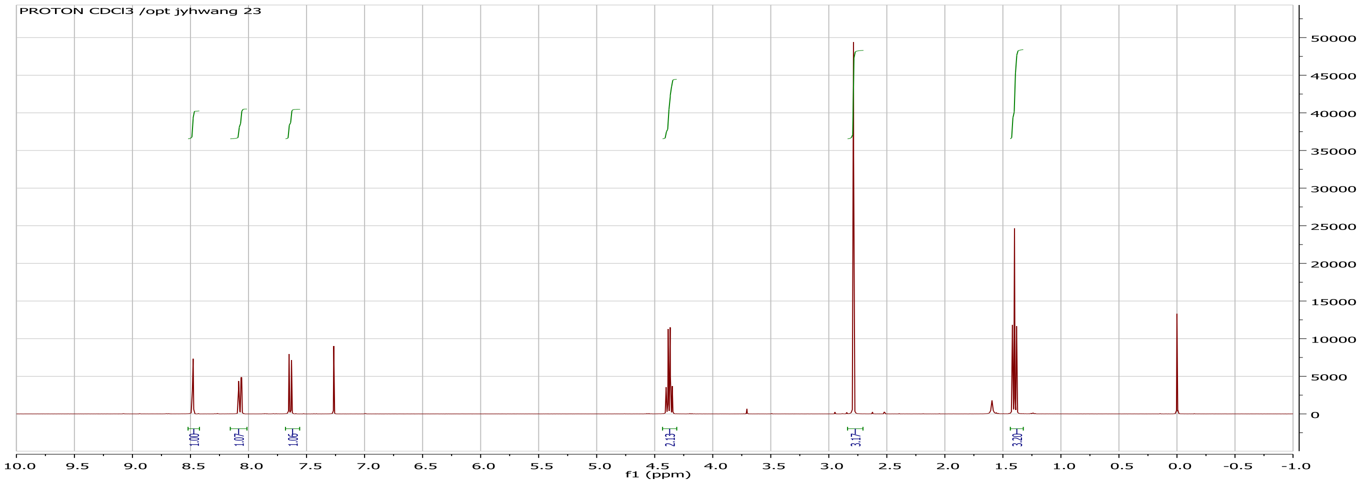

C13CPD CDCl3 /opt jyhwang 28
f1 (ppm)

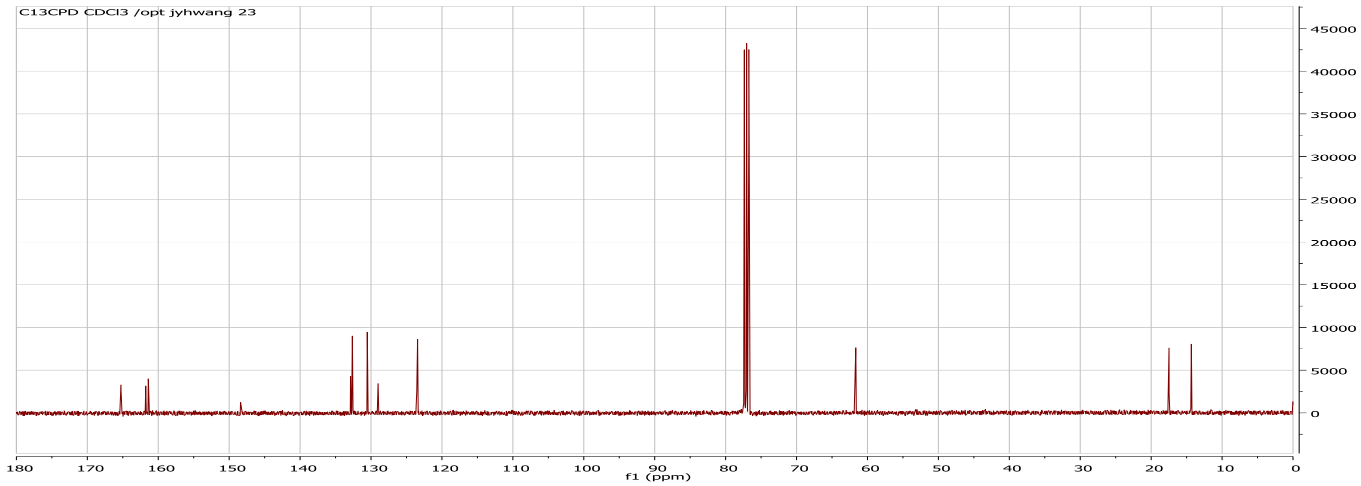
8{1}


PROTON CDCl3 /opt jyhwang 1
f1 (ppm)

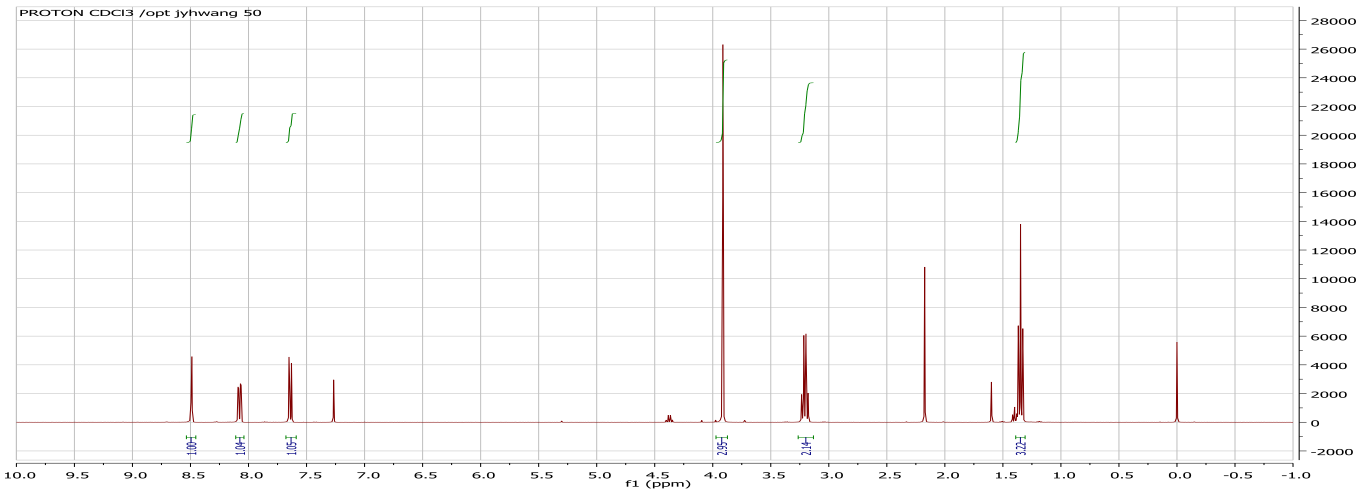

C13CPD CDCl3 /opt jyhwang 1
f1 (ppm)

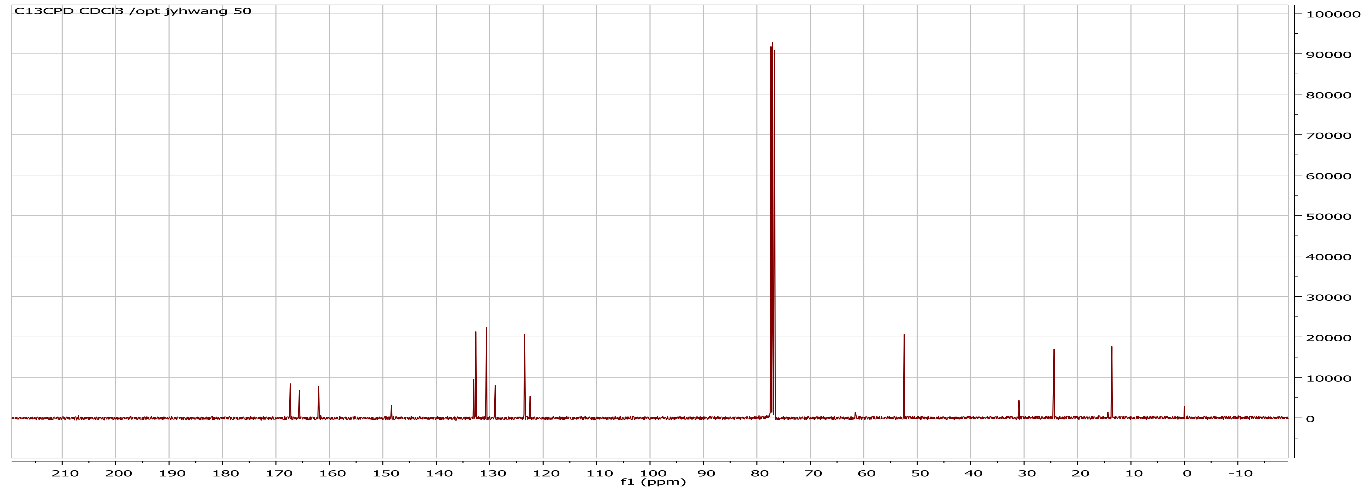
8{2}


PROTON CDCl3 /opt jyhwang 23
1.00
1.07
1.06
2.13
3.17
3.20
f1 (ppm)

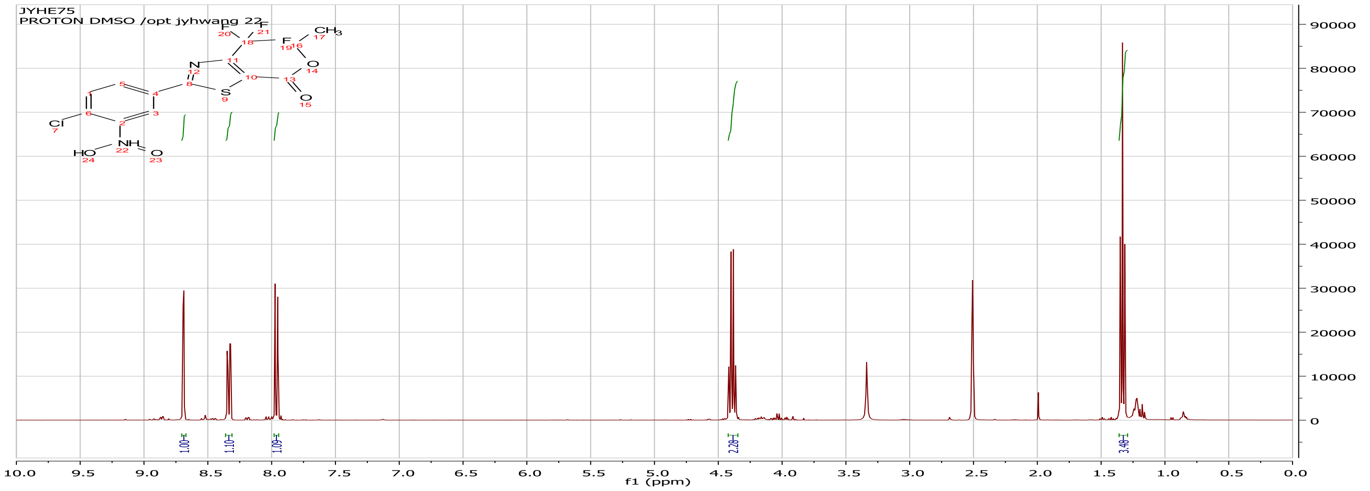

C13CPD CDCl3 /opt jyhwang 23
f1 (ppm)

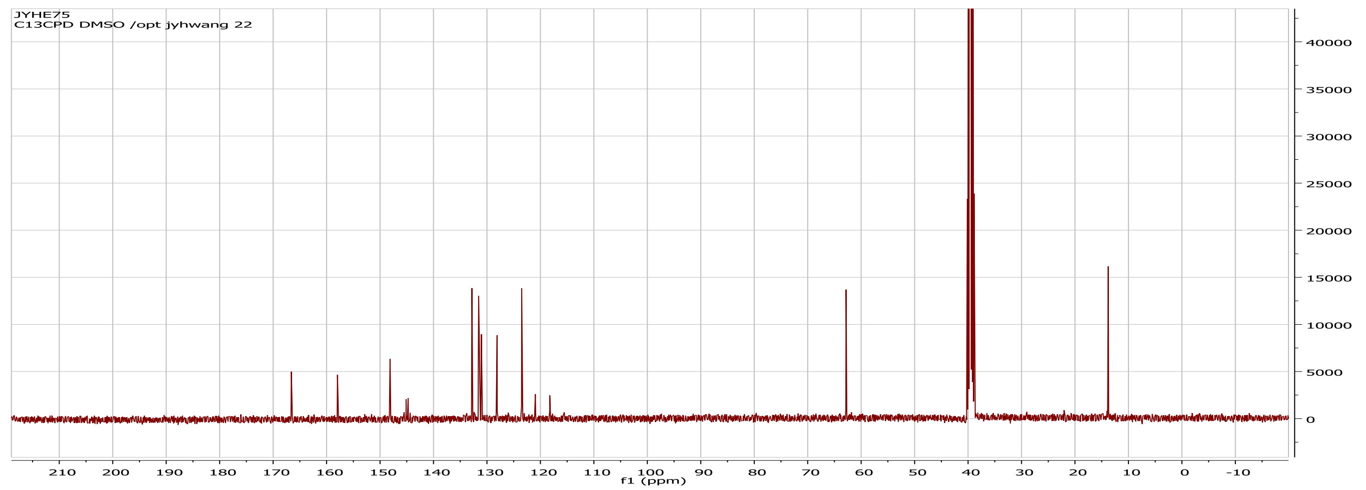
8{3}


PROTON CDCl3 /opt jyhwang 50
1.00
1.04
1.05
2.95
2.14
3.22
f1 (ppm)

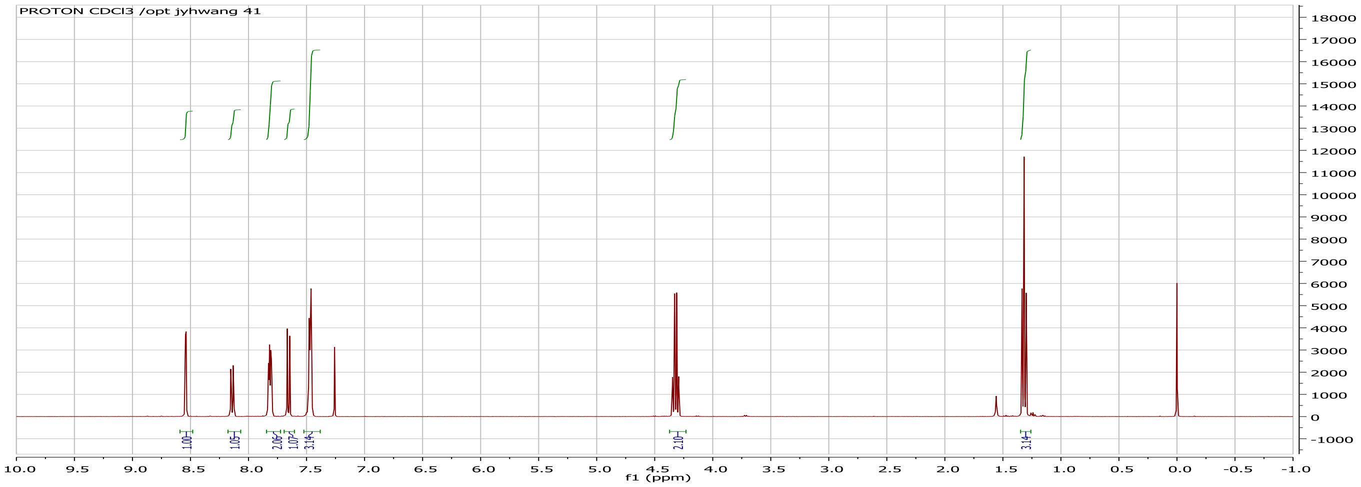

C13CPD CDCl3 /opt jyhwang 50
f1 (ppm)

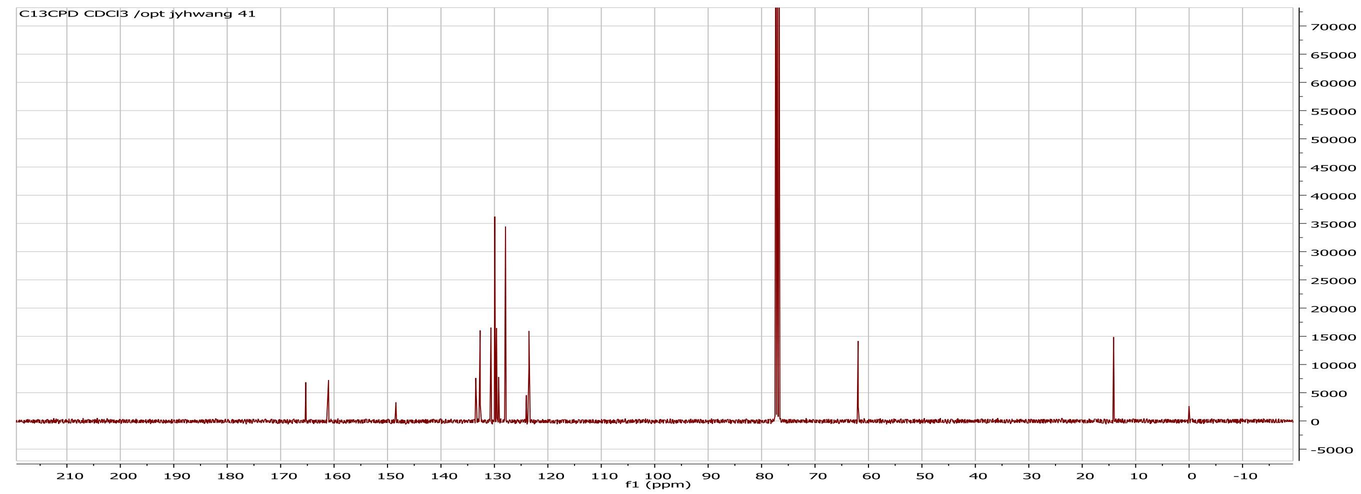
8{4}


JYHE75
PROTON DMSO /opt jyhwang 22
f1 (ppm)

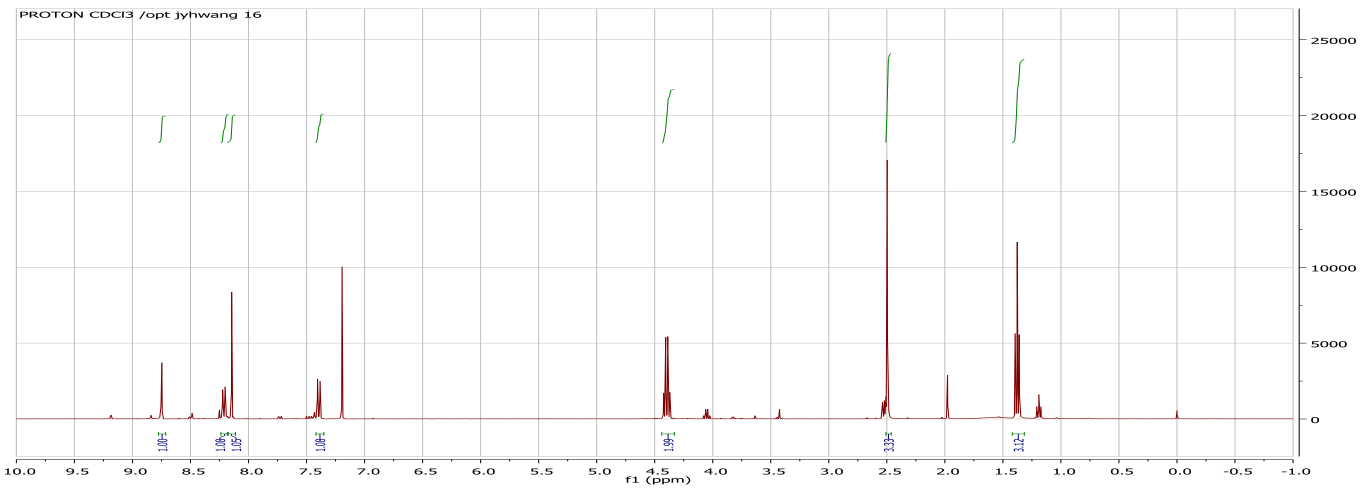

JYHE75
C13CPD DMSO /opt jyhwang 22
f1 (ppm)

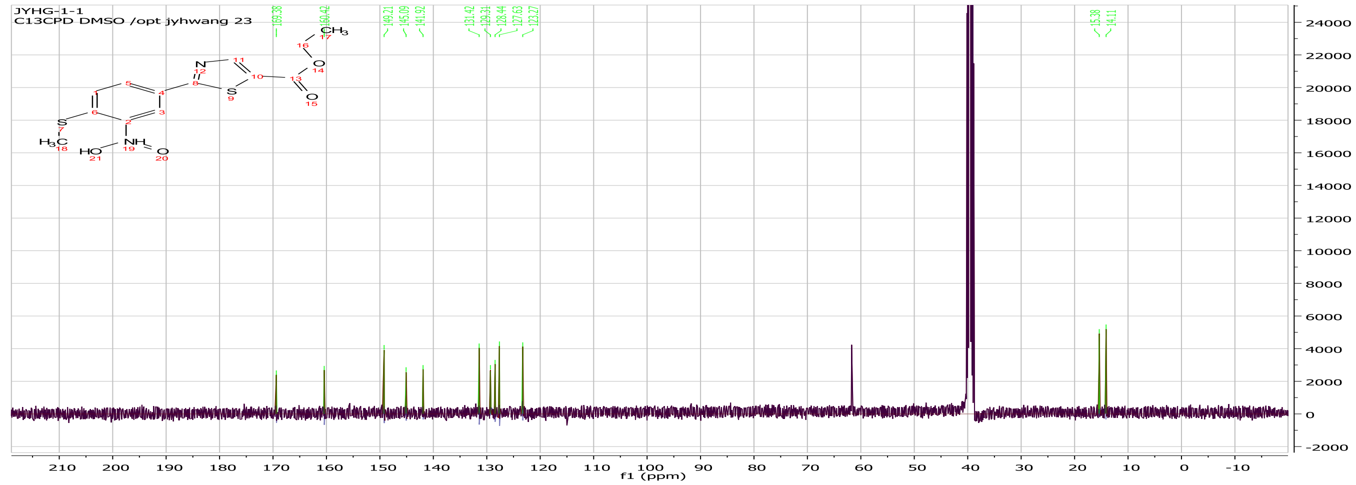
8{5}


PROTON CDCl3 /opt jyhwang 41
f1 (ppm)

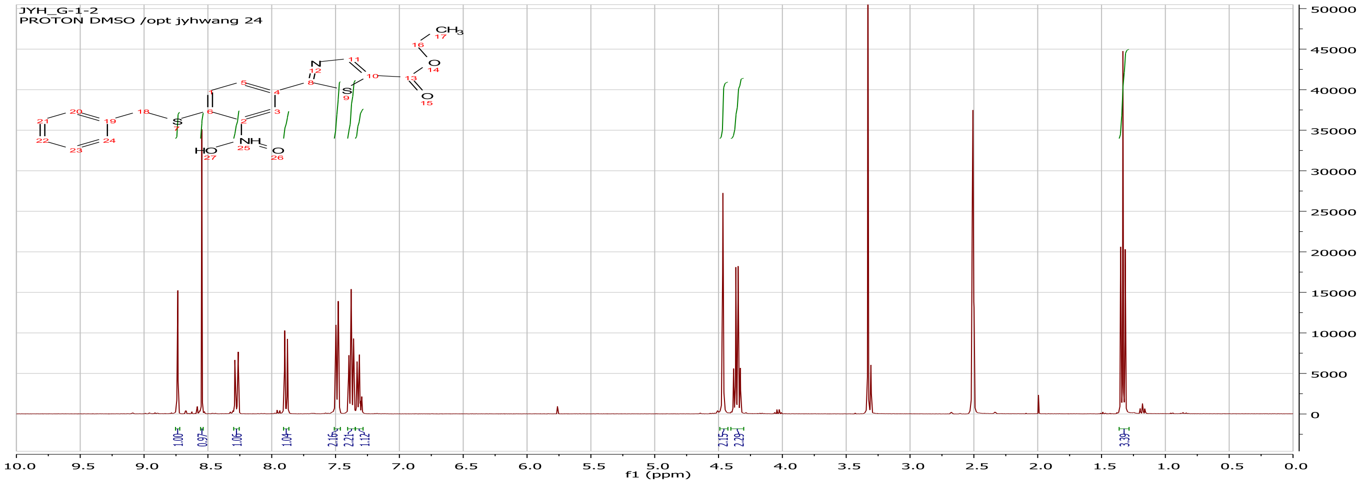

C13CPD CDCl3 /opt jyhwang 41
f1 (ppm)

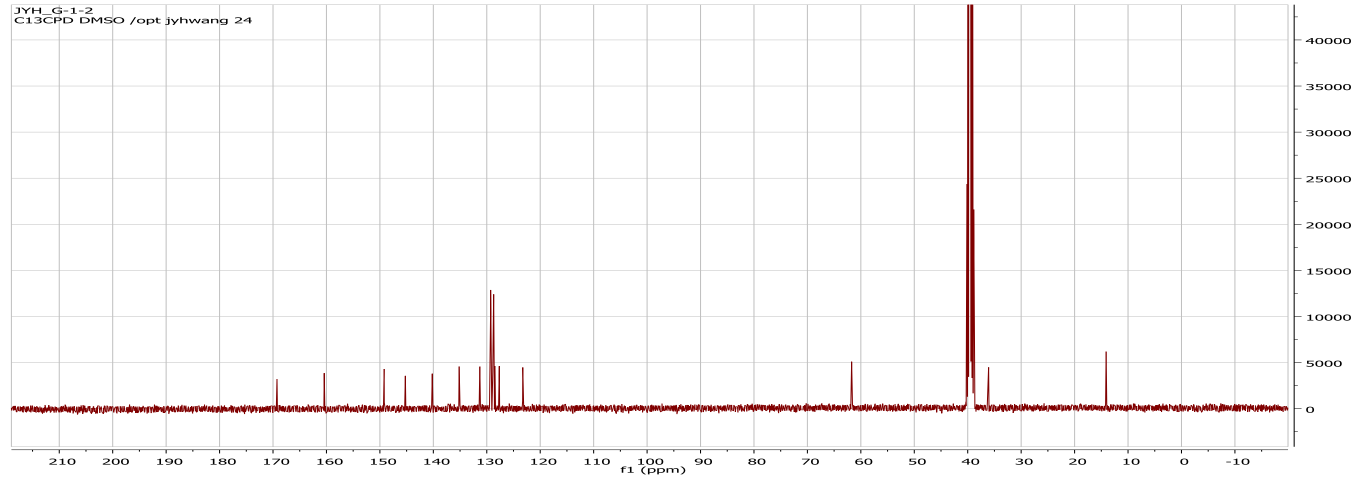
9{1,1}


PROTON CDCl3 /opt jyhwang 16
f1 (ppm)

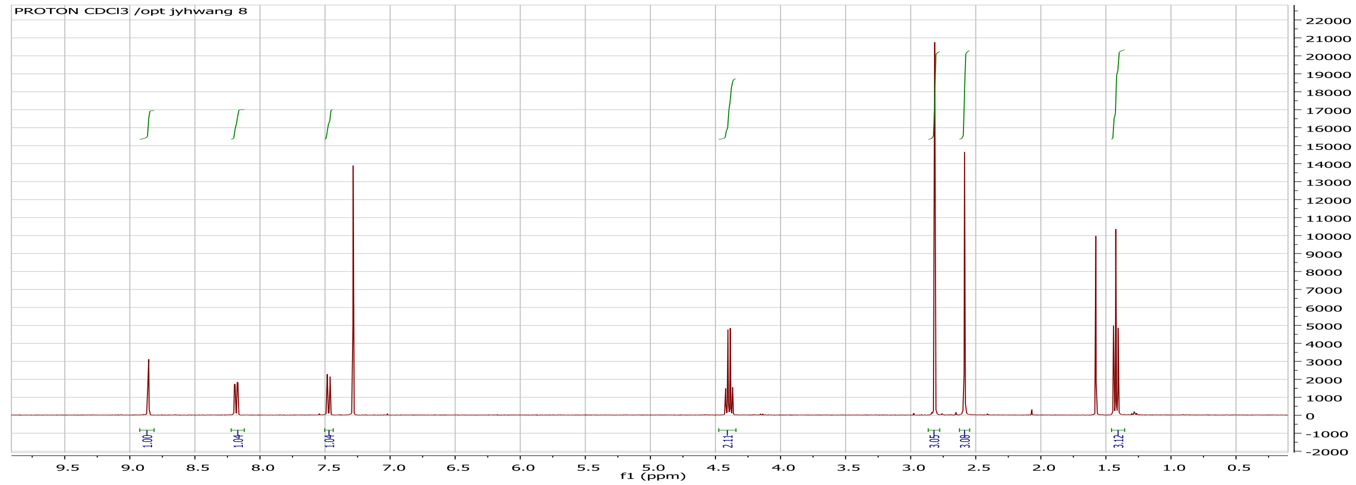

JYHG-1-1
C13CPD DMSO /opt jyhwang 23
f1 (ppm)

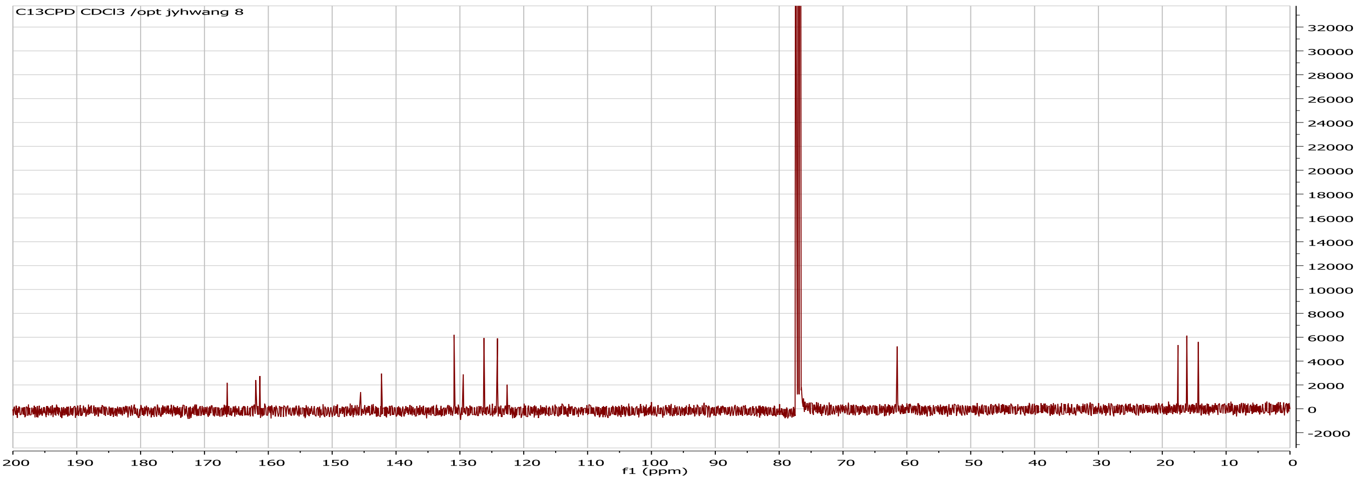
9{1,3}


JYH_G-1-2
PROTON DMSO /opt jyhwang 24
f1 (ppm)

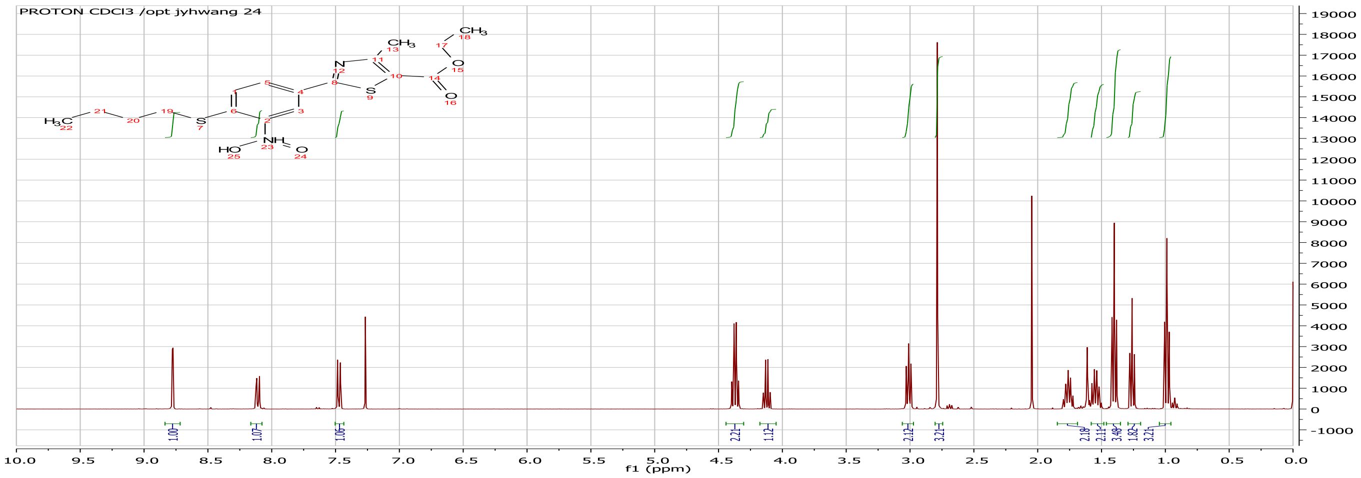

JYH_G-1-2
C13CPD DMSO /opt jyhwang 24
f1 (ppm)

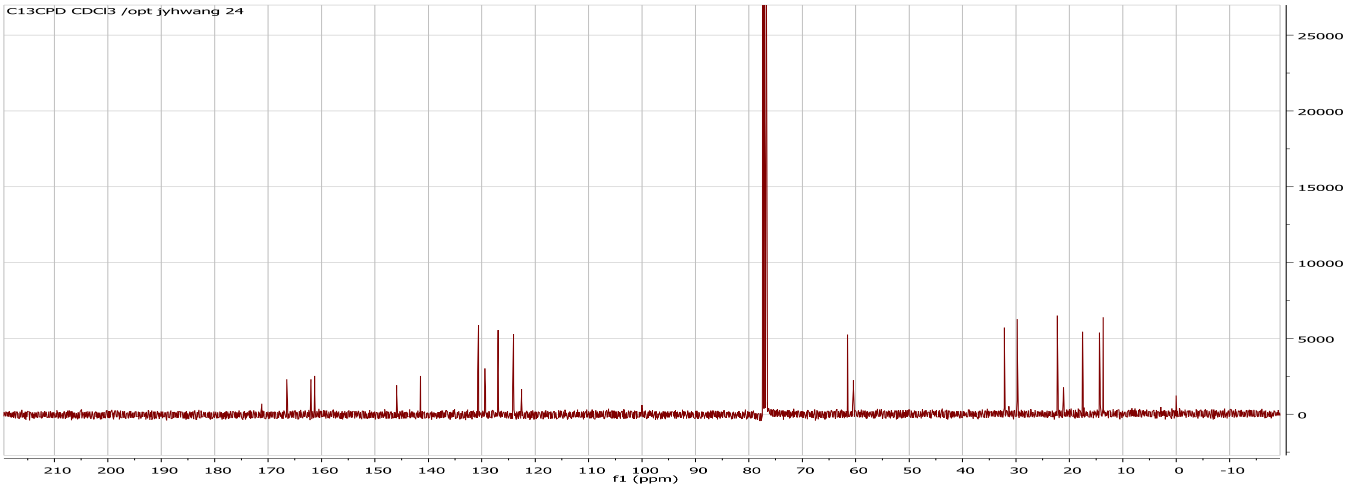
9{*2*,*1*}.


