SUPPORTING INFORMATION

Acyclic Nitronates Olefins Cycloaddition (ANOC): Regio- and Stereo-specific Synthesis of Isoxazolines

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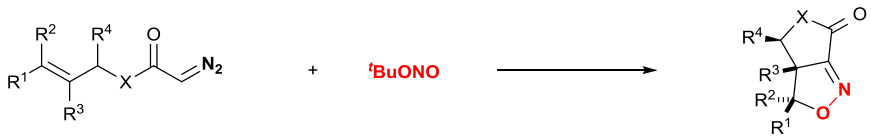
General information

Column chromatography was performed on silica gel (300-400 mesh) and reactions were monitored by thin layer chromatography (TLC) using UV light to visualize the course of the reactions. ^{1}H NMR (400 MHz), ^{13}C NMR (100 MHz) and ^{19}F NMR (376 MHz) spectra were acquired at various field strengths as indicated, and were referenced to $CHCl_3$ (7.26 and 77.0 ppm for ^{1}H and ^{13}C respectively) or DMSO (2.50 and 39.6 ppm for ^{1}H and ^{13}C respectively). The spectra were collected at 25 ^{o}C. ^{1}H NMR coupling constants are reported in Hertz and refer to apparent multiplicities and not true coupling constants. Collection parameters: Relaxation Delay- 1.0; Pulse Width- 10.0; Number of Scans- 1~16; Sweep Width- -3.84~16.19 (20.03) ppm. Data are reported as follows: chemical shift, multiplicity (s = singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, etc.), coupling constant and integration. All ^{13}C NMR spectra are ^{1}H decoupled. Collection parameters: Relaxation Delay- 2.0; Pulse Width- 8.8; Number of Scans- 10~100; Sweep Width- -19.47~219.45 (238.90) ppm. IR and HRMS were performed by the State-authorized Analytical Center in Soochow University.

Preparation of diazo compounds[1]

The corresponding alcohol (20 mmol) and $NaHCO_3$ (5.0 g, 60 mmol) were dissolved in acetonitrile (50 mL) and bromoacetyl bromide (2.6 mL, 30 mmol) was added slowly at 0 ℃. After stirring 30 min at the temperature, the reaction was quenched with H_2O. The solution was extracted with CH_2Cl_2 three times. The organic phase was washed with brine and dried over Na_2SO_4. The solvent was evaporated, and the residue was used in the next reaction without purification. The bromoacetate thus obtained and N, N'-ditosylhydrazine (13.6 g, 40 mmol) were dissolved in THF (50 mL) and cooled to 0 ℃. DBU (60 mL, 40 mmol) was added dropwise and stirred at the temperature for 30 minutes. After the quenching of the reaction by the addition of saturated $NaHCO_3$ solution, it was extracted with Et_2O three times. The organic phase was washed with brine, dried over Na_2SO_4 and evaporated to give the crude product. The crude product thus obtained was purified by chromatography over a column of silica gel using petroleum and ethyl acetate as eluent to afford the desired product.

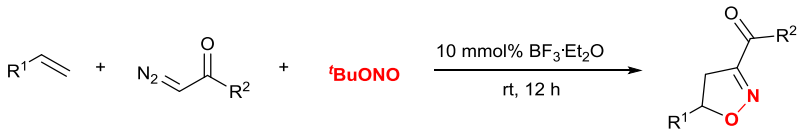
Intramolecular procedures for synthesis of isoxazolines



To a solution of diazo (0.2 mmol, 1.0 equiv) in *N*,*N*-dimethylformamide (2.0 mL) was added ^{t}BuONO (0.6 mmol, 3.0 equiv). The reaction mixture was vigorously stirred at 25 ℃ for 12 hours. After confirming the finish of the reaction by TLC, the resultant was diluted with brine, and extracted with

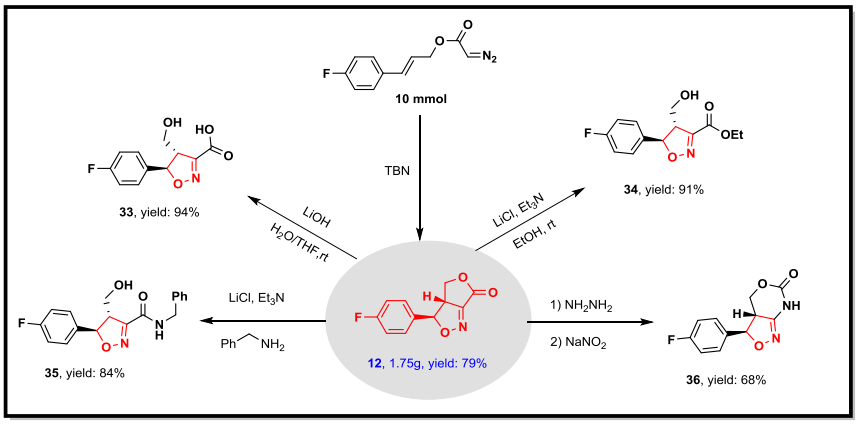
ethyl acetate three times. The combined organic phase was then dried over Na_2SO_4 and evaporated to give the crude product. The crude residue was purified by column chromatography on silica gel (ethyl acetate/petroleum ether = 1/5 to 1/1, v/v) to afford the desired products.

Intermolecular procedures for synthesis of isoxazolines



To a solution of alkenes (0.5 mmol, 1.0 equiv) in acetonitrile (2.0 mL) was added diazo compounds (1.0 mmol, 2.0 equiv), ^{t}BuONO (1.0 mmol, 2.0 equiv) and $BF_3{\cdot}Et_2O$ (0.05 mmol, 0.1 equiv) in turn. The reaction mixture was stirred at 25 ℃ for 12 hours. After confirming the finish of the reaction by TLC, the resultant was concentrated in vacuum and purified by column chromatography on silica gel (ethyl acetate/petroleum ether = 1/50 to 1/4, v/v) to afford the desired products.

General procedures for potential synthetic applications



The procedure for the hydrolysis of compound 12

To a solution of LiOH (5 equiv) in water:THF (1:5) at room temperature was slowly added the 3-(4-fluorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (**12**) (44.2 mg, 0.2 mmol, 1 equiv). The mixture was stirred at room temperature for overnight. Solvent was removed under reduced pressure. The residue was dissolved in water and acidified with 2M HCl to pH 1 followed by extraction with DCM. The crude product was purified by column chromatography on silica gel with methanol/DCM to afford the product **33** as a white solid, 45.1 mg, 94% yield.

The procedure for the esterification of compound 12[2]

To a stirred solution of 3-(4-fluorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (**12**)

(44.2 mg, 0.2 mmol, 1 equiv) in ethanol at 25 ℃ were added Et_3N (0.20 equiv) and LiCl (1 equiv). The reaction mixture was stirred at 25 ℃ for 12 h. Reaction mixture was quenched with 0.1 M HCl and diluted with EtOAc, then the organic layer was separated, and the aqueous layer was extracted with EtOAc. The combined organic extracts were washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with ethyl acetate/ petroleum ether to afford the expected product **34** as a colorless liquid, 48.6 mg, 91% yield.

The procedure for the ammonolysis of compound 12[3]

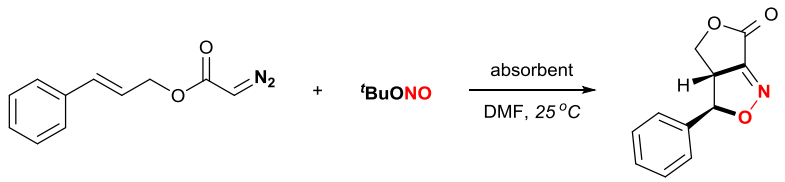
To a stirred solution of 3-(4-fluorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (**12**) (44.2 mg, 0.2 mmol, 1 equiv) and a benzylamine (1.2 equiv) in methanol at 25 ℃ were added Et_3N (0.20 equiv) and LiCl (1 equiv). The reaction mixture was stirred at 25 ℃ for 12 h. Reaction mixture was quenched with 0.1 M HCl and diluted with EtOAc, then the organic layer was separated, and the aqueous layer was extracted with EtOAc. The combined organic extracts were washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with ethyl acetate/ petroleum ether to afford the expected product **35** as a white solid, 54.9 mg, 84% yield.

The procedure for the ring expansion of compound 12[4]

To a solution of 3-(4-fluorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (**12**) (44.2 mg, 0.2 mmol, 1 equiv) in MeOH (5 mL) at 25 ℃ was added hydrazine monohydrate (10 equiv) over 15 min. The mixture was stirred at 25 ℃ for 12 h and was concentrated under reduced pressure to get the crude hydrazide as an off-white solid which was used in next step without any further purification. To a suspension of the crude acyl hydrazide in H_2O/Et_2O (1:1) at 0 ℃ was slowly added $NaNO_2$ (2.5 equiv). A solution of 6 N HCl (2.5 equiv) was then added dropwise. Upon completion of the addition, the mixture was stirred for 30 min at 0 ℃, and cold $CHCl_3$ was added. The layers were separated, and the aqueous layer was extracted with $CHCl_3$. The organic layers were combined and washed with aqueous $NaHCO_3$ and brine. The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure to half volume, whereupon a volume of toluene (5 mL) was added. The remaining chloroform was removed under reduced pressure, and an additional portion of toluene (5 mL) was added. The reaction mixture was heated at 80 ℃ for 16 h, whereupon the reaction mixture was concentrated under reduced pressure, and the crude yellow solid was purified by column chromatography on silica gel with ethyl acetate/ petroleum ether to afford the expected product **36** as a white solid, 32.3 mg, 68% yield.

Optimization of the reaction conditions

Table S1. Screenings of absorbent [a]

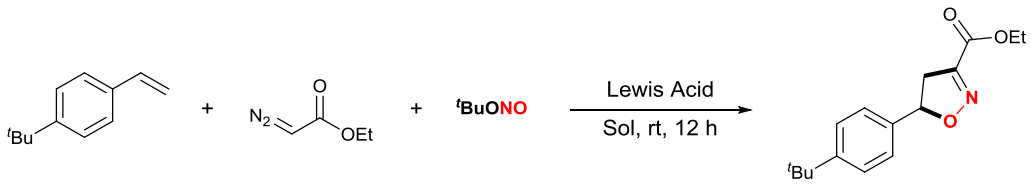


1 2 3

Entry	Absorbent (50 mg in 2 mL DMF)	Yield (%)[b]
1	Anhydrous magnesium sulfate	71%
2	Anhydrous sodium sulfate	68%
3	Pre-activated 4Å molecular sieves	74%

[a] Reaction conditions: : diazo compound 1 (0.2 mmol, 1.0 equiv), tert-butyl nitrite 2 (0.6 mmol, 3.0 equiv), absorbent (50 mg) and solvent (2.0 mL) at 25 ℃ for 12 h unless otherwise noted. [b] Isolated yields.

Table S2. Optimization for intermolecular Reaction[a]



entry	Lewis Acid	solvent	Yield (%)[b]
1	$BF_3{\cdot}Et_2O$	PE	41
2	$BF_3{\cdot}Et_2O$	EA	75
3	$BF_3{\cdot}Et_2O$	THF	55
4	$BF_3{\cdot}Et_2O$	CH_3CN	80
5	$BF_3{\cdot}Et_2O$	*i*-PrOH	8
6	$BF_3{\cdot}Et_2O$	CH_3NO_2	58
7	$BF_3{\cdot}Et_2O$	DMF	42
8	$BF_3{\cdot}Et_2O$	DMSO	56
9	$BF_3{\cdot}Et_2O$	NMP	19
10	$BF_3{\cdot}Et_2O$	Tol	71
11	$BF_3{\cdot}Et_2O$	DCE	70
12	$BF_3{\cdot}Et_2O$	cyclohexane	39
13	$BF_3{\cdot}Et_2O$	1,4-dioxane	40
14	$BF_3{\cdot}Et_2O$	DCM	69
15	$BF_3{\cdot}Et_2O$	Acetone	57
16	$Cu(OTf)_2$	CH_3CN	20

17	$Mg(OTf)_2$	CH_3CN	16
18	$FeCl_3·6H_2O$	CH_3CN	35
19	$ZnBr_2$	CH_3CN	20
20	$LiClO_4$	CH_3CN	21
21	—	CH_3CN	10

[a]Reaction conditions: **alkene** (0.5 mmol, 1.0 equiv), **diazo** (1.0 mmol, 2.0 equiv), **TBN** (1.0 mmol, 2.0 eqiuv), Lewis Acid (0.05 mmol, 10 mol %) and solvent (2.0 mL) at 25 ℃ under air for 12 h unless otherwise noted. [b]Isolated yields.

DFT calculations

Computational methods

The BP86 density functional method (DFT)[5] was employed to carry out all the calculations. The LANL2DZ[6] and 6-31G(d) basis sets[7] were used for Br and the other atoms, respectively. To consider solvation effects, geometry optimizations were performed with the SMD solvation model[8] (solvent = N,N-dimethylformamide or acetonitrile). Vibrational frequency analyses at the same level of the theory were performed on all the optimized geometries to characterize them as local minima (no imaginary frequency) or transition states (one imaginary frequency). In addition, intrinsic reaction coordinate (IRC) calculations were used to verify that the transition state connect with appropriate reactant and product.[9] The Gibbs energies for all species were obtained at 298.15 K and 1 atm at their respective optimized structures. The larger basis sets, SDD[10] for Br and 6-311++G(d,p) for other atoms, were utilized for single-point energy calculations with SMD solvation model. The solution-phase Gibbs energy was determined by adding the solvation single-point energy and the gas-phase thermal correction to the Gibbs energy obtained from the vibrational frequencies. The translational entropy in solution was corrected using the method proposed by Whitesides *et al*.[11] Unless otherwise specified, the solution-phase Gibbs energy was used in the present discussions. All calculations

were carried out with the Gaussian 09 suite of programs.[12]

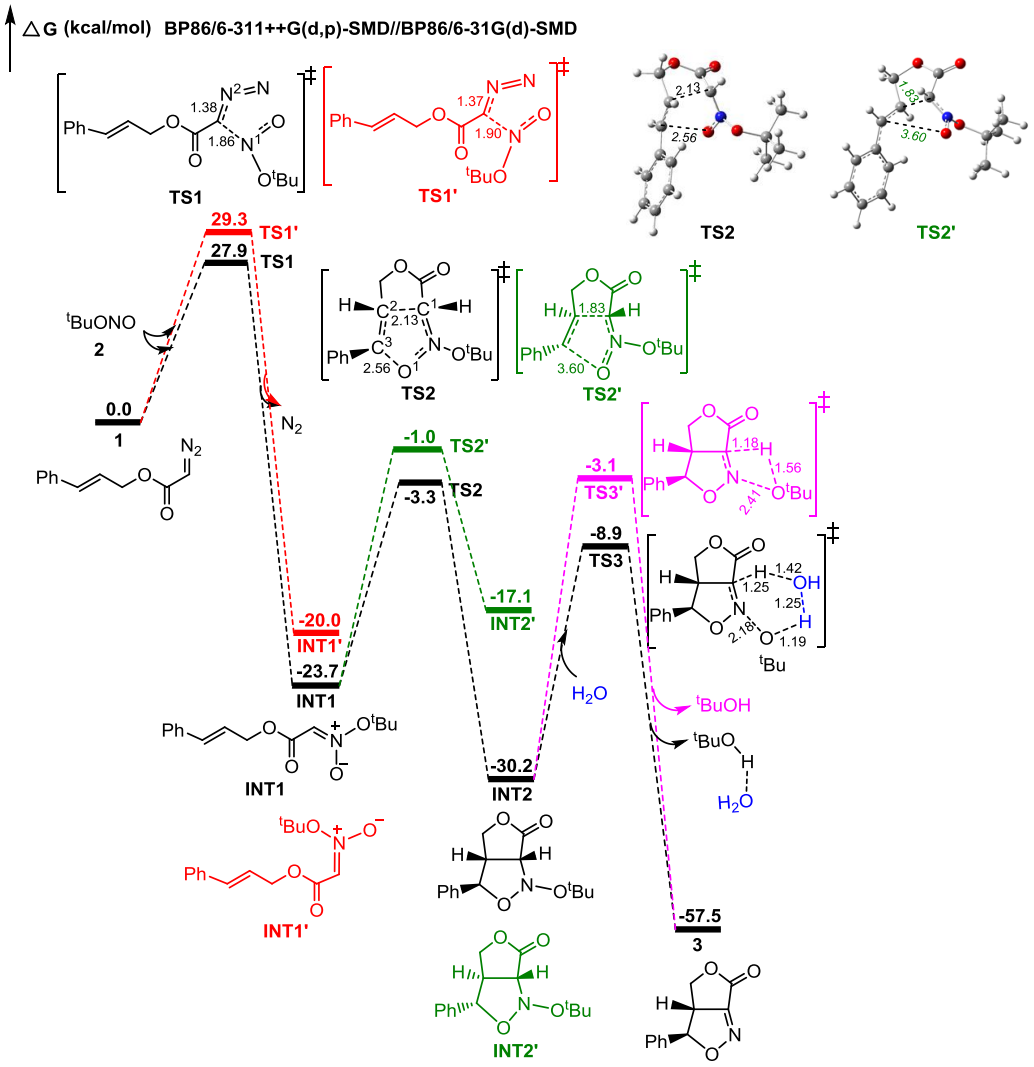


Figure S1. Energy profiles for the intramolecular acyclic nitronates olefins cycloaddition reaction. Bond lengths are shown in Å.

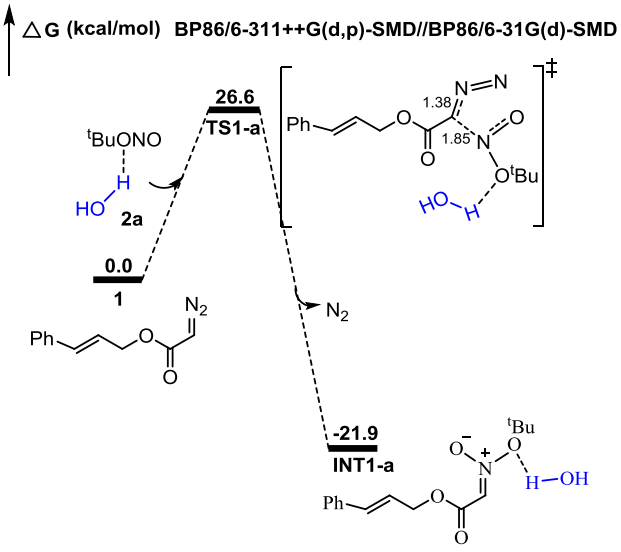


Figure S2. Energy profile for the formation of nitronate intermediate with the assistance of one water molecule. Bond lengths are shown in Å.

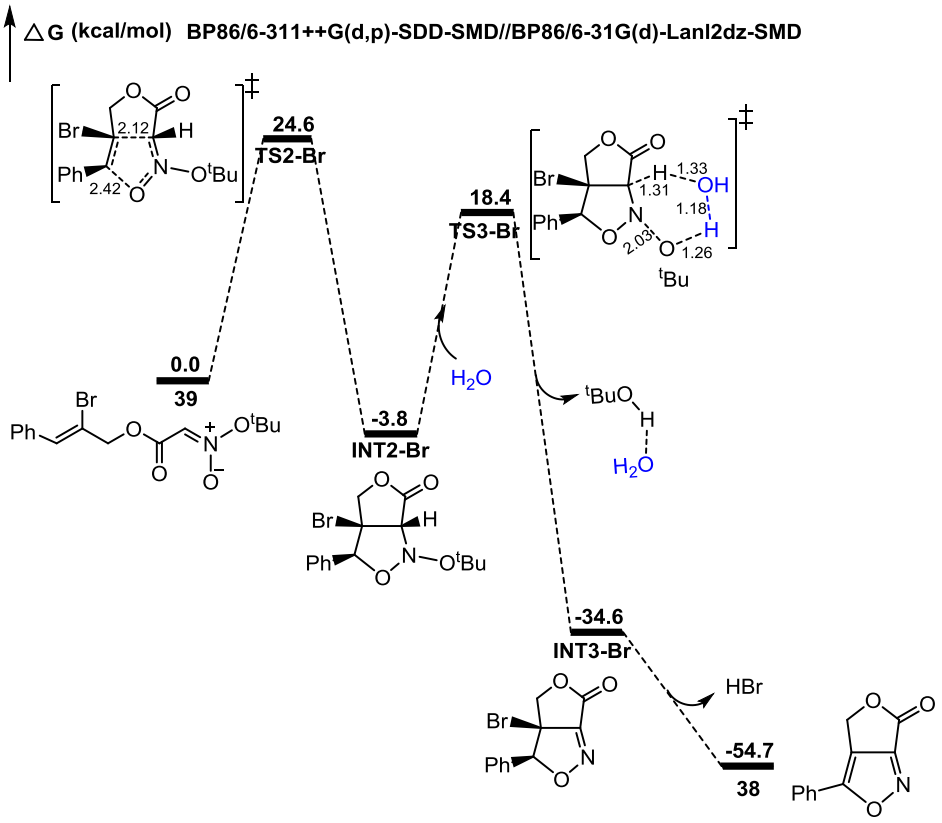


Figure S3. Energy profiles for the intramolecular acyclic nitronates olefins cycloaddition reaction for the substrate 37. Bond lengths are shown in Å.

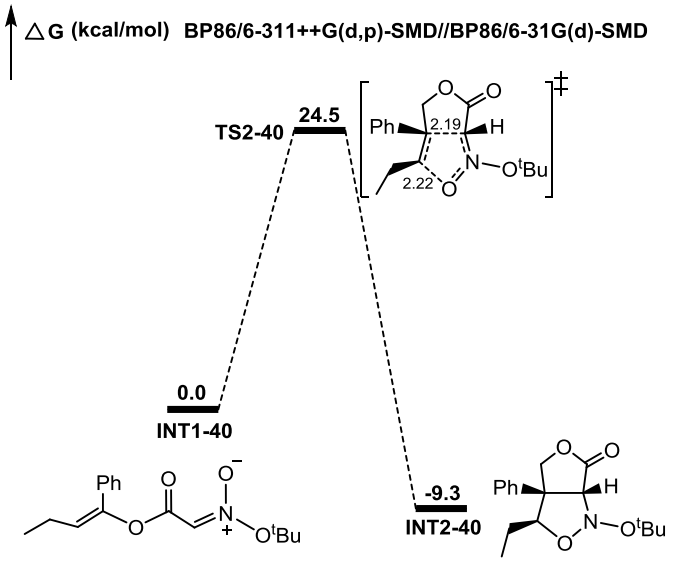


Figure S4. Energy profile for the intramolecular [3+2] cycloaddition after the formation of nitronate intermediate for the substrate **40**. Bond lengths are shown in Å.

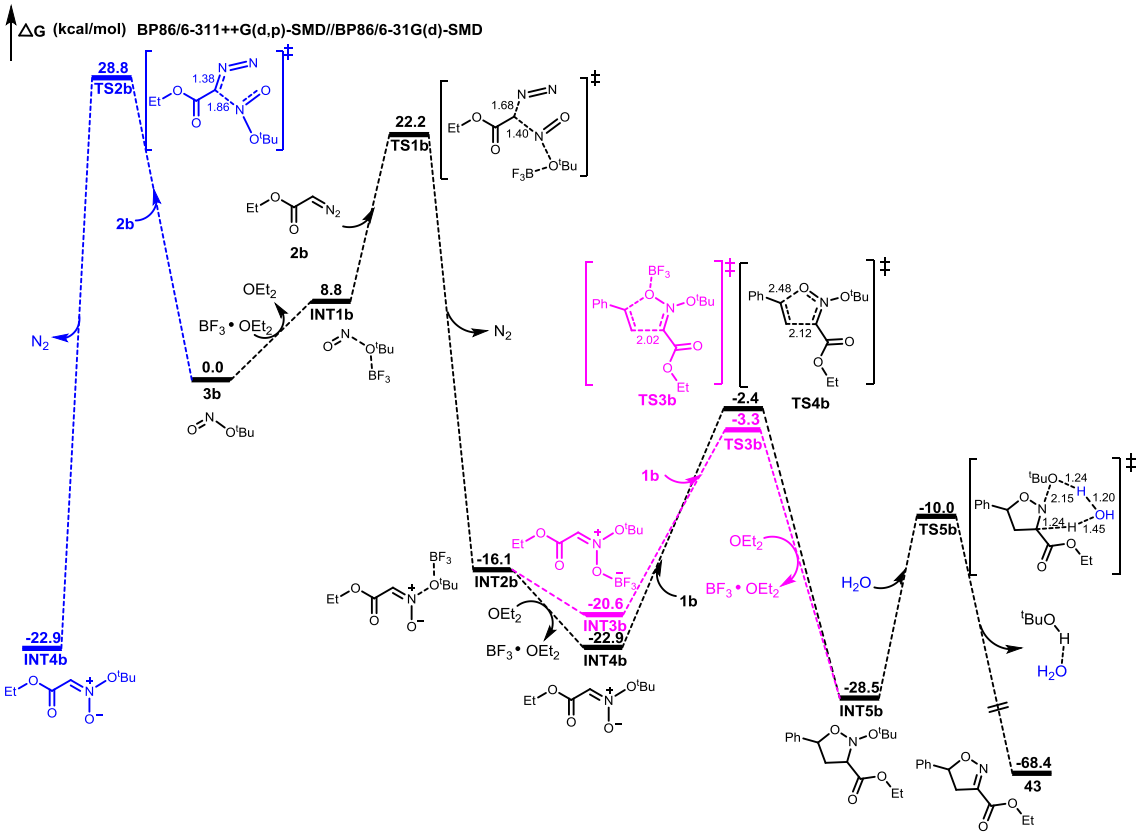
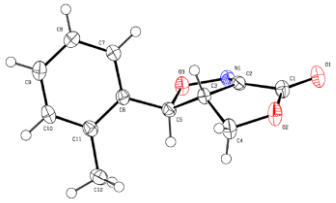
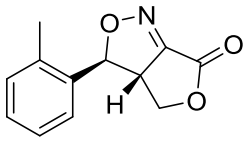


Figure S5. Energy profiles for the intermolecular acyclic nitronates olefins cycloaddition reaction with and without the assistance of $BF_3 \cdot OEt_2$. Bond lengths are shown in Å.

X-Ray diffraction analysis of compound 6, 16, 29 and 31





Structure of **6** (CCDC 2011281)

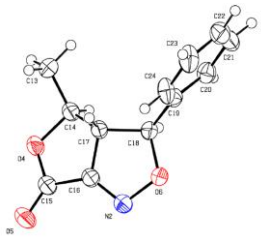
Table S3: Crystal data and structure refinement for **6 (**Molecular structure of **6** with ellipsoids at the 50% probability level.**)**

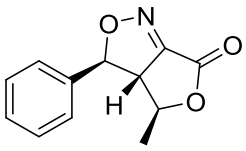
Empirical formula	$C_{12}H_{11}NO_3$
Formula weight	217.22
Temperature/K	119.99
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.4596(7)
b/Å	7.5335(5)
c/Å	10.8814(7)
α / °	90
β / °	92.749(2)
γ / °	90
Volume/Å^3	1020.20(11)
Z	4
ρ_{calc}g/cm^3	1.414
μ /mm^{-1}	0.103
F(000)	456.0
Crystal size/mm^3	0.4 × 0.4 × 0.4
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.548 to 55.092
Index ranges	-16 ⩽ h ⩽ 15, -9 ⩽ k ⩽ 9, -14 ⩽ l ⩽ 14
Reflections collected	15370
Independent reflections	2342 [R_{int} = 0.0696, R_{sigma} = 0.0447]
Data/restraints/parameters	2342/0/146
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0409, wR_2 = 0.1117
Final R indexes [all data]	R_1 = 0.0563, wR_2 = 0.1264

Largest diff. peak/hole / e Å^{-3}	0.26/-0.26

Table S4: Bond lengths [Å] and angles [°] for **6**

O3-N1	1.4145(15)	C6-C7	1.395(2)
O3-C5	1.4927(16)	C6-C11	1.3978(19)
O1-C1	1.1971(17)	C6-C5	1.5022(19)
O2-C1	1.3585(18)	C2-C1	1.480(2)
O2-C4	1.4736(17)	C10-C11	1.399(2)
N1-C2	1.2727(18)	C10-C9	1.378(2)
C3-C2	1.4858(18)	C7-C8	1.386(2)
C3-C5	1.5194(19)	C11-C12	1.506(2)
C3-C4	1.523(2)	C8-C9	1.386(2)
N1-O3-C5	108.45(10)	C8-C7-C6	120.97(14)
C1-O2-C4	112.01(11)	C6-C11-C10	117.79(14)
C2-N1-O3	106.42(11)	C6-C11-C12	122.43(13)
C2-C3-C5	99.24(11)	C10-C11-C12	119.76(13)
C2-C3-C4	99.75(11)	O3-C5-C3	102.46(10)
C5-C3-C4	122.62(13)	O3-C5-C6	108.36(11)
C7-C6-C11	120.15(13)	C6-C5-C3	116.93(11)
C7-C6-C5	118.37(12)	O1-C1-O2	123.01(14)
C11-C6-C5	121.44(13)	O1-C1-C2	131.91(14)
N1-C2-C3	117.04(13)	O2-C1-C2	105.07(12)
N1-C2-C1	130.93(13)	C7-C8-C9	119.20(15)
C1-C2-C3	110.11(12)	C10-C9-C8	119.95(14)
C9-C10-C11	121.93(14)	O2-C4-C3	104.38(12)





Structure of **16** (CCDC 2021609)

Table S5: Crystal data and structure refinement for **16 (**Molecular structure of **16** with ellipsoids at the 50% probability level.**)**

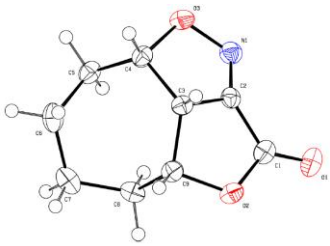
Empirical formula	$C_{24}H_{22}N_2O_6$
Formula weight	434.43
Temperature/K	120.04

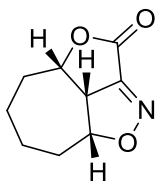
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.4978(7)
b/Å	19.9607(13)
c/Å	11.2962(8)
α / °	90
β / °	91.786(2)
γ / °	90
Volume/Å^3	2140.5(3)
Z	4
ρ_{calc}g/cm^3	1.348
μ /mm^{-1}	0.098
F(000)	912.0
Crystal size/mm^3	0.5 × 0.4 × 0.4
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/ °	4.144 to 55.04
Index ranges	-12 ⩽ h ⩽ 12, -25 ⩽ k ⩽ 25, -14 ⩽ l ⩽ 14
Reflections collected	43141
Independent reflections	4914 [R_{int} = 0.0753, R_{sigma} = 0.0415]
Data/restraints/parameters	4914/0/291
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0523, wR_2 = 0.1340
Final R indexes [all data]	R_1 = 0.0835, wR_2 = 0.1609
Largest diff. peak/hole / e Å^{-3}	0.47/-0.36

Table S6: Bond lengths [Å] and angles [°] for 1**6**

C1-C2	1.495(3)	C13-C14	1.498(3)
C2-C5	1.525(3)	C14-C17	1.523(3)
C2-O1	1.484(2)	C14-O4	1.494(2)
C3-C4	1.482(3)	C15-C16	1.483(3)
C3-O1	1.348(3)	C15-O4	1.341(3)
C3-O2	1.201(3)	C15-O5	1.198(3)
C4-C5	1.476(3)	C16-C17	1.481(3)
C4-N1	1.273(3)	C16-N2	1.270(3)
C5-C6	1.520(3)	C17-C18	1.512(3)
C6-C7	1.494(3)	C18-C19	1.502(3)
C6-O3	1.480(2)	C18-O6	1.496(2)
C7-C8	1.386(3)	C19-C20	1.384(3)
C7-C12	1.376(3)	C19-C24	1.384(3)
C8-C9	1.368(3)	C20-C21	1.394(3)

C9-C10	1.351(5)	C21-C22	1.374(4)
C10-C11	1.368(5)	C22-C23	1.380(4)
C11-C12	1.419(4)	C23-C24	1.371(3)
N1-O3	1.417(2)	N2-O6	1.413(2)
C1-C2-C5	116.69(17)	C13-C14-C17	117.06(18)
O1--C2-C1	107.74(16)	O4-C14-C13	107.42(16)
O1-C2-C5	104.24(15)	O4-C14-C17	103.67(15)
O1-C3-C4	105.71(17)	O4-C15-C16	105.63(17)
O2-C3-C4	131.3(2)	O5-C15-C16	131.2(2)
O2-C3-O1	123.0(2)	O5-C15-O4	123.12(19)
C5-C4-C3	110.23(17)	C17-C16-C15	110.11(16)
N1-C4-C3	130.28(19)	N2-C16-C15	130.18(19)
N1-C4-C5	116.98(18)	N2-C16-C17	117.18(17)
C4-C5-C2	101.14(15)	C16-C17-C14	100.82(15)
C4-C5-C6	98.52(15)	C16-C17-C18	98.85(15)
C6-C5-C2	122.13(16)	C18-C17-C14	122.25(17)
C7-C6-C5	116.18(16)	C19-C18-C17	117.70(16)
O3-C6-C5	102.17(14)	O6-C18-C17	102.18(14)
O3-C6-C7	111.05(16)	O6-C18-C19	109.55(15)
C8-C7-C6	117.28(19)	C20-C19-C18	117.81(18)
C12-C7-C6	123.3(2)	C24-C19-C18	122.79(18)
C12-C7-C8	119.3(2)	C24-C19-C20	119.39(19)
C9-C8-C7	121.5(3)	C19-C20-C21	120.1(2)
C10-C9-C8	120.0(3)	C22-C21-C20	119.8(2)
C9-C10-C11	120.4(3)	C21-C22-C23	119.8(2)
C10-C11-C12	120.5(3)	C24-C23-C22	120.7(2)
C7-C12-C11	118.3(3)	C23-C24-C19	120.2(2)
C4-N1-O3	106.00(16)	C16-N2-O6	106.11(16)
C3-O1-C2	112.39(15)	C15-O4-C14	112.40(15)
N1-O3-C6	107.51(14)	N2-O6-C18	107.39(13)





Structure of **29** (CCDC 2011280)

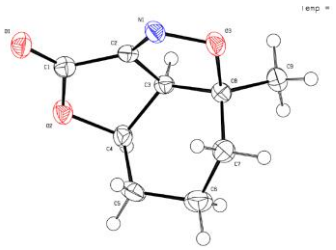
Table S7: Crystal data and structure refinement for **29 (**Molecular structure of **29** with ellipsoids at the 50% probability level.**)**

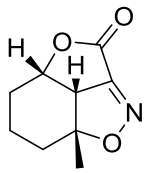
Empirical formula	$C_9H_{11}NO_3$
Formula weight	181.19
Temperature/K	120.03
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	10.2859(6)
b/Å	10.6455(6)
c/Å	7.6374(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	836.28(9)
Z	4
ρ_{calc}g/cm^3	1.439
μ/mm^{-1}	0.109
F(000)	384.0
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.508 to 54.944
Index ranges	$-13 \leq h \leq 11$, $-13 \leq k \leq 12$, $-9 \leq l \leq 9$
Reflections collected	6696
Independent reflections	1889 [R_{int} = 0.0630, R_{sigma} = 0.0663]
Data/restraints/parameters	1889/1/118
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0414, wR_2 = 0.0856
Final R indexes [all data]	R_1 = 0.0614, wR_2 = 0.0977
Largest diff. peak/hole / e Å^{-3}	0.17/-0.20
Flack parameter	-0.3(10)

Table S8: Bond lengths [Å] and angles [°] for **29**

O2-C9	1.491(3)	C3-C9	1.544(4)
O2-C1	1.358(3)	C3-C4	1.533(4)
O3-N1	1.406(3)	C9-C8	1.511(4)
O3-C4	1.493(3)	C4-C5	1.517(4)
O1-C1	1.205(3)	C8-C7	1.527(4)

N1-C2	1.271(4)	C5-C6	1.529(4)
C2-C3	1.478(4)	C6-C7	1.534(4)
C2-C1	1.475(4)		
C1-O2-C9	111.7(2)	C8-C9-C3	117.4(2)
N1-O3-C4	109.3(2)	O3-C4-C3	102.9(2)
C2-N1-O3	106.6(2)	O3-C4-C5	109.0(2)
N1-C2-C3	118.0(3)	C5-C4-C3	118.8(2)
N1-C2-C1	130.2(3)	C9-C8-C7	114.0(3)
C1-C2-C3	110.4(2)	O2-C1-C2	105.4(2)
C2-C3-C9	99.9(2)	O1-C1-O2	123.0(3)
C2-C3-C4	99.3(2)	O1-C1-C2	131.6(3)
C4-C3-C9	127.4(2)	C4-C5-C6	109.9(3)
O2-C9-C3	102.5(2)	C5-C6-C7	113.8(2)
O2-C9-C8	107.4(2)	C8-C7-C6	115.1(2)





Structure of **31** (CCDC 2011278)

Table S9: Crystal data and structure refinement for **31 (**Molecular structure of **31** with ellipsoids at the 50% probability level.**)**

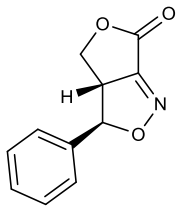
Empirical formula	$C_9H_{11}NO_3$
Formula weight	181.19
Temperature/K	119.98
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.0794(6)
b/Å	23.851(2)
c/Å	6.5545(6)
α/°	90
β/°	114.294(3)
γ/°	90
Volume/Å^3	866.26(15)
Z	4
ρ_{calc}g/cm^3	1.389
μ/mm^{-1}	0.105
F(000)	384.0

Crystal size/mm^3	0.5 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/ °	7.354 to 49.992
Index ranges	-7 ≤ h ≤ 7, -28 ≤ k ≤ 28, -7 ≤ l ≤ 7
Reflections collected	9883
Independent reflections	1516 [R_{int} = 0.0642, Rsigma = 0.0388]
Data/restraints/parameters	1516/0/135
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0473, wR_2 = 0.1141
Final R indexes [all data]	R_1 = 0.0515, wR_2 = 0.1184
Largest diff. peak/hole / e Å^{-3}	0.72/-0.24

Table S10: Bond lengths [Å] and angles [°] for **31**

O2-C1	1.348(2)	C3-C4	1.538(2)
O2-C4	1.489(2)	C3-C8	1.525(3)
O1-C1	1.204(2)	C4-C5	1.520(3)
O3-N1	1.412(2)	C8-C9	1.508(3)
O3-C8	1.504(2)	C8-C7	1.529(3)
N1-C2	1.275(2)	C7-C6	1.498(3)
C2-C3	1.476(3)	C5-C6	1.523(3)
C2-C1	1.476(3)		
C1-O2-C4	111.84(14)	O2-C4-C3	103.56(14)
N1-O3-C8	108.54(13)	O2-C4-C5	109.03(16)
C2-N1-O3	106.31(15)	C5-C4-C3	113.65(16)
N1-C2-C3	117.05(17)	O3-C8-C3	101.33(14)
N1-C2-C1	130.63(17)	O3-C8-C9	106.08(15)
C1-C2-C3	110.37(15)	O3-C8-C7	107.02(15)
C2-C3-C4	100.36(14)	C3-C8-C7	113.01(15)
C2-C3-C8	99.80(15)	C9-C8-C3	114.67(16)
C8-C3-C4	123.23(15)	C9-C8-C7	113.41(17)
O2-C1-C2	105.96(15)	C6-C7-C8	112.25(17)
O1-C1-O2	123.26(17)	C4-C5-C6	111.62(17)
O1-C1-C2	130.76(17)	C7-C6-C5	111.07(19)

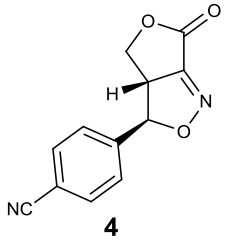
Compound characterisations



3

3-Phenyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (3)

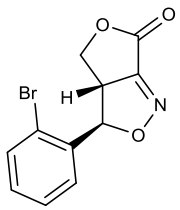
ethyl acetate/ petroleum ether =1:4; light yellow solid; 85% yield (34.6 mg); 10.0 mmol scale: 81% yield (1.64 g, 20 h); mp: 107-108℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.32 (m, 5H), 5.76 (d, *J* = 12.5, 1H), 4.76 (t, *J* = 8.6, 1H), 4.45 (t, *J* = 8.6, 1H), 4.37 (dt, *J* = 12.5, 8.6, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 157.2, 134.7, 129.7, 129.1, 126.8, 94.3, 69.9, 54.4; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_9NNaO_3^+$+MeOH: 258.0737, Found: 258.0752; IR (neat, cm^{-1}): υ 3035, 2919, 2850, 1781, 1622, 1077, 755, 696.



4

4-(-6-Oxo-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-3-yl)benzonitrile (4)

ethyl acetate/ petroleum ether =1:3; white solid; 90% yield (41.1 mg); mp: > 200℃; ^{1}H NMR (400 MHz, DMSO-d6) δ 7.92 (d, *J* = 8.3, 2H), 7.71 (d, *J* = 8.3, 2H), 6.03 (d, *J* = 12.2, 1H), 4.83 – 4.75 (m, 1H), 4.73 – 4.59 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 159.3, 159.1, 141.5, 132.8, 128.4, 118.6, 111.9, 91.8, 70.3, 54.2; Anal. Calcd. For $C_{12}H_8N_2NaO_3^+$+MeOH: 283.0689, Found: 283.0697; IR (neat, cm^{-1}): υ 2918, 2850, 2226, 1778, 1633, 1288, 1082, 851.

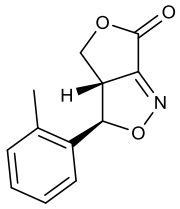


5

3-(2-Bromophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (5)

ethyl acetate/ petroleum ether =1:4; light yellow solid; 87% yield (49.1 mg); mp: 112-114℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.70 (m, 1H), 7.63 – 7.57 (m, 1H), 7.47 – 7.29 (m, 1H), 7.31 – 7.25 (m, 1H), 6.02 (d, *J* = 12.2, 1H), 4.90 (t, *J* = 9.0, 1H), 4.66 (t, *J* = 9.0, 1H), 4.11 (dt, *J* = 12.2, 9.0, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 157.0, 136.0, 132.7, 130.4 , 128.3, 126.9, 121.3, 92.6, 71.0, 55.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_8{}^{79}BrNNaO_3^+$+MeOH: 335.9842, $C_{11}H_8{}^{81}BrNNaO_3^+$+MeOH:

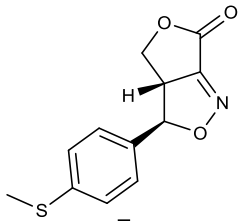
337.9821, Found: 335.9852, 337.9834; IR (neat, cm^{-1}): υ 2918, 2850, 1783, 1629, 1359, 1292, 1081, 925, 766.



6

3-(o-Tolyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (6)

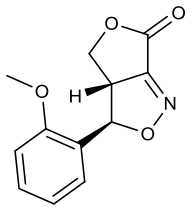
ethyl acetate/ petroleum ether =1:4; light yellow solid; 83% yield (36.1 mg); mp: 106-108℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.51 (m, 1H), 7.34 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 5.96 (d, *J* = 12.7, 1H), 4.78 (t, *J* = 8.8, 1H), 4.47 (t, *J* = 8.8, 1H), 4.29 (dt, *J* = 12.7, 8.8, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 157.0, 135.5, 133.2, 131.0, 129.3, 126.7, 125.8, 92.0, 70.2, 53.7, 19.3; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{11}NNaO_3^+$+MeOH: 272.0893, Found: 272.0906; IR (neat, cm^{-1}): υ 2912, 2851, 1782, 1635, 1290, 1063, 924, 840, 763.



7

3-(4-(Methylthio)phenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (7)

ethyl acetate/ petroleum ether =1:2; yellow solid; 97% yield (48.4 mg); mp: 147-148℃; ^{1}H NMR (400 MHz, DMSO-d6) δ 7.48 – 7.42 (m, 2H), 7.36 – 7.30 (m, 2H), 5.90 (d, *J* = 12.2, 1H), 4.79 – 4.71 (m, 1H), 4.69 – 4.58 (m, 2H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 159.38, 159.36, 139.8, 131.9, 128.2, 126.0, 92.9, 70.3, 53.3, 14.6; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{11}NNaO_3S^+$+MeOH: 304.0614, Found: 304.0618; IR (neat, cm^{-1}): υ 2919, 2850, 1779, 1717, 1636, 1288, 1083, 957, 919, 844.

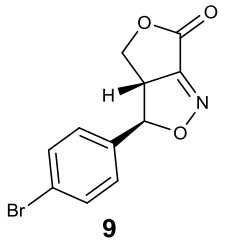


8

3-(2-Methoxyphenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (8)

ethyl acetate/ petroleum ether =1:4; light yellow solid; 67% yield (31.1 mg); mp: 97-99℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.4, 1H), 7.39 – 7.33 (m, 1H), 7.07 – 7.01 (m, 1H), 6.92 (d, *J* = 8.3, 1H), 5.84 (d, *J* = 12.9, 1H), 4.77 (t, *J* = 8.9, 1H), 4.52 (t, *J* = 8.9, 1H), 4.12 (dt, *J* = 12.9, 8.9, 1H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 158.0, 155.7, 129.8, 126.0, 124.4, 121.1, 110.2, 90.3, 71.0, 55.5,

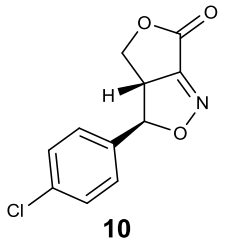
54.4; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{11}NNaO_4^+$+MeOH: 288.0842, Found: 288.0851; IR (neat, cm^{-1}): υ 2918, 2849, 1780, 1622, 1463, 1250, 1076, 985, 855, 763.



9

3-(4-Bromophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (9)

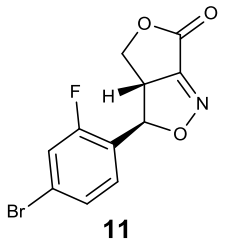
ethyl acetate/ petroleum ether =1:4; light yellow solid; 78% yield (44.0 mg); mp: 132-133℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.5, 2H), 7.31 (d, *J* = 8.5, 2H), 5.73 (d, *J* = 12.6, 1H), 4.77 (t, *J* = 8.8, 1H), 4.45 (t, *J* = 8.8, 1H), 4.33 (dt, *J* = 12.6, 8.8, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.2, 133.8, 132.3, 128.4, 123.8, 93.4, 69.8, 54.6; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_8{}^{79}BrNNaO_3^+$+MeOH: 335.9842, $C_{11}H_8{}^{81}BrNNaO_3^+$+MeOH: 337.9821, Found: 335.9850, 337.9837; IR (neat, cm^{-1}): υ 2920, 2851, 1776, 1630, 1490, 1290, 1081, 1068, 919, 847.



10

3-(4-Chlorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (10)

ethyl acetate/ petroleum ether =1:4; white solid; 89% yield (42.3 mg); mp: 112-114℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.29 (m, 4H), 5.74 (d, *J* = 12.6, 1H), 4.76 (t, *J* = 8.8, 1H), 4.45 (t, *J* = 8.8, 1H), 4.33 (dt, *J* = 12.6, 8.8, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 157.3, 135.6, 133.3, 129.3, 128.2, 93.4, 69.8, 54.5; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_8ClNNaO_3^+$+MeOH: 292.0347, Found: 292.0359; IR (neat, cm^{-1}): υ 2924, 2852, 1776, 1637, 1492, 1291, 1082, 848, 803.

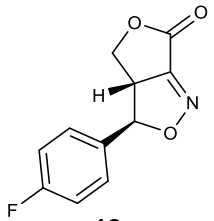


11

3-(4-Bromo-2-fluorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (11)

ethyl acetate/ petroleum ether =1:4; light yellow solid; 86% yield (51.7 mg); mp: 110-112℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (t, *J* = 8.0, 1H), 7.42 – 7.36 (m, 1H), 7.35 – 7.28 (m, 1H), 5.84 (d, *J* = 12.7, 1H), 4.82 (t, *J* = 8.9, 1H), 4.51 (t, *J* = 8.9, 1H), 4.28 (dt, *J* = 12.7, 8.9, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4 (d, *J* = 250.9), 157.75, 157.72, 128.5 (d, *J* = 3.9), 128.3 (d, *J* = 3.6), 123.5 (d, *J* = 9.6), 122.3 (d,

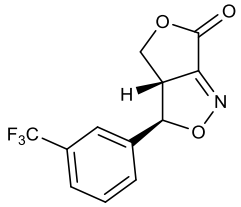
J = 12.9), 119.4 (d, *J* = 23.8), 87.7 (d, *J* = 2.4), 70.0 (d, *J* = 3.7), 54.2 (d, *J* = 1.7); ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_7{}^{79}BrFNNaO_3{}^+$+MeOH: 353.9748, $C_{11}H_7{}^{81}BrFNNaO_3{}^+$+MeOH: 355.9727, Found: 353.9733, 355.9745; IR (neat, cm^{-1}): υ 3077, 2958, 2925, 2852, 1790, 1640, 1487, 1286, 1066, 890, 850, 839, 808.



12

3-(4-Fluorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (12)

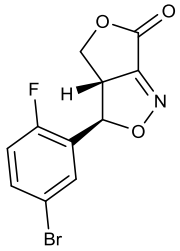
ethyl acetate/ petroleum ether =1:4; white solid; 84% yield (37.1 mg); 10.0 mmol scale: 79% yield (1.75 g, 16 h); mp: 100-102℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.33 (m, 2H), 7.21 – 7.00 (m, 2H), 5.75 (d, *J* = 12.6, 1H), 4.76 (t, *J* = 8.8, 1H), 4.45 (t, *J* = 8.8, 1H), 4.35 (dt, *J* = 12.6, 8.8, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3 (d, *J* = 249.4), 158.1, 157.3, 130.5 (d, *J* = 3.3), 128.9 (d, *J* = 8.6), 116.2 (d, *J* = 21.9), 93.5, 69.9, 54.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_8FNNaO_3{}^+$+MeOH: 276.0643, Found: 276.0657; IR (neat, cm^{-1}): υ 2919, 2850, 1774, 1634, 1510, 1228, 1081, 847, 800.



13

3-(3-(Trifluoromethyl)phenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (13)

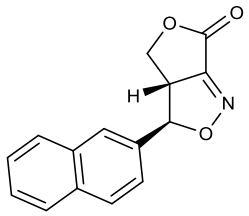
ethyl acetate/ petroleum ether =1:4; white solid; 70% yield (38.0 mg); mp: 118-119℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.67 (m, 2H), 7.67 – 7.57 (m, 2H), 5.83 (d, *J* = 12.5, 1H), 4.81 (t, *J* = 8.8, 1H), 4.50 (t, *J* = 8.8, 1H), 4.38 (dt, *J* = 12.5, 8.8, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 157.2, 136.1, 130.1, 129.8, 126.5 (q, *J* = 3.7), 123.7 (q, *J* = 3.8), 93.1, 69.7, 54.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_8F_3NNaO_3{}^+$+MeOH: 326.0611, Found: 326.0624; IR (neat, cm^{-1}): υ 2918, 2850, 1776, 1636, 1331, 1130, 1083, 1071, 895, 802, 705.



14

3-(5-Bromo-2-fluorophenyl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (14)

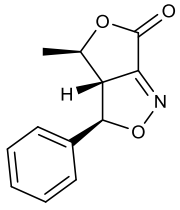
ethyl acetate/ petroleum ether =1:4; white solid; 92% yield (55.2 mg); mp: 124-126℃; ^{1}H NMR (400 MHz, DMSO-d6) δ 7.84 – 7.78 (m, 1H), 7.70 – 7.63 (m, 1H), 7.35 – 7.26 (m, 1H), 6.06 (d, *J* = 11.7, 1H), 4.91 – 4.57 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 159.49, 159.47 (d, *J* = 248.3), 159.1, 133.9 (d, *J* = 8.7), 131.4 (d, *J* = 3.6), 125.7 (d, *J* = 14.4), 118.3 (d, *J* = 22.6), 116.5 (d, *J* = 3.5), 86.7 (d, *J* = 2.0), 70.3 (d, *J* = 2.0), 53.0; ^{19}F NMR (376 MHz, DMSO-d6) δ -118.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_7{}^{79}BrFNNaO_3{}^{+}$+MeOH: 353.9748, $C_{11}H_7{}^{81}BrFNNaO_3{}^{+}$+MeOH: 355.9727, Found: 353.9733, 355.9744; IR (neat, cm^{-1}): υ 3066, 2922, 2851, 1785, 1635, 1481, 1289, 1079, 1067, 871, 825.



15

3-(Naphthalen-2-yl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (15)

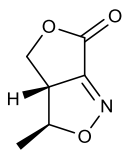
ethyl acetate/ petroleum ether =1:4; light yellow solid; 71% yield (36.0 mg); mp: 126-127℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.87 (m, 2H), 7.79 – 7.66 (m, 2H), 7.61 – 7.54 (m, 2H), 7.54 – 7.48 (m, 1H), 6.34 (d, *J* = 12.7, 1H), 4.77 (t, *J* = 8.8, 1H), 4.56 (t, *J* = 8.8, 1H), 4.41 (dt, *J* = 12.7, 8.8, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 157.3, 133.8, 130.5, 130.2, 130.1, 129.3, 127.1, 126.3, 125.3, 124.4, 122.2, 92.4, 70.3, 53.7; HRMS (ESI-TOF): Anal. Calcd. For $C_{15}H_{11}NNaO_3{}^{+}$+MeOH: 308.0893, Found: 308.0903; IR (neat, cm^{-1}): υ 3054, 2918, 2850, 1778, 1626, 1286, 1067, 929, 795, 779, 741.



16

4-Methyl-3-phenyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (16)

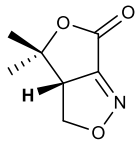
ethyl acetate/ petroleum ether =1:4; white solid; 80% yield (34.7 mg); mp: 114-115℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.35 (m, 5H), 5.77 (d, *J* = 12.4, 1H), 4.77 (dq, *J* = 8.0, 6.2, 1H), 3.90 (dd, *J* = 12.4, 8.0, 1H), 1.52 (d, *J* = 6.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 158.1, 135.3, 129.5, 129.2, 126.4, 93.0, 80.2, 61.7, 20.4; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{11}NNaO_3{}^{+}$+MeOH: 272.0893, Found: 272.0887; IR (neat, cm^{-1}): υ 2975, 2919, 2850, 1777, 1626, 1292, 1030, 887, 758, 703.



17

3-Methyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (17)

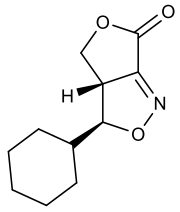
ethyl acetate/ petroleum ether =1:3; white solid; 76% yield (21.4 mg); mp: 73-75℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.91 (dq, *J* = 12.4, 6.2, 1H), 4.71 (t, *J* = 8.9, 1H), 4.29 (t, *J* = 8.9, 1H), 3.94 (dt, *J* = 12.4, 8.9, 1H), 1.64 (d, *J* = 6.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 157.6, 89.6, 69.8, 53.7, 18.2; HRMS (ESI-TOF): Anal. Calcd. For $C_6H_7NNaO_3^+$+MeOH: 196.0580, Found: 196.0576; IR (neat, cm^{-1}): υ 2986, 2918, 2850, 1771, 1633, 1292, 1076, 890, 847.



18

4,4-Dimethyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (18)

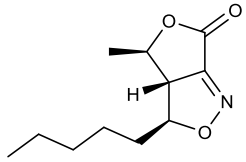
ethyl acetate/ petroleum ether =1:3; white solid; 71% yield (22.0 mg); mp: 64-65℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.84 (dd, *J* = 11.2, 9.1, 1H), 4.38 (dd, *J* = 12.2, 9.1, 1H), 4.22 (dd, *J* = 12.2, 11.2, 1H), 1.61 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 157.2, 85.6, 74.8, 59.1, 28.6, 23.4; HRMS (ESI-TOF): Anal. Calcd. For $C_7H_9NNaO_3^+$+MeOH: 210.0737, Found: 210.0750; IR (neat, cm^{-1}): υ 2920, 2850, 1765, 1637, 1295, 1265, 1053, 866, 843.



19

3-Cyclohexyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (19)

ethyl acetate/ petroleum ether =1:3; white solid; 61% yield (25.6 mg); mp: 62-64℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.66 (t, *J* = 8.9, 1H), 4.47 (dd, *J* = 12.8, 8.2, 1H), 4.23 (t, *J* = 8.9, 1H), 3.96 (dt, *J* = 12.8, 8.9, 1H), 2.03 – 1.95 (m, 1H), 1.84 – 1.68 (m, 3H), 1.61 – 1.48 (m, 1H), 1.37 – 1.14 (m, 4H), 1.09 – 0.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 157.1, 97.9, 70.1, 50.8, 40.4, 29.8, 28.9, 25.9, 25.4, 25.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_{15}NNaO_3^+$+MeOH: 264.1206, Found: 264.1218; IR (neat, cm^{-1}): υ 2924, 2853, 1778, 1621, 1292, 1071, 933, 892.

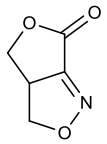


20

4-Methyl-3-pentyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (20)

ethyl acetate/ petroleum ether =1:4; colorless liquid; 66% yield (27.9 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (dt, *J* = 12.1, 6.8, 1H), 4.57 (dq, *J* = 8.1, 6.2, 1H), 3.47 (dd, *J* = 12.1, 8.1, 1H), 2.07 – 1.96 (m, 1H), 1.87 – 1.76 (m, 1H), 1.54 (d, *J* = 6.2, 3H), 1.47 – 1.29 (m, 6H), 0.97 – 0.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 158.4, 92.3, 80.1, 59.9, 32.9, 31.3, 25.5, 22.3, 20.5, 13.8; HRMS (ESI-TOF): Anal.

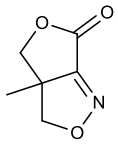
Calcd. For $C_{11}H_{17}NNaO_3^+$: 234.1101, Found: 234.1091; IR (neat, cm^{-1}): υ 2932, 2862, 1781, 1625, 1297, 1034, 890, 866.



21

3a,4-Dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (21)

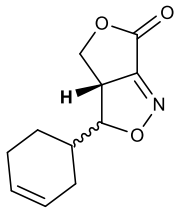
ethyl acetate/ petroleum ether =1:3; white solid; 67% yield (17.0 mg); mp: 59-60℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.00 – 4.92 (m, 1H), 4.84 – 4.73 (m, 1H), 4.51 – 4.25 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 156.5, 78.1, 70.4, 49.0; HRMS (ESI-TOF): Anal. Calcd. For $C_5H_5NNaO_3^+$+MeOH: 182.0424, Found: 182.0422; IR (neat, cm^{-1}): υ 2921, 2888, 2852, 1771, 1628, 1276, 1080, 888, 852, 824, 747.



22

3a-Methyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (22)

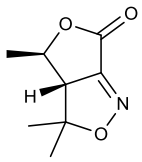
ethyl acetate/ petroleum ether =1:3; white solid; 51% yield (14.4 mg); mp: 64-65℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.55 (d, *J* = 9.0, 1H), 4.44 (d, *J* = 9.0, 1H), 4.41 (d, *J* = 9.0, 1H), 4.36 (d, *J* = 9.0, 1H), 1.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 158.0, 83.7, 76.6, 54.6, 20.7; HRMS (ESI-TOF): Anal. Calcd. For $C_6H_7NNaO_3^+$+MeOH: 196.0580, Found: 196.0585; IR (neat, cm^{-1}): υ 2922, 2850, 1779, 1761, 1629, 1291, 1065, 868, 844.



23

3-(Cyclohex-3-en-1-yl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (23)

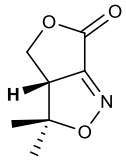
ethyl acetate/ petroleum ether =1:3; white solid; 65% yield (26.9 mg); mp: 105-106℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.16 – 5.50 (m, 3H), 4.72 – 4.64 (m, 1H), 4.60 (dt, *J* = 12.8, 7.9, 1H), 4.31 – 4.23 (m, 1H), 4.06 – 3.95 (m, 1H), 2.38 – 1.96 (m, 5H), 1.76 – 1.59 (m, 1H), 1.54 – 1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 157.2, 157.1, 127.9, 126.7, 124.9, 123.9, 97.3, 96.7, 70.1, 70.0, 50.95, 50.87, 36.6, 36.4, 28.3, 27.3, 25.2, 25.0, 24.2, 23.8; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_{13}NNaO_3^+$+MeOH: 262.1050, Found: 262.1060; IR (neat, cm^{-1}): υ 3024, 2922, 2849, 1786, 1720, 1632, 1292, 1068, 907, 849, 665.



24

3,3,4-Trimethyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (24)

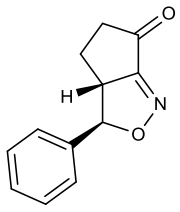
ethyl acetate/ petroleum ether =1:4; white solid; 73% yield (24.7 mg); mp: 99-101℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.72 (dq, *J* = 8.6, 6.2, 1H), 3.62 (d, *J* = 8.6, 1H), 1.68 (s, 3H), 1.52 (d, *J* = 6.2, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 157.0, 94.1, 76.3, 63.3, 27.5, 22.0, 20.9; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{11}NNaO_3^+$+MeOH: 272.0893, Found: 272.0887; IR (neat, cm^{-1}): υ 2986, 2918, 2850, 1772, 1637, 1319, 1153, 1097, 1035, 893, 882.



25

3,3-Dimethyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (25)

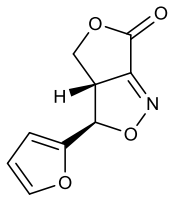
ethyl acetate/ petroleum ether =1:3; colorless liquid; 78% yield (24.2 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.60 (t, *J* = 9.2, 1H), 4.37 (t, *J* = 9.2, 1H), 4.12 (t, *J* = 9.2, 1H), 1.68 (s, 3H), 1.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 155.7, 95.2, 66.6, 55.5, 26.9, 21.9; HRMS (ESI-TOF): Anal. Calcd. For $C_7H_9NNaO_3^+$: 178.0475, Found: 178.0462; IR (neat, cm^{-1}): υ 2978, 2934, 1719, 1579, 1277, 1222, 1150, 949.



26

3-Phenyl-3,3a,4,5-tetrahydro-6H-cyclopenta[c]isoxazol-6-one (26)

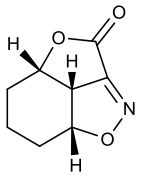
ethyl acetate/ petroleum ether =1:4; light yellow solid; 50% yield (20.1 mg); mp: 135-137℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.34 (m, 5H), 5.58 (d, *J* = 11.9, 1H), 3.97 (ddd, *J* = 11.9, 10.6, 7.7, 1H), 2.91 – 2.82 (m, 1H), 2.80 – 2.68 (m, 1H), 2.51 – 2.42 (m, 1H), 2.09 – 1.97 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.2, 165.1, 137.1, 128.92, 128.89, 126.5, 94.3, 56.8, 43.5, 25.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_9NNaO_3^+$+MeOH: 258.0737, Found: 258.0752; IR (neat, cm^{-1}): υ 3064, 3034, 2974, 2918, 2901, 1737, 1598, 1456, 1267, 1052, 840, 699.



27

3-(Furan-2-yl)-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (27)

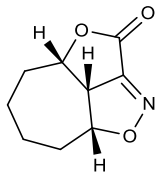
ethyl acetate/ petroleum ether =1:4; brownish liquid; 38% yield (14.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 1.8, 1H), 6.59 (d, *J* = 3.3, 1H), 6.45 (dd, *J* = 3.3, 1.8, 1H), 5.75 (d, *J* = 12.6, 1H), 4.81 – 4.67 (m, 2H), 4.45 – 4.34 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 157.0, 145.9, 144.4, 112.4, 111.1, 86.3, 69.7, 50.4; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_9NNaO_3^+$+MeOH: 248.0529, Found: 248.0521; IR (neat, cm^{-1}): υ 3150, 3126, 2972, 2916, 1779, 1725, 1627, 1287, 1073, 921, 743.



28

2a,2a1,3,4,5,5a-Hexahydro-7H-benzofuro[3,4-cd]isoxazol-7-one (28)

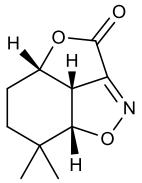
ethyl acetate/ petroleum ether =1:4; white solid; 74% yield (24.7 mg); mp: 74-76℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.23 (ddd, *J* = 10.9, 6.3, 4.9, 1H), 4.95 (ddd, *J* = 8.8, 7.0, 4.8, 1H), 4.38 (dd, *J* = 10.9, 8.8, 1H), 2.06 – 1.96 (m, 1H), 1.85 – 1.73 (m, 3H), 1.65 – 1.56 (m, 1H), 1.47 – 1.30 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 155.4, 85.0, 74.8, 48.1, 30.2, 29.3, 16.8; HRMS (ESI-TOF): Anal. Calcd. For $C_8H_9NNaO_3^+$: 190.0475, Found: 190.0481; IR (neat, cm^{-1}): υ 2930, 2851, 1784, 1621, 1297, 1086, 904, 723.



29

2a1,4a,6,7,8,8a-Hexahydro-2H,5H-1,4-dioxa-3-azacyclopenta[cd]azulen-2-one (29)

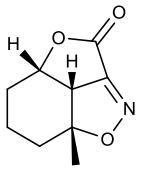
ethyl acetate/ petroleum ether =1:4; white solid; 82% yield (29.7 mg); mp: 65-66℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.12 (ddd, *J* = 11.8, 7.5, 4.0, 1H), 4.78 (ddd, *J* = 11.4, 8.0, 4.4, 1H), 4.47 (dd, *J* = 11.8, 8.0, 1H), 2.20 – 2.08 (m, 2H), 1.87 – 1.71 (m, 2H), 1.73 – 1.46 (m, 3H), 1.38 – 1.24 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 154.2, 86.7, 81.0, 54.8, 30.6, 28.3, 21.2, 21.0; HRMS (ESI-TOF): Anal. Calcd. For $C_9H_{11}NNaO_3^+$: 204.0631, Found: 204.0646; IR (neat, cm^{-1}): υ 2980, 2938, 2872, 1778, 1639, 1320, 1297, 1082, 955, 892, 874.



30

(3,3-Dimethyl-2a,2a1,3,4,5,5a-hexahydro-7H-benzofuro[3,4-cd]isoxazol-7-one (30)

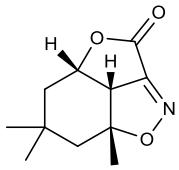
ethyl acetate/ petroleum ether =1:4; white solid; 83% yield (32.4 mg); mp: 55-56℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.93 (dt, *J* = 8.6, 2.1, 1H), 4.70 (dd, *J* = 11.4, 1.9, 1H), 4.45 (dd, *J* = 11.4, 8.6, 1H), 2.16 – 2.04 (m, 1H), 1.92 – 1.84 (m, 1H), 1.65 – 1.55 (m, 1H), 1.25 – 1.17 (m, 1H), 1.09 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 155.1, 91.8, 73.5, 48.5, 32.6, 28.7, 25.5, 25.4, 24.7; HRMS (ESI-TOF): Anal. Calcd. For $C_{10}H_{13}NNaO_3^+$+MeOH: 250.1050, Found: 250.1051; IR (neat, cm^{-1}): υ 2973, 2946, 2870, 1763, 1618, 1276, 1095, 966, 905, 895, 870.



31

2a-Methyl-2a,2a1,3,4,5,5a-hexahydro-7H-benzofuro[3,4-cd]isoxazol-7-one (31)

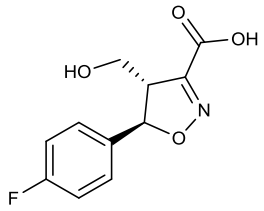
ethyl acetate/ petroleum ether =1:4; white solid; 79% yield (28.6 mg); mp: 67-69℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.93 (ddd, *J* = 8.8, 7.4, 5.5, 1H), 4.00 (d, *J* = 8.8, 1H), 2.16 – 2.01 (m, 1H), 1.99 – 1.89 (m, 1H), 1.81 – 1.60 (m, 6H), 1.37 – 1.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 156.2, 95.2, 75.4, 53.4, 36.0, 30.3, 26.2, 18.1; HRMS (ESI-TOF): Anal. Calcd. For $C_9H_{11}NNaO_3^+$: 204.0631, Found: 204.0644; IR (neat, cm^{-1}): υ 2960, 2938, 2872, 1772, 1629, 1295, 1089, 794.



32

2a,4,4-Trimethyl-2a,2a1,3,4,5,5a-hexahydro-7H-benzofuro[3,4-cd]isoxazol-7-one (32)

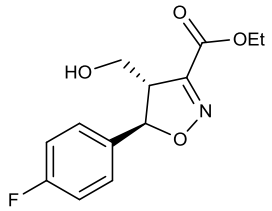
ethyl acetate/ petroleum ether =1:4; white solid; 77% yield (32.2 mg); mp: 95-97℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.93 (ddd, *J* = 10.3, 8.4, 7.3, 1H), 3.97 (d, *J* = 8.4, 1H), 2.14 – 2.03 (m, 1H), 1.75 – 1.69 (m, 5H), 1.35 – 1.19 (m, 1H), 1.00 (s, 3H), 0.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 156.5, 95.6, 76.4, 53.6, 48.4, 41.4, 32.7, 31.7, 28.3, 24.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_{15}NNaO_3^+$: 232.0944, Found: 232.0943; IR (neat, cm^{-1}): υ 2965, 2935, 2869, 1780, 1629, 1282, 1256, 1070, 959, 920, 896, 868.



33

5-(4-Fluorophenyl)-4-(hydroxymethyl)-4,5-dihydroisoxazole-3-carboxylic acid (33)

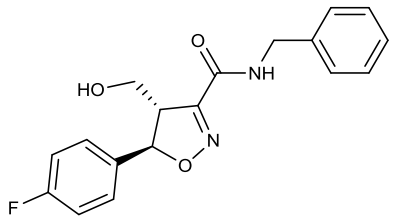
methanol/ DCM =1:10; white solid; 94% yield (45.1 mg); mp: 145-147℃; ^{1}H NMR (400 MHz, Methanol-d4) δ 7.40 – 7.30 (m, 2H), 7.16 – 7.06 (m, 2H), 5.69 (d, *J* = 7.4, 1H), 3.97 (dd, *J* = 11.2, 5.5, 1H), 3.85 (dd, *J* = 11.2, 3.4, 1H), 3.59 – 3.48 (m, 1H); ^{13}C NMR (100 MHz, Methanol-d4) δ 164.3 (d, *J* = 245.7) , 163.2, 153.3, 137.7 (d, *J* = 3.2), 129.1 (d, *J* = 8.5), 116.8 (d, *J* = 21.9), 88.8, 61.2, 59.7; ^{19}F NMR (376 MHz, Methanol-d4) δ -115.67; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_{10}FNNaO_4^+$: 262.0486, Found: 262.0481; IR (neat, cm^{-1}): υ 3321, 2952, 2921, 2899, 2852, 2759, 2573, 1712, 1591, 1511, 1261, 1221, 1080, 963, 905, 833, 749.



34

Ethyl (5-(4-fluorophenyl)-4-(hydroxymethyl)-4,5-dihydroisoxazole-3-carboxylate (34)

ethyl acetate/ petroleum ether =1:1; colorless liquid; 91% yield (48.6 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 2H), 7.09 – 7.01 (m, 2H), 5.60 (d, *J* = 7.7, 1H), 4.40 – 4.30 (m, 2H), 4.01 – 3.90 (m, 2H), 3.60 – 3.53 (m, 1H), 2.93 (s, 1H), 1.37 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.5), 161.1, 151.2, 134.9, 127.6 (d, *J* = 8.6), 115.8 (d, *J* = 21.5), 87.5, 62.5, 61.3, 58.0, 14.0; ^{19}F NMR (376 MHz, CDCl3) δ -112.97; HRMS (ESI-TOF): Anal. Calcd. For $C_{13}H_{14}FNNaO_4^+$: 290.0799, Found: 290.0791; IR (neat, cm^{-1}): υ 3446, 2986, 2941, 2902, 1717, 1606, 1587, 1511, 1226, 1128, 1017, 833.

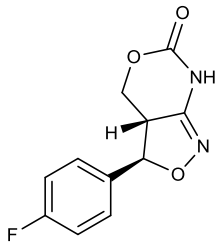


35

N-Benzyl-5-(4-fluorophenyl)-4-(hydroxymethyl)-4,5-dihydroisoxazole-3-carboxamide (35)

ethyl acetate/ petroleum ether =1:1; white solid; 84% yield (54.9 mg); mp: 87-89℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.26 (m, 7H), 7.23 (s, 1H), 7.11 – 7.03 (m, 2H), 5.33 (d, *J* = 9.3, 1H), 4.65 – 4.47 (m, 2H), 4.36 (s, 1H), 3.99 – 3.82 (m, 2H), 3.63 (ddd, *J* = 9.3, 7.3, 4.5, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, *J* = 248.2)., 160.4, 154.2, 136.8, 134.31 (d, *J* = 2.8), 128.9, 127.91, 127.86, 127.8 (d, *J* = 8.4),

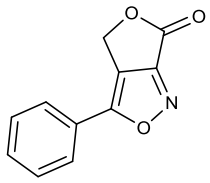
115.93 (d, *J* = 21.8), 87.5, 62.2, 58.2, 43.7; ^{19}F NMR (376 MHz, CDCl3) δ -112.54; HRMS (ESI-TOF): Anal. Calcd. For $C_{18}H_{18}FN_2O_3^+$: 329.1296, Found: 329.1294; IR (neat, cm^{-1}): υ 3361, 3306, 3069, 3035, 2943, 2880, 1725, 1650, 1593, 1545, 1510, 1225, 1074, 832, 701.



36

3-(4-Fluorophenyl)-3a,4-dihydro-3H-isoxazolo[3,4-d][1,3]oxazin-6(7H)-one (36)

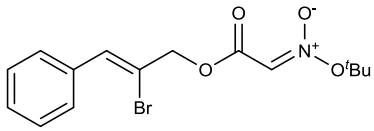
ethyl acetate/ petroleum ether =1.5:1; white solid; 68% yield (32.3 mg); mp: > 200℃; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.13 (s, 1H), 7.59 – 7.50 (m, 2H), 7.29 – 7.21 (m, 2H), 5.27 (d, *J* = 12.7, 1H), 4.54 (d, *J* = 9.4, 2H), 4.05 (dt, *J* = 12.7, 9.4, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 162.4 (d, *J* = 245.0), 155.7, 149.4, 132.5 (d, *J* = 3.0), 129.7 (d, *J* = 8.5), 115.6 (d, *J* = 21.6), 83.6, 67.2, 46.3; ^{19}F NMR (376 MHz, DMSO-d6) δ -113.02; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_{10}FN_2O_3^+$: 237.0670, Found: 237.0681; IR (neat, cm^{-1}): υ 3394, 3187, 3060, 2921, 2884, 2848, 1712, 1665, 1511, 1409, 1269, 1226, 1051, 754.



38

3-Phenyl-4H,6H-furo[3,4-c]isoxazol-6-one (38)

ethyl acetate/ petroleum ether =1:10; white solid; 13% yield (5.2 mg); mp: 158-160℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.61 (m, 2H), 7.57 – 7.49 (m, 3H), 5.48 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 159.1, 131.4, 129.5, 126.3, 125.6, 120.1, 64.6; ^{1}HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_7NNaO_3^+$: 224.0318, Found: 224.0315; IR (neat, cm^{-1}): υ 2918, 2850, 1794, 1775, 1649, 1489, 1454, 1066, 961, 776, 690, 661.

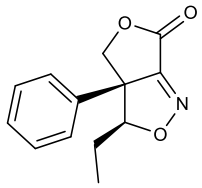


39

(Z)-2-Bromo-3-phenylallyl (E)-2-(tert-butoxyoxidoazanylidene)acetate (39)

ethyl acetate/ petroleum ether =1:15; white solid; 5% yield (3.6 mg); mp: 70-72℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.59 (m, 2H), 7.41 – 7.30 (m, 3H), 7.11 (s, 1H), 7.09 (s, 1H), 4.97 (d, *J* = 0.7, 2H), 1.50 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2, 149.2, 134.4, 132.1, 129.1, 128.6, 128.2, 118.2, 82.8, 71.1, 28.0; ^{1}HRMS (ESI-TOF): Anal. Calcd. For $C_{15}H_{18}{}^{79}BrNNaO_4^+$: 378.0311, $C_{15}H_{18}{}^{81}BrNNaO_4^+$:

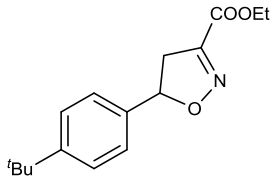
380.0291, Found: 378.0328, 380.0289; IR (neat, cm^{-1}): υ 2979, 2932, 1780, 1718, 1519, 1492, 1148, 1079, 692.



41

3-Ethyl-3a-phenyl-3a,4-dihydro-3H,6H-furo[3,4-c]isoxazol-6-one (41)

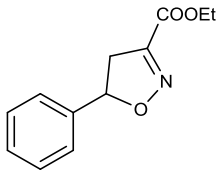
ethyl acetate/ petroleum ether =1:5; colorless liquid; 28% yield (13.0 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.41 (m, 3H), 7.21 – 7.16 (m, 2H), 5.12 (d, *J* = 9.3, 1H), 4.83 (dd, *J* = 7.8, 6.2, 1H), 4.63 (d, *J* = 9.3, 1H), 1.37 – 1.29 (m, 2H), 0.92 (t, *J* = 7.4, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 158.2, 132.0, 129.4, 129.1, 127.2, 97.5, 76.1, 62.4, 22.1, 10.4; HRMS (ESI-TOF): Anal. Calcd. For $C_{13}H_{13}NNaO_3^+$: 254.0788, Found: 254.0792; IR (neat, cm^{-1}): υ 2973, 2937, 2881, 1785, 1733, 1076, 934, 873, 734, 699.



42

Ethyl 5-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (42)

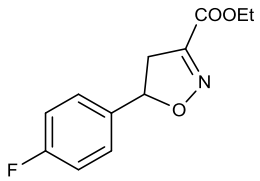
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 80% yield (110.1 mg); 20.0 mmol scale: 80% yield (4.41 g); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.4, 2H), 7.26 (d, *J* = 8.4, 2H), 5.76 (dd, *J* = 11.6, 9.0, 1H), 4.36 (q, *J* = 7.1, 2H), 3.60 (dd, *J* = 17.8, 11.6, 1H), 3.23 (dd, *J* = 17.8, 9.0, 1H), 1.37 (t, *J* = 7.1, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 151.7, 151.1, 136.3, 125.69, 125.66, 84.9, 62.0, 41.1, 34.5, 31.2, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{22}NO_3^+$: 276.1594, Found: 276.1612 ($M+H^+$); IR (neat, cm^{-1}): υ 2963, 2906, 2870, 1717, 1589, 1245, 1119, 1110, 923, 832, 749.



43

Ethyl 5-phenyl-4,5-dihydroisoxazole-3-carboxylate (43)

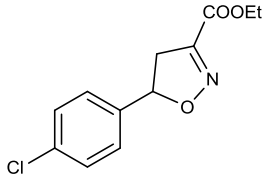
ethyl acetate/ petroleum ether =1:20; light yellow solid; 74% yield (81.1 mg); mp: 28-30℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.21 (m, 5H), 5.77 (dd, *J* = 11.6, 8.9, 1H), 4.35 (q, *J* = 7.1, 2H), 3.62 (dd, *J* = 17.8, 11.6, 1H), 3.20 (dd, *J* = 17.8, 8.9, 1H), 1.36 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.0, 139.4, 128.7, 128.5, 125.7, 84.8, 62.0, 41.3, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{13}NNaO_3^+$: 242.0788, Found: 242.0797 ($M+Na^+$); IR (neat, cm^{-1}): υ 3064, 2981, 2936, 2875, 1713, 1592, 1250, 1112, 920, 760, 743, 694.



44

Ethyl 5-(4-fluorophenyl)-4,5-dihydroisoxazole-3-carboxylate (44)

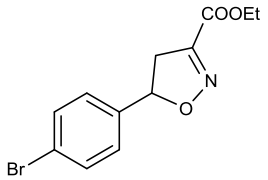
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 67% yield (79.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.28 (m, 2H), 7.14-7.00 (m, 2H), 5.77 (dd, *J* = 11.6, 8.9, 1H), 4.36 (q, *J* = 7.1, 2H), 3.64 (dd, *J* = 17.8, 11.6, 1H), 3.18 (dd, *J* = 17.8, 8.9, 1H), 1.38 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 247.7), 160.3, 151.1, 135.2 (d, *J* = 3.1), 127.7 (d, *J* = 8.1), 115.7 (d, *J* = 21.8), 84.2, 62.1, 41.4, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.08; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{13}FNO_3^+$: 238.0874, Found: 238.0870 ($M+H^+$); IR (neat, cm^{-1}): υ 2985, 2939, 2909, 1719, 1512, 1243, 1120, 920, 835, 751.



45

Ethyl 5-(4-chlorophenyl)-4,5-dihydroisoxazole-3-carboxylate (45)

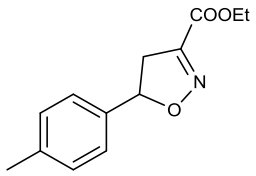
ethyl acetate/ petroleum ether =1:20; light yellow solid; 75% yield (95.1 mg); mp: 53-54℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.4, 2H), 7.24 (d, *J* = 8.4, 2H), 5.74 (dd, *J* = 11.6, 8.7, 1H), 4.34 (q, *J* = 7.1, 2H), 3.62 (dd, *J* = 17.8, 11.6, 1H), 3.15 (dd, *J* = 17.8, 8.7, 1H), 1.35 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 151.0, 138.0, 134.4, 128.9, 127.2, 84.0, 62.1, 41.4, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{12}ClNNaO_3^+$: 276.0398, Found: 276.0391 ($M+Na^+$); IR (neat, cm^{-1}): υ 2985, 2964, 2938, 2853, 1713, 1594, 1252, 1113, 1091, 920, 831.



46

Ethyl 5-(4-bromophenyl)-4,5-dihydroisoxazole-3-carboxylate (46)

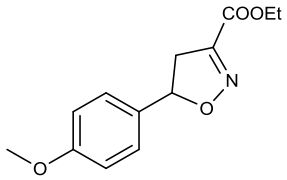
ethyl acetate/ petroleum ether =1:20; light yellow solid; 50% yield (74.5 mg); mp: 58-60℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.5, 2H), 7.19 (d, *J* = 8.5, 2H), 5.73 (dd, *J* = 11.6, 8.6, 1H), 4.35 (q, *J* = 7.1, 2H), 3.63 (dd, *J* = 17.8, 11.6, 1H), 3.15 (dd, *J* = 17.8, 8.6, 1H), 1.36 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 151.0, 138.5, 131.9, 127.5, 122.6, 84.0, 62.2 , 41.4, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{12}{}^{79}BrNNaO_3^+$: 319.9893, $C_{12}H_{12}{}^{81}BrNNaO_3^+$: 321.9872, Found: 319.9875, 321.9852 ($M+Na^+$); IR (neat, cm-1): υ 2984, 2964, 2937, 2850, 1712, 1594, 1253, 1113, 920, 818, 747.



47

Ethyl 5-(p-tolyl)-4,5-dihydroisoxazole-3-carboxylate (47)

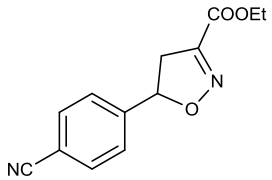
ethyl acetate/ petroleum ether =1:20; light yellow solid; 75% yield (87.5 mg); mp: 52-54℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.14 (m, 4H), 5.73 (dd, *J* = 11.6, 9.0, 1H), 4.35 (q, *J* = 7.1, 2H), 3.60 (dd, *J* = 17.8, 11.6, 1H), 3.19 (dd, *J* = 17.8, 9.0, 1H), 2.34 (s, 3H), 1.37 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 151.0, 138.4, 136.4, 129.4, 125.8, 84.9, 62.0, 41.2, 21.0, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{13}H_{15}NNaO_3^+$: 256.0944, Found: 256.0953 ($M+Na^+$); IR (neat, cm^{-1}): υ 3014, 2981, 2920, 2874, 1713, 1593, 1273, 1252, 1112, 921, 812, 749.



48

Ethyl 5-(4-methoxyphenyl)-4,5-dihydroisoxazole-3-carboxylate (48)

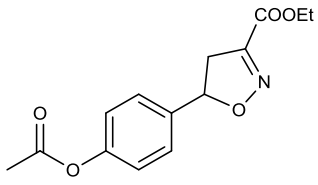
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 38% yield (47.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.8, 2H), 6.90 (d, *J* = 8.8, 2H), 5.73 (dd, *J* = 11.5, 9.2, 1H), 4.36 (q, *J* = 7.1, 2H), 3.81 (s, 3H), 3.59 (dd, *J* = 17.8, 11.5, 1H), 3.20 (dd, *J* = 17.8, 9.2, 1H), 1.38 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 159.8, 151.1, 131.3, 127.4, 114.1, 84.9, 62.0, 55.3, 41.0, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{13}H_{15}NNaO_4^+$: 272.0893, Found: 272.0892 ($M+Na^+$); IR (neat, cm^{-1}): υ 2981, 2961, 2935, 2840, 1717, 1613, 1587, 1515, 1246, 1177, 1119, 926, 831, 750.



49

Ethyl 5-(4-cyanophenyl)-4,5-dihydroisoxazole-3-carboxylate (49)

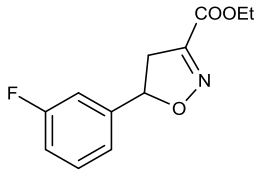
ethyl acetate/ petroleum ether =1:7; white solid; 69% yield (84.3 mg); mp: 113-115℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.2, 2H), 7.43 (d, *J* = 8.2, 2H), 5.82 (dd, *J* = 11.7, 8.3, 1H), 4.33 (q, *J* = 7.1, 2H), 3.70 (dd, *J* = 17.8, 11.7, 1H), 3.15 (dd, *J* = 17.8, 8.3, 1H), 1.34 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 151.0, 144.7, 132.6, 126.3, 118.2, 112.3, 83.4, 62.3, 41.6, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{13}H_{12}N_2NaO_3^+$: 267.0740, Found: 267.0756 ($M+Na^+$); IR (neat, cm^{-1}): υ 3095, 2959, 2922, 2852, 2225, 1717, 1268, 1234, 1151, 1116, 910, 828, 749.



50

Ethyl 5-(4-acetoxyphenyl)-4,5-dihydroisoxazole-3-carboxylate (50)

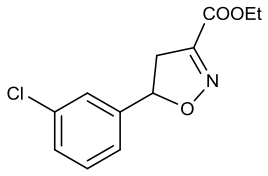
ethyl acetate/ petroleum ether =1:10; light yellow solid; 75% yield (104.0 mg); mp: 79-81℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.5, 2H), 7.07 (d, *J* = 8.5, 2H), 5.74 (dd, *J* = 11.6, 8.7, 1H), 4.32 (q, *J* = 7.1, 2H), 3.60 (dd, *J* = 17.8, 11.6, 1H), 3.16 (dd, *J* = 17.8, 8.7, 1H), 2.25 (s, 3H), 1.33 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 160.2, 151.0, 150.6, 136.9, 126.9, 121.9, 84.1, 62.0, 41.3, 20.9, 13.9; HRMS (ESI-TOF): Anal. Calcd. For $C_{14}H_{16}NO_5^+$: 278.1023, Found: 278.1028 ($M+H^+$); IR (neat, cm^{-1}): υ 3070, 2988, 2939, 2911, 1747, 1711, 1249, 1222, 1194, 1132, 1114, 935, 916, 843, 752.



51

Ethyl 5-(3-fluorophenyl)-4,5-dihydroisoxazole-3-carboxylate (51)

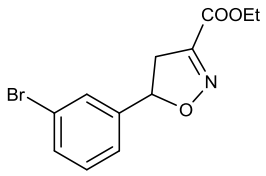
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 68% yield (80.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.30 (m, 1H), 7.10-7.06 (m, 1H), 7.06-6.98 (m, 2H), 5.76 (dd, *J* = 11.6, 8.5, 1H), 4.35 (q, *J* = 7.1, 2H), 3.65 (dd, *J* = 17.8, 11.6, 1H), 3.18 (dd, *J* = 17.8, 8.5, 1H), 1.36 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, *J* = 247.1), 160.3, 151.0, 142.1 (d, *J* = 7.2), 130.5 (d, *J* = 8.2), 121.3 (d, *J* = 3.0), 115.5 (d, *J* = 21.2), 112.7 (d, *J* = 22.6), 83.8 (d, *J* = 1.9), 62.2, 41.5, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.87; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{12}FNNaO_3^+$: 260.0693, Found: 260.0688 ($M+Na^+$); IR (neat, cm^{-1}): υ 3068, 2985, 2917, 2850, 1718, 1591, 1246, 1120, 922, 786, 749.



52

Ethyl 5-(3-chlorophenyl)-4,5-dihydroisoxazole-3-carboxylate (52)

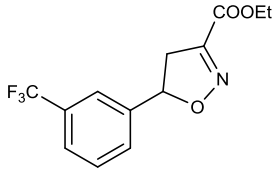
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 75% yield (95.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.25 (m, 3H), 7.21-7.16 (m, 1H), 5.74 (dd, *J* = 11.6, 8.5, 1H), 4.35 (q, *J* = 7.1, 2H), 3.64 (dd, *J* = 17.8, 11.6, 1H), 3.17 (dd, *J* = 17.8, 8.5, 1H), 1.36 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 151.0, 141.6, 134.7, 130.1, 128.7, 125.9, 123.8, 83.8, 62.2, 41.5, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{12}ClNNaO_3^+$: 276.0398, Found: 276.0401 ($M+Na^+$); IR (neat, cm^{-1}): υ 3069, 2984, 2938, 2873, 1718, 1591, 1245, 1120, 919, 785, 747, 692.



53

Ethyl 5-(3-bromophenyl)-4,5-dihydroisoxazole-3-carboxylate (53)

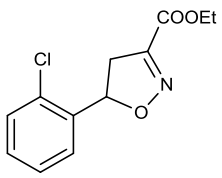
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 62% yield (92.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.41 (m, 2H), 7.25-7.20 (m, 2H), 5.73 (dd, *J* = 11.6, 8.5, 1H), 4.34 (q, *J* = 7.1, 2H), 3.64 (dd, *J* = 17.8, 11.6, 1H), 3.17 (dd, *J* = 17.8, 8.5, 1H), 1.36 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 151.0, 141.8, 131.6, 130.4, 128.7, 124.3, 122.8, 83.7, 62.2, 41.5, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{12}{}^{79}BrNNaO_3{}^{+}$: 319.9893, $C_{12}H_{12}{}^{81}BrNNaO_3{}^{+}$: 321.9872, Found: 319.9895, 321.9887 ($M+Na^{+}$); IR (neat, cm^{-1}): υ 3064, 2983, 2938, 2907, 1717, 1591, 1245, 1120, 919, 783, 746, 691.



54

Ethyl 5-(3-(trifluoromethyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (54)

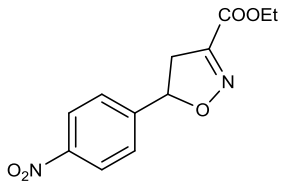
ethyl acetate/ petroleum ether =1:15; light yellow liquid; 66% yield (94.8 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.55 (m, 2H), 7.54-7.48 (m, 2H), 5.83 (dd, *J* = 11.6, 8.6, 1H), 4.35 (q, *J* = 7.1, 2H), 3.70 (dd, *J* = 17.8, 11.6, 1H), 3.20 (dd, *J* = 17.8, 8.6, 1H), 1.36 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 151.1, 140.6, 131.2 (q, *J* = 32.5), 129.4, 129.08, 129.06, 125.4 (q, *J* = 3.7), 122.6 (q, *J* = 3.8), 83.8, 62.2, 41.6, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.72; HRMS (ESI-TOF): Anal. Calcd. For $C_{13}H_{12}F_3NNaO_3{}^{+}$: 310.0661, Found: 310.0658 ($M+Na^{+}$); IR (neat, cm^{-1}): υ 2986, 2937, 2878, 2851, 1720, 1593, 1326, 1247, 1119, 1073, 920, 803, 702.



55

Ethyl 5-(2-chlorophenyl)-4,5-dihydroisoxazole-3-carboxylate (55)

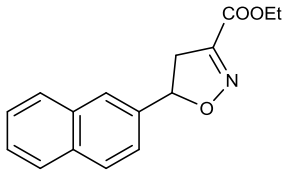
ethyl acetate/ petroleum ether =1:20; white solid; 63% yield (79.9 mg); mp: 39-41℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.41 (m, 1H), 7.40-7.33 (m, 1H), 7.30-7.21 (m, 2H), 6.05 (dd, *J* = 11.7, 7.8, 1H), 4.33 (q, *J* = 7.1, 2H), 3.77 (dd, *J* = 17.9, 11.7, 1H), 3.07 (dd, *J* = 17.9, 7.8, 1H), 1.35 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 151.2, 137.6, 131.0, 129.6, 129.4, 127.2, 126.3, 81.7, 62.1, 41.2, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{12}ClNNaO_3{}^{+}$: 276.0398, Found: 276.0408 ($M+Na^{+}$); IR (neat, cm^{-1}): υ 3068, 2978, 2937, 2911, 1719, 1598, 1252, 1133, 1112, 926, 749, 689.



56

Ethyl 5-(4-nitrophenyl)-4,5-dihydroisoxazole-3-carboxylate (56)

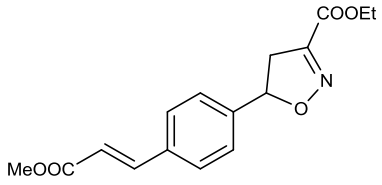
ethyl acetate/ petroleum ether =1:5; light yellow solid; 61% yield (80.6 mg); mp: 85-86℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.6, 2H), 7.49 (d, *J* = 8.6, 2H), 5.88 (dd, *J* = 11.8, 8.2, 1H), 4.33 (q, *J* = 7.1, 2H), 3.74 (dd, *J* = 17.8, 11.8, 1H), 3.17 (dd, *J* = 17.8, 8.2, 1H), 1.34 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 151.0, 147.8, 146.6, 126.5, 124.0, 83.2, 62.3, 41.7, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{12}N_2NaO_5^+$: 287.0638, Found: 287.0640 (M+Na$^+$); IR (neat, cm^{-1}): υ 3112, 2984, 2918, 2850, 1718, 1518, 1339, 1327, 1270, 1234, 906, 855.



57

Ethyl 5-(naphthalen-2-yl)-4,5-dihydroisoxazole-3-carboxylate (57)

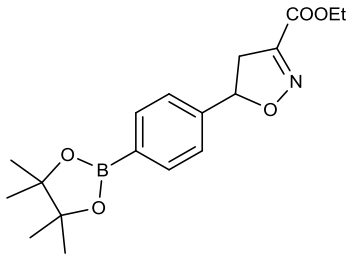
ethyl acetate/ petroleum ether =1:20; yellow solid; 74% yield (99.6 mg); mp: 82-84℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.78 (m, 4H), 7.53-7.47 (m, 2H), 7.39 (dd, *J* = 8.5, 1.8, 1H), 5.93 (dd, *J* = 11.6, 8.8, 1H), 4.37 (q, *J* = 7.2, 2H), 3.69 (dd, *J* = 17.8, 11.6, 1H), 3.29 (dd, *J* = 17.8, 8.8, 1H), 1.39 (t, *J* = 7.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.1, 136.6, 133.1, 132.9, 128.9, 127.9, 127.6, 126.5, 126.4, 125.1, 123.1, 85.0, 62.1, 41.3, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{15}NNaO_3^+$: 292.0944, Found: 292.0948 (M+Na$^+$); IR (neat, cm^{-1}): υ 3055, 3020, 2981, 2940, 1730, 1594, 1242, 1132, 927, 824, 750, 740.



58

Ethyl (E)-5-(4-(2-(propionyloxy)vinyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (58)

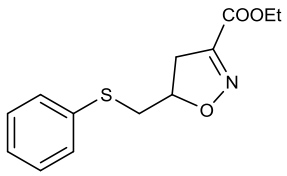
ethyl acetate/ petroleum ether =1:7; light yellow solid; 64% yield (97.1 mg); mp: 76-78℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 16.0, 1H), 7.50 (d, *J* = 8.1, 2H), 7.32 (d, *J* = 8.1, 2H), 6.41 (d, *J* = 16.0, 1H), 5.77 (dd, *J* = 11.6, 8.6, 1H), 4.33 (q, *J* = 7.2, 2H), 3.77 (s, 3H), 3.63 (dd, *J* = 17.8, 11.6, 1H), 3.17 (dd, *J* = 17.8, 8.6, 1H), 1.34 (t, *J* = 7.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 160.3, 151.0, 143.8, 141.58, 134.6, 128.4, 126.2, 118.4, 84.2, 62.1, 51.6, 41.4, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{17}NNaO_5^+$: 326.0999, Found: 326.0982 (M+Na$^+$); IR (neat, cm^{-1}): υ 2984, 2948, 2907, 2845, 1713, 1638, 1251, 1164, 1109, 917, 822.



59

Ethyl 5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (59)

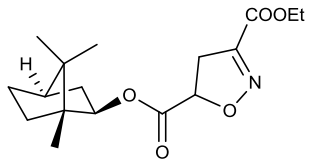
ethyl acetate/ petroleum ether =1:10; white solid; 55% yield (94.9 mg); mp: 91-93℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.1, 2H), 7.32 (d, *J* = 8.1, 2H), 5.78 (dd, *J* = 11.6, 8.8, 1H), 4.34 (q, *J* = 7.1, 2H), 3.63 (dd, *J* = 17.8, 11.6, 1H), 3.18 (dd, *J* = 17.8, 8.8, 1H), 1.36 (t, *J* = 7.1, 3H), 1.33 (s, 12H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.0, 142.4, 135.2, 125.0, 84.7, 83.9, 62.1, 41.5, 24.8, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{18}H_{25}BNO_5^+$: 346.1820, Found: 346.1811 ($M+H^+$); IR (neat, cm^{-1}): υ 2978, 2935, 1719, 1613, 1400, 1360, 1343, 1252, 1141, 1089, 858, 657.



60

Ethyl 5-((phenylthio)methyl)-4,5-dihydroisoxazole-3-carboxylate (60)

ethyl acetate/ petroleum ether =1:10; light yellow liquid; 40% yield (53.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 2H), 7.34 – 7.26 (m, 2H), 7.26 – 7.21 (m, 1H), 4.90 (dddd, *J* = 10.9, 8.6, 7.4, 4.6, 1H), 4.33 (q, *J* = 7.1, 2H), 3.36 – 3.23 (m, 2H), 3.12 (dd, *J* = 17.9, 7.4, 1H), 2.95 (dd, *J* = 13.8, 8.6, 1H), 1.35 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.2, 134.1, 130.4, 129.2, 127.1, 82.0, 62.1, 38.1, 37.6, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{13}H_{16}NO_3S^+$: 266.0845, Found: 266.0861 ($M+H^+$); IR (neat, cm^{-1}): υ 3058, 2982, 2930, 1716, 1586, 1255, 1123, 923, 740, 691.

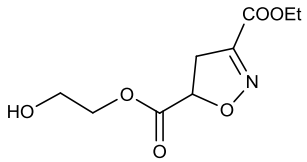


61

3-Ethyl 5-((1R,2R,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl) 4,5-dihydroisoxazole-3,5-dicarboxylate (61)

ethyl acetate/ petroleum ether =1:10; colorless liquid; 76% yield (122.9 mg); ^{1}H NMR (400 MHz, DMSO-d6) δ 5.31 (dd, *J* = 12.1, 6.6, 1H), 4.62 (td, *J* = 7.3, 4.0, 1H), 4.26 (q, *J* = 7.1, 2H), 3.55 (ddd, *J* = 17.8, 12.1, 4.2, 1H), 3.37-3.28 (m, 1H), 1.82-1.69 (m, 3H), 1.64 (td, *J* = 11.6, 11.2, 5.3, 1H), 1.52 (td, *J* = 11.6, 10.7, 3.2, 1H), 1.26 (t, *J* = 7.1, 3H), 1.16-1.04 (m, 2H), 0.91 (d, *J* = 2.7, 3H), 0.83-0.74 (m, 6H); ^{13}C NMR (100 MHz, DMSO-d6) δ 168.3, 168.2, 159.5, 151.64, 151.61, 81.70, 81.65, 79.8, 79.7, 61.7,

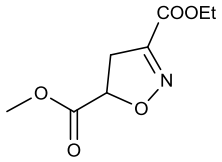
48.52, 48.47, 46.6, 44.4, 38.1, 38.0, 37.4, 37.3, 33.1, 26.6, 19.9, 19.7, 14.0, 11.24, 11.18; HRMS (ESI-TOF): Anal. Calcd. For $C_{17}H_{25}NNaO_5^+$: 346.1625, Found: 346.1614 ($M+Na^+$); IR (neat, cm^{-1}): υ 2956, 2878, 1723, 1597, 1252, 1208, 1121, 1051, 1013, 917.



62

3-Ethyl 5-(2-hydroxyethyl) 4,5-dihydroisoxazole-3,5-dicarboxylate (62)

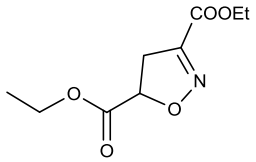
ethyl acetate/ petroleum ether =1:1; light yellow liquid; 51% yield (59.0 mg); ^{1}H NMR (400 MHz, DMSO-d6) δ 5.36 (dd, *J* = 12.3, 7.0, 1H), 4.88 (t, *J* = 5.6, 1H), 4.26 (q, *J* = 7.1, 2H), 4.24 – 4.06 (m, 2H), 3.76 – 3.47 (m, 3H), 3.49 – 3.38 (m, 1H), 1.26 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 169.3, 159.6, 151.7, 79.4, 67.2, 61.9, 58.9, 37.6, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_9H_{13}NNaO_6^+$: 254.0635, Found: 254.0645 ($M+Na^+$); IR (neat, cm^{-1}): υ 3383, 2924, 2853, 1731, 1648, 1047, 1024, 992.



63

3-Ethyl 5-methyl 4,5-dihydroisoxazole-3,5-dicarboxylate (63)

ethyl acetate/ petroleum ether =1:10; light yellow liquid; 70% yield (70.4 mg); ^{1}H NMR (400 MHz, DMSO-d6) δ 5.37 (dd, *J* = 12.2, 6.9, 1H), 4.26 (q, *J* = 7.1, 2H), 3.71 (s, 3H), 3.56 (dd, *J* = 17.8, 12.2, 1H), 3.39 (dd, *J* = 17.8, 6.9, 1H), 1.26 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 169.6, 159.5, 151.7, 79.4, 61.8, 52.6, 37.5, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_8H_{11}NNaO_5^+$: 224.0529, Found: 224.0521 ($M+Na^+$); IR (neat, cm^{-1}): υ 2986, 2959, 2852, 1739, 1720, 1598, 1252, 1216, 1122, 1017, 916.

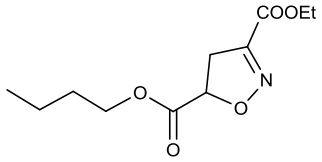


64

Diethyl 4,5-dihydroisoxazole-3,5-dicarboxylate (64)

ethyl acetate/ petroleum ether =1:10; light yellow liquid; 75% yield (80.7 mg); ^{1}H NMR (400 MHz, DMSO-d6) δ 5.34 (dd, *J* = 12.2, 7.0, 1H), 4.26 (q, *J* = 7.1, 2H), 4.17 (q, *J* = 7.1, 2H), 3.56 (dd, *J* = 17.8, 12.2, 1H), 3.38 (dd, *J* = 17.8, 7.0, 1H), 1.27 (t, *J* = 7.1, 3H), 1.23 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 169.1, 159.6, 151.6, 79.5, 61.8, 61.5, 37.4, 13.910, 13.907; HRMS (ESI-TOF): Anal. Calcd.

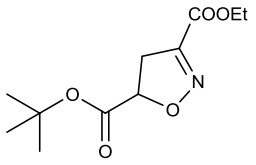
For $C_9H_{13}NNaO_5^+$: 238.0686, Found: 238.0679 ($M+Na^+$); IR (neat, cm^{-1}): υ 2985, 2941, 2912, 1721, 1598, 1253, 1206, 1122, 1018, 917.



65

5-Butyl 3-ethyl 4,5-dihydroisoxazole-3,5-dicarboxylate (65)

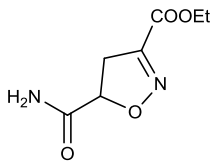
ethyl acetate/ petroleum ether =1:10; light yellow liquid; 75% yield (91.2 mg); ^{1}H NMR (400 MHz, DMSO-d6) δ 5.35 (dd, *J* = 12.2, 6.9, 1H), 4.26 (q, *J* = 7.1, 2H), 4.12 (t, *J* = 6.6, 2H), 3.56 (dd, *J* = 17.8, 12.2, 1H), 3.36 (dd, *J* = 17.8, 6.9, 1H), 1.63-1.54 (m, 2H), 1.39-1.30 (m, 2H), 1.26 (t, *J* = 7.1, 3H), 0.89 (t, *J* = 7.4, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 169.1, 159.5, 151.7, 79.5, 65.1, 61.8, 37.4, 30.1, 18.6, 13.9, 13.5; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_{17}NNaO_5^+$: 266.0999, Found: 266.0982 ($M+Na^+$); IR (neat, cm^{-1}): υ 2962, 2937, 2875, 1737, 1722, 1597, 1253, 1204, 1122, 1016, 918.



66

5-(tert-Butyl) 3-ethyl 4,5-dihydroisoxazole-3,5-dicarboxylate (66)

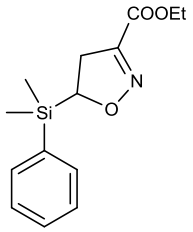
ethyl acetate/ petroleum ether =1:10; light yellow liquid; 76% yield (92.4 mg); ^{1}H NMR (400 MHz, DMSO-d6) δ 5.20 (dd, *J* = 12.3, 7.2, 1H), 4.26 (q, *J* = 7.1, 2H), 3.53 (dd, *J* = 17.8, 12.3, 1H), 3.29 (dd, *J* = 17.8, 7.2, 1H), 1.44 (s, 9H), 1.26 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 168.1, 159.6, 151.5, 82.3, 80.0, 61.7, 37.3, 27.6, 13.9; HRMS (ESI-TOF): Anal. Calcd. For $C_{11}H_{17}NNaO_5^+$: 266.0999, Found: 266.0980 ($M+Na^+$); IR (neat, cm^{-1}): υ 2982, 2938, 1722, 1596, 1370, 1250, 1150, 1122, 918.



67

Ethyl 5-carbamoyl-4,5-dihydroisoxazole-3-carboxylate (67)

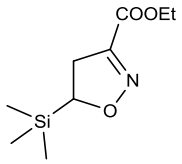
ethyl acetate/ petroleum ether =1:1; white solid; 55% yield (51.2 mg); mp: 120-122℃; ^{1}H NMR (400 MHz, DMSO-d6) δ 7.69 (s, 1H), 7.45 (s, 1H), 5.12 (dd, *J* = 12.0, 7.2, 1H), 4.25 (q, *J* = 7.1, 2H), 3.45 (dd, *J* = 17.7, 12.0, 1H), 3.28 (dd, *J* = 17.7, 7.2, 1H), 1.26 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 170.8, 159.8, 151.8, 80.8, 61.8, 37.3, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_7H_{10}N_2NaO_4^+$: 209.0533, Found: 209.0537 ($M+Na^+$); IR (neat, cm^{-1}): υ 3425, 3197, 2988, 2959, 2919, 2854, 1722, 1632, 1605, 1260, 1129, 910, 893.



68

Ethyl 5-(dimethyl(phenyl)silyl)-4,5-dihydroisoxazole-3-carboxylate (68)

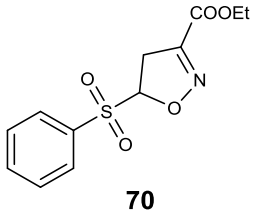
ethyl acetate/ petroleum ether =1:40; colorless liquid; 61% yield (84.3 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.51 (m, 2H), 7.48 – 7.31 (m, 3H), 4.37 (dd, *J* = 15.7, 12.3, 1H), 4.32 (q, *J* = 7.1, 2H), 3.30 (dd, *J* = 16.9, 12.3, 1H), 2.94 (dd, *J* = 16.9, 15.7, 1H), 1.35 (t, *J* = 7.1, 3H), 0.44 (s, 3H), 0.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 151.5, 134.6, 134.0, 129.9, 128.1, 77.0, 61.9, 36.5, 14.1, -5.3, -5.8; HRMS (ESI-TOF): Anal. Calcd. For $C_{14}H_{19}NNaO_3Si^+$: 300.1026, Found: 300.1029 ($M+Na^+$); IR (neat, cm^{-1}): υ 3071, 3050, 2982, 2961, 2907, 2853, 1716, 1626, 1585, 1251, 1228, 1113, 805, 735, 700.



69

Ethyl 5-(trimethylsilyl)-4,5-dihydroisoxazole-3-carboxylate (69)

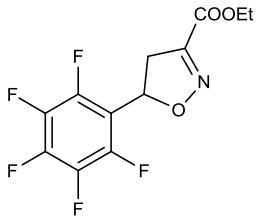
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 55% yield (59.2 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.32 (q, *J* = 7.1, 2H), 4.16 (dd, *J* = 15.6, 12.4, 1H), 3.32 (dd, *J* = 16.8, 12.4, 1H), 2.93 (dd, *J* = 16.8, 15.6, 1H), 1.34 (t, *J* = 7.1, 3H), 0.11 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 151.3, 77.3, 61.9, 36.2, 14.1, -4.2; HRMS (ESI-TOF): Anal. Calcd. For $C_9H_{17}NNaO_sSi^+$: 238.0875, Found: 238.0878 ($M+Na^+$); IR (neat, cm^{-1}): υ 2984, 2959, 2902, 1717, 1584, 1250, 1228, 1114, 840, 815.



70

Ethyl 5-(phenylsulfonyl)-4,5-dihydroisoxazole-3-carboxylate (70)

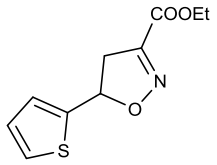
ethyl acetate/ petroleum ether =1:2; white solid; 28% yield (40.1 mg); mp: 96-98℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.91 (m, 2H), 7.75 – 7.69 (m, 1H), 7.63 – 7.56 (m, 2H), 5.55 (dd, *J* = 11.3, 5.1, 1H), 4.32 (q, *J* = 7.1, 2H), 3.92 (dd, *J* = 19.4, 5.1, 1H), 3.64 (dd, *J* = 19.4, 11.3, 1H), 1.34 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 151.9, 134.8, 134.7, 129.7, 129.4, 94.0, 62.7, 35.6, 13.9; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{13}NNaO_5S^+$: 306.0407, Found: 306.0413 ($M+Na^+$); IR (neat, cm^{-1}): υ 3064, 3053, 2958, 2933, 2911, 2869, 1692, 1574, 1304, 1152, 1087, 914, 823, 727, 687.



71

Ethyl 5-(perfluorophenyl)-4,5-dihydroisoxazole-3-carboxylate (71)

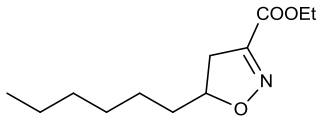
ethyl acetate/ petroleum ether =1:12; white solid; 56% yield (87.1 mg); mp: 66-68℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.05 (dd, *J* = 12.5, 8.9, 1H), 4.36 (q, *J* = 7.1, 2H), 3.65 (dd, *J* = 17.9, 12.5, 1H), 3.35 (dd, *J* = 17.9, 8.9, 1H), 1.38 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 150.7, 112.6, 74.2, 62.4, 39.4, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -140.62 – -143.49 (m, 2F), -150.57 – -153.36 (m, 1F), -158.22 – -162.43 (m, 2F); HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_9F_5NO_3^+$: 310.0497, Found: 310.0479 ($M+H^+$); IR (neat, cm^{-1}): υ 2988, 2937, 2916, 1720, 1601, 1505, 1258, 1125, 1018, 968, 918.



72

Ethyl 5-(thiophen-2-yl)-4,5-dihydroisoxazole-3-carboxylate (72)

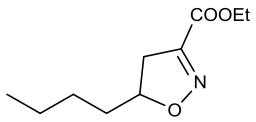
ethyl acetate/ petroleum ether =1:10; yellow liquid; 64% yield (72.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 5.0, 1.0, 1H), 7.09 (dd, *J* = 3.5, 1.0, 1H), 6.99 (dd, *J* = 5.0, 3.5, 1H), 5.99 (dd, *J* = 11.2, 8.8, 1H), 4.36 (q, *J* = 7.1, 2H), 3.62 (dd, *J* = 17.8, 11.2, 1H), 3.35 (dd, *J* = 17.8, 8.8, 1H), 1.38 (t, *J* = 7.1, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.1, 141.6, 127.0, 126.4, 126.1, 80.7, 62.2, 41.2, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{10}H_{11}NNaO_3S^+$: 248.0352, Found: 248.0356 ($M+Na^+$); IR (neat, cm^{-1}): υ 3111, 2985, 2939, 2907, 1718, 1590, 1249, 1121, 908, 726, 706.



73

Ethyl 5-hexyl-4,5-dihydroisoxazole-3-carboxylate (73)

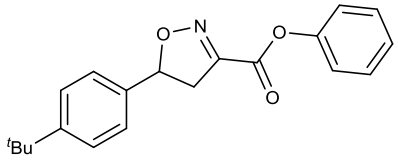
ethyl acetate/ petroleum ether =1:30; light yellow liquid; 33% yield (37.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.77 (ddt, *J* = 11.0, 8.6, 6.5, 1H), 4.32 (q, *J* = 7.1, 2H), 3.23 (dd, *J* = 17.5, 11.0, 1H), 2.82 (dd, *J* = 17.5, 8.6, 1H), 1.81 – 1.70 (m, 1H), 1.64 – 1.51 (m, 1H), 1.49 – 1.23 (m, 12H), 1.00 – 0.79 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 151.3, 84.1, 61.9, 38.3, 35.0, 31.6, 28.9, 25.0, 22.5, 14.1, 14.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{12}H_{21}NNaO_3^+$: 250.1414, Found: 250.1410 ($M+Na^+$); IR (neat, cm^{-1}): υ 2956, 2930, 2858, 1741, 1717, 1587, 1250, 1123, 931, 748.



74

Ethyl 5-butyl-4,5-dihydroisoxazole-3-carboxylate (74)

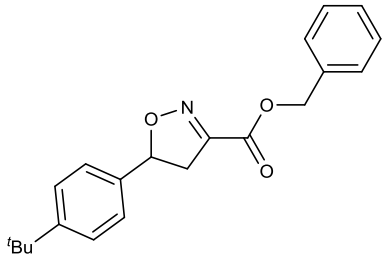
ethyl acetate/ petroleum ether =1:50; light yellow liquid; 48% yield (48.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.79 (ddt, *J* = 11.0, 8.5, 6.5, 1H), 4.34 (q, *J* = 7.1, 2H), 3.24 (dd, *J* = 17.5, 11.0, 1H), 2.84 (dd, *J* = 17.5, 8.5, 1H), 1.84 – 1.72 (m, 1H), 1.65 – 1.56 (m, 2H), 1.40 – 1.33 (m, 6H), 0.91 (t, *J* = 7.0, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 151.3, 84.2, 62.0, 38.3, 34.7, 27.2, 22.4, 14.1, 13.9; HRMS (ESI-TOF): Anal. Calcd. For $C_{10}H_{17}NNaO_3^+$: 222.1101, Found: 222.1106 ($M+Na^+$); IR (neat, cm^{-1}): υ 2987, 2940, 2875, 1745, 1622, 1478, 1332, 1240, 1195, 1064, 1021, 754.



75

Phenyl 5-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (75)

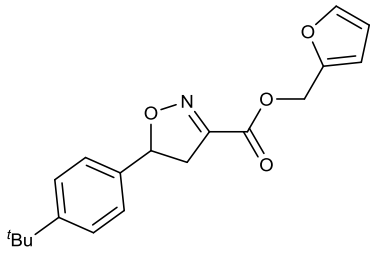
ethyl acetate/ petroleum ether =1:20; light yellow solid; 67% yield (108.3 mg); mp: 104-105℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.41 (m, 4H), 7.36-7.27 (m, 3H), 7.27-7.19 (m, 2H), 5.87 (dd, *J* = 11.6, 9.1, 1H), 3.73 (dd, *J* = 17.8, 11.6, 1H), 3.35 (dd, *J* = 17.8, 9.1, 1H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 151.8, 150.7, 150.0, 136.1, 129.5, 126.3, 125.75, 125.71, 121.3, 85.4, 40.9, 34.5, 31.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{20}H_{21}NNaO_3^+$: 346.1414, Found: 346.1402 ($M+Na^+$); IR (neat, cm^{-1}): υ 3064, 2964, 2903, 2868, 1749, 1588, 1340, 1235, 1193, 1119, 940, 923, 823, 750, 737, 689.



76

Benzyl 5-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (76)

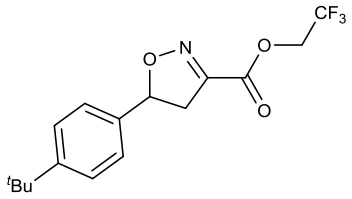
ethyl acetate/ petroleum ether =1:20; light yellow solid; 92% yield (155.2 mg); mp: 66-68℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.30 (m, 7H), 7.24 (d, *J* = 8.1, 2H), 5.73 (dd, *J* = 11.6, 9.0, 1H), 5.31 (s, 2H), 3.58 (dd, *J* = 17.8, 11.6, 1H), 3.20 (dd, *J* = 17.8, 9.0, 1H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 151.7, 150.9, 136.2, 134.8, 128.53, 128.49, 128.46, 125.662, 125.658, 85.0, 67.4, 41.0, 34.5, 31.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{21}H_{23}NNaO_3^+$: 360.1570, Found: 360.1577 ($M+Na^+$); IR (neat, cm^{-1}): υ 3066, 3041, 2967, 2951, 2869, 1709, 1272, 1245, 1105, 918, 896, 745, 693.



77

Furan-2-ylmethyl 5-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (77)

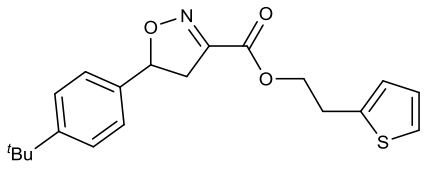
ethyl acetate/ petroleum ether =1:20; yellow liquid; 45% yield (73.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 1.9, 1H), 7.39 (d, *J* = 8.4, 2H), 7.24 (d, *J* = 8.4, 2H), 6.48 (d, *J* = 3.2, 1H), 6.36 (dd, *J* = 3.2, 1.9, 1H), 5.74 (dd, *J* = 11.6, 9.1, 1H), 5.27 (s, 2H), 3.59 (dd, *J* = 17.8, 11.6, 1H), 3.21 (dd, *J* = 17.8, 9.1, 1H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 151.8, 150.7, 148.3, 143.5, 136.2, 125.71, 125.69, 111.62, 110.59, 85.1, 59.1, 41.0, 34.5, 31.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{19}H_{21}NNaO_4^+$: 350.1363, Found: 350.1360 ($M+Na^+$); IR (neat, cm^{-1}): υ 2962, 2925, 2869, 1720, 1588, 1242, 1152, 1107, 919, 825, 744.



78

2,2,2-Trifluoroethyl 5-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (78)

ethyl acetate/ petroleum ether =1:20; light yellow solid; 66% yield (109.5 mg); mp: 60-61℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.5, 2H), 7.26 (d, *J* = 8.5, 2H), 5.81 (dd, *J* = 11.6, 9.2, 1H), 4.66 (q, *J* = 8.2, 2H), 3.62 (dd, *J* = 17.8, 11.6, 1H), 3.24 (dd, *J* = 17.8, 9.2, 1H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 152.0, 149.7, 135.8, 125.8, 125.7, 85.6, 61.00 (q, *J* = 37.3), 40.6, 34.6, 31.2; ^{19}F NMR (376 MHz, CDCl3) δ -73.49; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{18}F_3NNaO_3^+$: 352.1131, Found: 352.1150 ($M+Na^+$); IR (neat, cm^{-1}): υ 2970, 2908, 2871, 1749, 1734, 1586, 1279, 1166, 1147, 1123, 938.

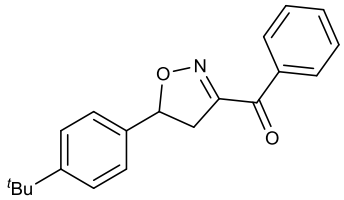


79

2-(Thiophen-2-yl)ethyl 5-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (79)

ethyl acetate/ petroleum ether =1:20; white solid; 66% yield (153.8 mg); mp: 54-56℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.39 (m, 2H), 7.29-7.25 (m, 2H), 7.17 (dd, *J* = 5.1, 1.2, 1H), 6.95 (dd, *J* = 5.1, 3.4, 1H), 6.91 (dd, *J* = 3.4, 1.2, 1H), 5.77 (dd, *J* = 11.5, 9.1, 1H), 4.51 (t, *J* = 6.9, 2H), 3.61 (dd, *J* = 17.7, 11.5, 1H), 3.30 – 3.20 (m, 3H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 156.1, 150.9, 139.0, 136.2, 127.0, 125.82, 125.76, 125.73, 124.2, 85.1, 66.0, 41.0, 34.6, 31.2, 29.0; HRMS (ESI-TOF): Anal. Calcd.

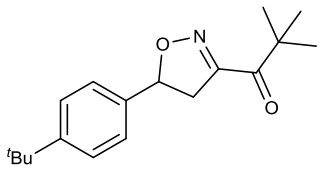
For $C_{20}H_{23}NNaO_3S^+$: 380.1291, Found: 380.1303 ($M+Na^+$); IR (neat, cm^{-1}): υ 3106, 3091, 2966, 2928, 2860, 1714, 1590, 1270, 1247, 1110, 915, 830, 708.



80

(5-(4-(tert-Butyl)phenyl)-4,5-dihydroisoxazol-3-yl)(phenyl)methanone (80)

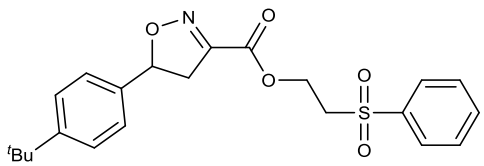
ethyl acetate/ petroleum ether =1:20; light yellow liquid; 69% yield (106.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32-8.23 (m, 2H), 7.66-7.59 (m, 1H), 7.54-7.46 (m, 2H), 7.45-7.41 (m, 2H), 7.33 (d, *J* = 8.3, 2H), 5.78 (dd, *J* = 11.5, 8.9, 1H), 3.77 (dd, *J* = 17.7, 11.5, 1H), 3.43 (dd, *J* = 17.7, 8.9, 1H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.2, 157.4, 151.7, 136.5, 135.7, 133.5, 130.3, 128.3, 125.731, 125.728, 84.1, 41.5, 34.5, 31.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{20}H_{21}NNaO_2^+$: 330.1465, Found: 330.1459 ($M+Na^+$); IR (neat, cm^{-1}): υ 2959, 2904, 2867, 1652, 1563, 1245, 930, 909, 704, 689, 674.



81

1-(5-(4-(tert-Butyl)phenyl)-4,5-dihydroisoxazol-3-yl)-2,2-dimethylpropan-1-one (81)

ethyl acetate/ petroleum ether =1:50; yellow liquid; 31% yield (44.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.3, 2H), 7.24 (d, *J* = 8.3, 2H), 5.62 (dd, *J* = 11.5, 8.9, 1H), 3.55 (dd, *J* = 17.7, 11.5, 1H), 3.19 (dd, *J* = 17.7, 8.9, 1H), 1.37 (s, 9H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 155.4, 151.7, 136.7, 125.8, 125.7, 83.4, 44.7, 41.8, 34.6, 31.3, 27.0; HRMS (ESI-TOF): Anal. Calcd. For $C_{18}H_{25}NNaO_2^+$: 310.1778, Found: 310.1780 ($M+Na^+$); IR (neat, cm^{-1}): υ 2959, 2906, 2870, 1665, 1572, 1478, 1338, 1200, 922, 822, 790.



82

2-(Phenylsulfonyl)ethyl 5-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazole-3-carboxylate (82)

ethyl acetate/ petroleum ether =1:4; white solid; 72% yield (143.9 mg); mp: 86-88℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.7, 2H), 7.64 (t, *J* = 7.4, 1H), 7.55 (t, *J* = 7.6, 2H), 7.39 (d, *J* = 8.0, 2H), 7.21 (d, *J* = 8.0, 2H), 5.72 (dd, *J* = 11.5, 8.9, 1H), 3.52 (t, *J* = 7.3, 2H), 3.49-3.40 (m, 1H), 3.36 (t, *J* = 6.8, 2H), 3.08 (dd, *J* = 17.7, 8.9, 1H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.6, 156.9, 151.8, 138.3, 135.9, 133.8, 129.3, 128.0, 125.63, 125.59, 85.5, 50.2, 39.0, 34.4, 32.3, 31.1; HRMS (ESI-TOF):

Anal. Calcd. For $C_{22}H_{25}NNaO_4S^+$: 422.1346, Found: 422.1340 ($M+Na^+$); IR (neat, cm^{-1}): υ 3064, 2958, 2933, 2869, 1692, 1574, 1304, 1152, 1087, 914, 823, 727, 687.

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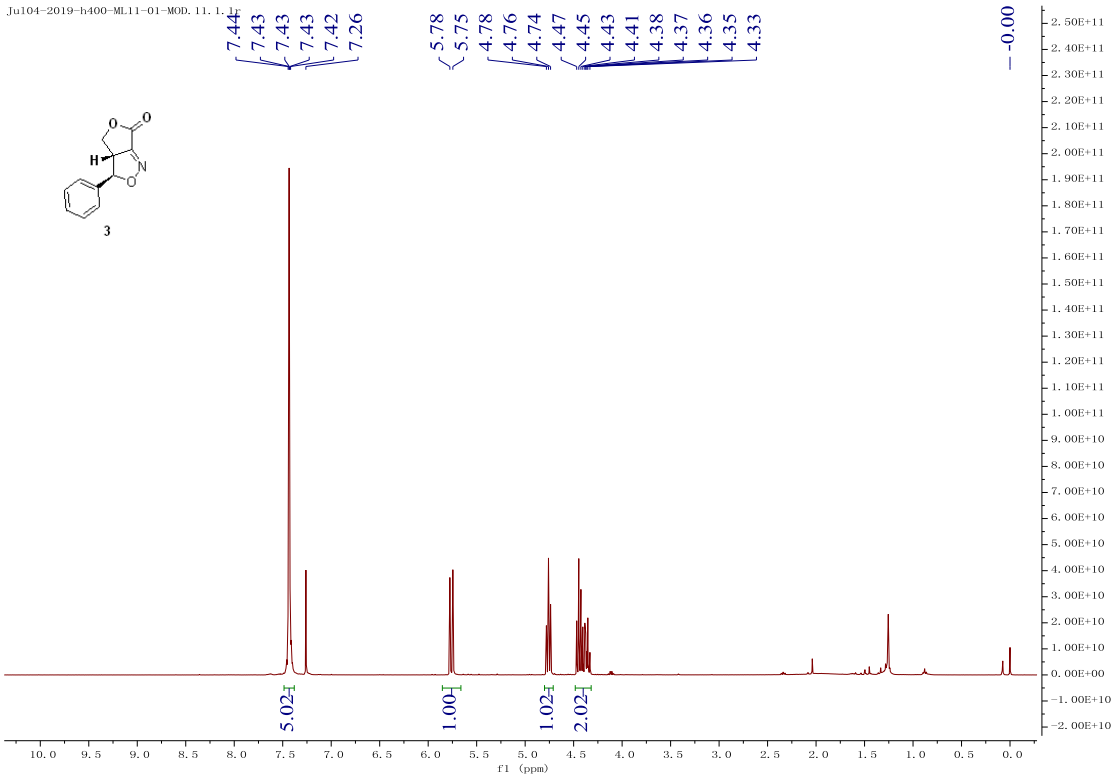
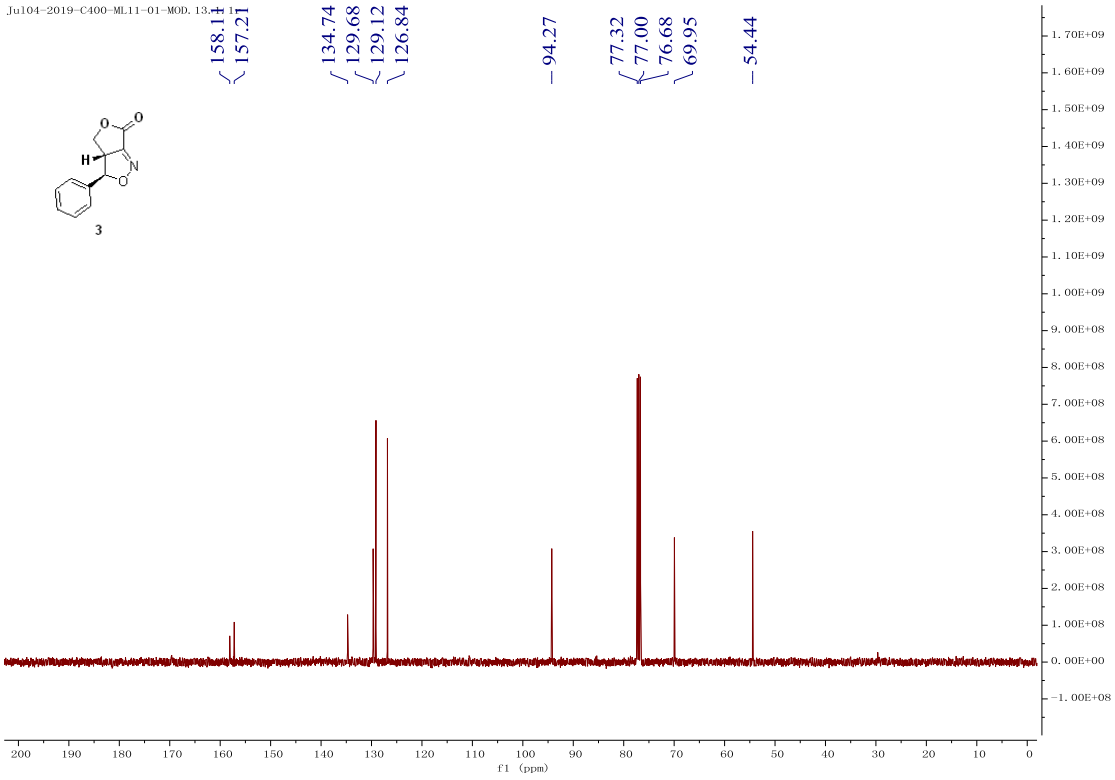
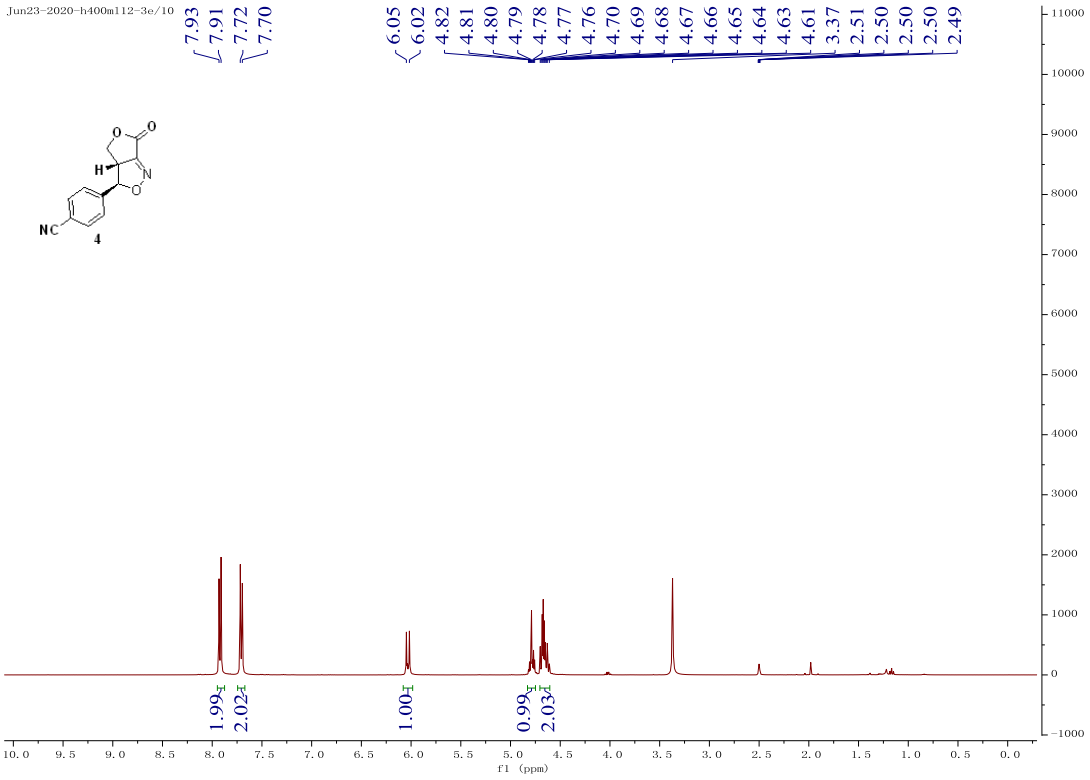
Spectroscopic data for substrates and products