PROTON CDCl3 /opt jyhwang 8
f1 (ppm)

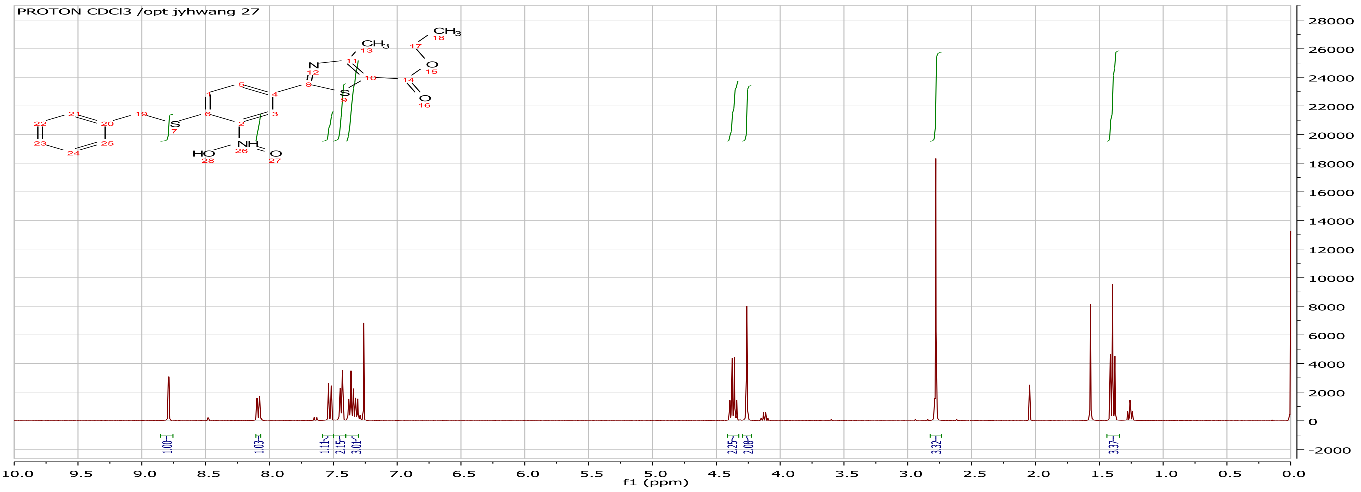

C13CPD CDCl3 /opt jyhwang 8
f1 (ppm)

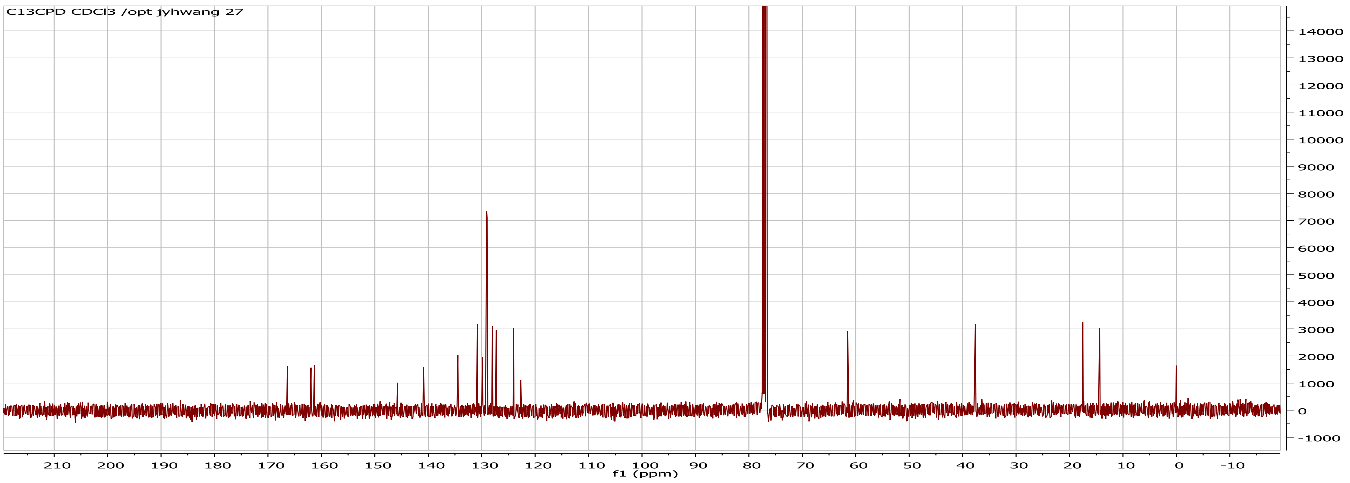
9{*2,2*}


PROTON CDCl3 /opt jyhwang 24
f1 (ppm)

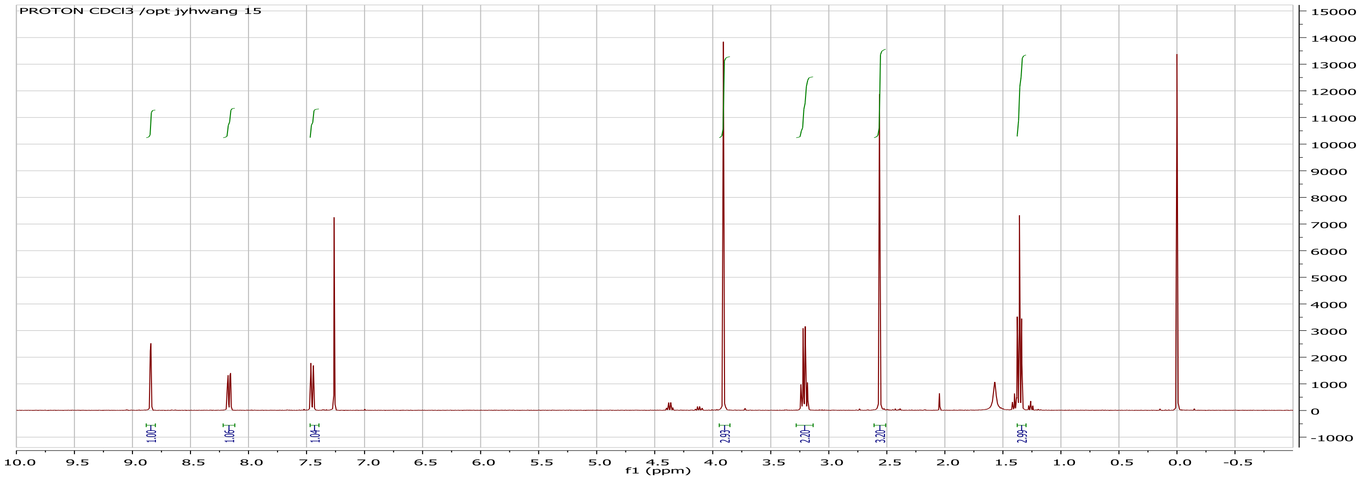

C13CPD CDCl3 /opt jyhwang 24
f1 (ppm)

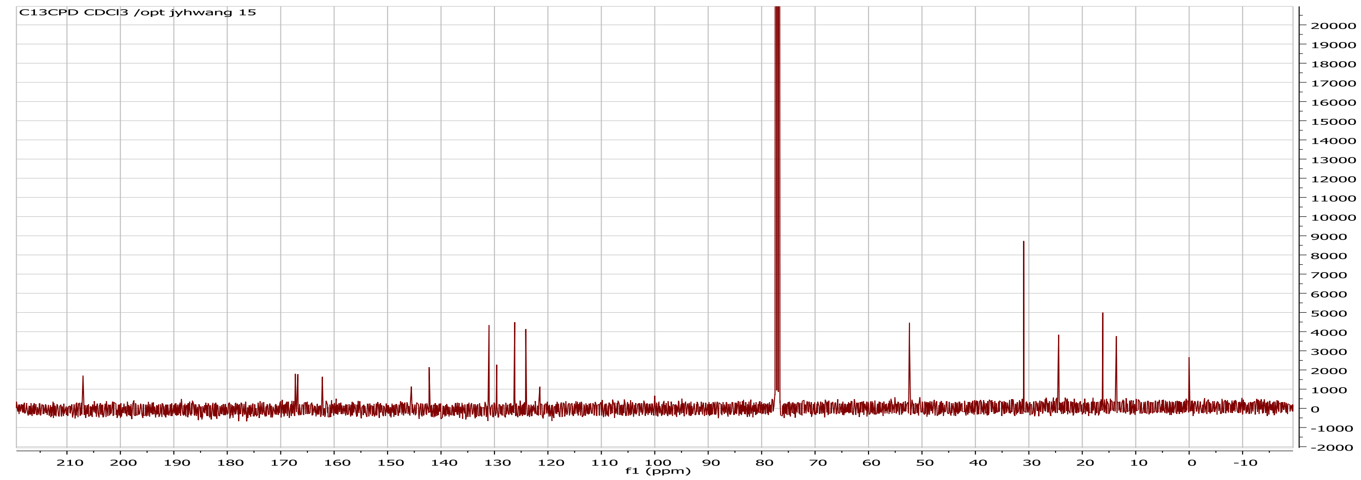
9{*2,3*}


PROTON CDCl3 /opt jyhwang 27
f1 (ppm)

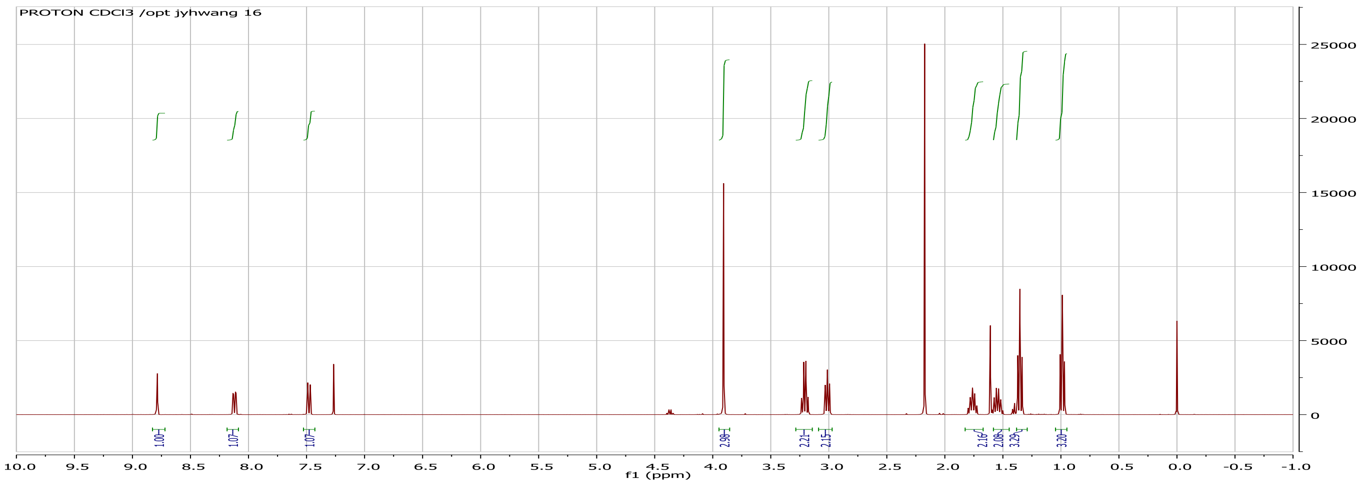

C13CPD CDCl3 /opt jyhwang 27
f1 (ppm)

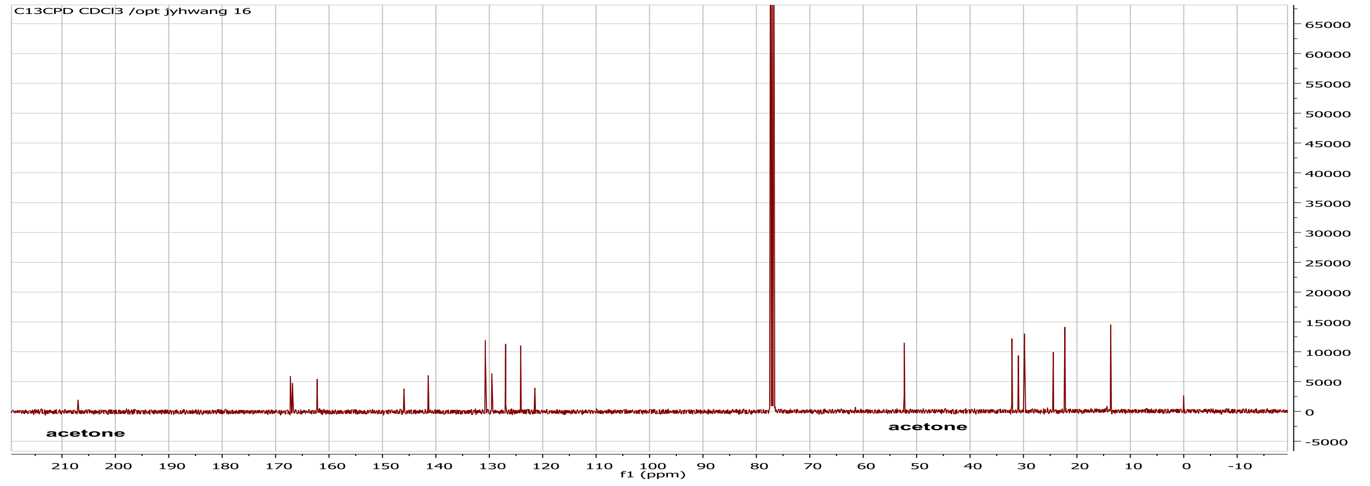
9{3,1}


PROTON CDCl3 /opt jyhwang 15
f1 (ppm)

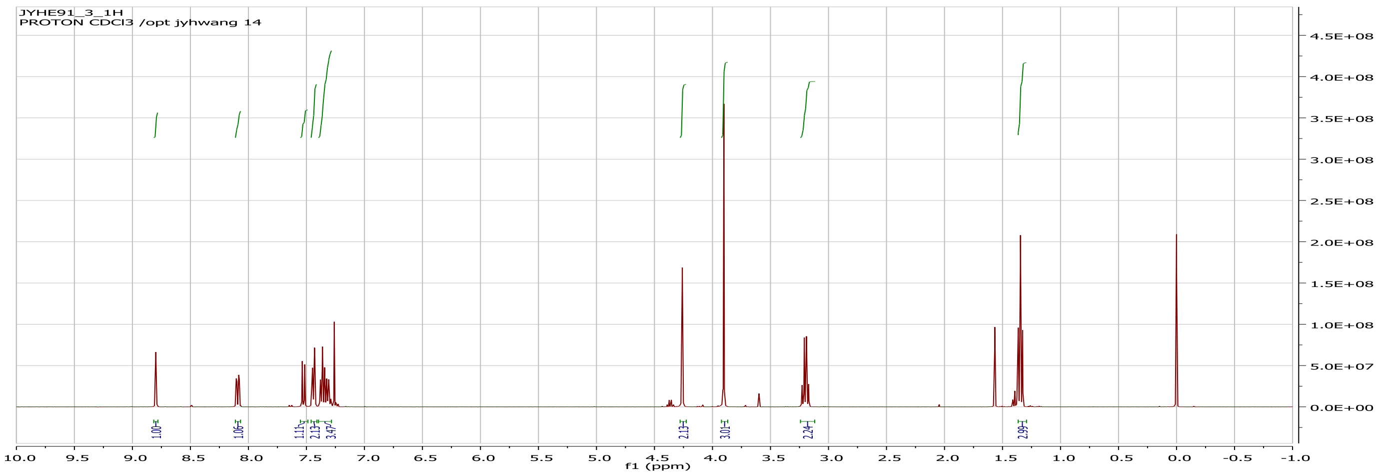

C13CPD CDCl3 /opt jyhwang 15
f1 (ppm)

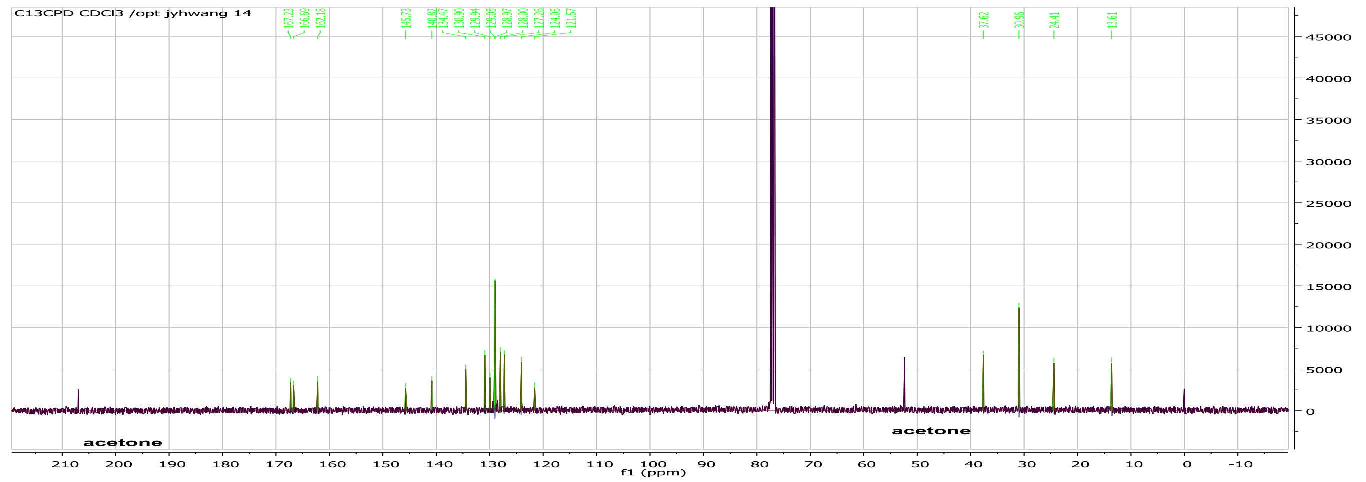
9{3,2}


PROTON CDCl3 /opt jyhwang 16
f1 (ppm)

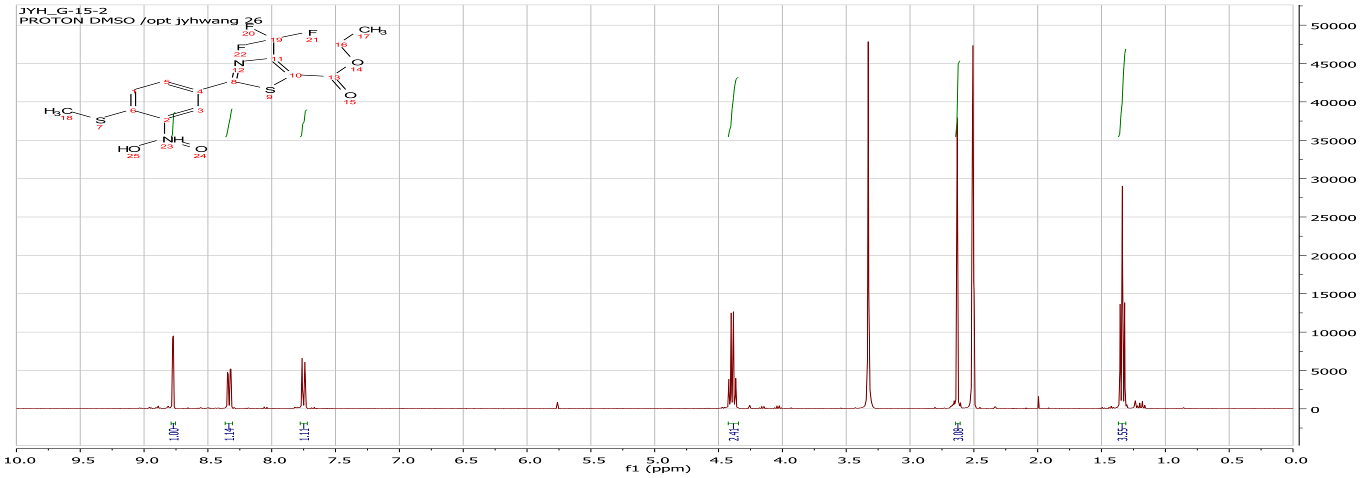

C13CPD CDCl3 /opt jyhwang 16
acetone
acetone
f1 (ppm)

9{3,3}

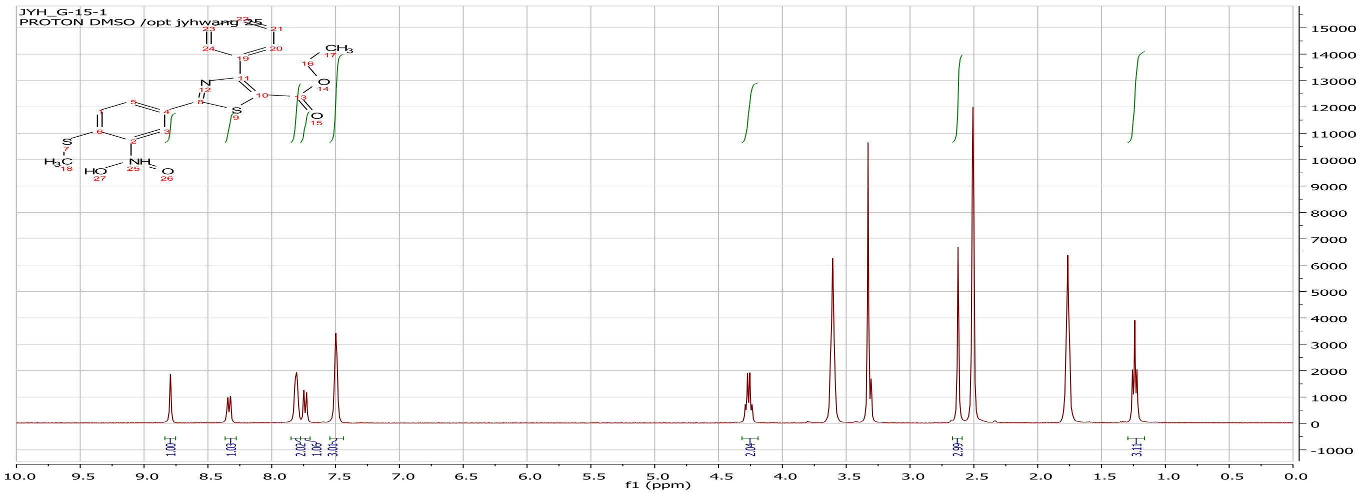

JYHE91_3_1H
PROTON CDCl3 /opt jyhwang 14
f1 (ppm)


C13CPD CDCl3 /opt jyhwang 14
acetone
acetone
f1 (ppm)

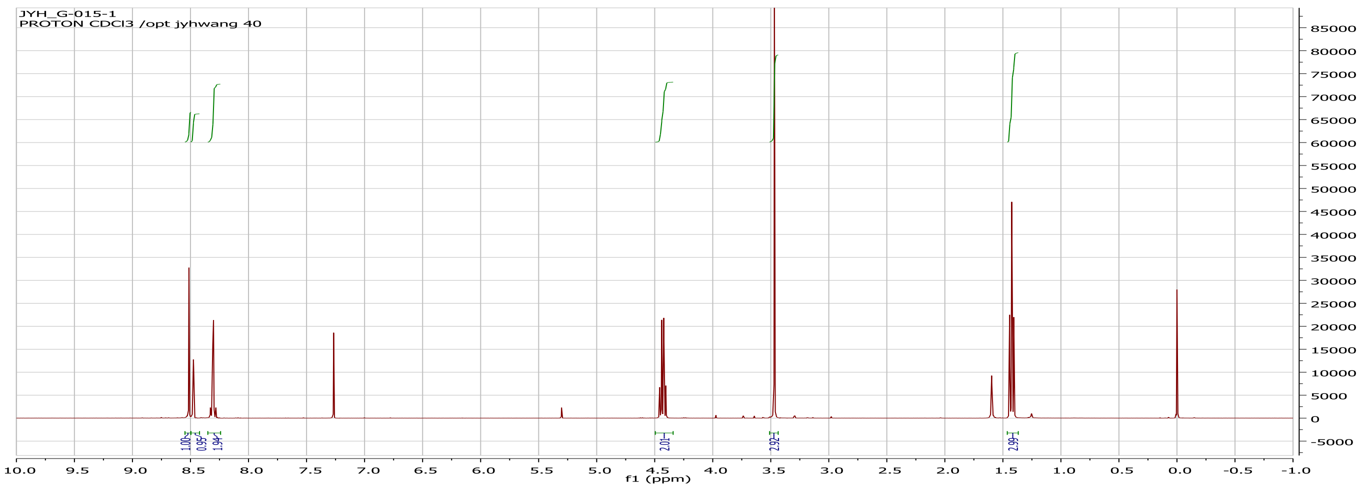
9{4,1}

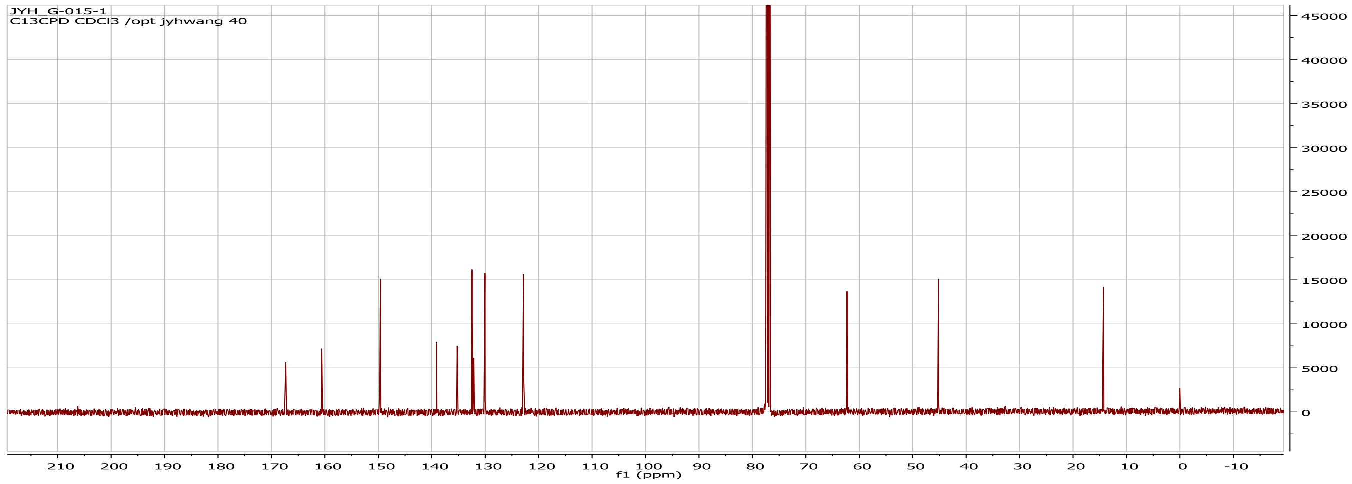

JYH_G-15-2
PROTON DMSO /opt jyhwang 26
f1 (ppm)

9{5,1}

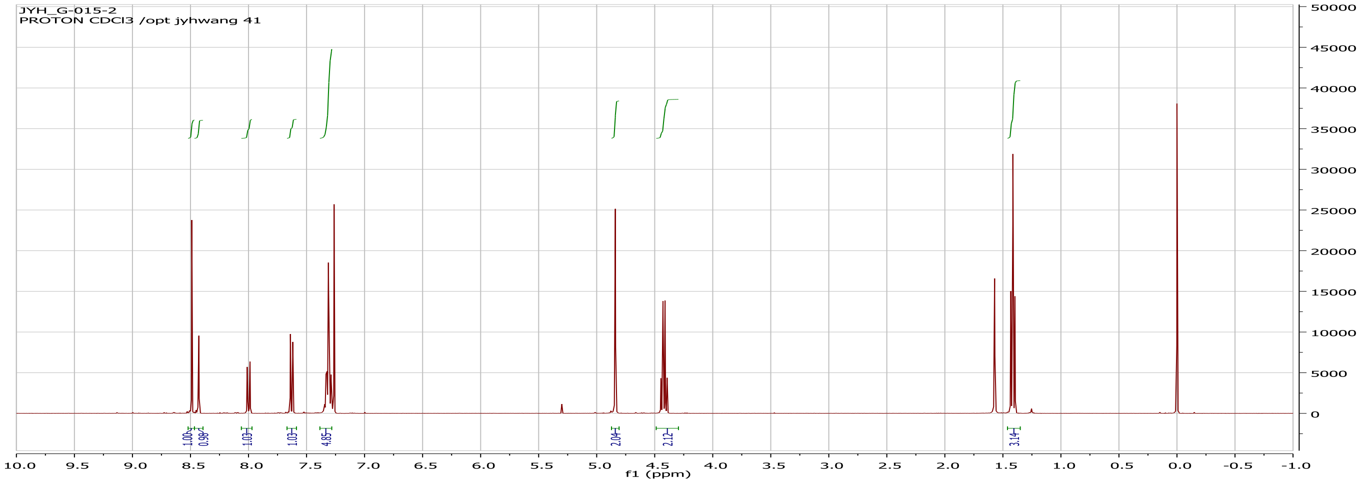

JYH_G-15-1
PROTON DMSO /opt jyhwang 25
f1 (ppm)

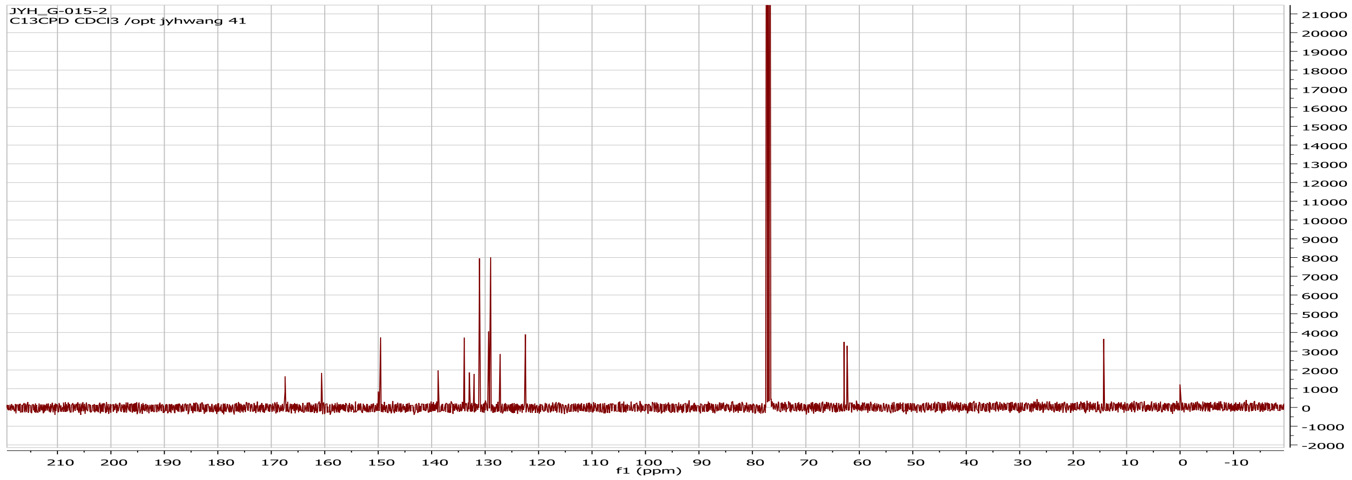
10{1,1}


JYH_G-015-1
PROTON CDCl3 /opt jyhwang 40
f1 (ppm)

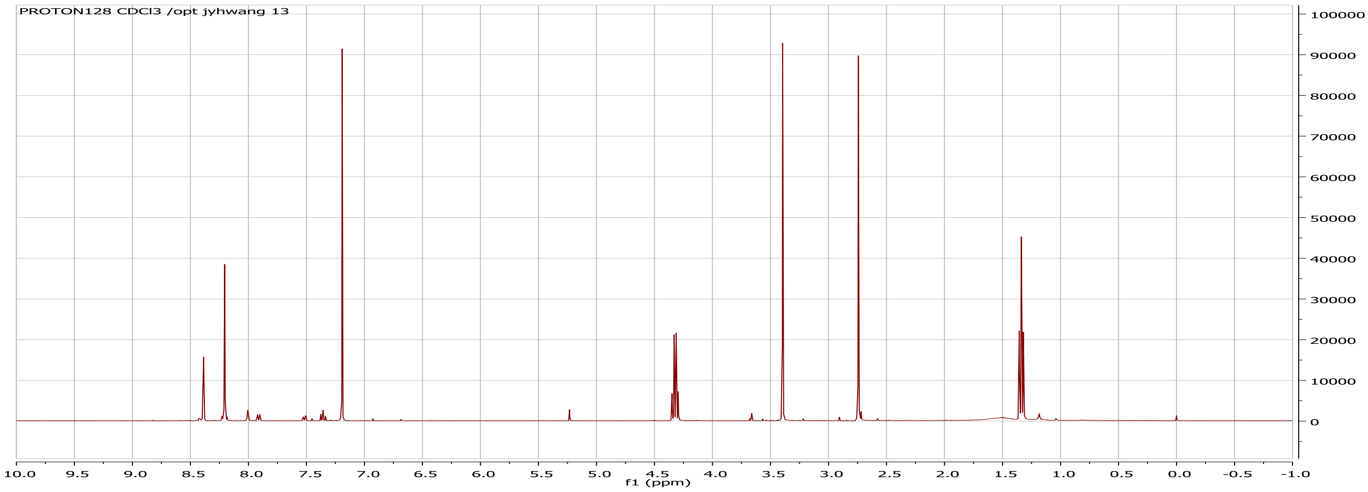

JYH_G-015-1
C13CPD CDCl3 /opt jyhwang 40
f1 (ppm)

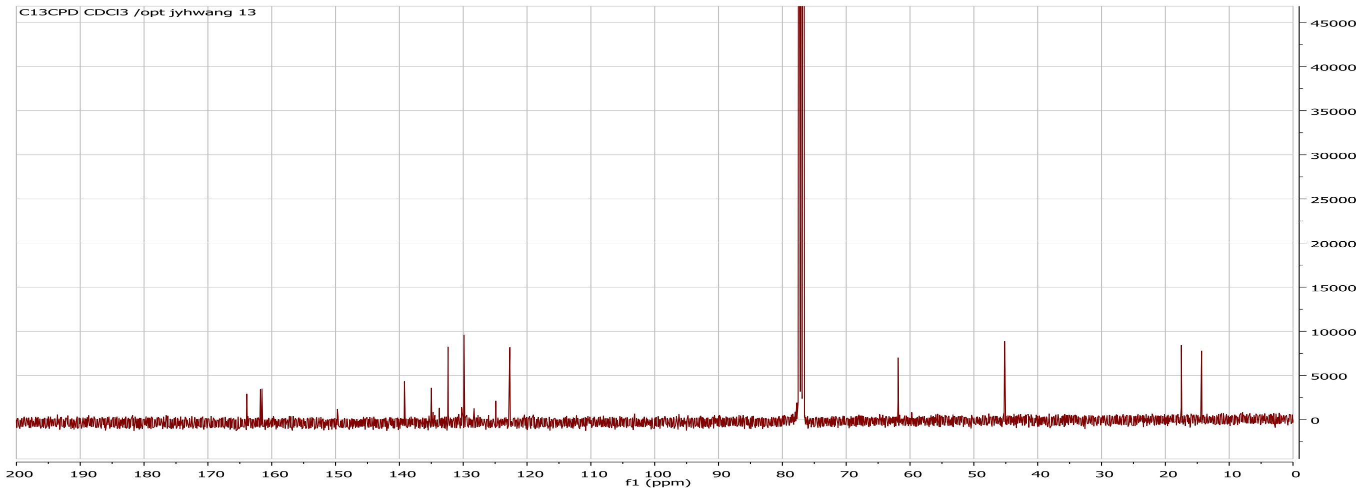
10{1,3}


JYH_G-015-2
PROTON CDCl3 /opt jyhwang 41
f1 (ppm)

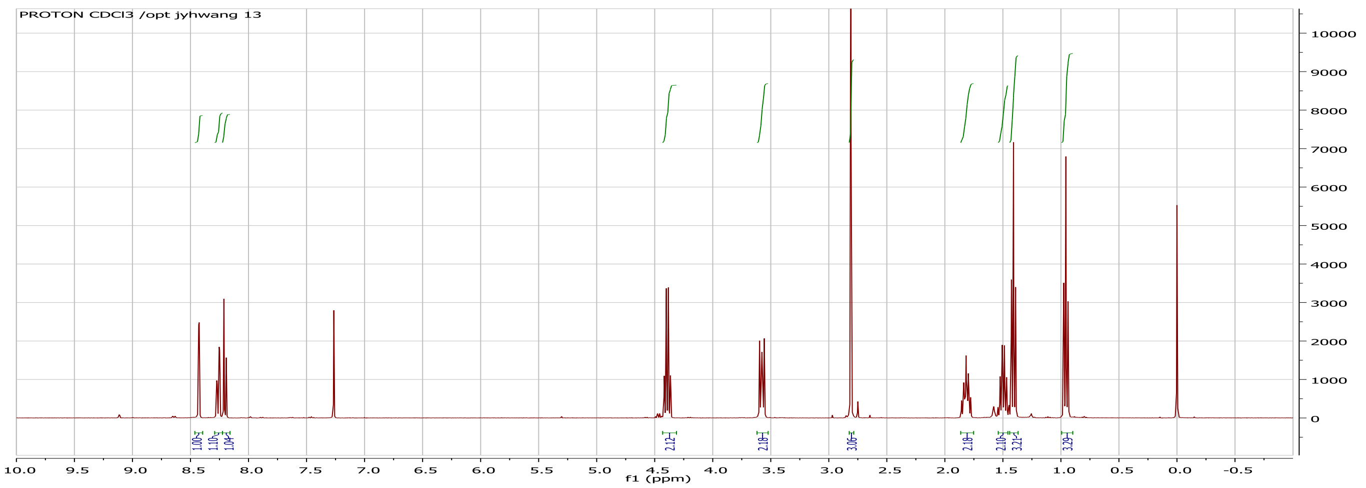

JYH_G-015-2
C13CPD CDCl3 /opt jyhwang 41
f1 (ppm)

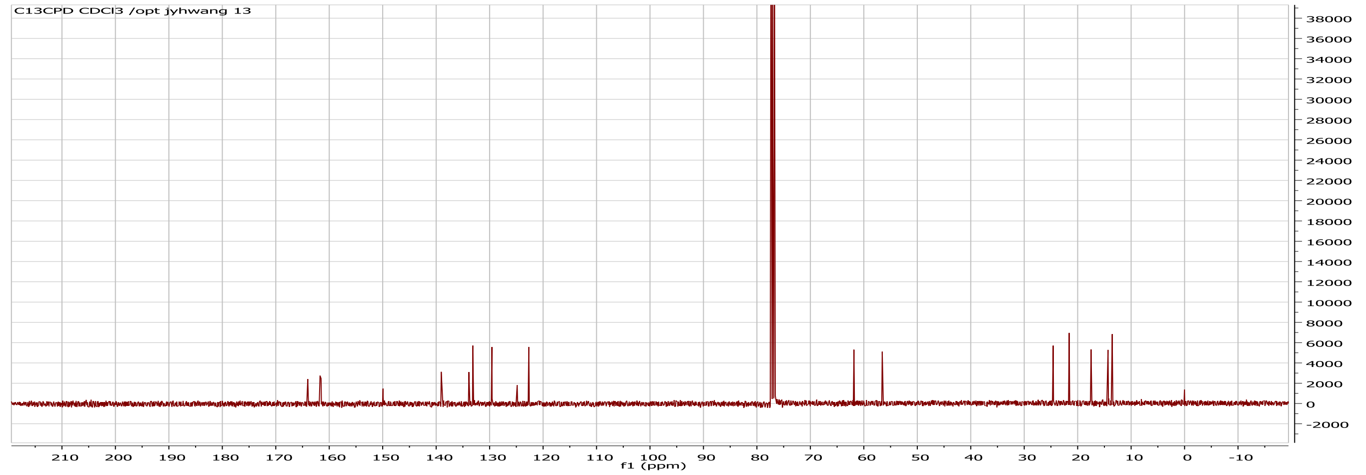
10{2,1}


PROTON128 CDCl3 /opt jyhwang 13
f1 (ppm)