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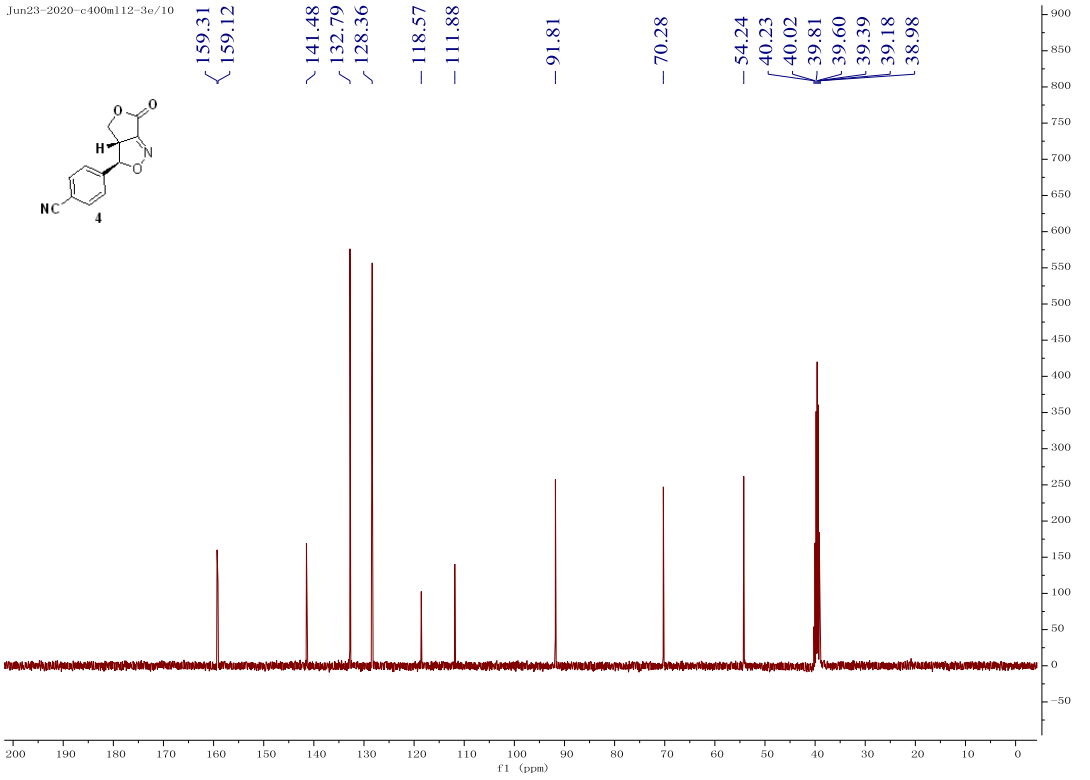
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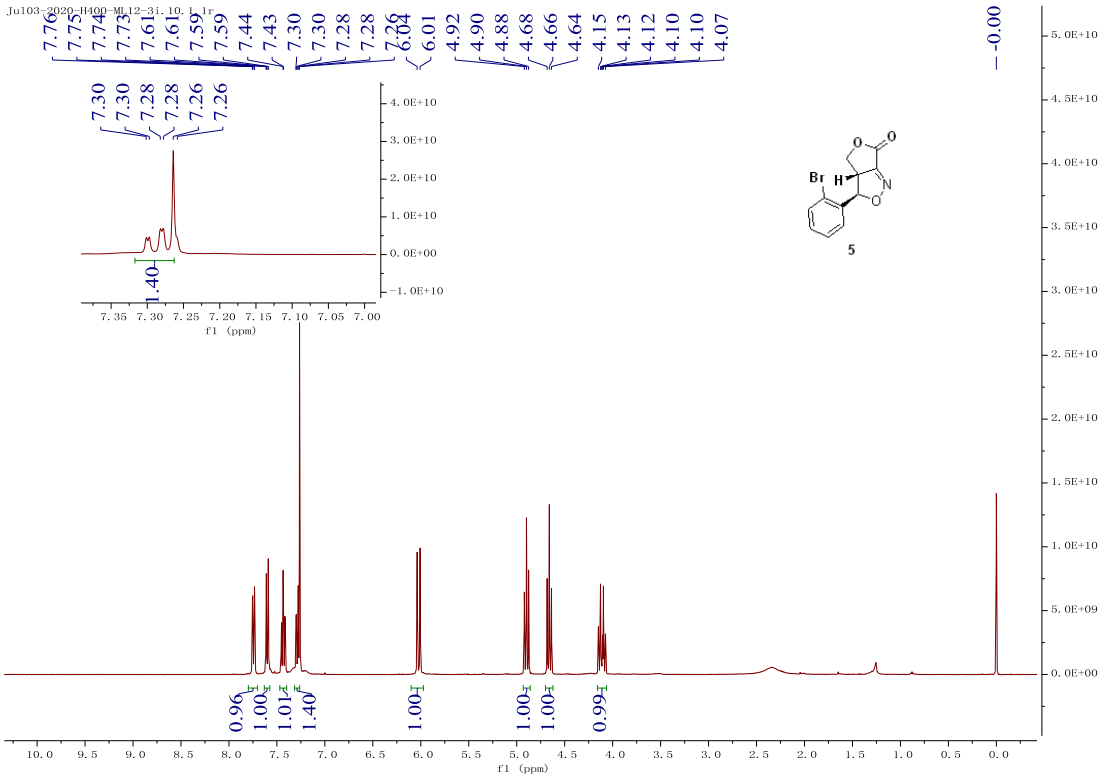
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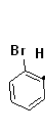
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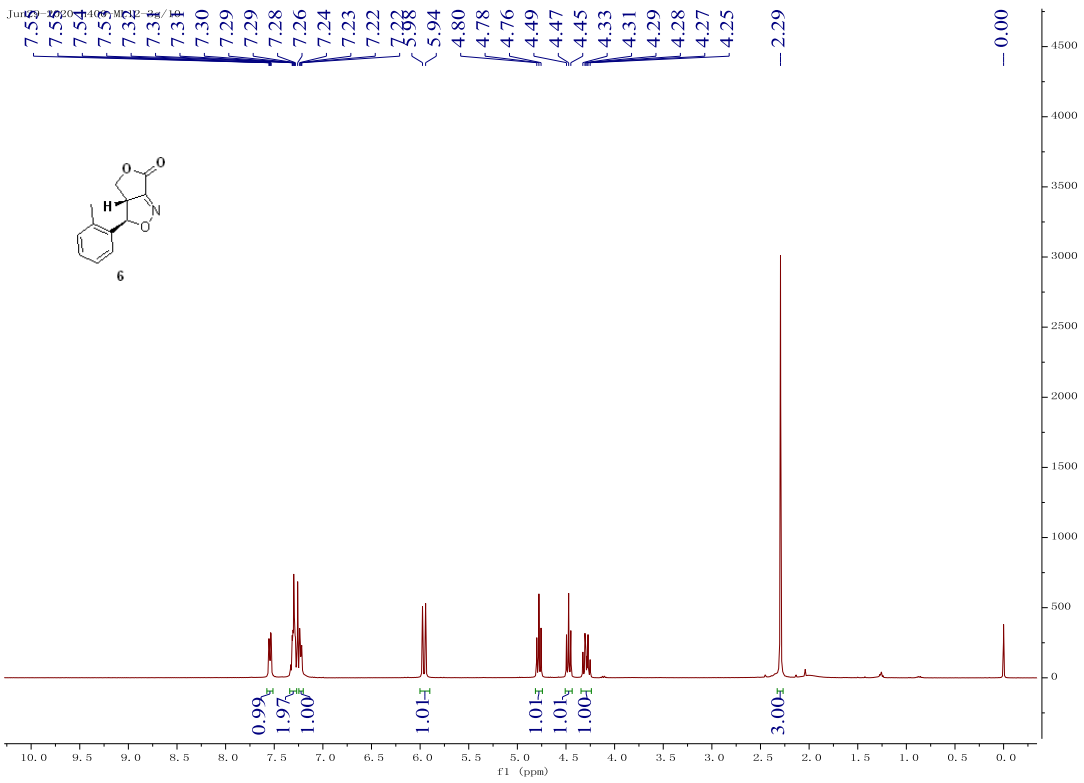
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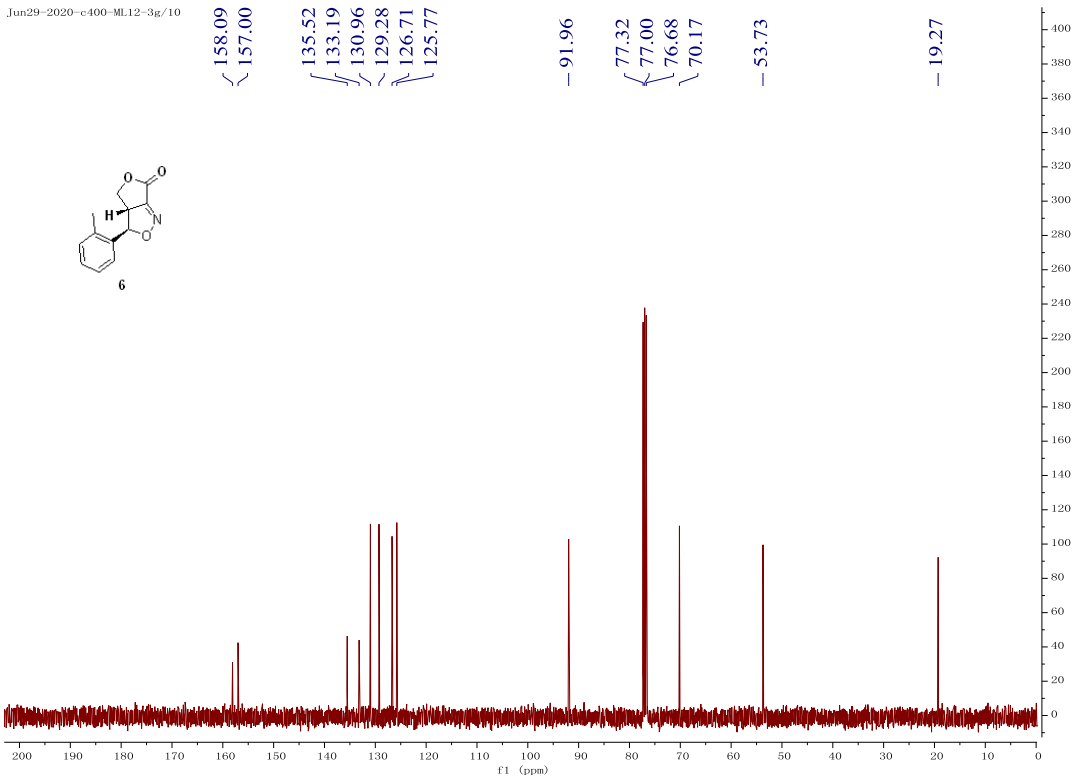
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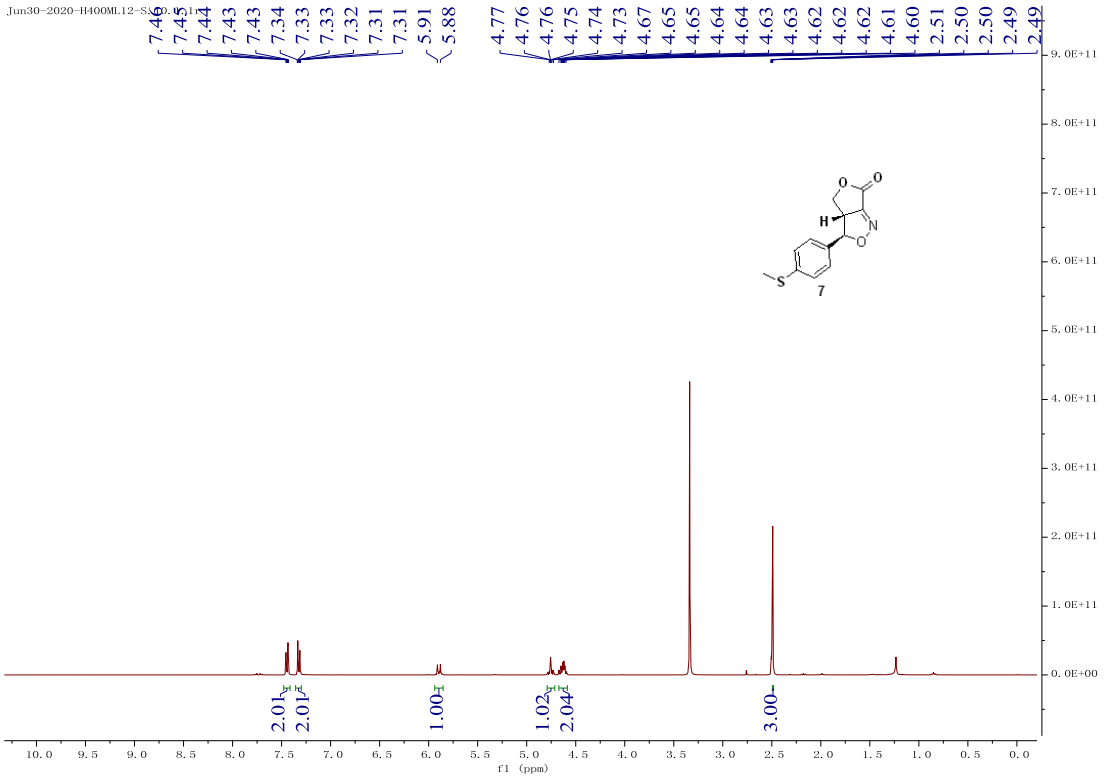
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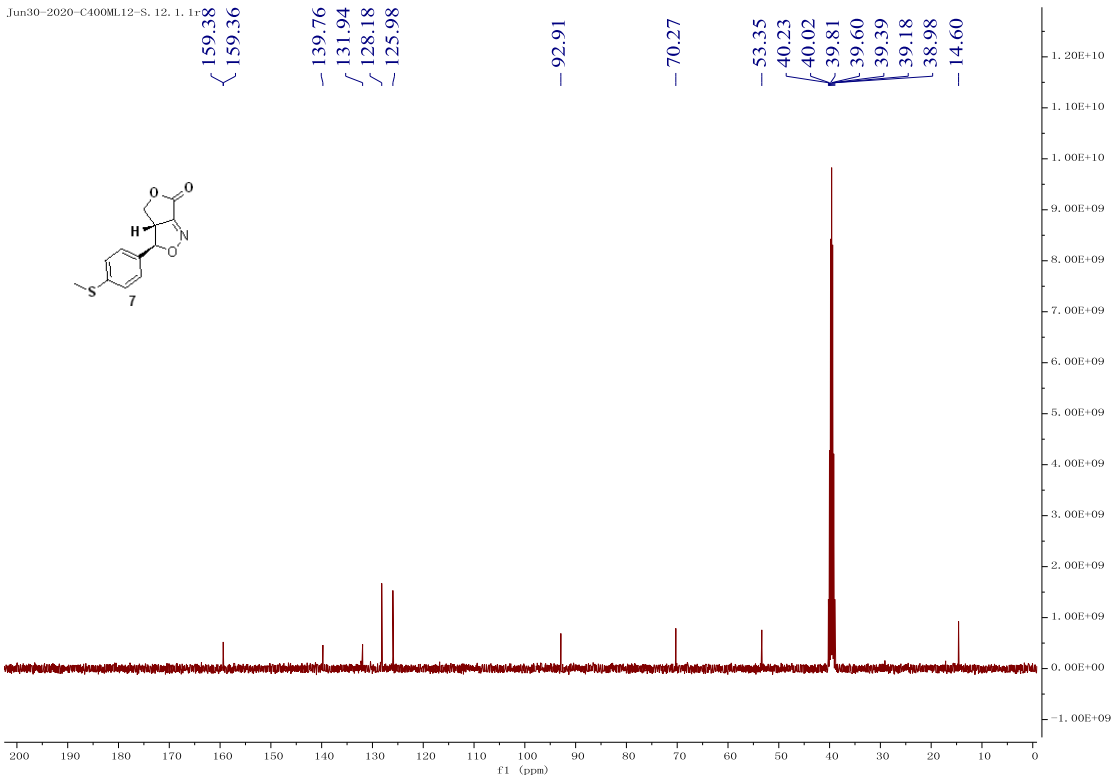
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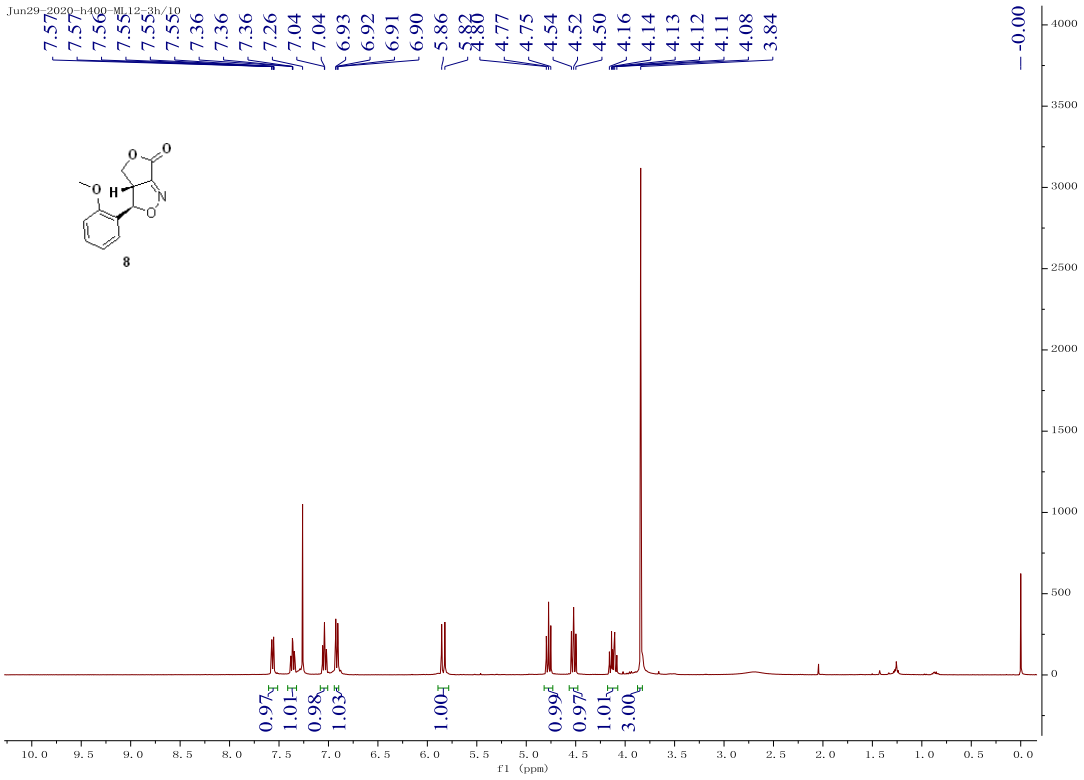
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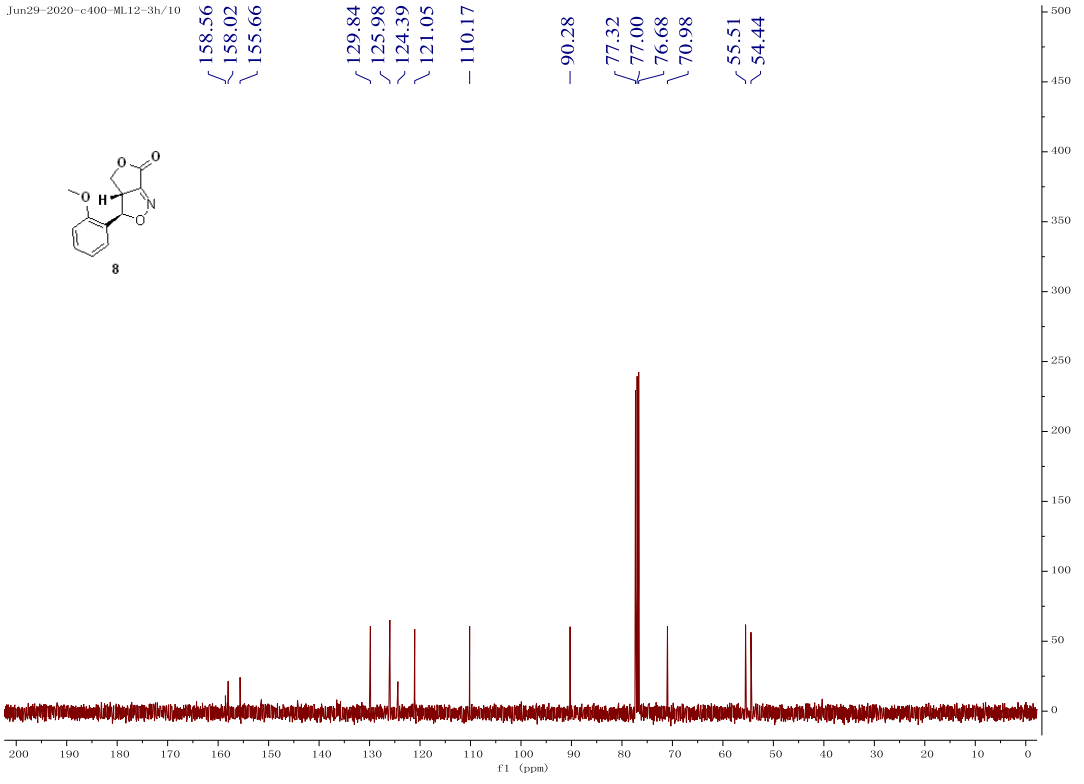
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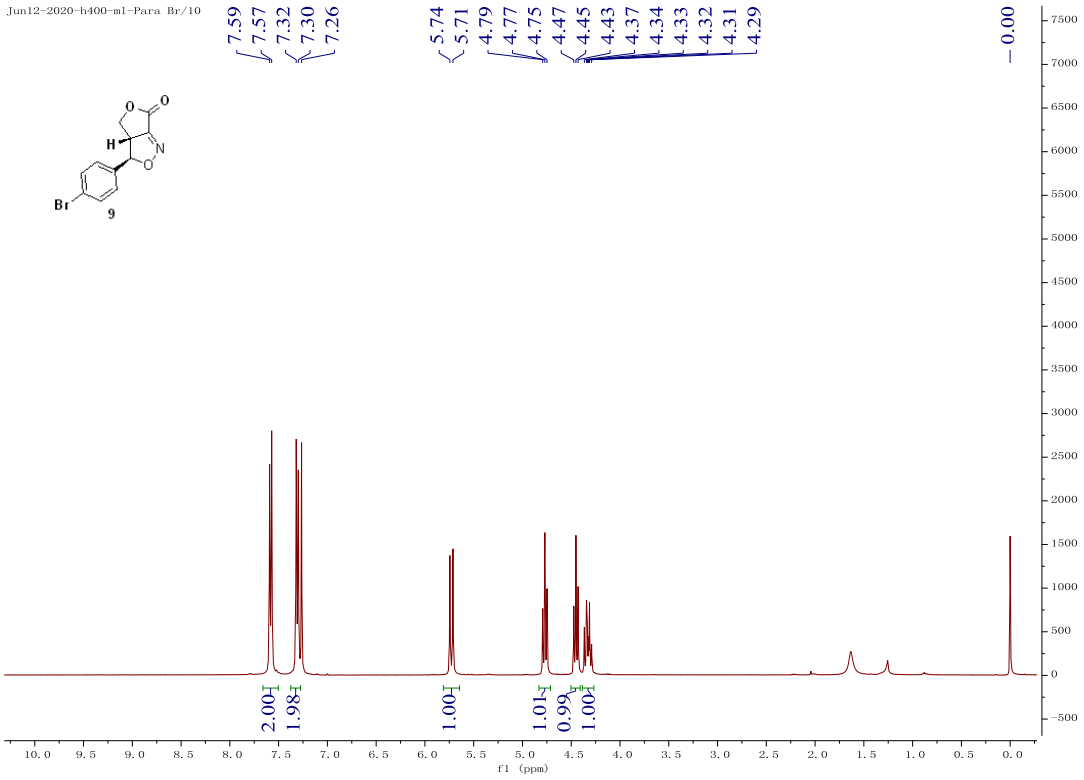
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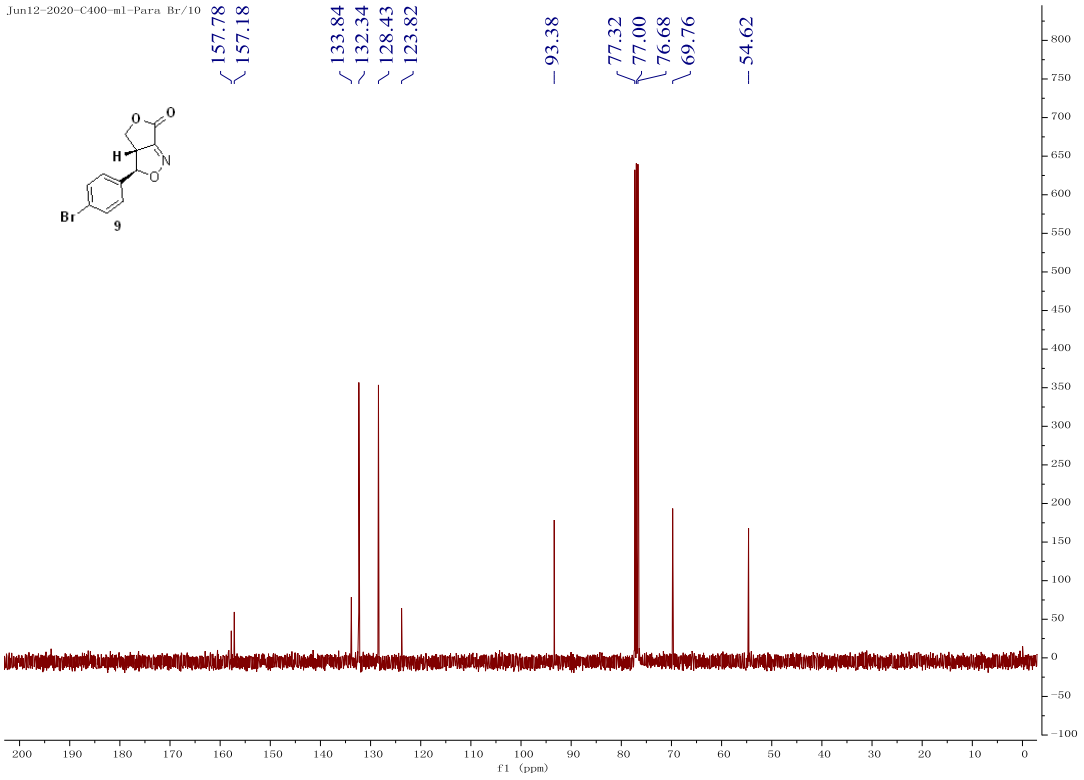
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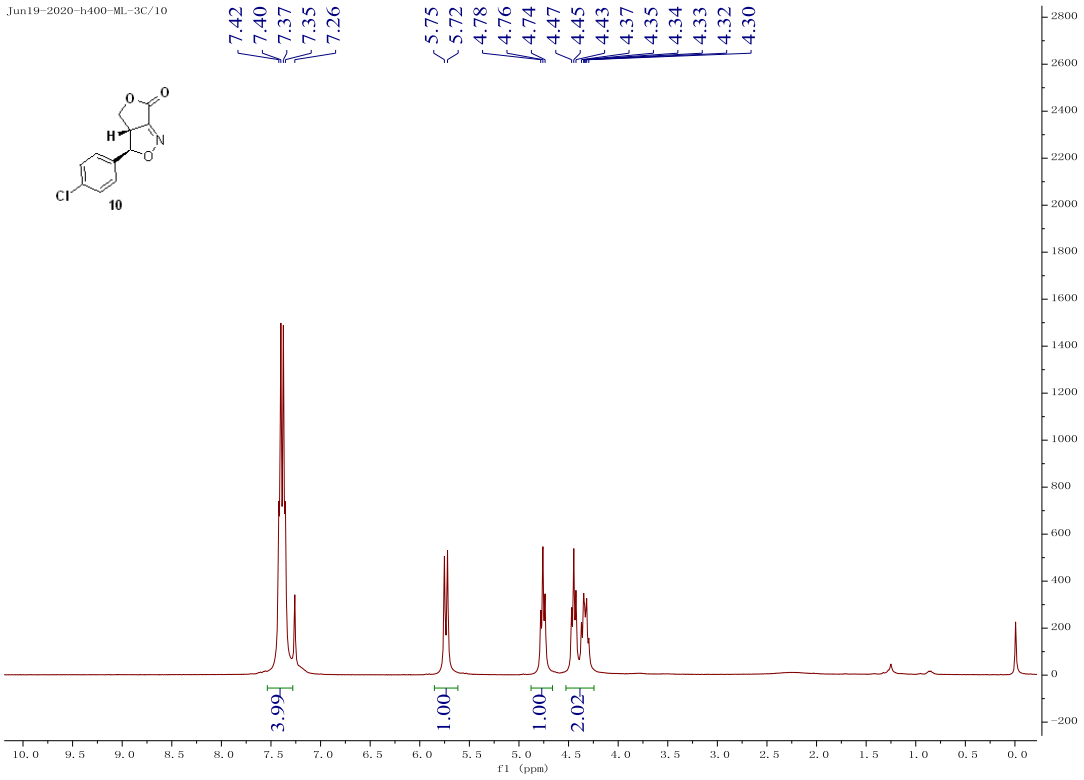
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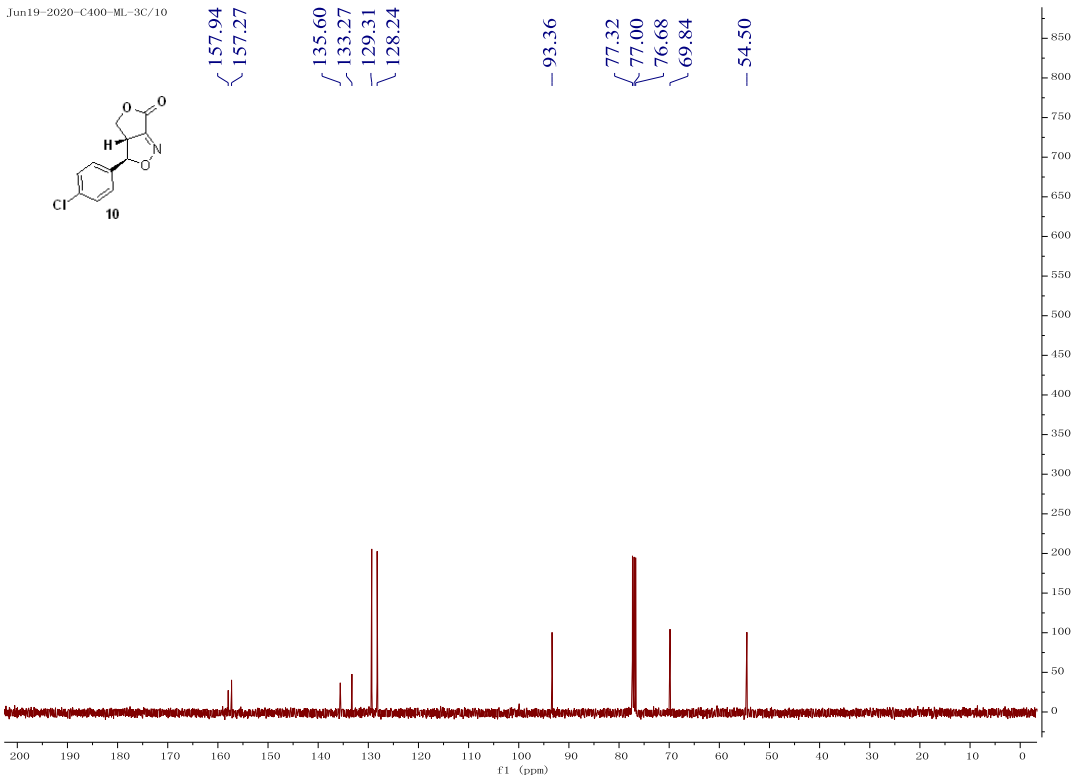
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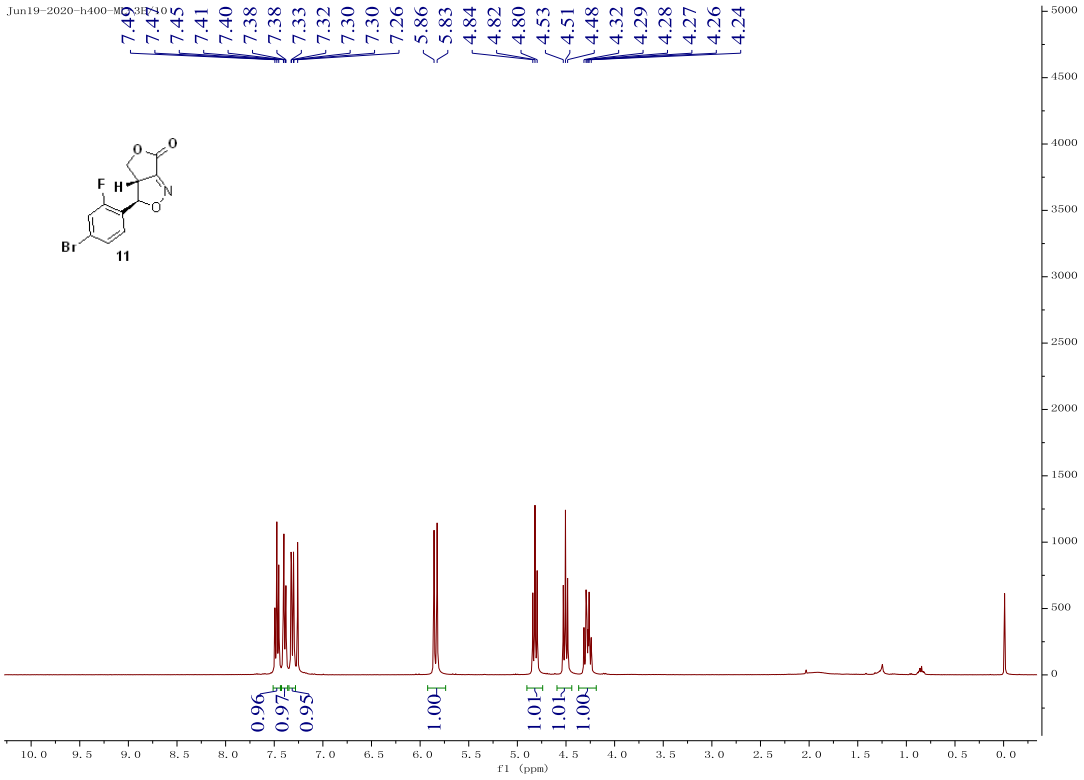
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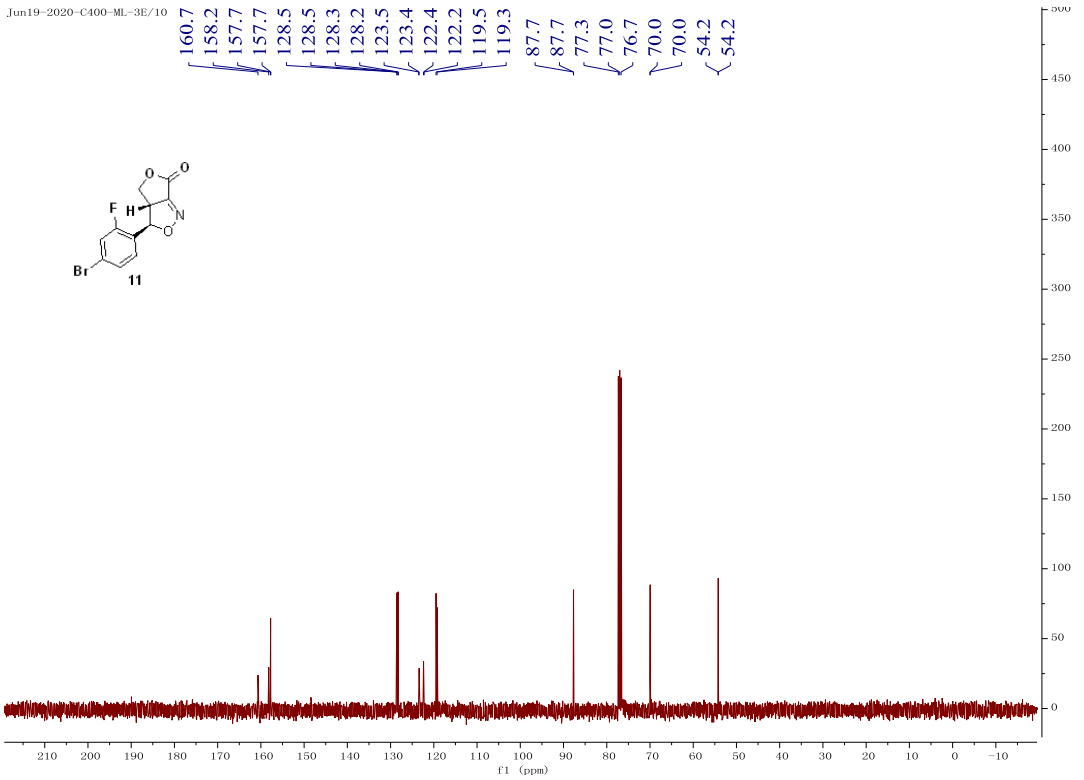
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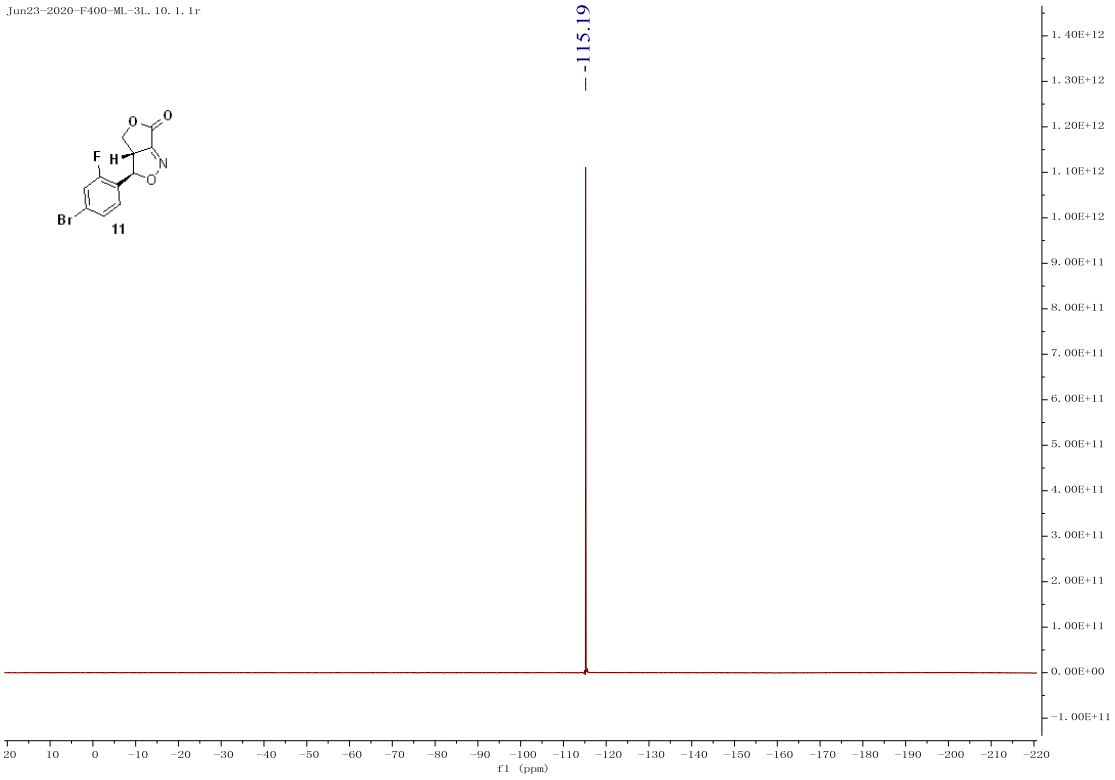
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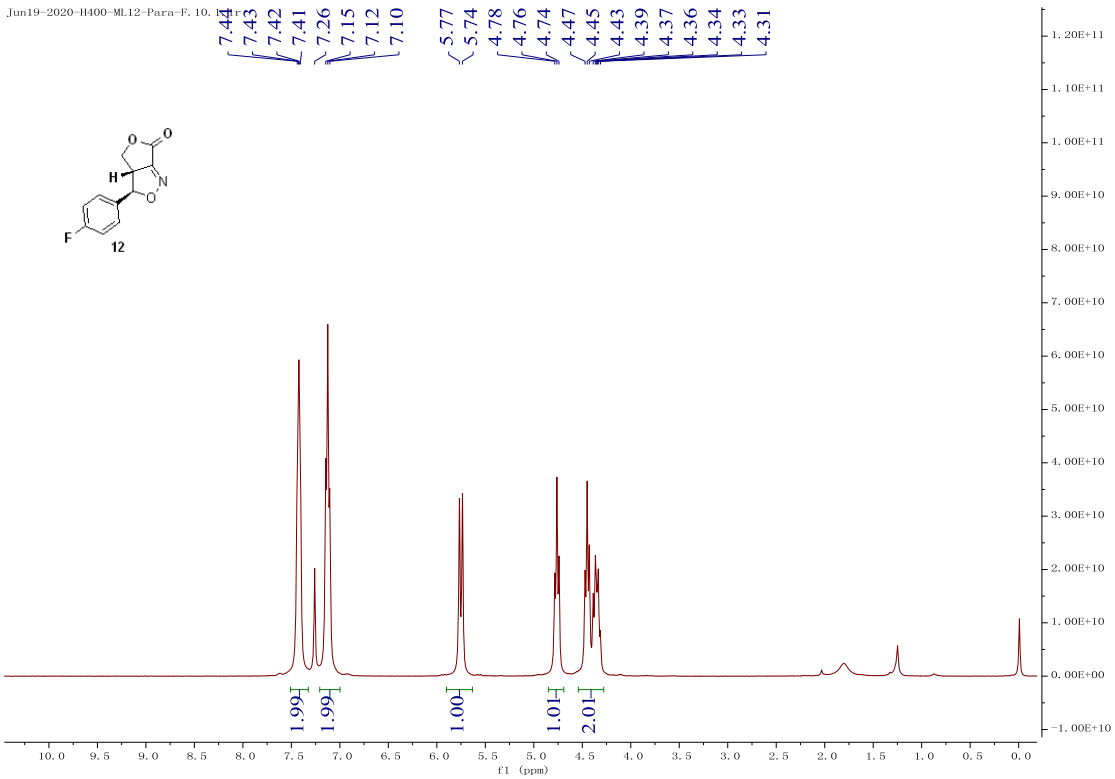
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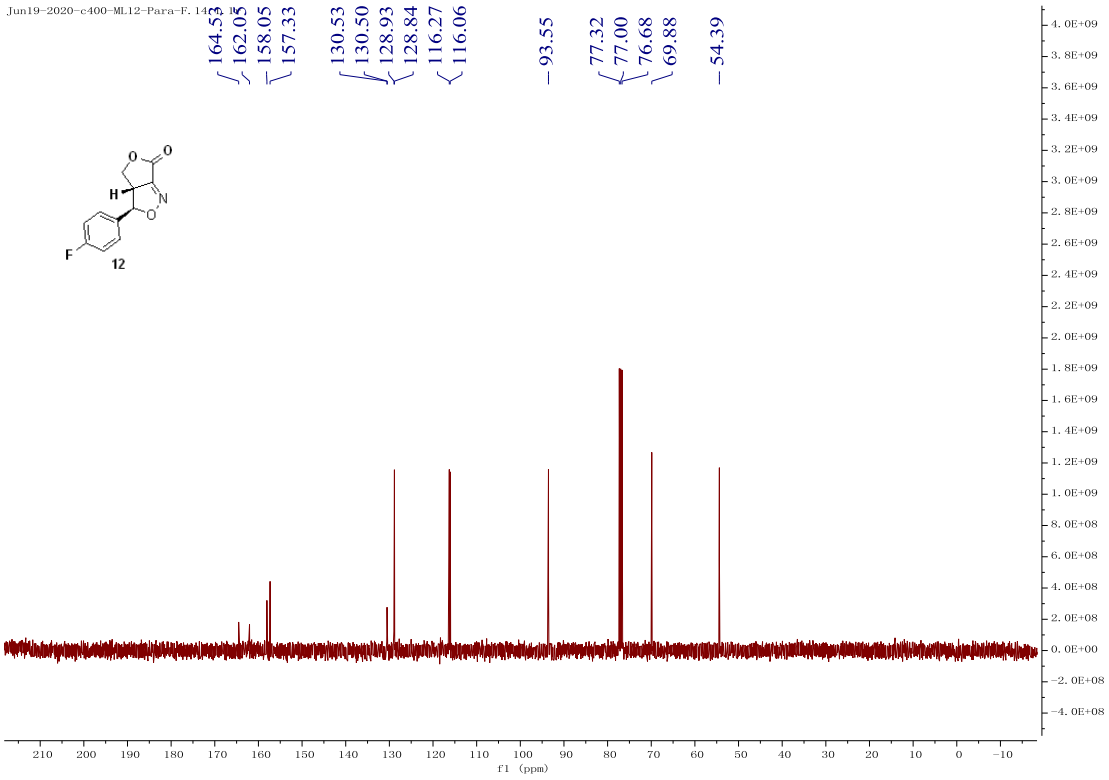
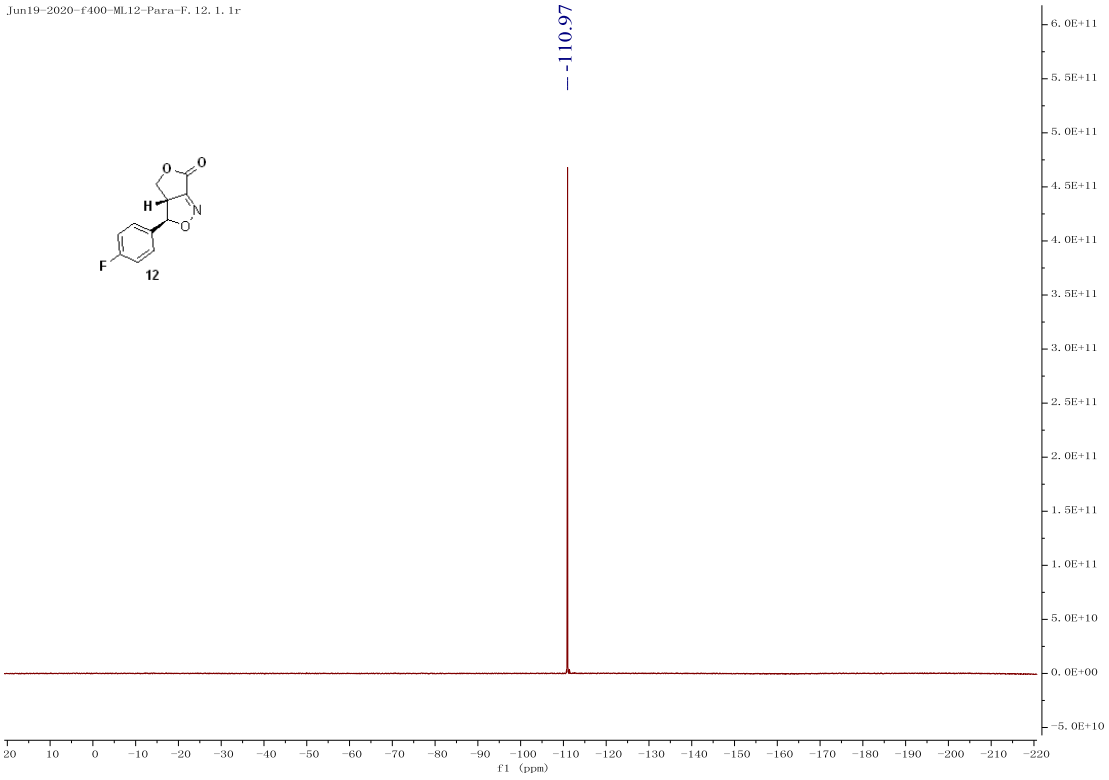
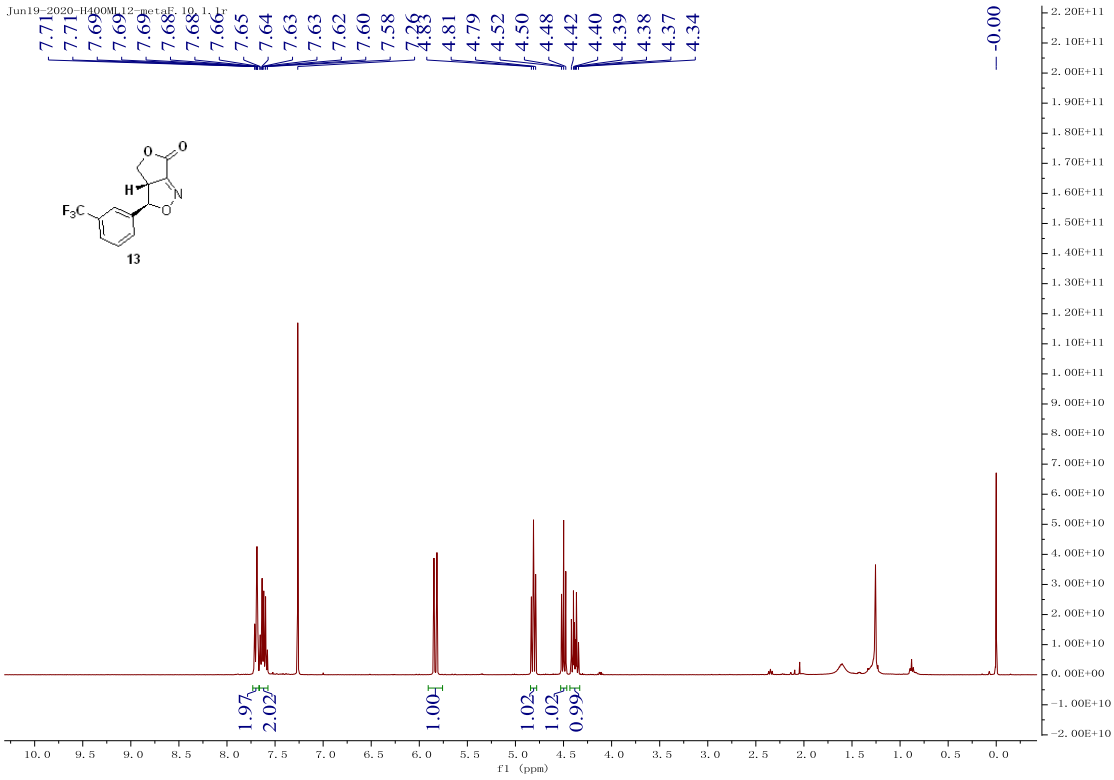
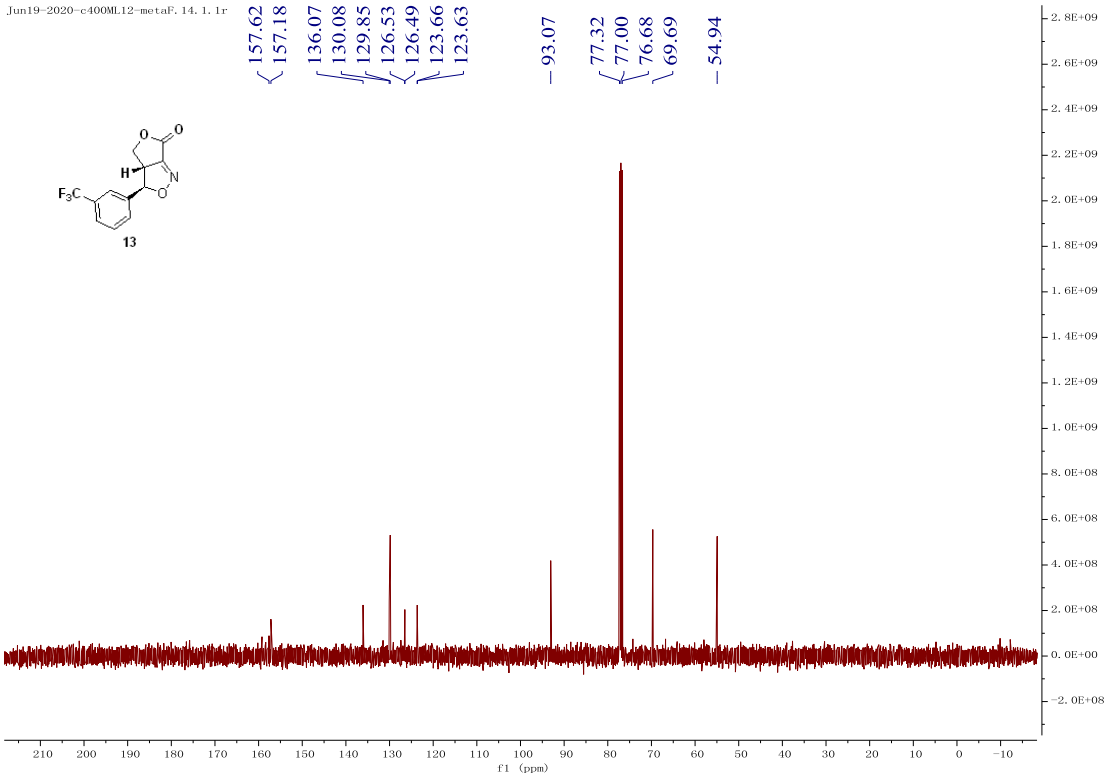
4.74
4.47
4.45
4.43
4.39
4.37
4.36
4.34
4.33
4.31
H
O
O
N
O
F
12
1.99
1.99
1.00
1.01
2.01
f1 (ppm)


Jun19-2020-c400-ML12-Para-F. 14.1.1r
164.53
162.05
158.05
157.33
130.53
130.50
128.93
128.84
116.27
116.06
93.55
77.32
77.00
76.68
69.88
54.39
12
f1 (ppm)


Jun19-2020-f400-ML12-Para-F. 12.1.1r
-110.97
12
f1 (ppm)


Jun19-2020-H400ML12-metaF. 10. 1. 1r
7.71
7.71
7.69
7.69
7.69
7.68
7.68
7.66
7.65
7.64
7.63
7.63
7.62
7.60
7.58
7.26
4.83
4.81
4.79
4.52
4.50
4.48
4.42
4.40
4.39
4.38
4.37
4.34
-0.00
13
1.97
2.02
1.00
1.02
1.02
0.99
f1 (ppm)


Jun19-2020-c400ML12-metaF. 14. 1. 1r
157.62
157.18
136.07
130.08
129.85
126.53
126.49
123.66
123.63
93.07
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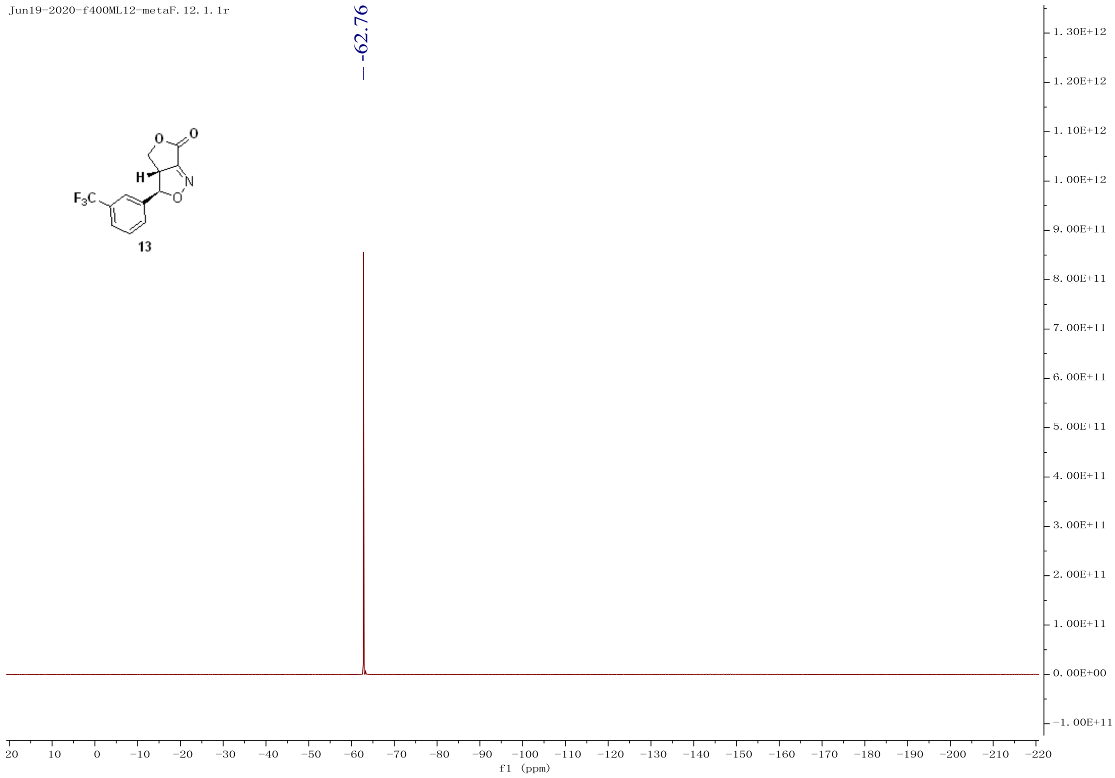
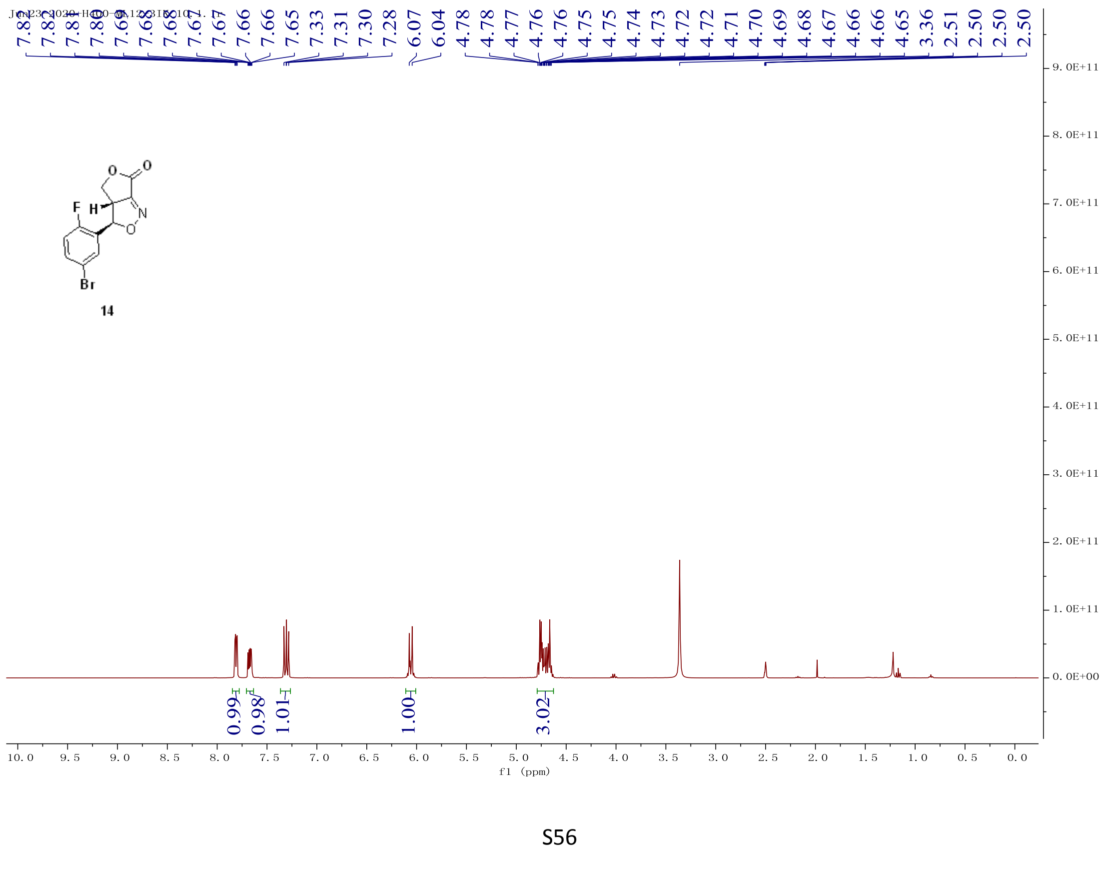
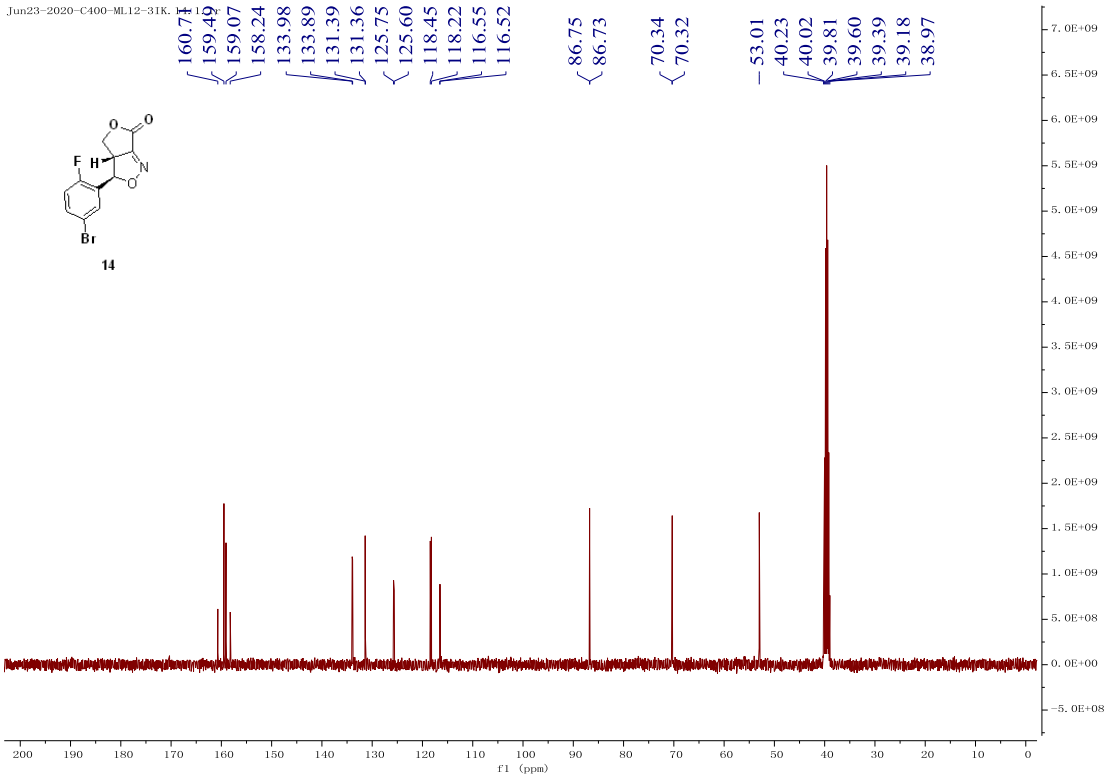
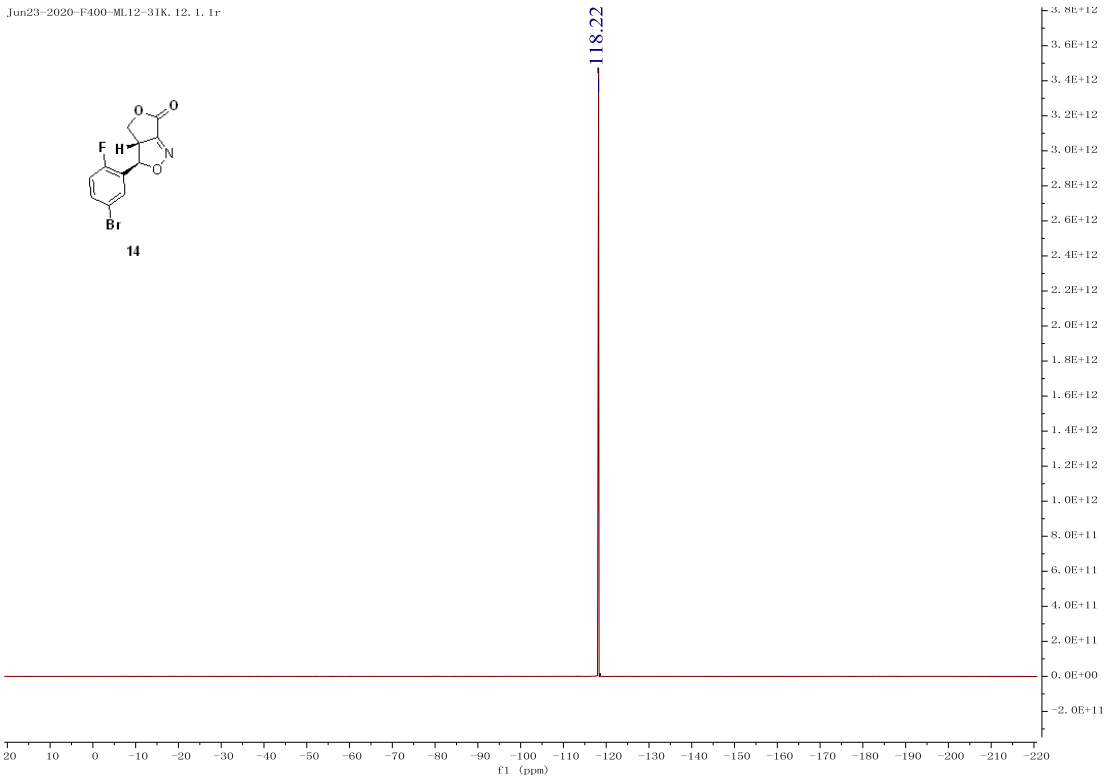
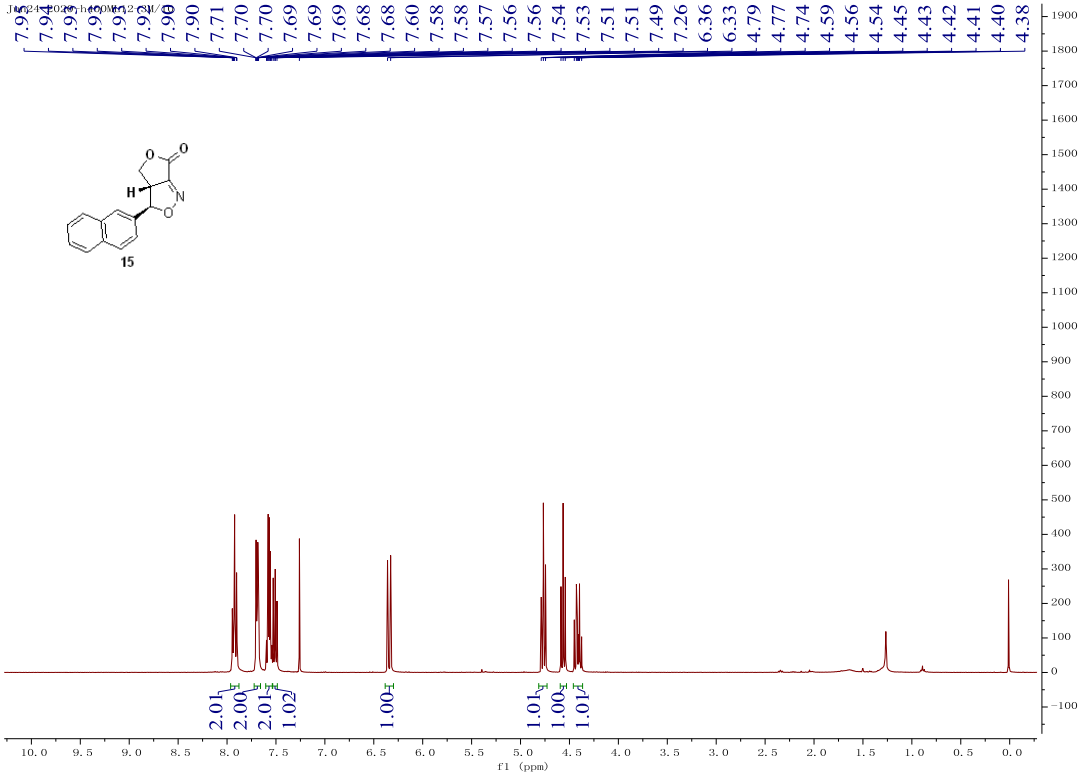
77.00
76.68
69.69
54.94
13
f1 (ppm)

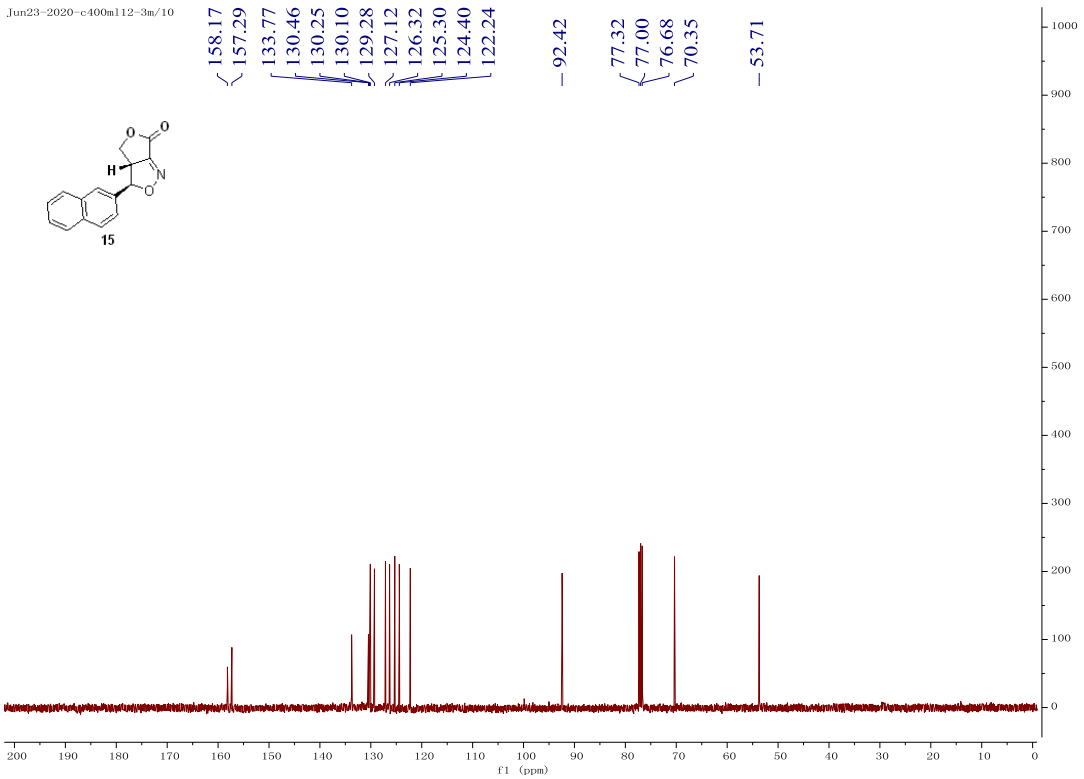

Jun19-2020-f400ML12-metaF.12.1.1r
-62.76
13
f1 (ppm)