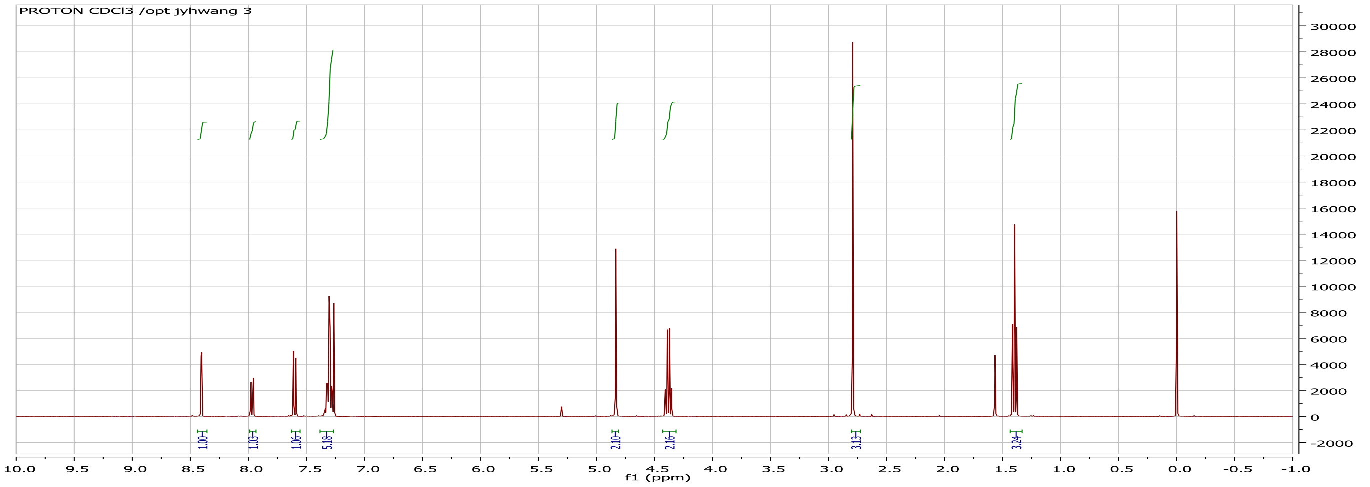

C13CPD CDCl3 /opt jyhwang 13
f1 (ppm)

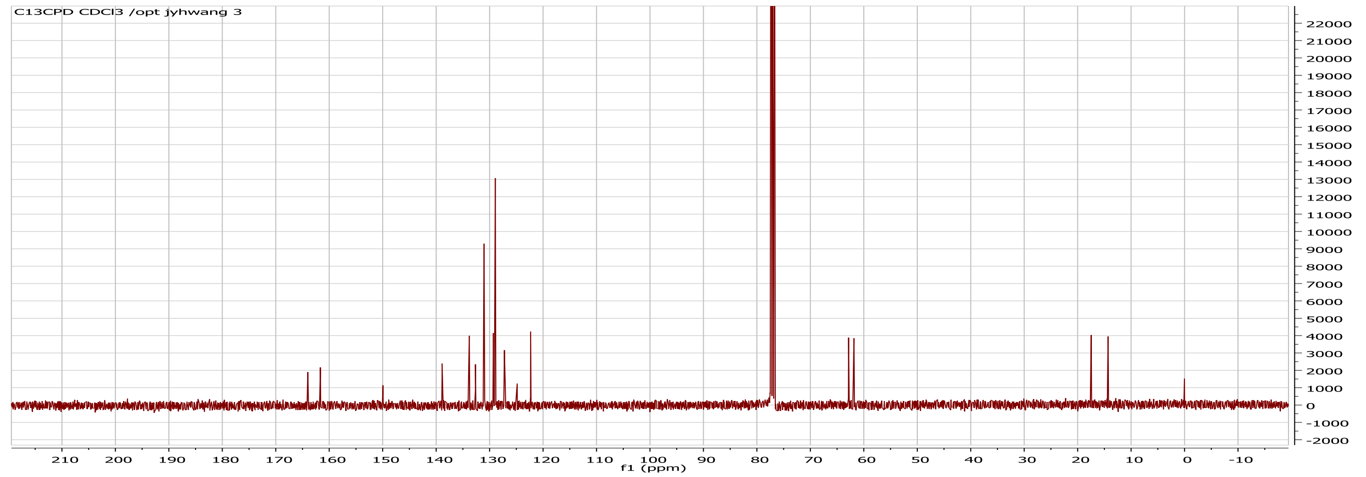
10{2,2}


PROTON CDCl3 /opt jyhwang 13
f1 (ppm)

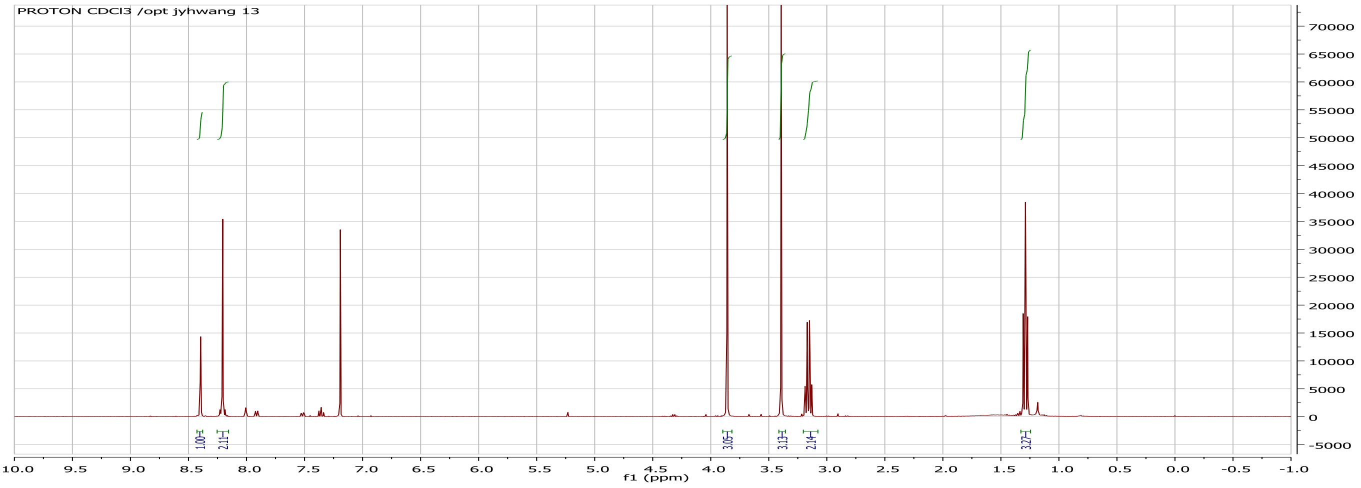

C13CPD CDCl3 /opt jyhwang 13
f1 (ppm)

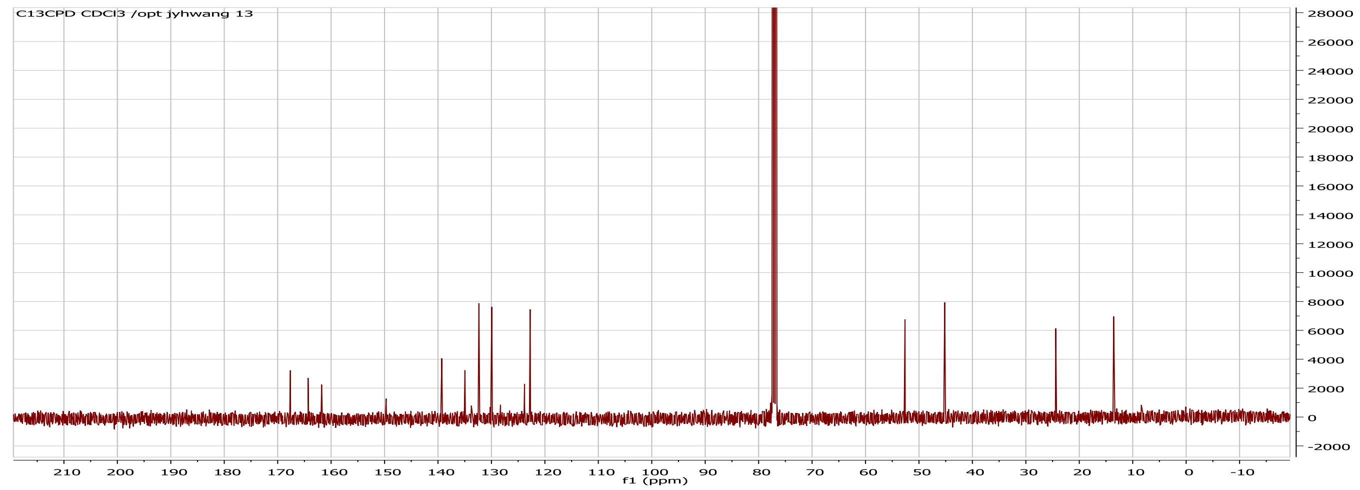
10{2,3}


PROTON CDCl3 /opt jyhwang 3
1.00
1.03
1.06
5.18
2.10
2.16
3.13
3.24
f1 (ppm)

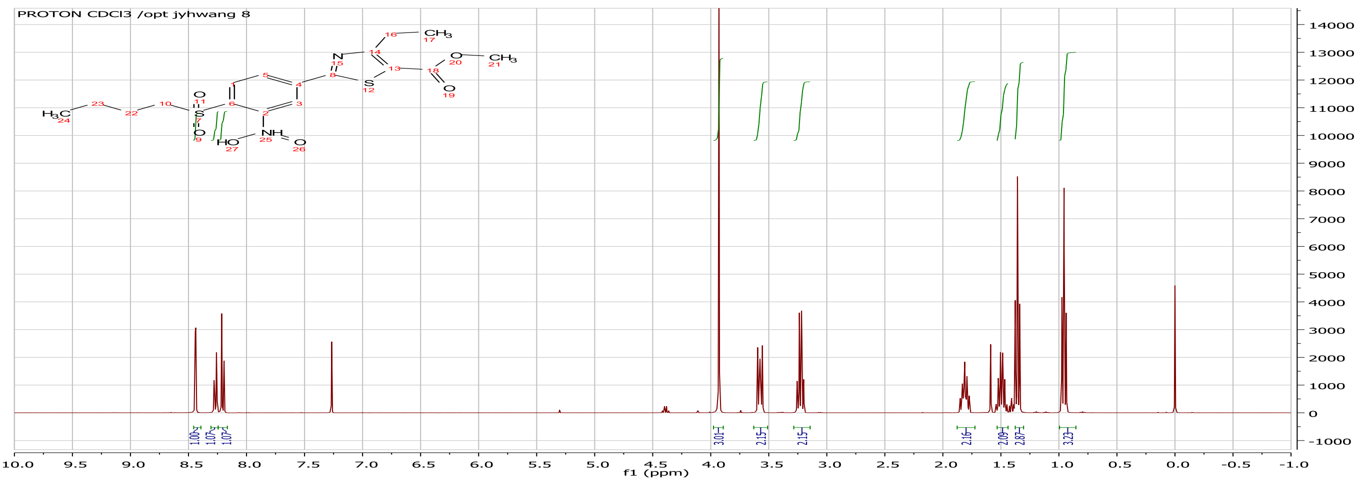

C13CPD CDCl3 /opt jyhwang 3
f1 (ppm)

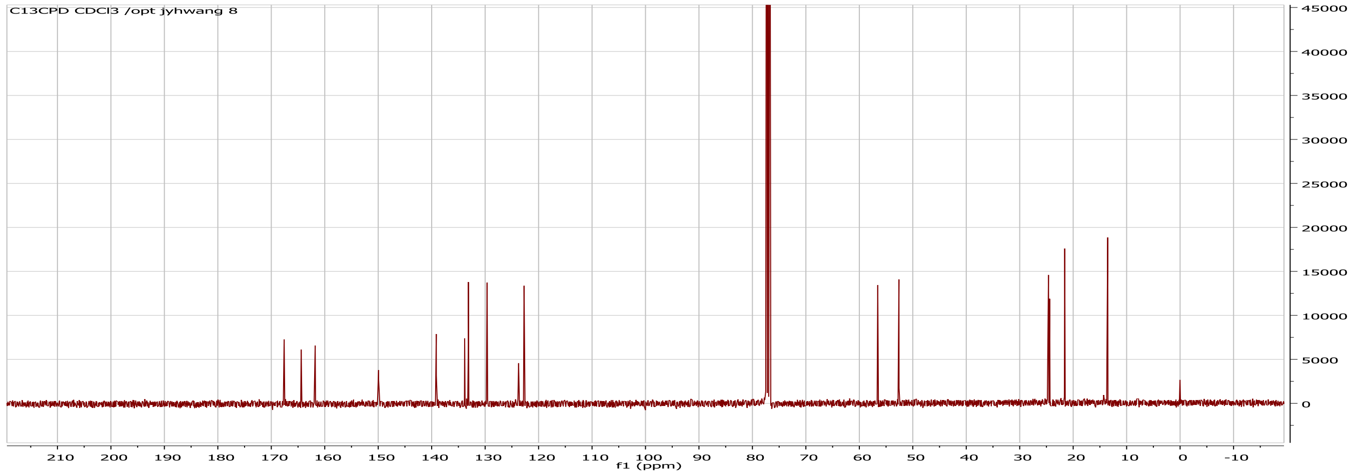
10{3,1}


PROTON CDCl3 /opt jyhwang 13
f1 (ppm)

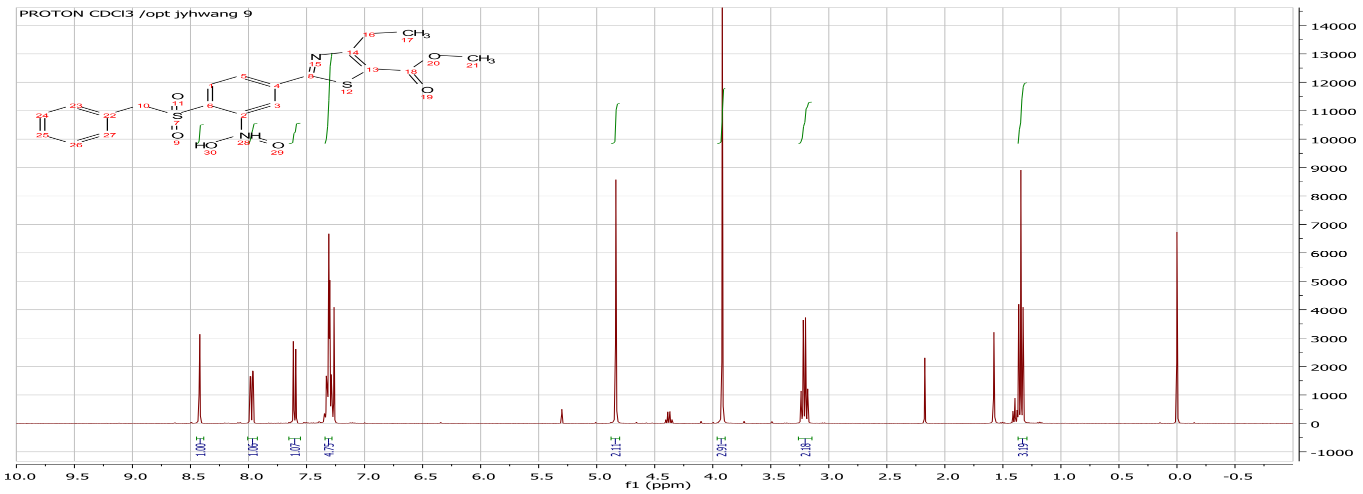

C13CPD CDCl3 /opt jyhwang 13
f1 (ppm)

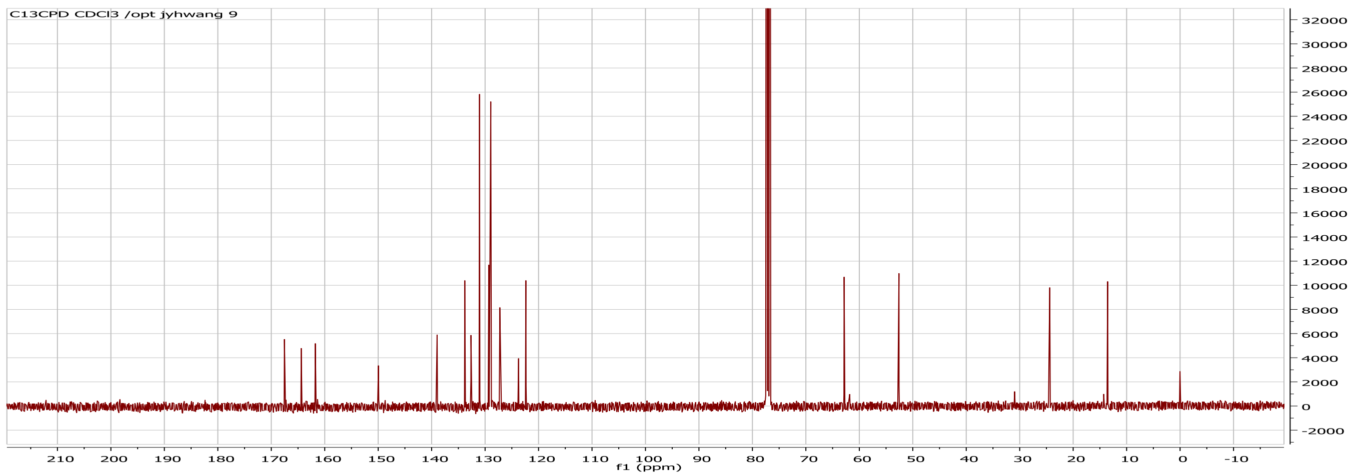
10{3,2}


PROTON CDCl3 /opt jyhwang 8
f1 (ppm)

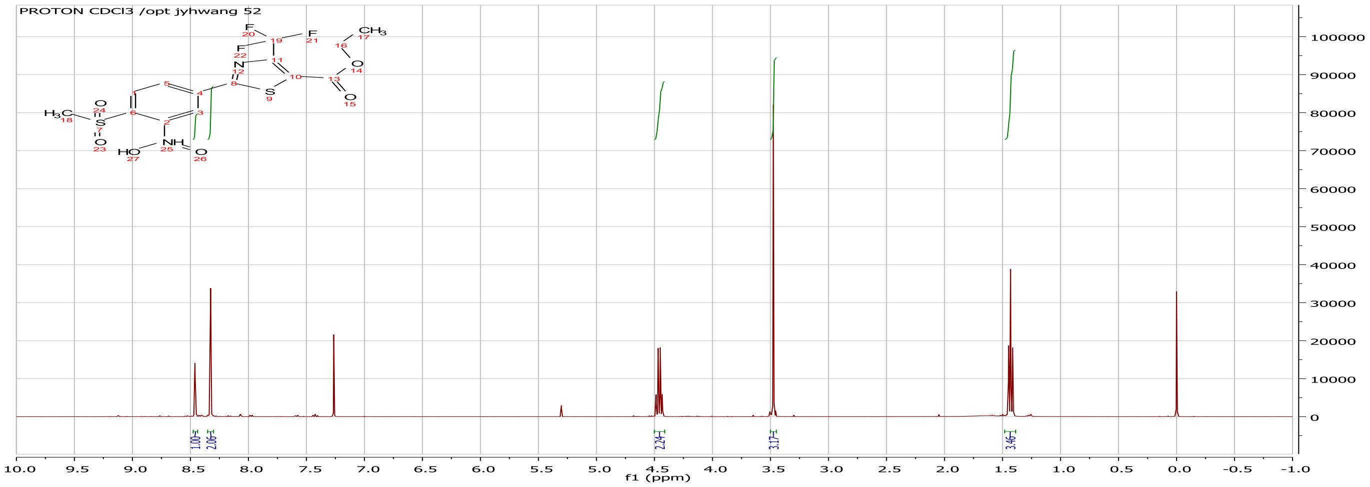

C13CPD CDCl3 /opt jyhwang 8
f1 (ppm)

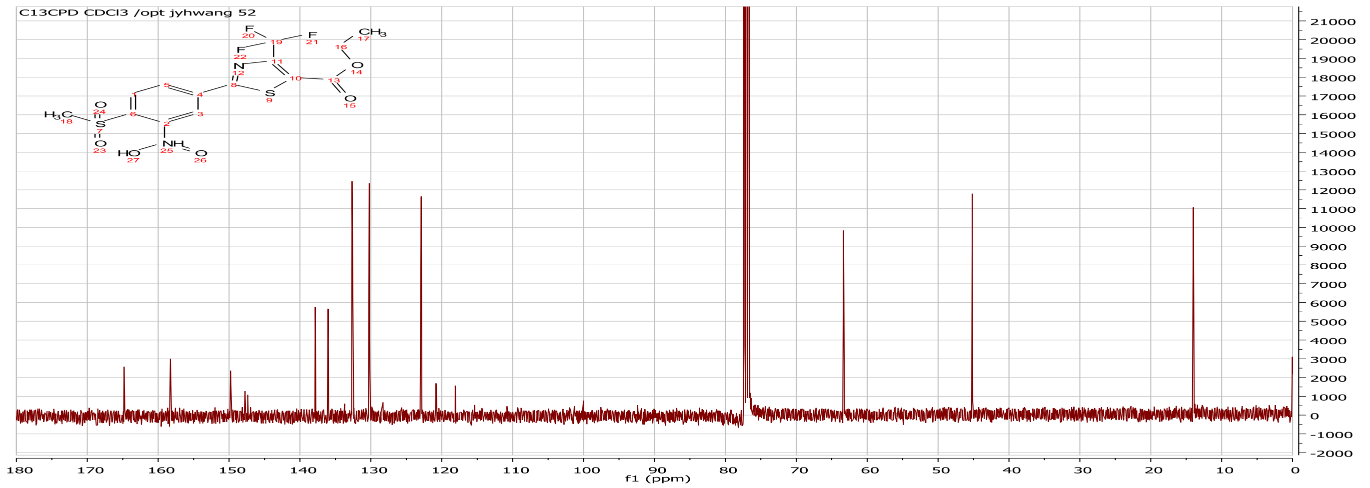
10{3,3}


PROTON CDCl3 /opt jyhwang 9
f1 (ppm)

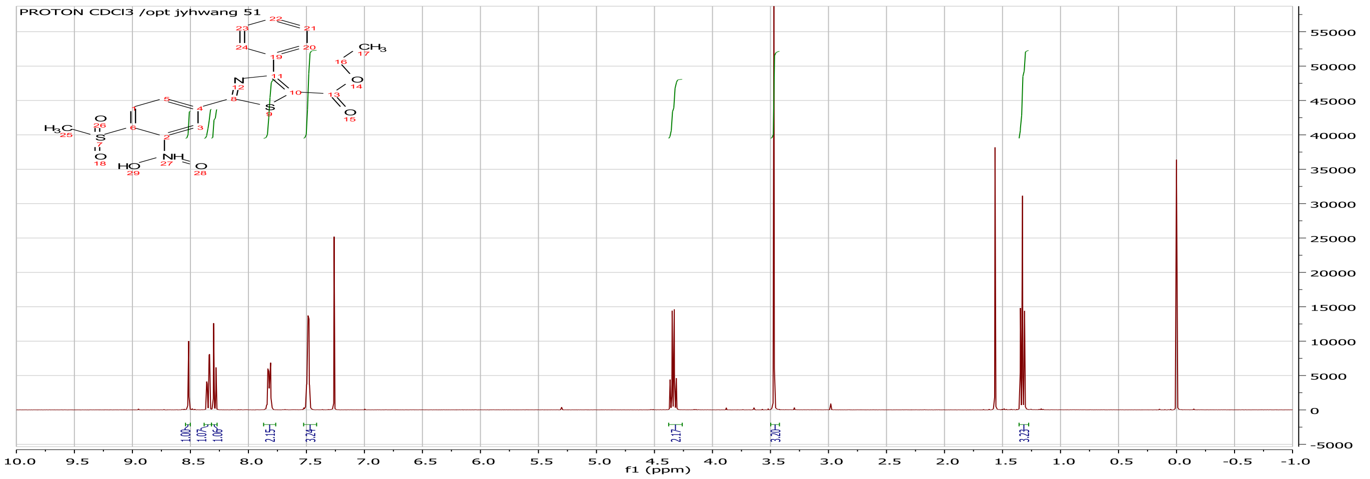

C13CPD CDCl3 /opt jyhwang 9
f1 (ppm)

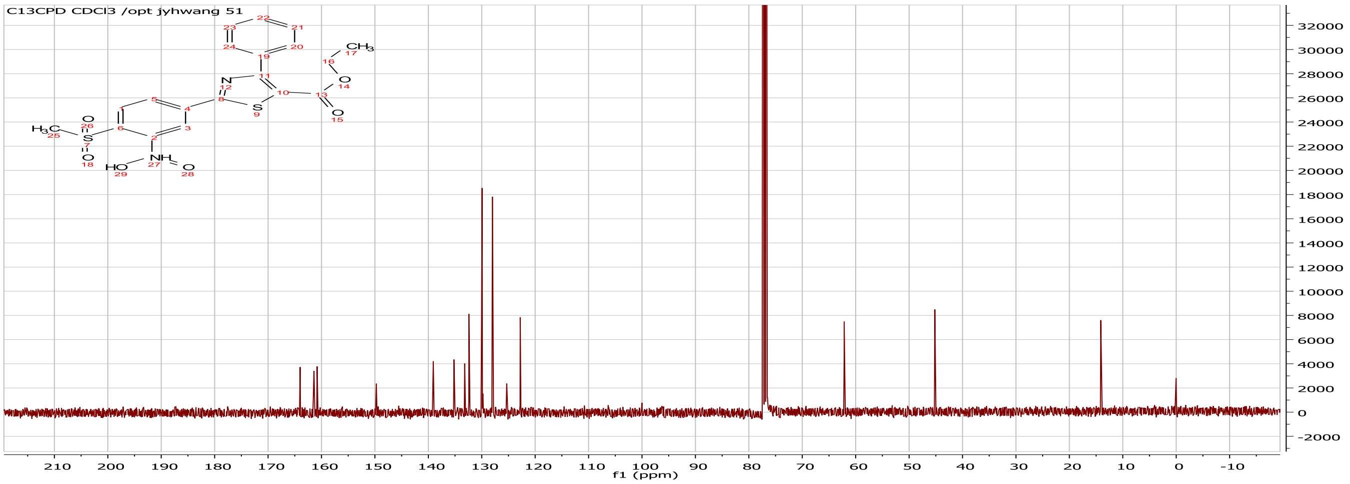
10{4,1}


PROTON CDCl3 /opt jyhwang 52
f1 (ppm)

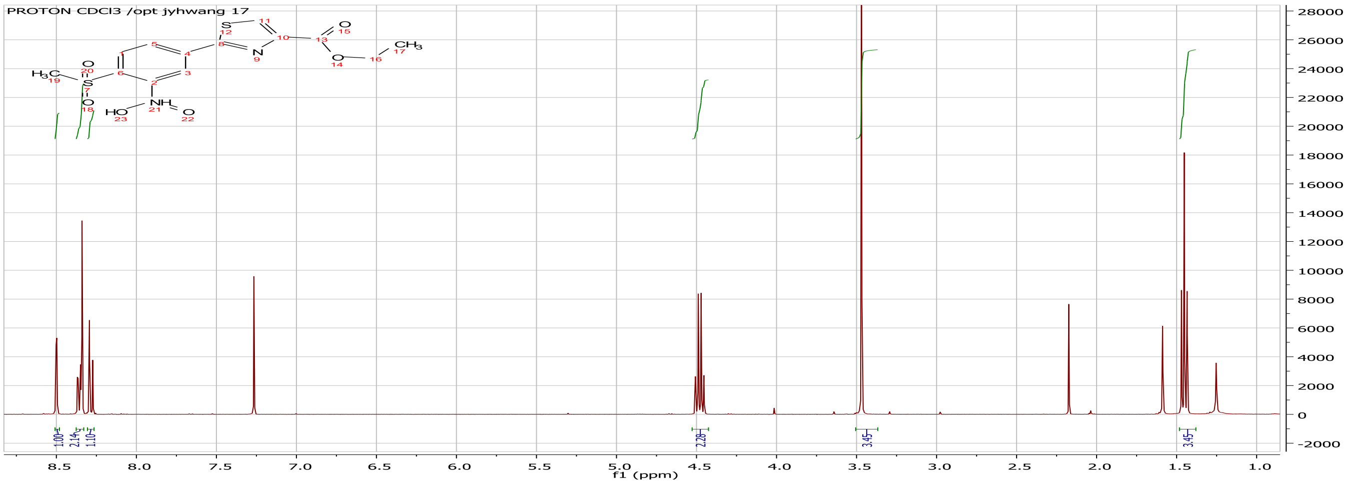

C13CPD CDCl3 /opt jyhwang 52
f1 (ppm)

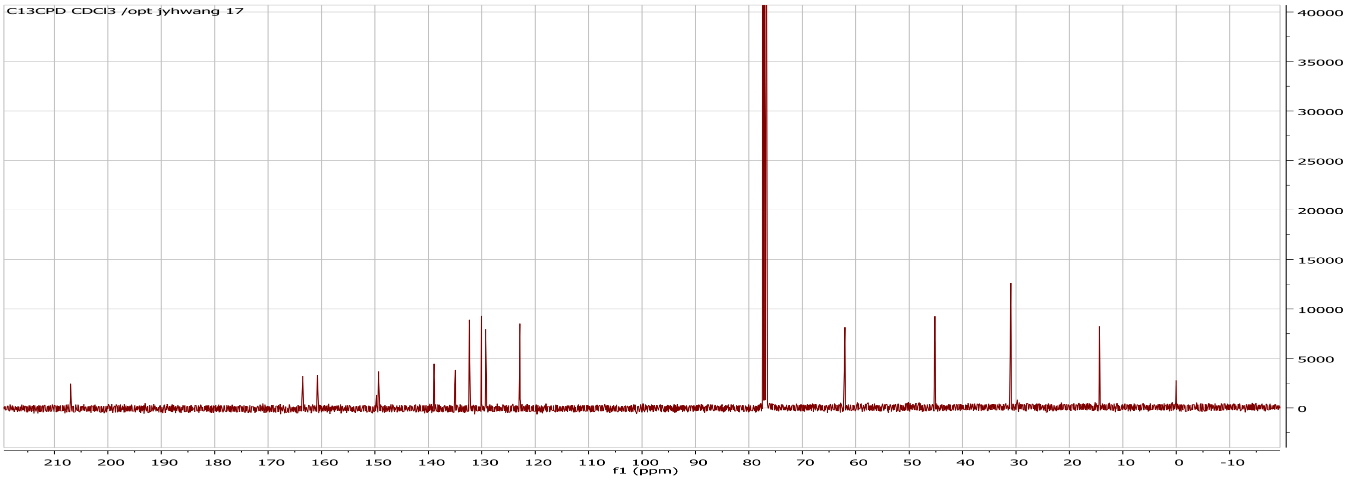
10{5,1}


PROTON CDCl3 /opt jyhwang 51
f1 (ppm)

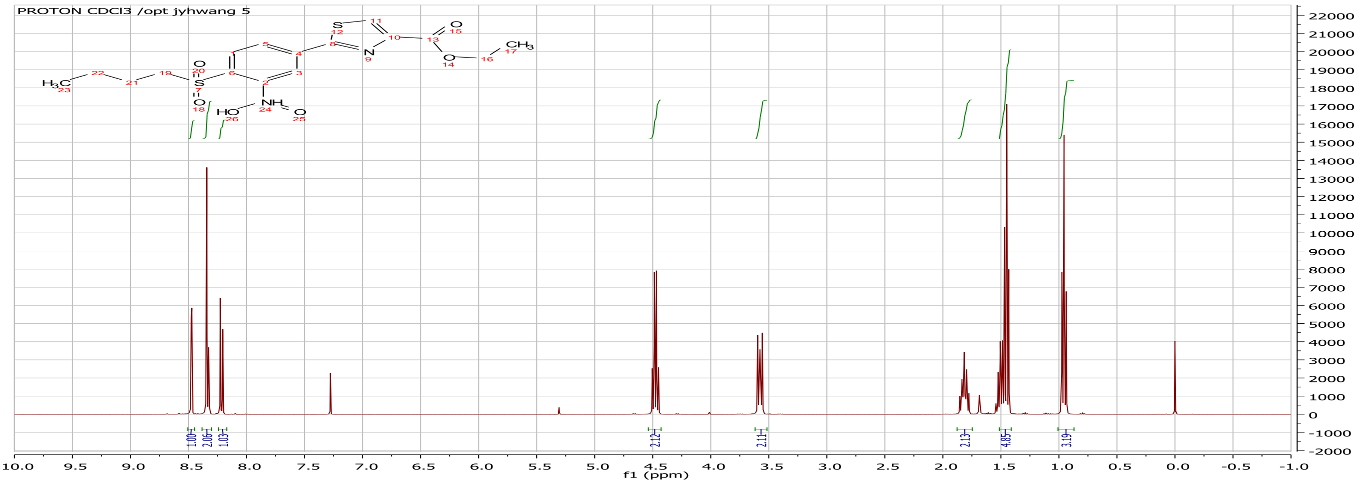

C13CPD CDCl3 /opt jyhwang 51
f1 (ppm)

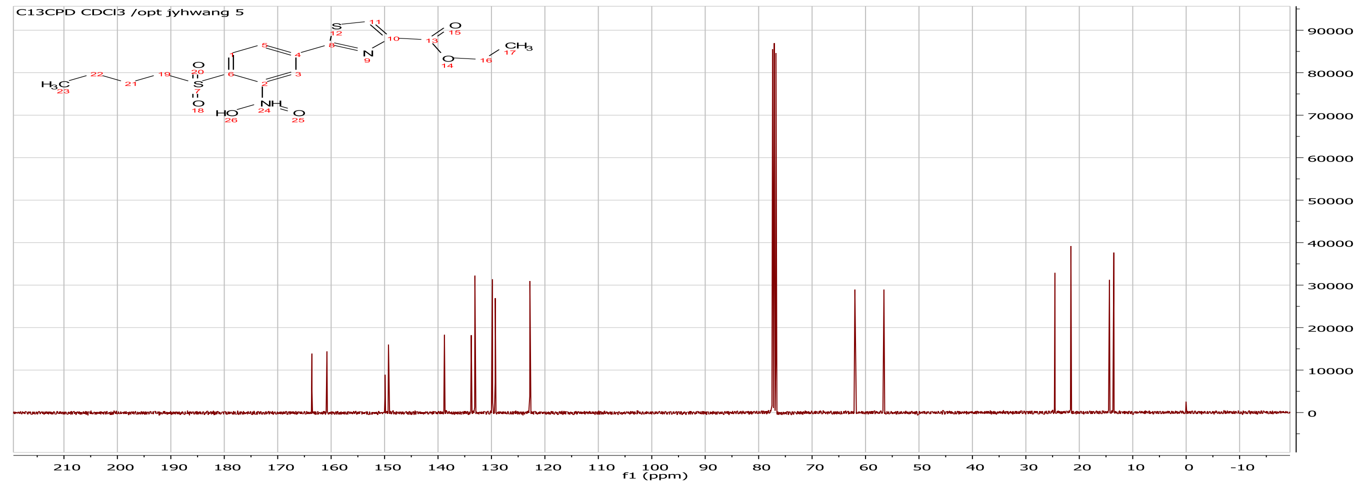
15{6,1}


PROTON CDCl3 /opt jyhwang 17
f1 (ppm)

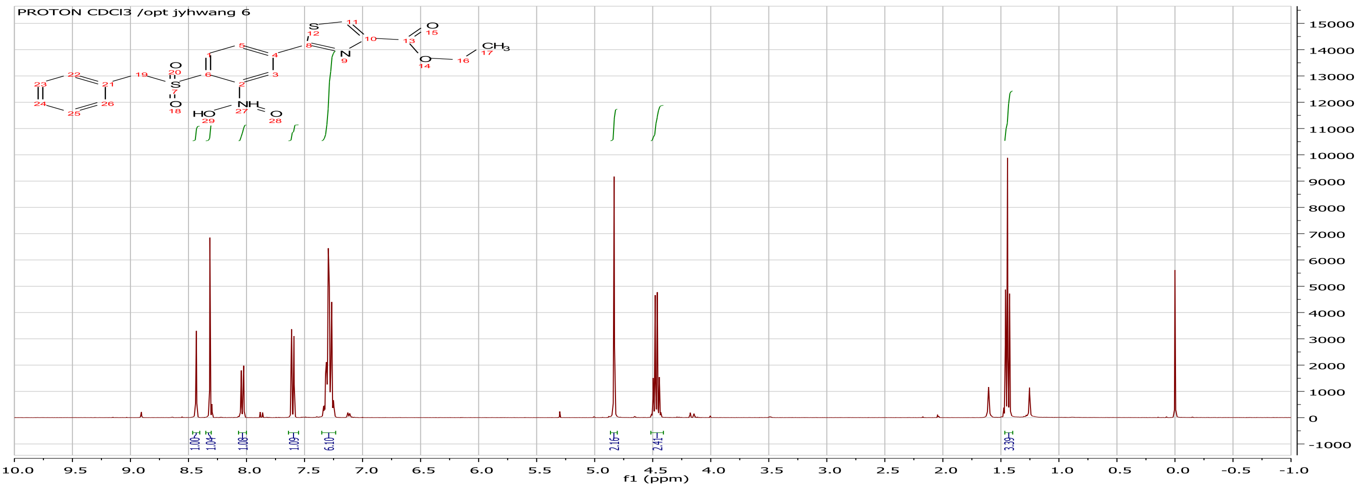

C13CPD CDCl3 /opt jyhwang 17
f1 (ppm)

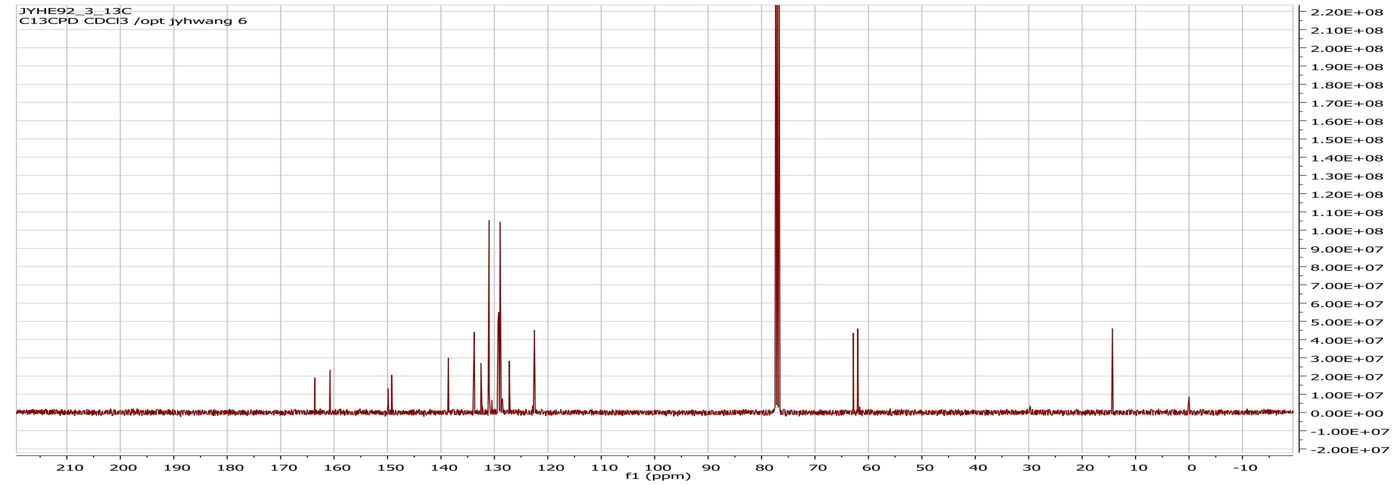
15{6,2}


PROTON CDCl3 /opt jyhwang 5
f1 (ppm)

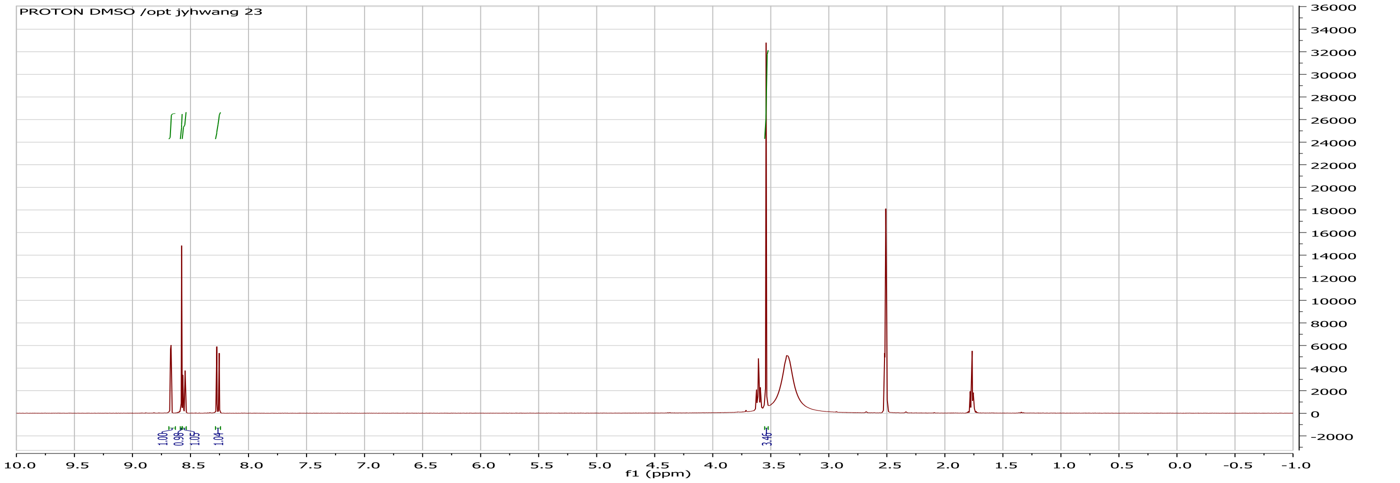

C13CPD CDCl3 /opt jyhwang 5
f1 (ppm)

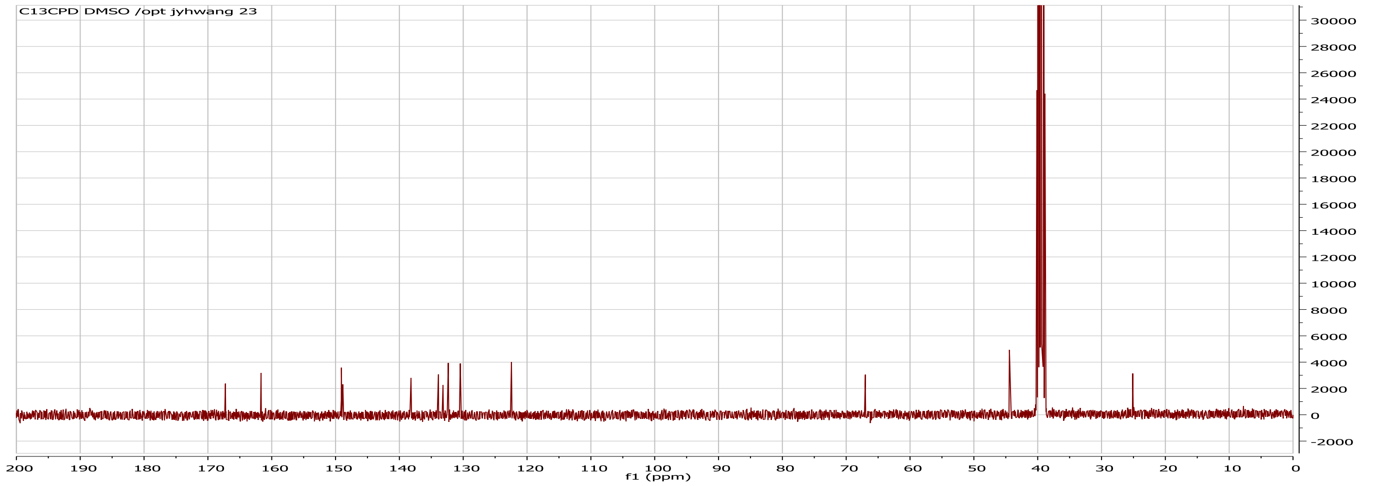
15{6,3}


PROTON CDCl3 /opt jyhwang 6
f1 (ppm)

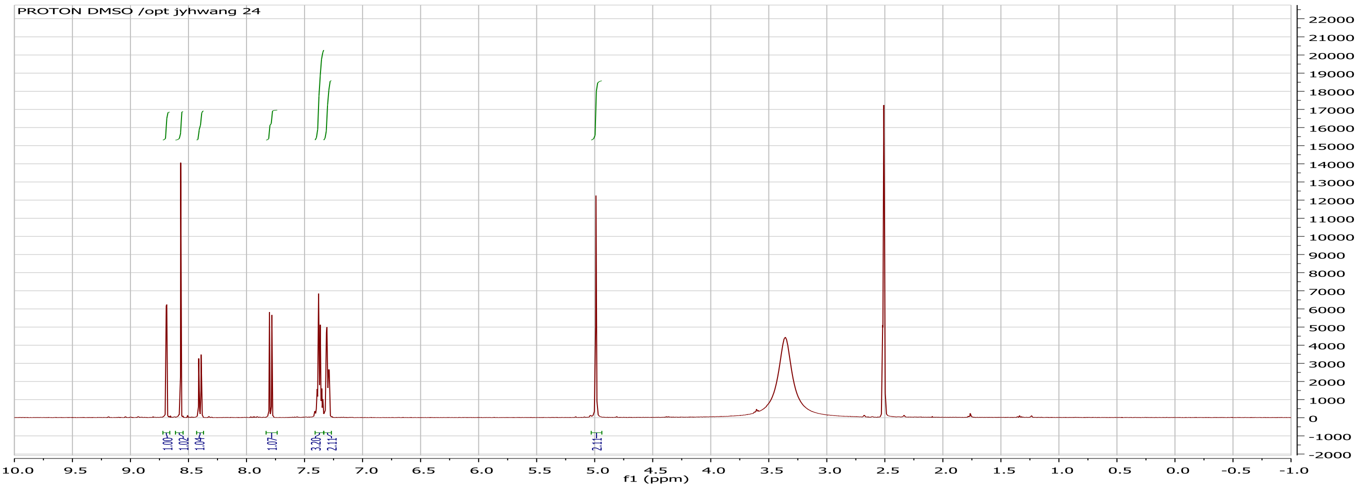

JYHE92_3_13C
C13CPD CDCl3 /opt jyhwang 6
f1 (ppm)

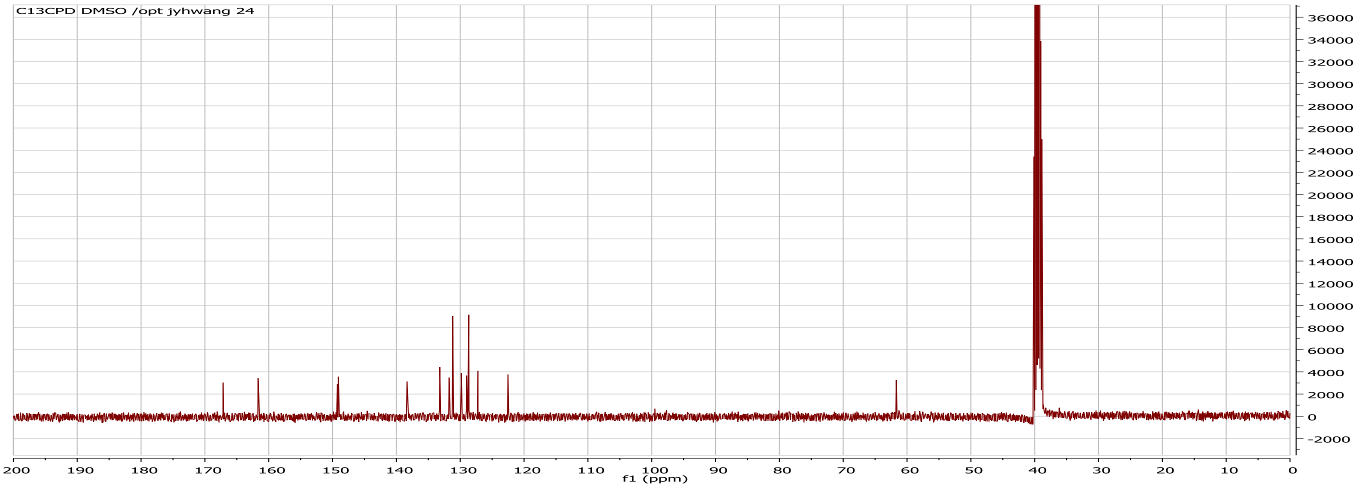
11{*1,1*}


PROTON DMSO /opt jyhwang 23
f1 (ppm)

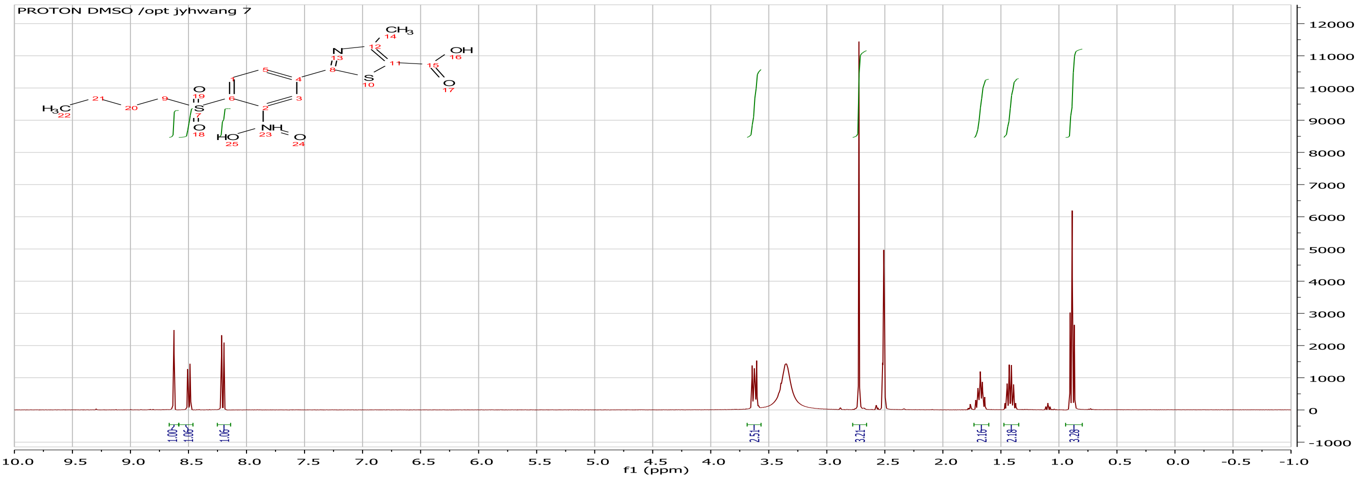

C13CPD DMSO /opt jyhwang 23
f1 (ppm)

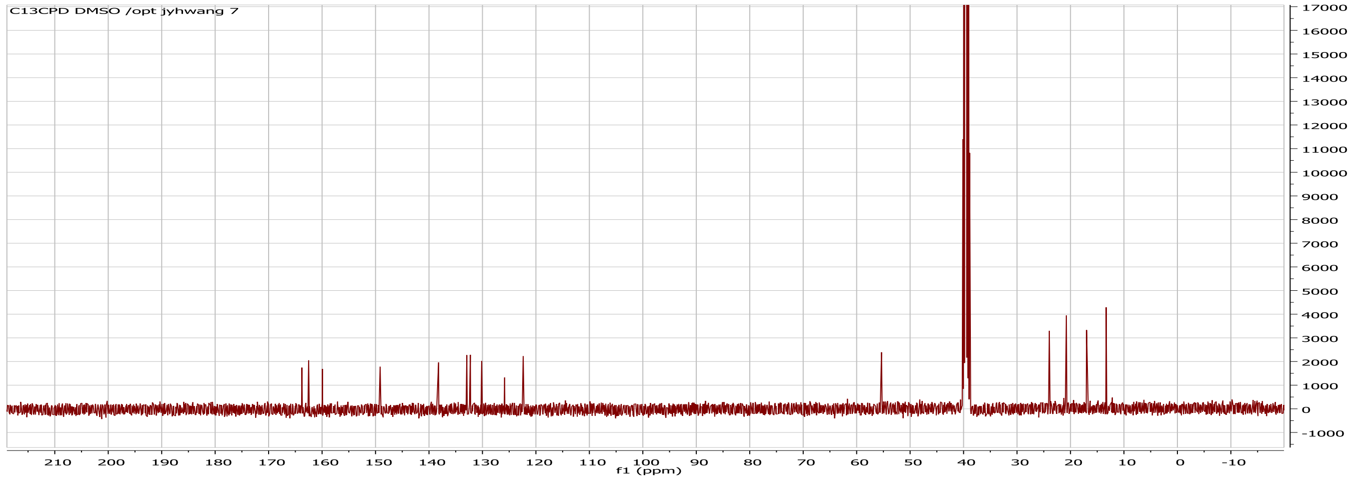
11{1,3}


PROTON DMSO /opt jyhwang 24
f1 (ppm)

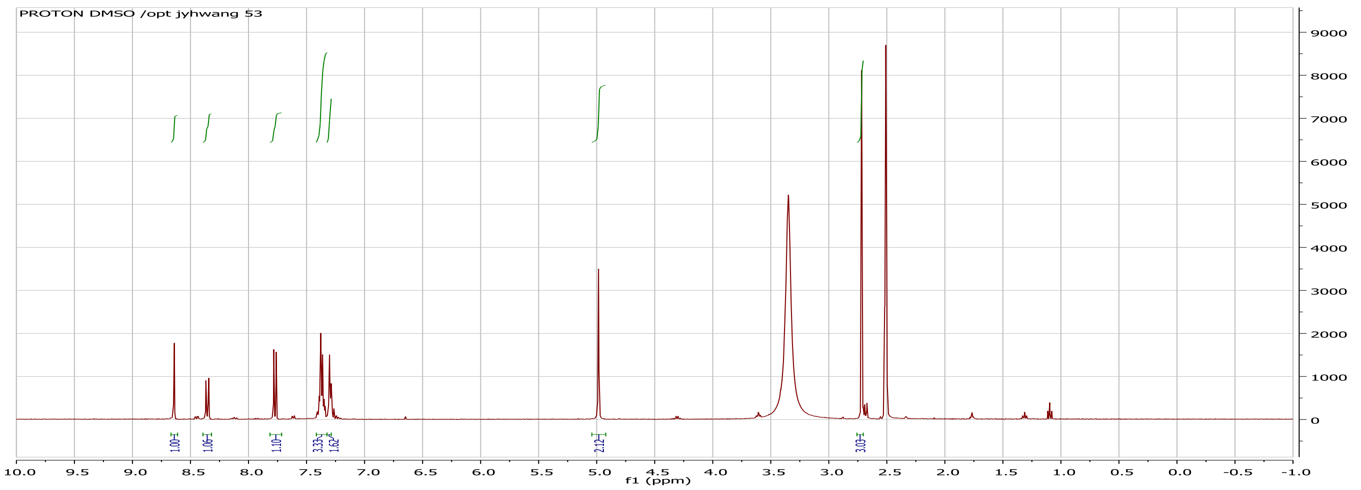

C13CPD DMSO /opt jyhwang 24
f1 (ppm)

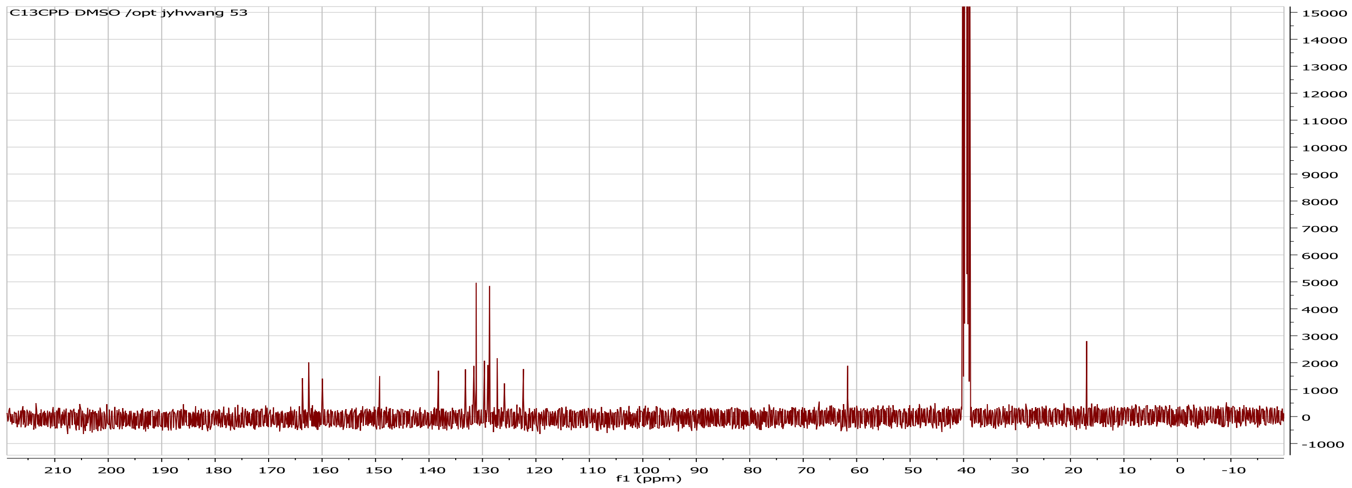
11{2,2}


PROTON DMSO /opt jyhwang 7
f1 (ppm)

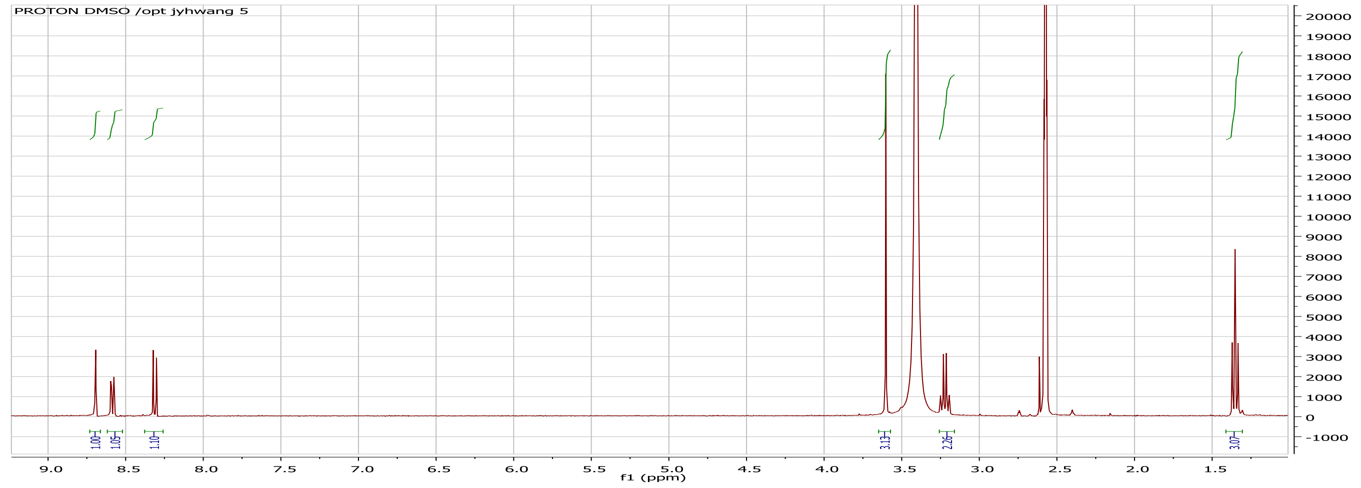

C13CPD DMSO /opt jyhwang 7
f1 (ppm)

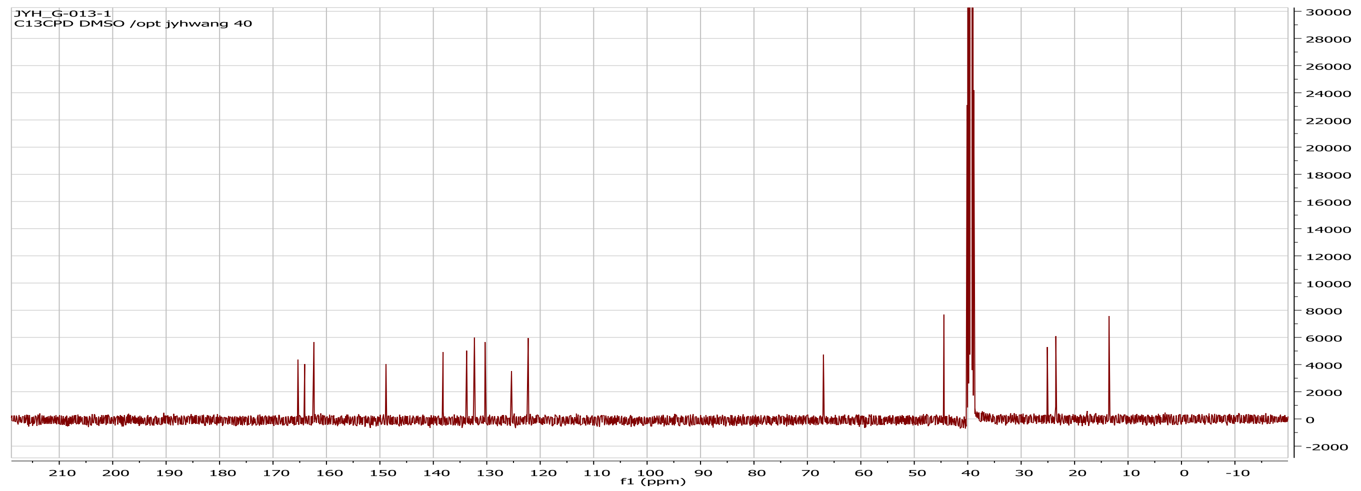
11{2,3}


PROTON DMSO /opt jyhwang 53
1.00
1.06
1.10
3.33
1.62
2.12
3.03
f1 (ppm)

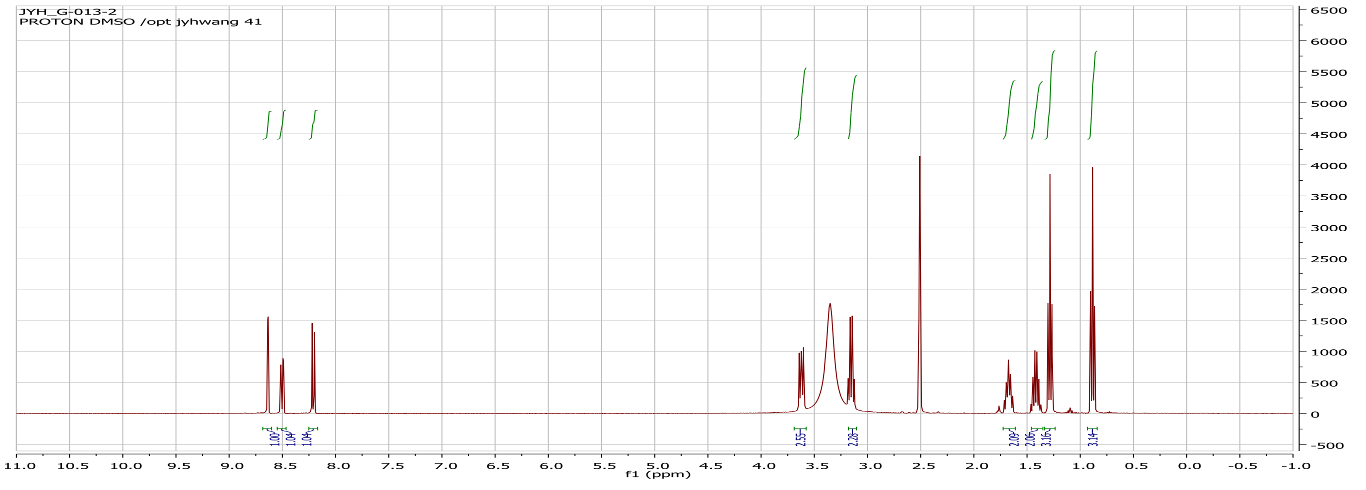

C13CPD DMSO /opt jyhwang 53
f1 (ppm)

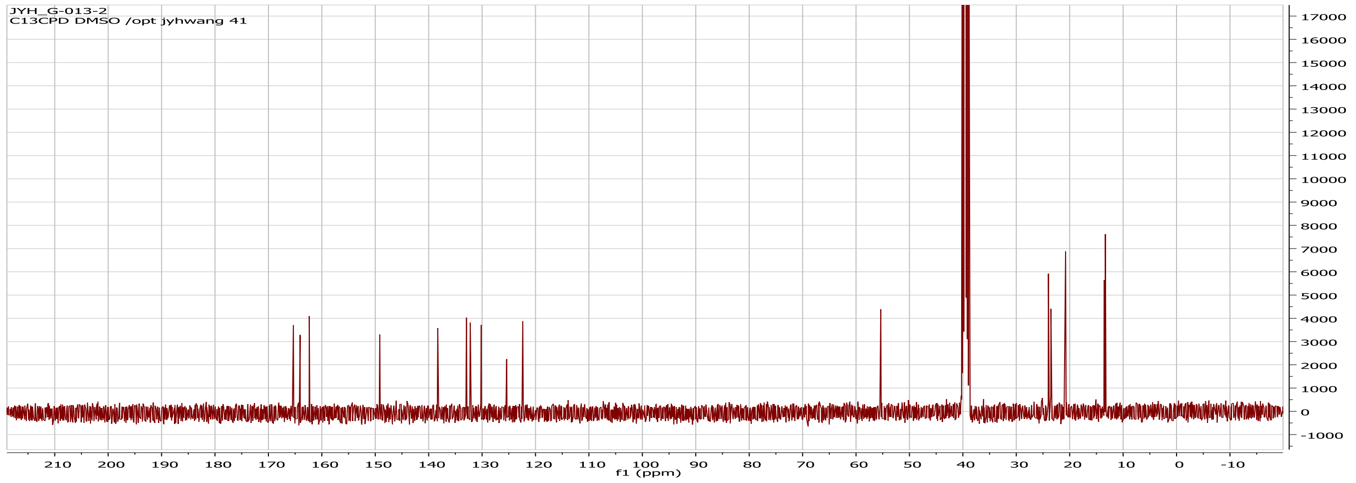
11{3,1}


PROTON DMSO /opt jyhwang 5
f1 (ppm)

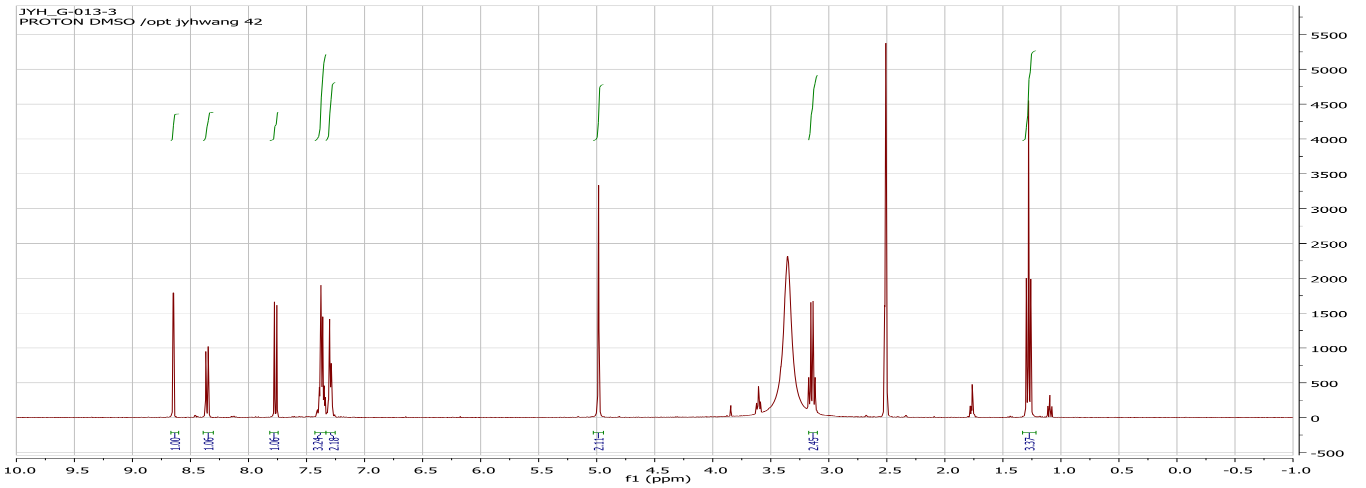

JYH_G-013-1
C13CPD DMSO /opt jyhwang 40
f1 (ppm)

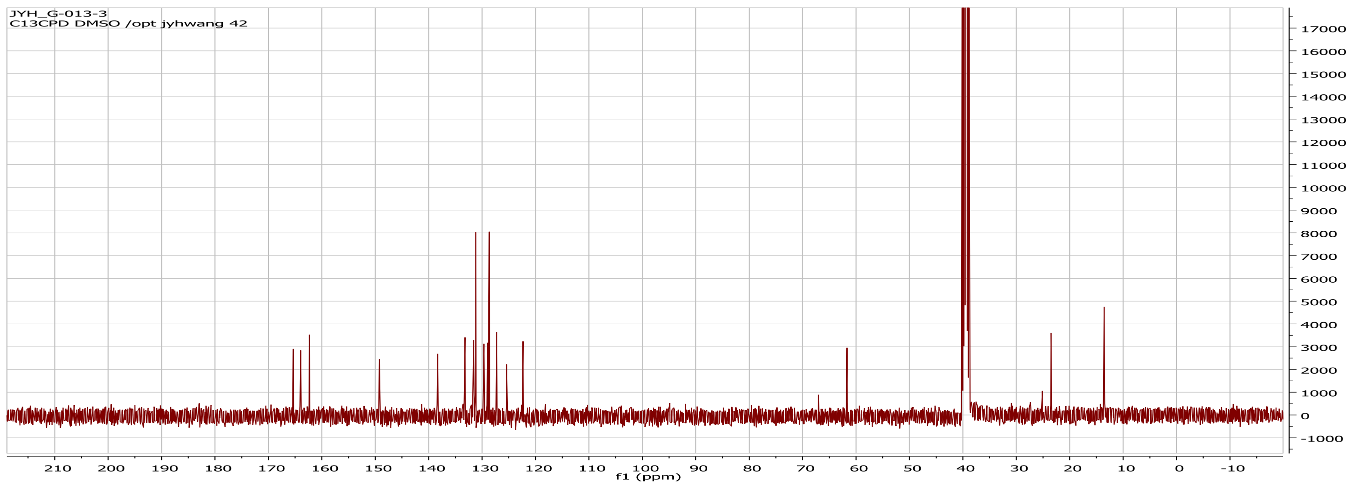
11{3,2}


JYH_G-013-2
PROTON DMSO /opt jyhwang 41
f1 (ppm)

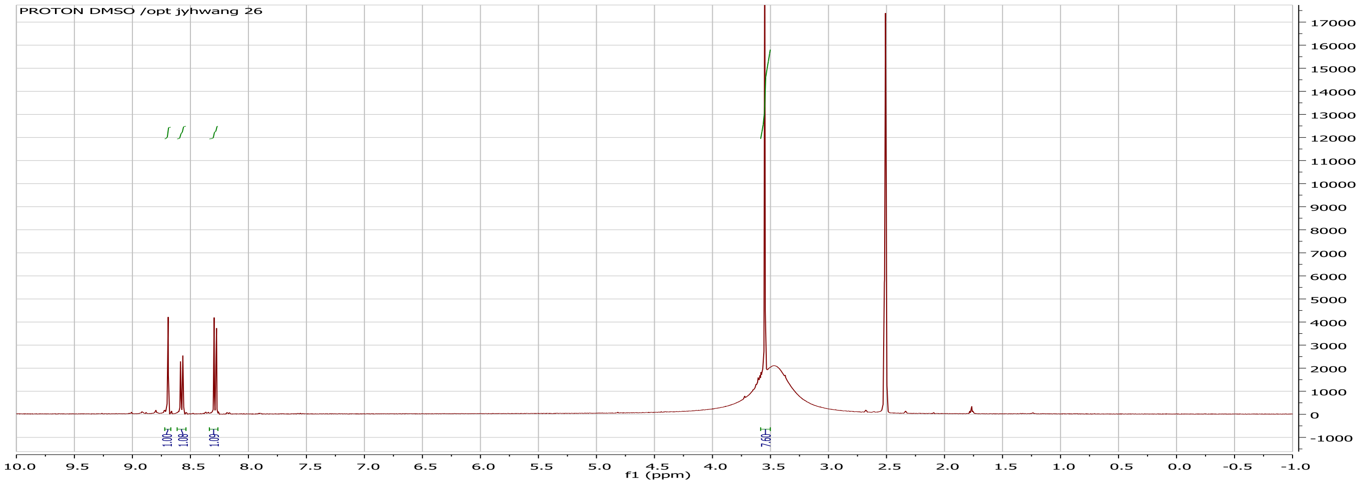

JYH_G-013-2
C13CPD DMSO /opt jyhwang 41
f1 (ppm)

11{3,3}

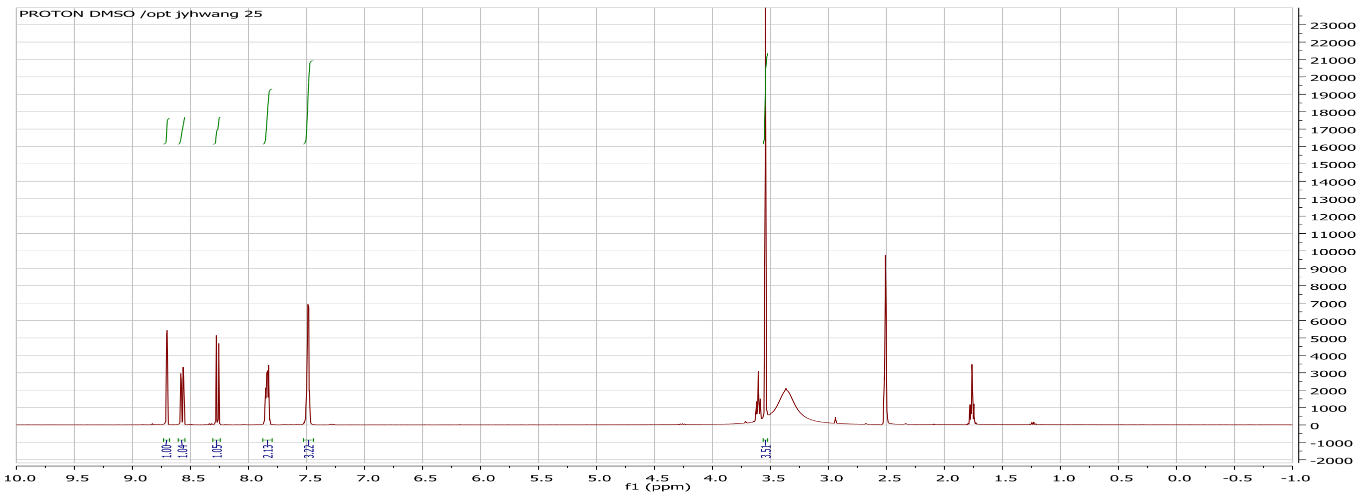

JYH_G-013-3
PROTON DMSO /opt jyhwang 42
1.00
1.06
1.06
3.24
2.18
2.11
2.45
3.37
f1 (ppm)

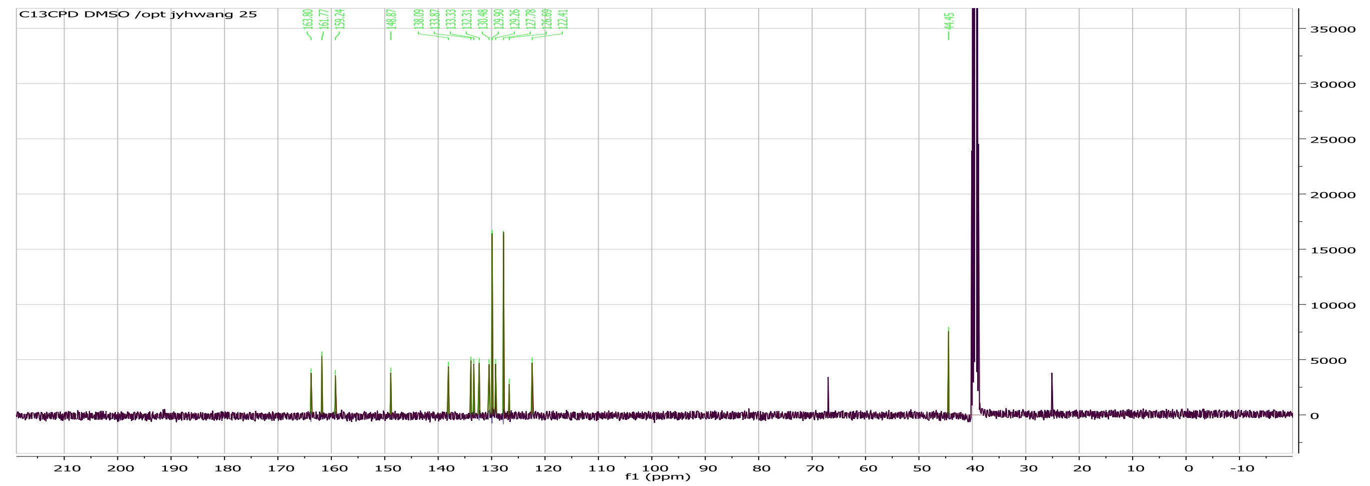

JYH_G-013-3
C13CPD DMSO /opt jyhwang 42
f1 (ppm)