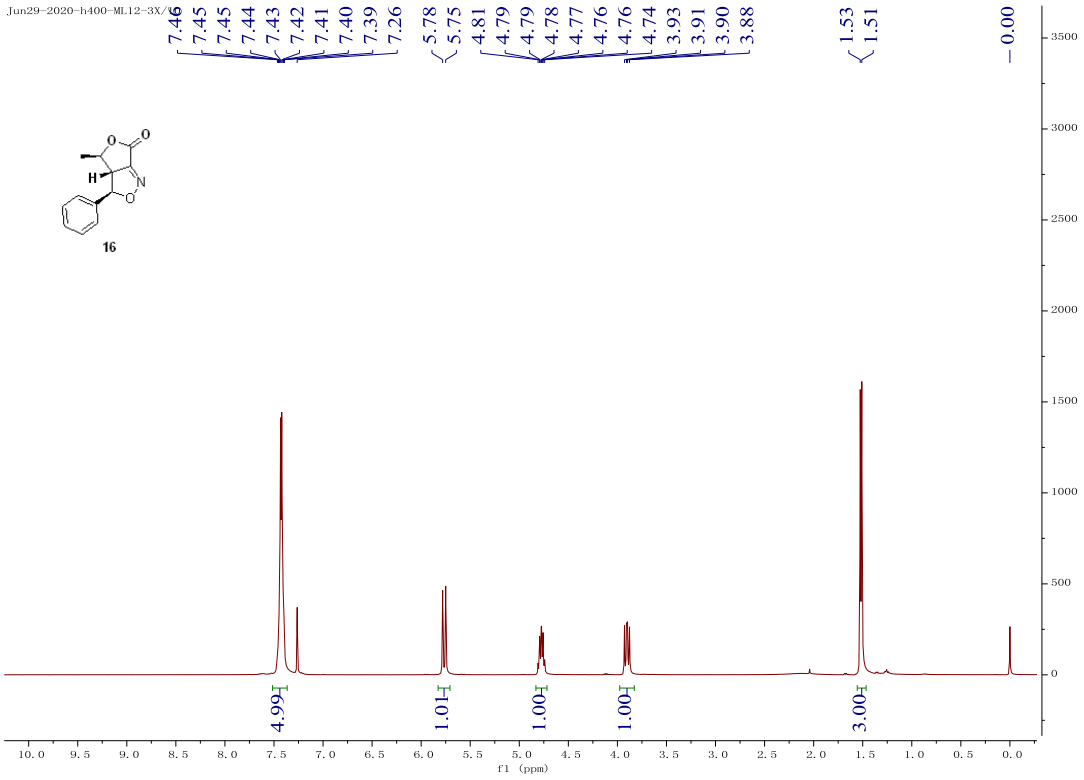

7.82 7.82 7.81 7.80 7.69 7.68 7.68 7.67 7.67 7.66 7.66 7.65 7.33 7.31 7.30 7.28 6.07 6.04 4.78 4.78 4.77 4.76 4.76 4.75 4.75 4.74 4.73 4.72 4.72 4.71 4.70 4.69 4.68 4.67 4.66 4.66 4.65 3.36 2.51 2.50 2.50 2.50
14
0.99 0.98 1.01 1.00 3.02
f1 (ppm)

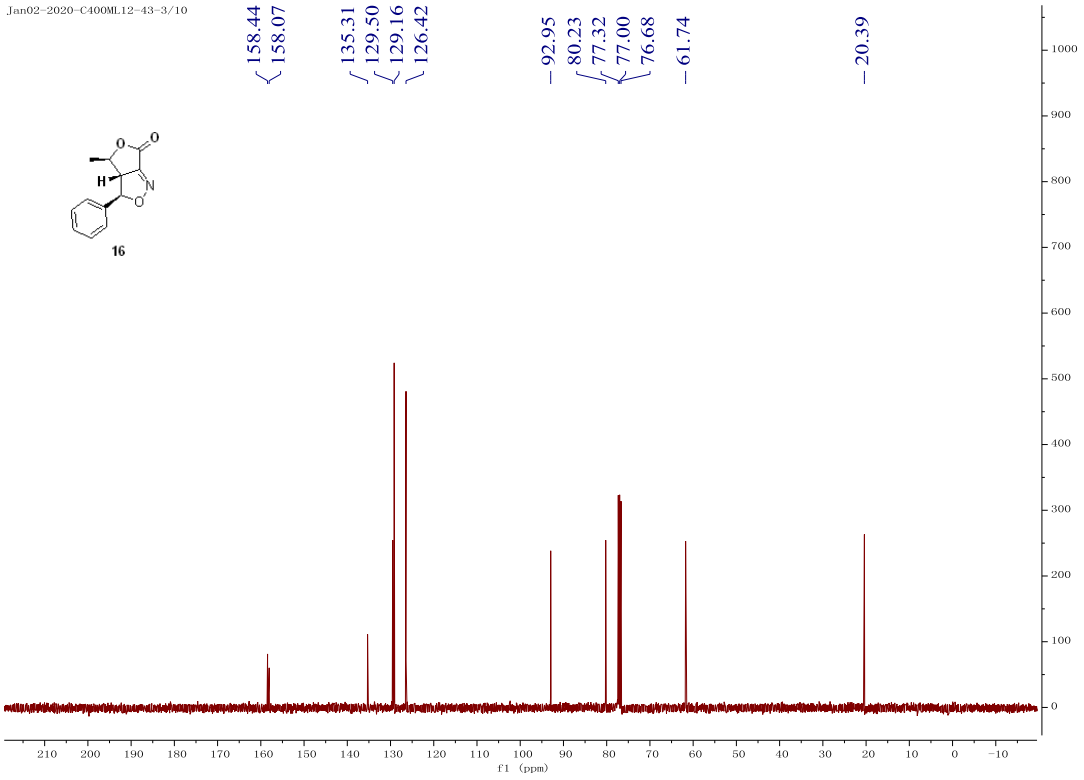

Jun23-2020-C400-ML12-31K.
160.71
159.49
159.07
158.24
133.98
133.89
131.39
131.36
125.75
125.60
118.45
118.22
116.55
116.52
86.75
86.73
70.34
70.32
53.01
40.23
40.02
39.81
39.60
39.39
39.18
38.97
14
f1 (ppm)

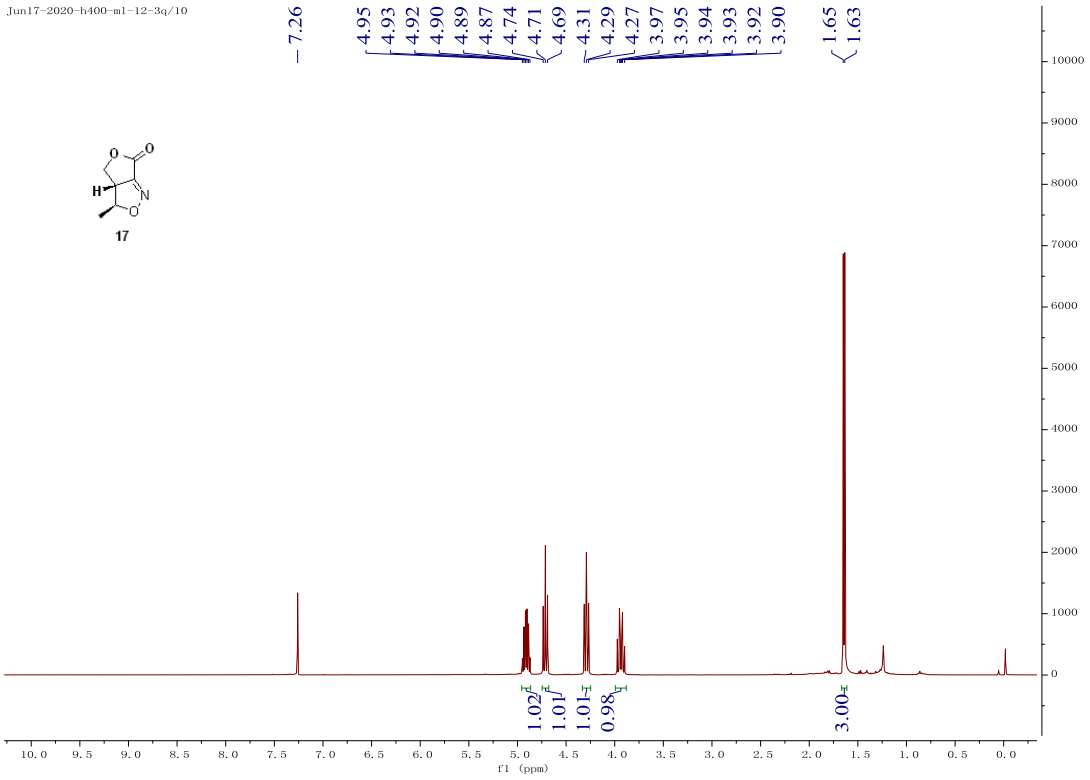

Jun23-2020-F400-ML12-31K.12.1.1r
118.22
14
f1 (ppm)

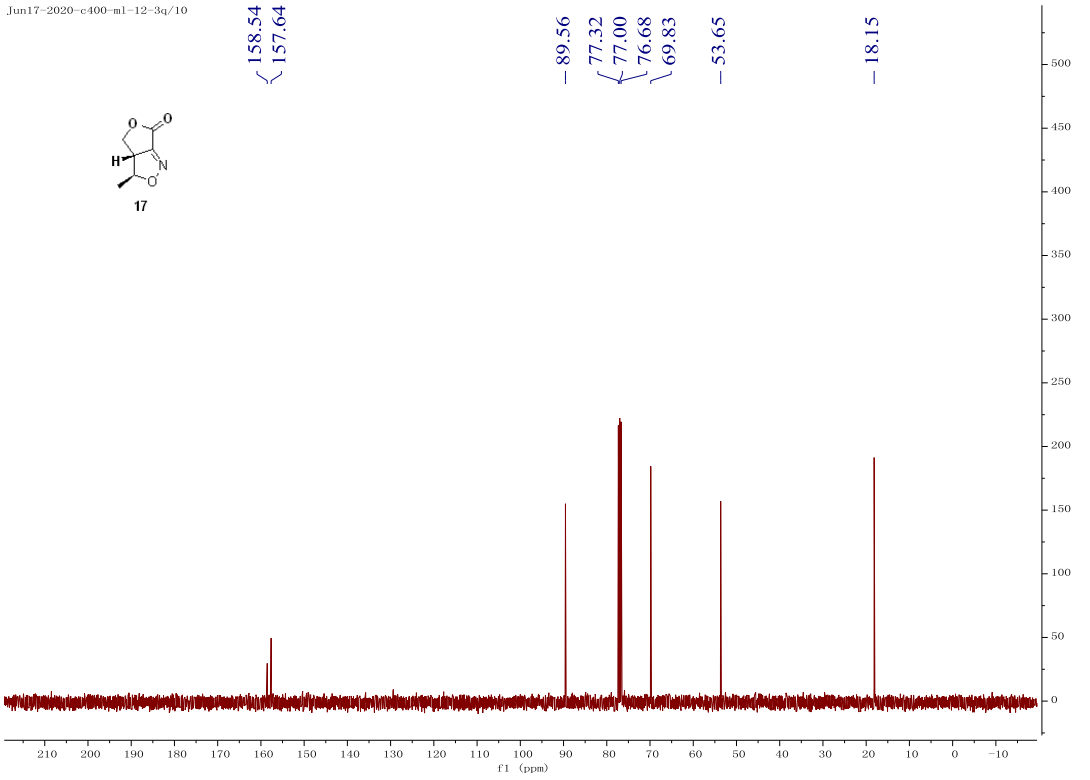

7.94 7.94 7.93 7.93 7.92 7.92 7.90 7.90 7.71 7.70 7.70 7.69 7.69 7.69 7.68 7.68 7.60 7.58 7.58 7.57 7.56 7.56 7.54 7.53 7.51 7.51 7.49 7.26 6.36 6.33 4.79 4.77 4.74 4.59 4.56 4.54 4.45 4.43 4.42 4.41 4.40 4.38
O
O
H
N
O
15
2.01 2.00 2.01 1.02 1.00 1.01 1.00 1.01
f1 (ppm)

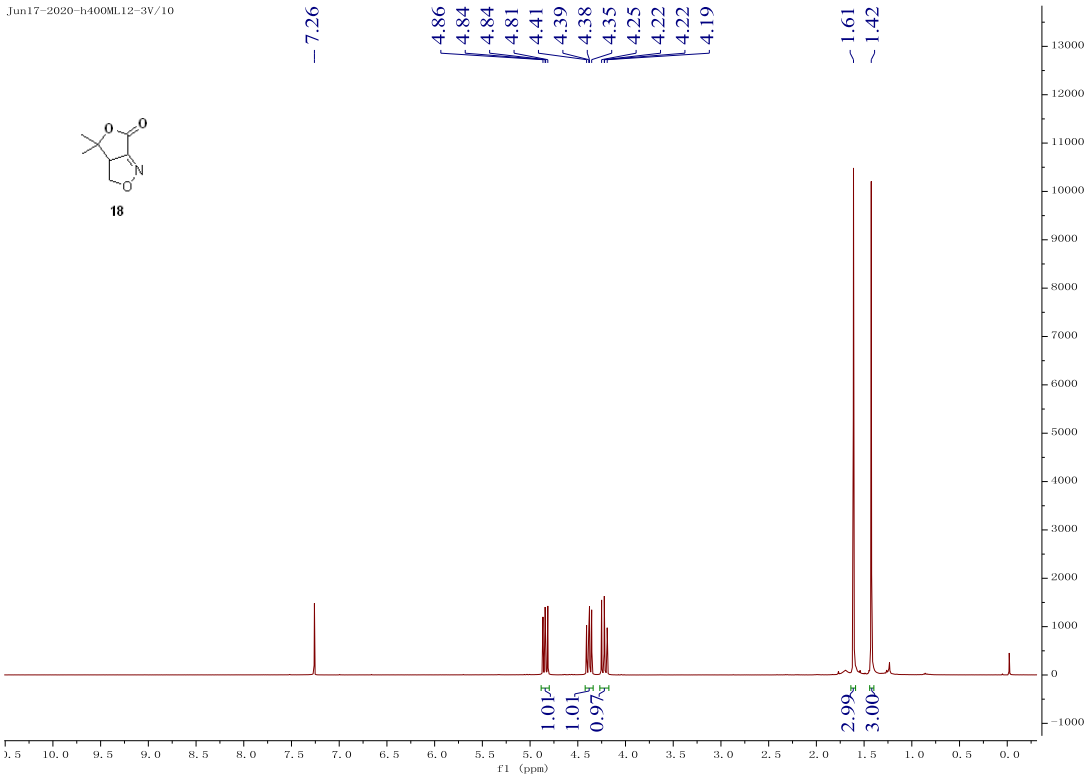

Jun23-2020-c400m112-3m/10
158.17 157.29 133.77 130.46 130.25 130.10 129.28 127.12 126.32 125.30 124.40 122.24 92.42 77.32 77.00 76.68 70.35 53.71
O
O
H
N
O
15
f1 (ppm)

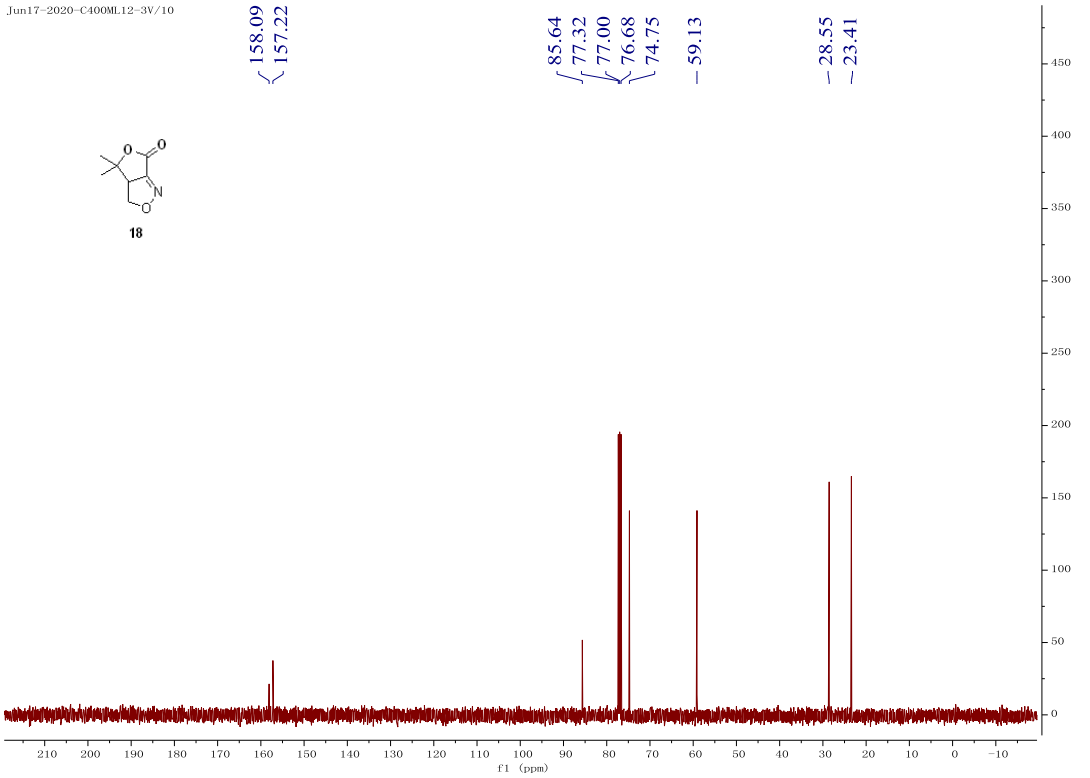

Jun29-2020-h400-ML12-3X/6
7.46
7.45
7.45
7.44
7.43
7.42
7.41
7.40
7.39
7.26
5.78
5.75
4.81
4.79
4.79
4.78
4.77
4.76
4.76
4.74
3.93
3.91
3.90
3.88
1.53
1.51
0.00
16
4.99
1.01
1.00
1.00
3.00
f1 (ppm)

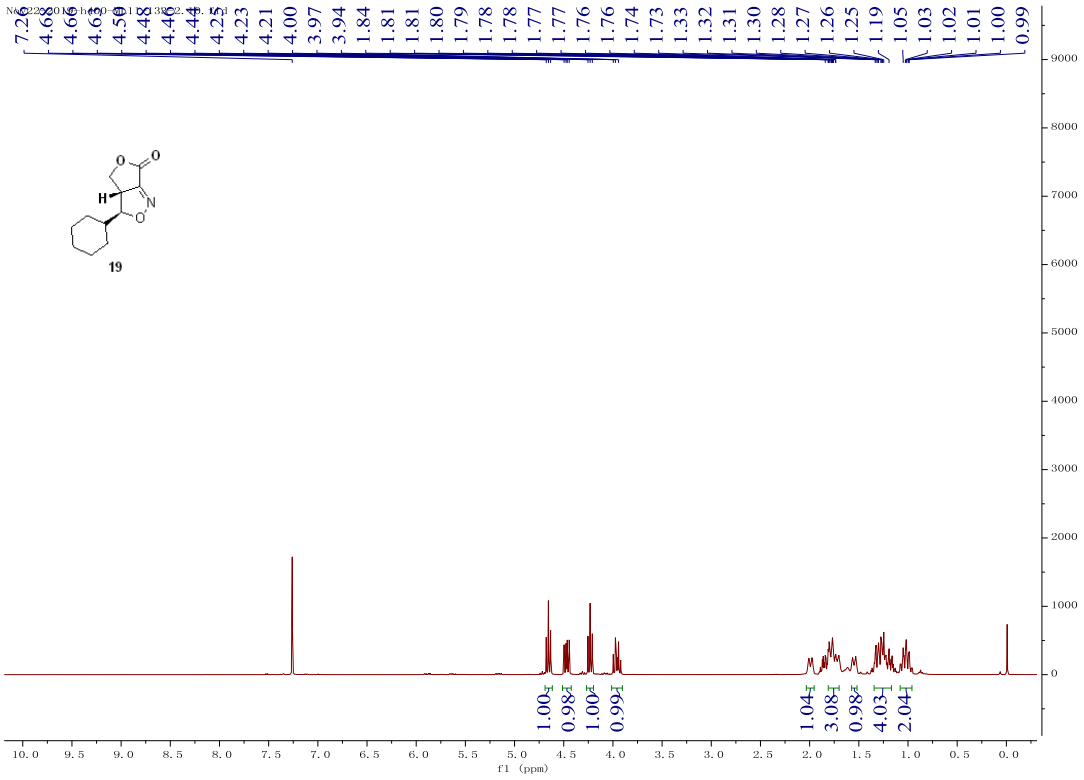

Jan02-2020-C400ML12-43-3/10
158.44
158.07
135.31
129.50
129.16
126.42
92.95
80.23
77.32
77.00
76.68
61.74
20.39
16
f1 (ppm)

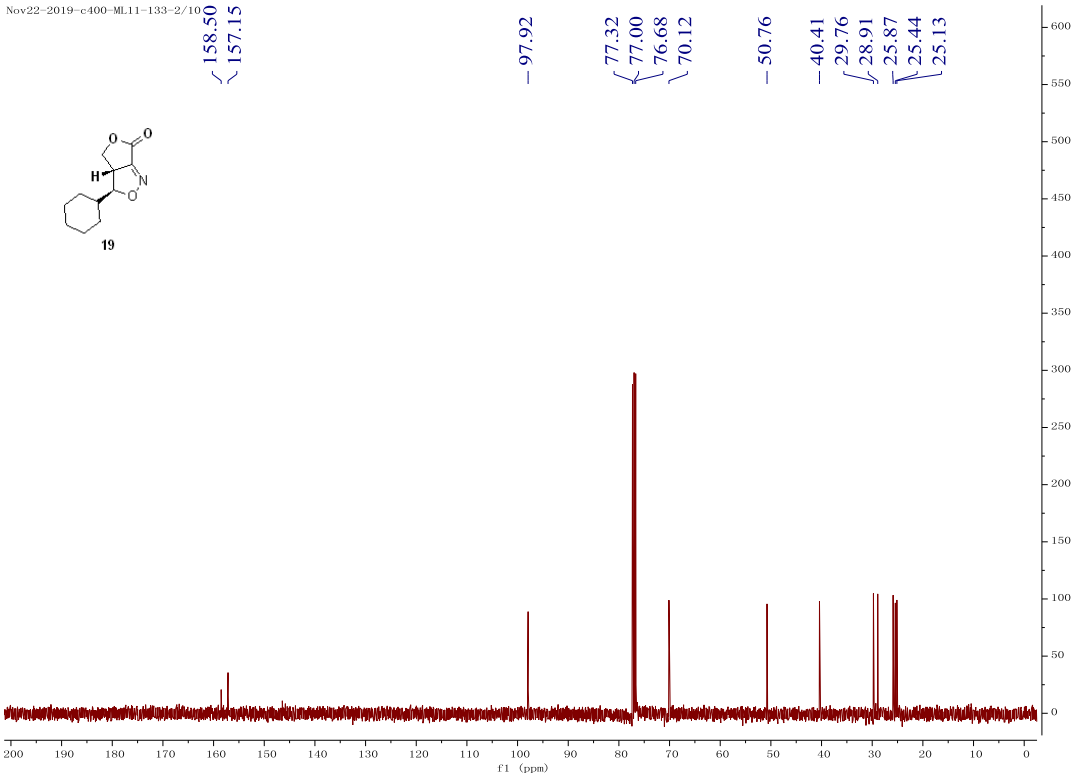

Jun17-2020-h400-ml-12-3q/10
7.26
4.95
4.93
4.92
4.90
4.89
4.87
4.74
4.71
4.69
4.31
4.29
4.27
3.97
3.95
3.94
3.93
3.92
3.90
1.65
1.63
17
1.02
1.01
1.01
0.98
3.00
f1 (ppm)

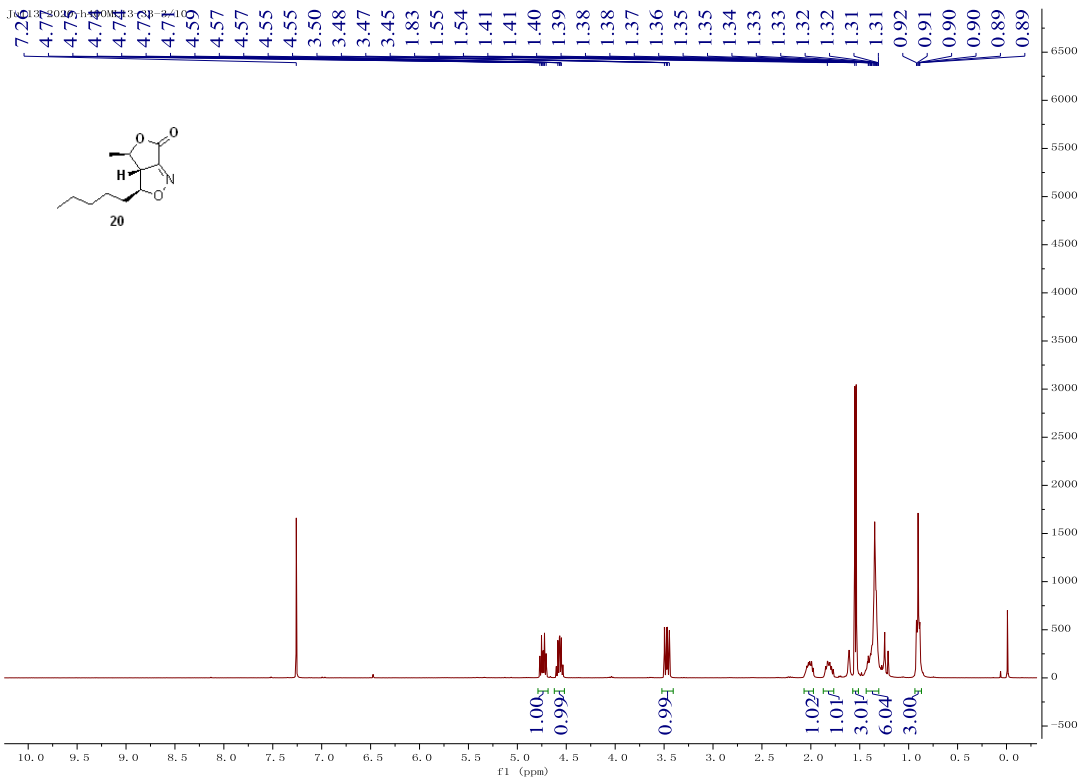

Jun17-2020-c400-ml-12-3q/10
158.54
157.64
89.56
77.32
77.00
76.68
69.83
53.65
18.15
17
f1 (ppm)

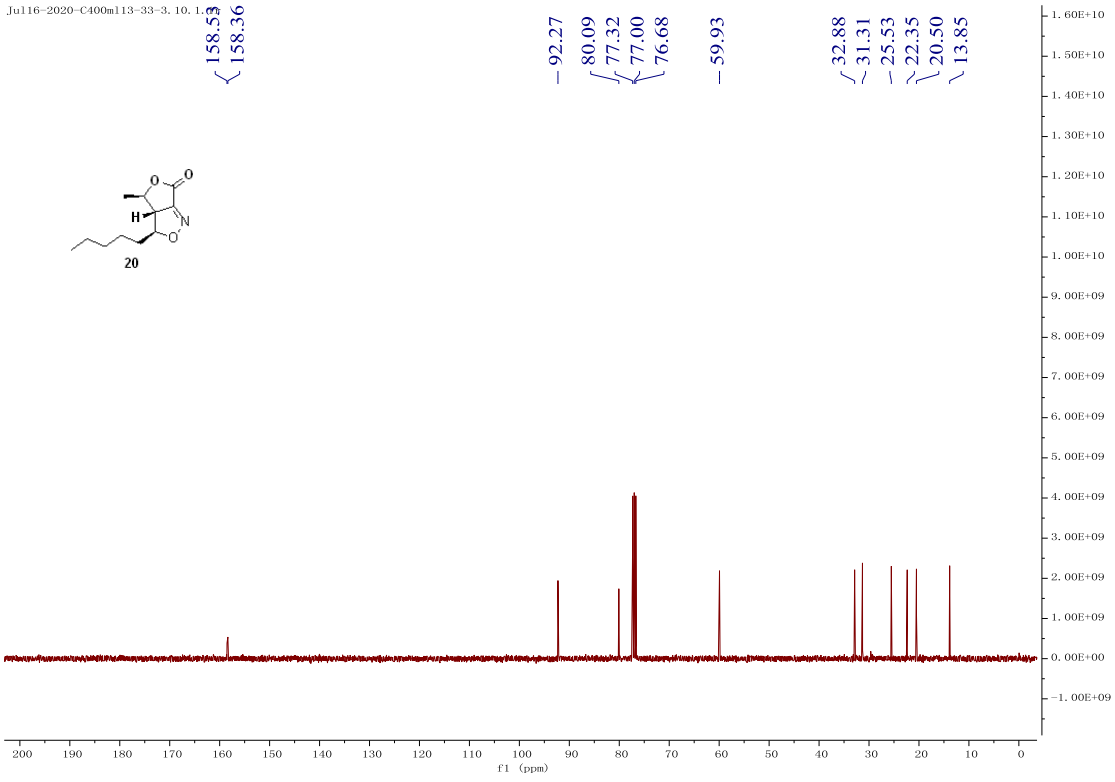

Jun17-2020-h400ML12-3V/10
7.26
4.86
4.84
4.84
4.81
4.41
4.39
4.38
4.35
4.25
4.22
4.22
4.19
1.61
1.42
18
1.01
1.01
0.97
2.99
3.00
f1 (ppm)

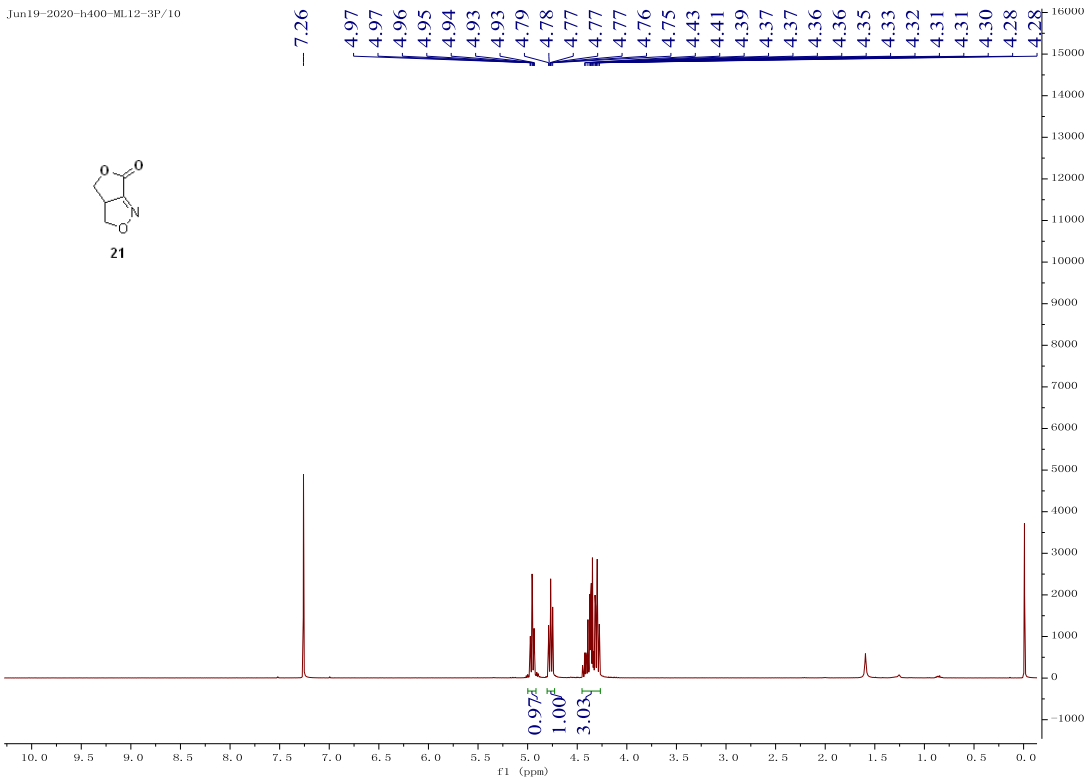

Jun17-2020-C400ML12-3V/10
158.09
157.22
85.64
77.32
77.00
76.68
74.75
59.13
28.55
23.41
18
f1 (ppm)

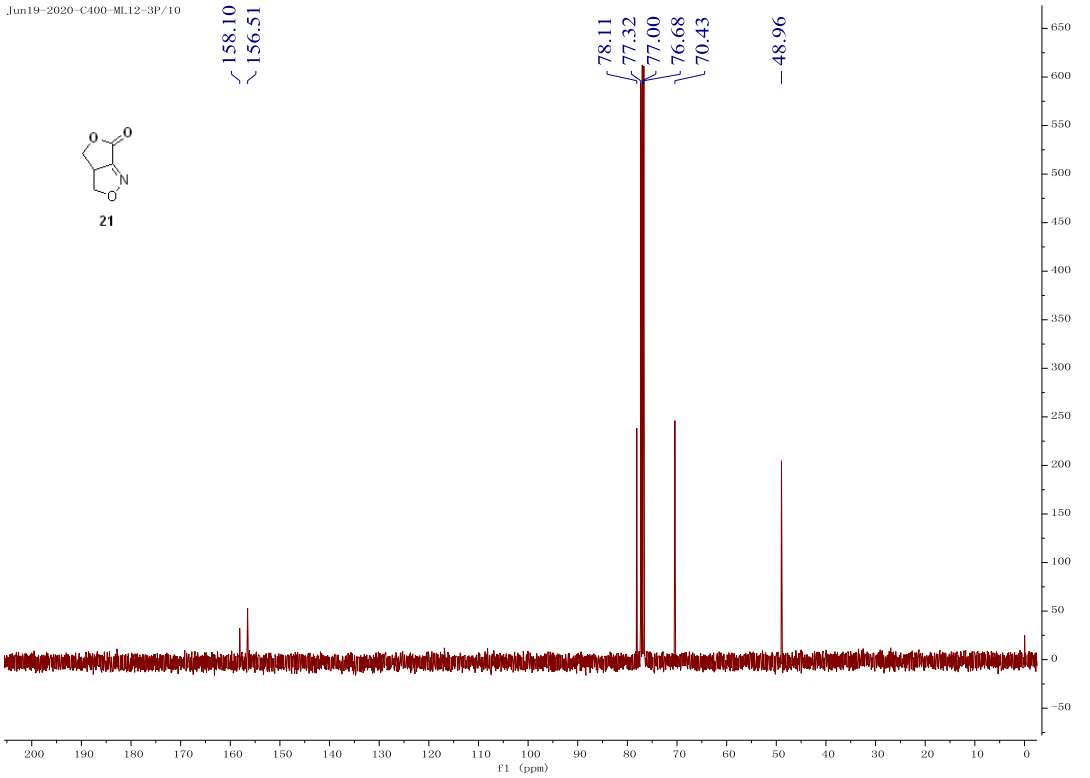

7.26
4.68
4.66
4.63
4.50
4.48
4.46
4.44
4.25
4.23
4.21
4.00
3.97
3.94
1.84
1.81
1.81
1.80
1.79
1.78
1.78
1.77
1.77
1.76
1.76
1.74
1.73
1.33
1.32
1.31
1.30
1.28
1.27
1.26
1.25
1.19
1.05
1.03
1.02
1.01
1.00
0.99
19
1.00
0.98
1.00
0.99
1.04
3.08
0.98
4.03
2.04
f1 (ppm)

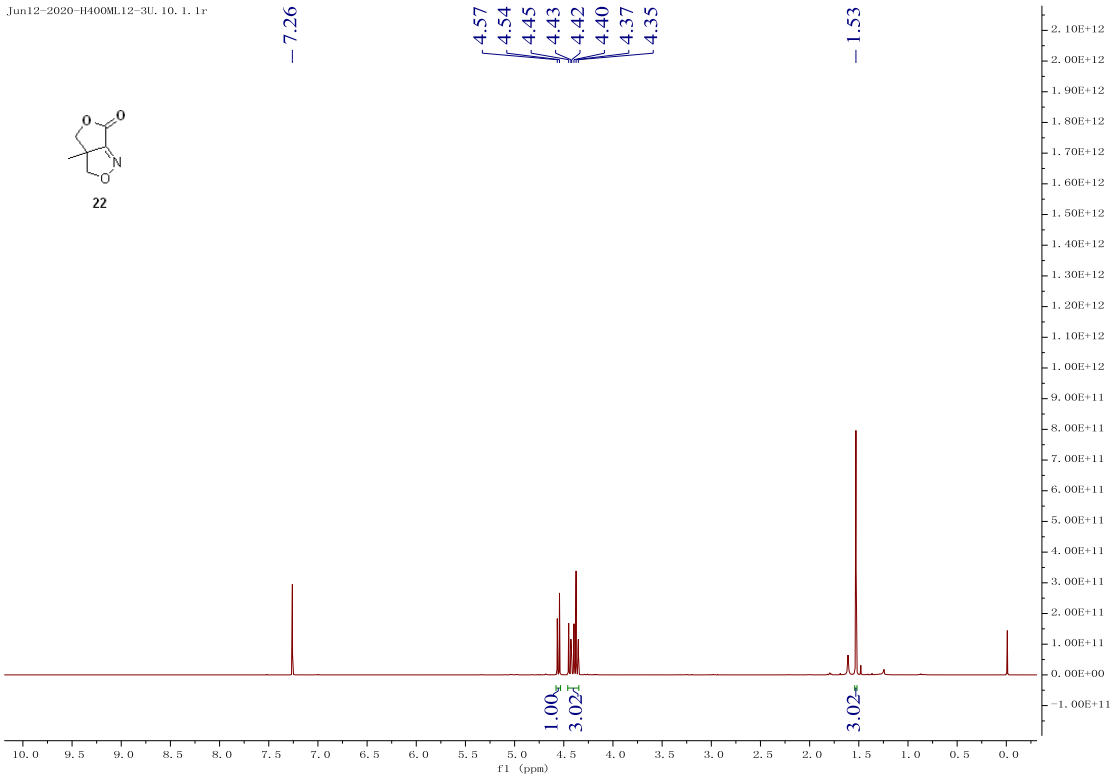

158.50
157.15
97.92
77.32
77.00
76.68
70.12
50.76
40.41
29.76
28.91
25.87
25.44
25.13
19
f1 (ppm)

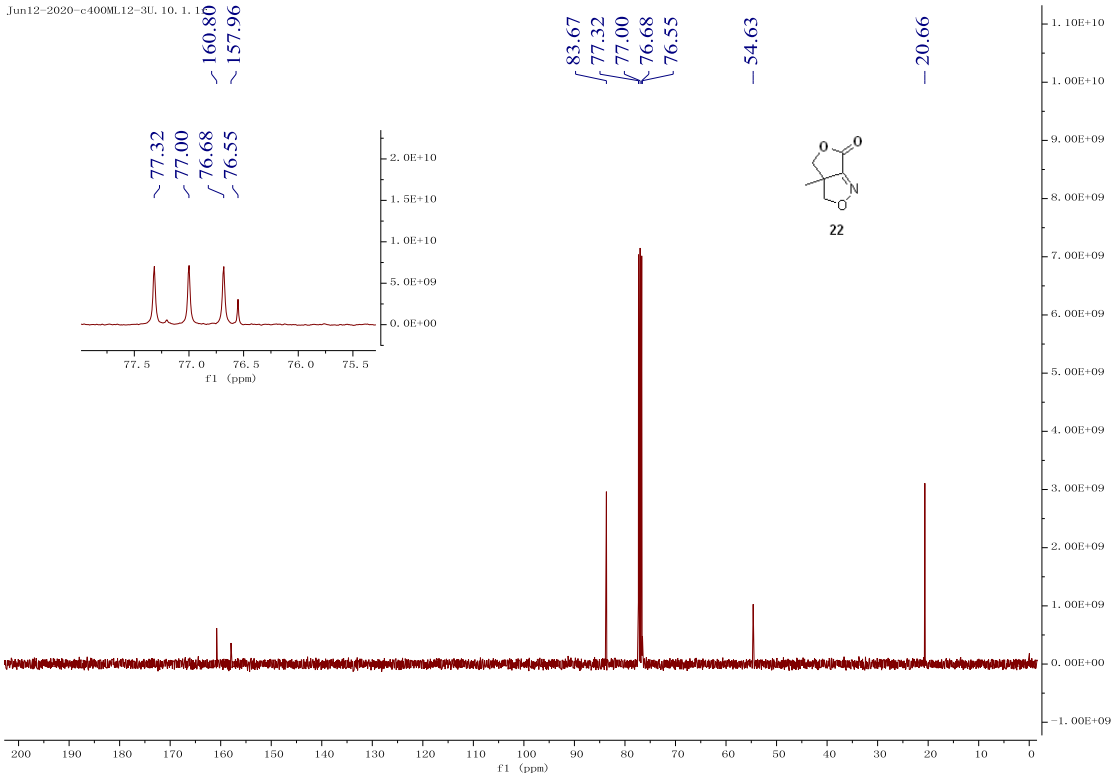

7.26
4.77
4.76
4.75
4.74
4.73
4.72
4.71
4.59
4.57
4.57
4.55
4.55
3.50
3.48
3.47
3.45
1.83
1.55
1.54
1.41
1.41
1.40
1.39
1.38
1.38
1.37
1.36
1.35
1.35
1.34
1.33
1.33
1.32
1.32
1.31
1.31
0.92
0.91
0.90
0.90
0.89
0.89
20
1.00
0.99
0.99
1.02
1.01
3.01
6.04
3.00
f1 (ppm)

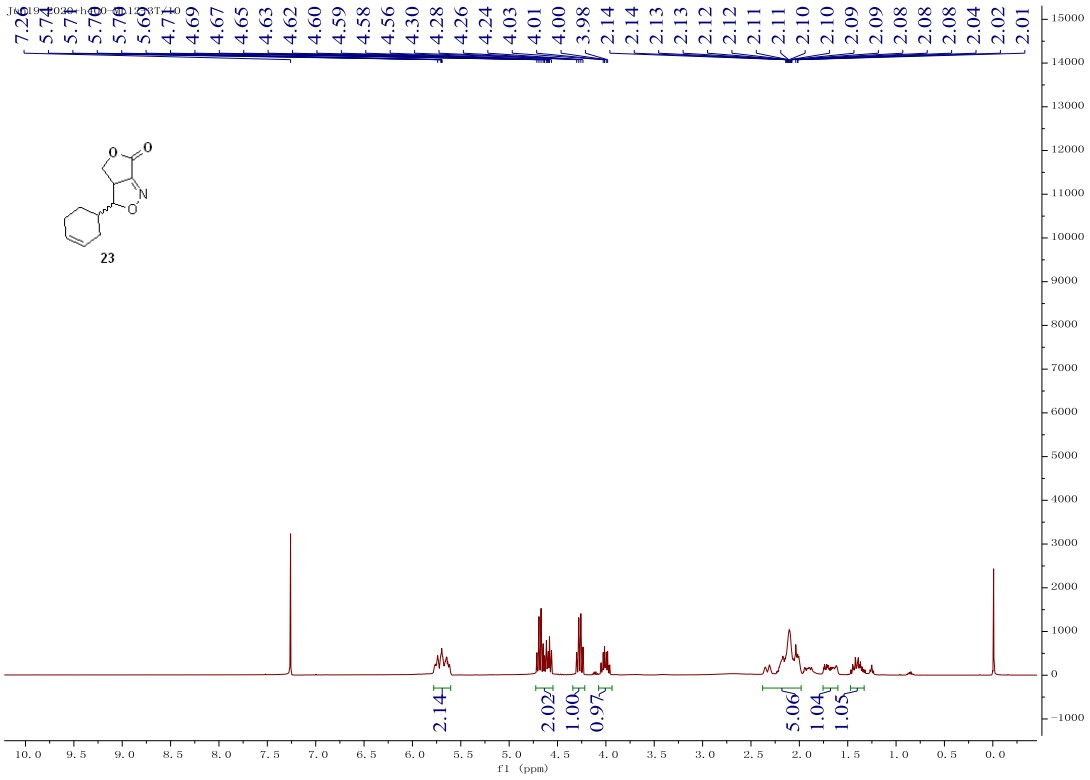

158.53
158.36
92.27
80.09
77.32
77.00
76.68
59.93
32.88
31.31
25.53
22.35
20.50
13.85
20
f1 (ppm)

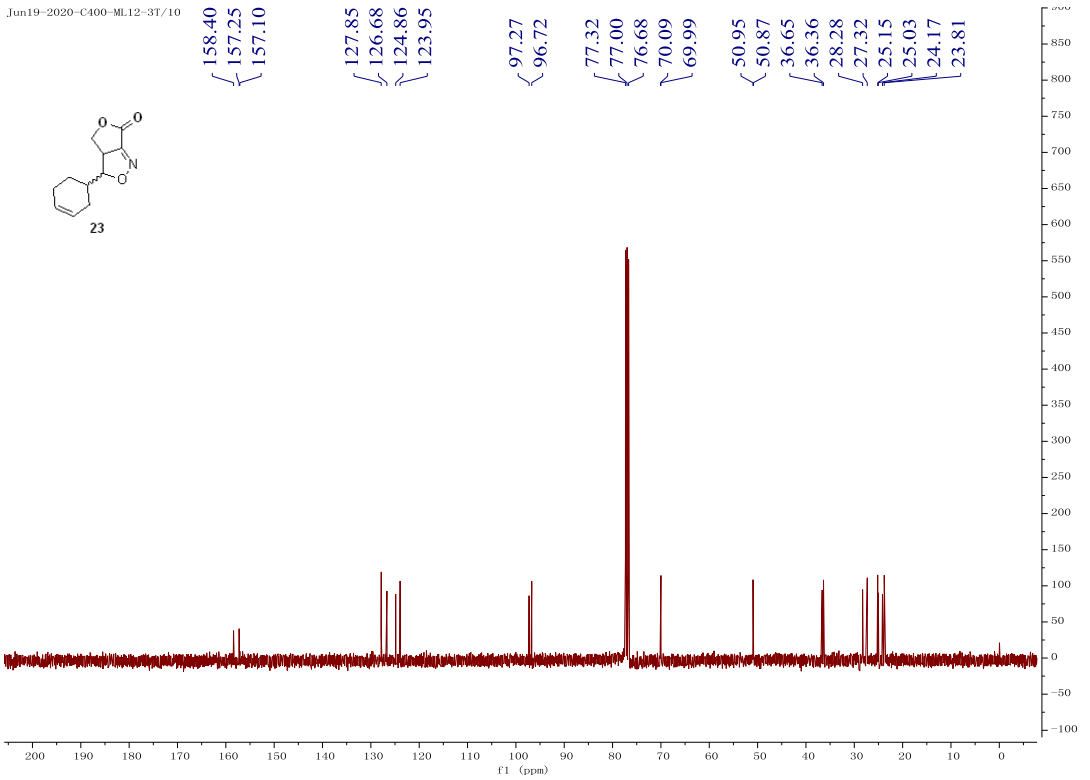

Jun19-2020-h400-ML12-3P/10
7.26
4.97
4.97
4.96
4.95
4.94
4.93
4.93
4.79
4.78
4.77
4.77
4.77
4.76
4.75
4.43
4.41
4.39
4.37
4.37
4.36
4.36
4.35
4.33
4.32
4.31
4.31
4.30
4.28
4.28
21
0.97
1.00
3.03
f1 (ppm)

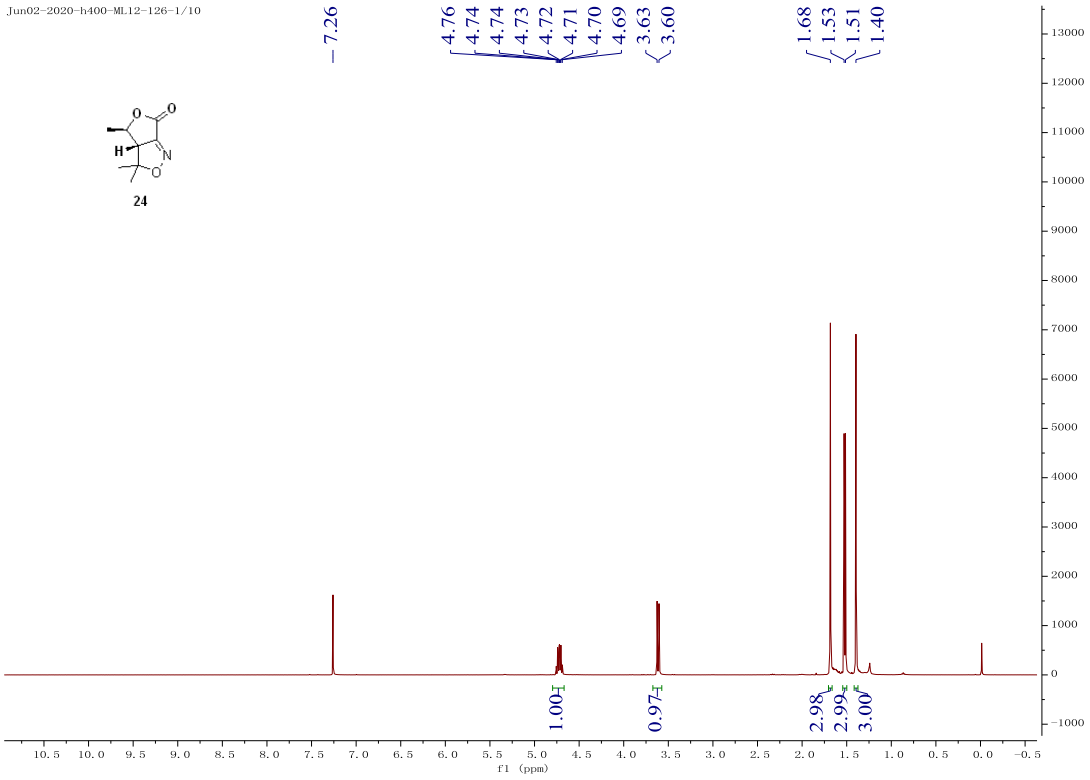

Jun19-2020-C400-ML12-3P/10
158.10
156.51
78.11
77.32
77.00
76.68
70.43
48.96
21
f1 (ppm)

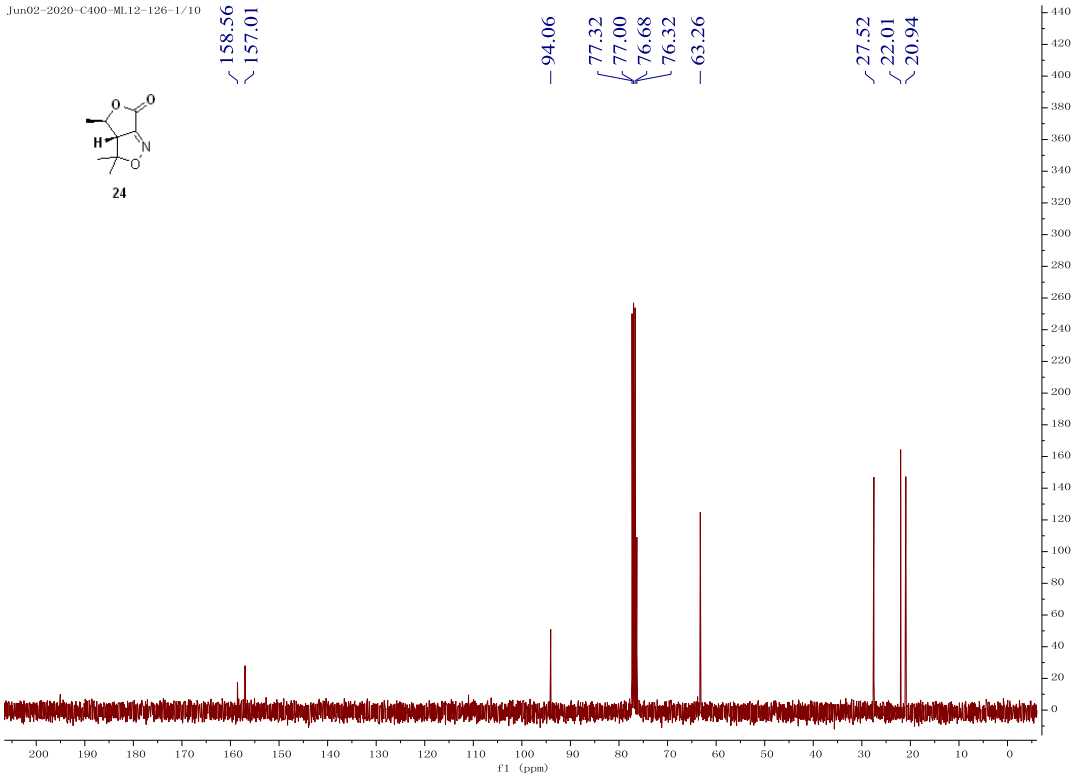

Jun12-2020-H400ML12-3U. 10. 1. 1r
7.26
4.57
4.54
4.45
4.43
4.42
4.40
4.37
4.35
1.53
22
1.00
3.02
3.02
f1 (ppm)

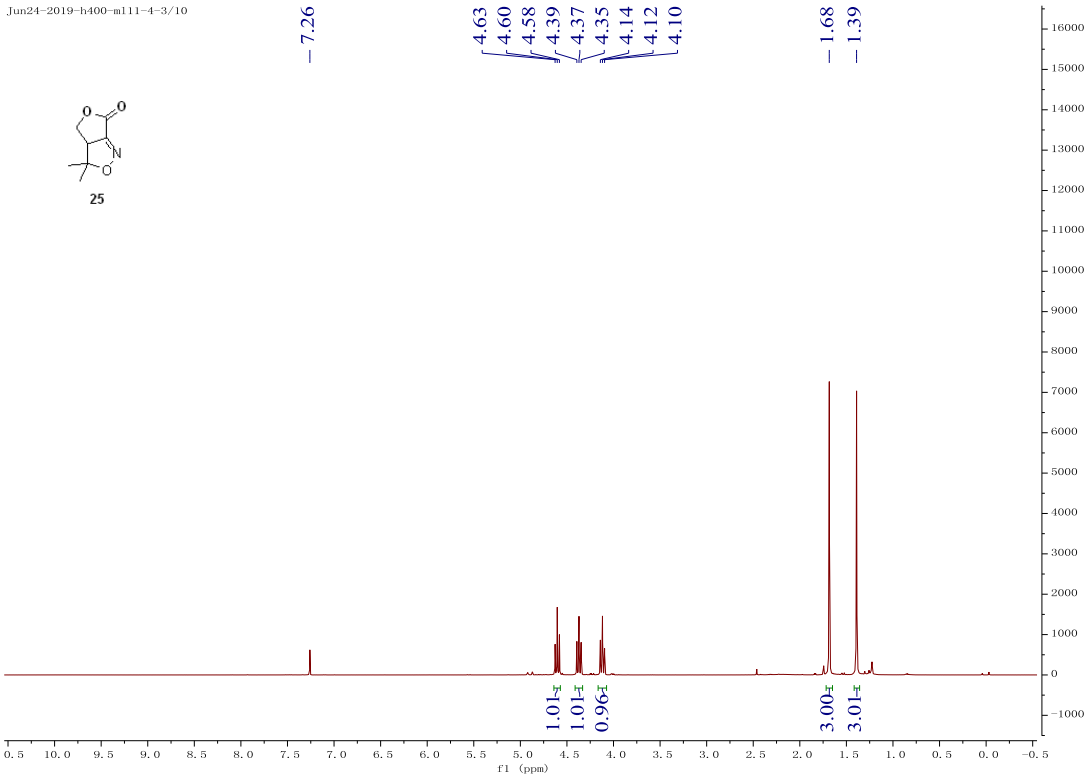

Jun12-2020-c400ML12-3U. 10. 1. 1
160.80
157.96
83.67
77.32
77.00
76.68
76.55
54.63
20.66
22
f1 (ppm)


7.26
5.74
5.71
5.70
5.70
5.68
4.71
4.69
4.67
4.65
4.63
4.62
4.60
4.59
4.58
4.56
4.30
4.28
4.26
4.24
4.03
4.01
4.00
3.98
2.14
2.14
2.13
2.13
2.12
2.12
2.11
2.11
2.10
2.10
2.09
2.09
2.08
2.08
2.08
2.04
2.02
2.01
23
2.14
2.02
1.00
0.97
5.06
1.04
1.05
f1 (ppm)

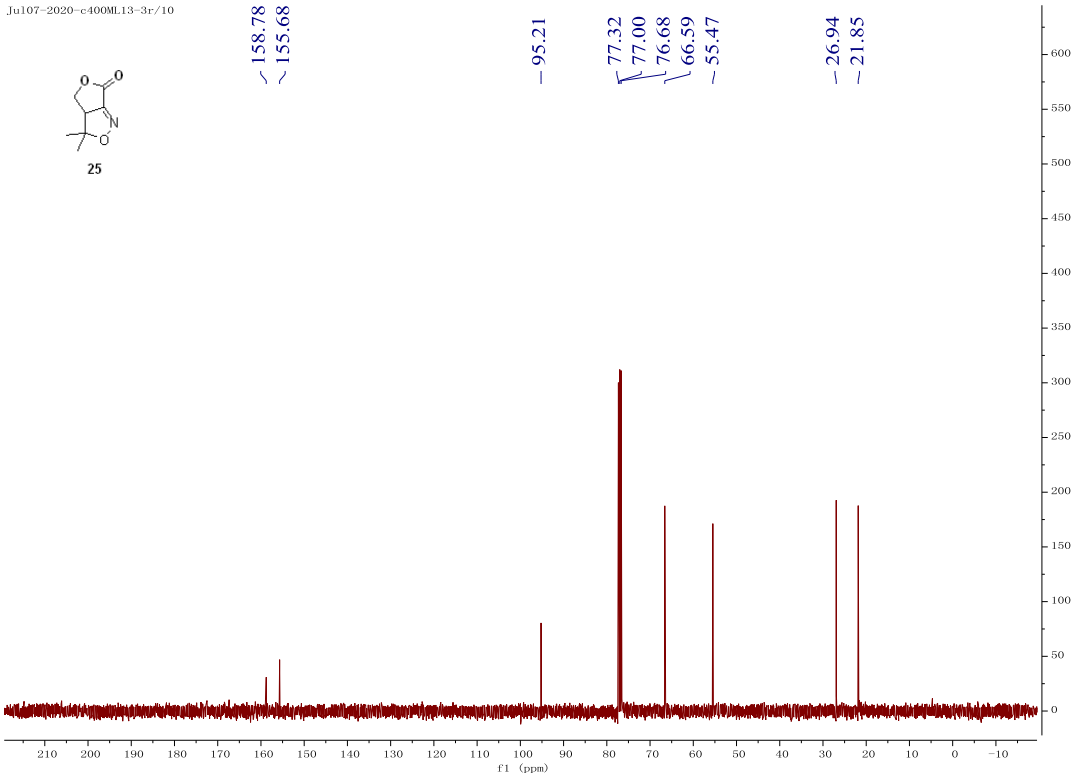

Jun19-2020-C400-ML12-3T/10
158.40
157.25
157.10
127.85
126.68
124.86
123.95
97.27
96.72
77.32
77.00
76.68
70.09
69.99
50.95
50.87
36.65
36.36
28.28
27.32
25.15
25.03
24.17
23.81
23
f1 (ppm)


Jun02-2020-h400-ML12-126-1/10
7.26
4.76
4.74
4.74
4.73
4.72
4.71
4.70
4.69
3.63
3.60
1.68
1.53
1.51
1.40
24
1.00
0.97
2.98
2.99
3.00
f1 (ppm)

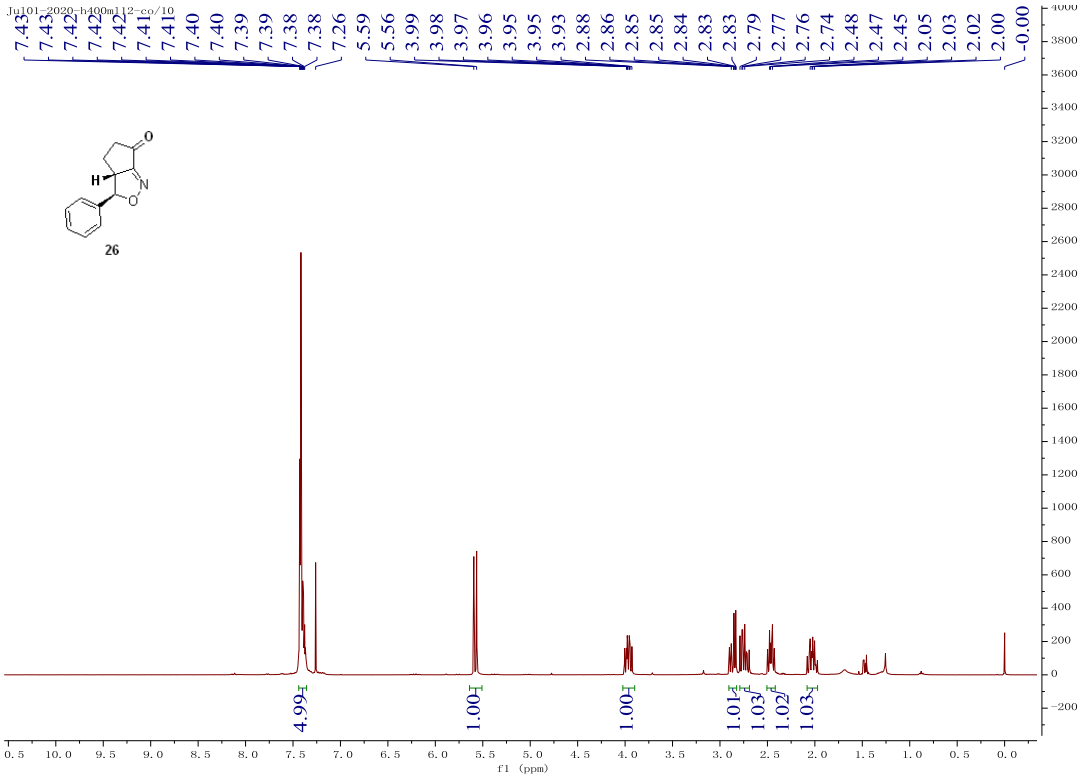

Jun02-2020-C400-ML12-126-1/10
158.56
157.01
94.06
77.32
77.00
76.68
76.32
63.26
27.52
22.01
20.94
24
f1 (ppm)

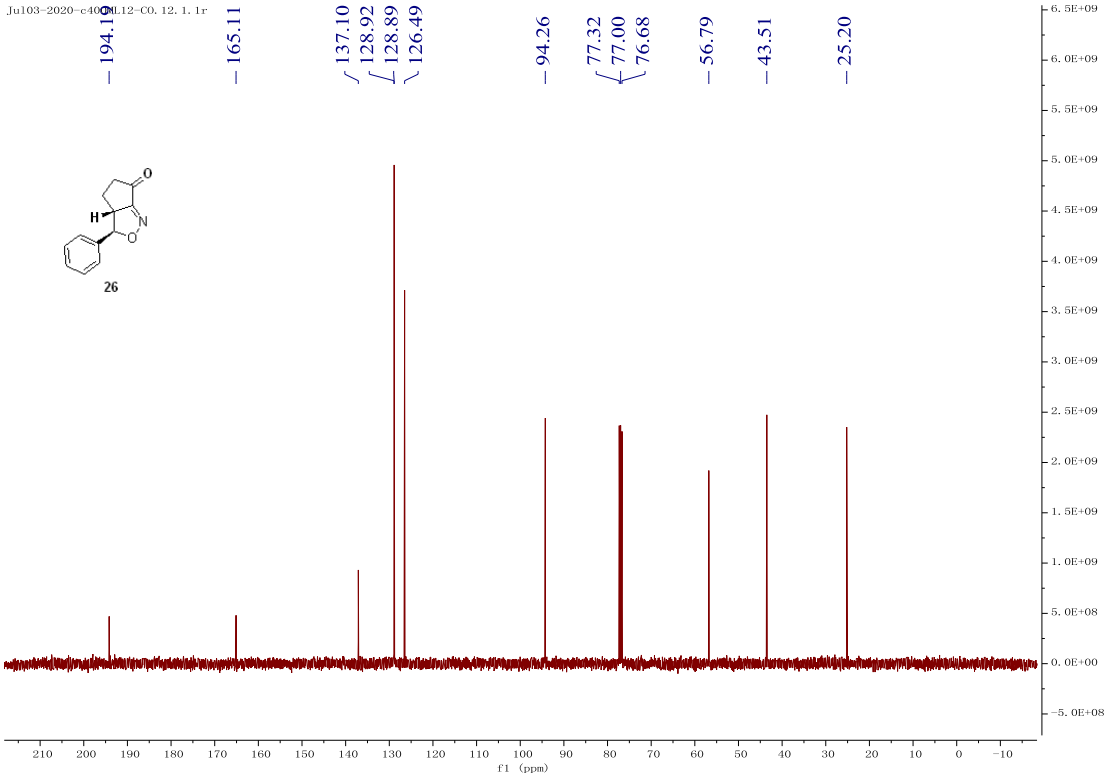

Jun24-2019-h400-m111-4-3/10
7.26
4.63
4.60
4.58
4.39
4.37
4.35
4.14
4.12
4.10
1.68
1.39
1.01
1.01
0.96
3.00
3.01
f1 (ppm)