11{4,1}

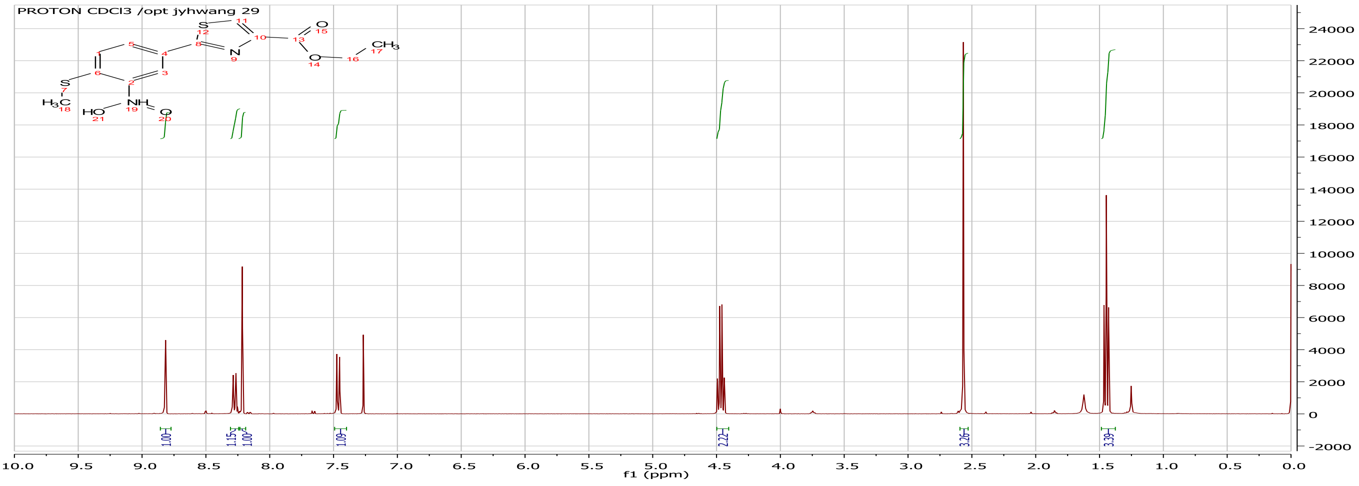

PROTON DMSO /opt jyhwang 26
f1 (ppm)

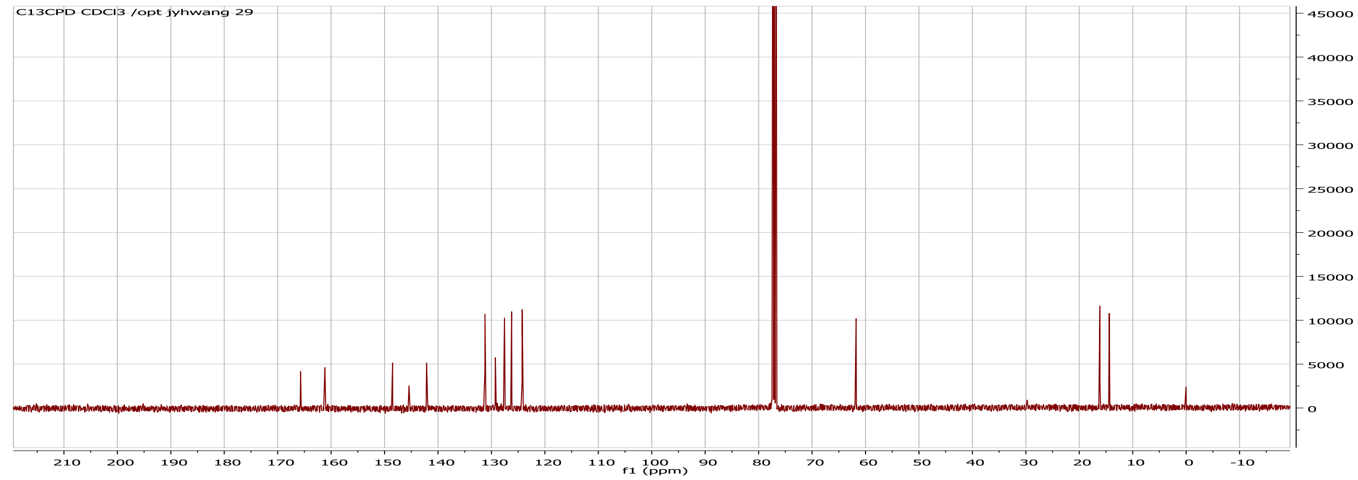
11{5,1}


PROTON DMSO /opt jyhwang 25
f1 (ppm)

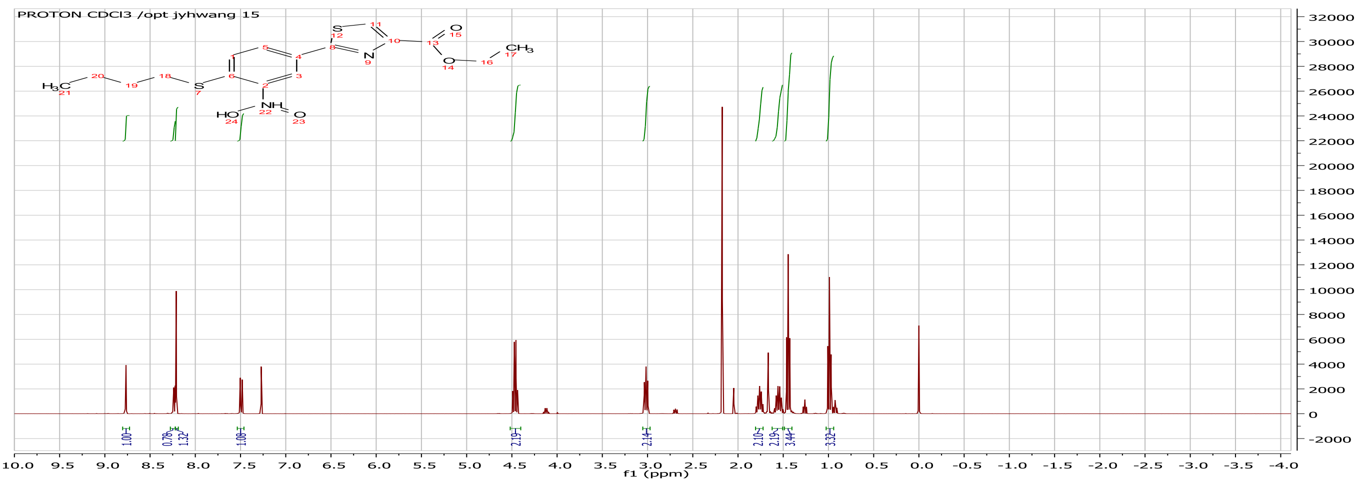

C13CPD DMSO /opt jyhwang 25
f1 (ppm)

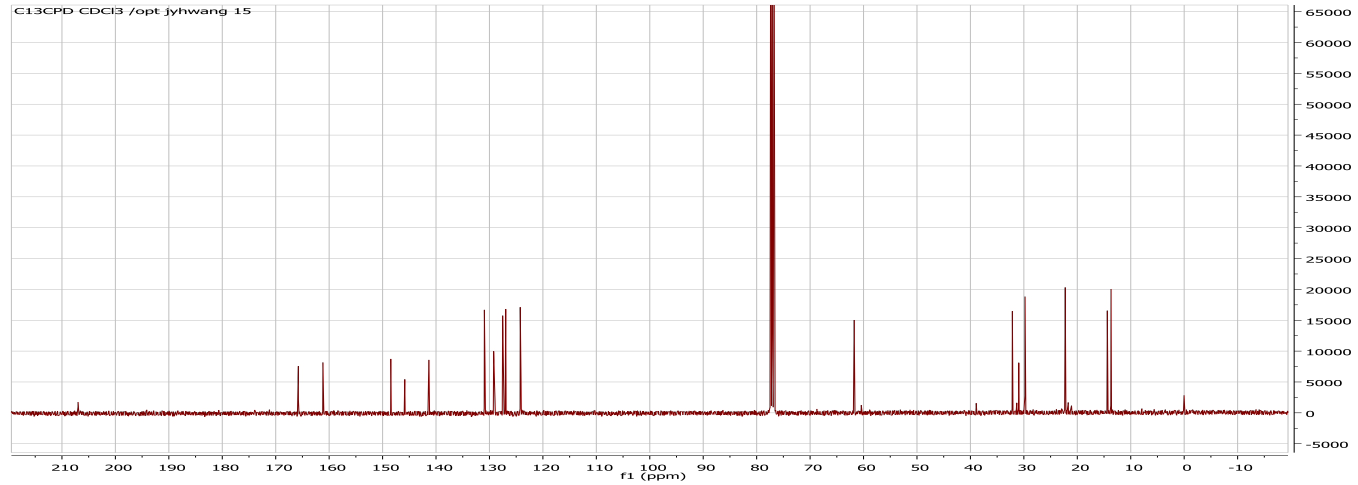
14{6,1}


PROTON CDCl3 /opt jyhwang 29
f1 (ppm)

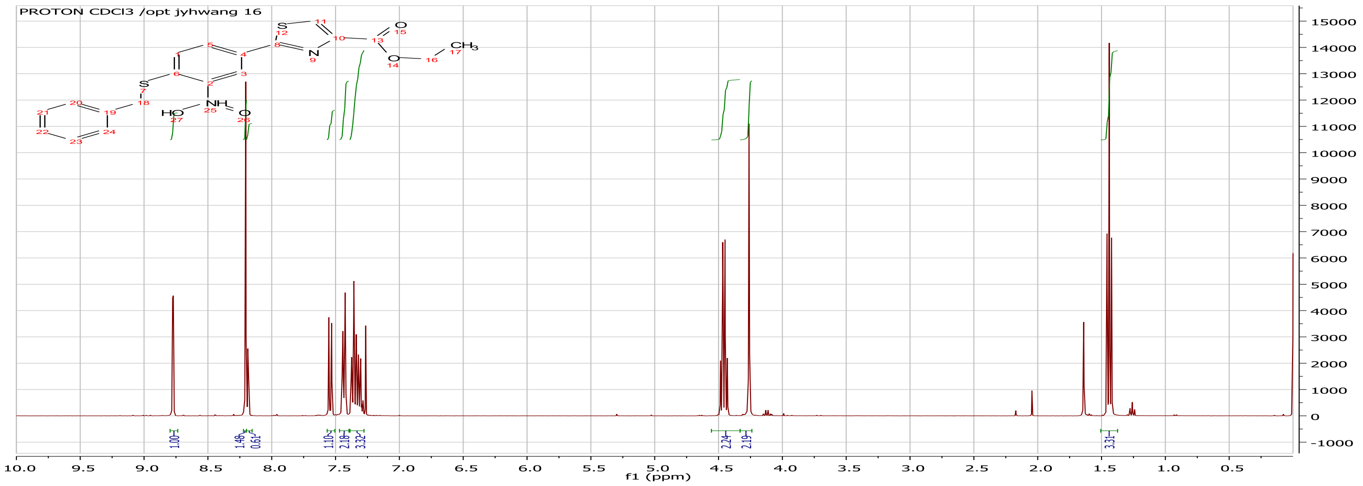

C13CPD CDCl3 /opt jyhwang 29
f1 (ppm)

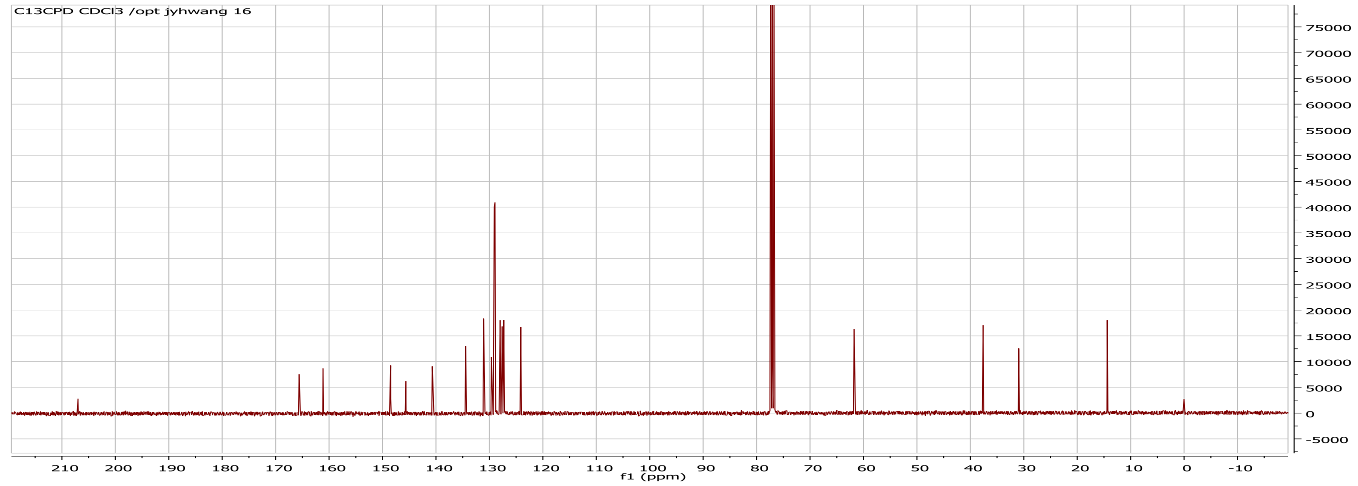
14{6,2}


PROTON CDCl3 /opt jyhwang 15
f1 (ppm)

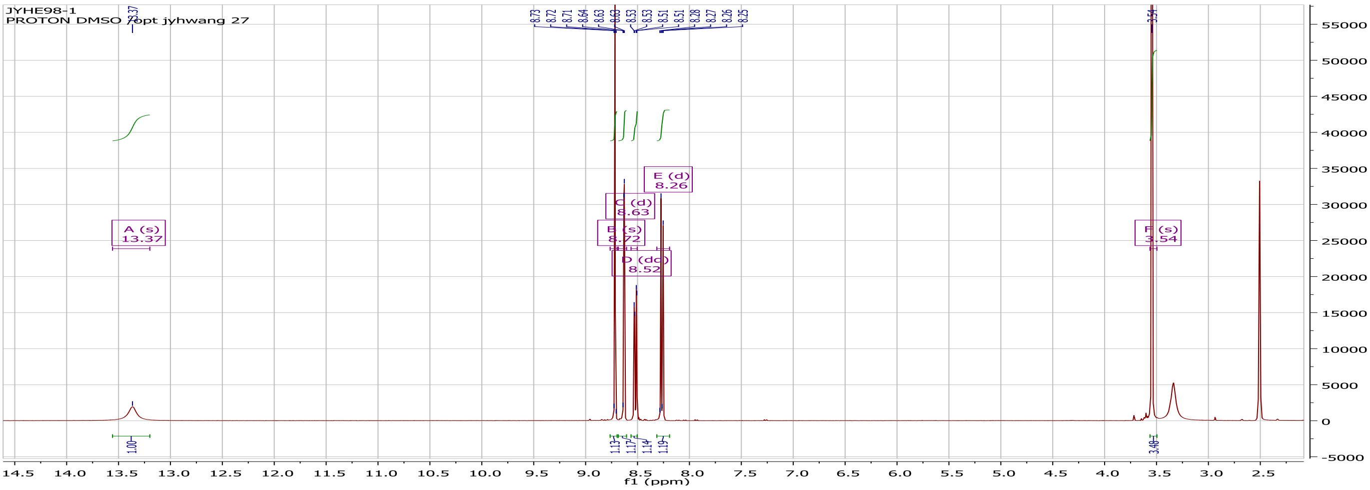

C13CPD CDCl3 /opt jyhwang 15
f1 (ppm)

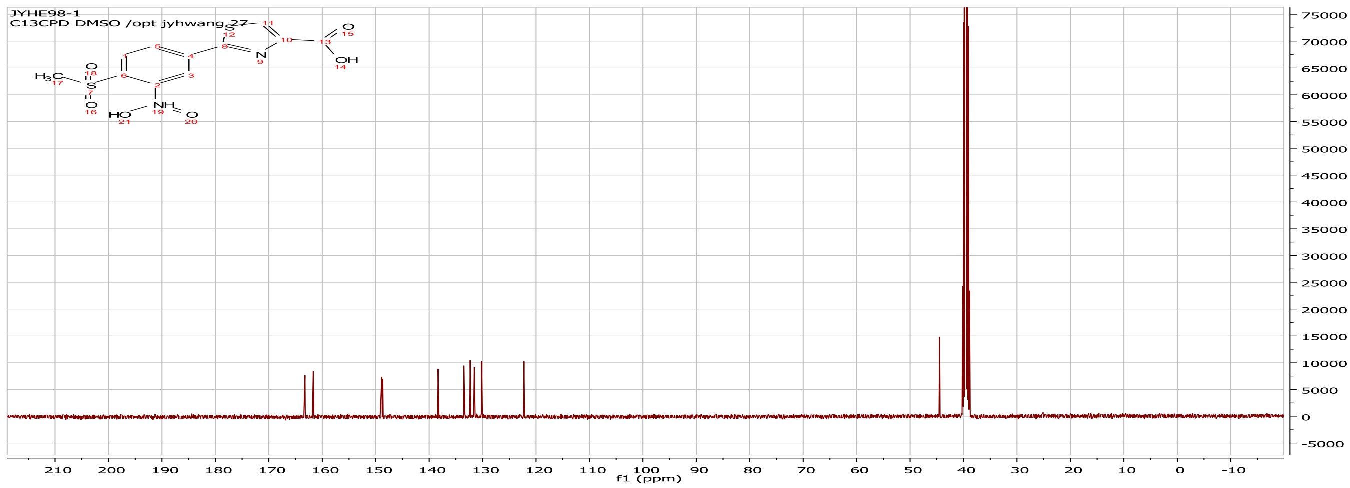
14{6,3}


PROTON CDCl3 /opt jyhwang 16
f1 (ppm)

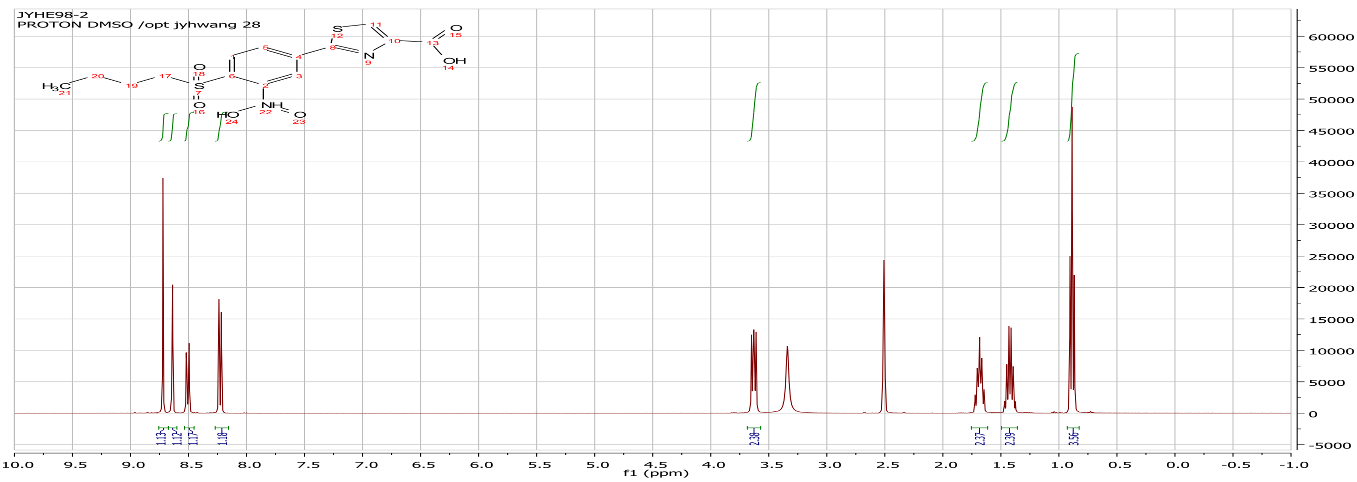

C13CPD CDCl3 /opt jyhwang 16
f1 (ppm)

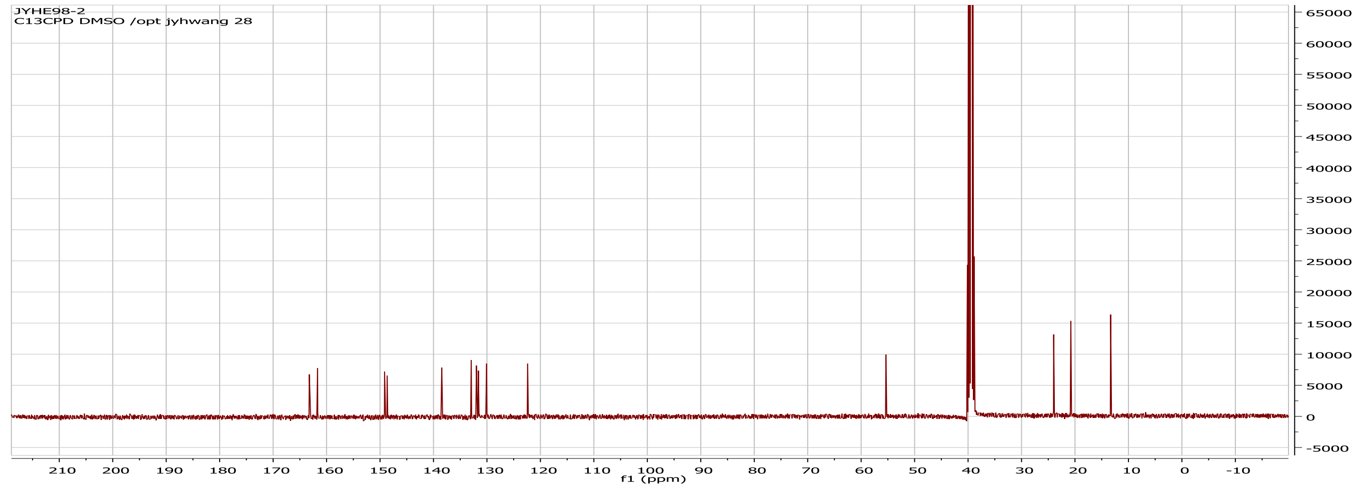
16{6,1}


JYHE98-1
PROTON DMSO /opt jyhwang 27
A (s)
13.37
B (s)
8.72
C (d)
8.63
D (dd)
8.52
E (d)
8.26
F (s)
3.54
f1 (ppm)

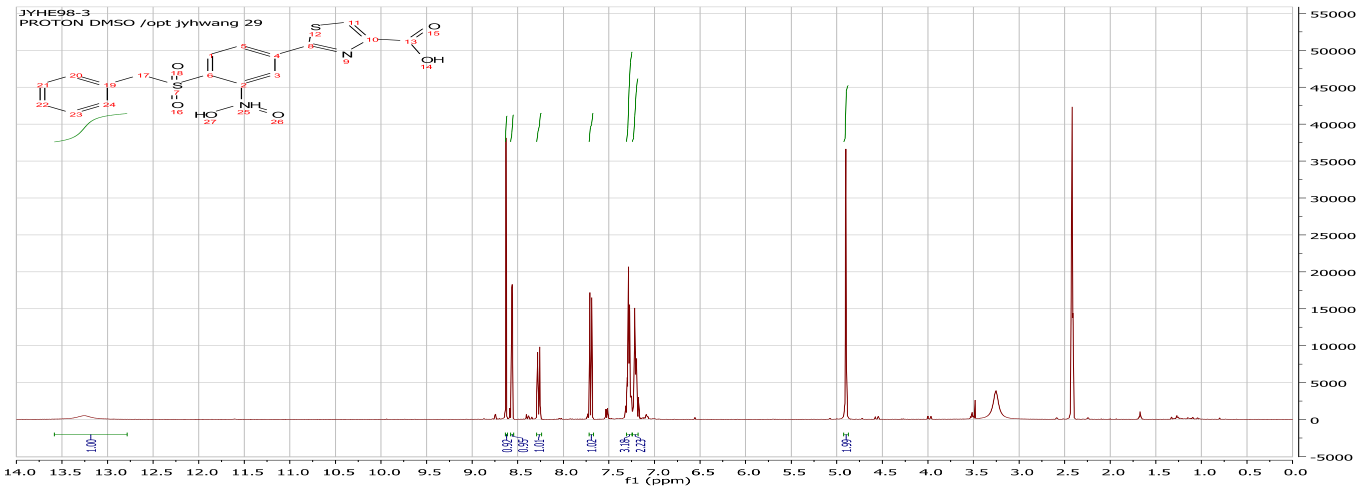

JYHE98-1
C13CPD DMSO /opt jyhwang 27
f1 (ppm)

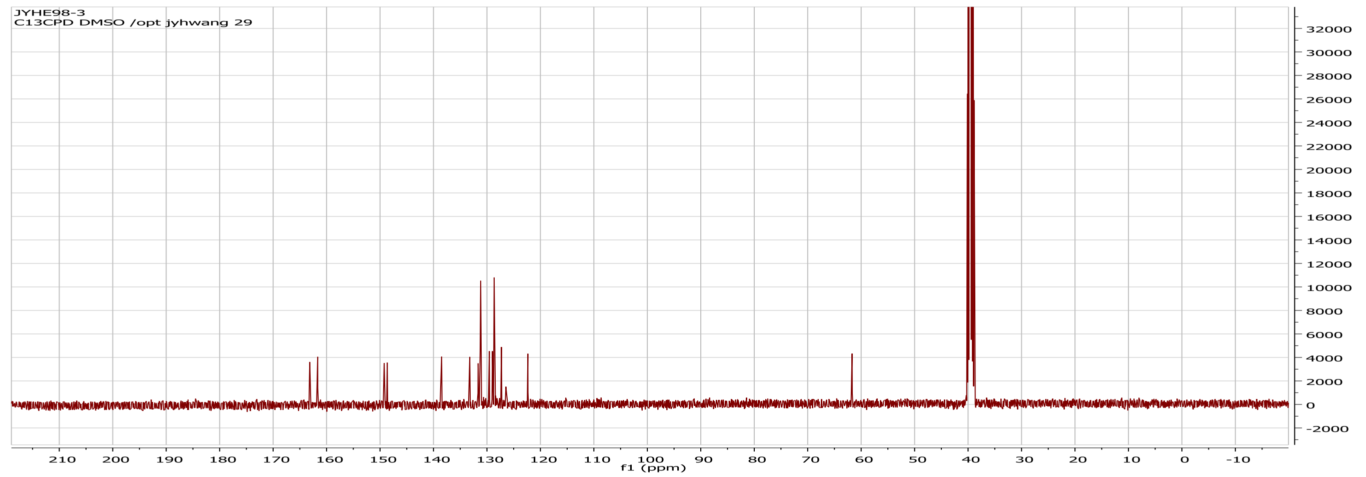
16{6,2}

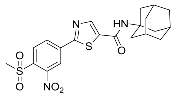

JYHE98-2
PROTON DMSO /opt jyhwang 28
f1 (ppm)


JYHE98-2
C13CPD DMSO /opt jyhwang 28
f1 (ppm)

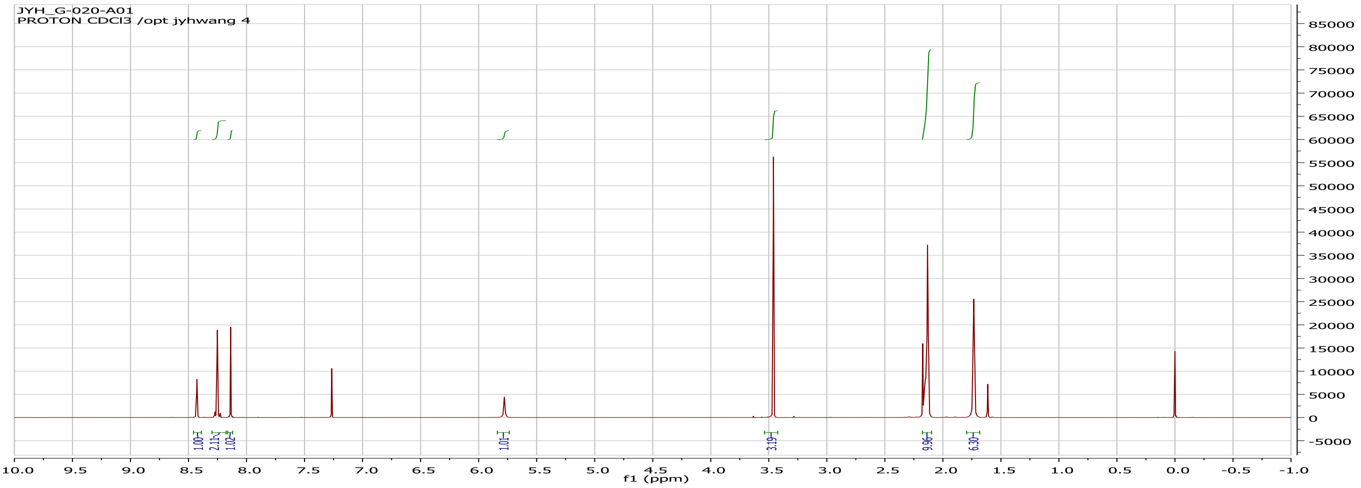
16{6,3}


JYHE98-3
PROTON DMSO /opt jyhwang 29
f1 (ppm)

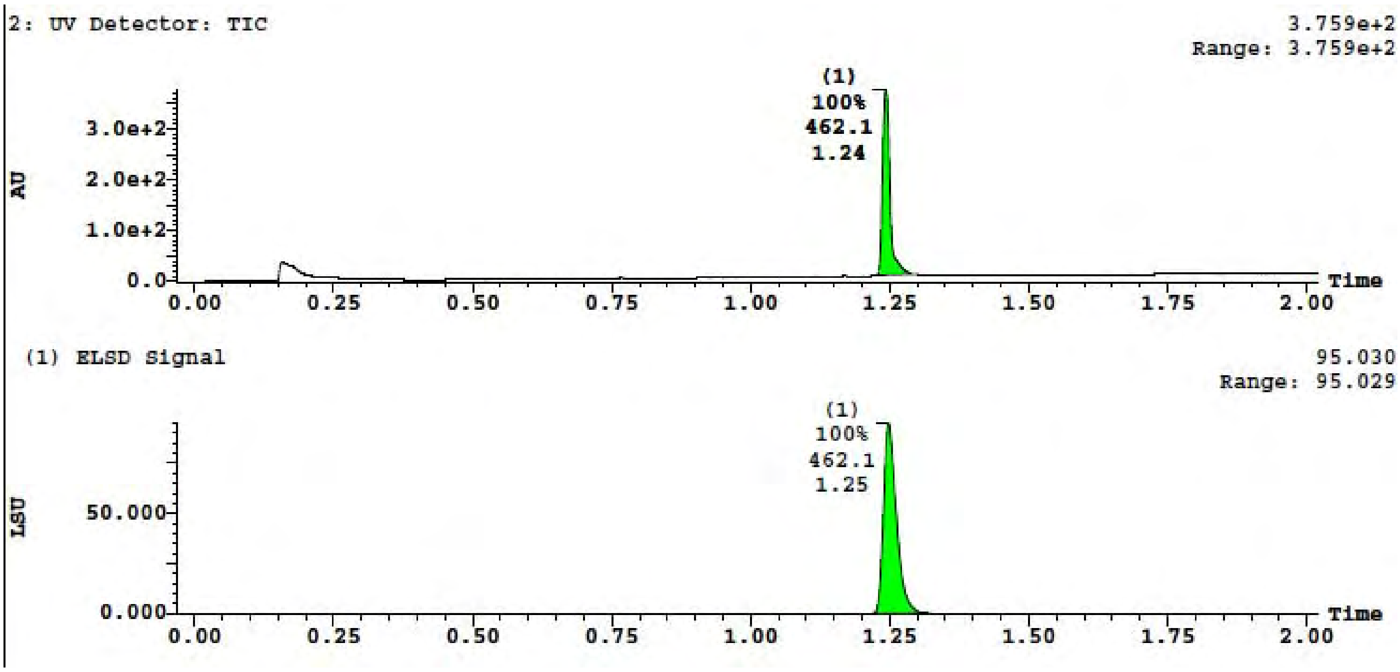

JYHE98-3
C13CPD DMSO /opt jyhwang 29
f1 (ppm)

2{*1,1,1*}	

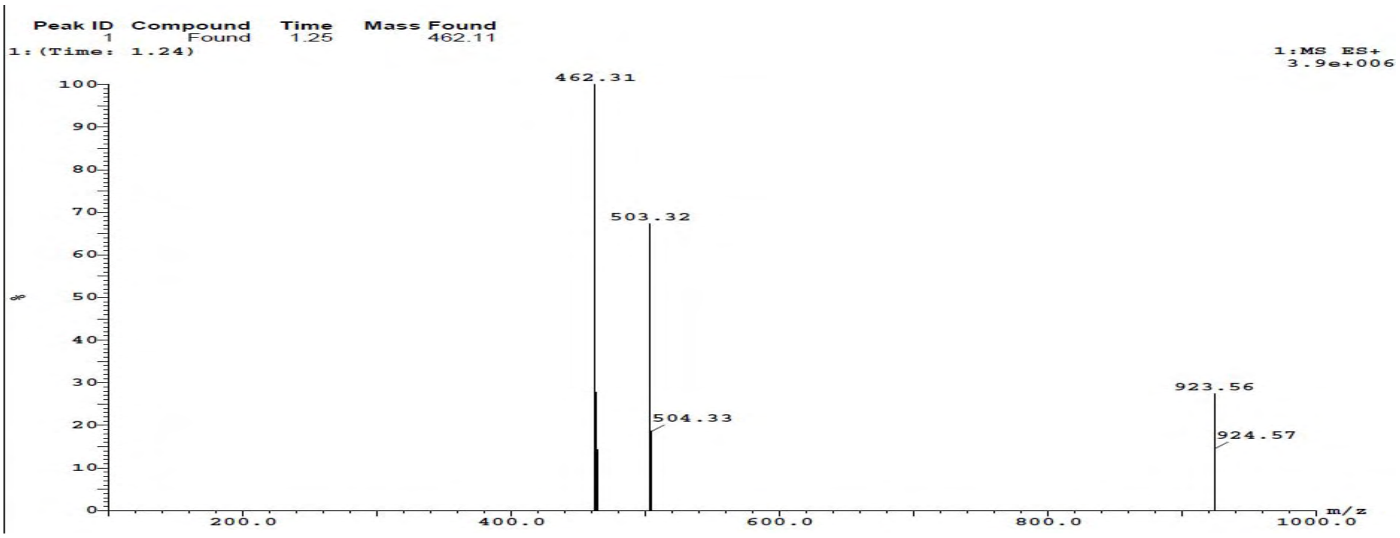
N
S
HN
O
O
S
O
NO2



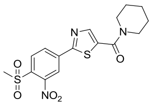
JYH_G-020-A01
PROTON CDCl3 /opt jyhwang 4
1.00
2.11
1.02
1.01
3.19
9.96
6.30
f1 (ppm)

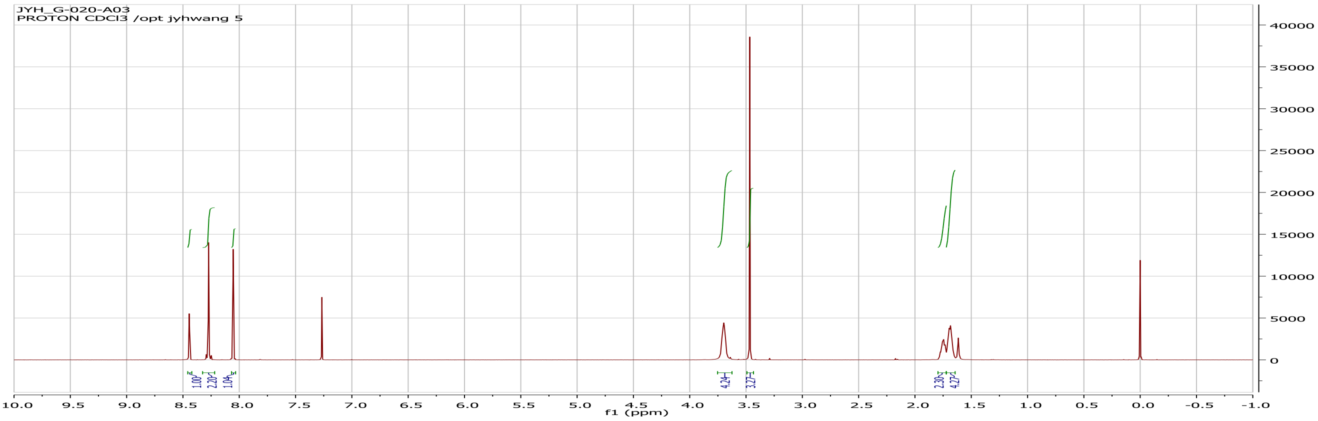


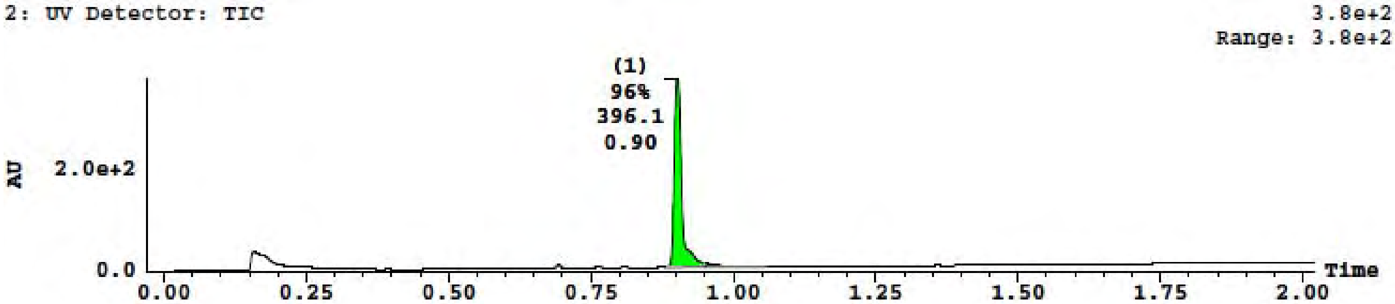
2: UV Detector: TIC
3.759e+2
Range: 3.759e+2
(1)
100%
462.1
1.24
AU
Time
(1) ELSD Signal
95.030
Range: 95.029
(1)
100%
462.1
1.25
LSU
Time

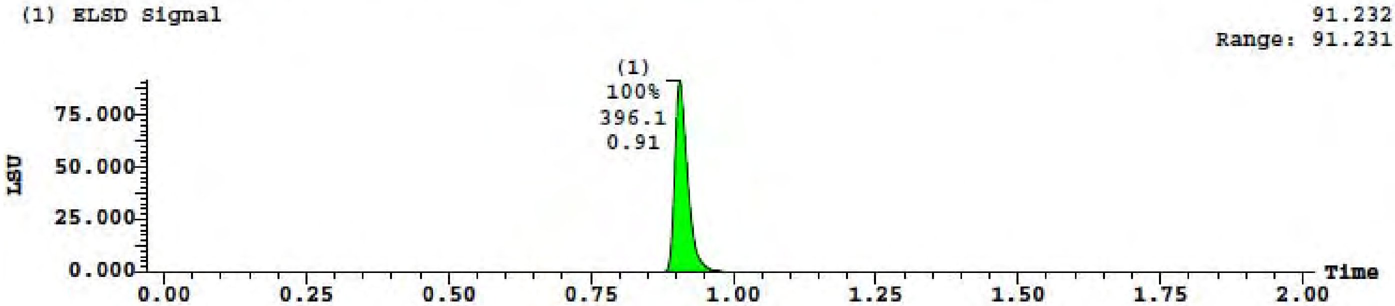


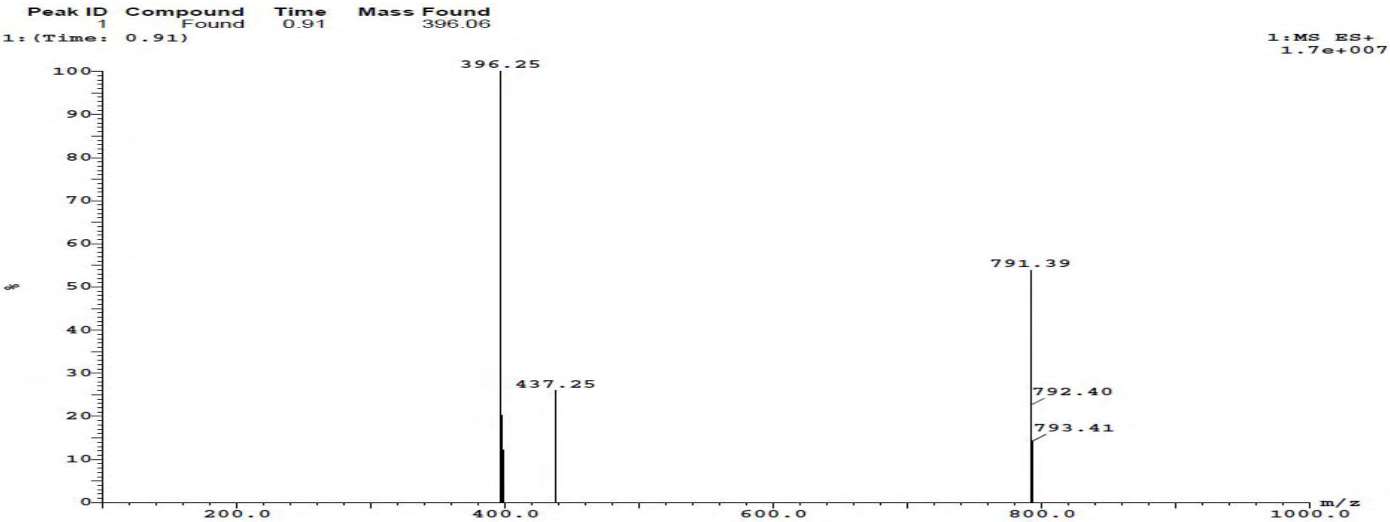
Peak ID Compound Time Mass Found
1 Found 1.25 462.11
1: (Time: 1.24)
1:MS ES+
3.9e+006
462.31
503.32
504.33
923.56
924.57
%
m/z

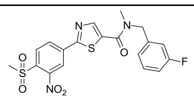
2{*1,1,4*}	

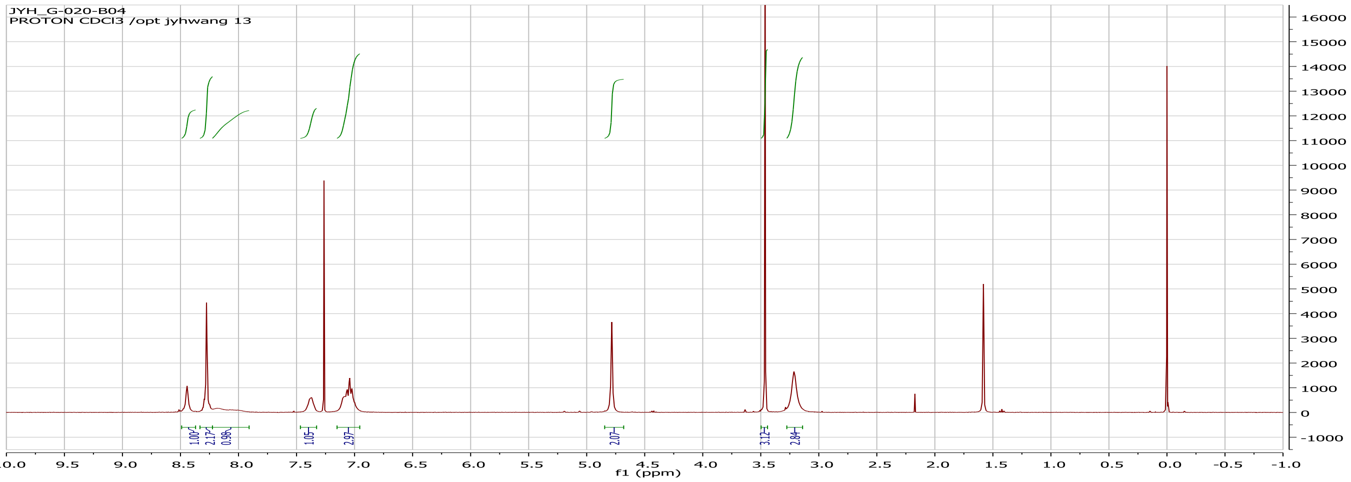

JYH_G-020-A03
PROTON CDCl3 /opt jyhwang 5
f1 (ppm)

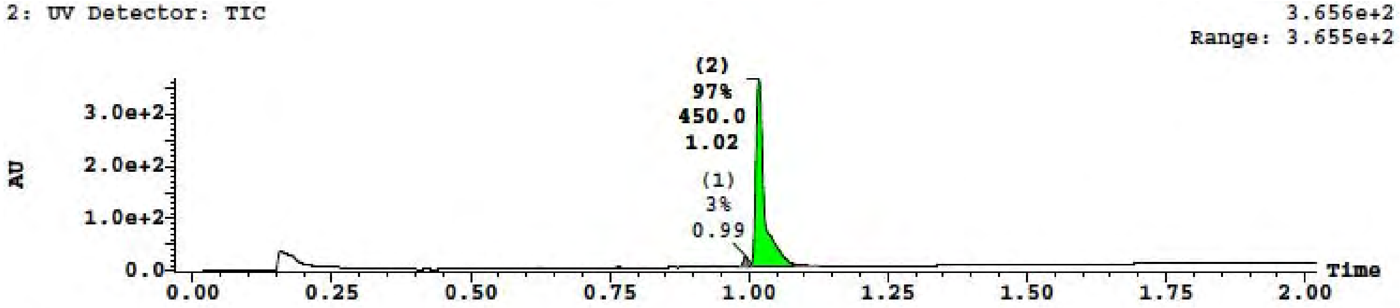

2: UV Detector: TIC
3.8e+2
Range: 3.8e+2
(1)
96%
396.1
0.90
AU
2.0e+2
0.0
Time

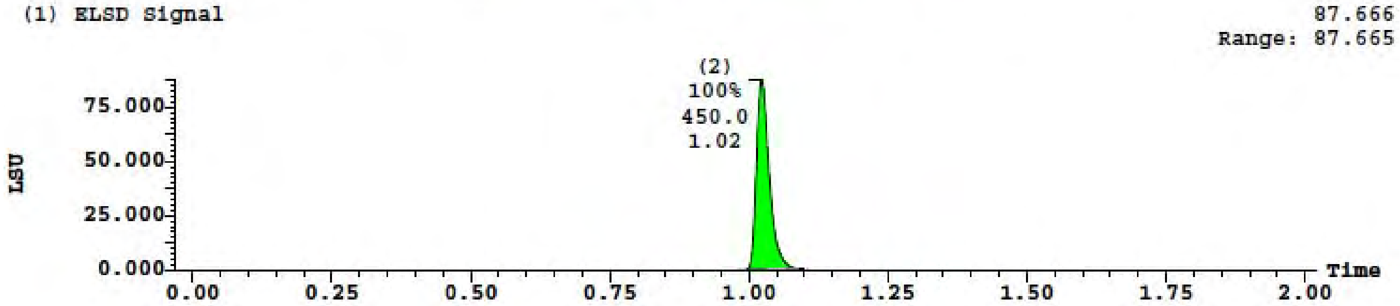

(1) ELSD Signal
91.232
Range: 91.231
(1)
100%
396.1
0.91
LSU
Time


Peak ID Compound Time Mass Found
1 Found 0.91 396.06
1: (Time: 0.91)
1:MS ES+
1.7e+007
396.25
437.25
791.39
792.40
793.41
%
m/z

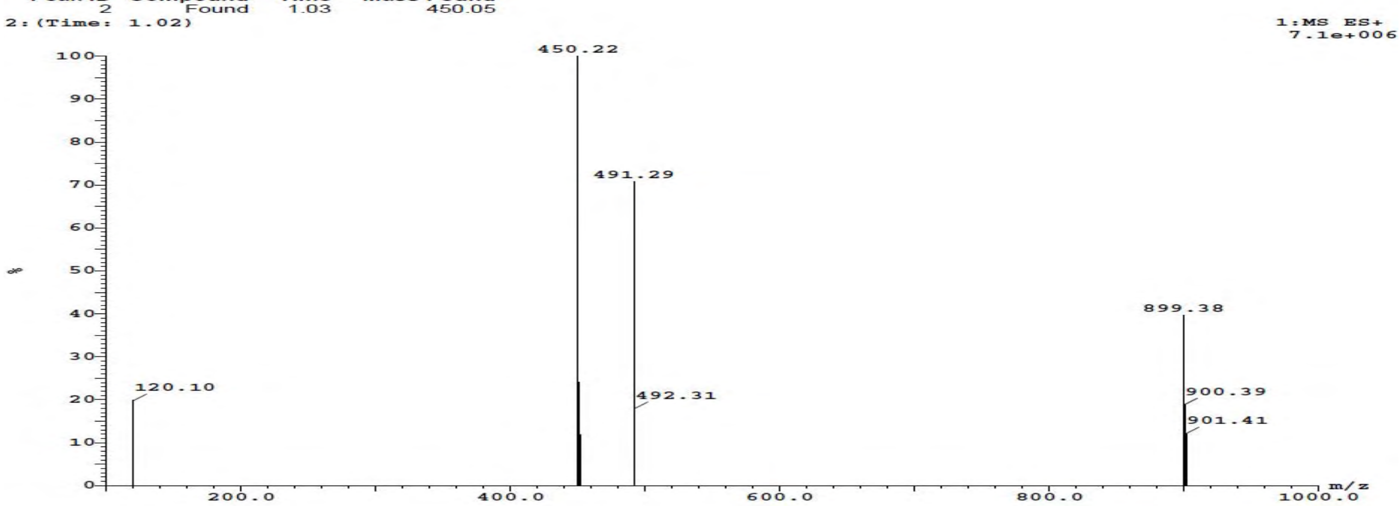
2{*1,1,16*}	

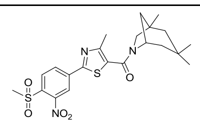


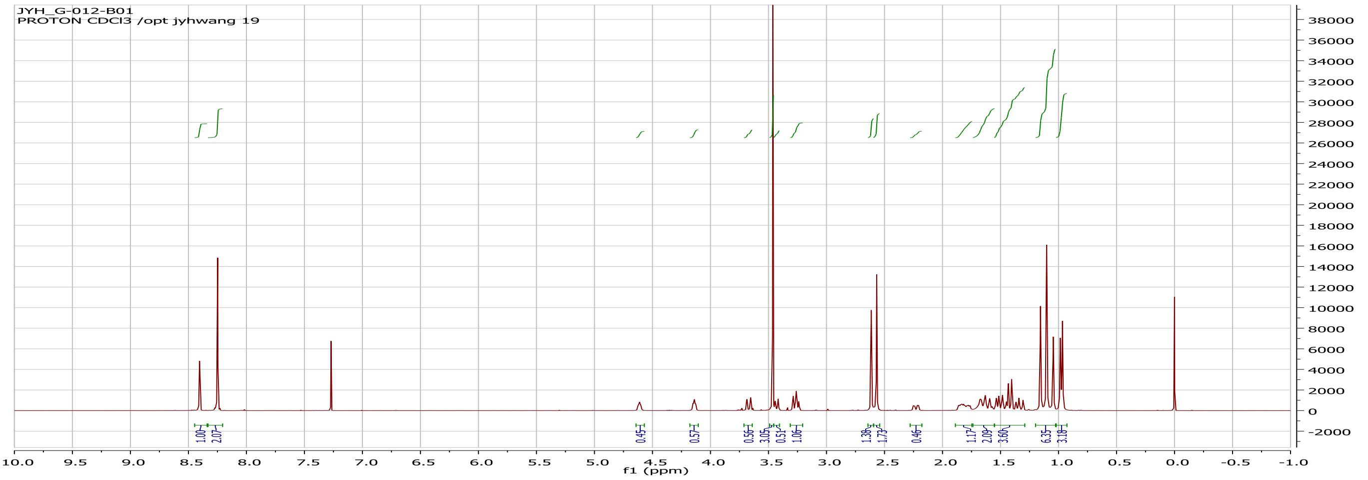


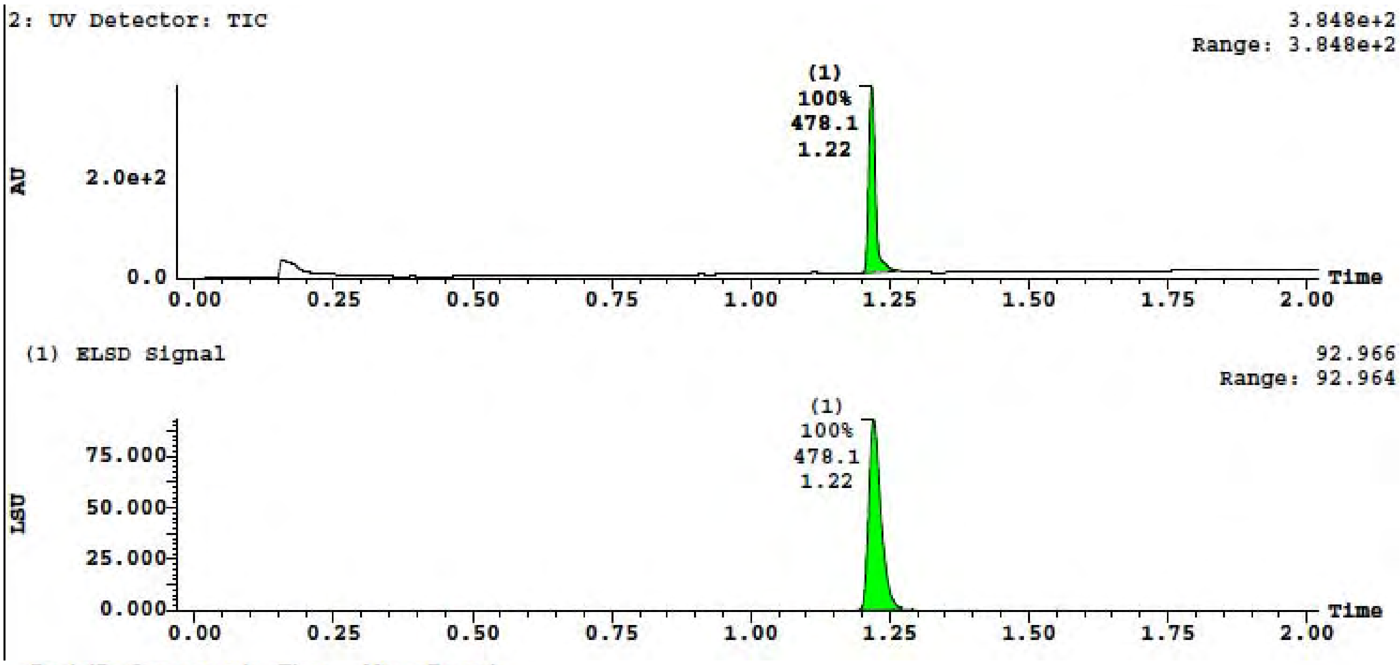


Peak ID	Compound	Time	Mass Found
2	Found	1.03	450.05



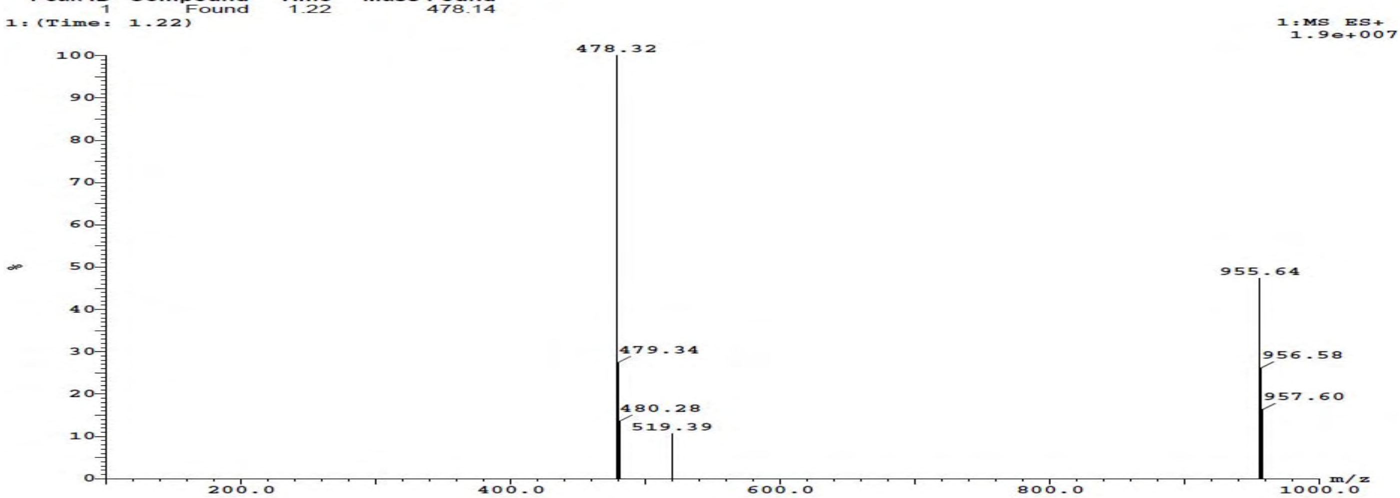
2{*2,1,2*}	

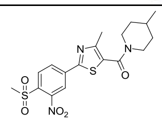


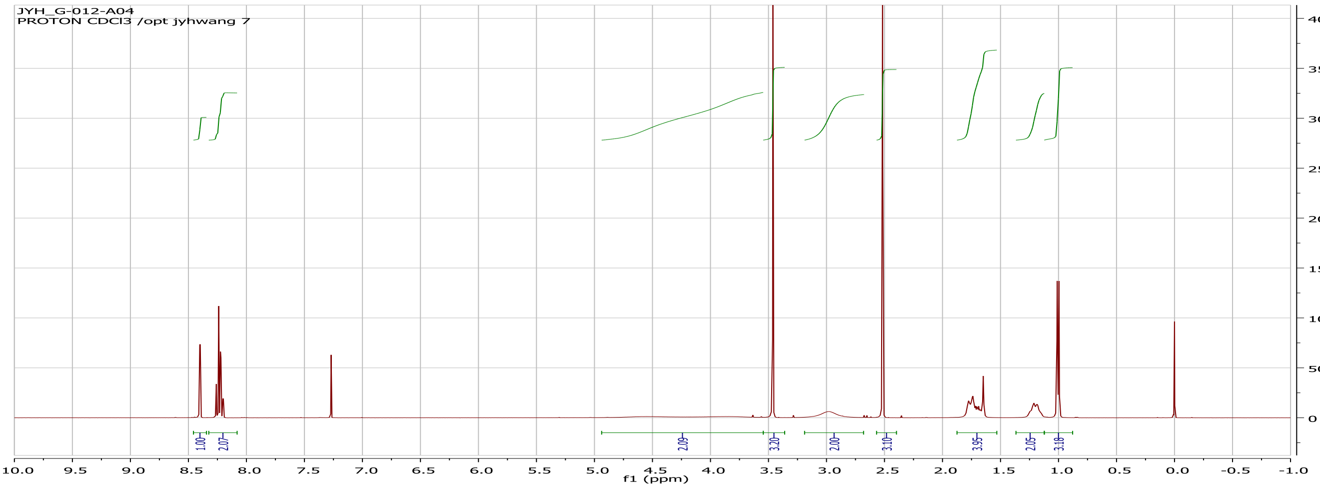


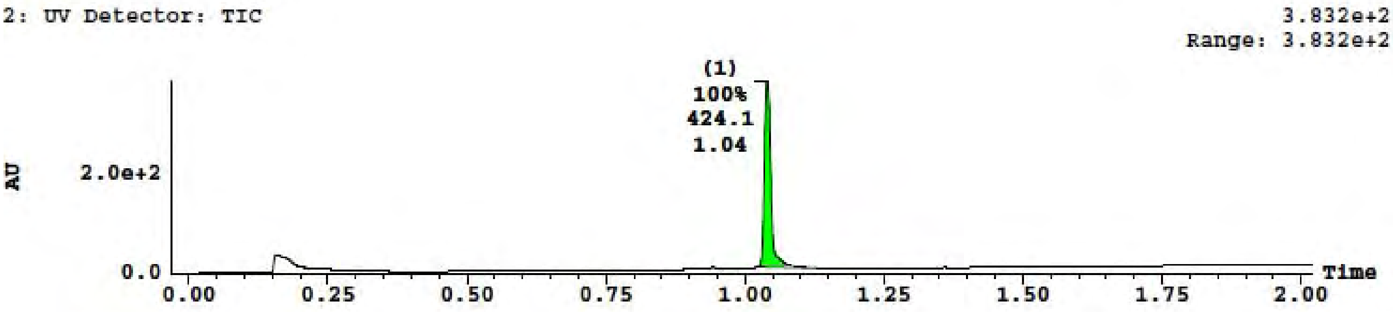
Peak ID	Compound	Time	Mass Found
1	Found	1.22	478.14

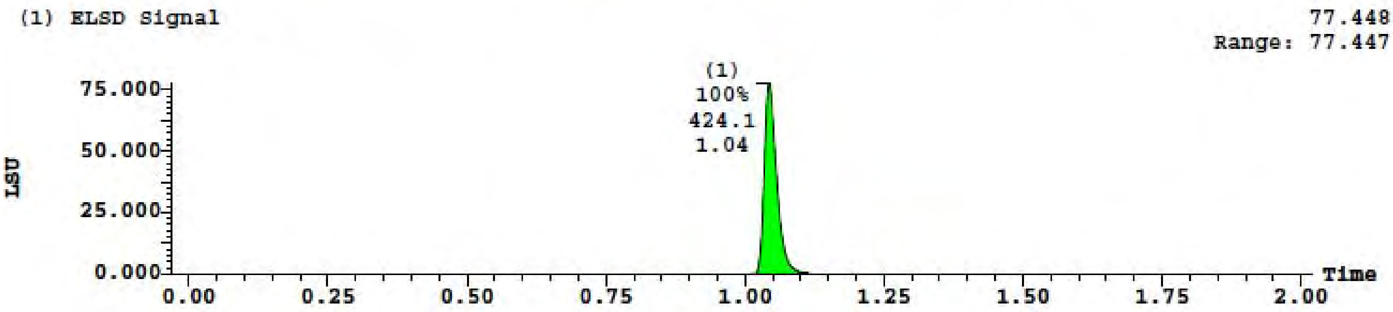
1: (Time: 1.22)

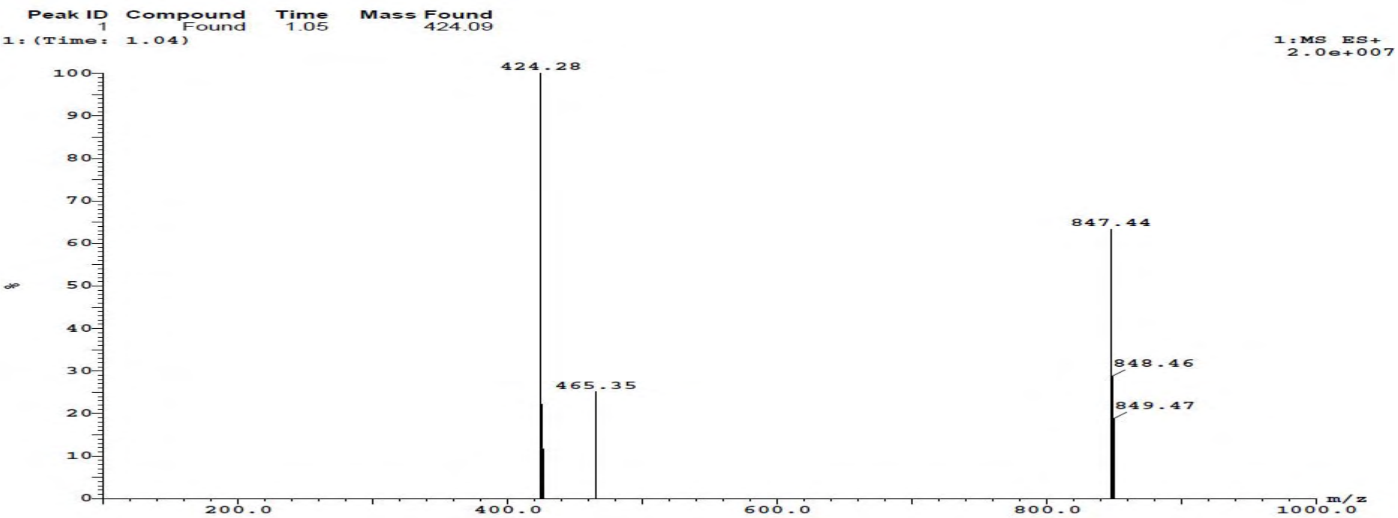


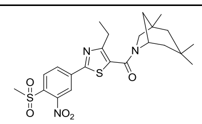
2{*2,1,5*}	

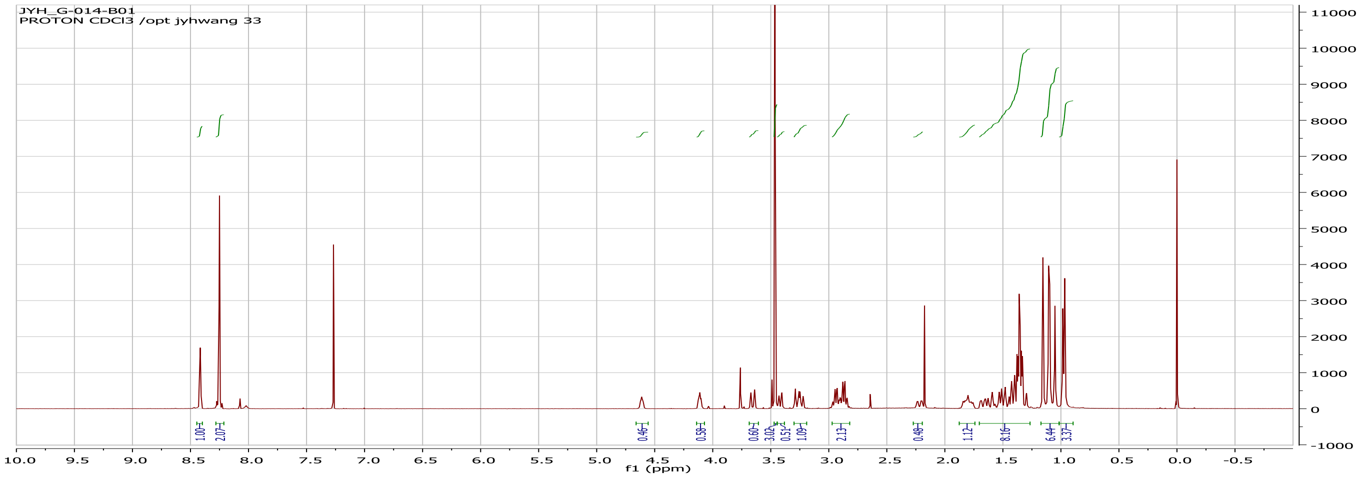

JYH_G-012-A04
PROTON CDCl3 /opt jyhwang 7
f1 (ppm)
1.00
2.07
2.09
3.20
2.00
3.10
3.95
2.05
3.18

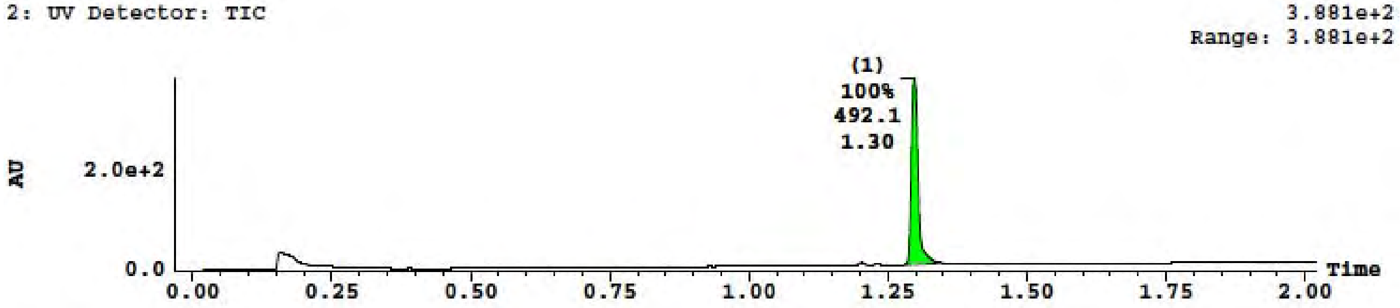

2: UV Detector: TIC
3.832e+2
Range: 3.832e+2
(1)
100%
424.1
1.04
AU
2.0e+2
0.0
Time

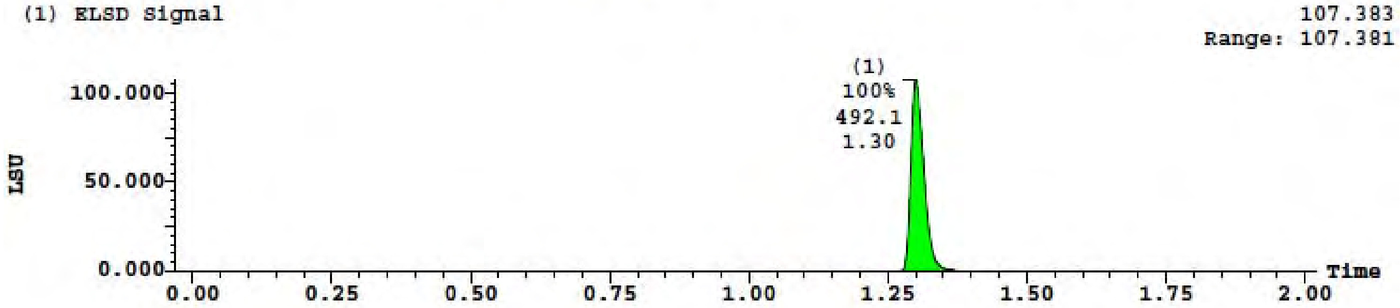

(1) ELSD Signal
77.448
Range: 77.447
(1)
100%
424.1
1.04
LSU
Time


Peak ID Compound Time Mass Found
1 Found 1.05 424.09
1: (Time: 1.04)
1: MS ES+
2.0e+007
424.28
465.35
847.44
848.46
849.47
%
m/z

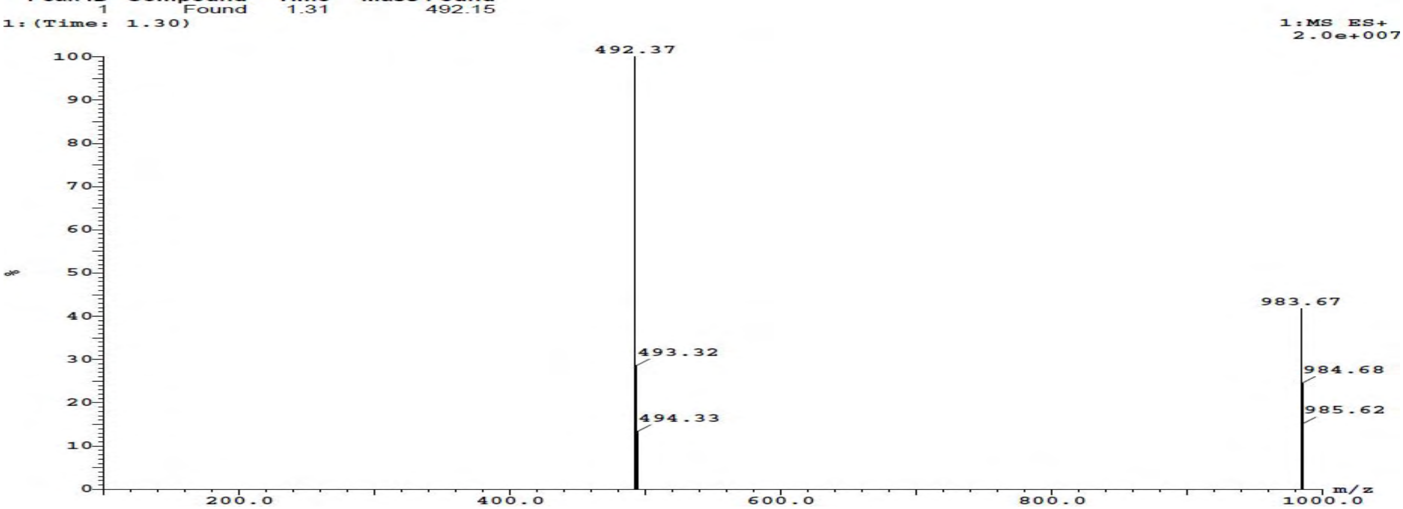
2{*3*,*1*,*2*}	

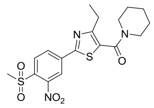


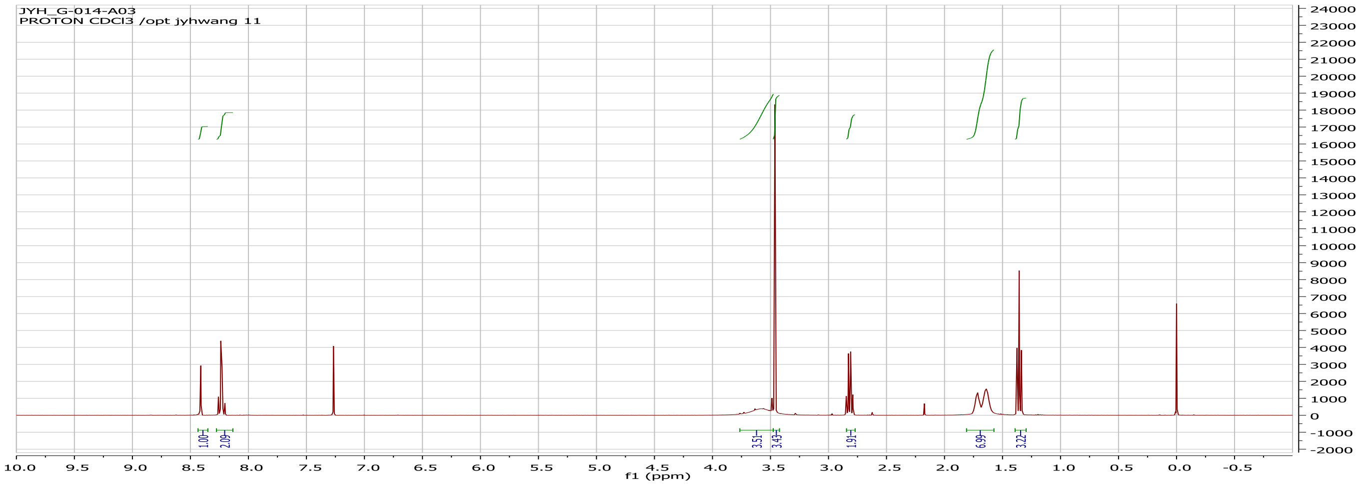


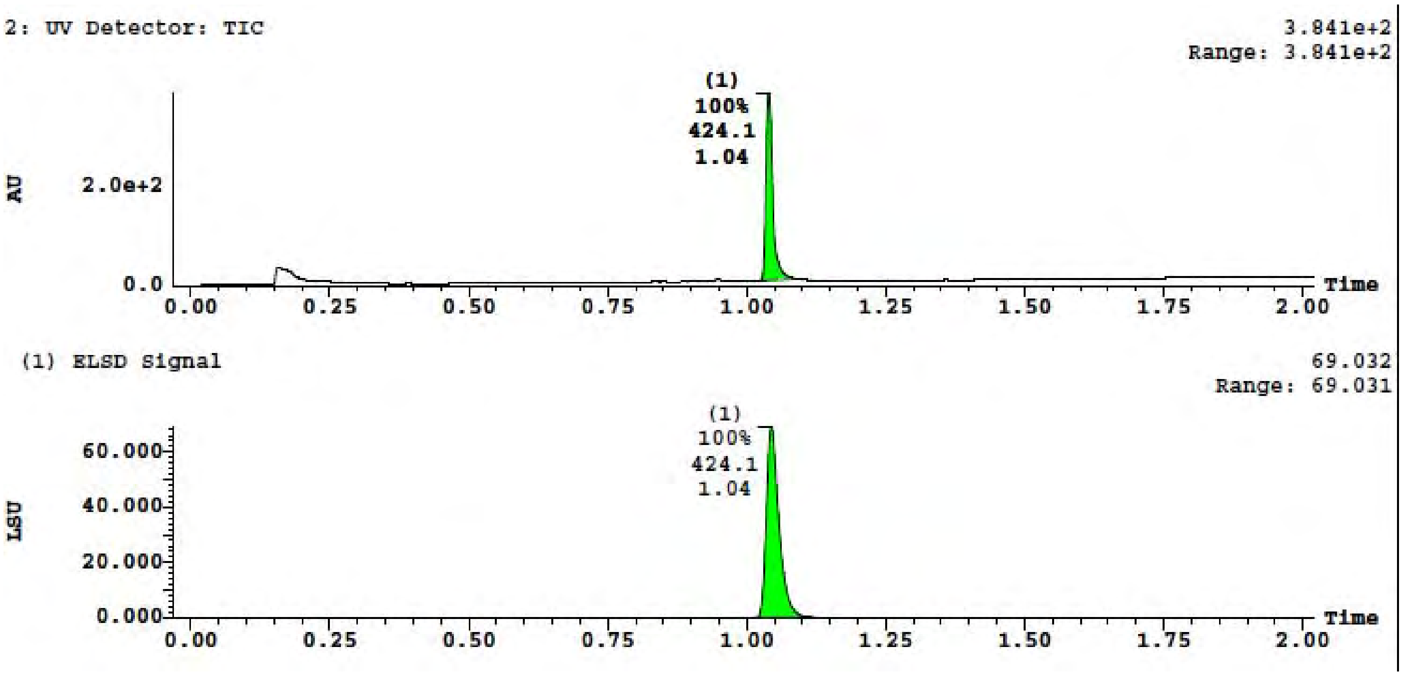


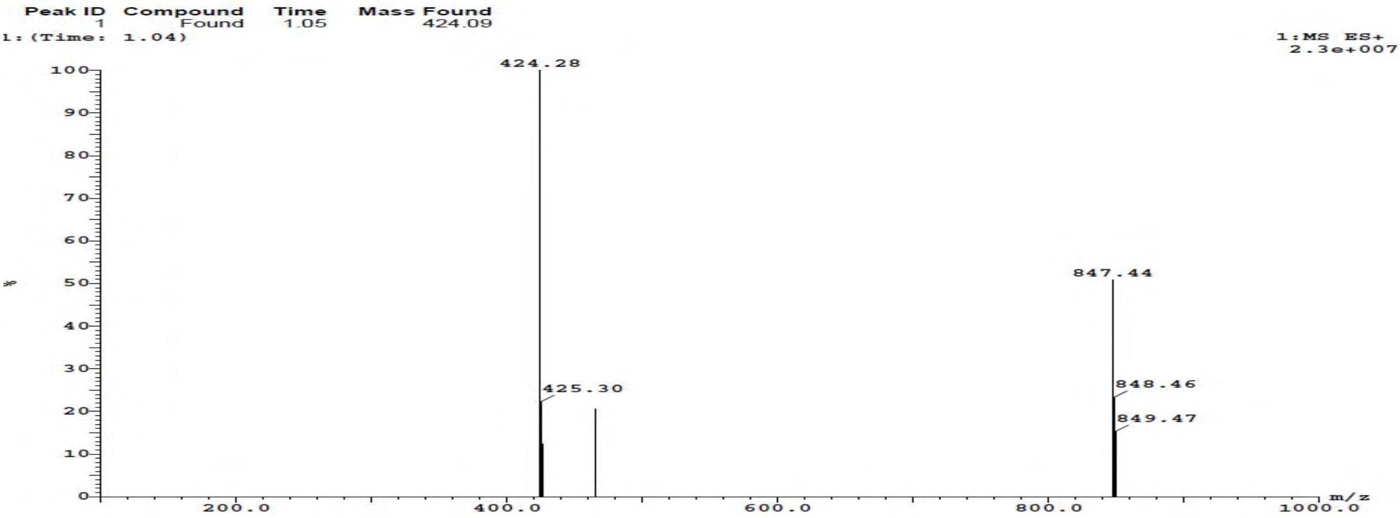
Peak ID	Compound	Time	Mass Found
1	Found	1.31	492.15