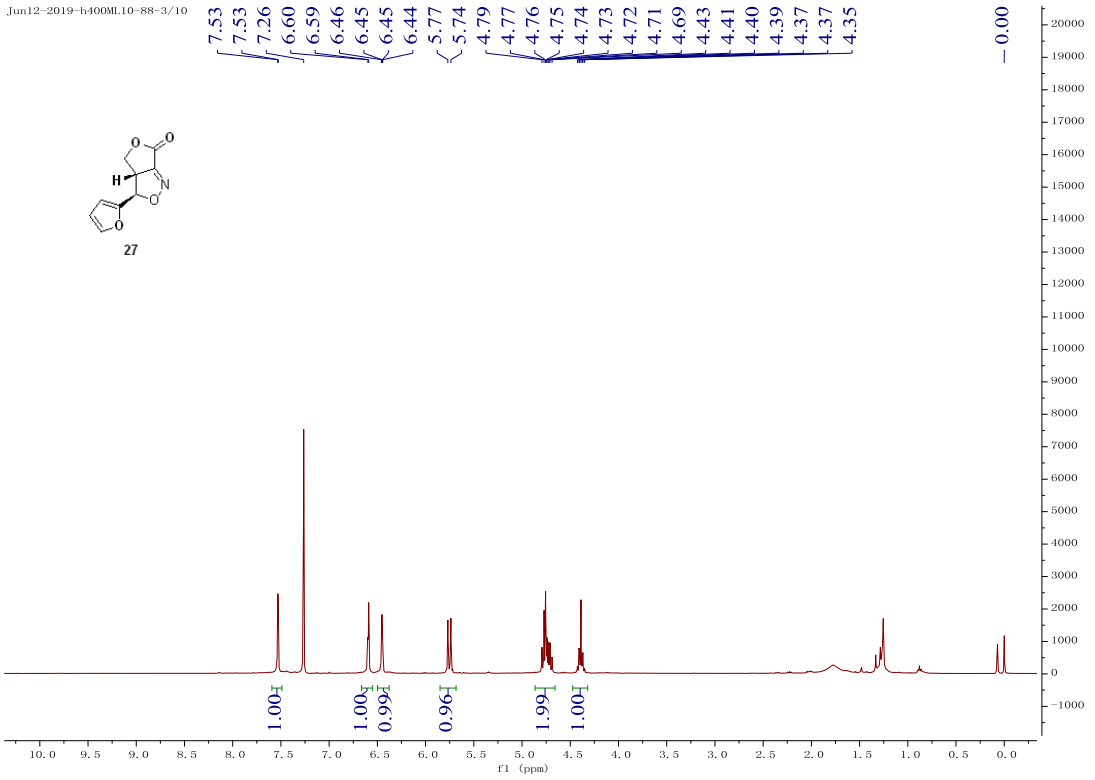
25

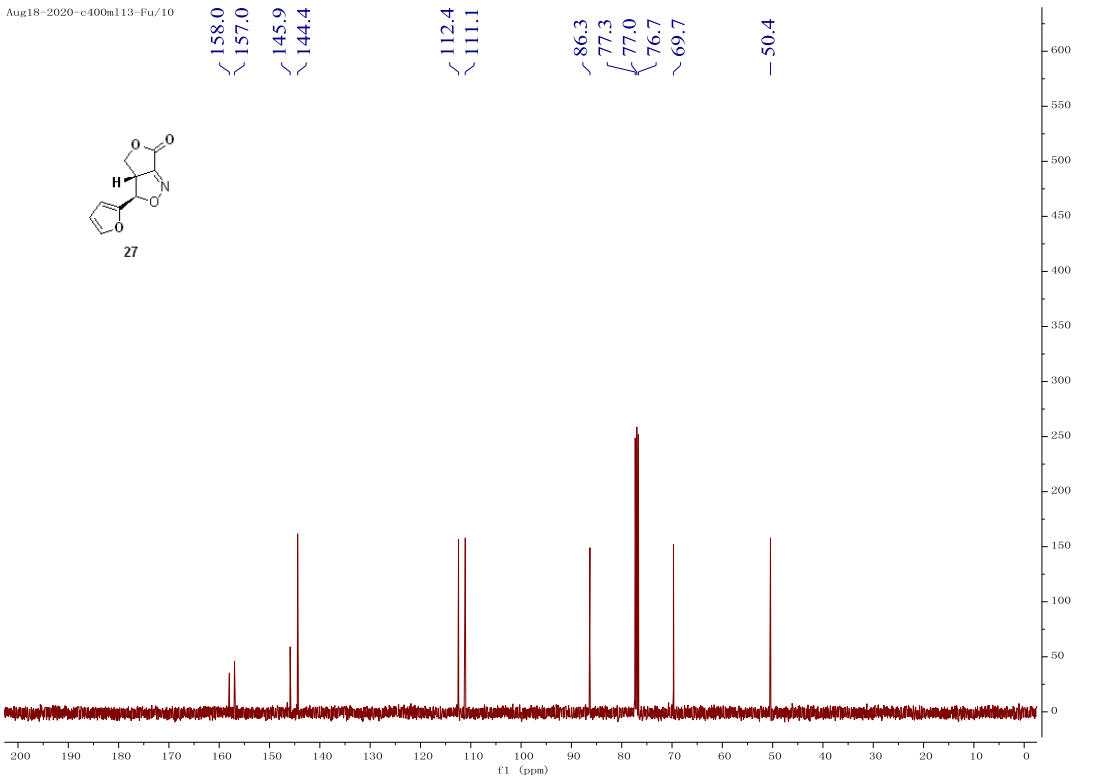

Ju107-2020-c400ML13-3r/10
158.78
155.68
95.21
77.32
77.00
76.68
66.59
55.47
26.94
21.85
f1 (ppm)

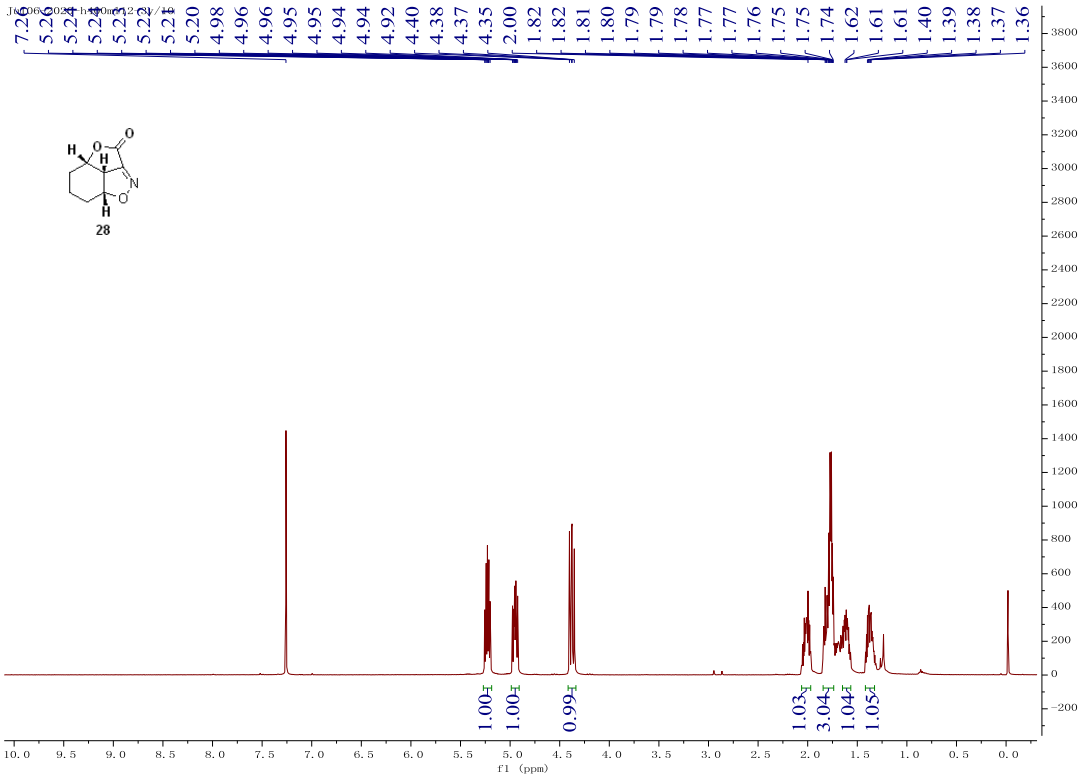
25

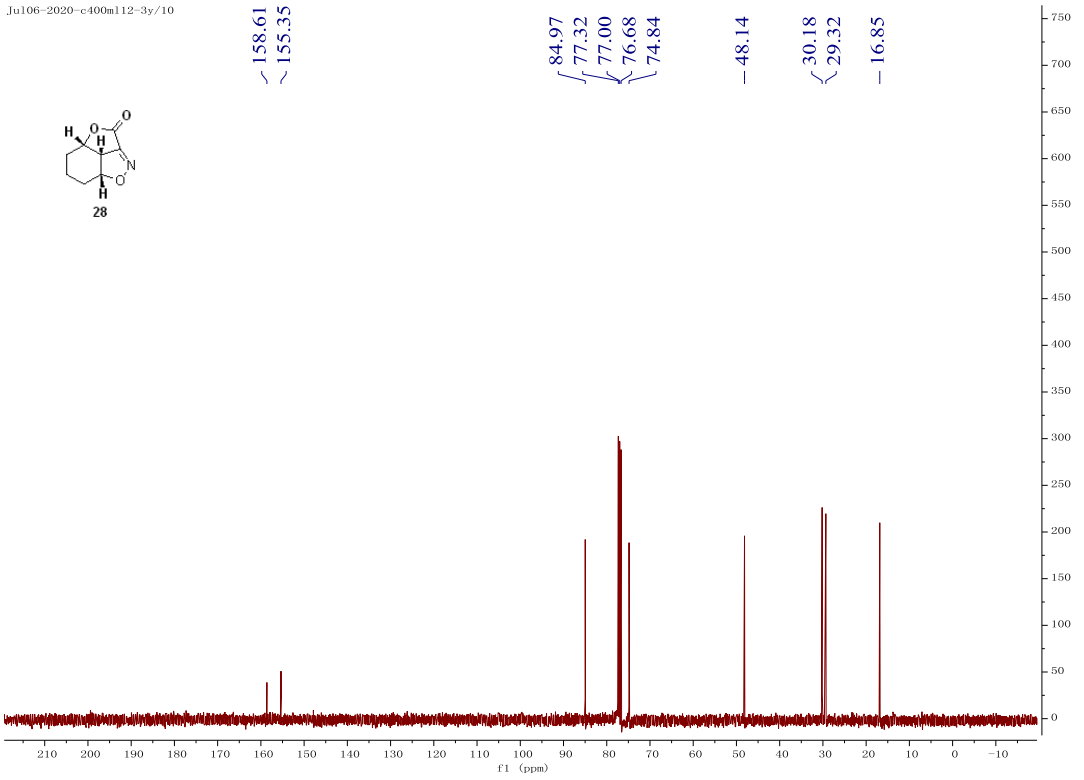

Ju101-2020-h400m112-co/10
7.43
7.43
7.42
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.26
5.59
5.56
3.99
3.98
3.97
3.96
3.95
3.95
3.93
2.88
2.86
2.85
2.85
2.84
2.83
2.83
2.79
2.77
2.76
2.74
2.48
2.47
2.45
2.05
2.03
2.02
2.00
-0.00
O
H
N
O
26
4.99
1.00
1.00
1.01
1.03
1.02
1.03
f1 (ppm)

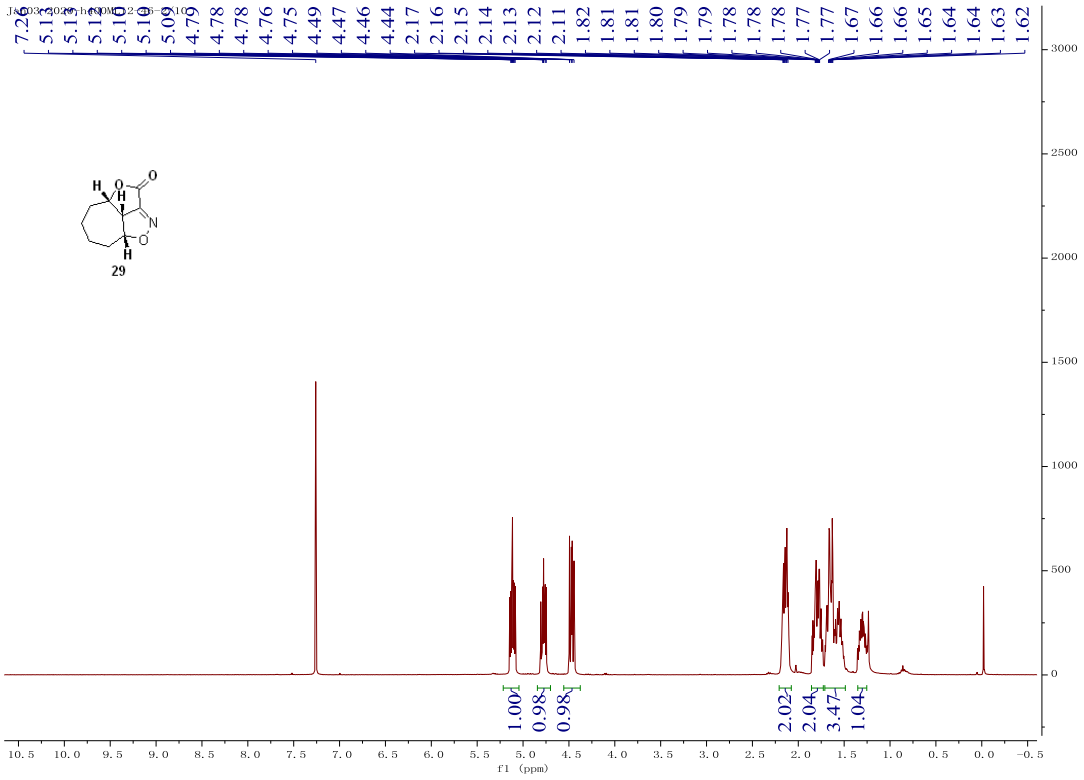

Ju103-2020-c400ML12-CO. 12. 1. 1r
194.19
165.11
137.10
128.92
128.89
126.49
94.26
77.32
77.00
76.68
56.79
43.51
25.20
O
H
N
O
26
f1 (ppm)

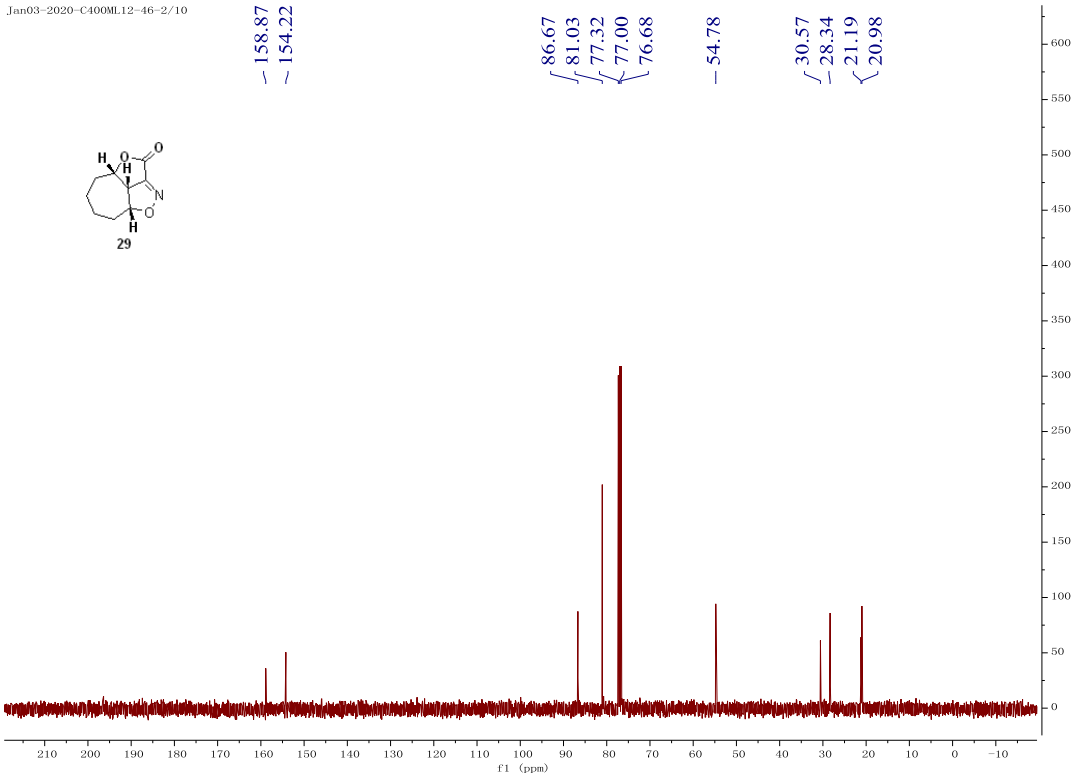

Jun12-2019-h400ML10-88-3/10
7.53
7.53
7.26
6.60
6.59
6.46
6.45
6.45
6.44
5.77
5.74
4.79
4.77
4.76
4.75
4.74
4.73
4.72
4.71
4.69
4.43
4.41
4.40
4.39
4.37
4.37
4.35
0.00
27
1.00
1.00
0.99
0.96
1.99
1.00
f1 (ppm)

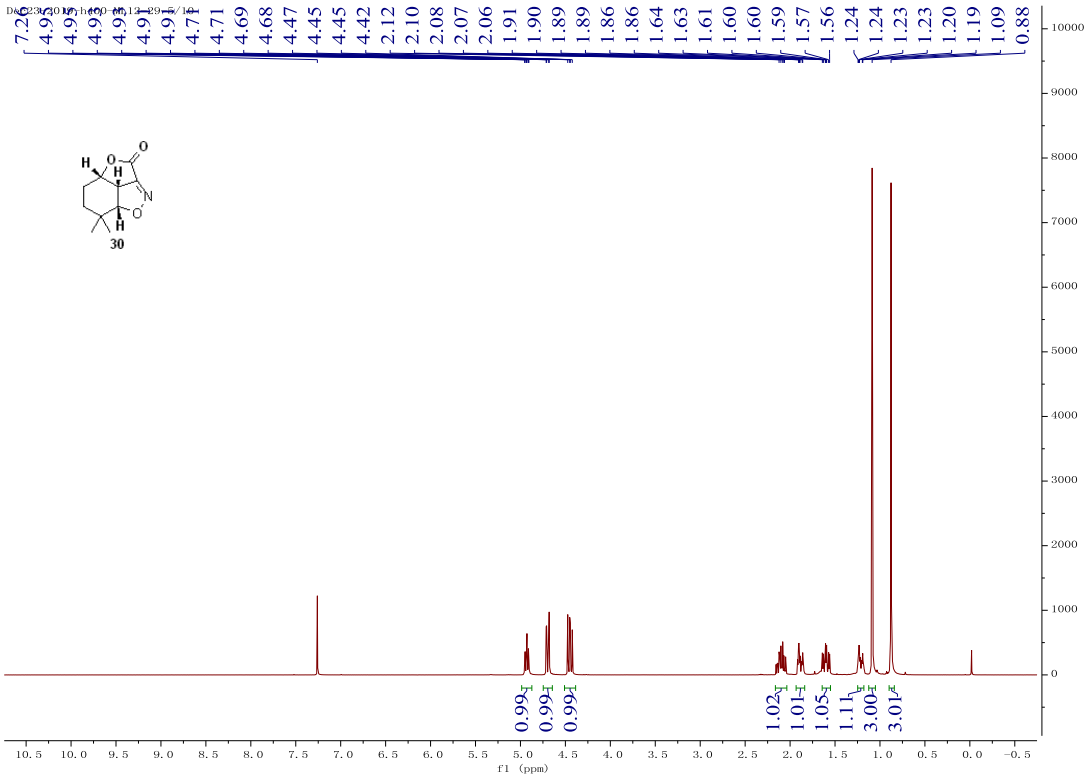

Aug18-2020-c400ml13-Fu/10
158.0
157.0
145.9
144.4
112.4
111.1
86.3
77.3
77.0
76.7
69.7
50.4
27
f1 (ppm)

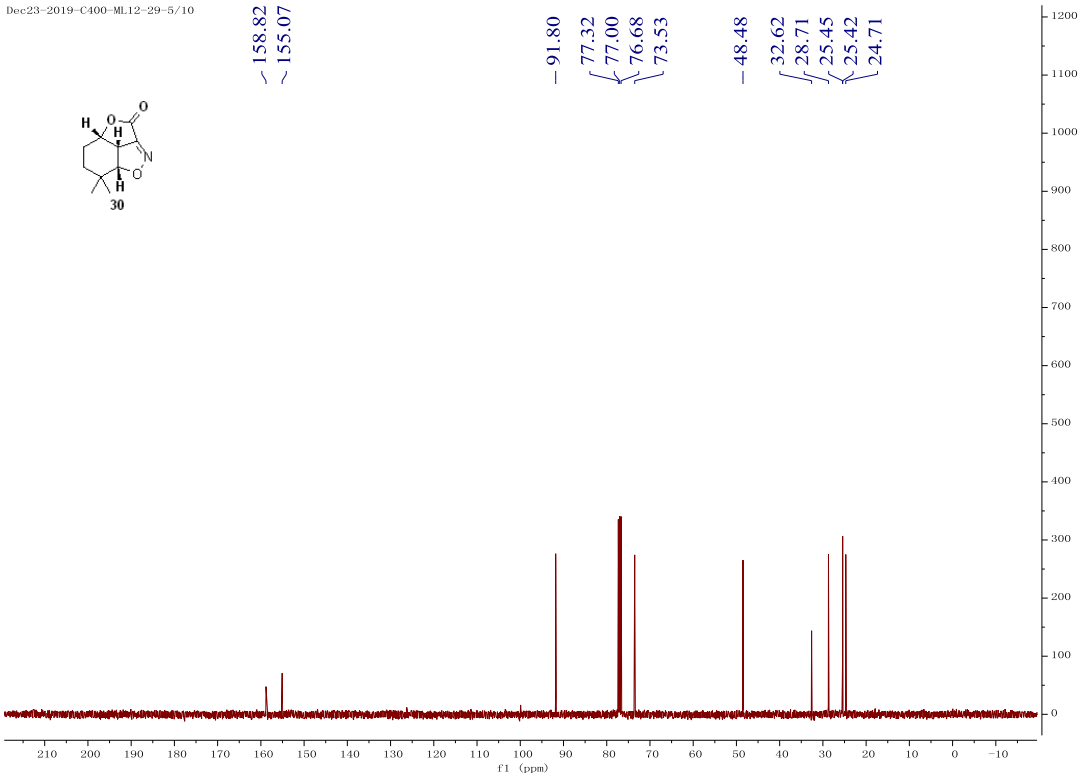

7.26
5.26
5.24
5.23
5.23
5.22
5.21
5.20
4.98
4.96
4.96
4.95
4.95
4.94
4.94
4.92
4.40
4.38
4.37
4.35
2.00
1.82
1.82
1.81
1.80
1.79
1.79
1.78
1.77
1.77
1.76
1.75
1.75
1.74
1.62
1.61
1.61
1.40
1.39
1.38
1.37
1.36
28
1.00
1.00
0.99
1.03
3.04
1.04
1.05
f1 (ppm)

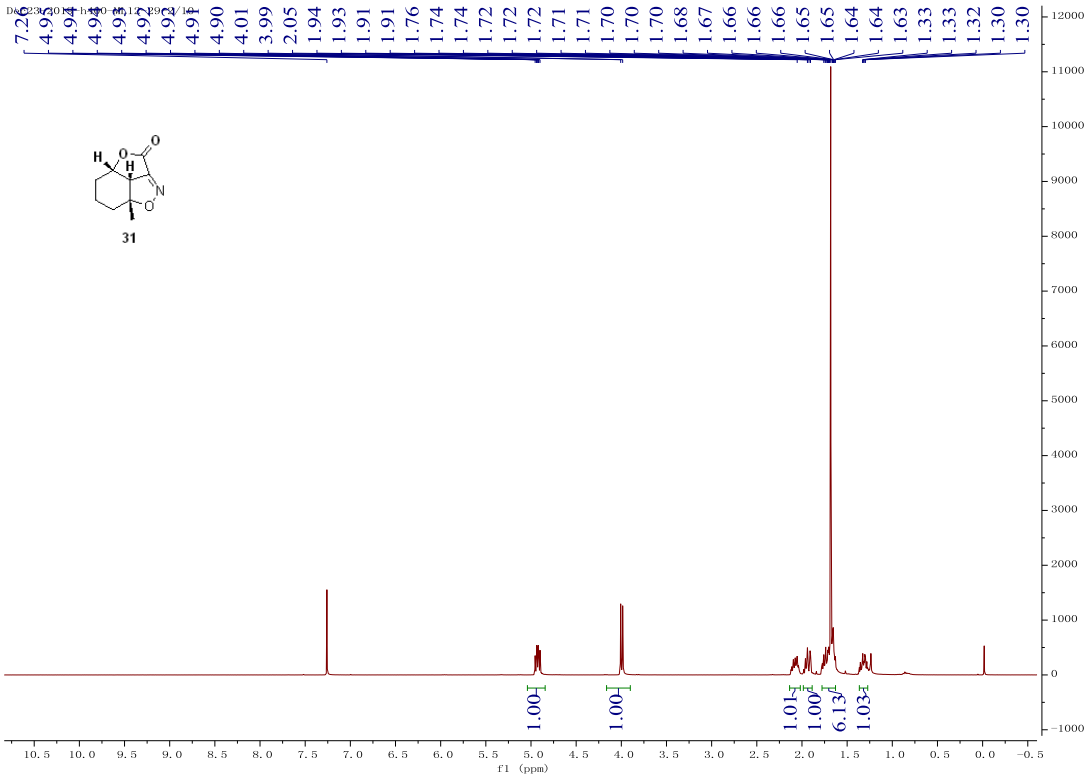

Ju106-2020-c400m112-3y/10
158.61
155.35
84.97
77.32
77.00
76.68
74.84
48.14
30.18
29.32
16.85
28
f1 (ppm)


7.26
5.13
5.12
5.12
5.10
5.10
5.09
4.79
4.78
4.78
4.76
4.75
4.49
4.47
4.46
4.44
2.17
2.16
2.15
2.14
2.13
2.12
2.11
1.82
1.81
1.81
1.80
1.79
1.79
1.78
1.78
1.78
1.77
1.77
1.67
1.66
1.66
1.65
1.64
1.64
1.63
1.62
29
1.00
0.98
0.98
2.02
2.04
3.47
1.04
f1 (ppm)

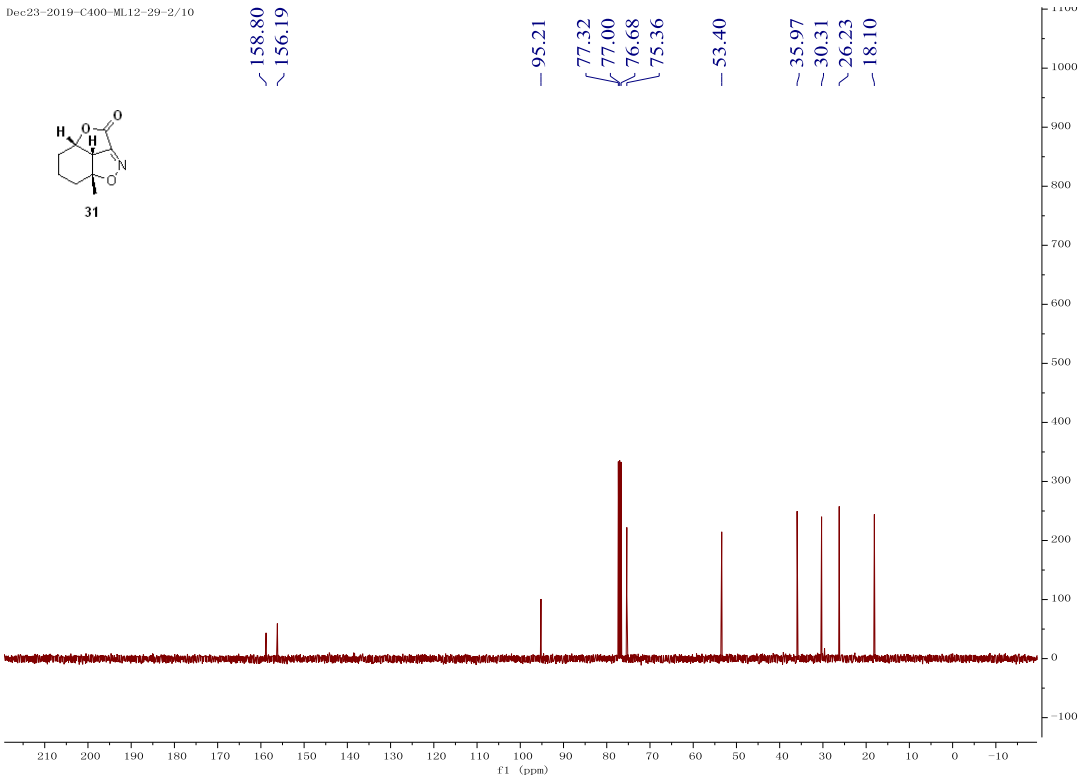

Jan03-2020-C400ML12-46-2/10
158.87
154.22
86.67
81.03
77.32
77.00
76.68
54.78
30.57
28.34
21.19
20.98
29
f1 (ppm)


7.26
4.93
4.93
4.93
4.92
4.91
4.91
4.71
4.71
4.69
4.68
4.47
4.45
4.45
4.42
2.12
2.10
2.08
2.07
2.06
1.91
1.90
1.89
1.89
1.86
1.86
1.64
1.63
1.61
1.60
1.60
1.59
1.57
1.56
1.24
1.24
1.23
1.23
1.20
1.19
1.09
0.88
30
0.99
0.99
0.99
1.02
1.01
1.05
1.11
3.00
3.01
f1 (ppm)

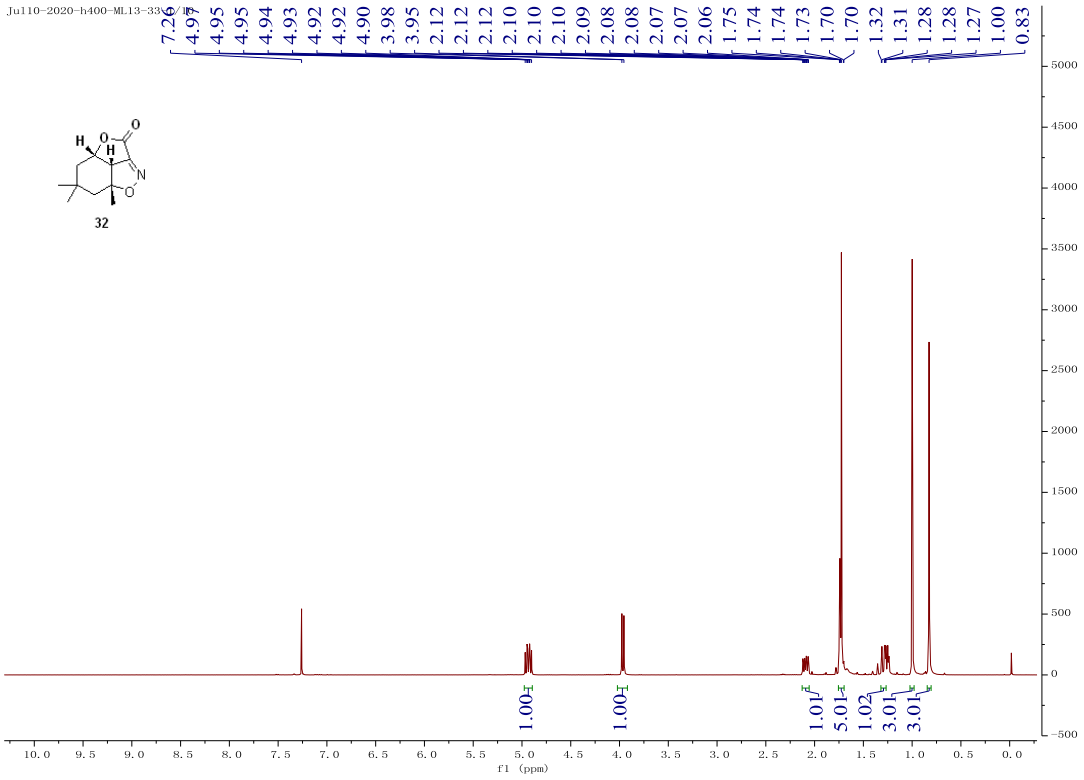

Dec23-2019-C400-ML12-29-5/10
158.82
155.07
91.80
77.32
77.00
76.68
73.53
48.48
32.62
28.71
25.45
25.42
24.71
30
f1 (ppm)

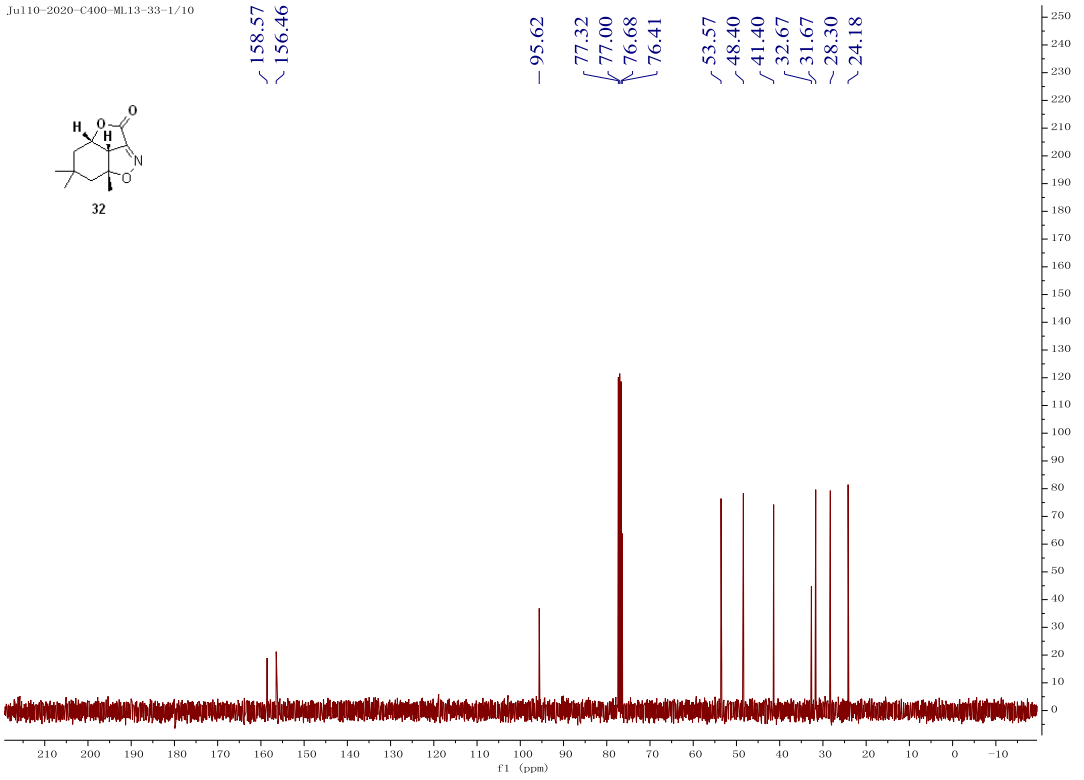

7.26
4.93
4.93
4.93
4.92
4.92
4.92
4.91
4.91
4.90
4.01
3.99
2.05
1.94
1.93
1.91
1.91
1.76
1.74
1.74
1.72
1.72
1.72
1.71
1.71
1.70
1.70
1.70
1.68
1.67
1.66
1.66
1.66
1.65
1.65
1.64
1.64
1.63
1.33
1.33
1.32
1.30
1.30
1.00
1.00
1.01
1.00
6.13
1.03
f1 (ppm)

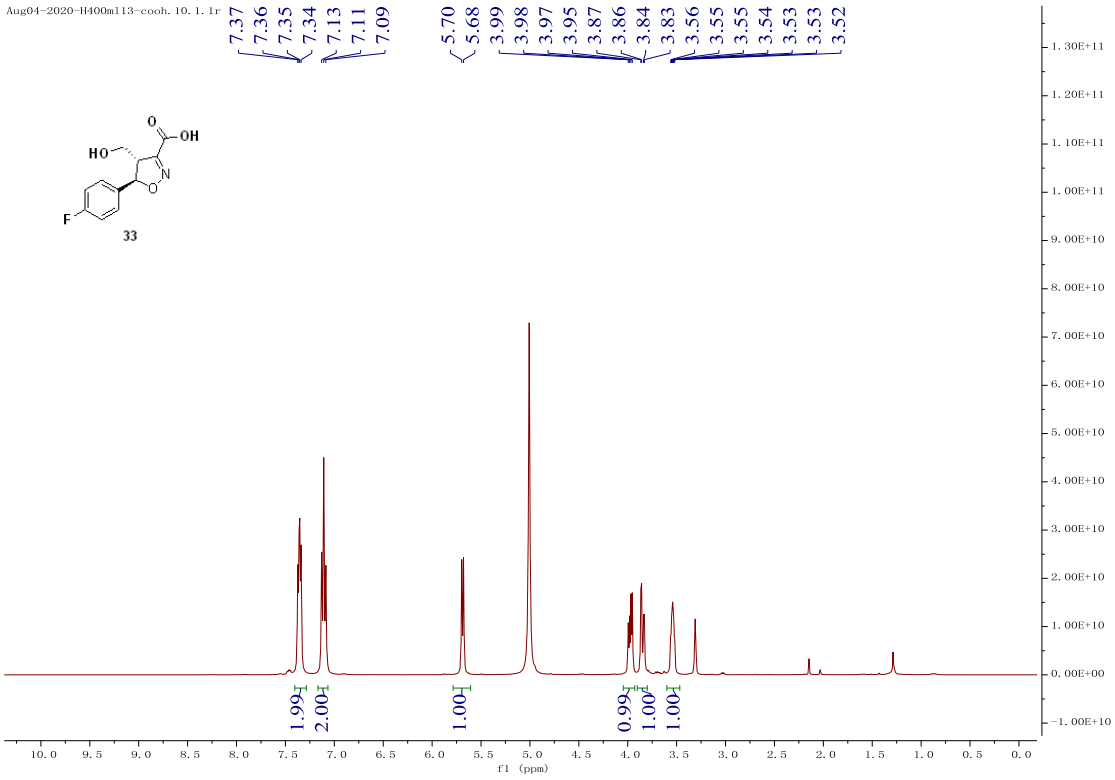
31

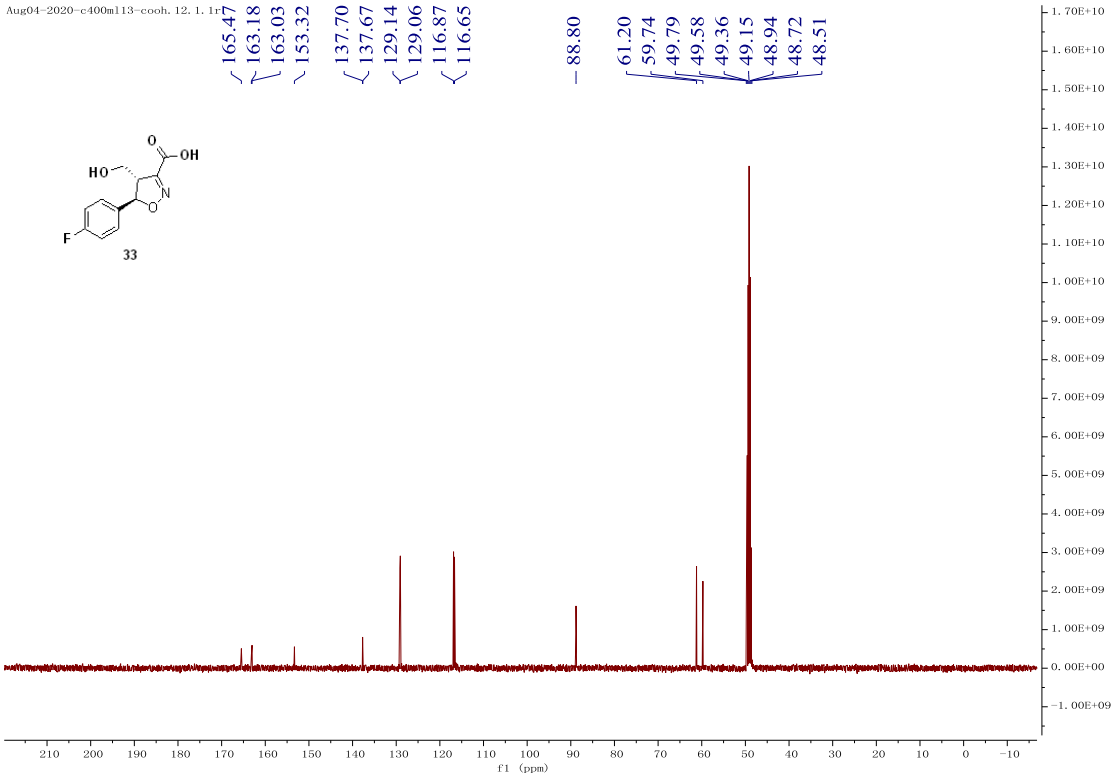

Dec23-2019-C400-ML12-29-2/10
158.80
156.19
95.21
77.32
77.00
76.68
75.36
53.40
35.97
30.31
26.23
18.10
f1 (ppm)

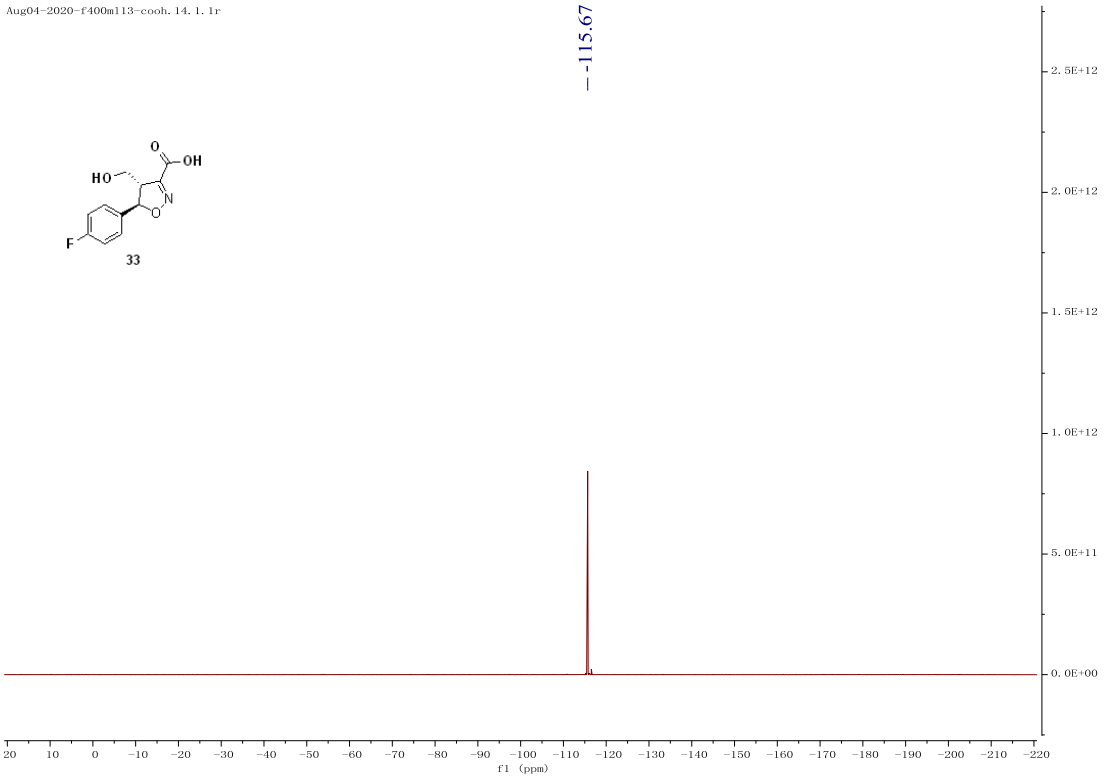
31

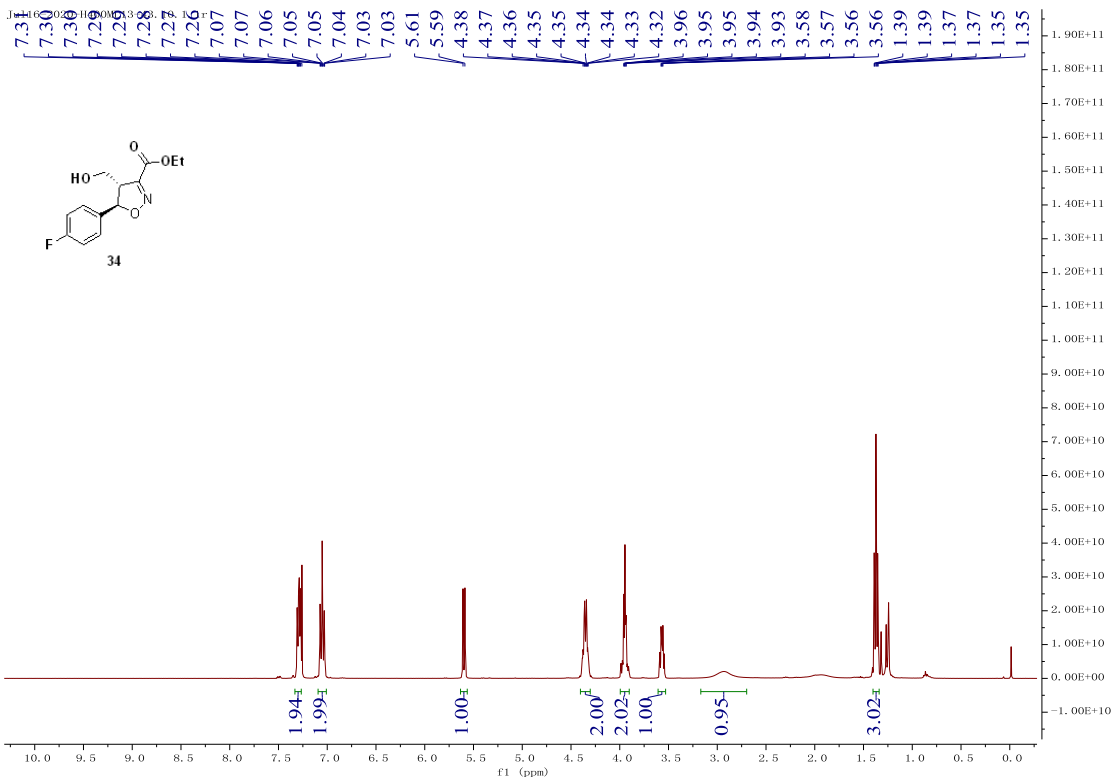

Jul10-2020-h400-ML13-33-1/10
7.26
4.97
4.95
4.95
4.94
4.93
4.92
4.92
4.90
3.98
3.95
2.12
2.12
2.12
2.10
2.10
2.10
2.09
2.08
2.08
2.07
2.07
2.06
1.75
1.74
1.74
1.73
1.70
1.70
1.32
1.31
1.28
1.28
1.27
1.00
0.83
32
1.00
1.00
1.01
5.01
1.02
3.01
3.01
f1 (ppm)

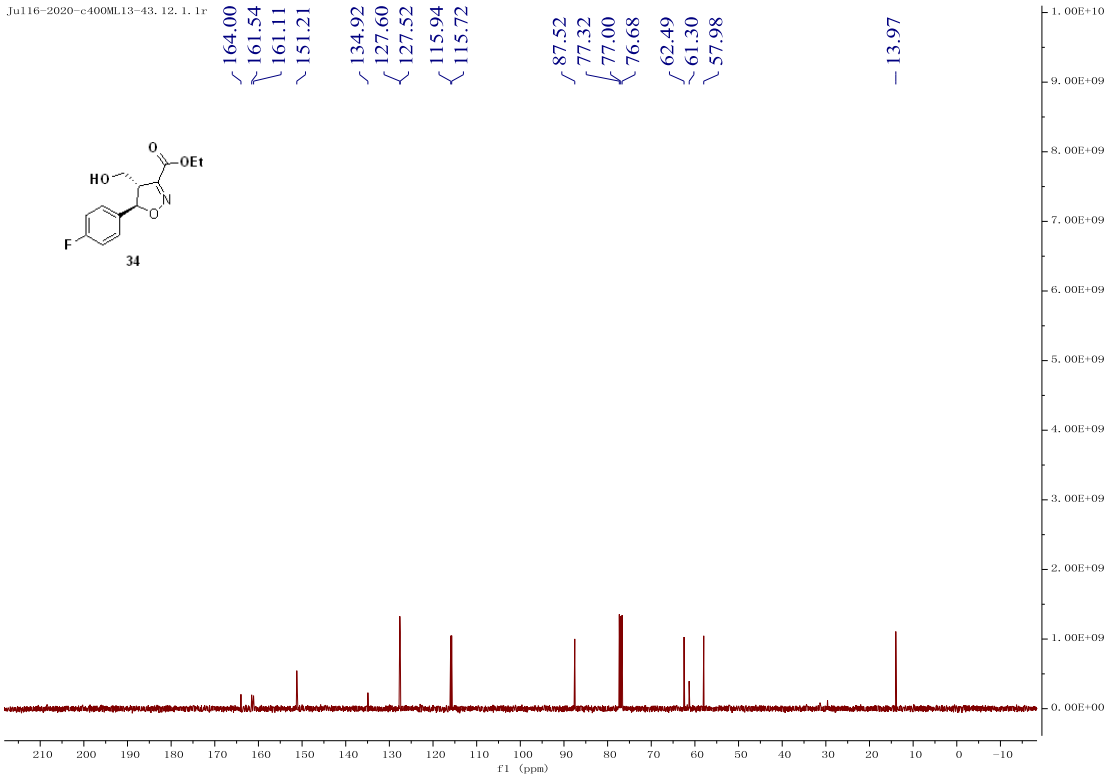

Jul10-2020-C400-ML13-33-1/10
158.57
156.46
95.62
77.32
77.00
76.68
76.41
53.57
48.40
41.40
32.67
31.67
28.30
24.18
32
f1 (ppm)

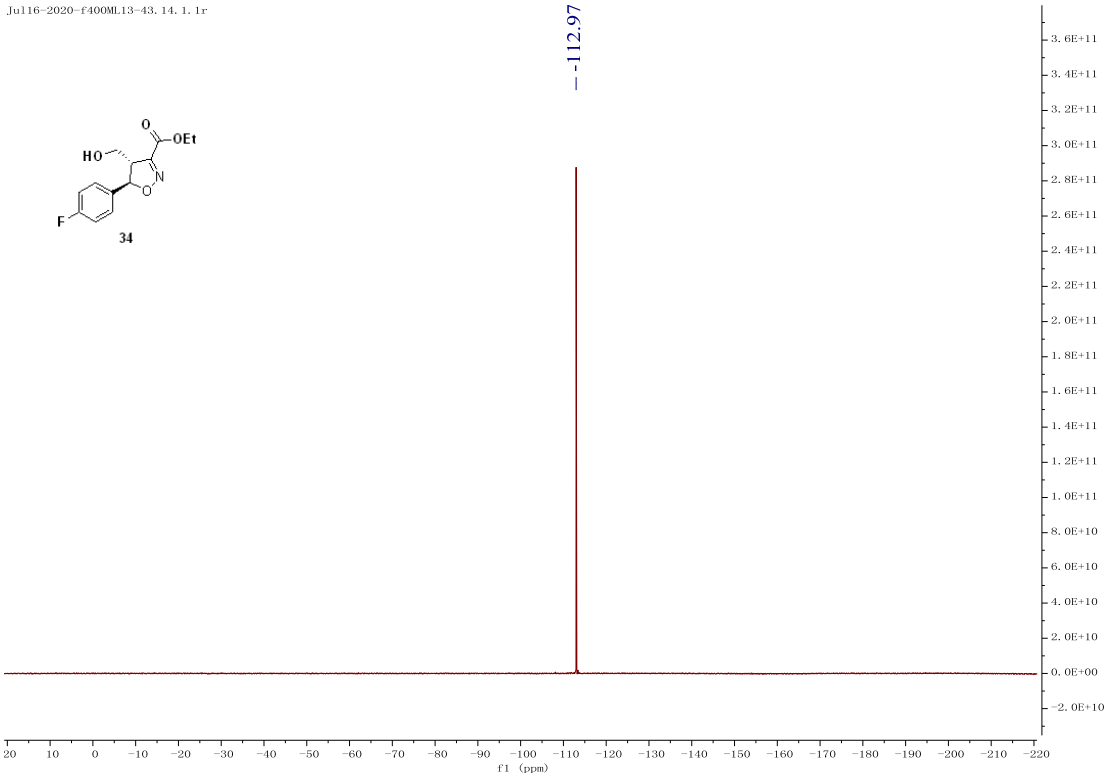

Aug04-2020-H400m113-cooh. 10. 1. 1r
7.37
7.36
7.35
7.34
7.13
7.11
7.09
5.70
5.68
3.99
3.98
3.97
3.95
3.87
3.86
3.84
3.83
3.56
3.55
3.55
3.54
3.53
3.53
3.52
HO
O
OH
N
O
F
33
1.99
2.00
1.00
0.99
1.00
1.00
f1 (ppm)

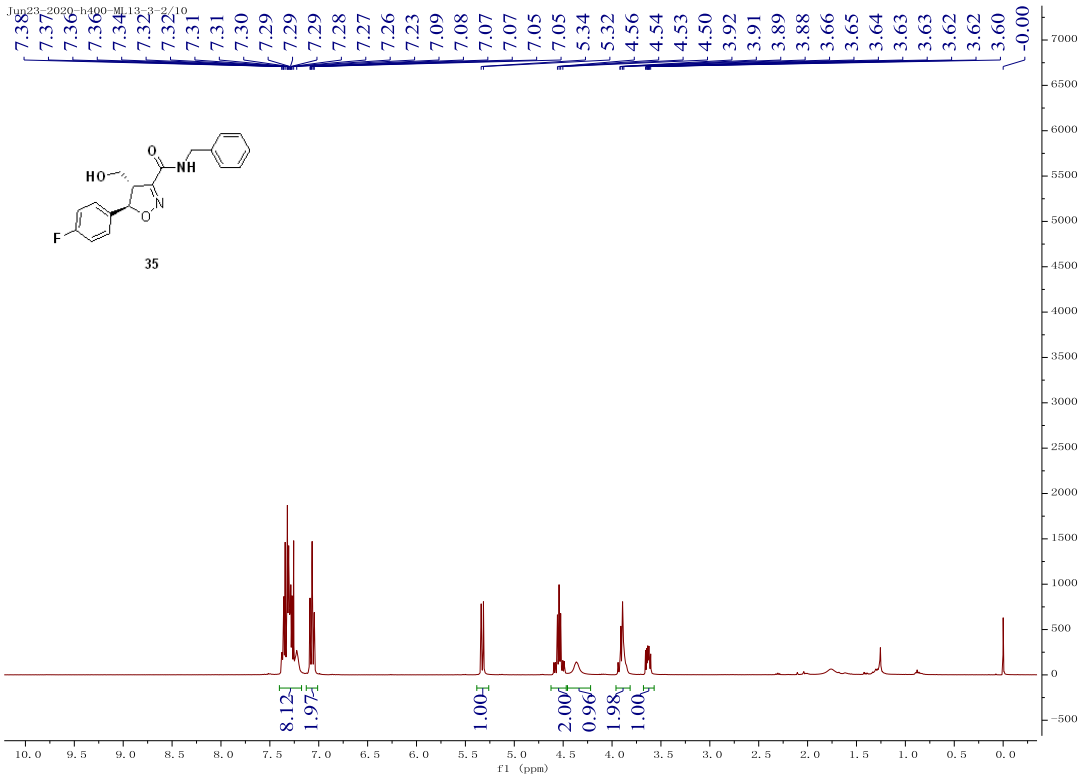

Aug04-2020-c400m113-cooh. 12. 1. 1r
165.47
163.18
163.03
153.32
137.70
137.67
129.14
129.06
116.87
116.65
88.80
61.20
59.74
49.79
49.58
49.36
49.15
48.94
48.72
48.51
HO
O
OH
N
O
F
33
f1 (ppm)

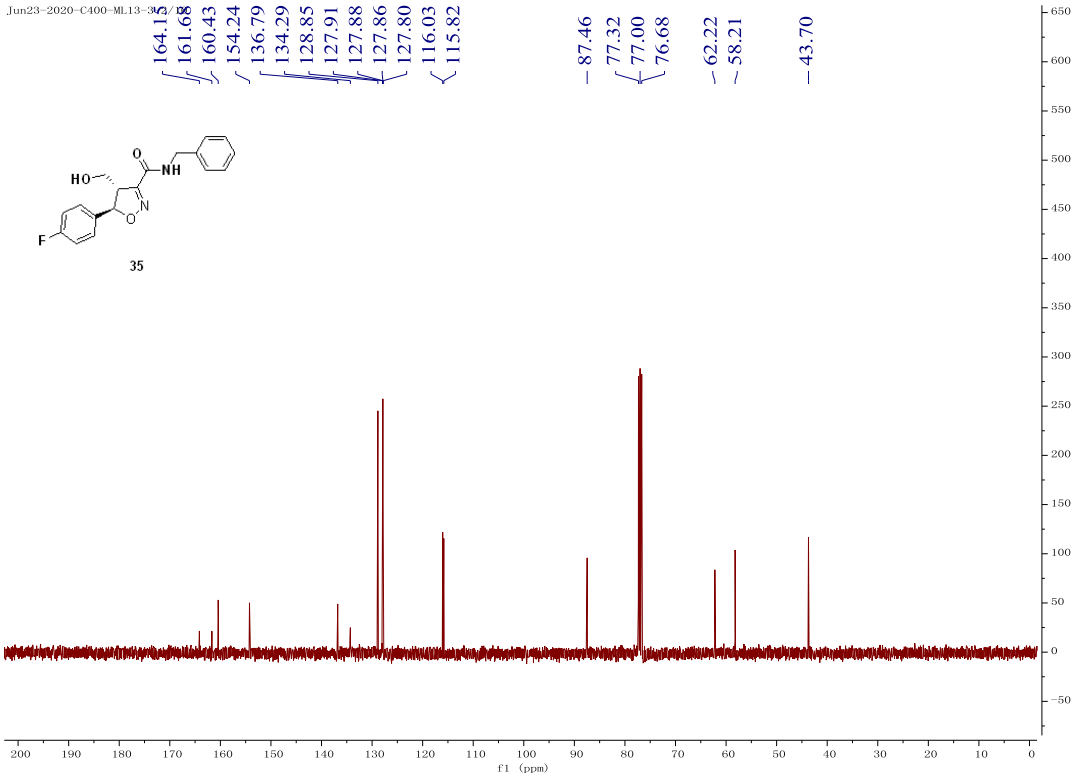

Aug04-2020-f400m113-cooh.14.1.1r
-115.67
HO
O
OH
N
O
F
33
2.5E+12
2.0E+12
1.5E+12
1.0E+12
5.0E+11
0.0E+00
f1 (ppm)

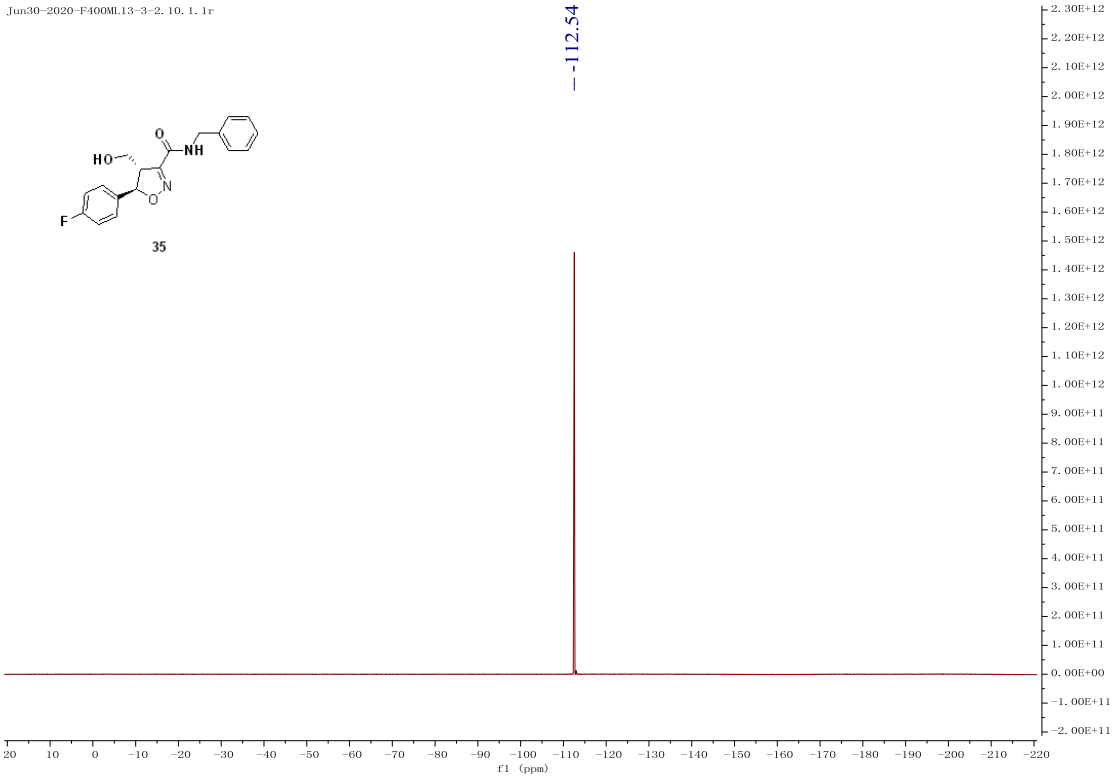

7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.26
7.07
7.07
7.06
7.05
7.05
7.04
7.03
7.03
5.61
5.59
4.38
4.37
4.36
4.35
4.35
4.34
4.34
4.33
4.32
3.96
3.95
3.95
3.94
3.93
3.58
3.57
3.56
3.56
1.39
1.39
1.37
1.37
1.35
1.35
HO
O
OEt
N
O
F
34
1.94
1.99
1.00
2.00
2.02
1.00
0.95
3.02
f1 (ppm)

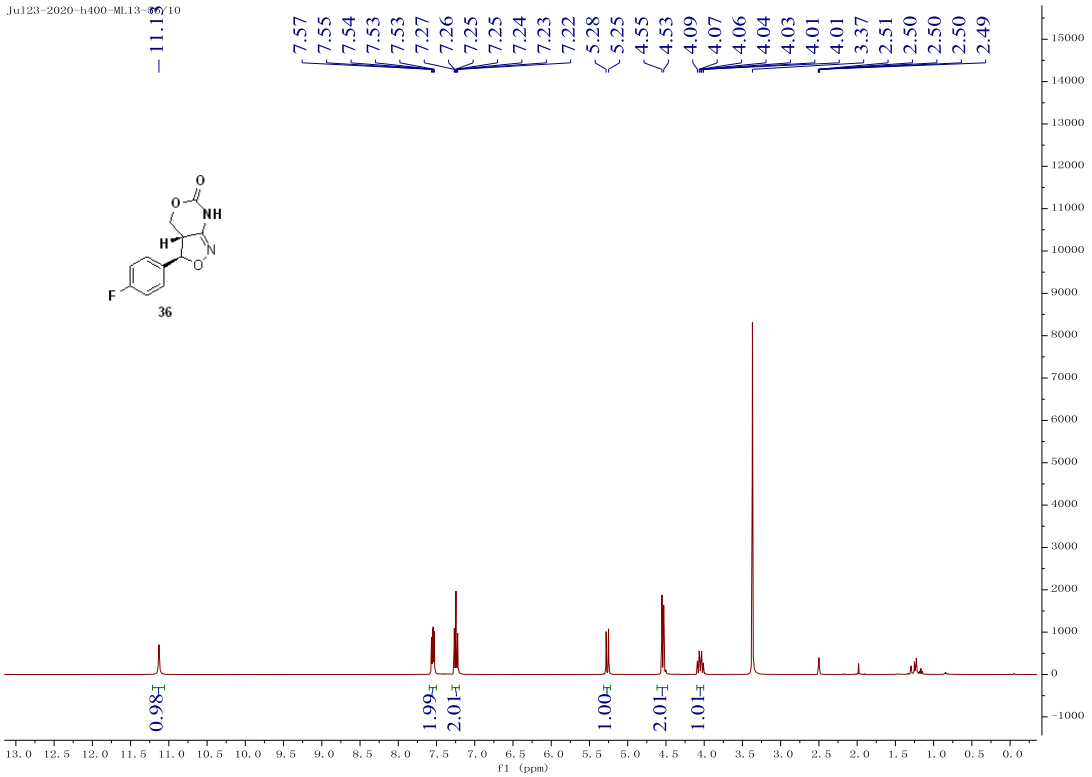

Jul16-2020-c400ML13-43.12.1.1r
164.00
161.54
161.11
151.21
134.92
127.60
127.52
115.94
115.72
87.52
77.32
77.00
76.68
62.49
61.30
57.98
13.97
HO
O
OEt
N
O
F
34
f1 (ppm)

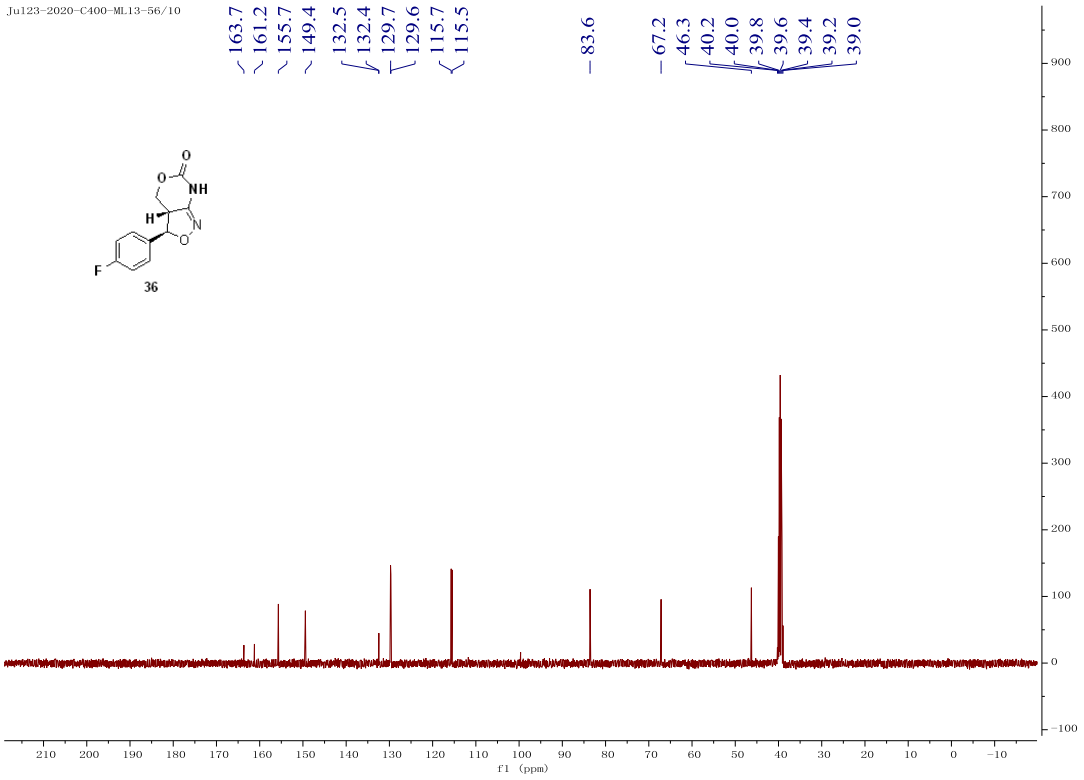

Jul16-2020-f400ML13-43.14.1.1r
-112.97
HO
O
OEt
N
O
F
34
f1 (ppm)

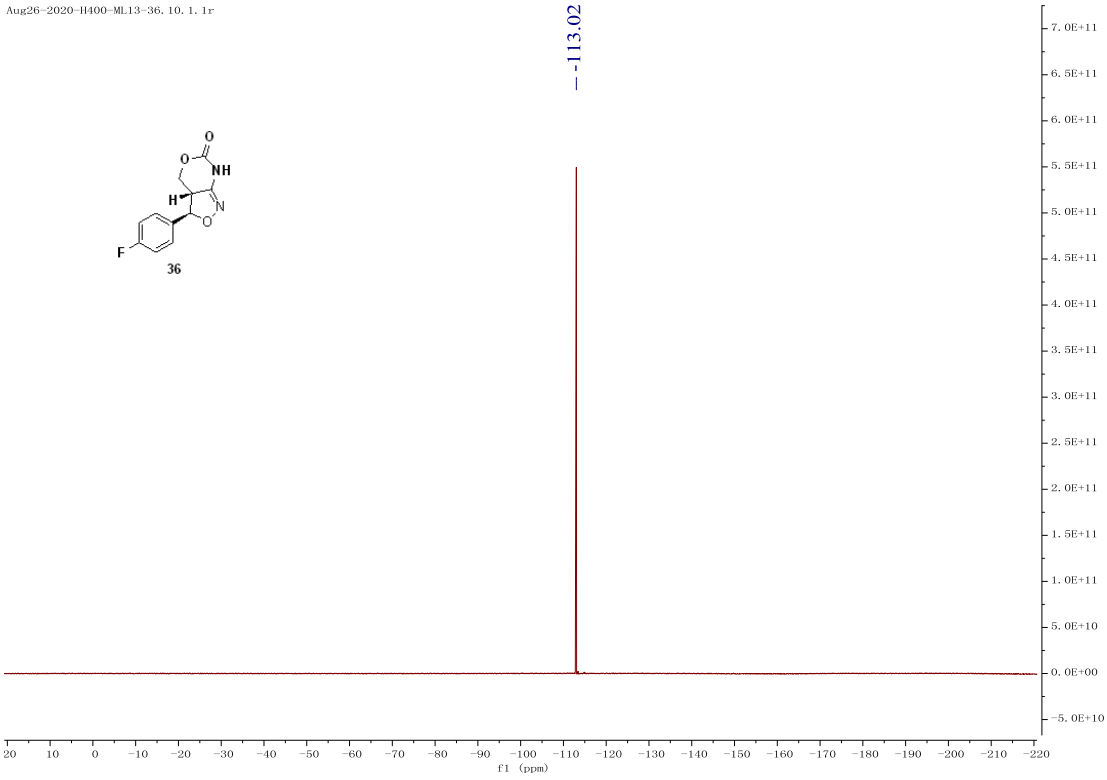

Jun23-2020-h400-ML13-3-2/10
7.38
7.37
7.36
7.36
7.34
7.32
7.32
7.31
7.31
7.30
7.29
7.29
7.29
7.28
7.27
7.26
7.23
7.09
7.08
7.07
7.07
7.05
7.05
5.34
5.32
4.56
4.54
4.53
4.50
3.92
3.91
3.89
3.88
3.66
3.65
3.64
3.63
3.63
3.62
3.62
3.60
-0.00
HO
O
NH
N
O
F
35
8.12
1.97
1.00
2.00
0.96
1.98
1.00
f1 (ppm)