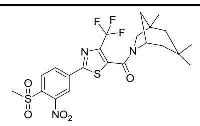


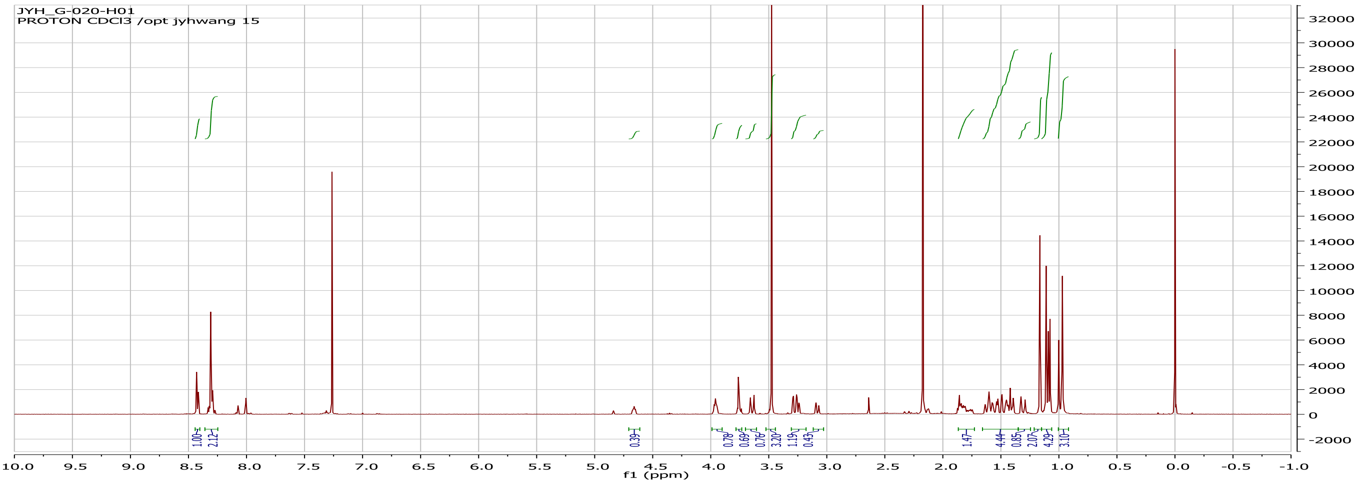
2{*3,1,4*}	

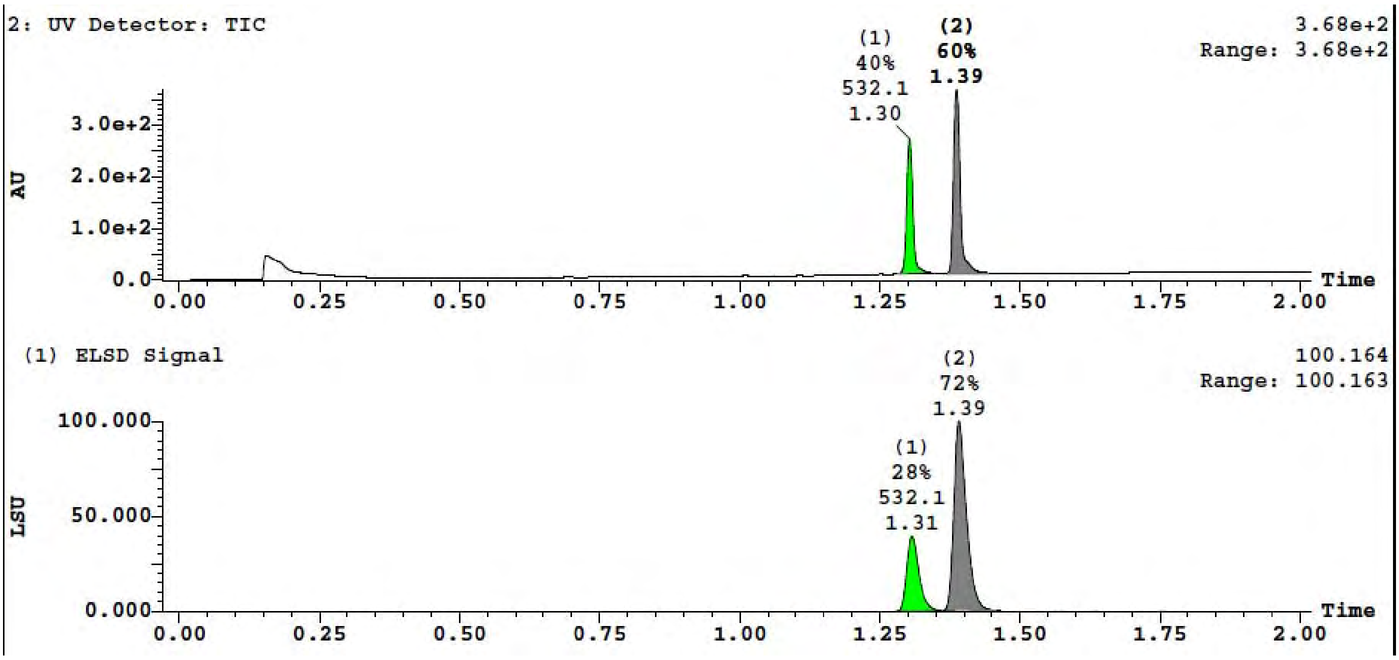

JYH_G-014-A03
PROTON CDCl3 /opt jyhwang 11
1.00
2.09
3.51
3.43
1.91
6.99
3.22
f1 (ppm)


2: UV Detector: TIC
3.841e+2
Range: 3.841e+2
(1)
100%
424.1
1.04
AU
2.0e+2
0.0
Time
(1) ELSD Signal
69.032
Range: 69.031
(1)
100%
424.1
1.04
LSU
60.000
40.000
20.000
0.000
Time

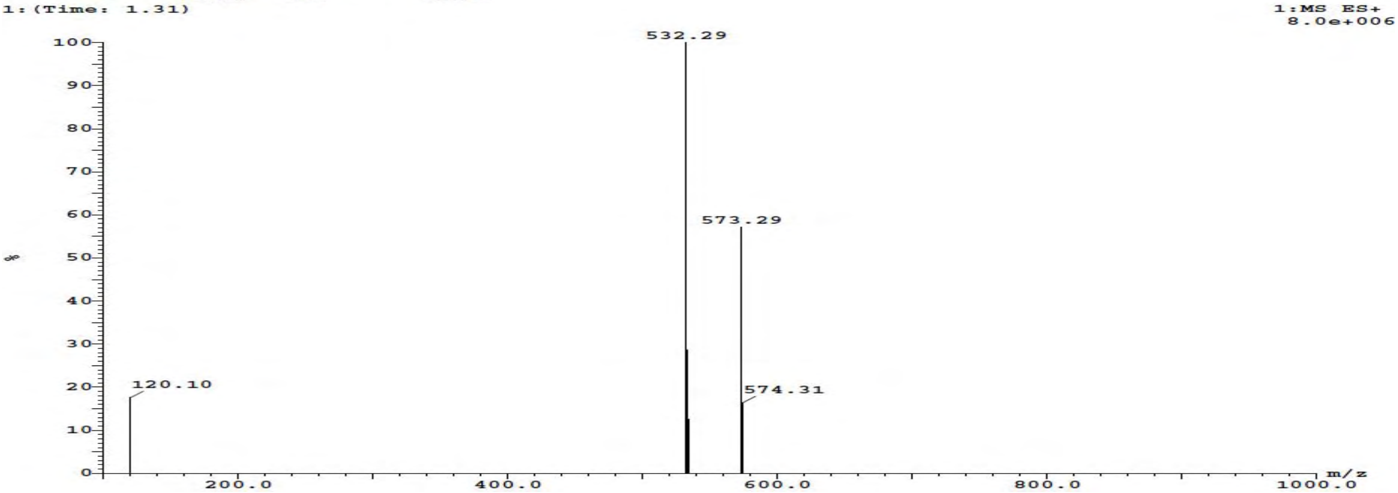

Peak ID Compound Time Mass Found
1 Found 1.05 424.09
1: (Time: 1.04)
1:MS ES+
2.3e+007
424.28
425.30
847.44
848.46
849.47
%
m/z

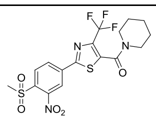
2{*4,1,2*}	

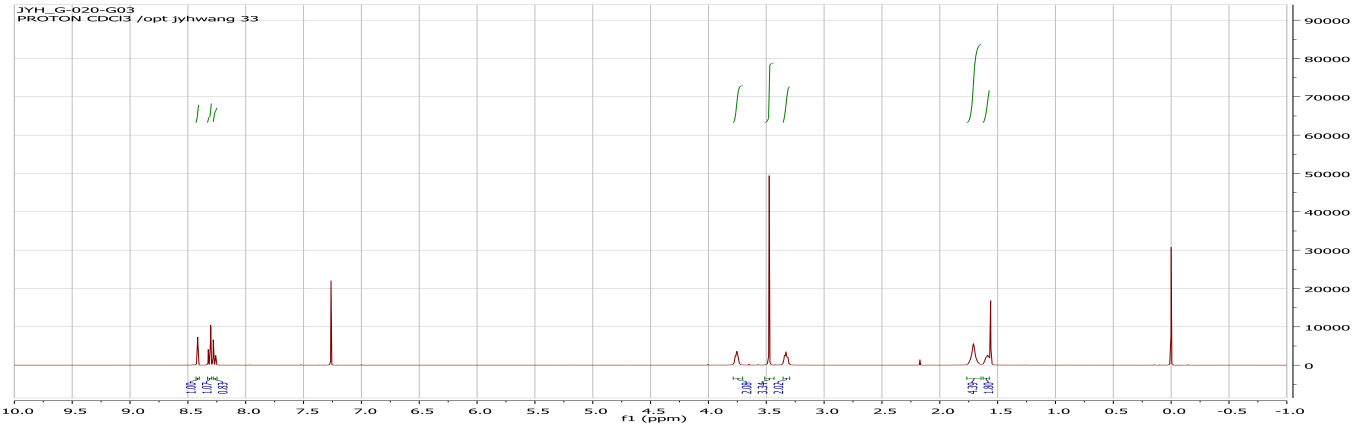


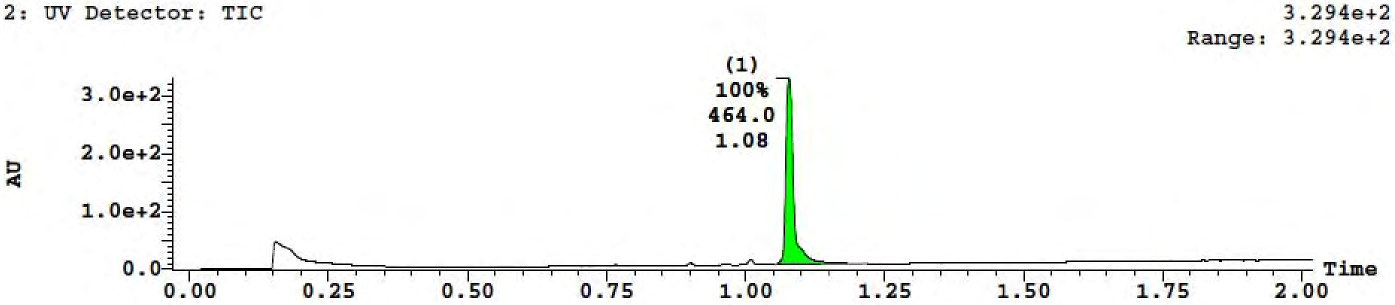


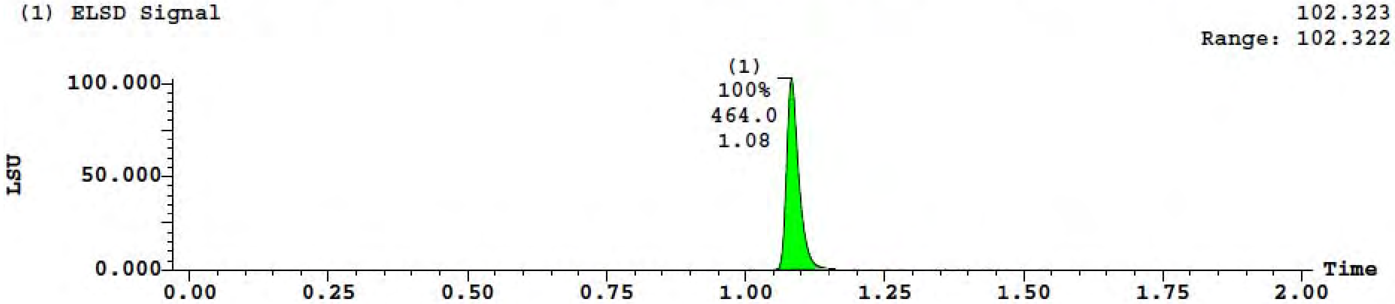
Peak ID	Compound Found	Time	Mass Found
1		1.31	532.11



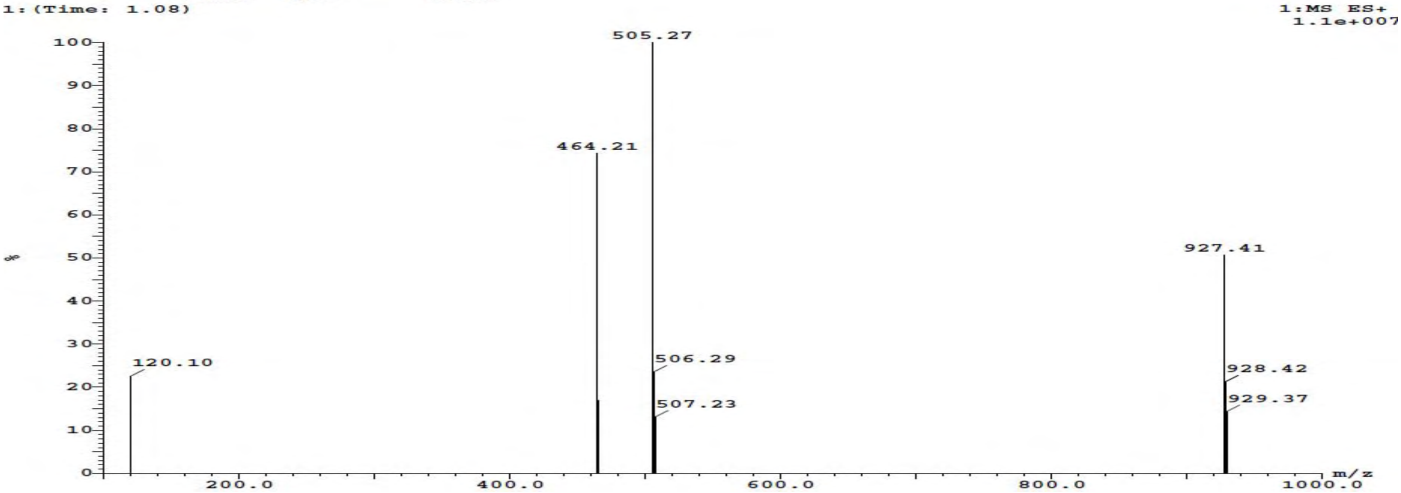
2{*4*,*1*,*4*}	

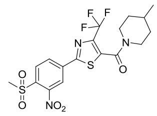


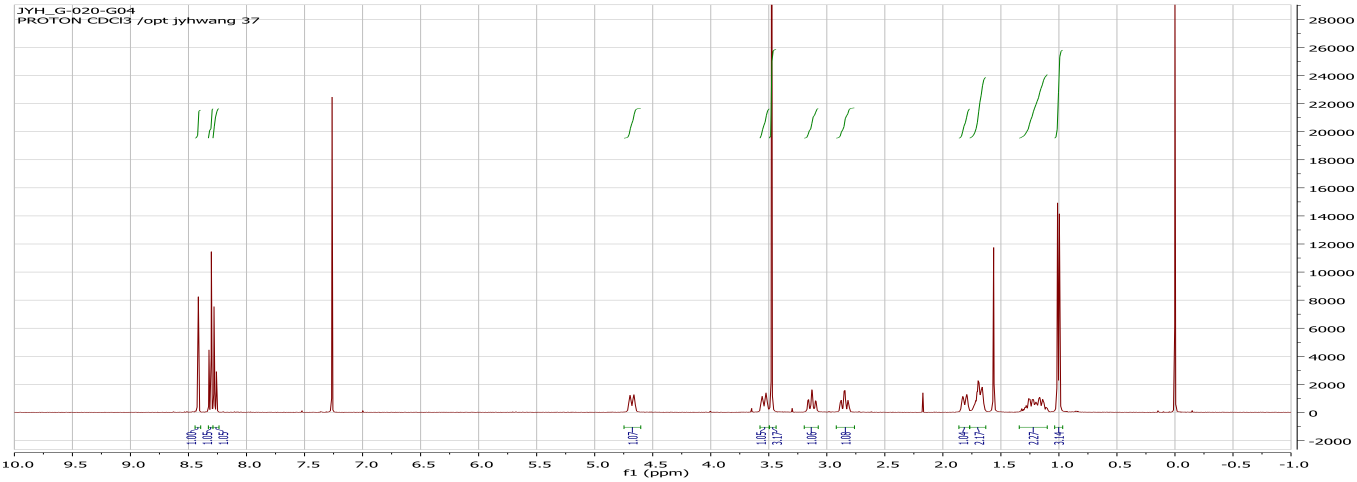


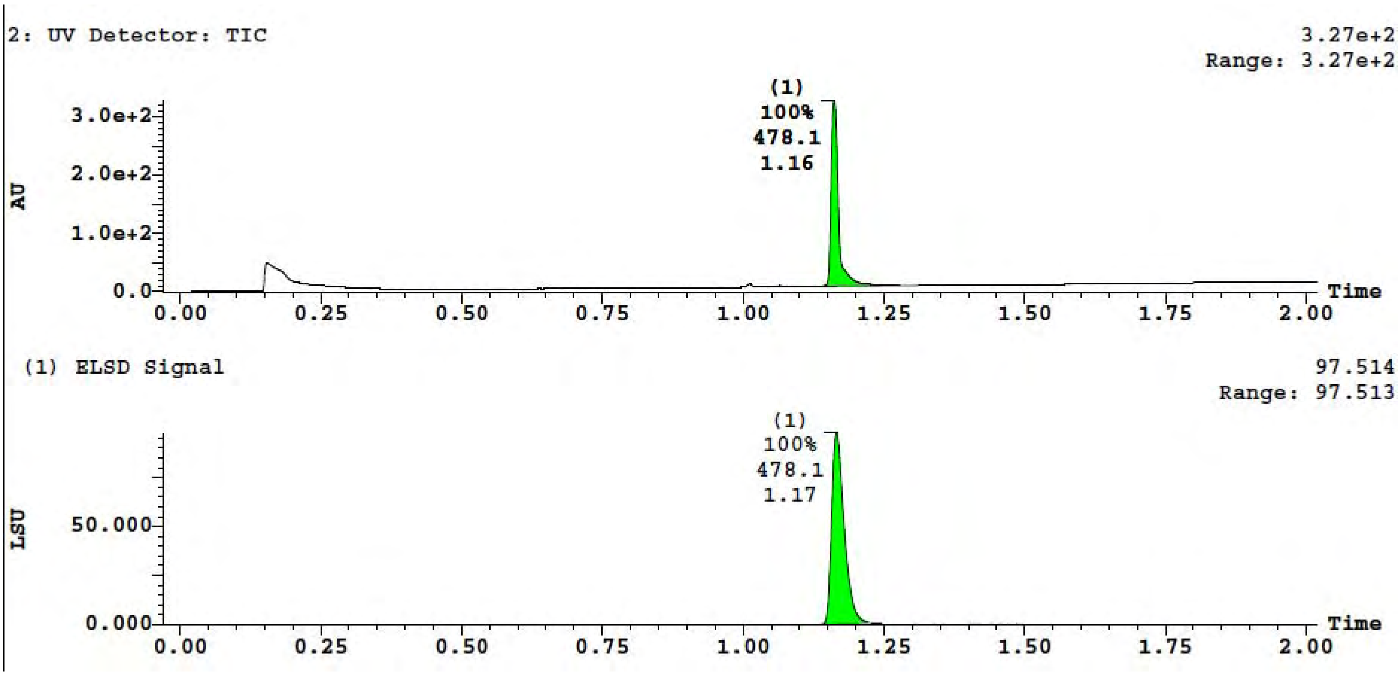


Peak ID	Compound	Time	Mass Found
1	Found	1.08	464.05

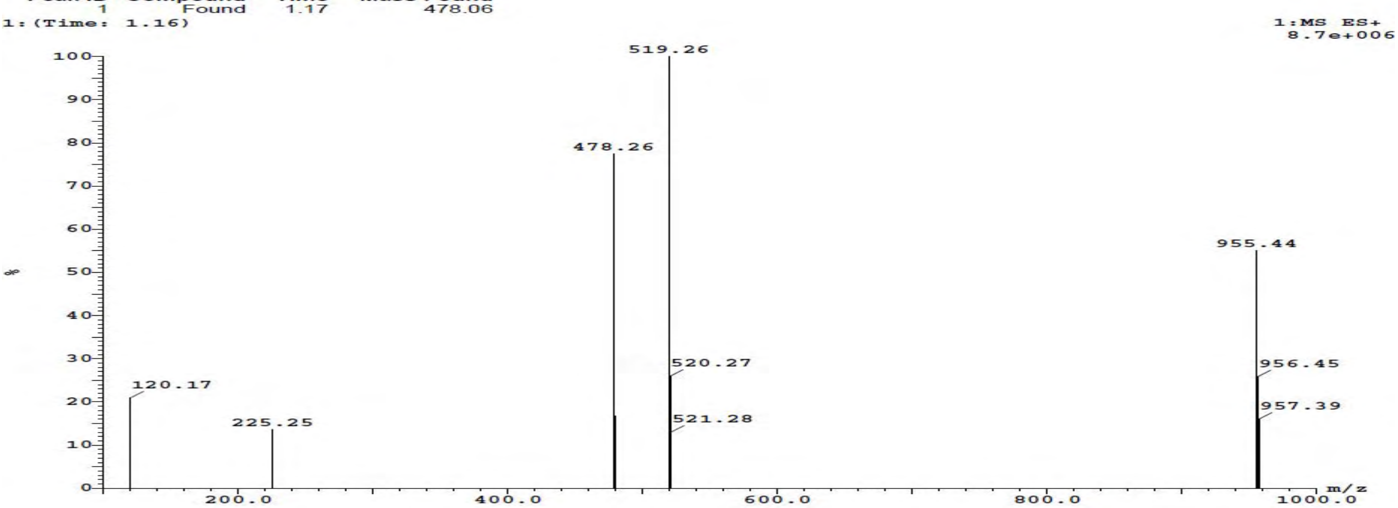


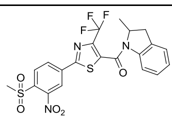
2{*4,1,5*}	

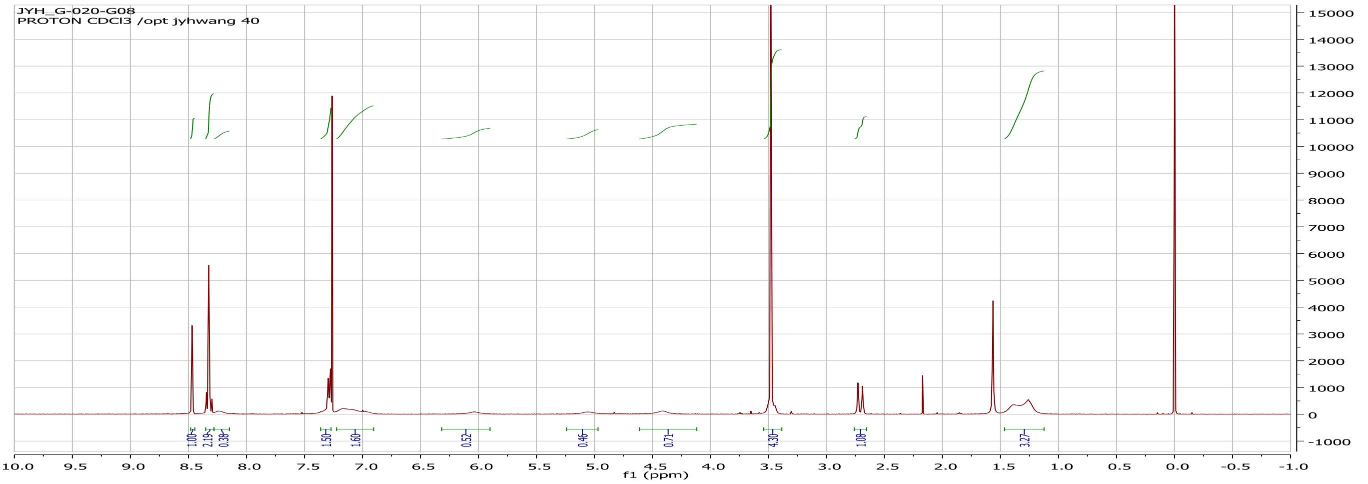


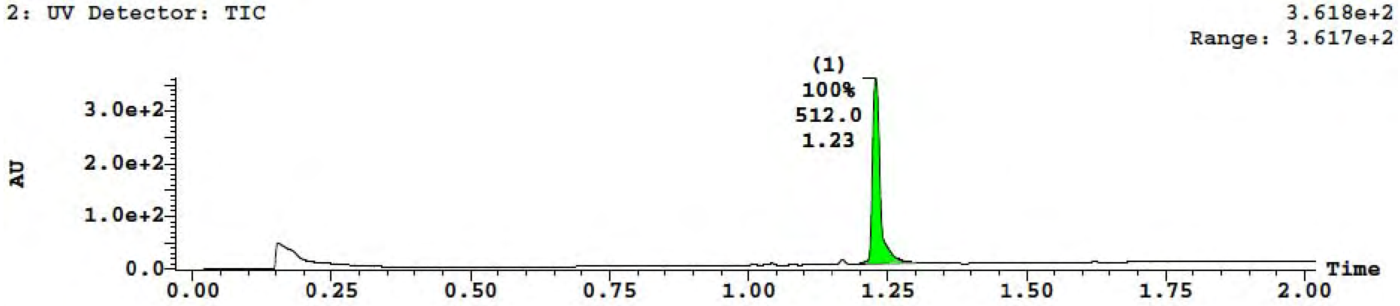


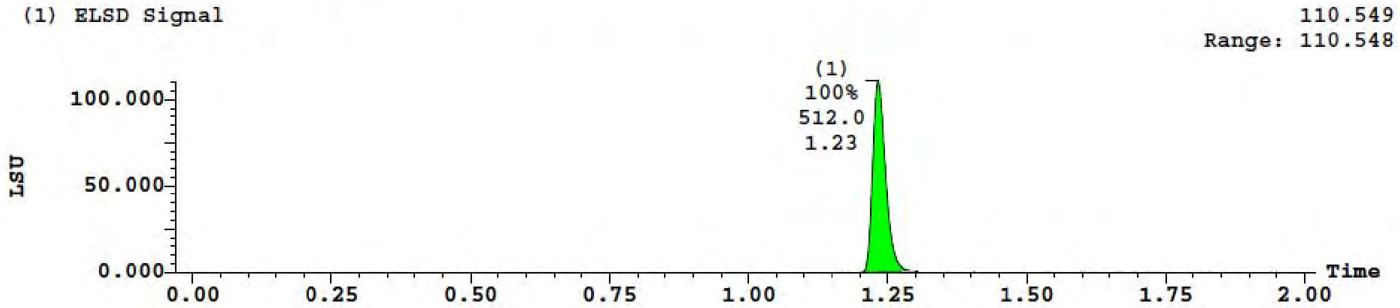
Peak ID	Compound	Time	Mass Found
1	Found	1.17	478.06



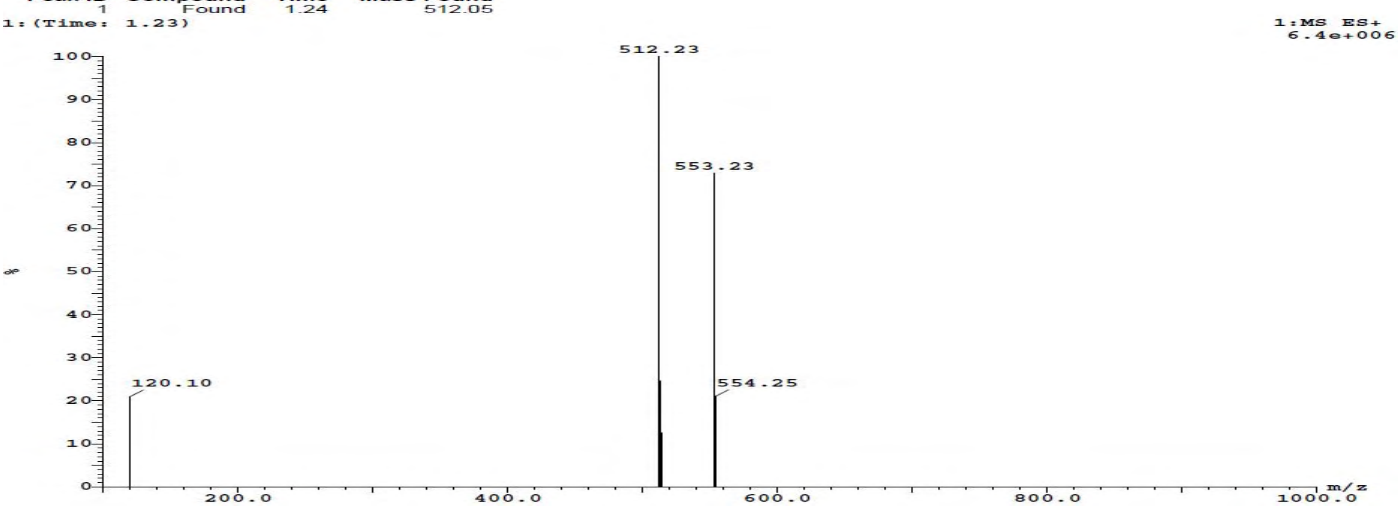
2{*4,1,9*}	

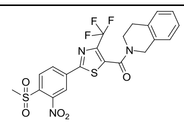


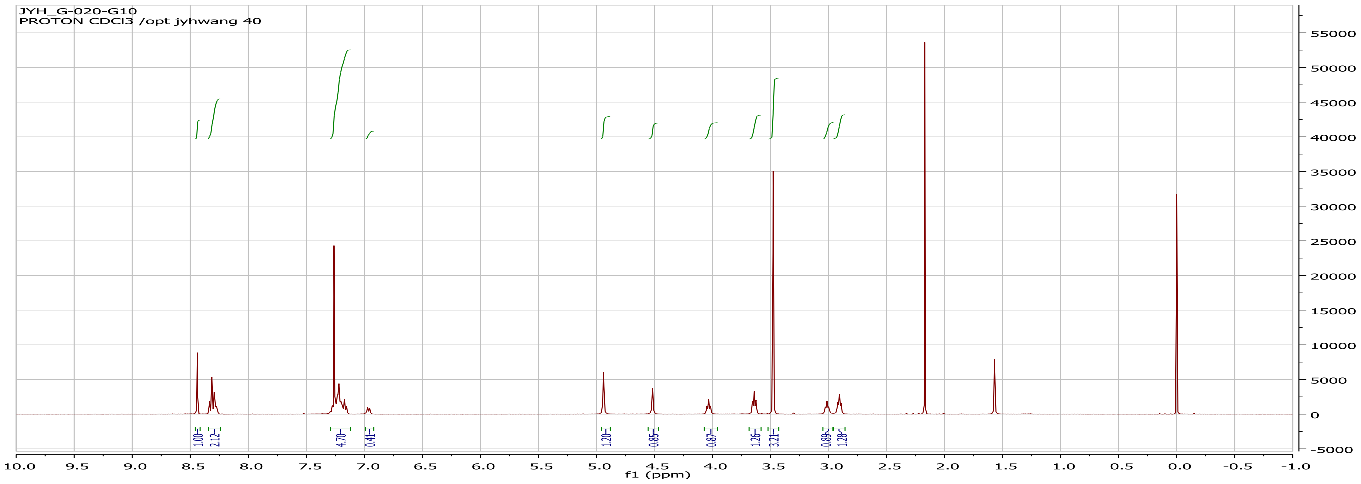


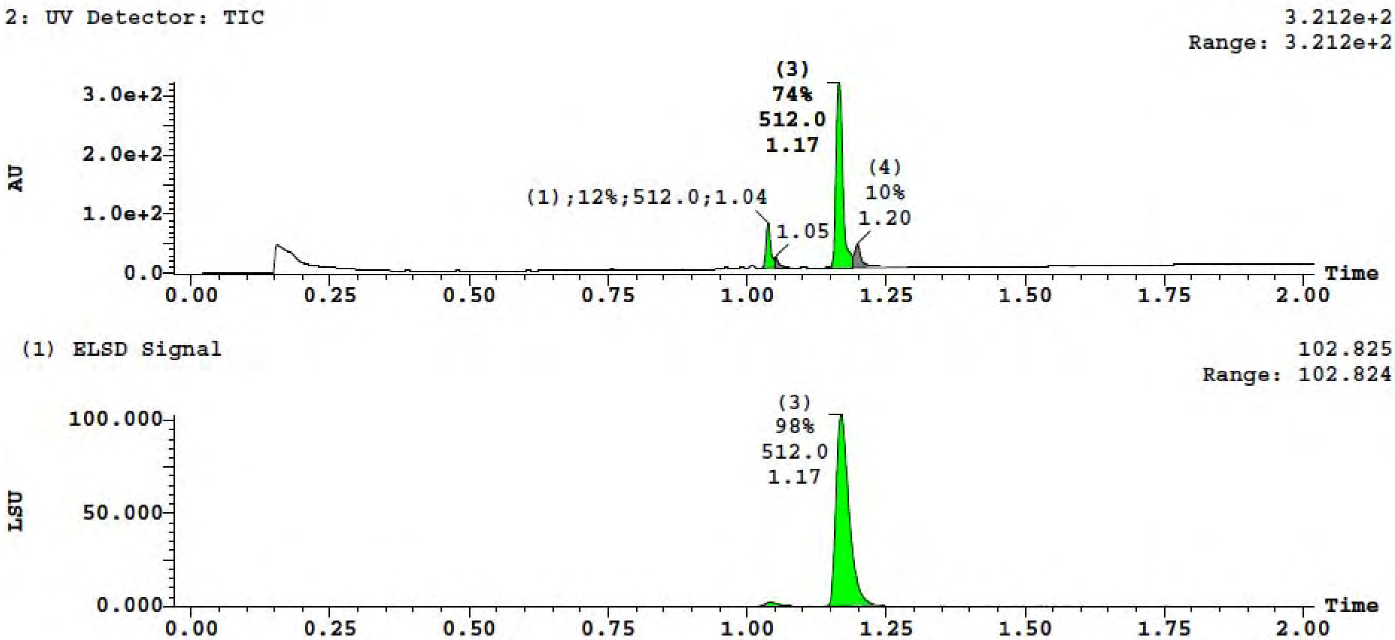


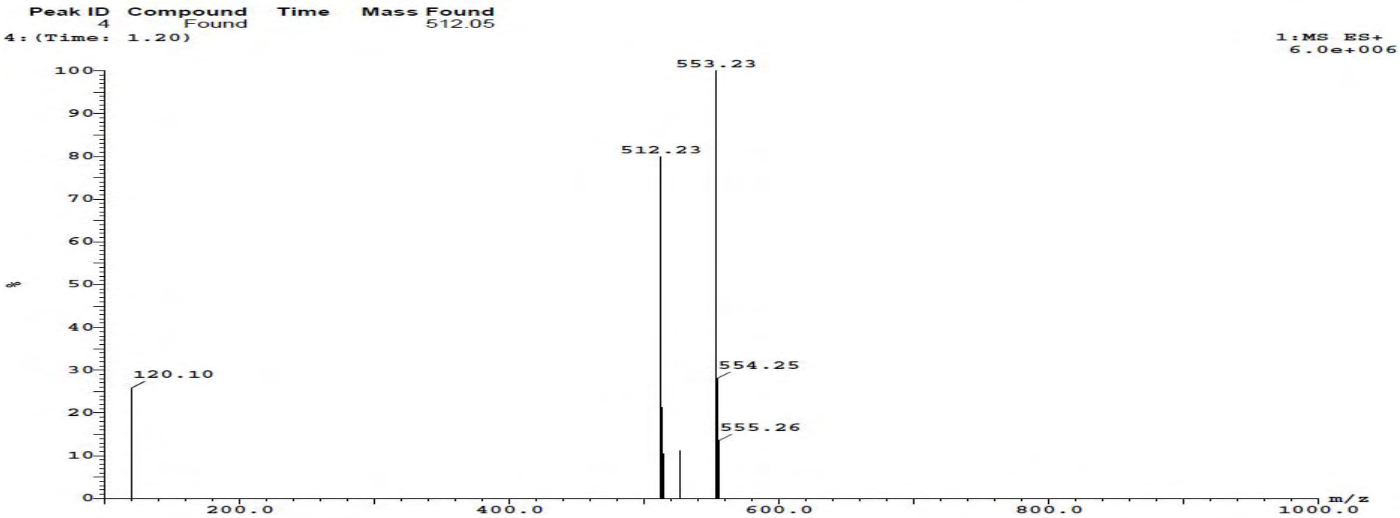
Peak ID	Compound Found	Time	Mass Found
1		1.24	512.05