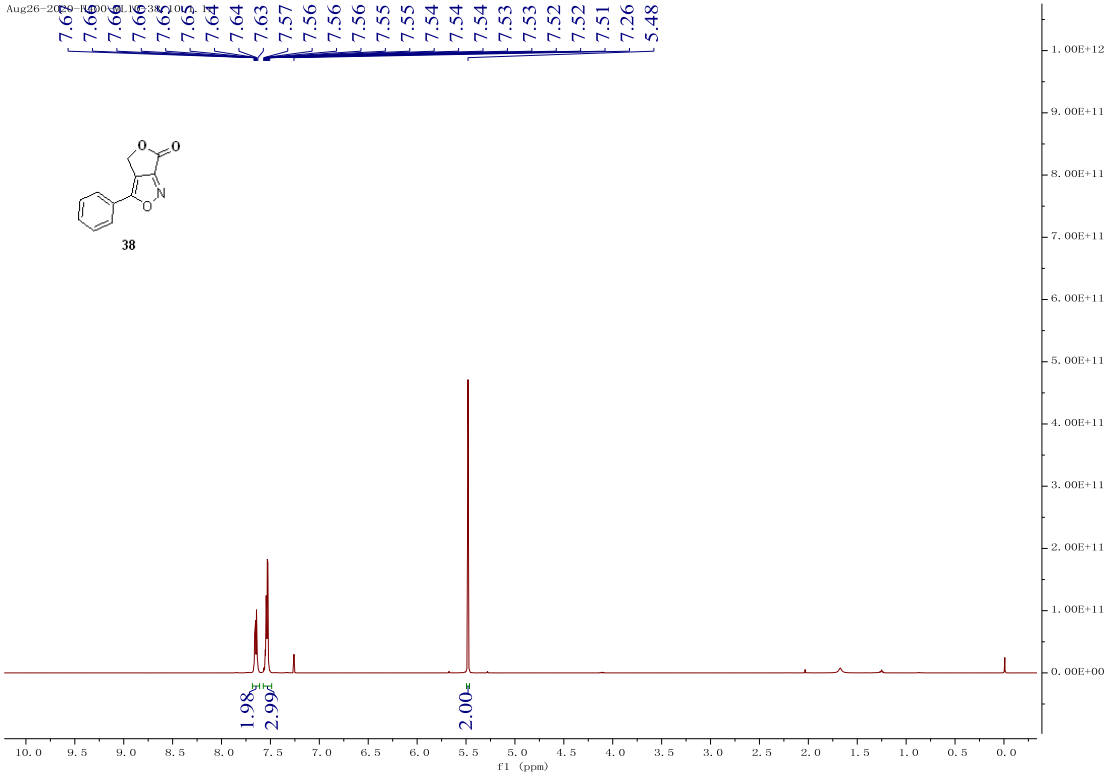

Jun23-2020-C400-ML13-3
164.15
161.68
160.43
154.24
136.79
134.29
128.85
127.91
127.88
127.86
127.80
116.03
115.82
87.46
77.32
77.00
76.68
62.22
58.21
43.70
HO
O
NH
N
O
F
35
f1 (ppm)

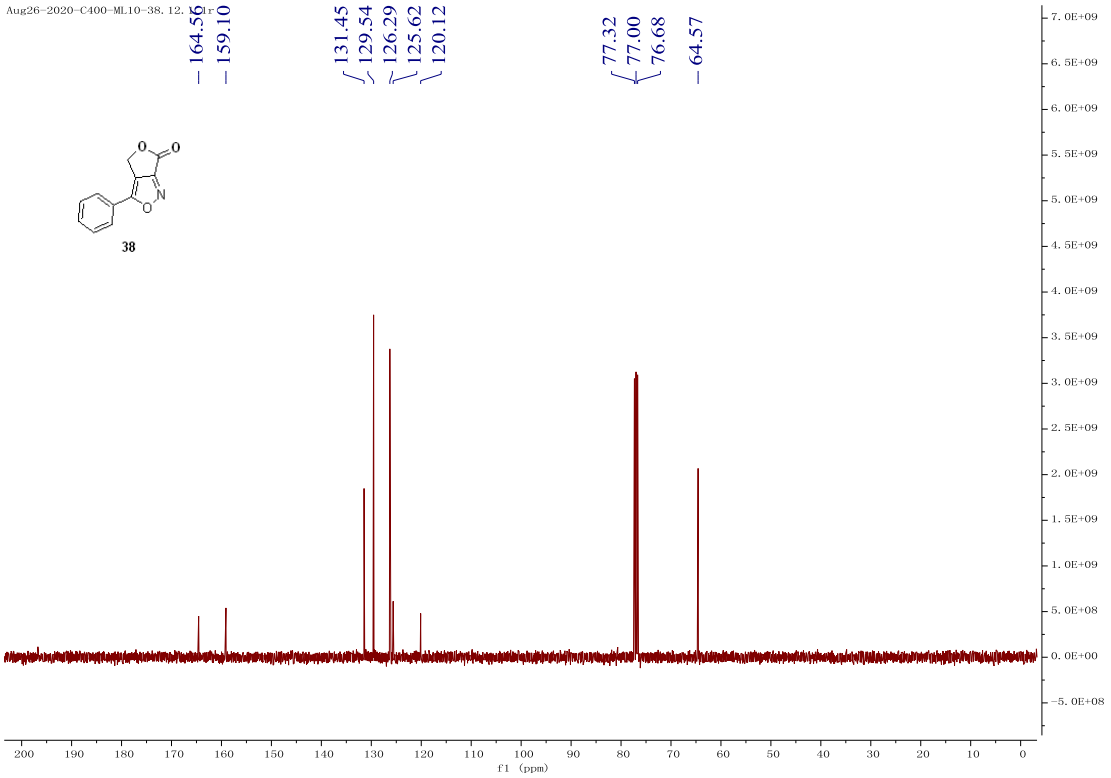

Jun30-2020-F400ML13-3-2. 10. 1. 1r
-112.54
HO
O
NH
N
O
F
35
f1 (ppm)

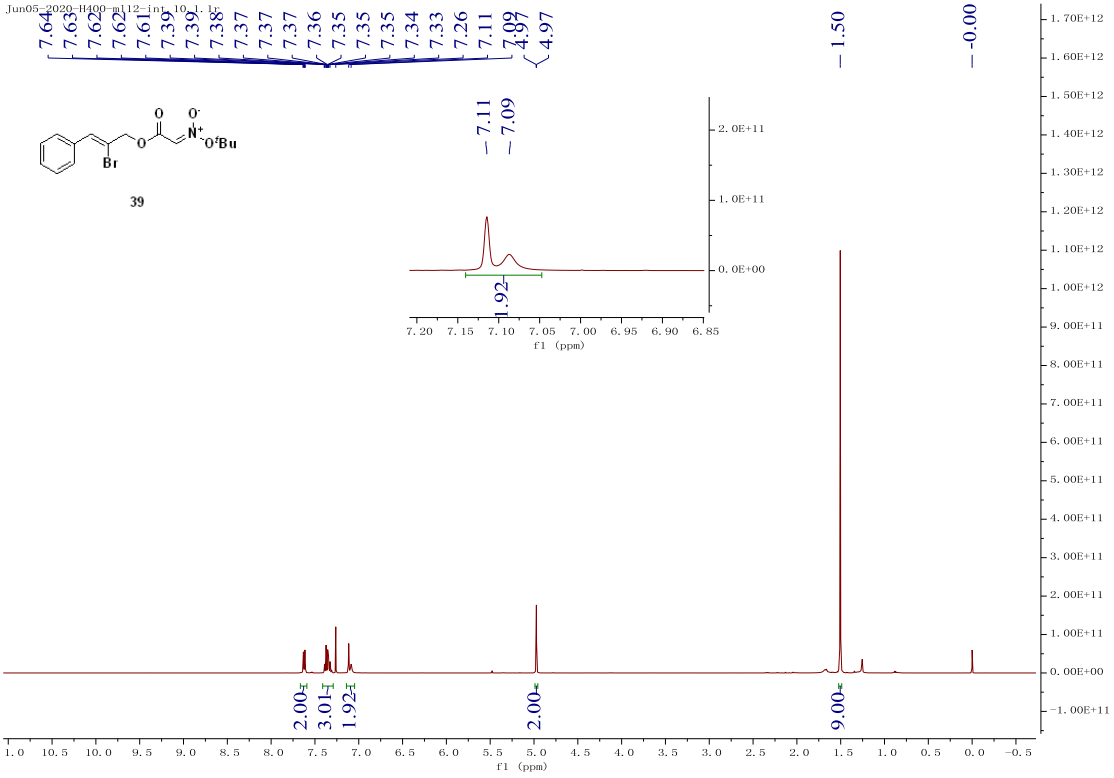

Ju123-2020-h400-ML13-
11.13
7.57
7.55
7.54
7.53
7.53
7.27
7.26
7.25
7.25
7.24
7.23
7.22
5.28
5.25
4.55
4.53
4.09
4.07
4.06
4.04
4.03
4.01
4.01
3.37
2.51
2.50
2.50
2.50
2.49
O
O
NH
H
N
O
F
36
0.98
1.99
2.01
1.00
2.01
1.01
f1 (ppm)

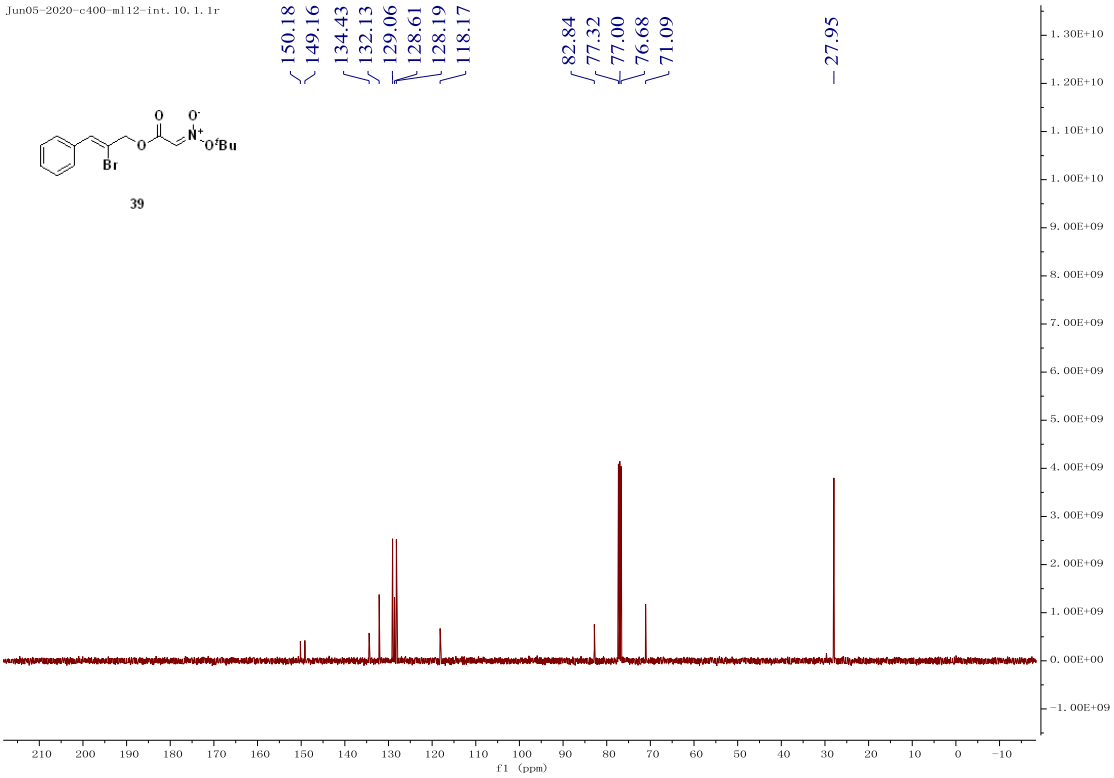

Ju123-2020-C400-ML13-56/10
163.7
161.2
155.7
149.4
132.5
132.4
129.7
129.6
115.7
115.5
83.6
67.2
46.3
40.2
40.0
39.8
39.6
39.4
39.2
39.0
O
O
NH
H
N
O
F
36
f1 (ppm)

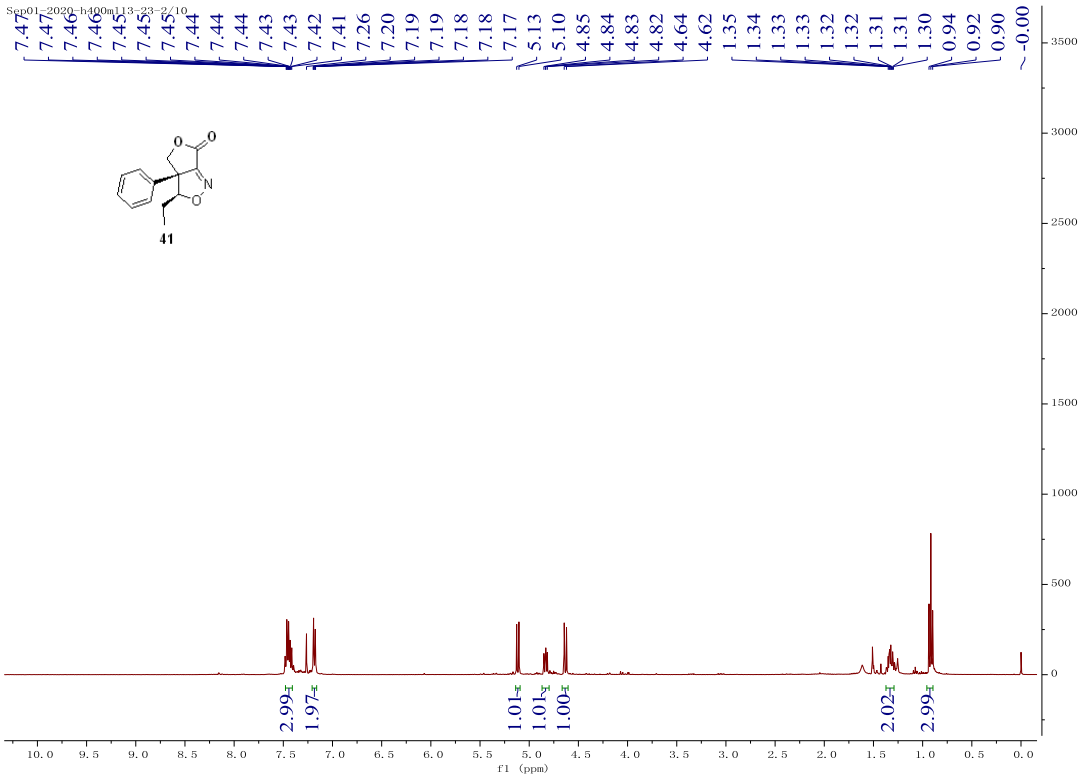

Aug26-2020-H400-ML13-36.10.1.1r
-113.02
O
O
NH
H
N
O
F
36
f1 (ppm)


7.67
7.66
7.66
7.66
7.65
7.65
7.64
7.64
7.63
7.57
7.56
7.56
7.56
7.55
7.55
7.54
7.54
7.54
7.53
7.53
7.52
7.52
7.51
7.26
5.48
38
1.98
2.99
2.00
f1 (ppm)


164.56
159.10
131.45
129.54
126.29
125.62
120.12
77.32
77.00
76.68
64.57
38
f1 (ppm)


Jun05-2020-H400-ml12-int.10.1.1r
7.64
7.63
7.62
7.62
7.61
7.39
7.39
7.38
7.37
7.37
7.37
7.36
7.35
7.35
7.35
7.34
7.33
7.26
7.11
7.09
4.97
4.97
1.50
-0.00
39
7.11
7.09
1.92
f1 (ppm)
2.00
3.01
1.92
2.00
9.00
f1 (ppm)


Jun05-2020-c400-ml12-int.10.1.1r
150.18
149.16
134.43
132.13
129.06
128.61
128.19
118.17
82.84
77.32
77.00
76.68
71.09
27.95
39
f1 (ppm)


Sep01-2020-h400m113-23-2/10
7.47
7.47
7.46
7.46
7.45
7.45
7.45
7.44
7.44
7.44
7.43
7.43
7.42
7.41
7.26
7.20
7.19
7.19
7.18
7.18
7.17
5.13
5.10
4.85
4.84
4.83
4.82
4.64
4.62
1.35
1.34
1.33
1.33
1.32
1.32
1.31
1.31
1.30
0.94
0.92
0.90
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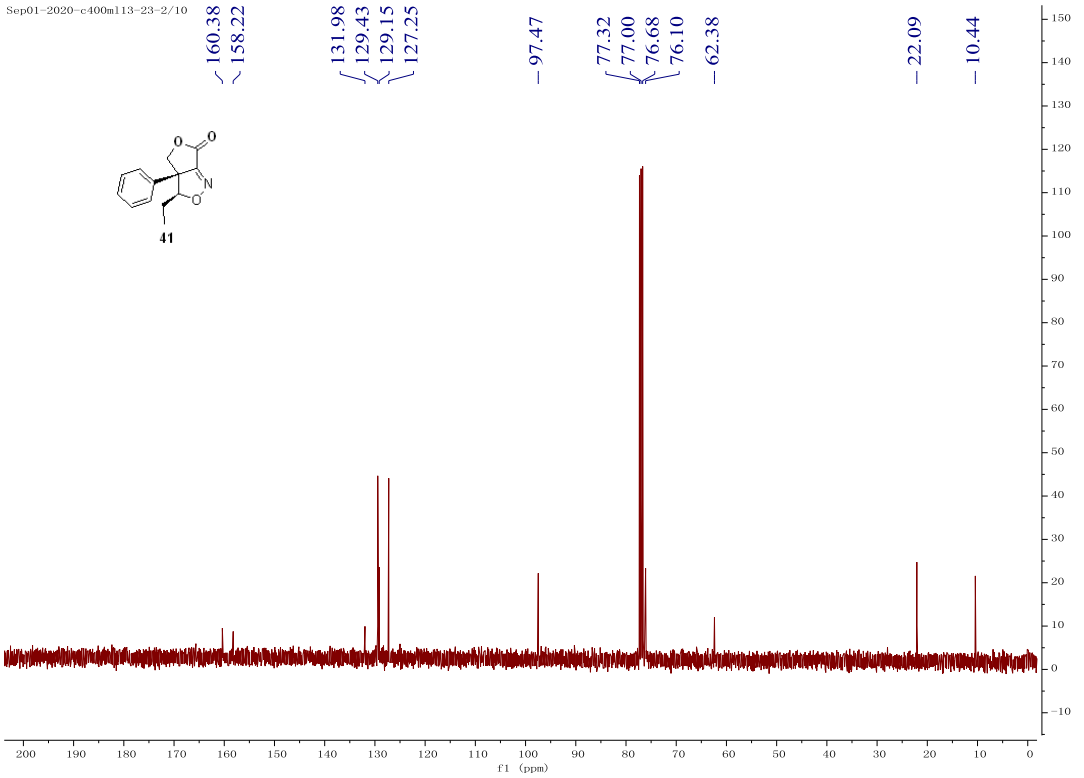
41
2.99
1.97
1.01
1.01
1.00
2.02
2.99
f1 (ppm)


Sep01-2020-c400m113-23-2/10
160.38
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129.15
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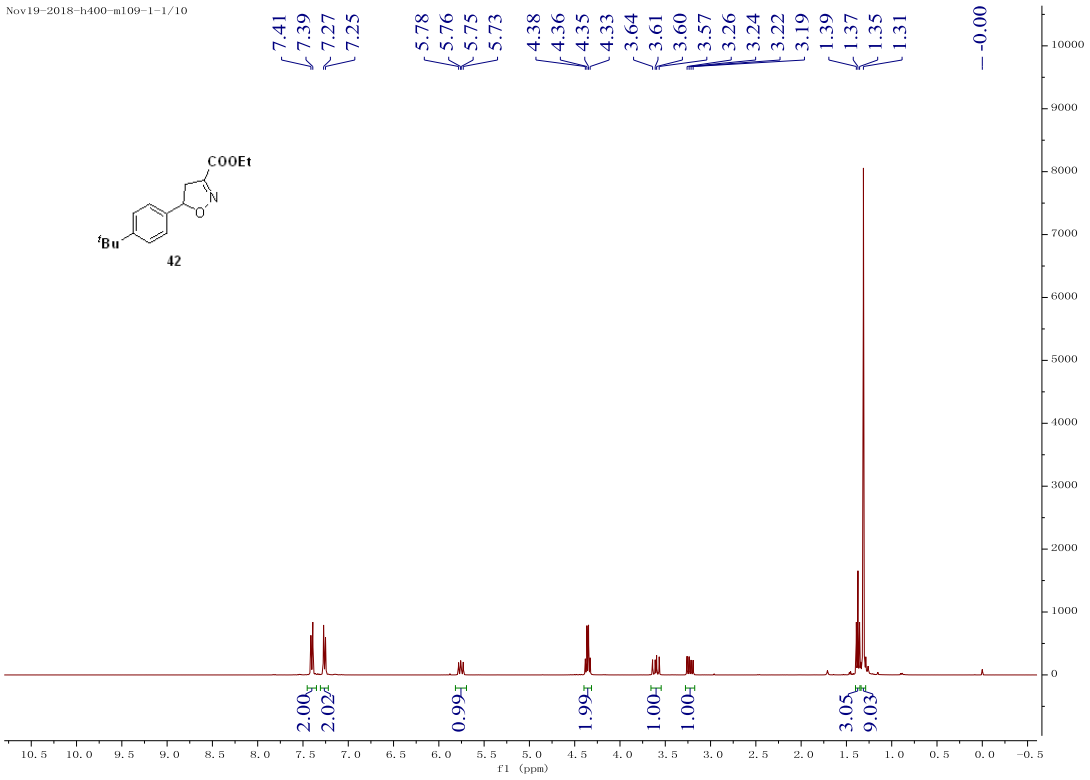
77.32
77.00
76.68
76.10
62.38
22.09
10.44
41
f1 (ppm)


Nov19-2018-h400-m109-1-1/10
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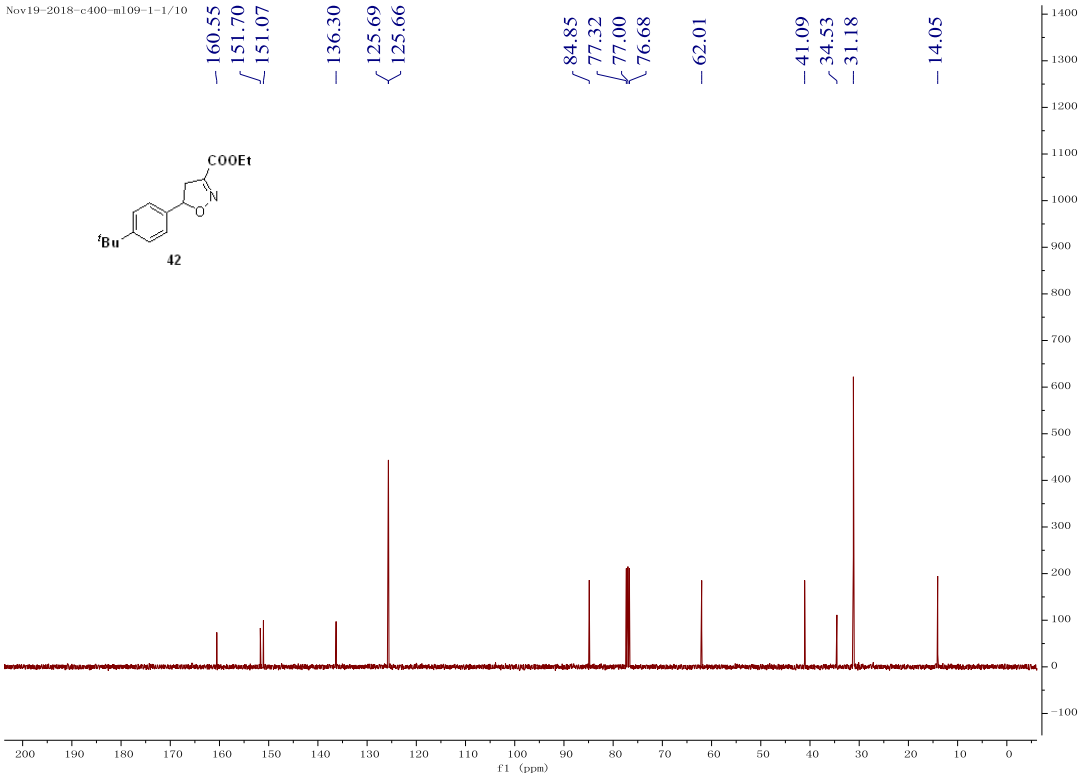
7.39
7.27
7.25
5.78
5.76
5.75
5.73
4.38
4.36
4.35
4.33
3.64
3.61
3.60
3.57
3.26
3.24
3.22
3.19
1.39
1.37
1.35
1.31
-0.00
COOEt
tBu
42
2.00
2.02
0.99
1.99
1.00
1.00
3.05
9.03
f1 (ppm)


Nov19-2018-c400-m109-1-1/10
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151.07
136.30
125.69
125.66
84.85
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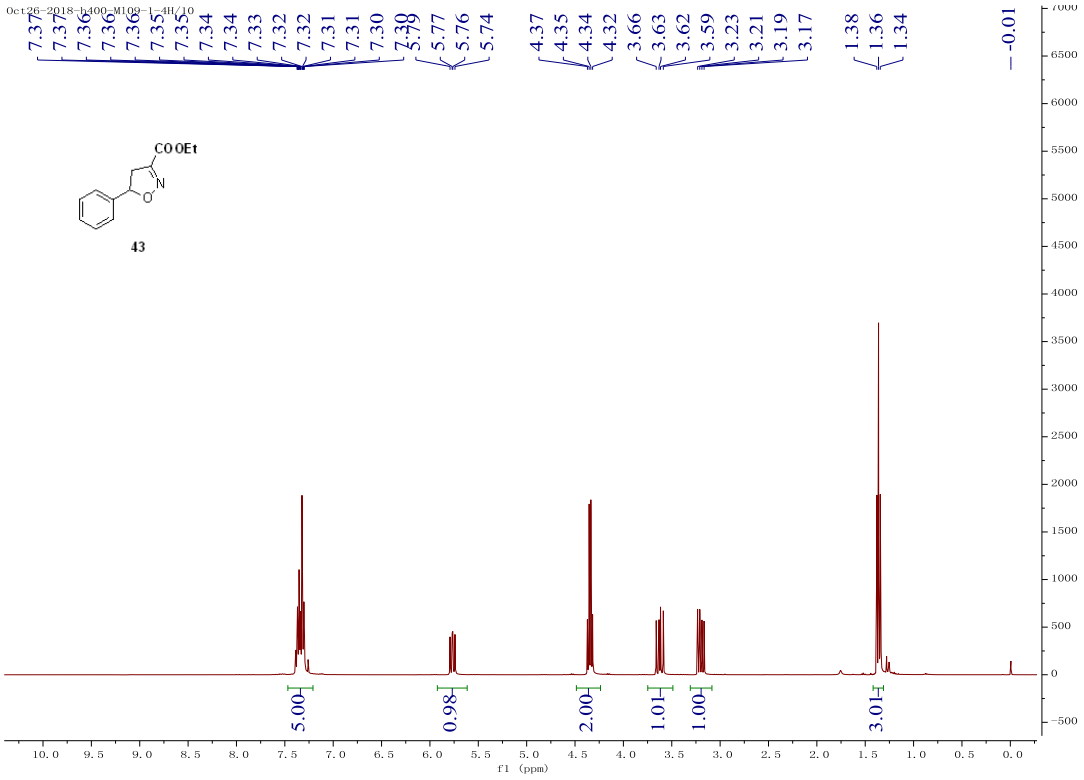
77.00
76.68
62.01
41.09
34.53
31.18
14.05
COOEt
tBu
42
f1 (ppm)


Oct26-2018-c400-M109-1-4H/10
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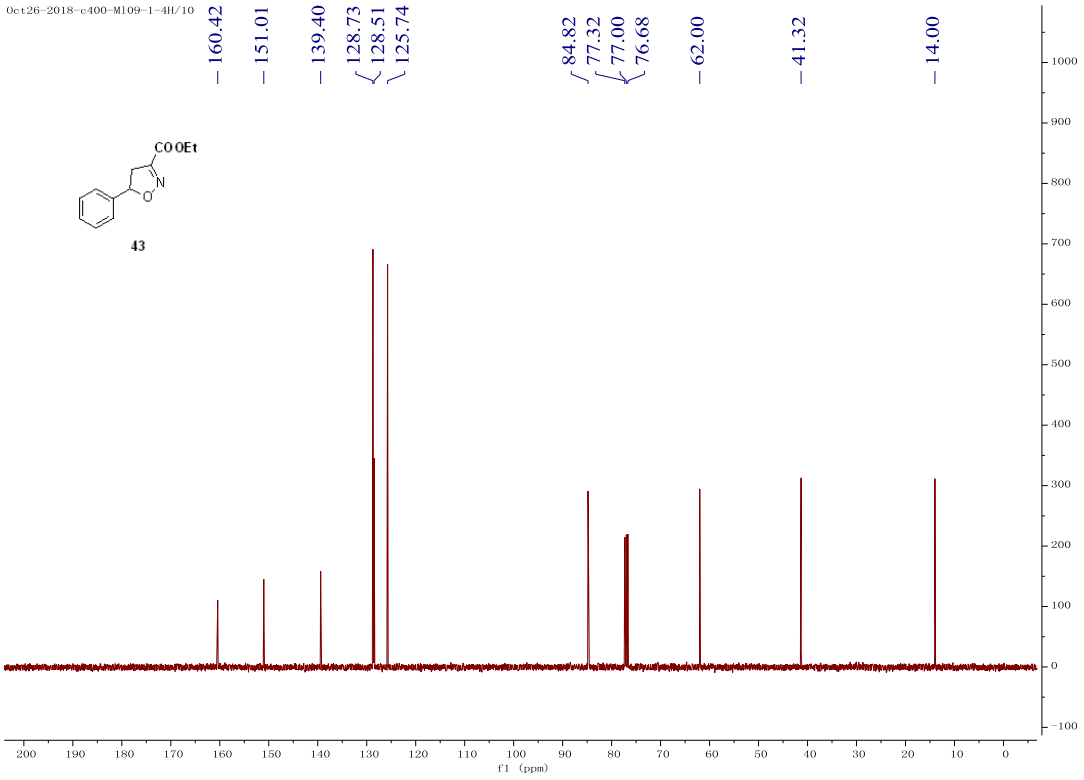
7.37
7.36
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.32
7.32
7.31
7.31
7.30
7.30
5.79
5.77
5.76
5.74
4.37
4.35
4.34
4.32
3.66
3.63
3.62
3.59
3.23
3.21
3.19
3.17
1.38
1.36
1.34
-0.01
COOEt
43
5.00
0.98
2.00
1.01
1.00
3.01
f1 (ppm)


Oct26-2018-c400-M109-1-4H/10
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151.01
139.40
128.73
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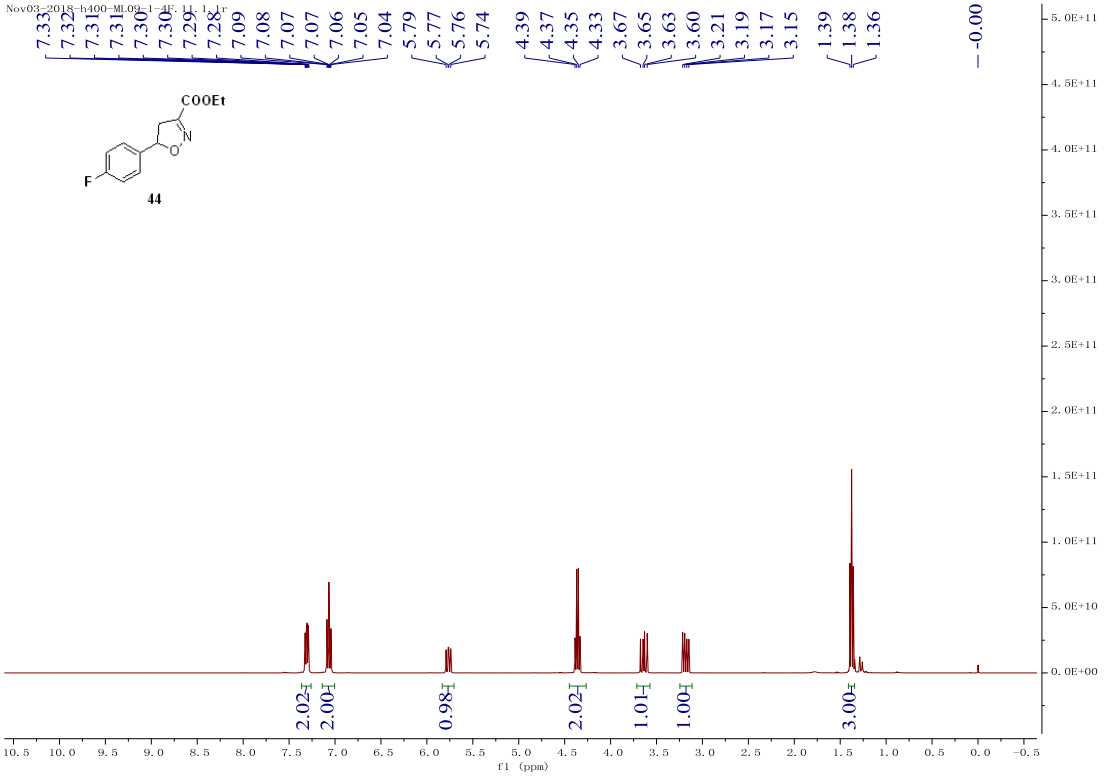
84.82
77.32
77.00
76.68
62.00
41.32
14.00
COOEt
43
f1 (ppm)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7.32
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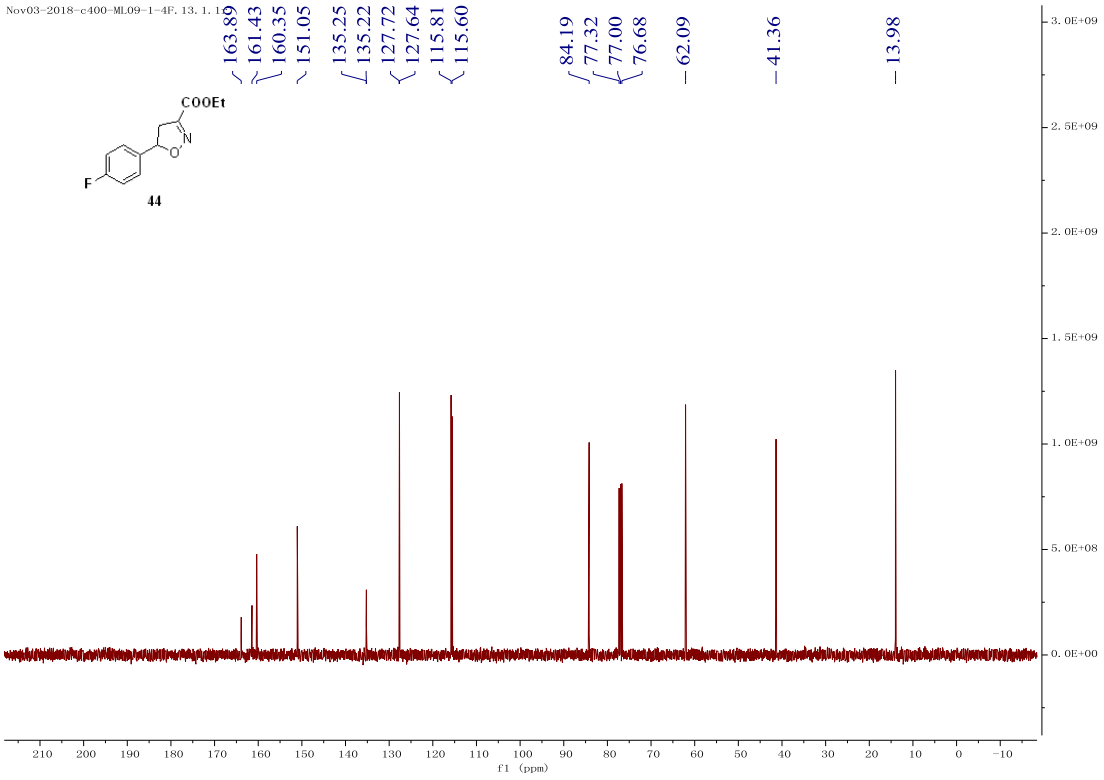
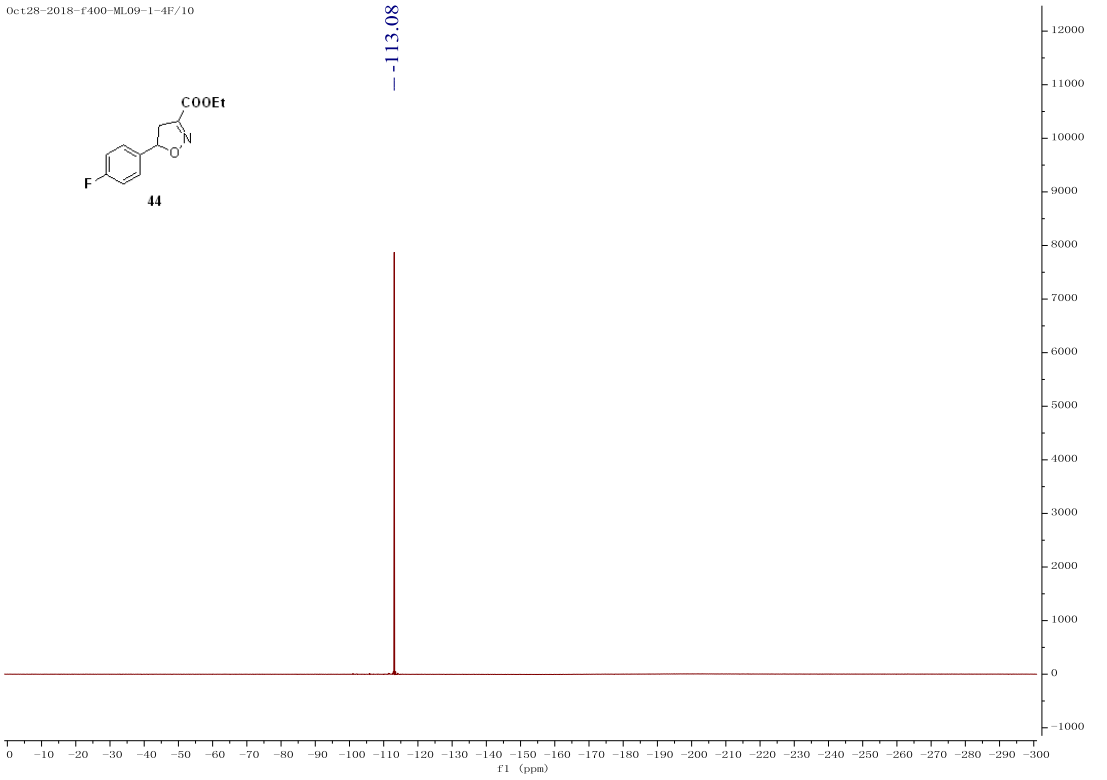
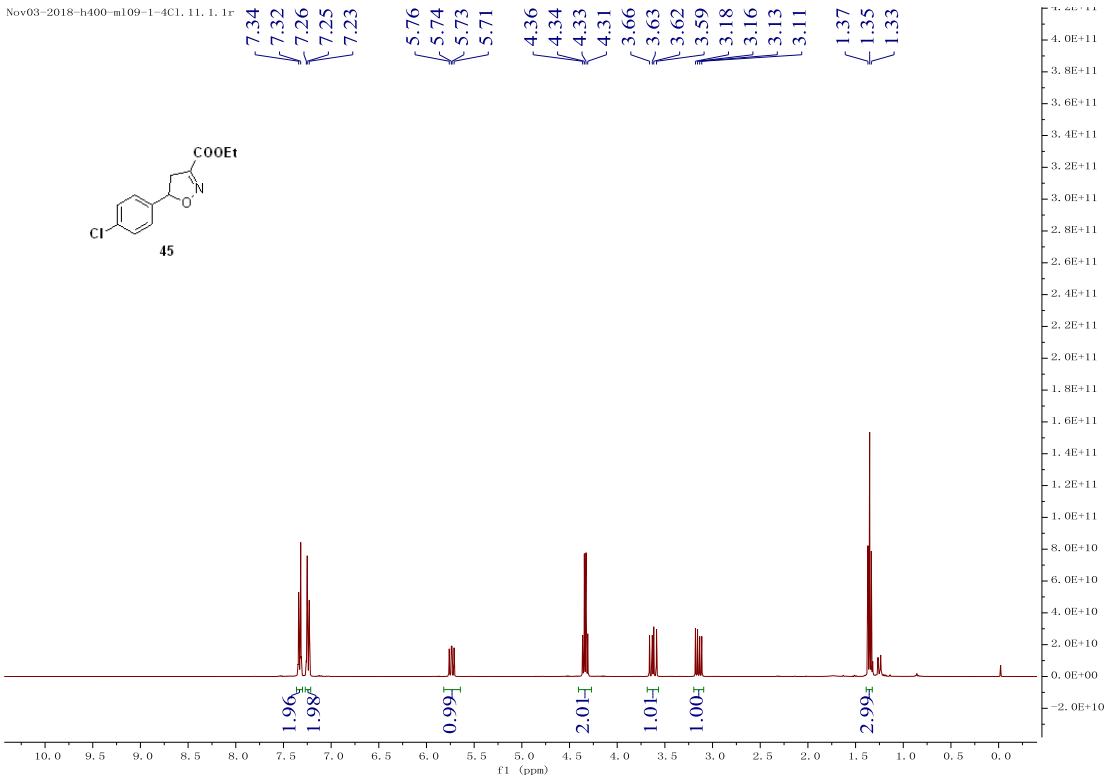
7.29
7.28
7.09
7.08
7.07
7.07
7.06
7.05
7.04
5.79
5.77
5.76
5.74
4.39
4.37
4.35
4.33
3.67
3.65
3.63
3.60
3.21
3.19
3.17
3.15
1.39
1.38
1.36
-0.00
COOEt
F
44
2.02
2.00
0.98
2.02
1.01
1.00
3.00
f1 (ppm)


163.89
161.43
160.35
151.05
135.25
135.22
127.72
127.64
115.81
115.60
84.19
77.32
77.00
76.68
62.09
41.36
13.98
COOEt
F
44
f1 (ppm)


Oct28-2018-f400-ML09-1-4F/10
-113.08
COOEt
F
44
f1 (ppm)


Nov03-2018-h400-ml09-1-4Cl.11.1.1r
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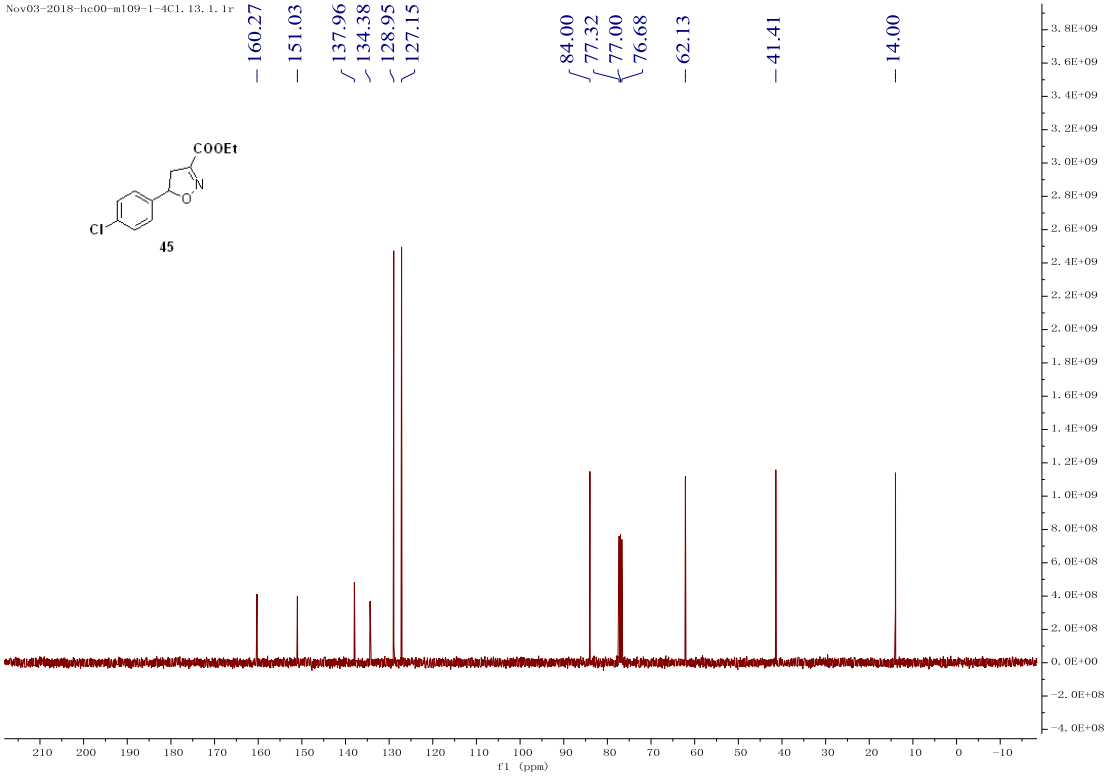
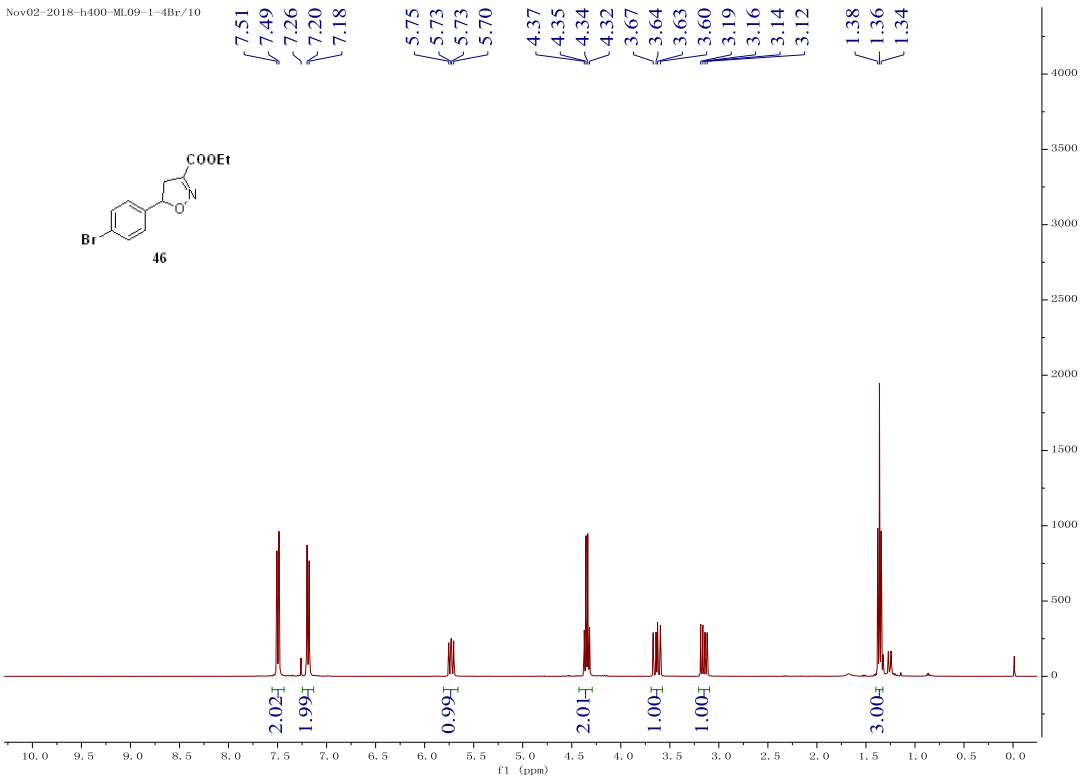
7.32
7.26
7.25
7.23
5.76
5.74
5.73
5.71
4.36
4.34
4.33
4.31
3.66
3.63
3.62
3.59
3.18
3.16
3.13
3.11
1.37
1.35
1.33
COOEt
Cl
45
1.96
1.98
0.99
2.01
1.01
1.00
2.99
f1 (ppm)


Nov03-2018-hc00-m109-1-4Cl.13.1.1r
160.27
151.03
137.96
134.38
128.95
127.15
84.00
77.32
77.00
76.68
62.13
41.41
14.00
COOEt
Cl
45
f1 (ppm)


Nov02-2018-h400-ML09-1-4Br/10
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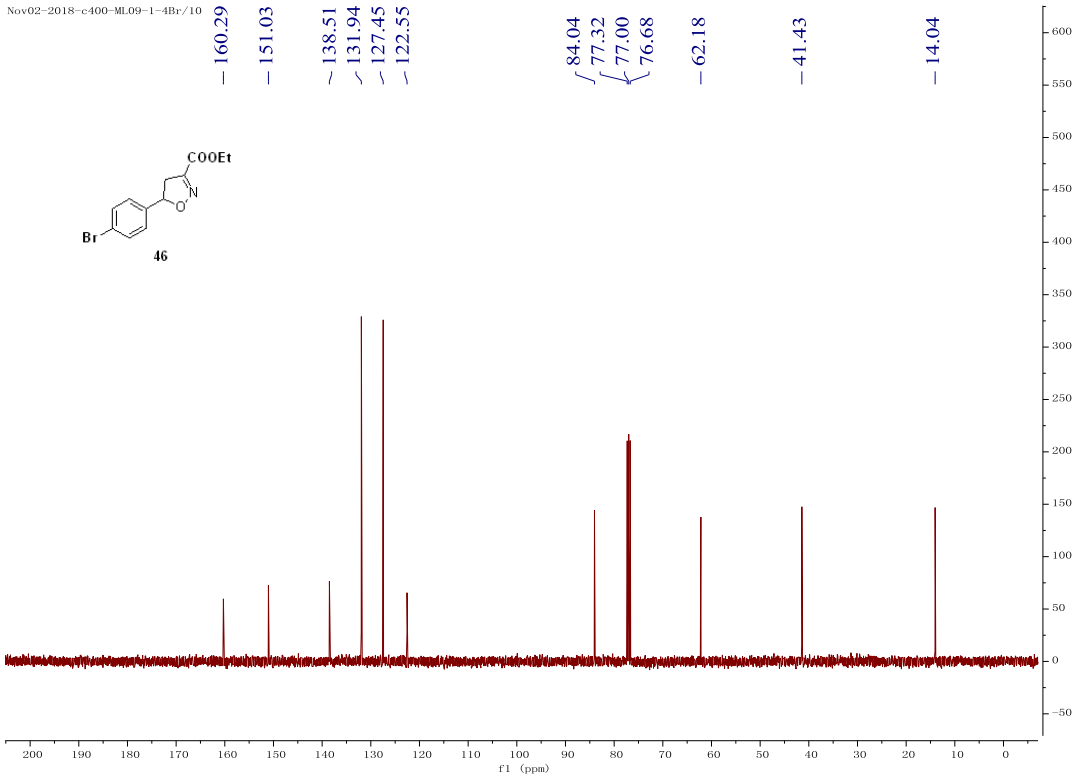
7.49
7.26
7.20
7.18
5.75
5.73
5.73
5.70
4.37
4.35
4.34
4.32
3.67
3.64
3.63
3.60
3.19
3.16
3.14
3.12
1.38
1.36
1.34
COOEt
Br
46
2.02
1.99
0.99
2.01
1.00
1.00
3.00
f1 (ppm)


Nov02-2018-c400-ML09-1-4Br/10
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151.03
138.51
131.94
127.45
122.55
84.04
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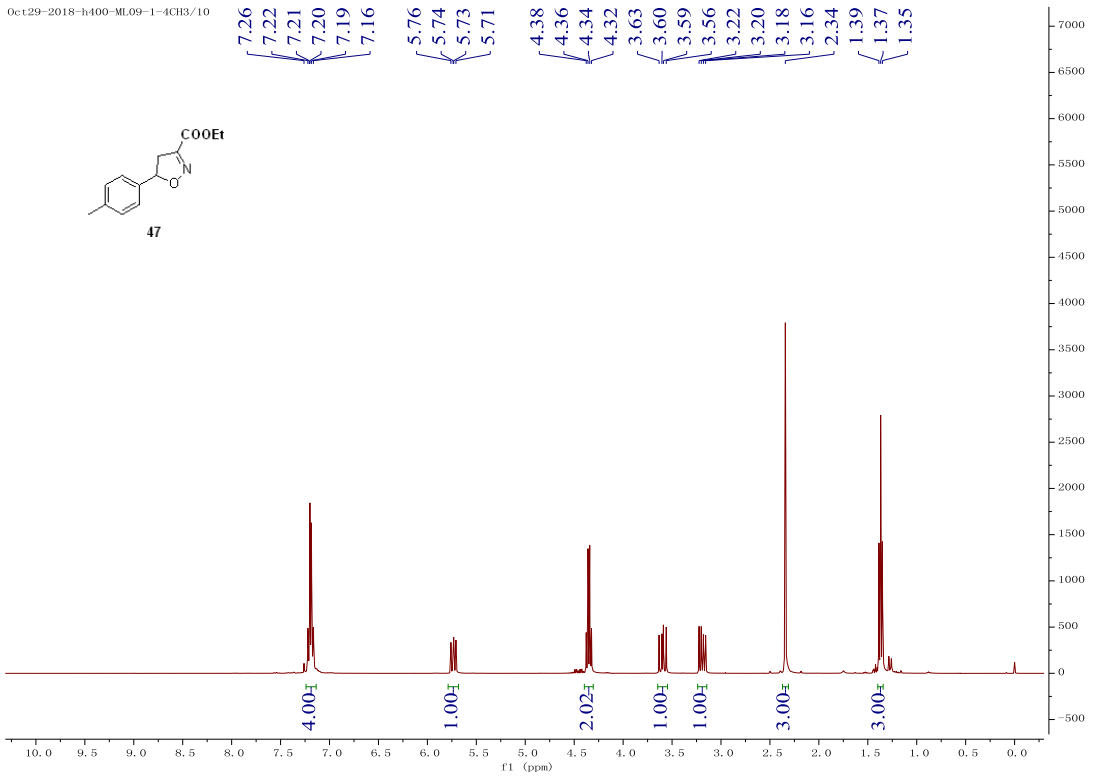
77.00
76.68
62.18
41.43
14.04
COOEt
N
O
Br
46
f1 (ppm)


Oct29-2018-h400-ML09-1-4CH3/10
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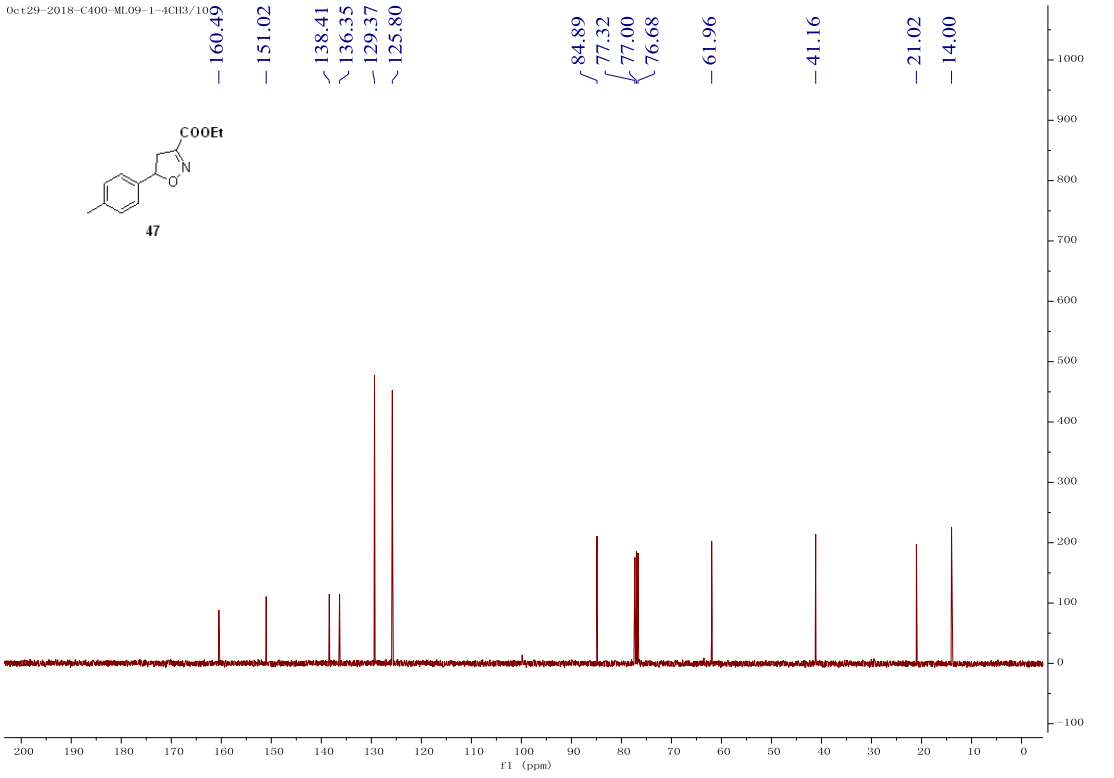
7.22
7.21
7.20
7.19
7.16
5.76
5.74
5.73
5.71
4.38
4.36
4.34
4.32
3.63
3.60
3.59
3.56
3.22
3.20
3.18
3.16
2.34
1.39
1.37
1.35
COOEt
N
O
47
4.00
1.00
2.02
1.00
1.00
3.00
3.00
f1 (ppm)


Oct29-2018-C400-ML09-1-4CH3/10
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138.41
136.35
129.37
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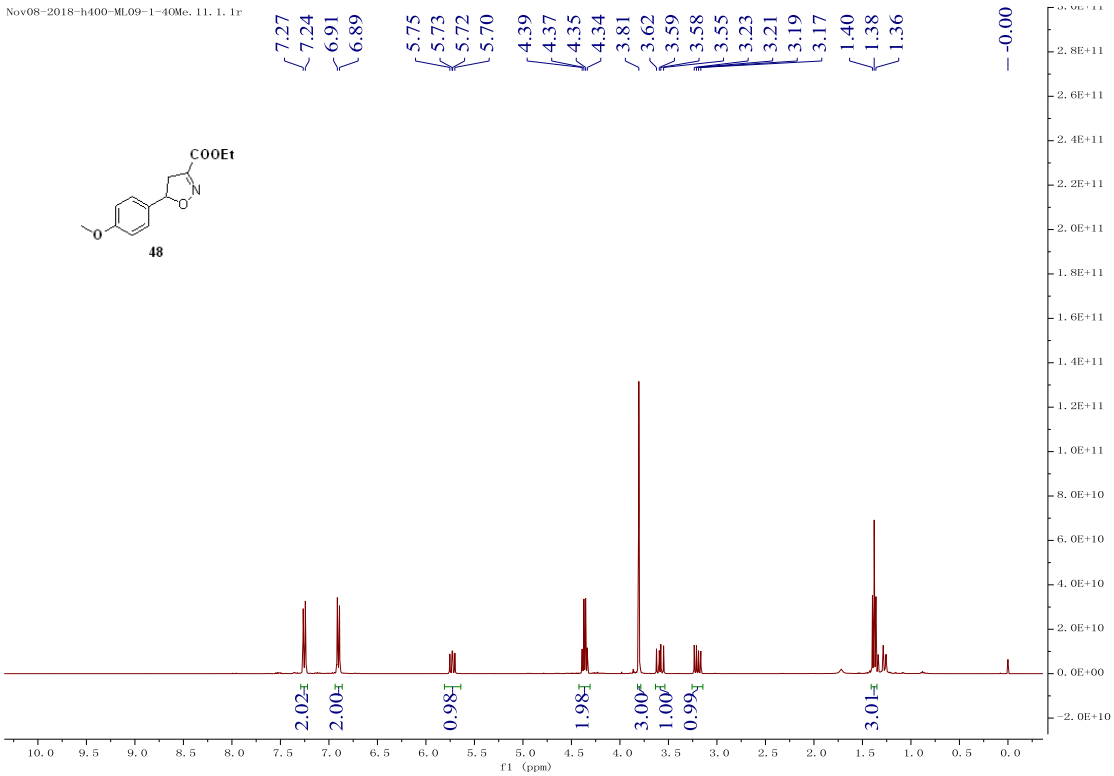
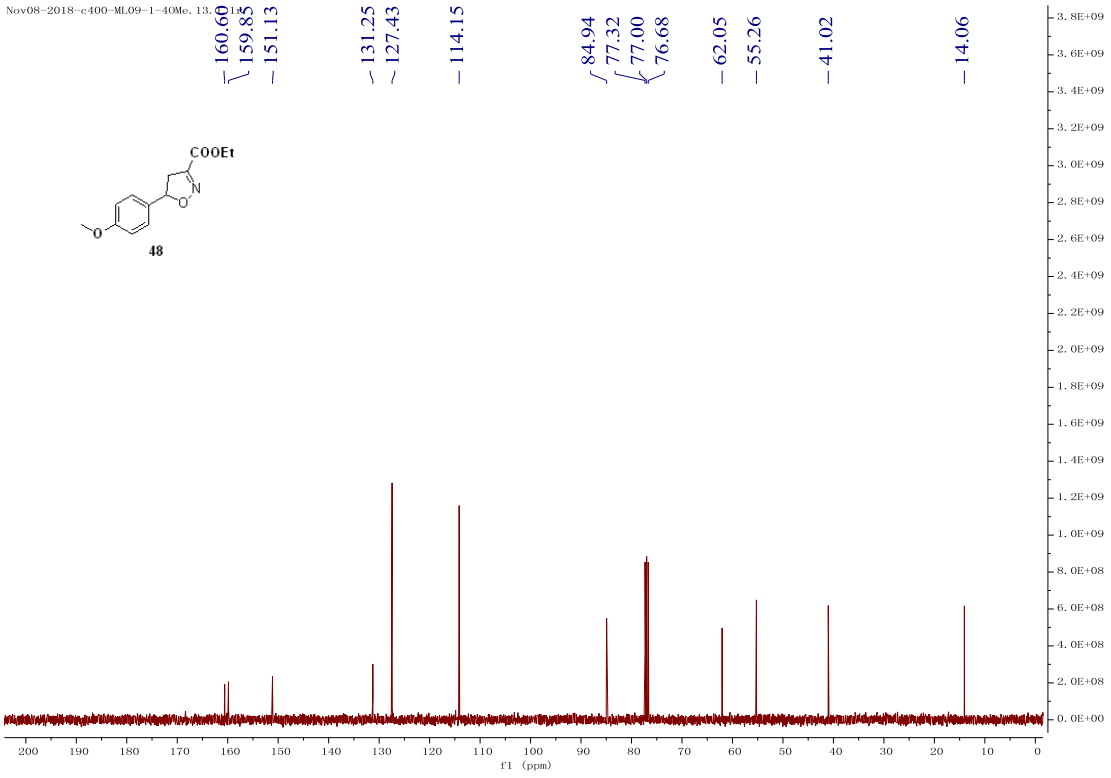
84.89
77.32
77.00
76.68
61.96
41.16
21.02
14.00
COOEt
47
f1 (ppm)


Nov08-2018-h400-ML09-1-40Me. 11. 1. 1r
7.27
7.24
6.91
6.89
5.75
5.73
5.72
5.70
4.39
4.37
4.35
4.34
3.81
3.62
3.59
3.58
3.55
3.23
3.21
3.19
3.17
1.40
1.38
1.36
-0.00
COOEt
48
2.02
2.00
0.98
1.98
3.00
1.00
0.99
3.01
f1 (ppm)


Nov08-2018-c400-ML09-1-40Me. 13.
160.66
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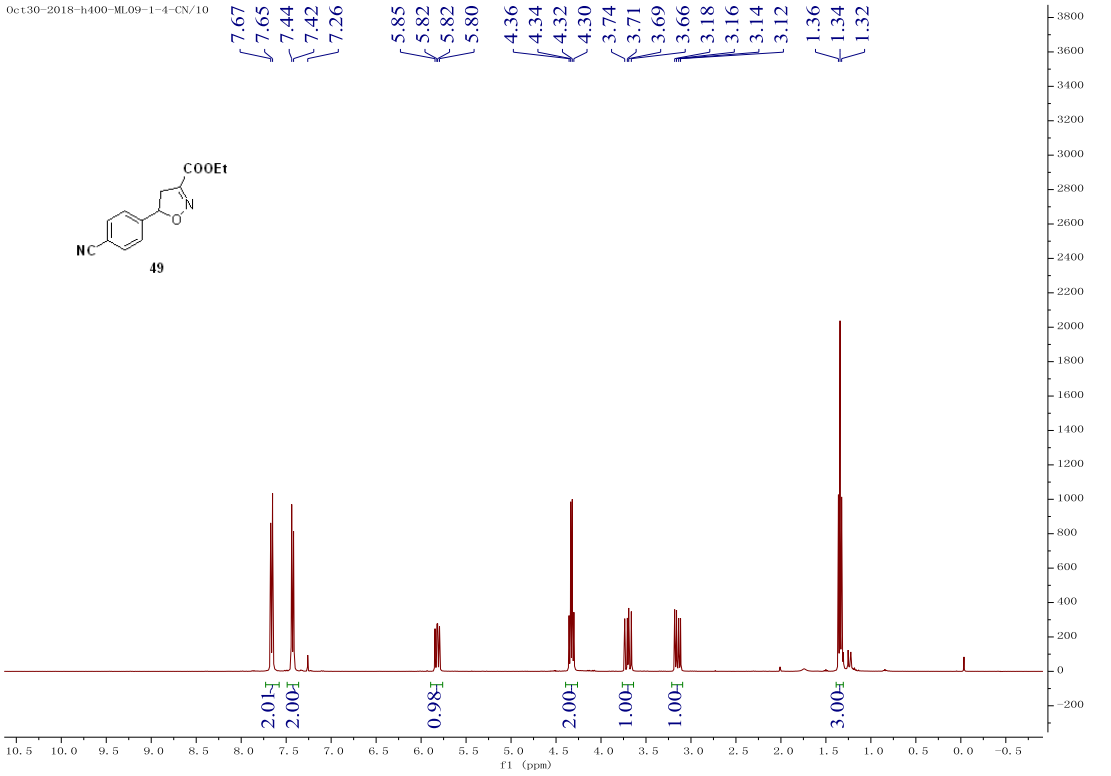
151.13
131.25
127.43
114.15
84.94
77.32
77.00
76.68
62.05
55.26
41.02
14.06
COOEt
O
N
O
48
f1 (ppm)


Oct30-2018-h400-ML09-1-4-CN/10
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7.44
7.42
7.26
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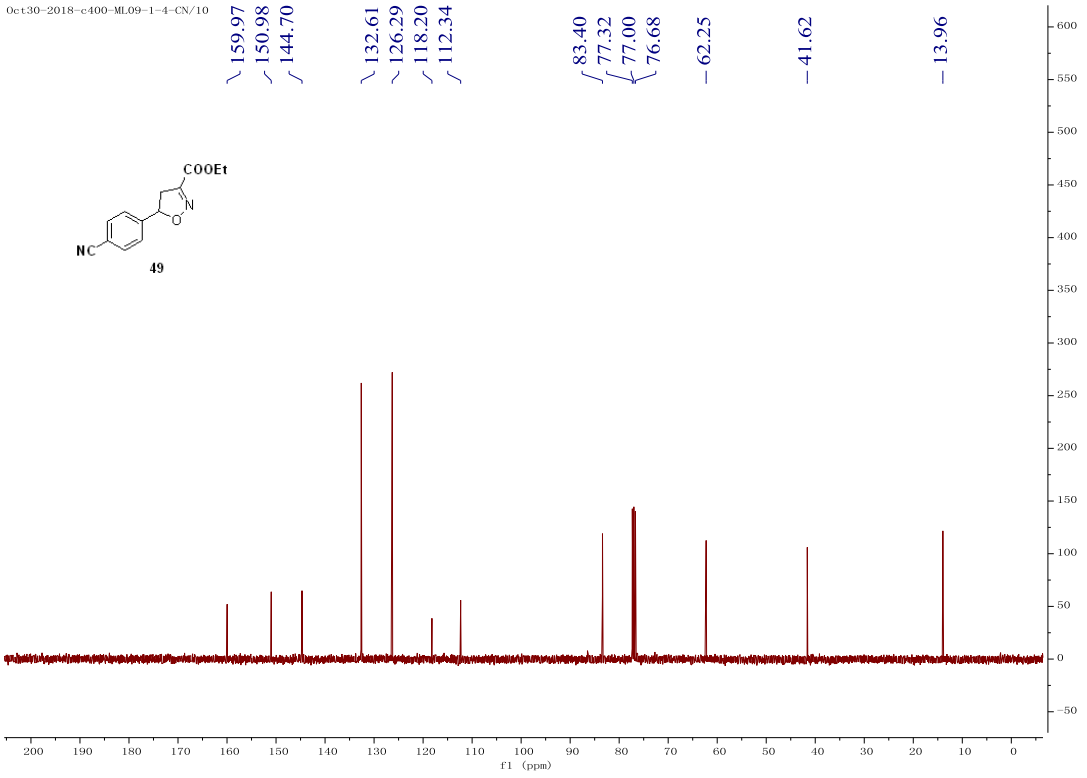
5.82
5.82
5.80
4.36
4.34
4.32
4.30
3.74
3.71
3.69
3.66
3.18
3.16
3.14
3.12
1.36
1.34
1.32
COOEt
N
O
NC
49
2.01
2.00
0.98
2.00
1.00
1.00
3.00
f1 (ppm)


Oct30-2018-c400-ML09-1-4-CN/10
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144.70
132.61
126.29
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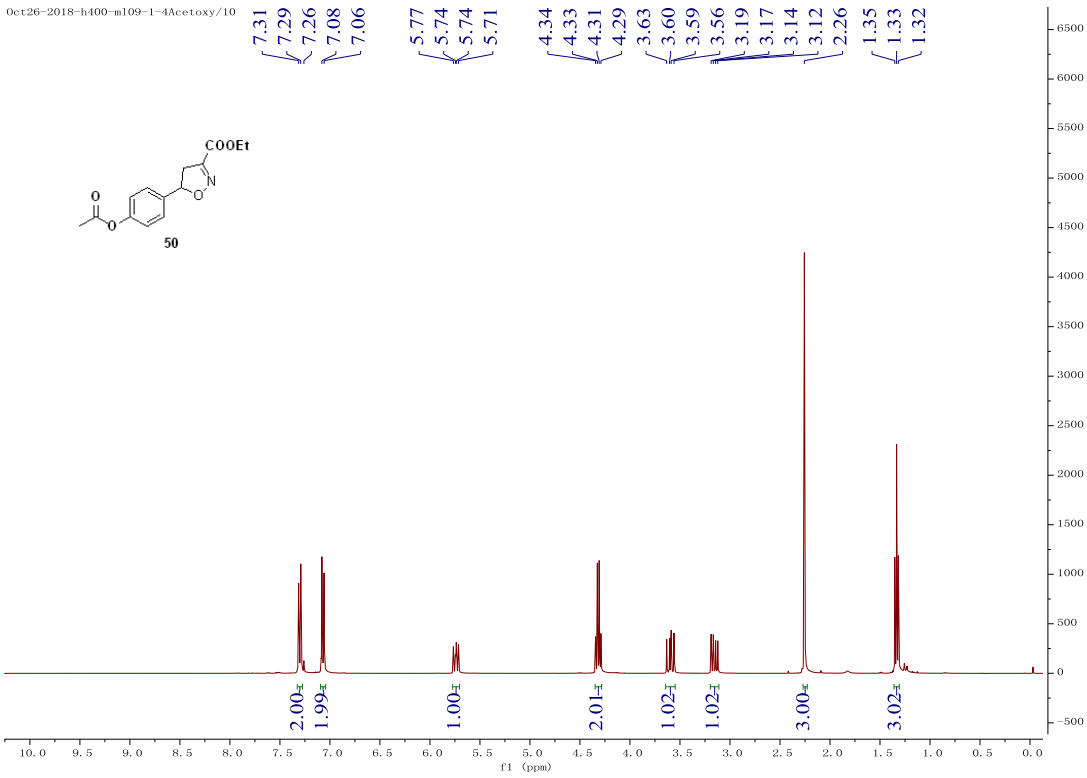
77.00
76.68
62.25
41.62
13.96
COOEt
NC
49
f1 (ppm)


Oct26-2018-h400-ml09-1-4Acetoxy/10
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5.74
5.71
4.34
4.33
4.31
4.29
3.63
3.60
3.59
3.56
3.19
3.17
3.14
3.12
2.26
1.35
1.33
1.32
COOEt
O
O
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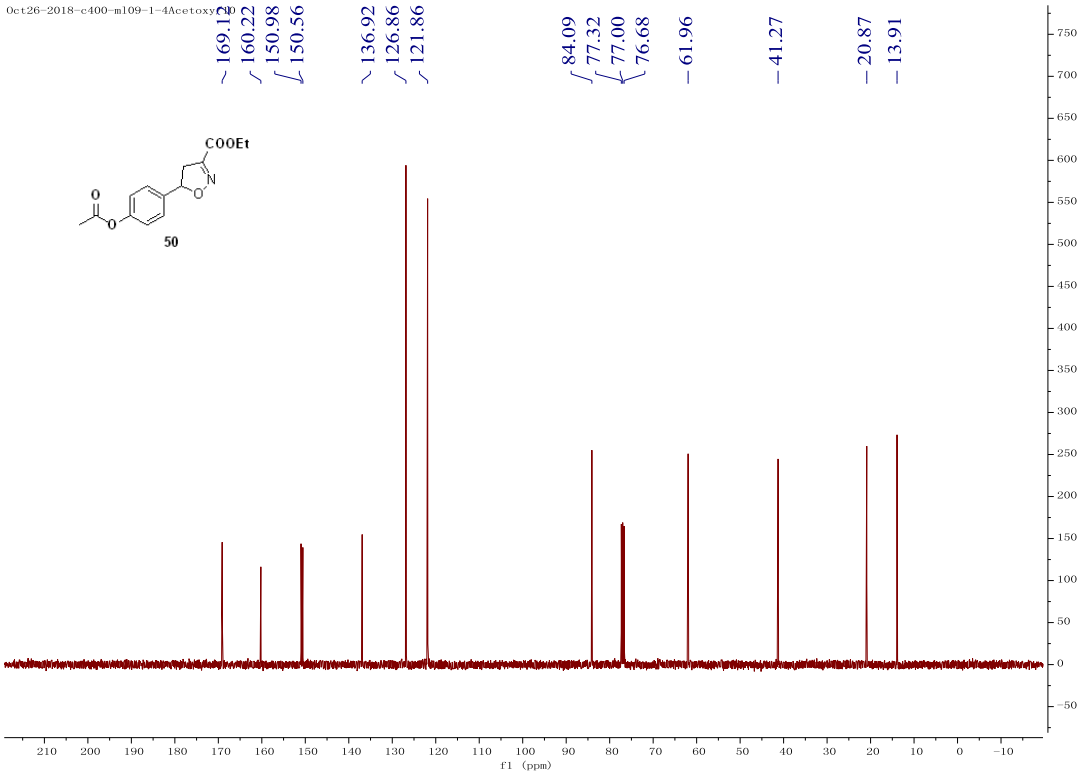
2.00
1.99
1.00
2.01
1.02
1.02
3.00
3.02
f1 (ppm)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121.86
84.09
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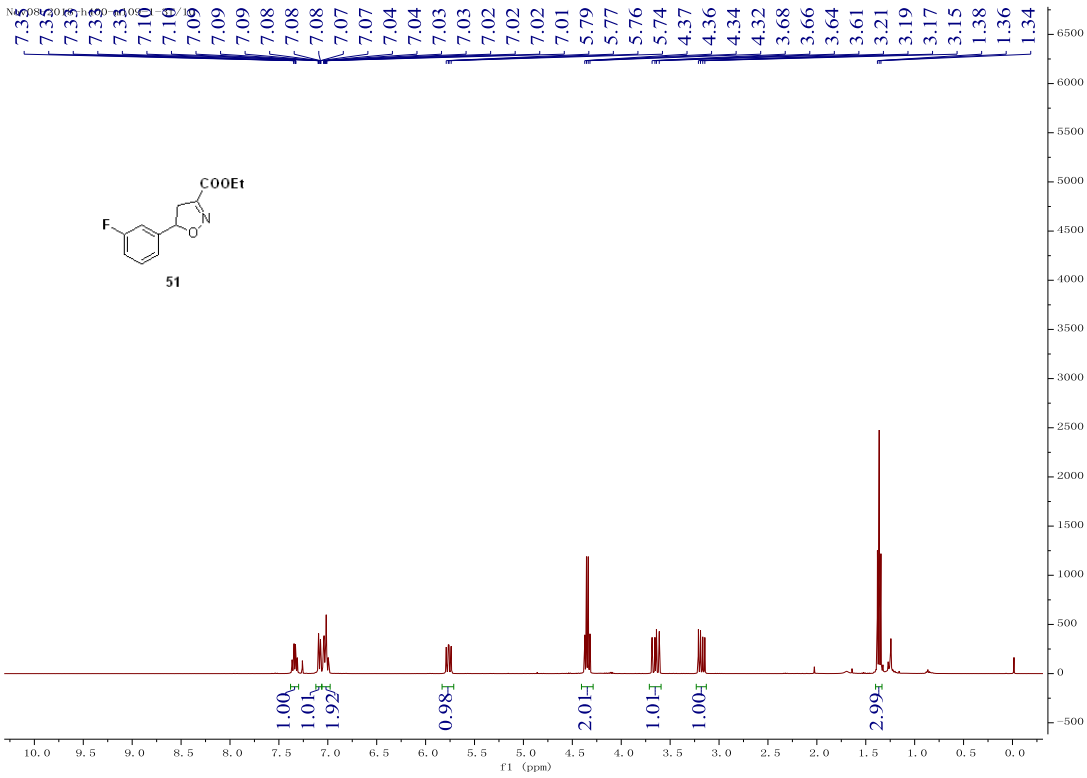
41.27
20.87
13.91
COOEt
O
O
N
O
50
f1 (ppm)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7.08
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7.04
7.04
7.03
7.03
7.02
7.02
7.02
7.01
5.79
5.77
5.76
5.74
4.37
4.36
4.34
4.32
3.68
3.66
3.64
3.61
3.21
3.19
3.17
3.15
1.38
1.36
1.34
COOEt
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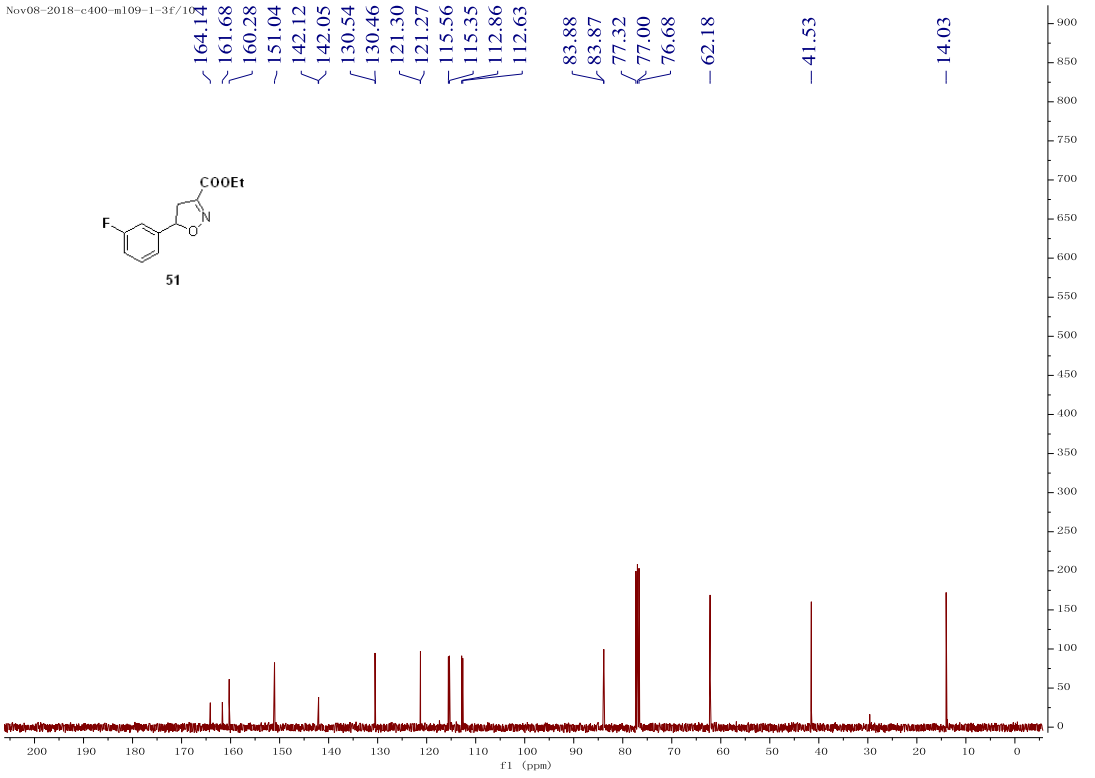
0.98
2.01
1.01
1.00
2.99
f1 (ppm)


Nov08-2018-c400-m109-1-3f/10
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142.05
130.54
130.46
121.30
121.27
115.56
115.35
112.86
112.63
83.88
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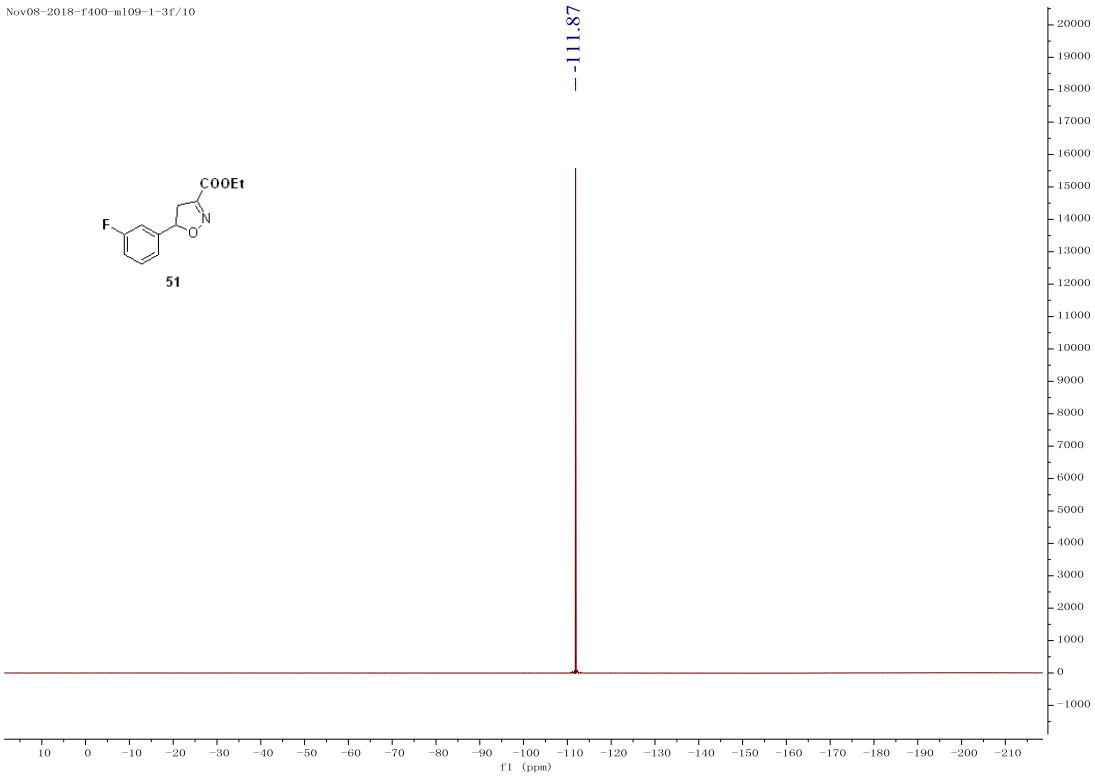
77.00
76.68
62.18
41.53
14.03
COOEt
F
N
O
51
f1 (ppm)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O
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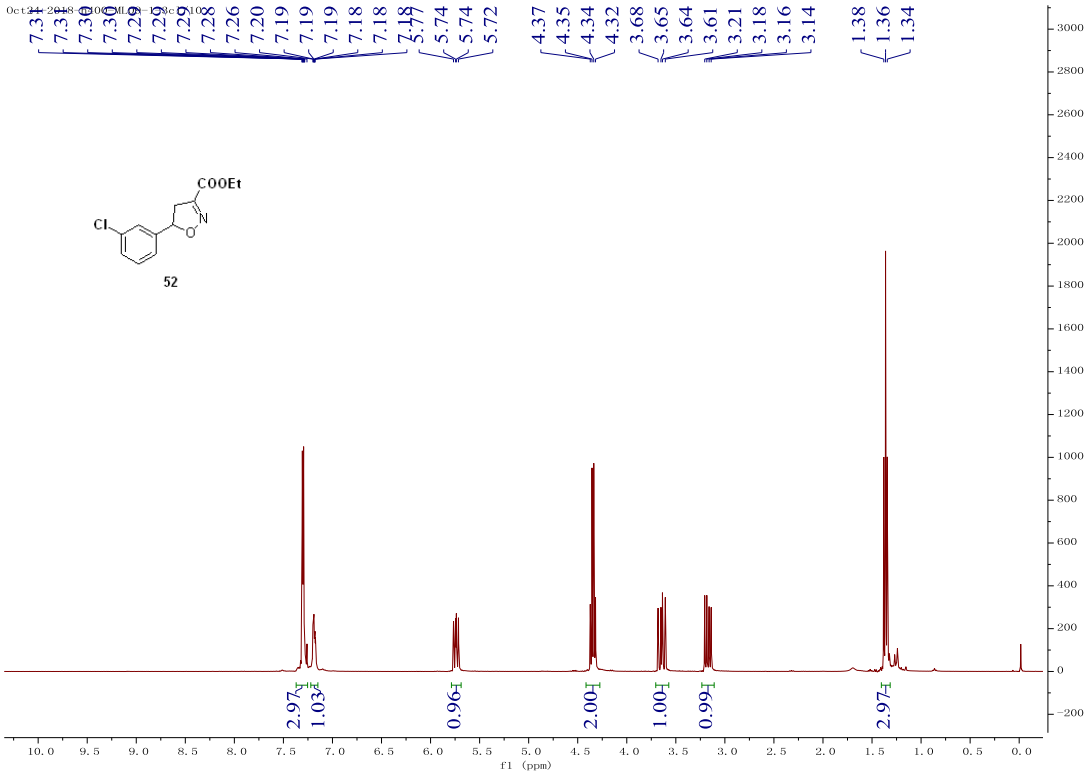
f1 (ppm)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7.18
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5.74
5.72
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4.35
4.34
4.32
3.68
3.65
3.64
3.61
3.21
3.18
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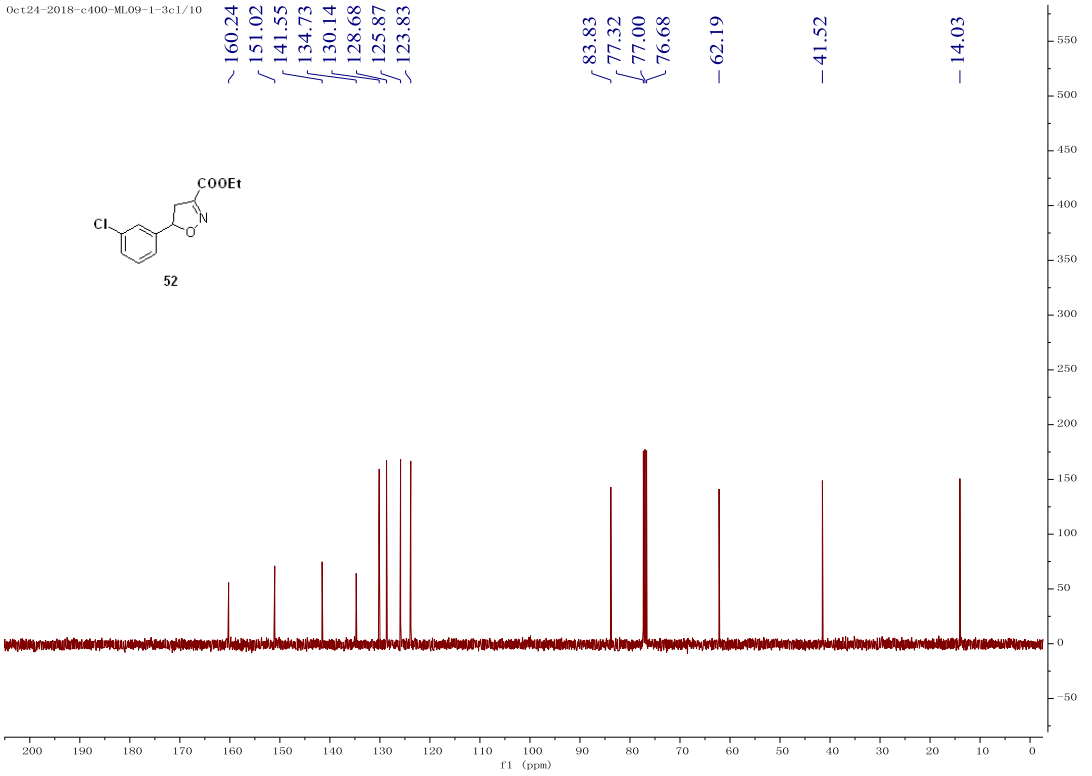
3.14
1.38
1.36
1.34
COOEt
Cl
O
N
52
2.97
1.03
0.96
2.00
1.00
0.99
2.97
f1 (ppm)


Oct24-2018-c400-ML09-1-3c1/10
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130.14
128.68
125.87
123.83
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77.00
76.68
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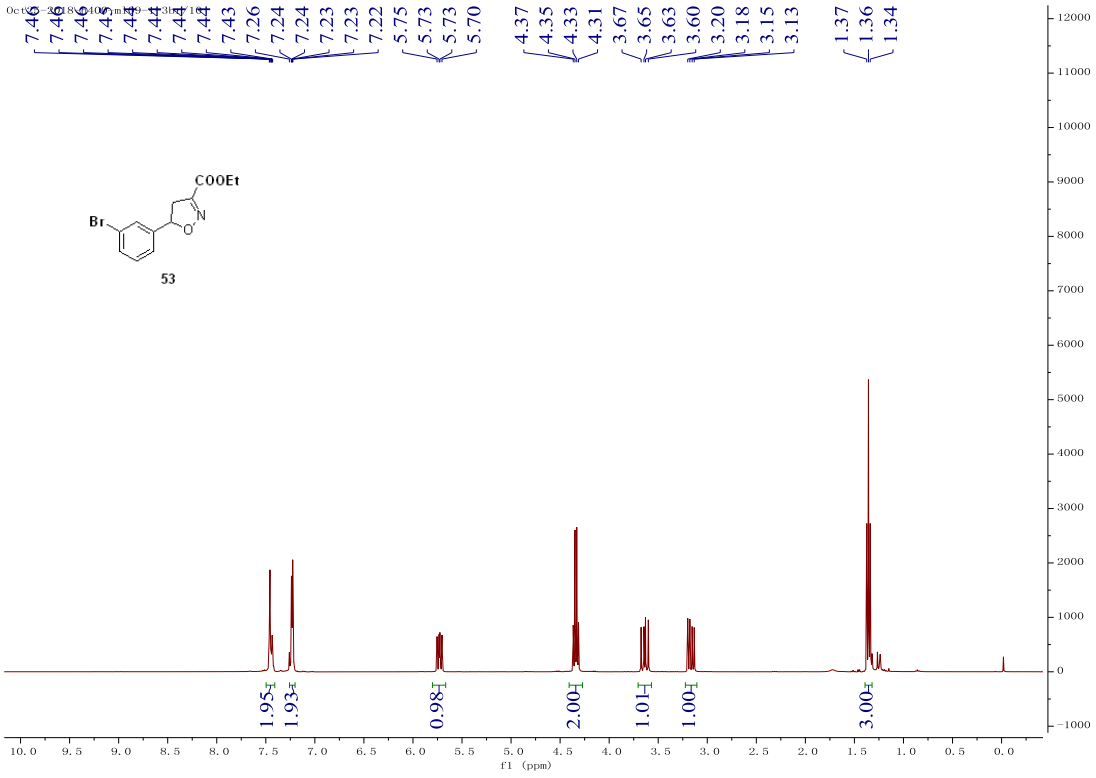
41.52
14.03
COOEt
Cl
O
N
52
f1 (ppm)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7.22
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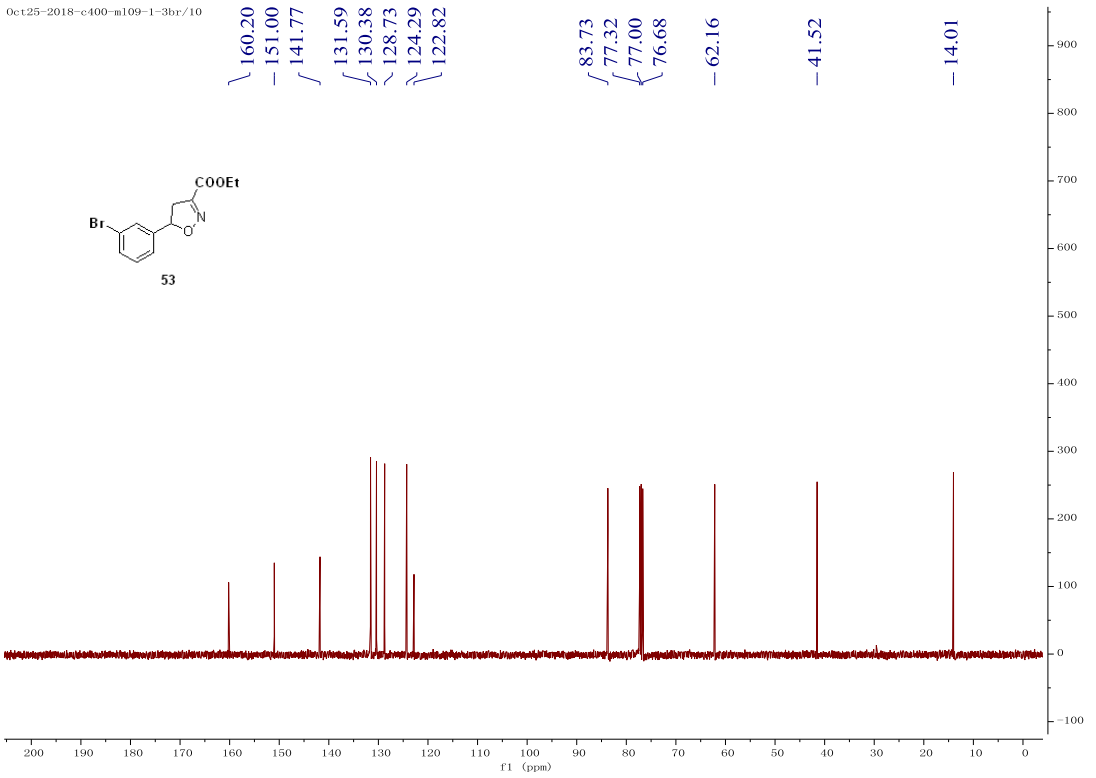
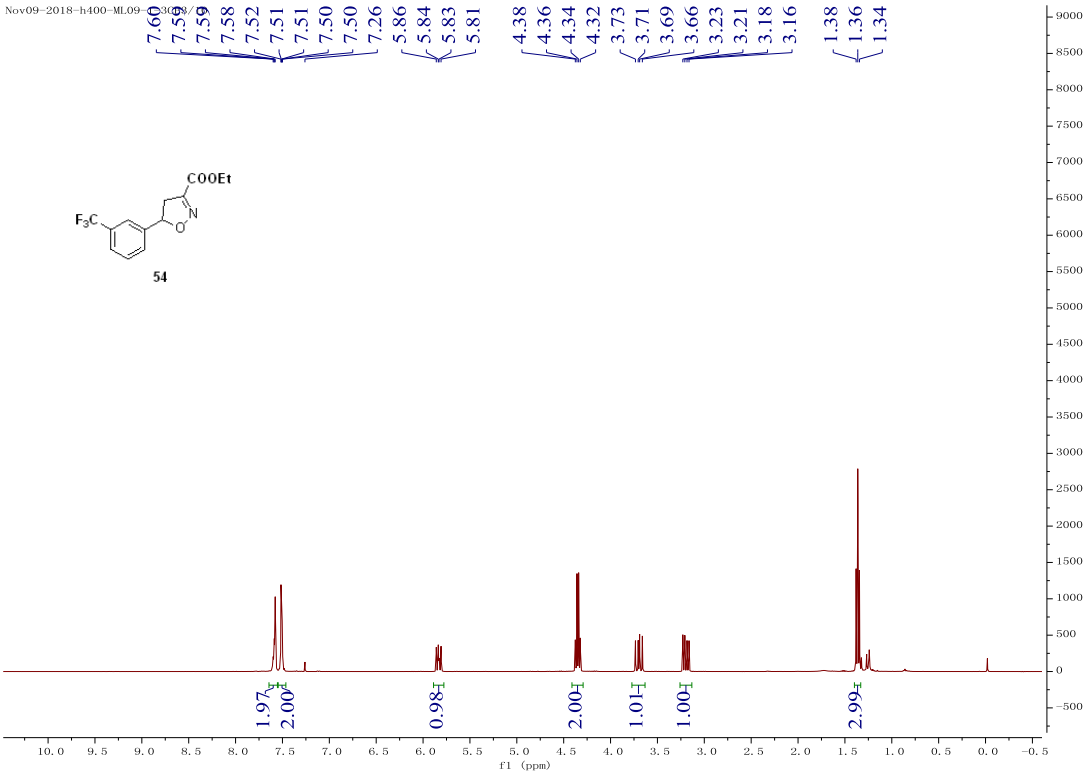
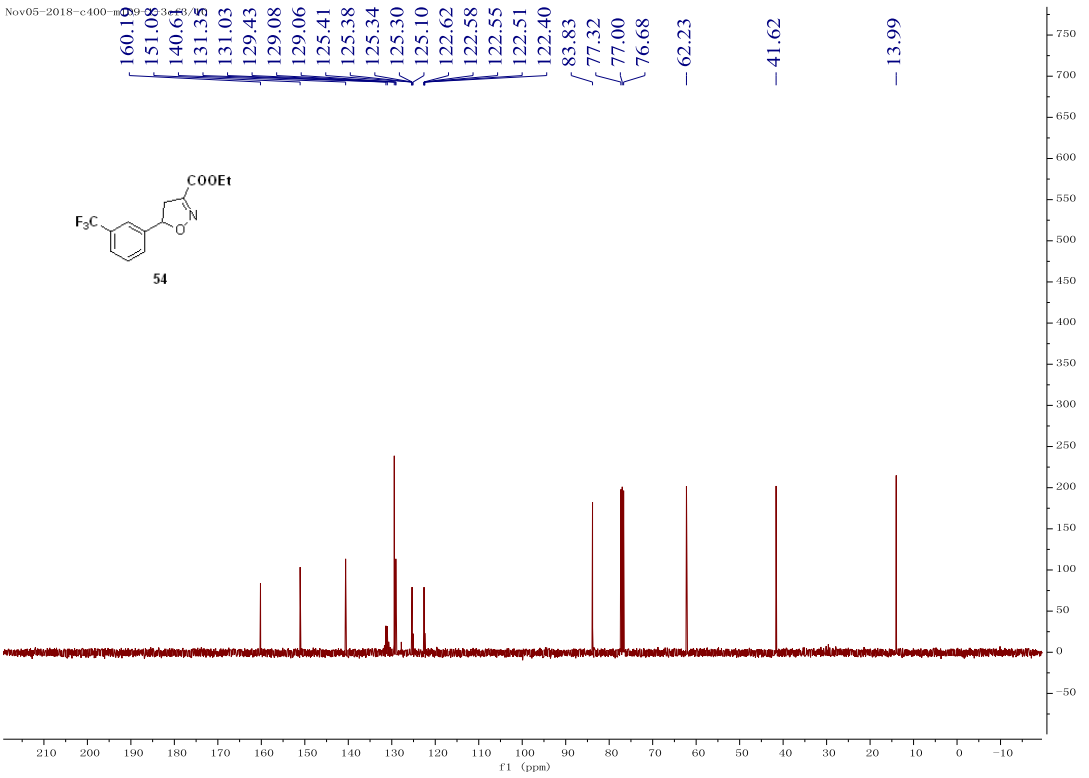
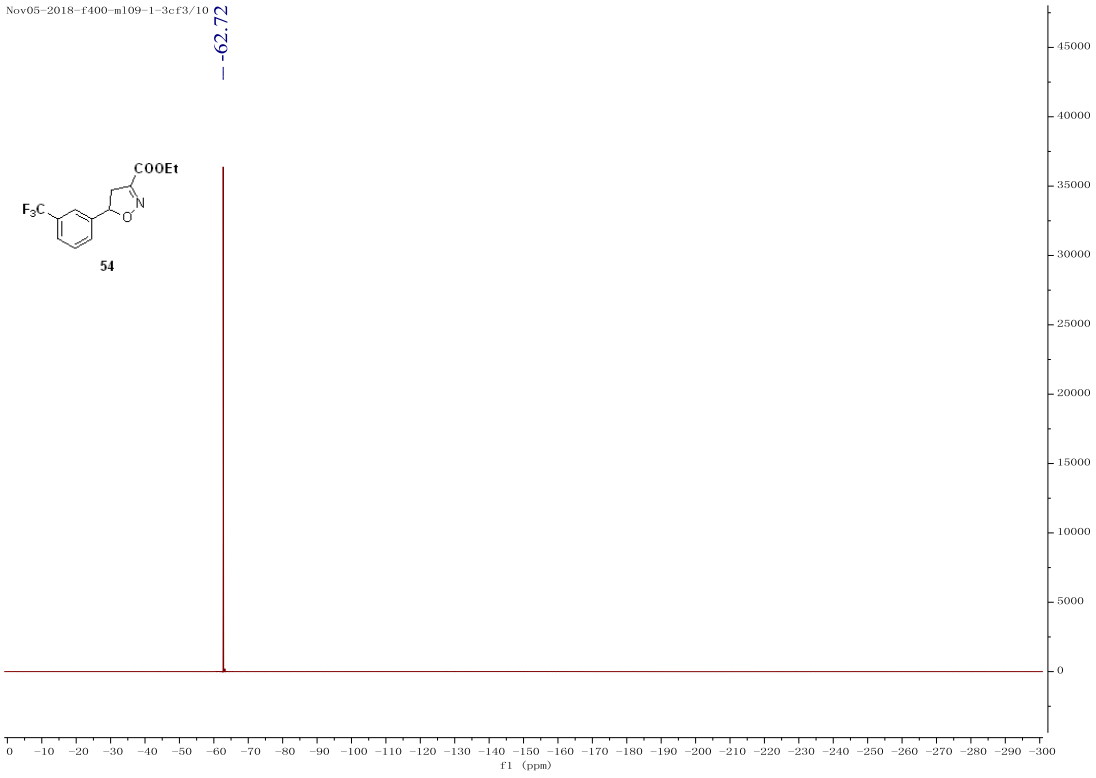
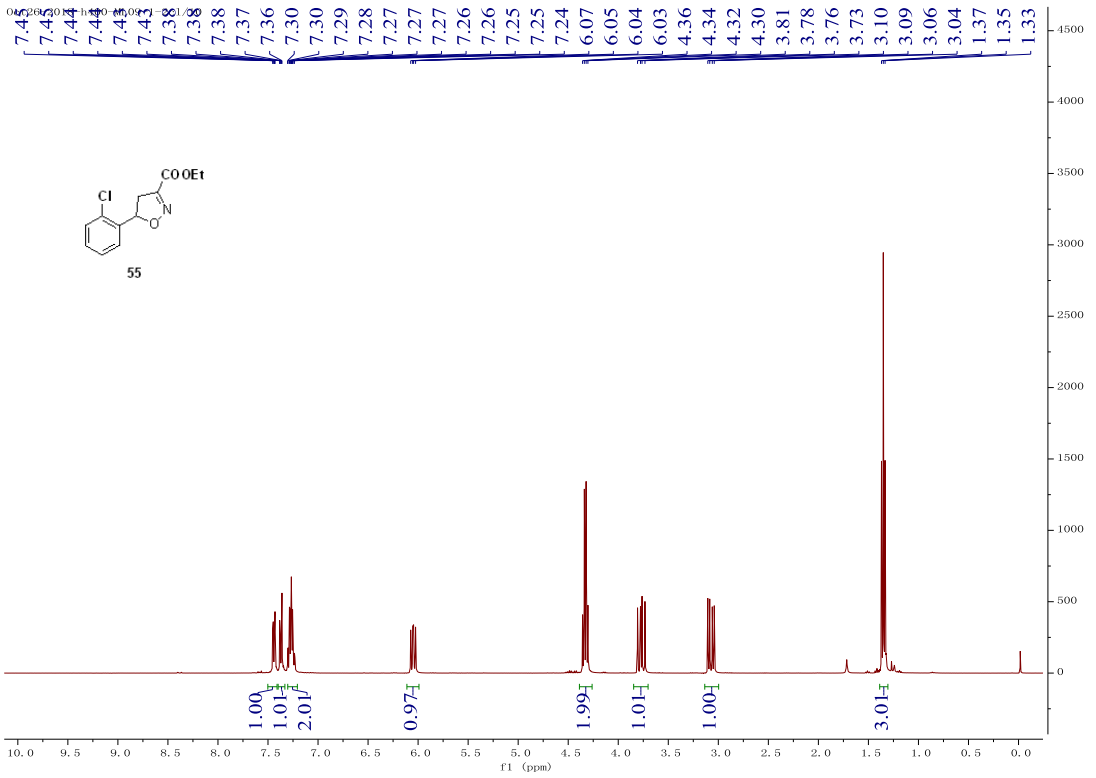
5.73
5.73
5.70
4.37
4.35
4.33
4.31
3.67
3.65
3.63
3.60
3.20
3.18
3.15
3.13
1.37
1.36
1.34
COOEt
Br
N
O
53
1.95
1.93
0.98
2.00
1.01
1.00
3.00
f1 (ppm)

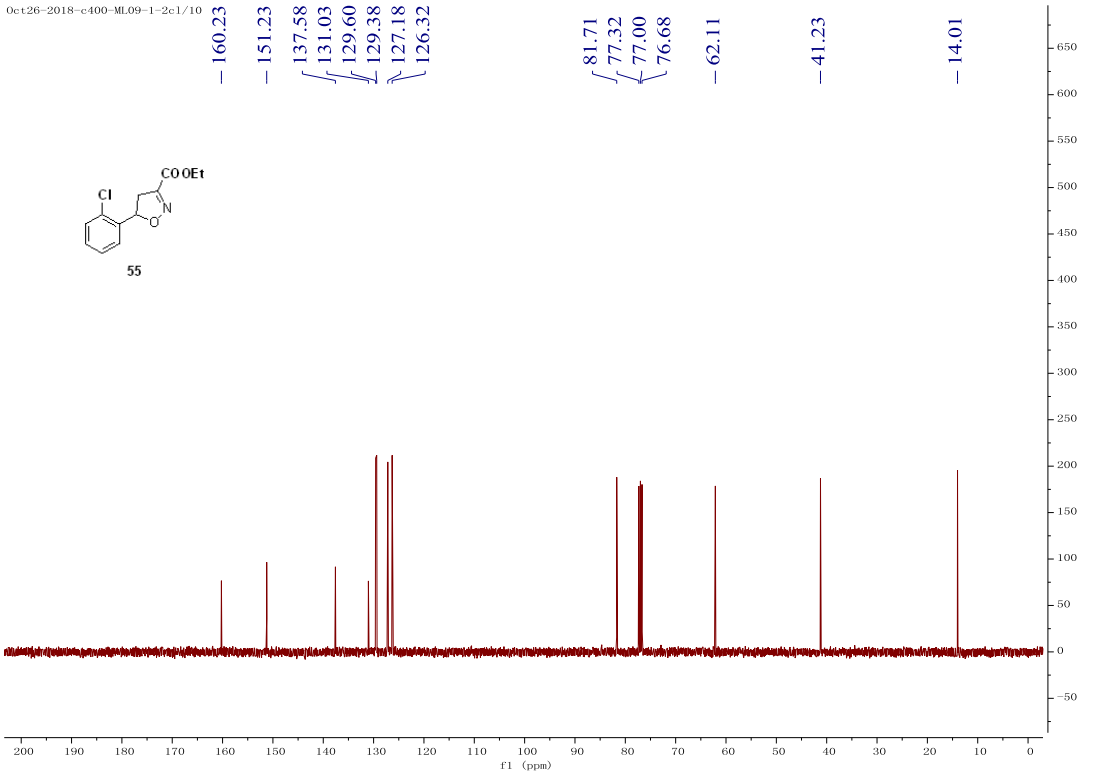

Oct25-2018-c400-ml09-1-3br/10
160.20
151.00
141.77
131.59
130.38
128.73
124.29
122.82
83.73
77.32
77.00
76.68
62.16
41.52
14.01
COOEt
Br
N
O
53
f1 (ppm)

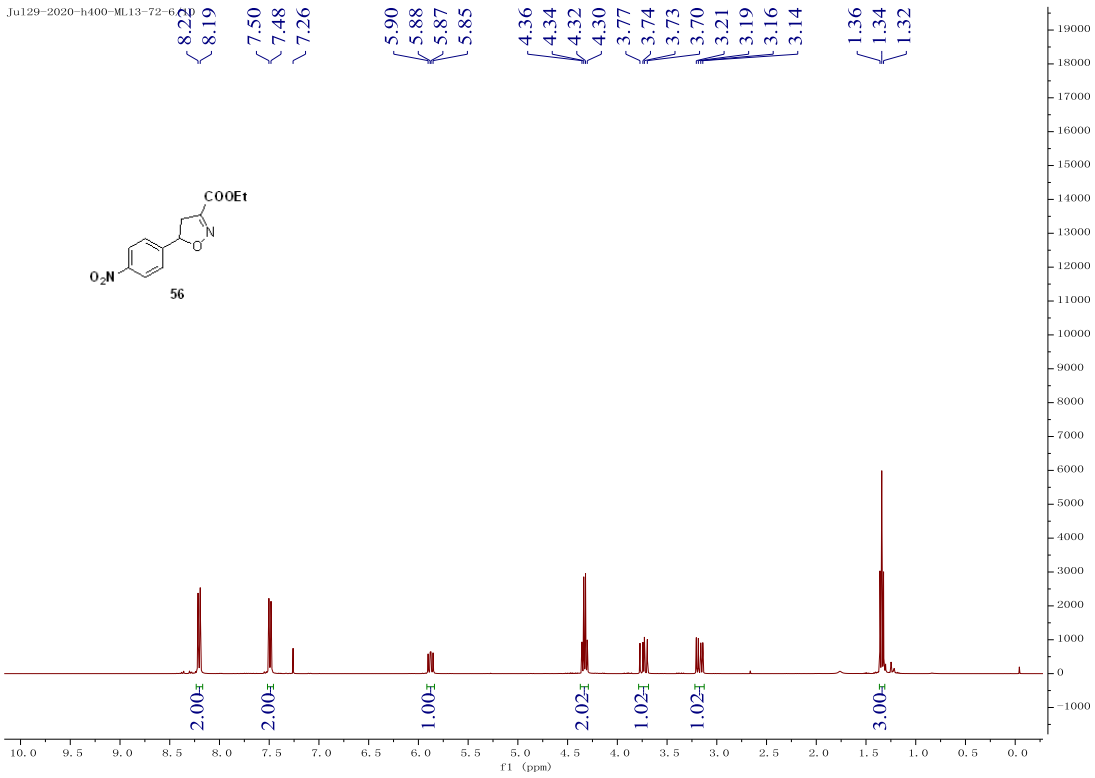

7.60
7.59
7.59
7.58
7.52
7.51
7.51
7.50
7.50
7.26
5.86
5.84
5.83
5.81
4.38
4.36
4.34
4.32
3.73
3.71
3.69
3.66
3.23
3.21
3.18
3.16
1.38
1.36
1.34
COOEt
F3C
N
O
54
1.97
2.00
0.98
2.00
1.01
1.00
2.99
f1 (ppm)

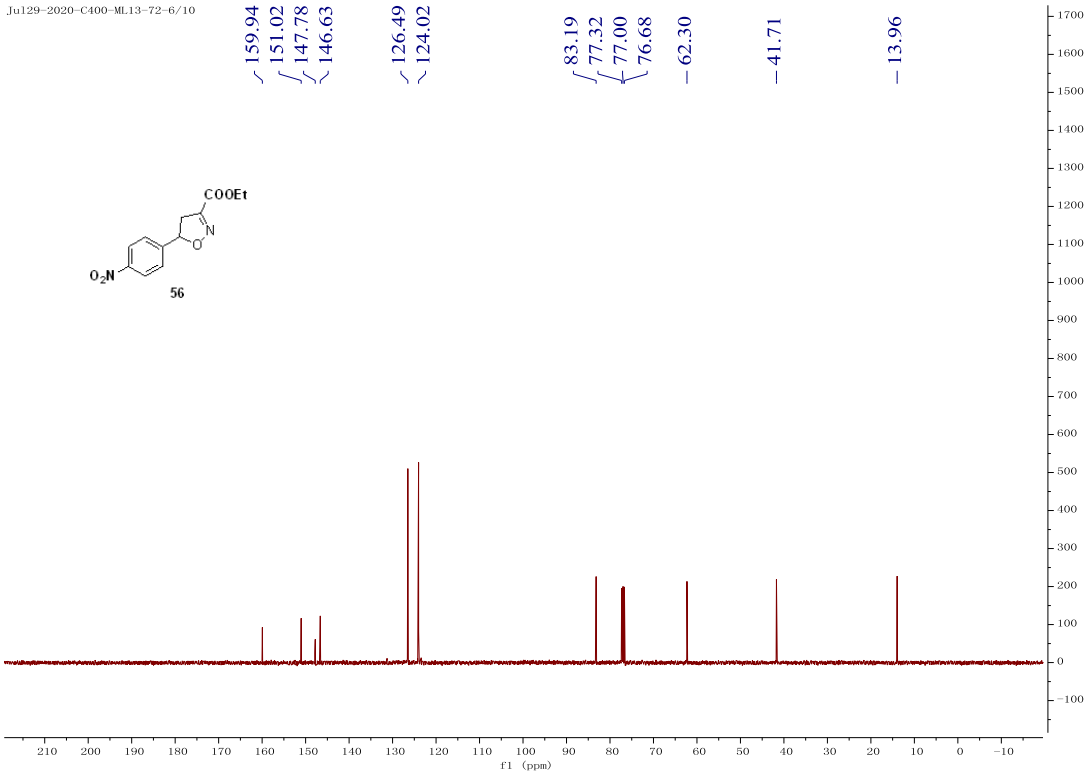

160.10
151.08
140.61
131.35
131.03
129.43
129.08
129.06
125.41
125.38
125.34
125.30
125.10
122.62
122.58
122.55
122.51
122.40
83.83
77.32
77.00
76.68
62.23
41.62
13.99
COOEt
F3C
N
O
54
f1 (ppm)

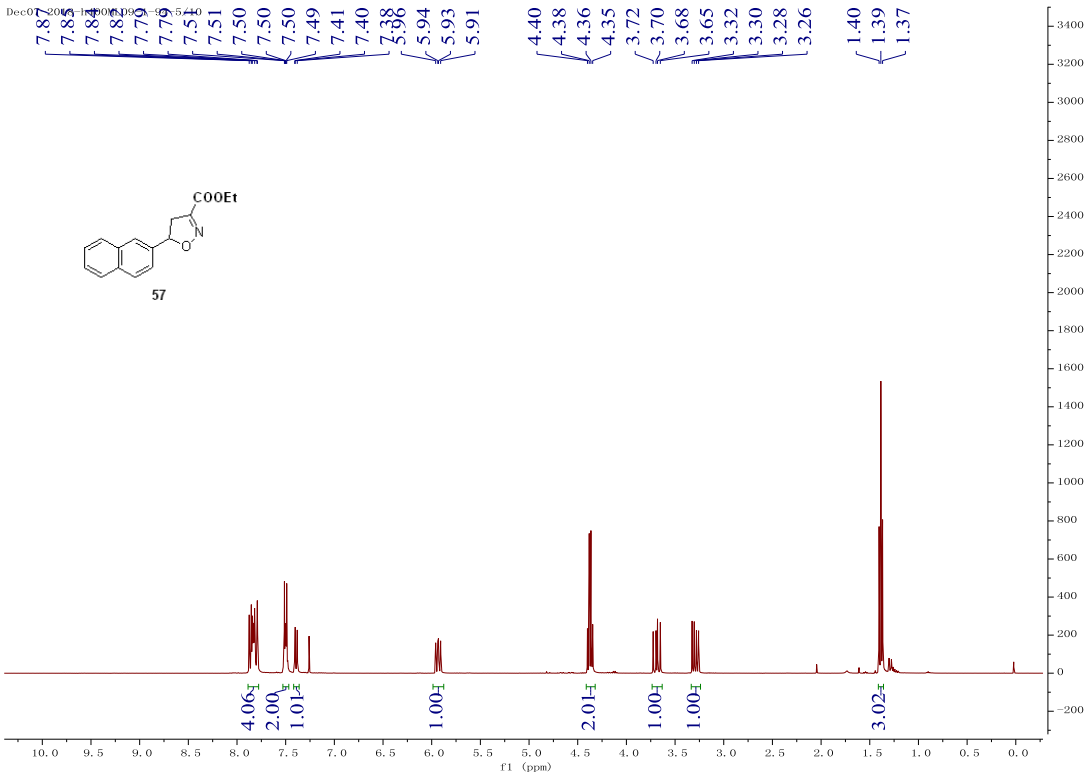

Nov05-2018-f400-m109-1-3cf3/10
-62.72
COOEt
F3C
N
O
54
f1 (ppm)

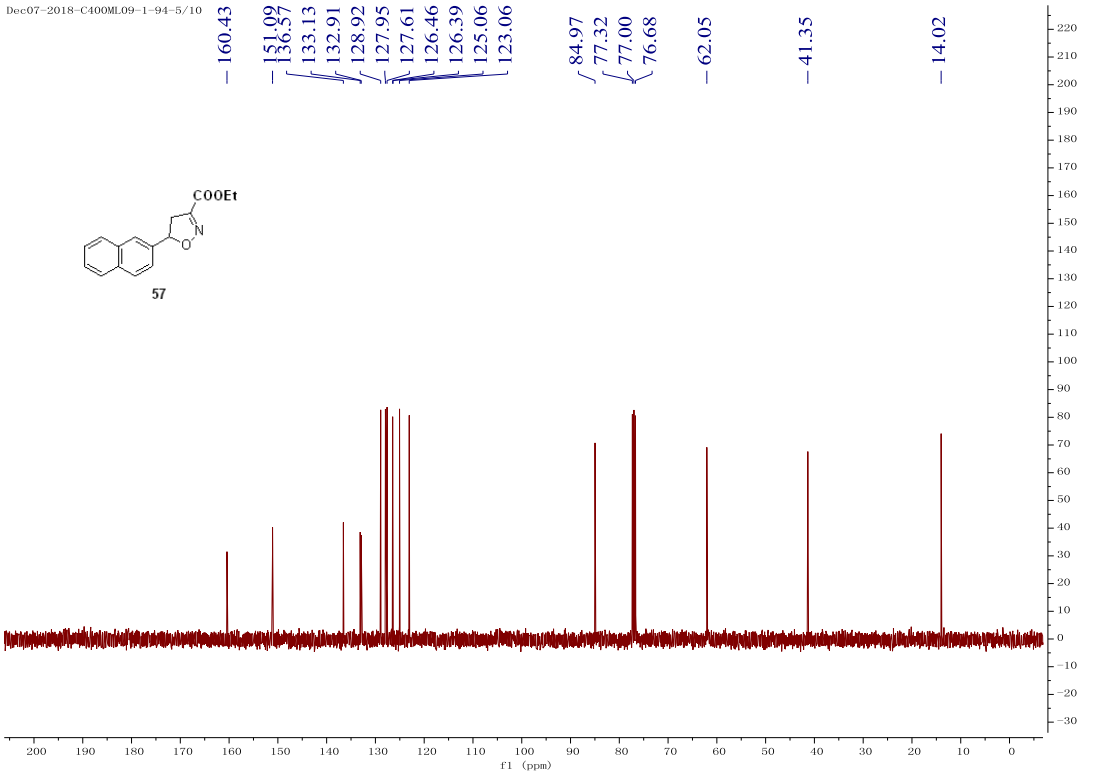

7.45 7.44 7.44 7.44 7.44 7.43 7.43 7.38 7.38 7.38 7.37 7.36 7.30 7.30 7.29 7.28 7.27 7.27 7.27 7.26 7.26 7.25 7.25 7.24 6.07 6.05 6.04 6.03 4.36 4.34 4.32 4.30 3.81 3.78 3.76 3.73 3.10 3.09 3.06 3.04 1.37 1.35 1.33
COOEt
Cl
N
O
55
1.00 1.01 2.01 0.97 1.99 1.01 1.00 3.01
f1 (ppm)

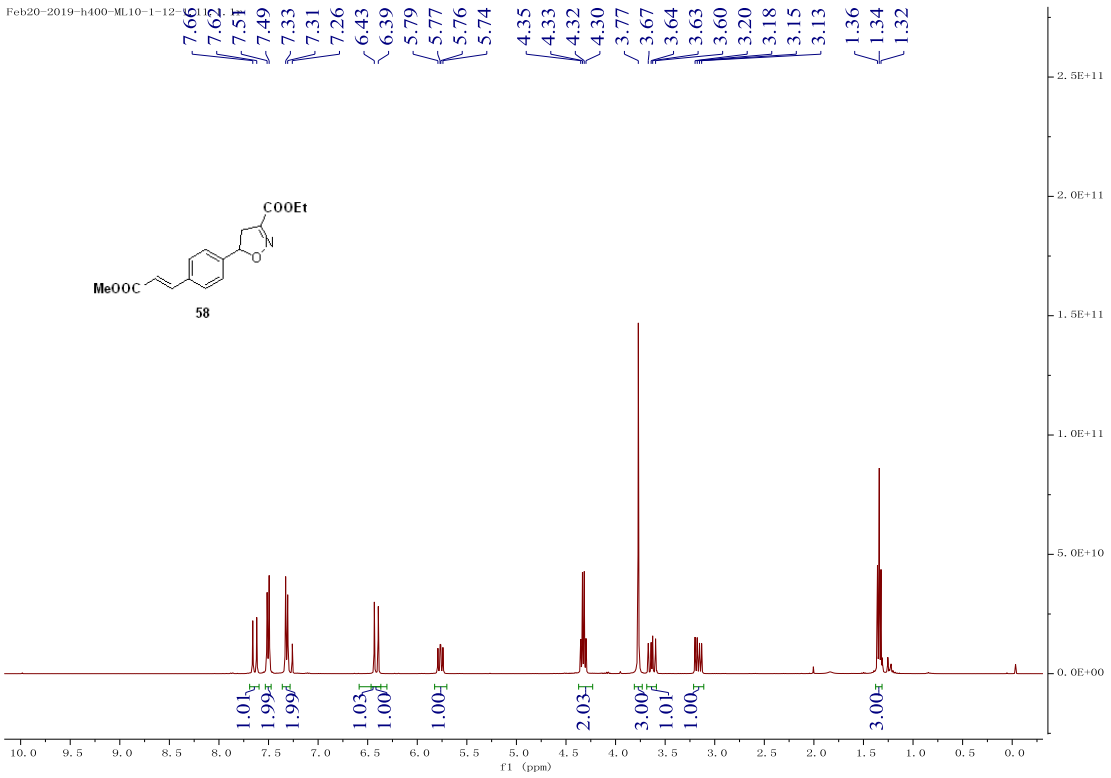

Oct26-2018-c400-ML09-1-2c1/10
160.23
151.23
137.58
131.03
129.60
129.38
127.18
126.32
81.71
77.32
77.00
76.68
62.11
41.23
14.01
COOEt
Cl
N
O
55
f1 (ppm)

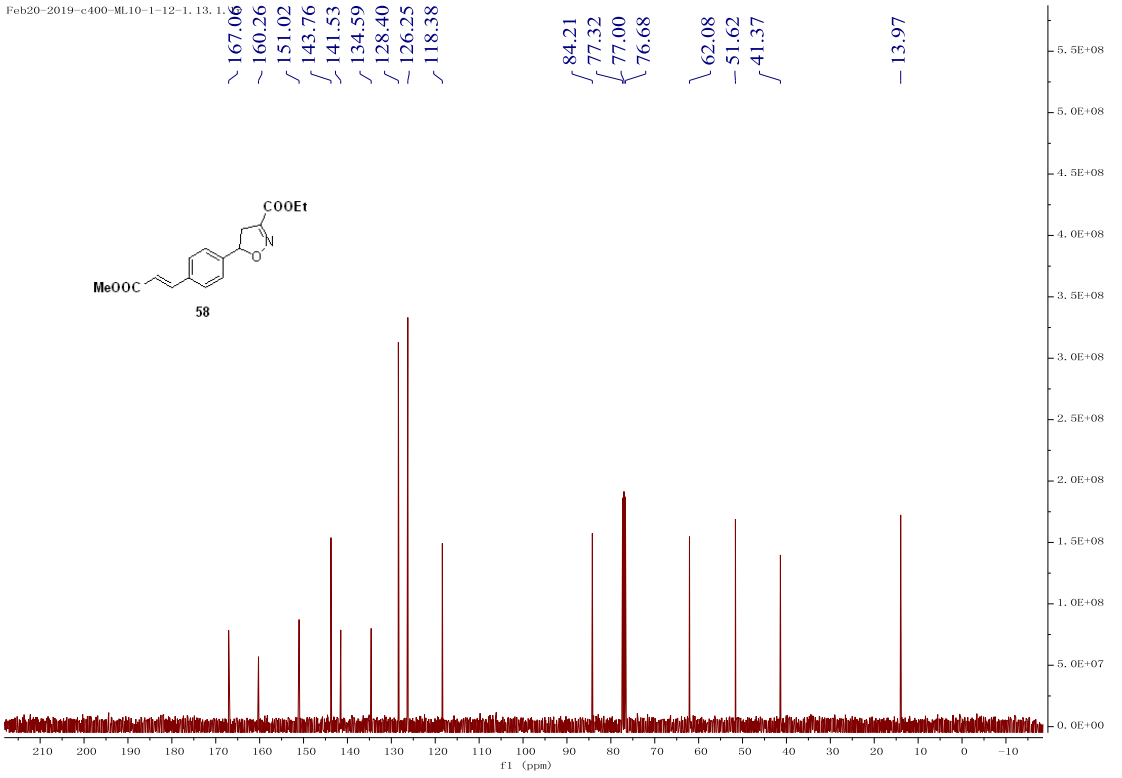

Ju129-2020-h400-ML13-72-6
8.22
8.19
7.50
7.48
7.26
5.90
5.88
5.87
5.85
4.36
4.34
4.32
4.30
3.77
3.74
3.73
3.70
3.21
3.19
3.16
3.14
1.36
1.34
1.32
COOEt
N
O
O2N
56
2.00
2.00
1.00
2.02
1.02
1.02
3.00
f1 (ppm)

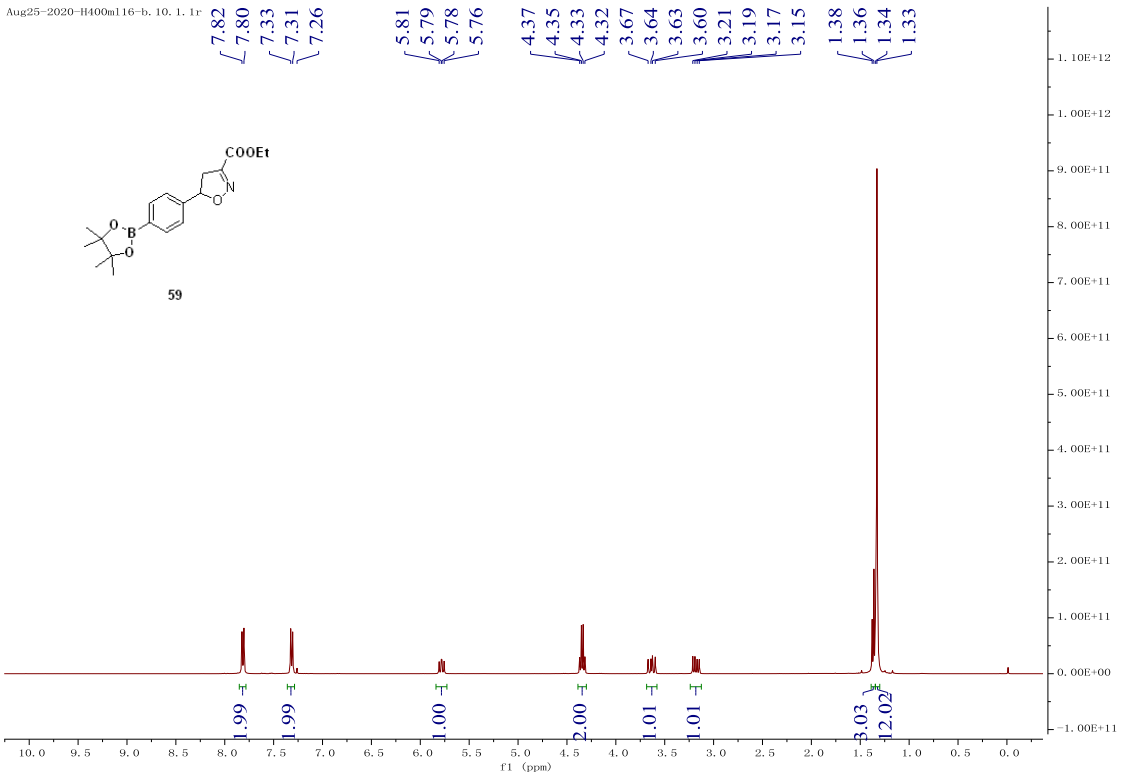

Ju129-2020-C400-ML13-72-6/10
159.94
151.02
147.78
146.63
126.49
124.02
83.19
77.32
77.00
76.68
62.30
41.71
13.96
COOEt
O2N
56
f1 (ppm)

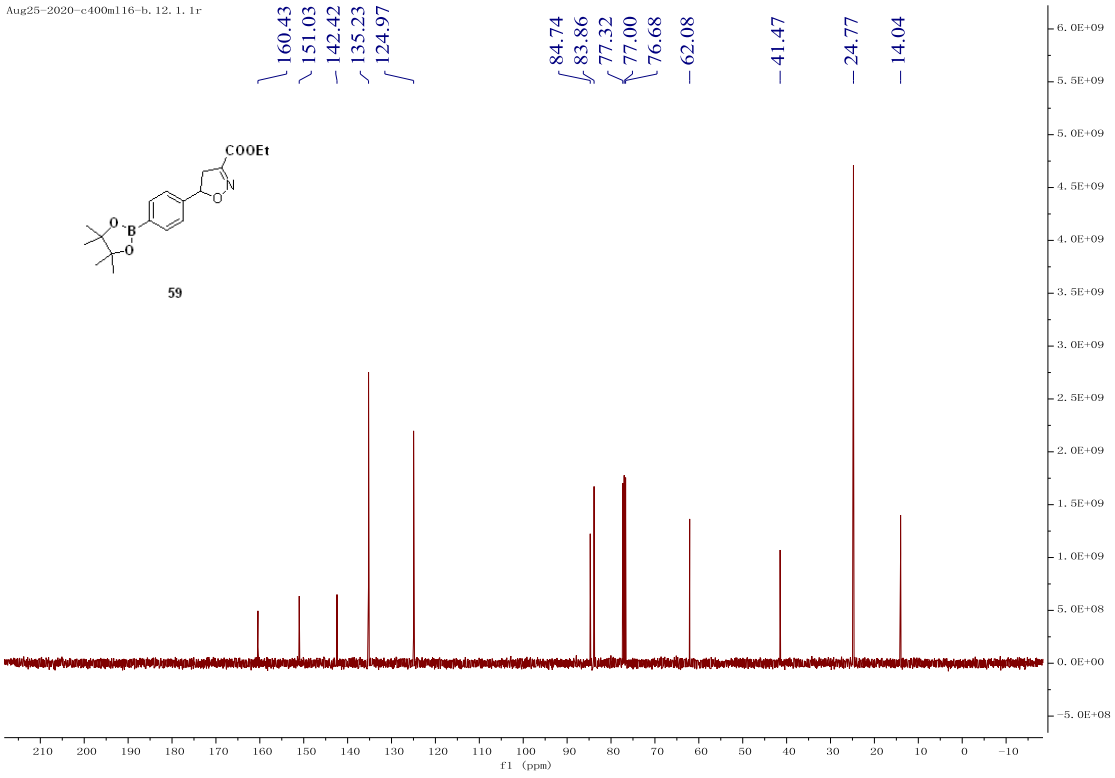

7.87
7.85
7.84
7.83
7.79
7.79
7.51
7.51
7.50
7.50
7.50
7.49
7.41
7.40
7.38
5.96
5.94
5.93
5.91
4.40
4.38
4.36
4.35
3.72
3.70
3.68
3.65
3.32
3.30
3.28
3.26
1.40
1.39
1.37
COOEt
57
4.06
2.00
1.01
1.00
2.01
1.00
1.00
3.02
f1 (ppm)