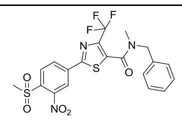


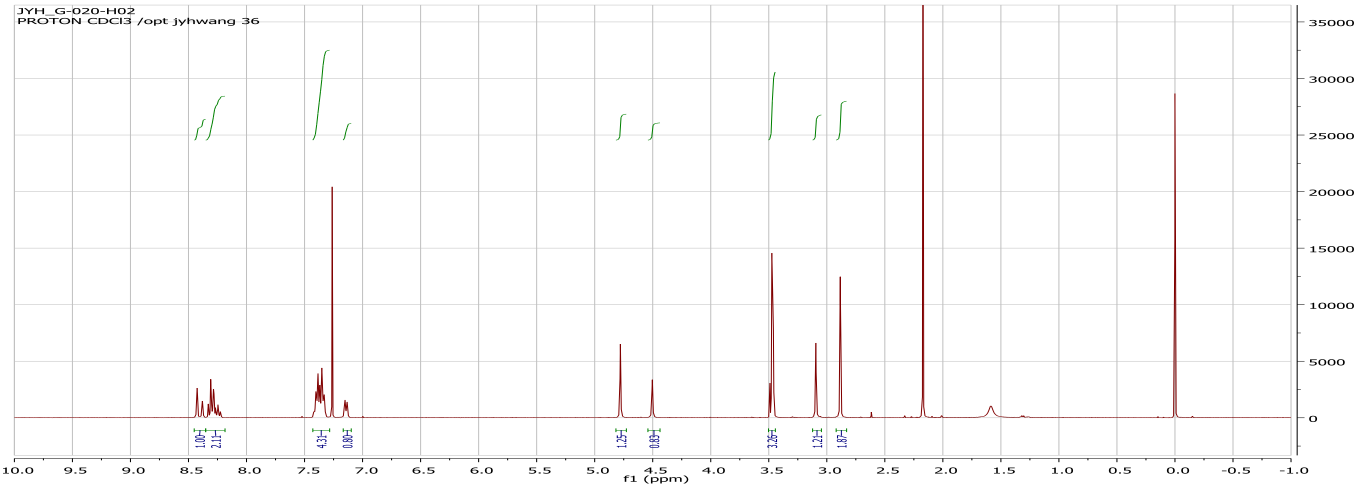
2{*4,1,11*}	

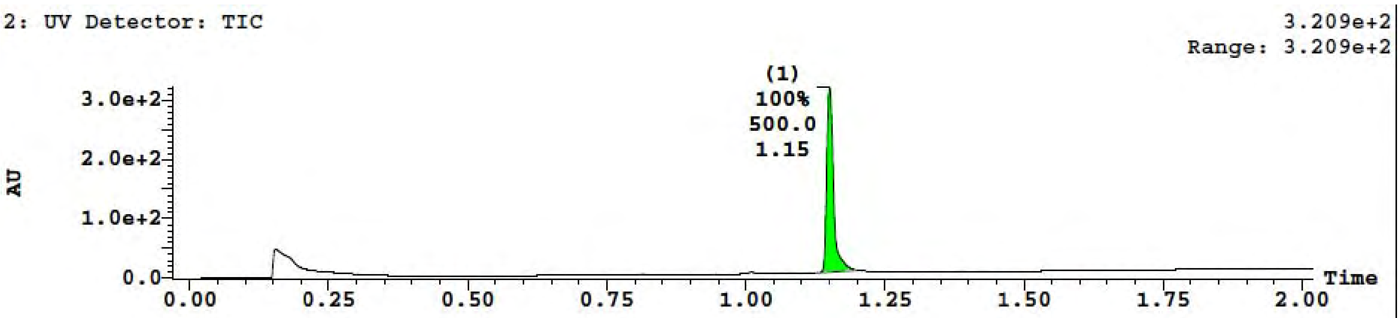

JYH_G-020-G10
PROTON CDCl3 /opt jyhwang 40
f1 (ppm)

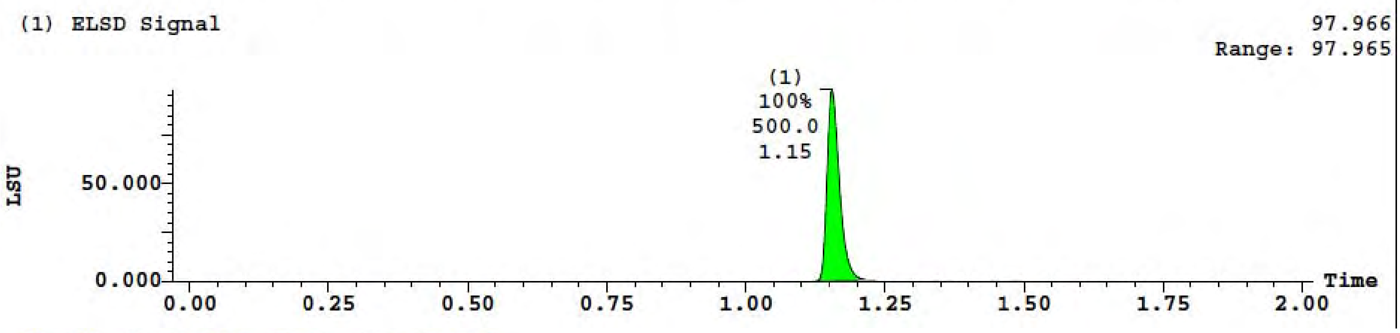

2: UV Detector: TIC
3.212e+2
Range: 3.212e+2
(3)
74%
512.0
1.17
(1);12%;512.0;1.04
1.05
(4)
10%
1.20
AU
Time
(1) ELSD Signal
102.825
Range: 102.824
(3)
98%
512.0
1.17
LSU
Time


Peak ID Compound Time Mass Found
4 Found 512.05
4: (Time: 1.20)
1:MS ES+
6.0e+006
553.23
512.23
554.25
555.26
120.10
%
m/z

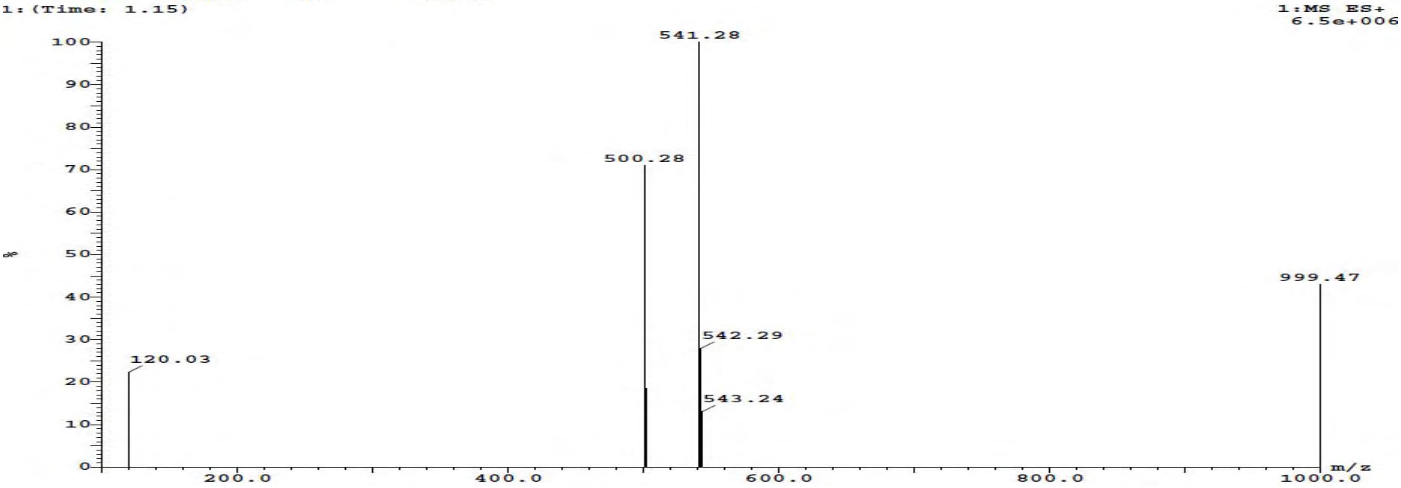
2{*4,1,14*}	

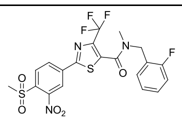


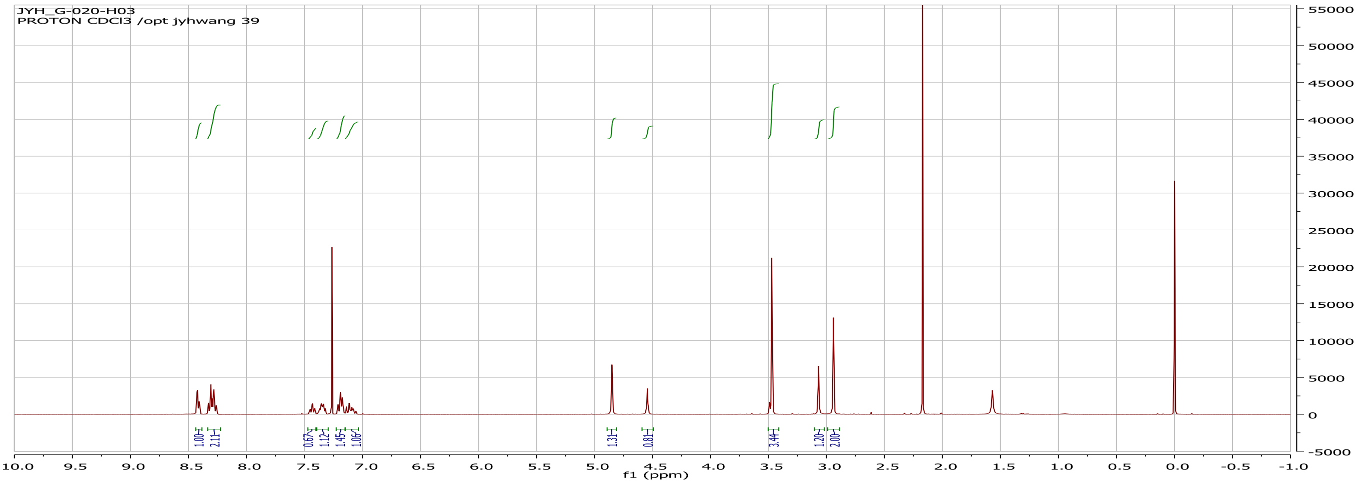


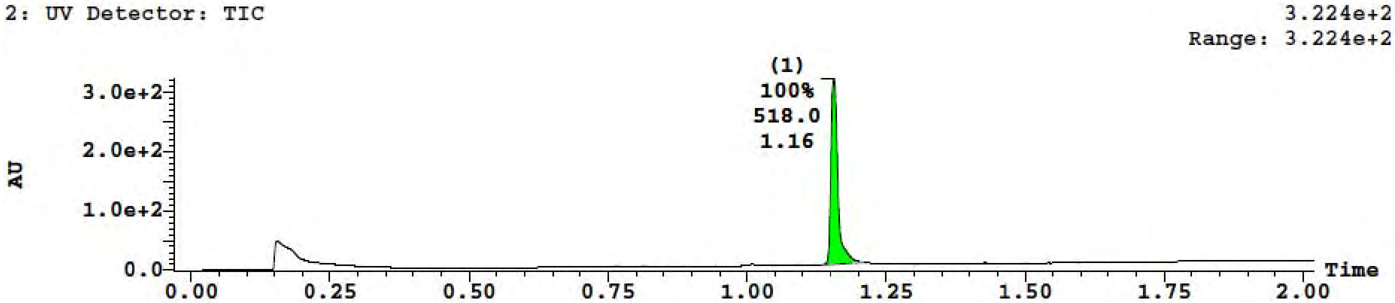


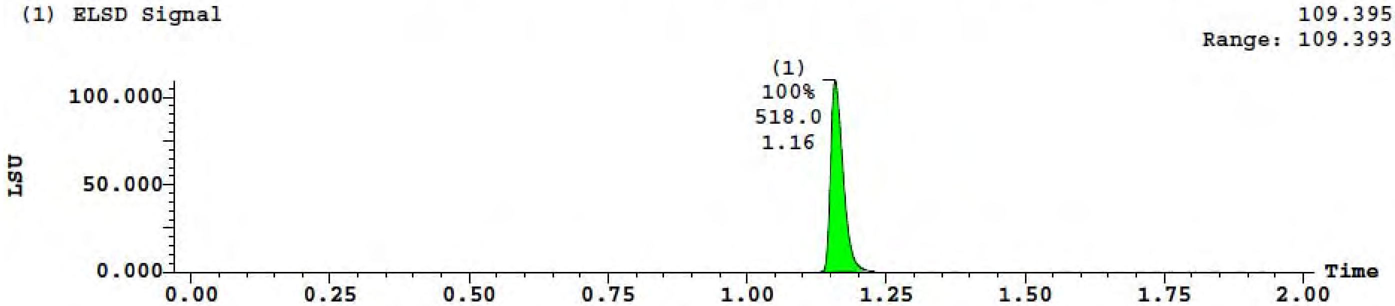
Peak ID	Compound	Time	Mass Found
1	Found	1.16	500.05



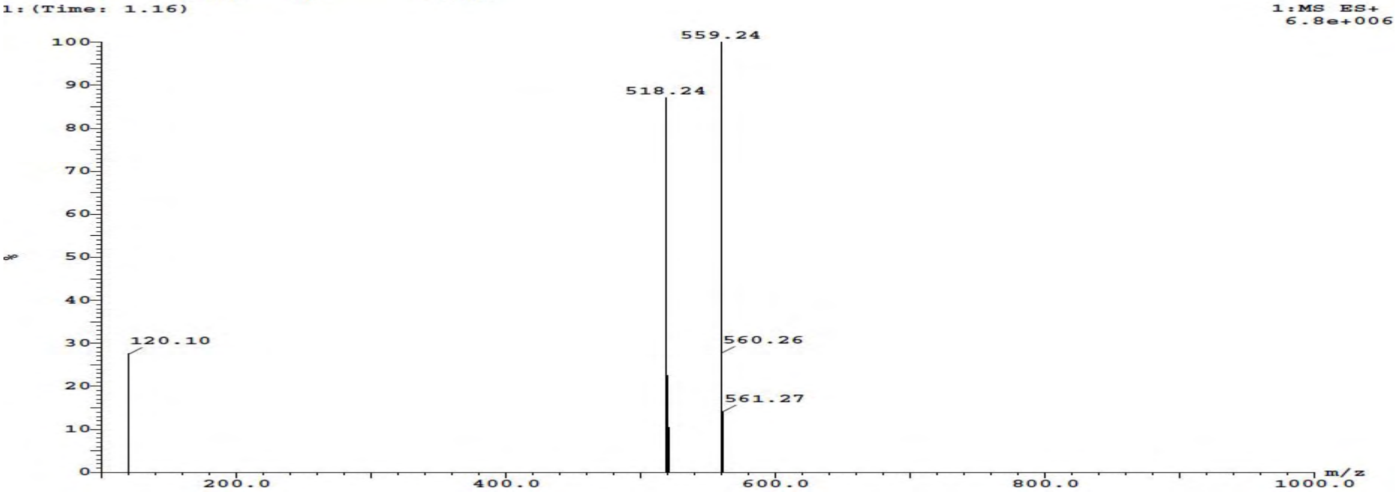
2{*4,1,15*}		3.4±2.5

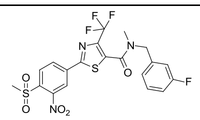


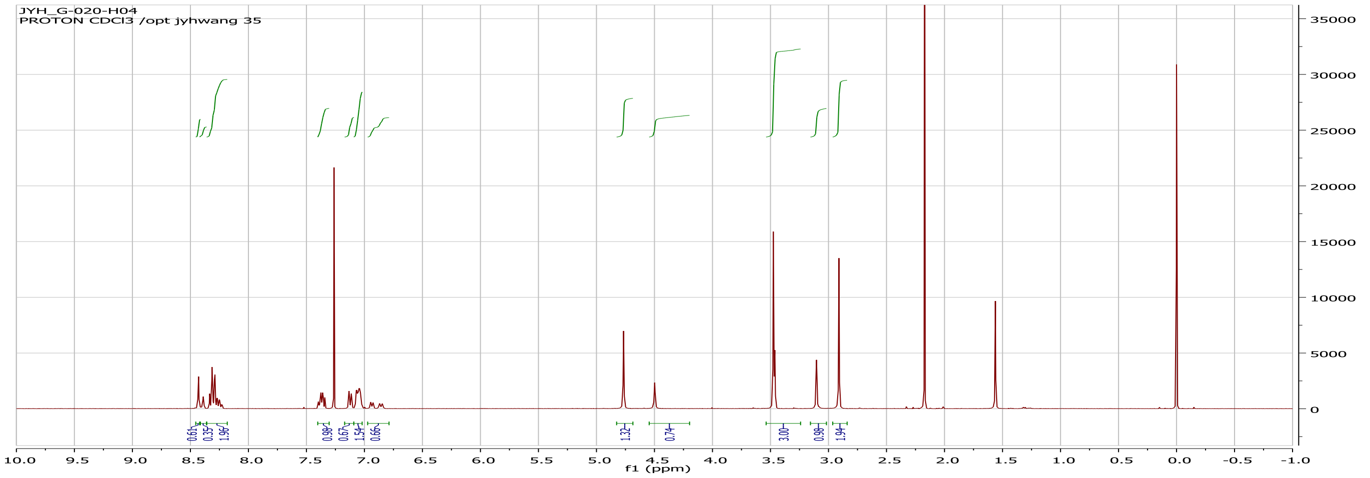


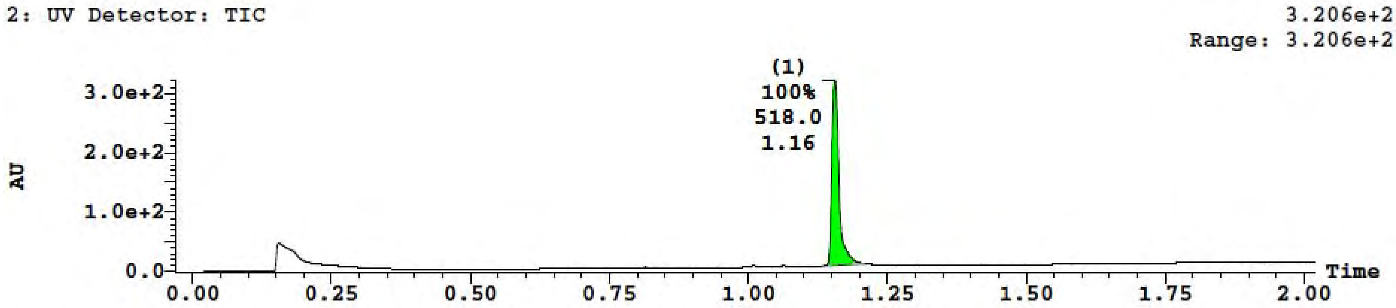


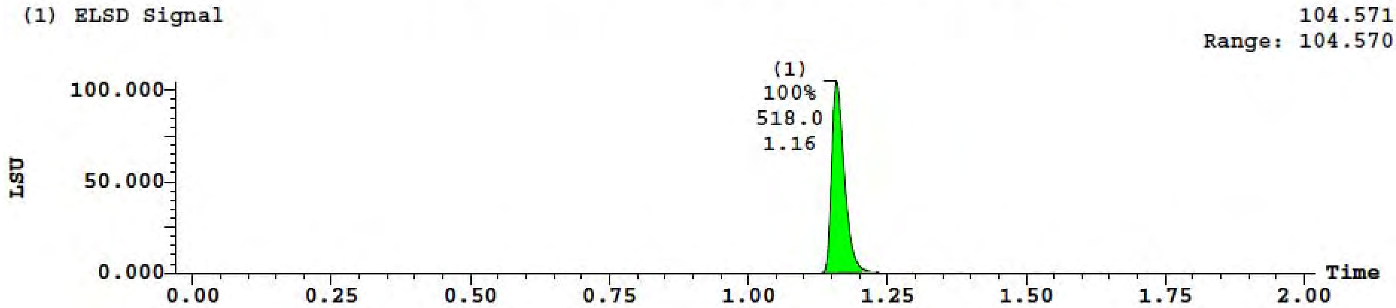
Peak ID	Compound Found	Time	Mass Found
1		1.16	518.04



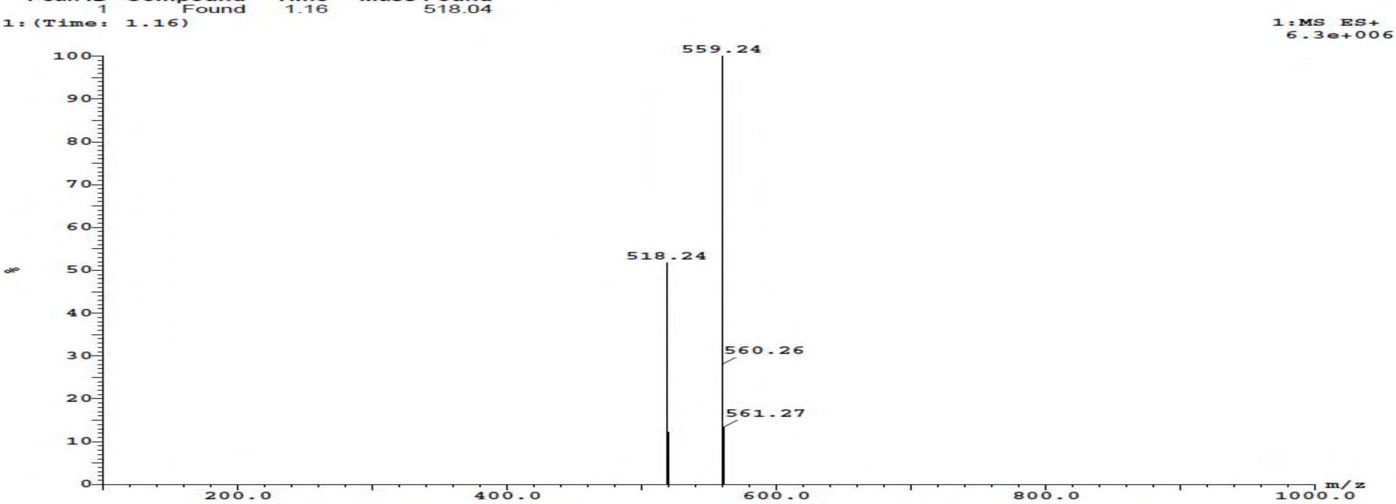
2{4,1,16}	

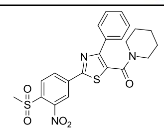


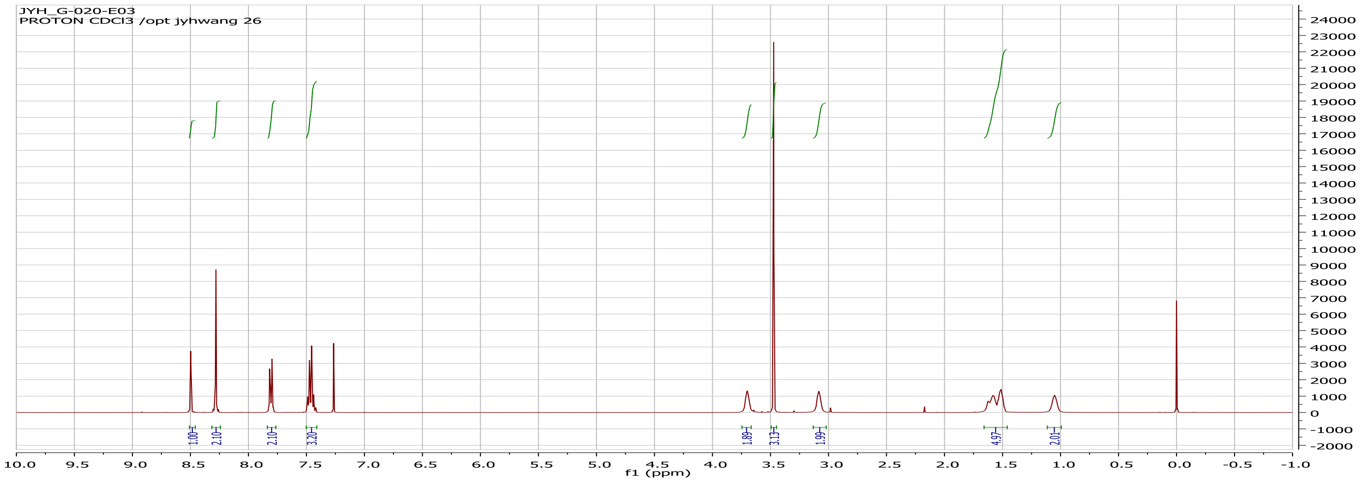


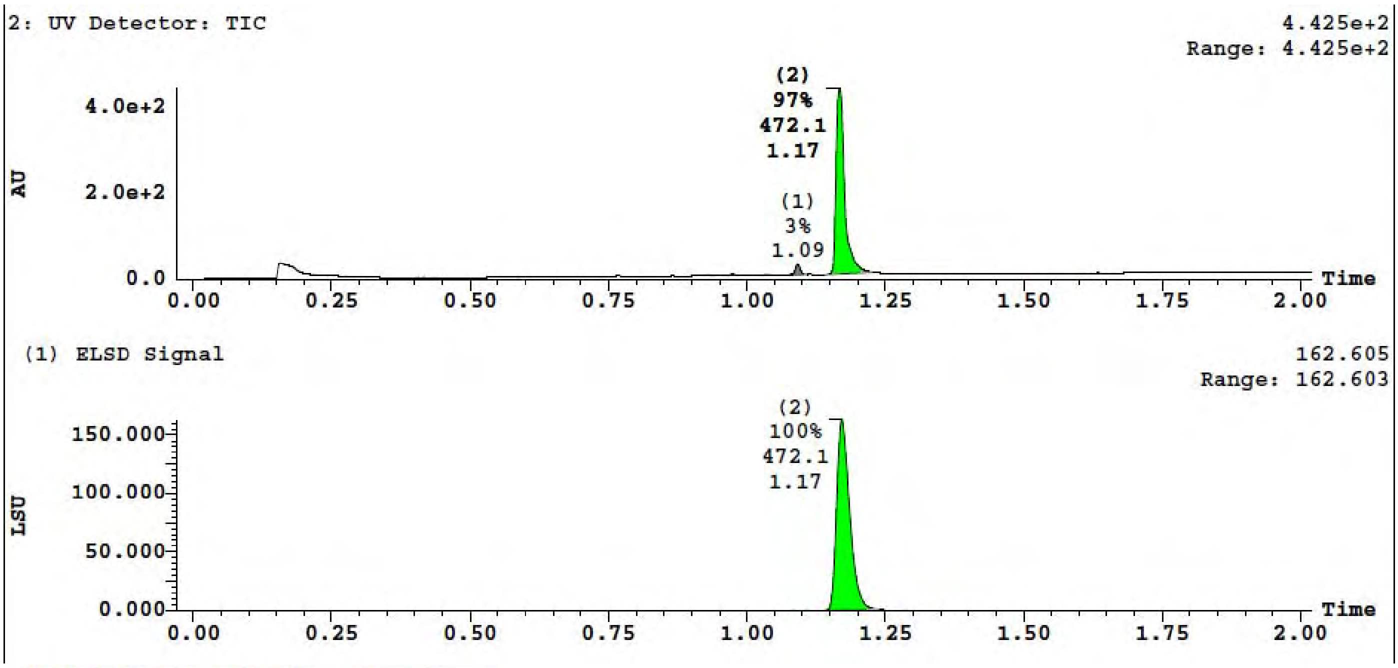


Peak ID	Compound Found	Time	Mass Found
1		1.16	518.04

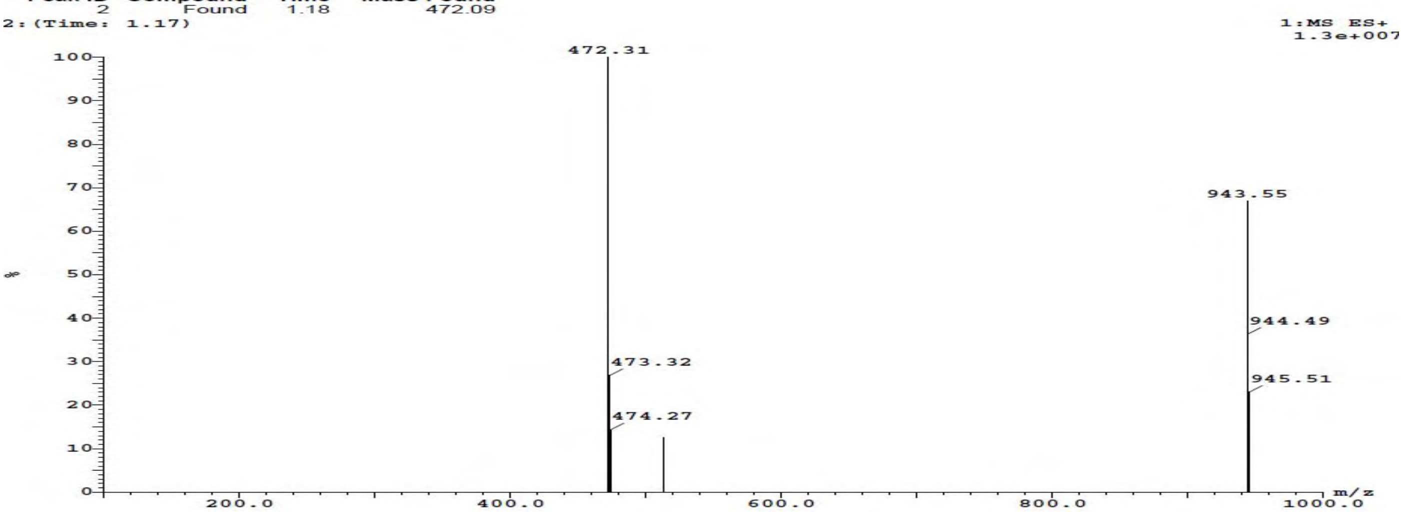


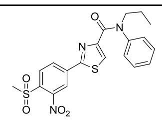
2{*5*,*1*,*4*}	

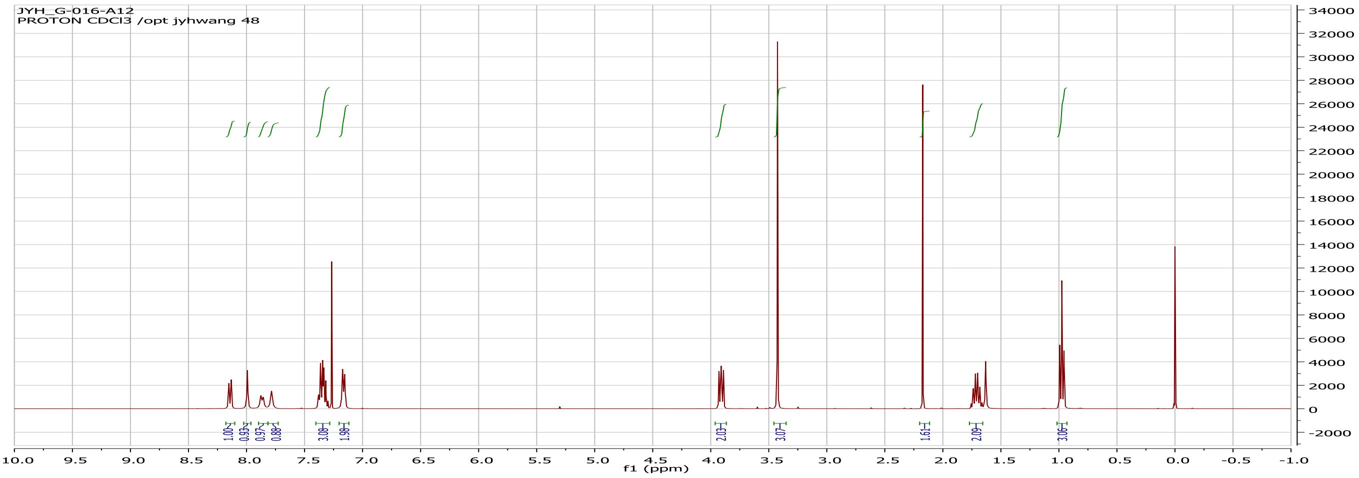


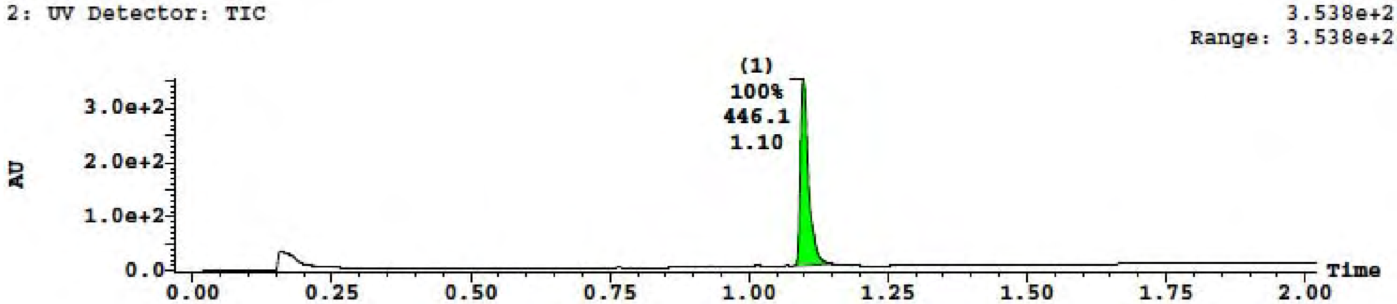


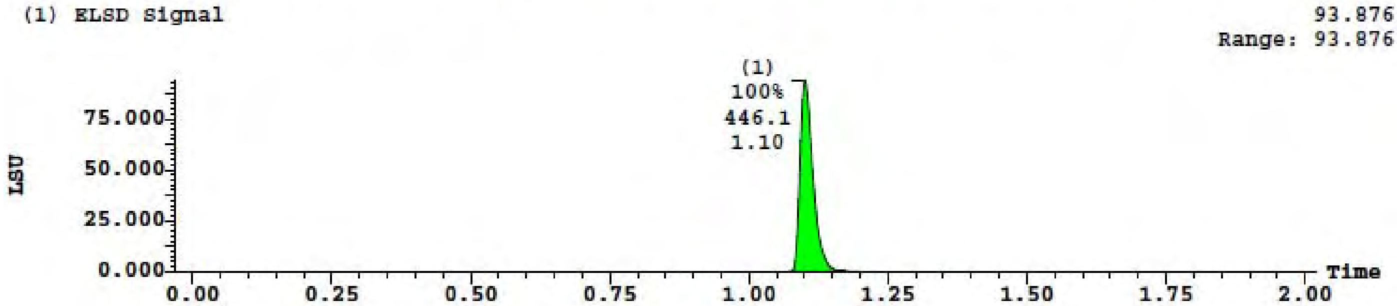
Peak ID	Compound	Time	Mass Found
2	Found	1.18	472.09



3{*6*,*1*,*13*}	







Peak ID	Compound	Time	Mass Found
1	Found	1.11	446.08