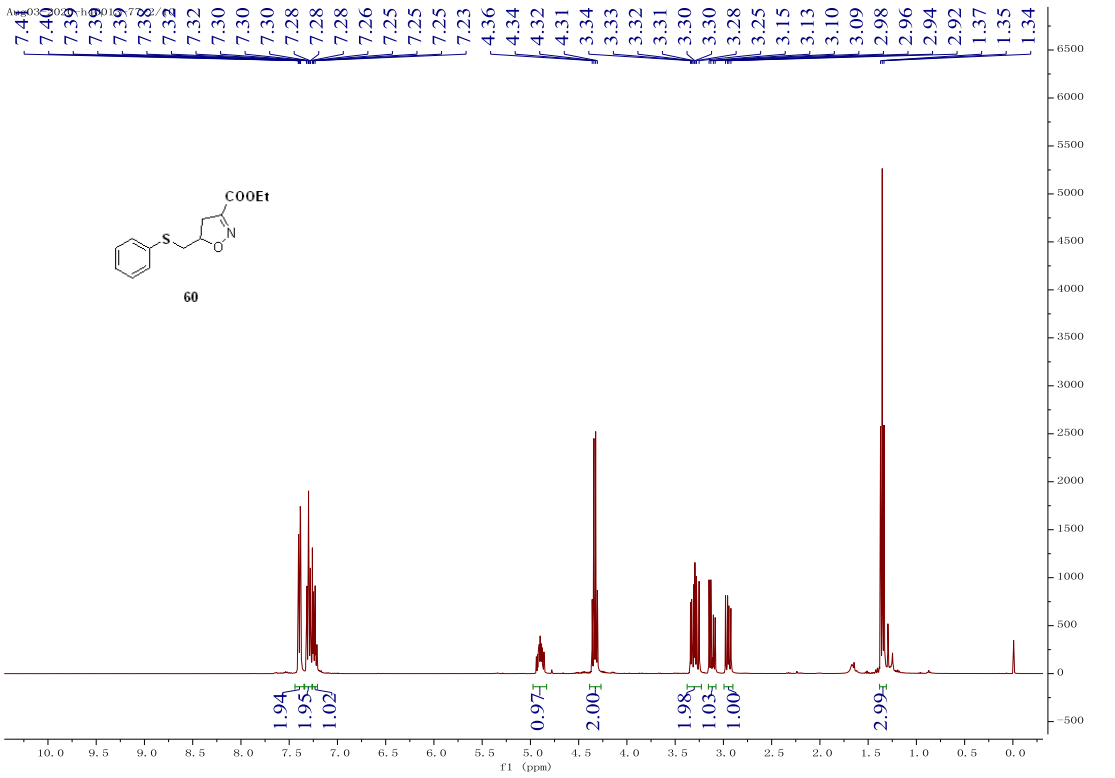

Dec07-2018-C400ML09-1-94-5/10
160.43
151.09
136.57
133.13
132.91
128.92
127.95
127.61
126.46
126.39
125.06
123.06
84.97
77.32
77.00
76.68
62.05
41.35
14.02
COOEt
N
O
57
f1 (ppm)


Feb20-2019-h400-ML10-1-12-1
7.66
7.62
7.51
7.49
7.33
7.31
7.26
6.43
6.39
5.79
5.77
5.76
5.74
4.35
4.33
4.32
4.30
3.77
3.67
3.64
3.63
3.60
3.20
3.18
3.15
3.13
1.36
1.34
1.32
COOEt
N
O
MeOOC
58
1.01
1.99
1.99
1.03
1.00
1.00
2.03
3.00
1.01
1.00
3.00
f1 (ppm)


Feb20-2019-c400-ML10-1-12-1.13.1.fid
167.06
160.26
151.02
143.76
141.53
134.59
128.40
126.25
118.38
84.21
77.32
77.00
76.68
62.08
51.62
41.37
13.97
COOEt
MeOOC
58
f1 (ppm)


Aug25-2020-H400ml16-b.10.1.1r
7.82
7.80
7.33
7.31
7.26
5.81
5.79
5.78
5.76
4.37
4.35
4.33
4.32
3.67
3.64
3.63
3.60
3.21
3.19
3.17
3.15
1.38
1.36
1.34
1.33
COOEt
59
1.99
1.99
1.00
2.00
1.01
1.01
3.03
12.02
f1 (ppm)


Aug25-2020-c400ml16-b. 12. 1. 1r
160.43
151.03
142.42
135.23
124.97
84.74
83.86
77.32
77.00
76.68
62.08
41.47
24.77
14.04
COOEt
59
f1 (ppm)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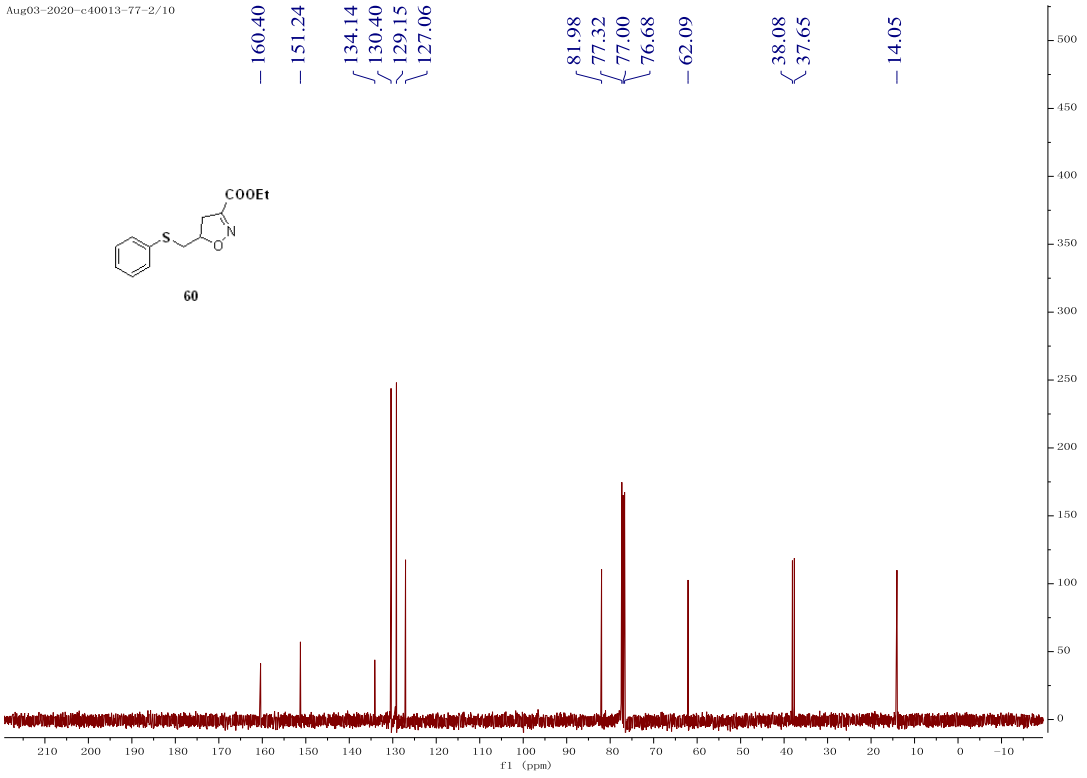
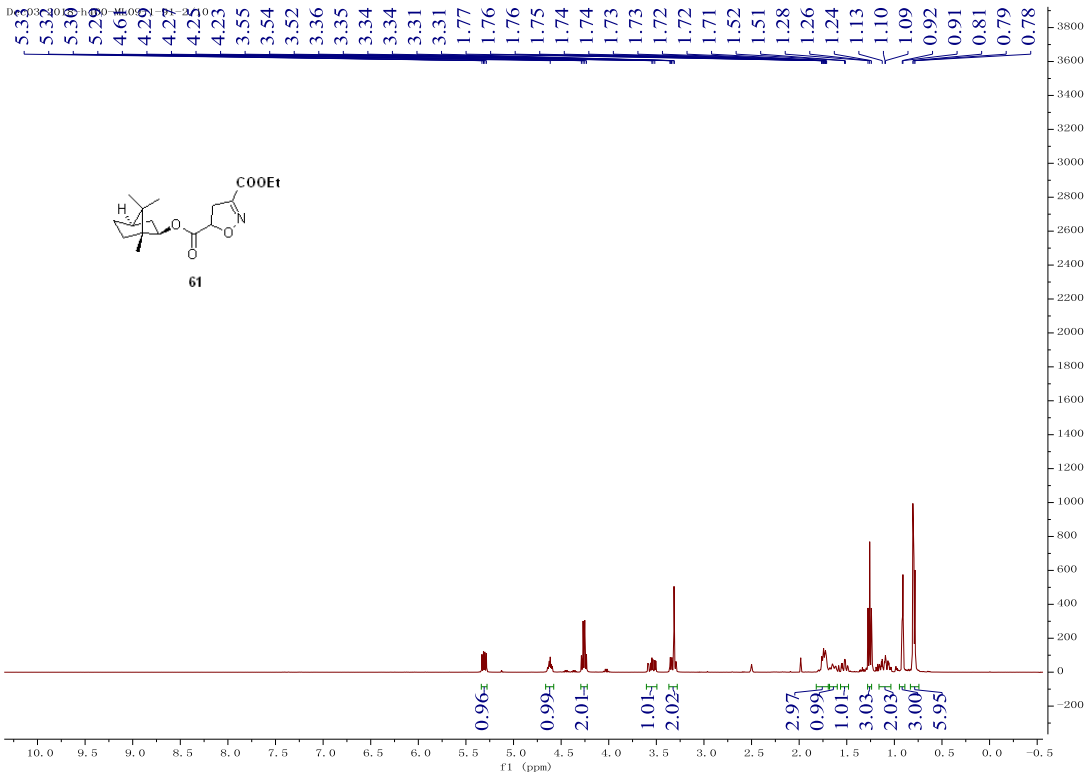
7.38
7.32
7.30
7.28
7.26
7.25
7.23
4.36
4.34
4.32
4.31
3.34
3.33
3.32
3.31
3.30
3.28
3.25
3.15
3.13
3.10
3.09
2.98
2.96
2.94
2.92
1.37
1.35
1.34
COOEt
60
1.94
1.95
1.02
0.97
2.00
1.98
1.03
1.00
2.99
f1 (ppm)


Aug03-2020-c40013-77-2/10
160.40
151.24
134.14
130.40
129.15
127.06
81.98
77.32
77.00
76.68
62.09
38.08
37.65
14.05
COOEt
S
N
O
60
f1 (ppm)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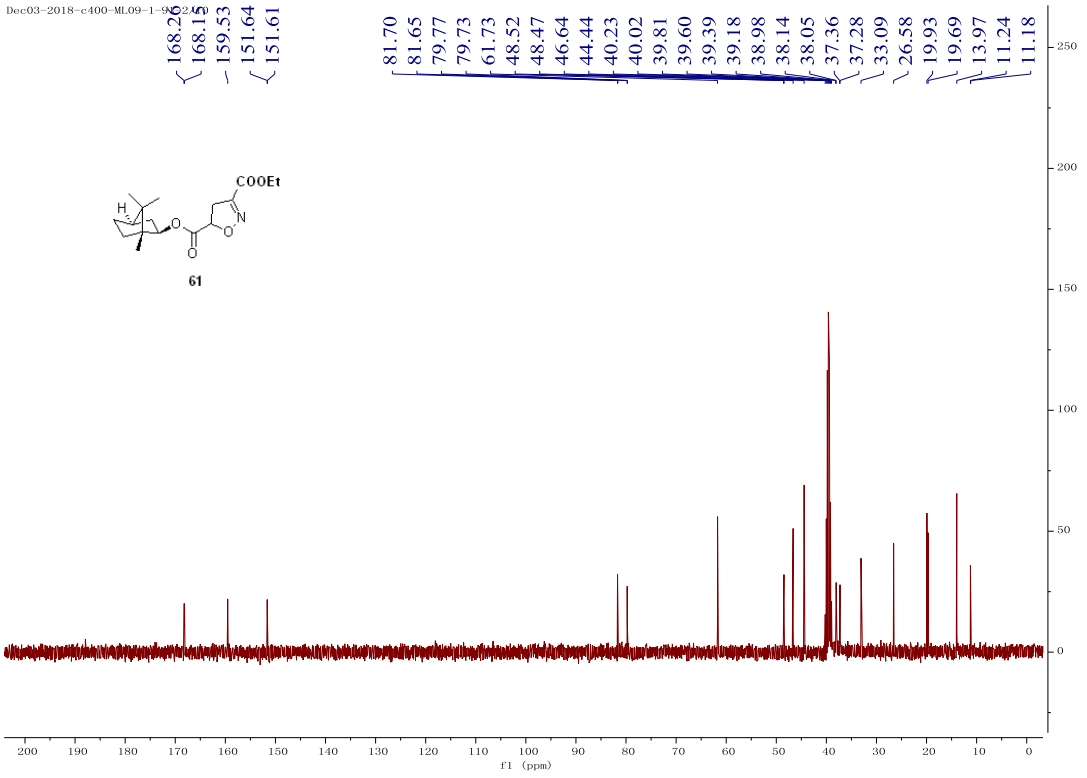
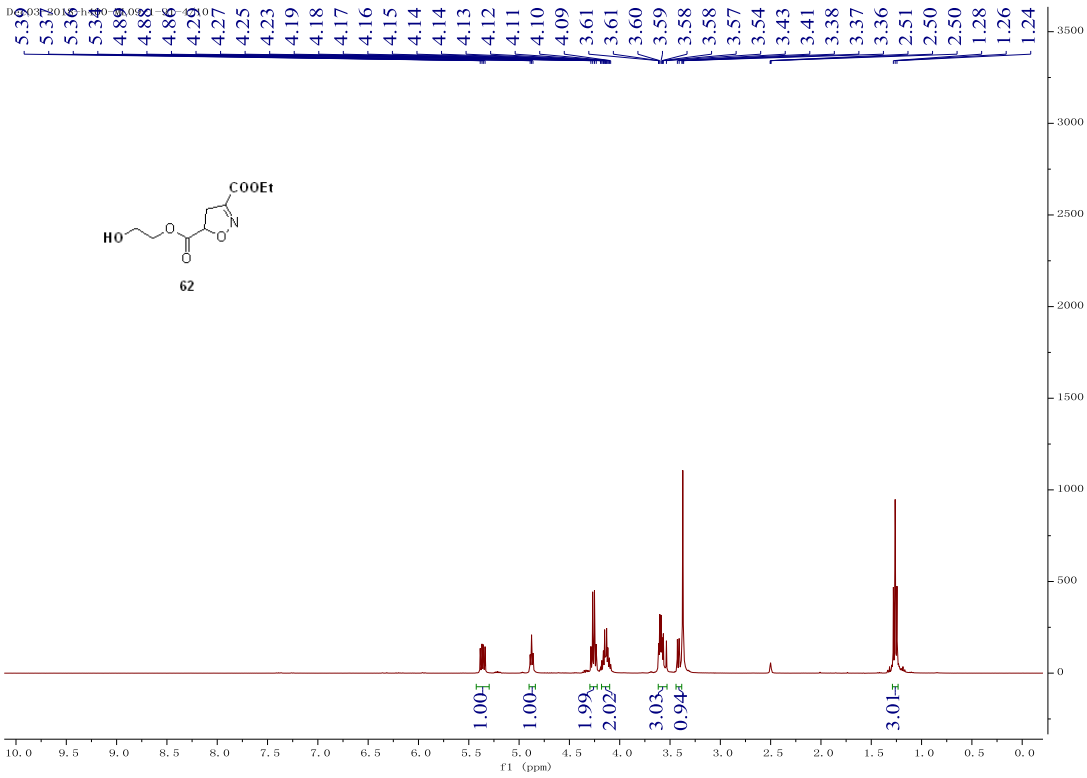
5.32
5.30
5.29
4.63
4.29
4.27
4.25
4.23
3.55
3.54
3.52
3.36
3.35
3.34
3.34
3.31
3.31
1.77
1.76
1.76
1.75
1.74
1.74
1.73
1.73
1.72
1.72
1.71
1.52
1.51
1.28
1.26
1.24
1.13
1.10
1.09
0.92
0.91
0.81
0.79
0.78
COOEt
H
O
N
O
O
61
0.96
0.99
2.01
1.01
2.02
2.97
0.99
1.01
3.03
2.03
3.00
5.95
f1 (ppm)


168.26
168.15
159.53
151.64
151.61
81.70
81.65
79.77
79.73
61.73
48.52
48.47
46.64
44.44
40.23
40.02
39.81
39.60
39.39
39.18
38.98
38.14
38.05
37.36
37.28
33.09
26.58
19.93
19.69
13.97
11.24
11.18
COOEt
61
f1 (ppm)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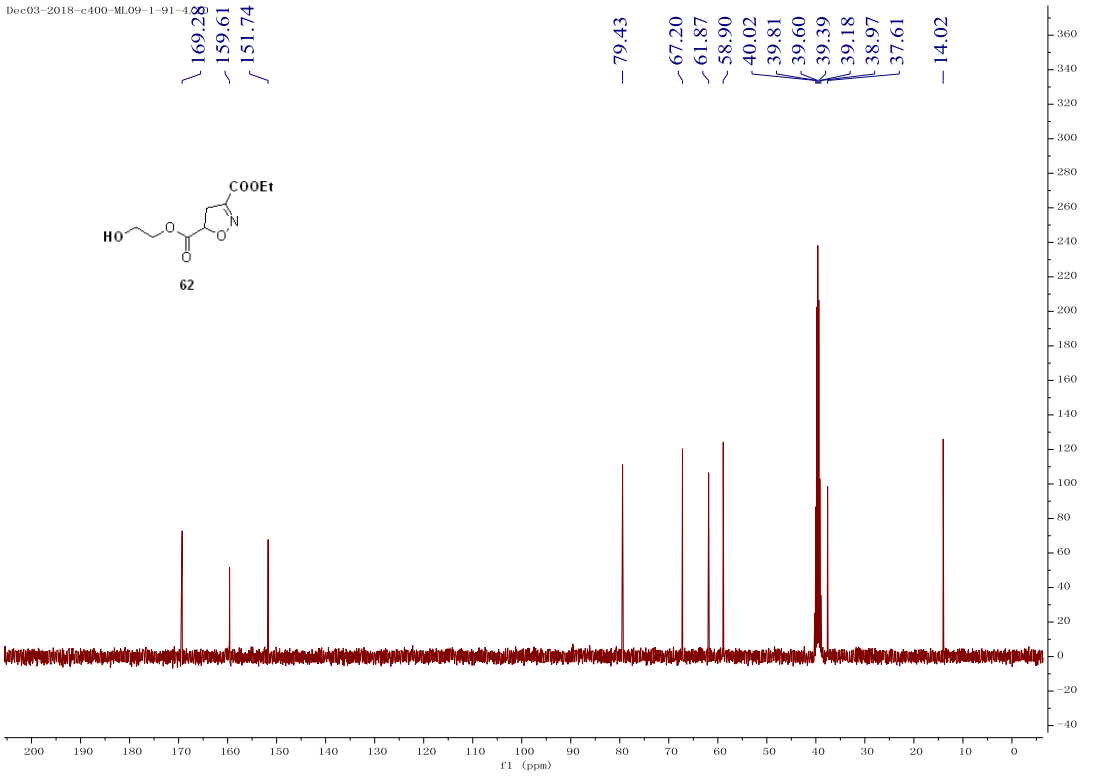
4.29
4.27
4.25
4.23
4.19
4.18
4.17
4.16
4.15
4.14
4.14
4.13
4.12
4.11
4.10
4.09
3.61
3.61
3.60
3.59
3.58
3.58
3.57
3.54
3.43
3.41
3.38
3.37
3.36
2.51
2.50
2.50
1.28
1.26
1.24
COOEt
HO
62
1.00
1.00
1.99
2.02
3.03
0.94
3.01
f1 (ppm)


Dec03-2018-c400-ML09-1-91-4
169.28
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151.74
79.43
67.20
61.87
58.90
40.02
39.81
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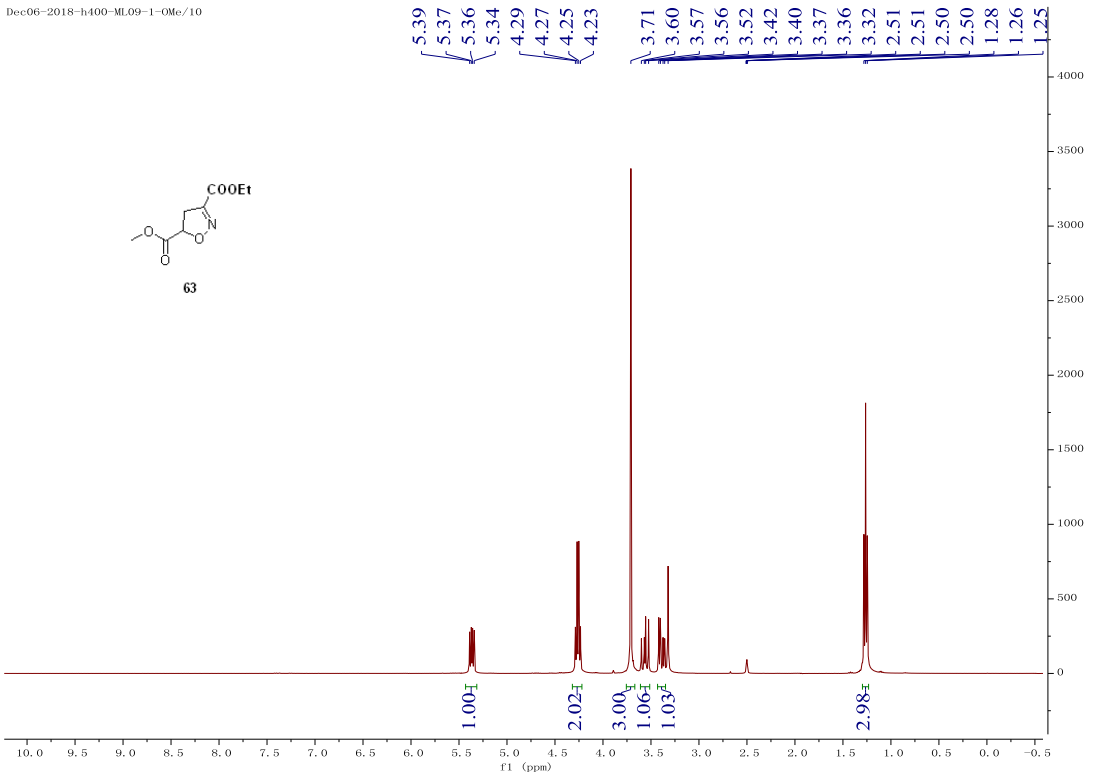
39.39
39.18
38.97
37.61
14.02
COOEt
HO
O
N
O
O
62
f1 (ppm)


Dec06-2018-h400-ML09-1-OMe/10
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5.37
5.36
5.34
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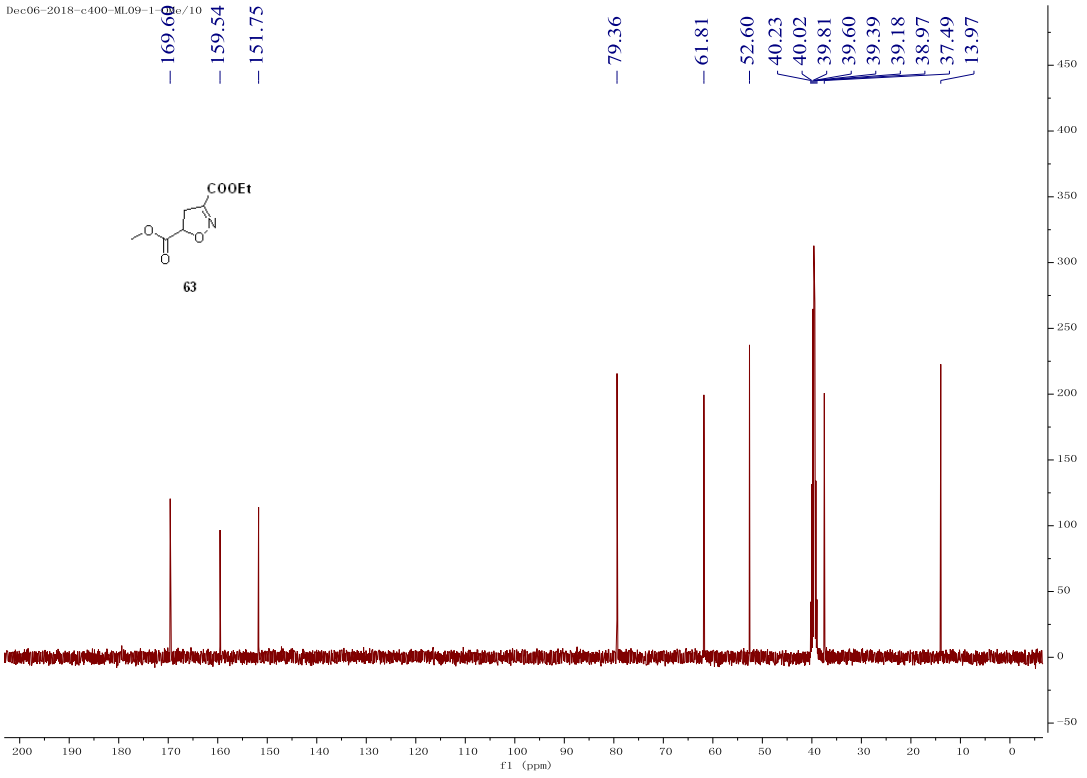
4.27
4.25
4.23
3.71
3.60
3.57
3.56
3.52
3.42
3.40
3.37
3.36
3.32
2.51
2.51
2.50
2.50
1.28
1.26
1.25
COOEt
O
N
O
O
63
1.00
2.02
3.00
1.06
1.03
2.98
f1 (ppm)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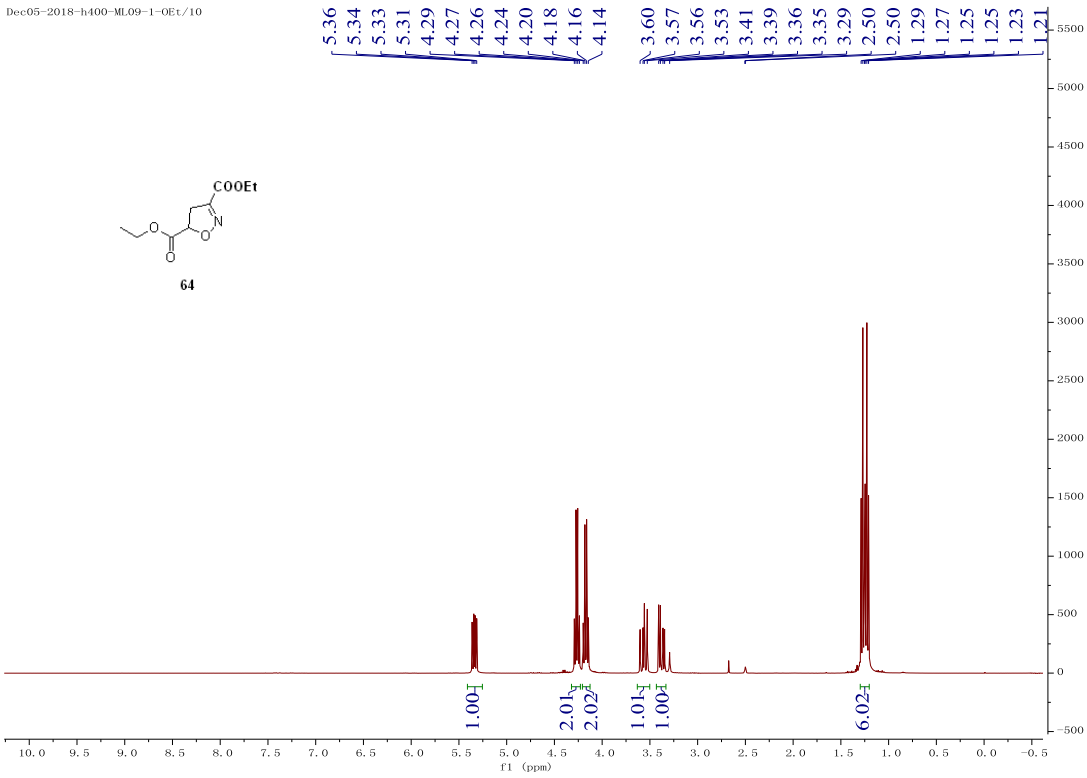
61.81
52.60
40.23
40.02
39.81
39.60
39.39
39.18
38.97
37.49
13.97
COOEt
63
f1 (ppm)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5.31
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4.27
4.26
4.24
4.20
4.18
4.16
4.14
3.60
3.57
3.56
3.53
3.41
3.39
3.36
3.35
3.29
2.50
2.50
1.29
1.27
1.25
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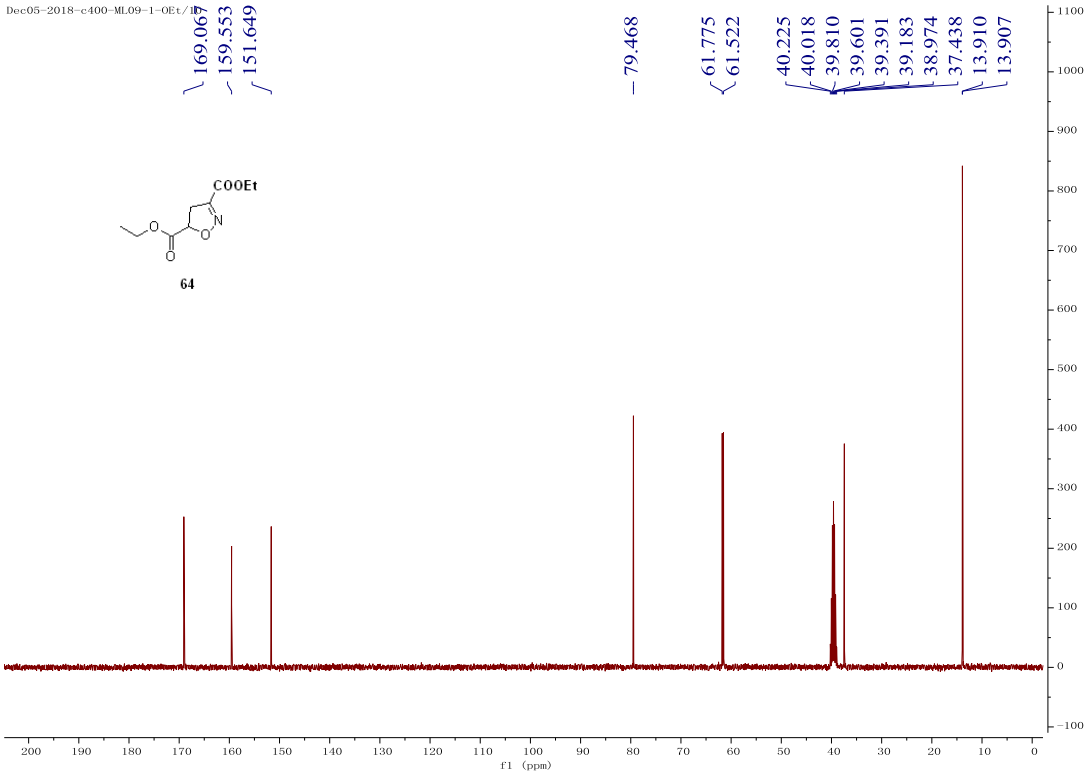
1.01
1.00
6.02
COOEt
64
f1 (ppm)


Dec05-2018-c400-ML09-1-OEt/1
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79.468
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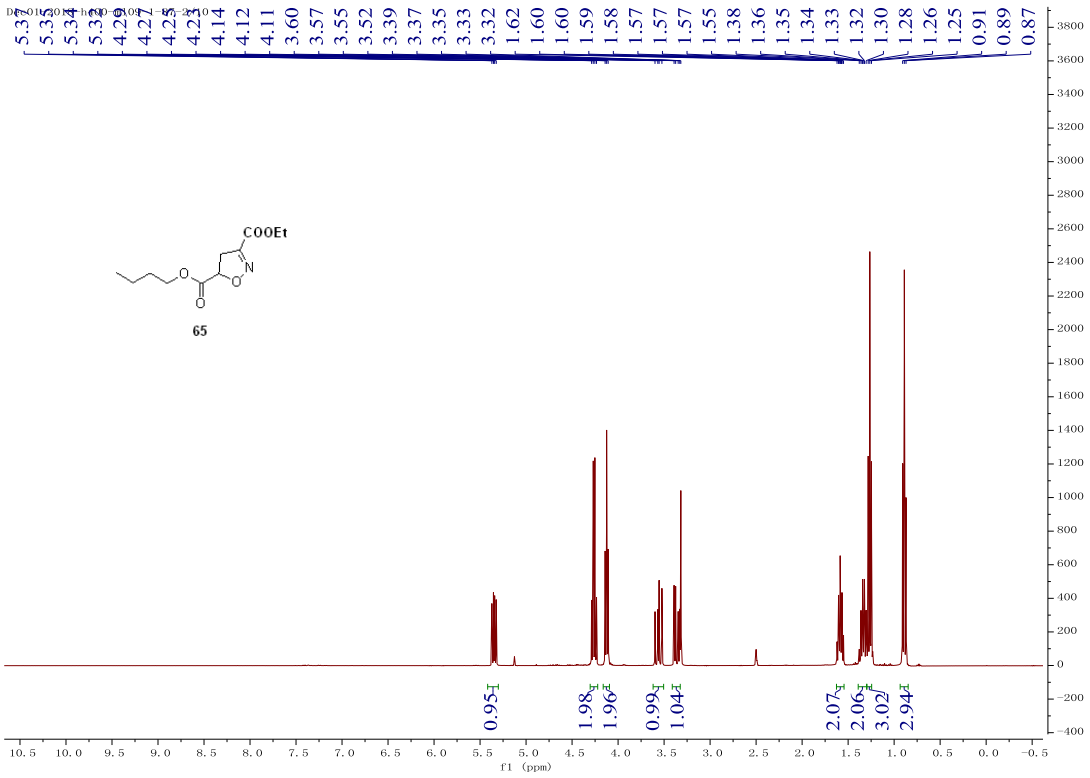
61.522
40.225
40.018
39.810
39.601
39.391
39.183
38.974
37.438
13.910
13.907
COOEt
64
f1 (ppm)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5.32
4.29
4.27
4.25
4.23
4.14
4.12
4.11
3.60
3.57
3.55
3.52
3.39
3.37
3.35
3.33
3.32
1.62
1.60
1.60
1.59
1.58
1.57
1.57
1.57
1.55
1.38
1.36
1.35
1.34
1.33
1.32
1.30
1.28
1.26
1.25
0.91
0.89
0.87
COOEt
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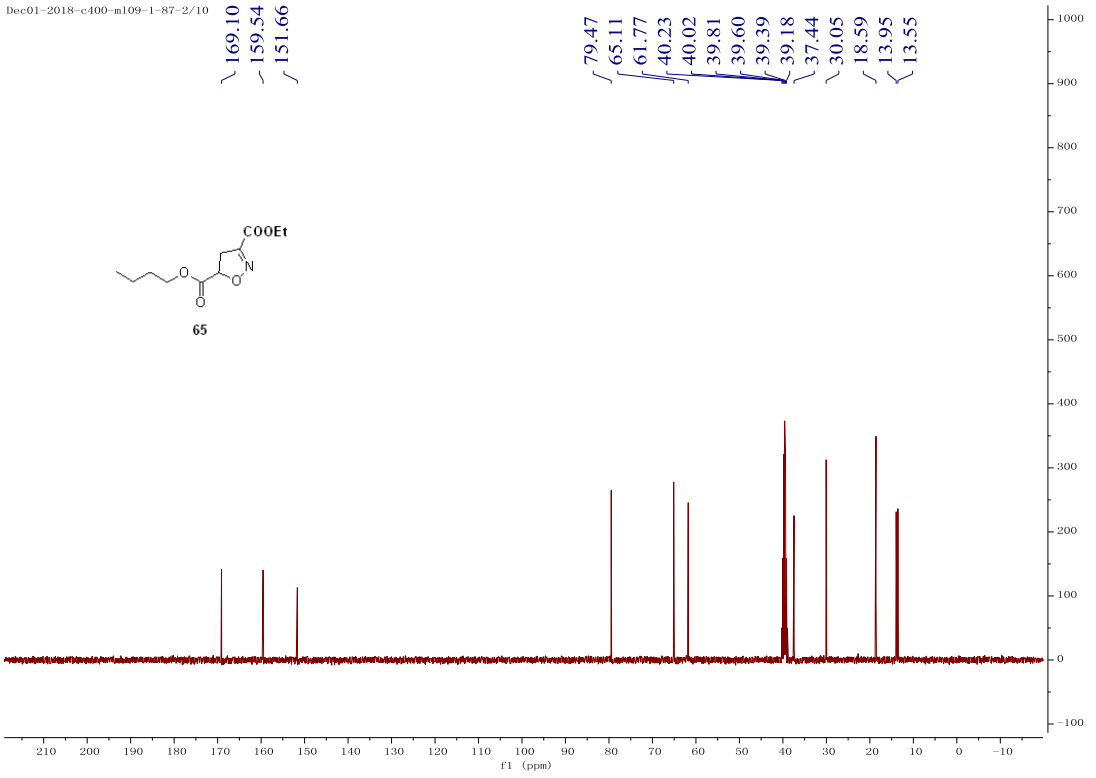
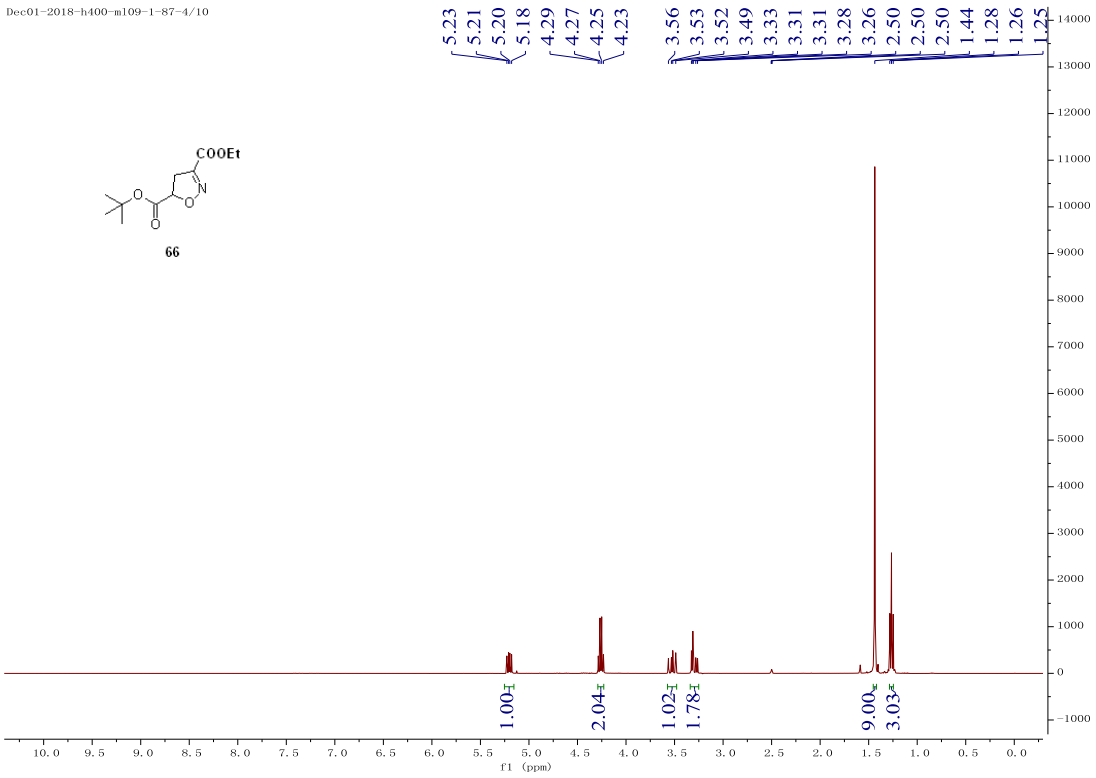
1.98
1.96
0.99
1.04
2.07
2.06
3.02
2.94
f1 (ppm)


Dec01-2018-c400-m109-1-87-2/10
169.10
159.54
151.66
79.47
65.11
61.77
40.23
40.02
39.81
39.60
39.39
39.18
37.44
30.05
18.59
13.95
13.55
COOEt
65
f1 (ppm)


Dec01-2018-h400-m109-1-87-4/10
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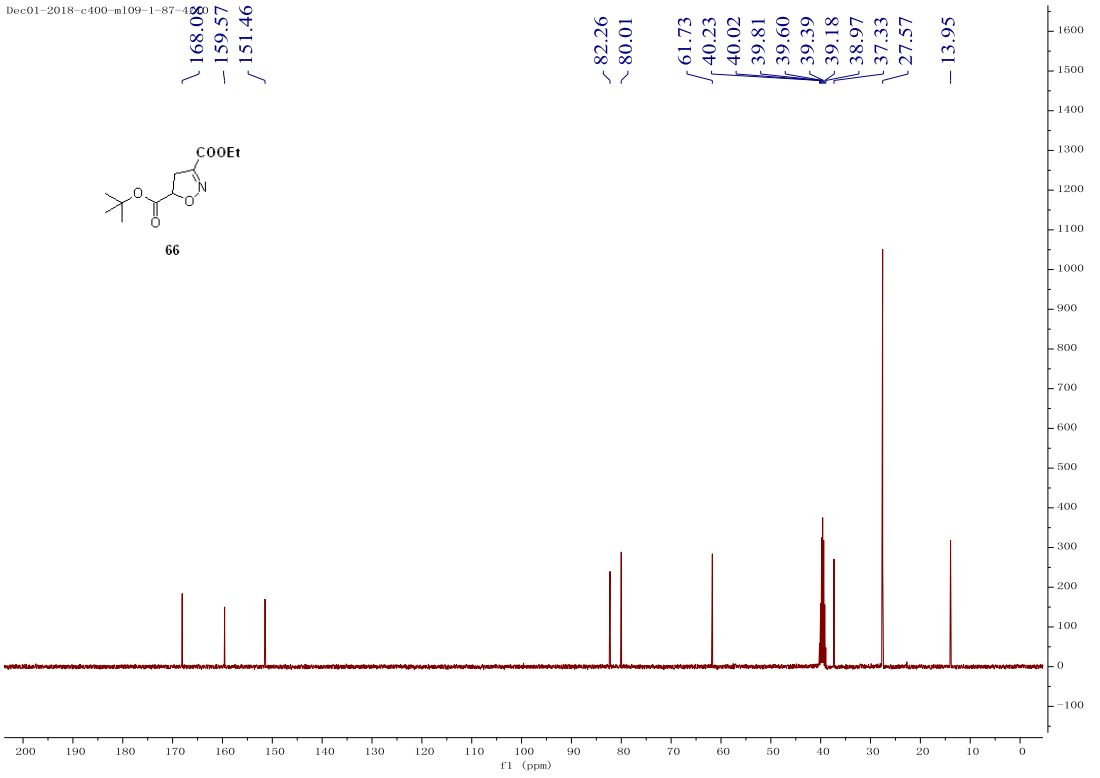
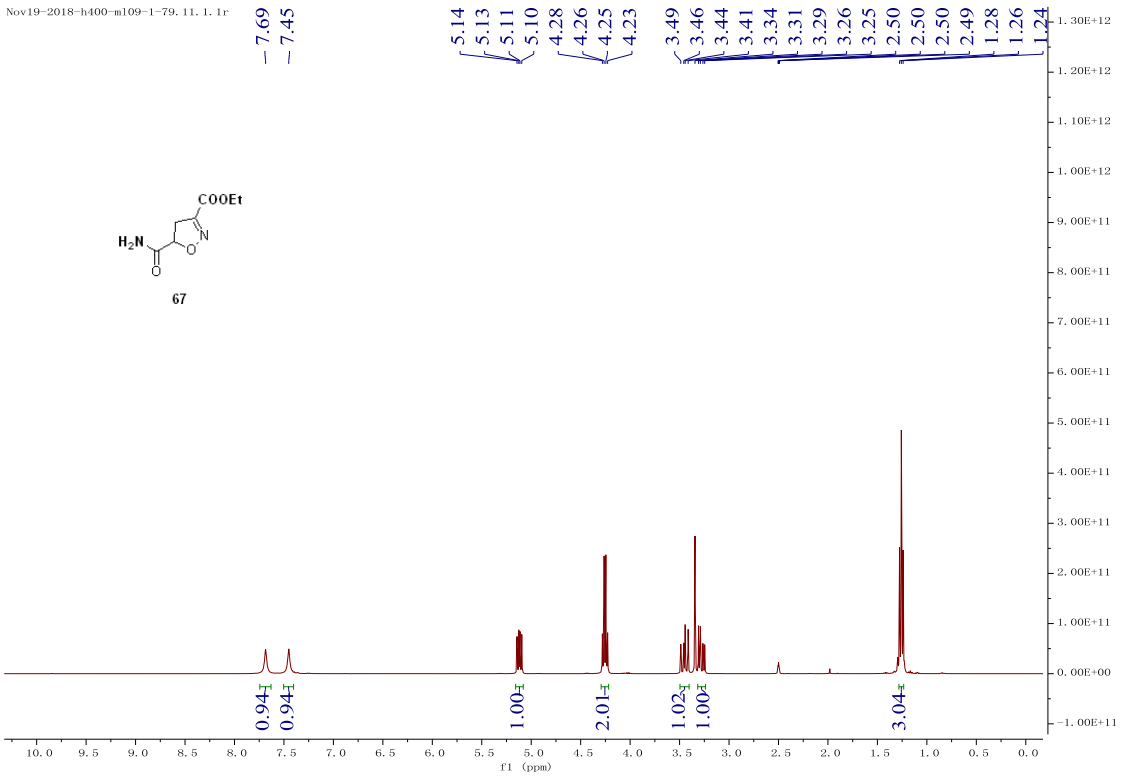
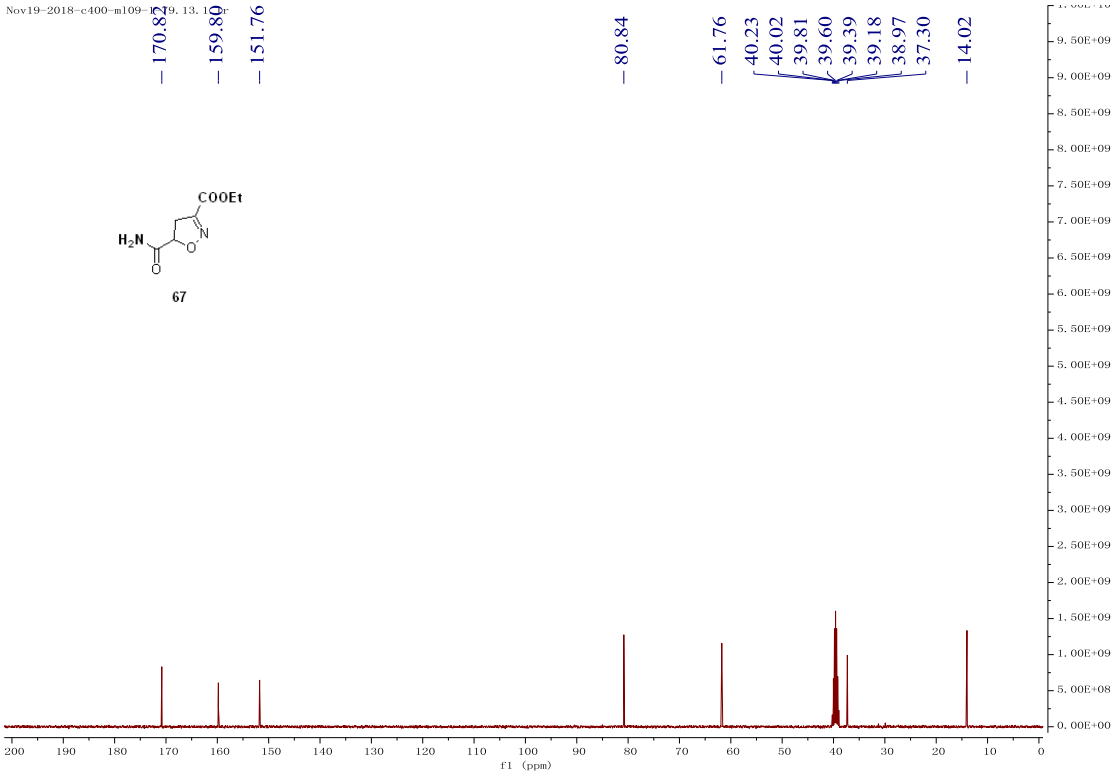
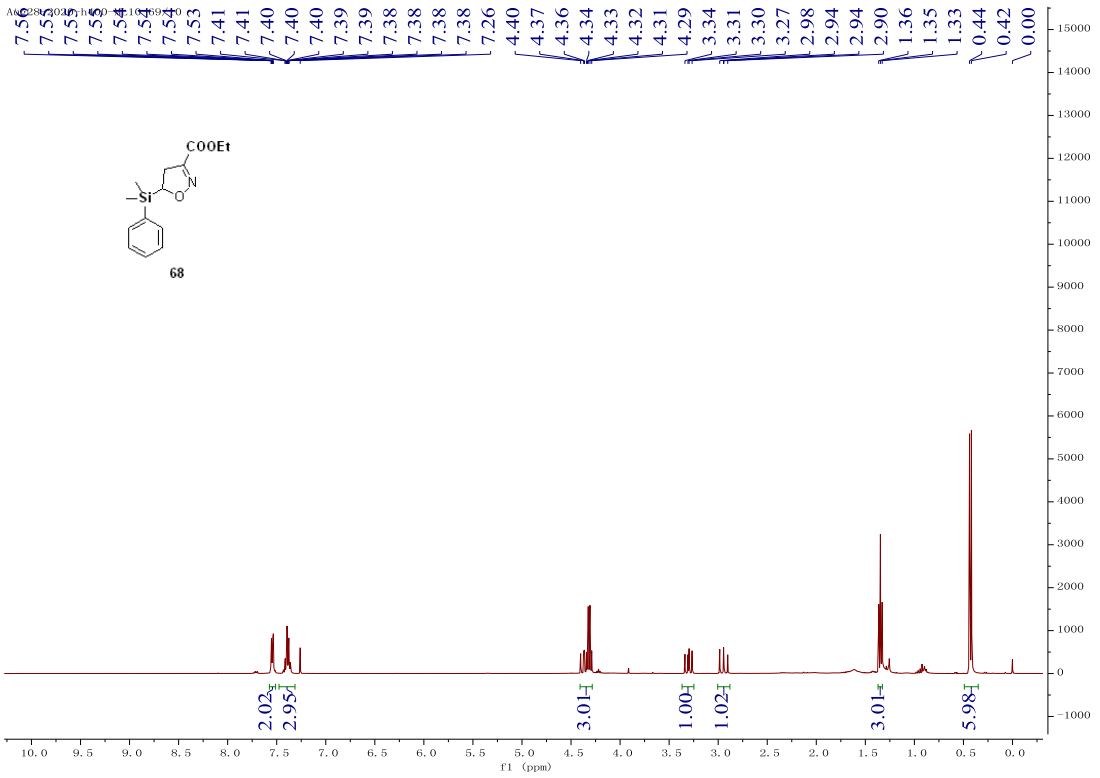
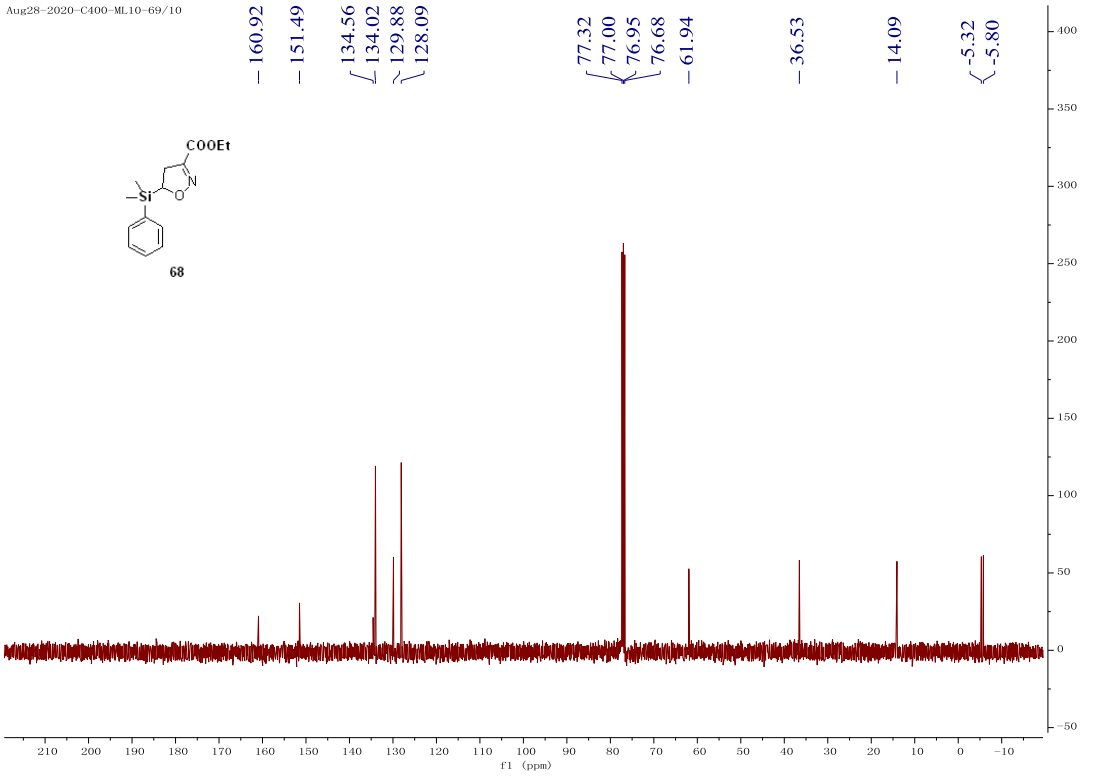
5.20
5.18
4.29
4.27
4.25
4.23
3.56
3.53
3.52
3.49
3.33
3.31
3.31
3.28
3.26
2.50
2.50
2.50
1.44
1.28
1.26
1.25
COOEt
66
1.00
2.04
1.02
1.78
9.00
3.03
f1 (ppm)

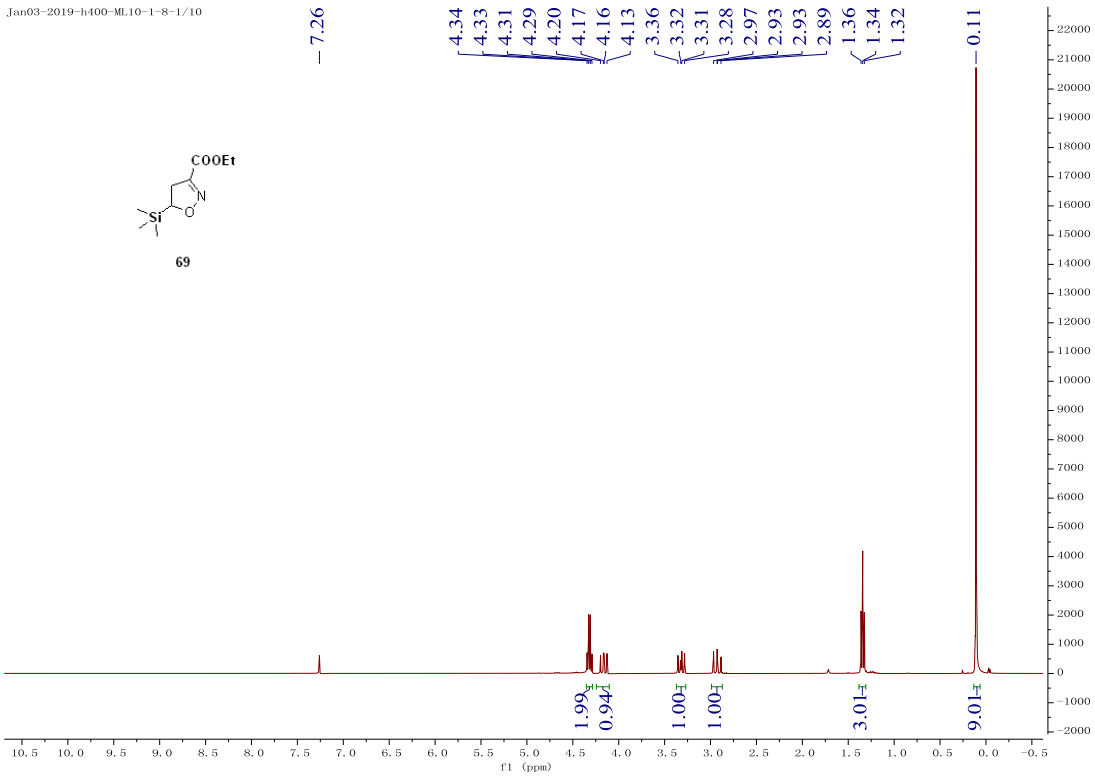

168.08
159.57
151.46
82.26
80.01
61.73
40.23
40.02
39.81
39.60
39.39
39.18
38.97
37.33
27.57
13.95
COOEt
66
f1 (ppm)

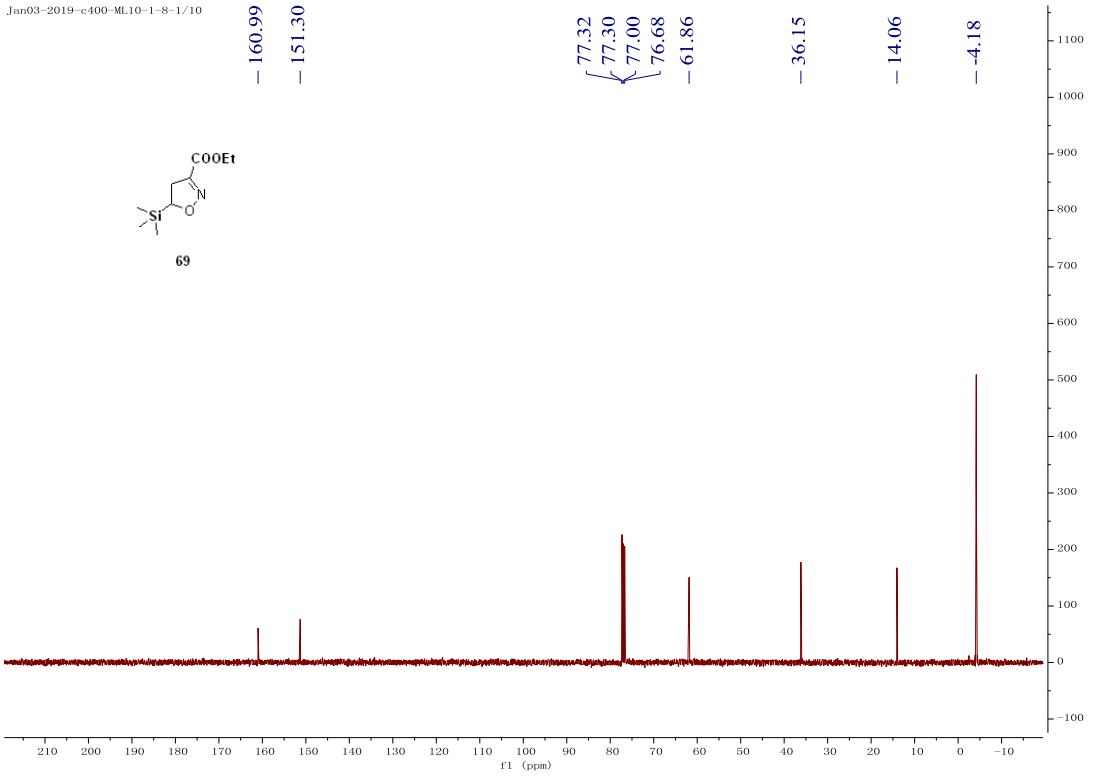

7.69
7.45
5.14
5.13
5.11
5.10
4.28
4.26
4.25
4.23
3.49
3.46
3.44
3.41
3.34
3.31
3.29
3.26
3.25
2.50
2.50
2.50
2.49
1.28
1.26
1.24
COOEt
67
0.94
0.94
1.00
2.01
1.02
1.00
3.04
f1 (ppm)

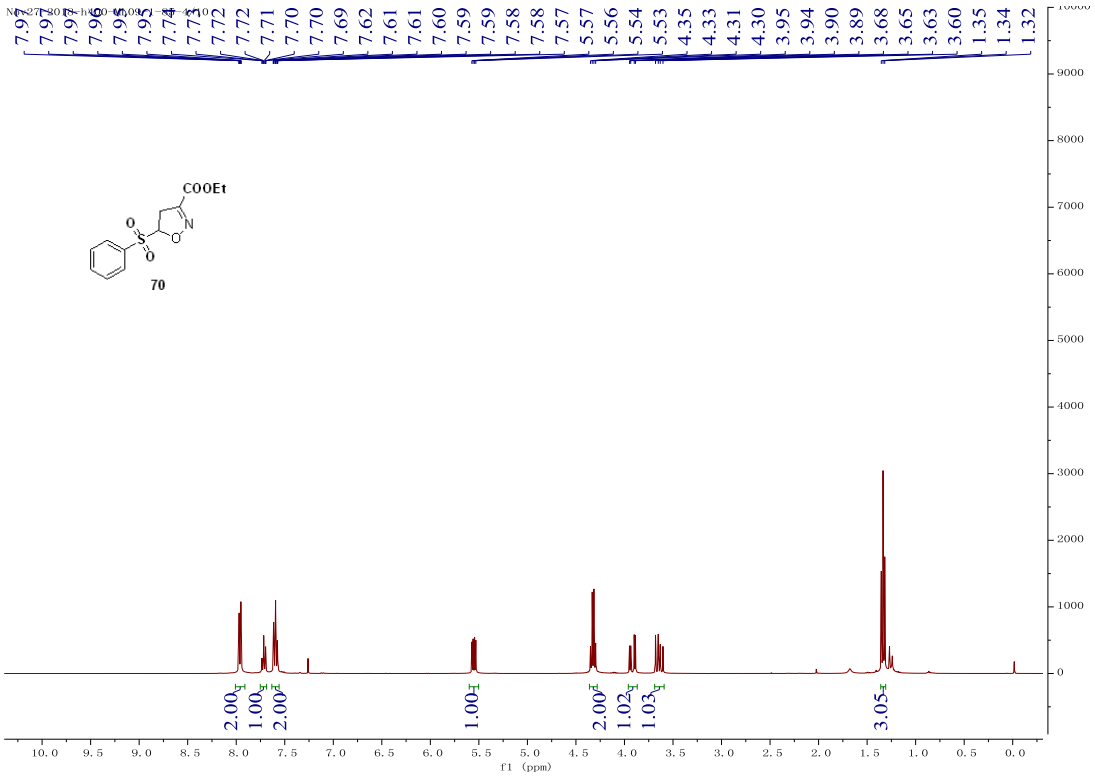

170.82
159.80
151.76
80.84
61.76
40.23
40.02
39.81
39.60
39.39
39.18
38.97
37.30
14.02
COOEt
H2N
O
N
O
67
f1 (ppm)

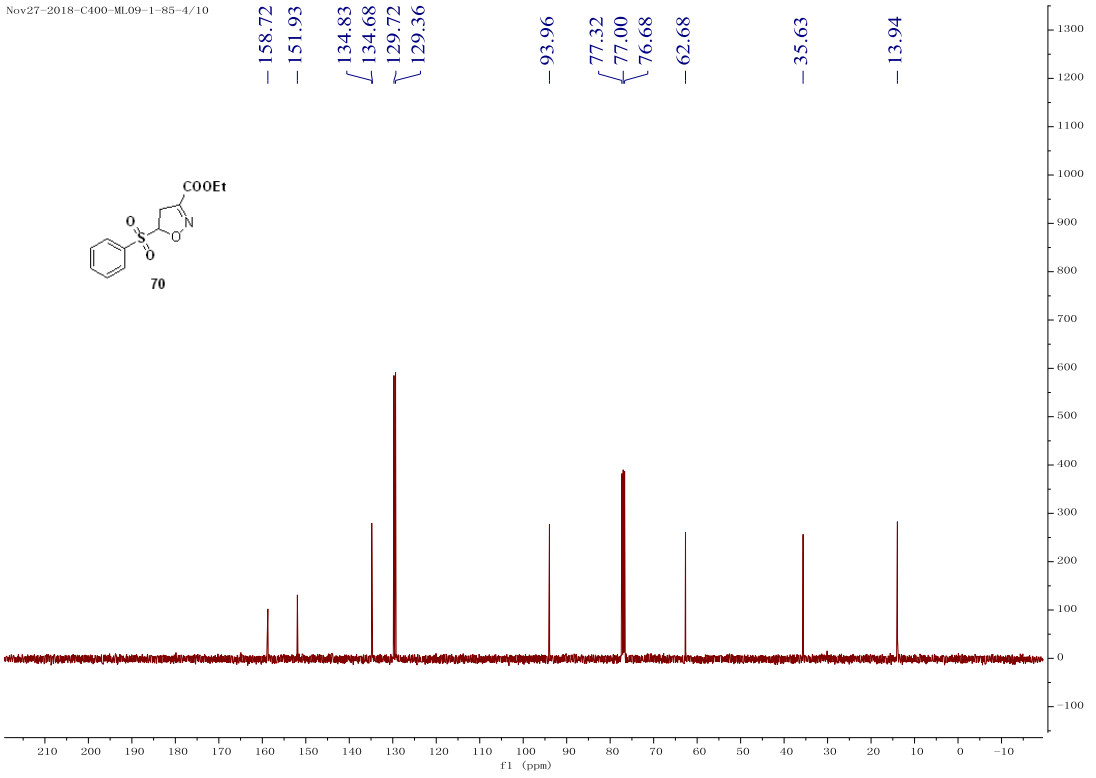

7.56
7.55
7.55
7.55
7.54
7.54
7.54
7.53
7.41
7.41
7.40
7.40
7.40
7.39
7.39
7.38
7.38
7.38
7.26
4.40
4.37
4.36
4.34
4.33
4.32
4.31
4.29
3.34
3.31
3.30
3.27
2.98
2.94
2.94
2.90
1.36
1.35
1.33
0.44
0.42
0.00
COOEt
Si
O
N
68
2.02
2.95
3.01
1.00
1.02
3.01
5.98
f1 (ppm)

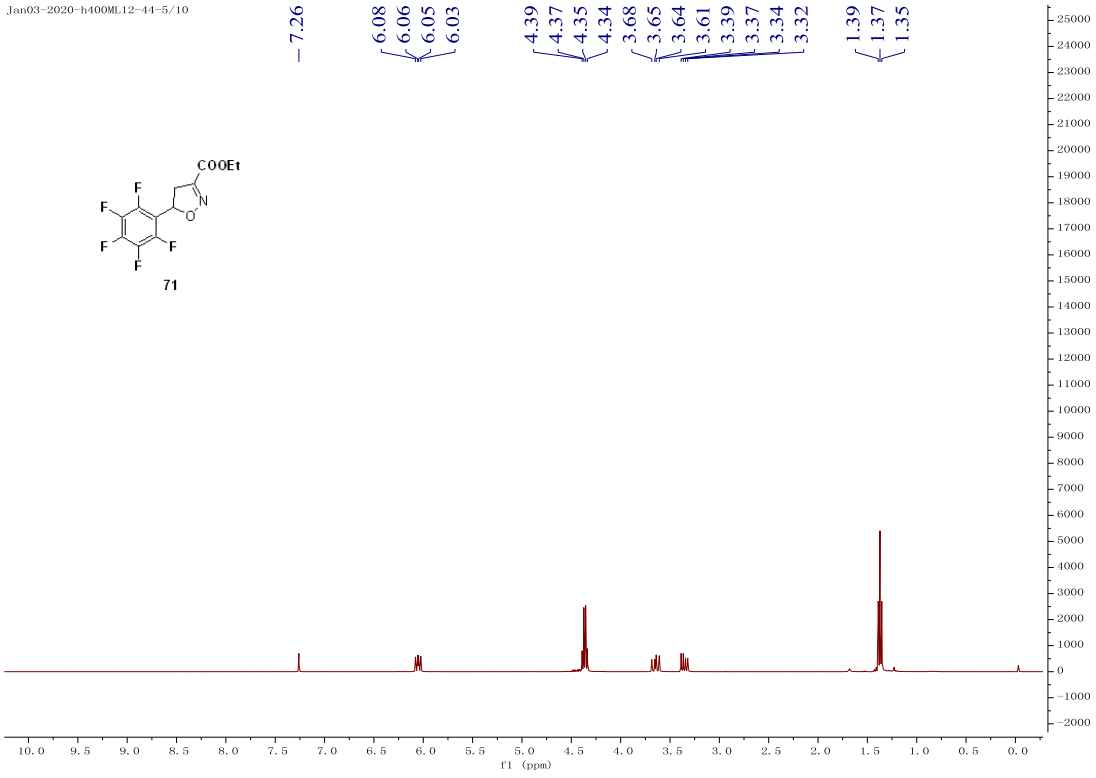

Aug28-2020-C400-ML10-69/10
160.92
151.49
134.56
134.02
129.88
128.09
77.32
77.00
76.95
76.68
61.94
36.53
14.09
-5.32
-5.80
COOEt
Si
O
N
68
f1 (ppm)

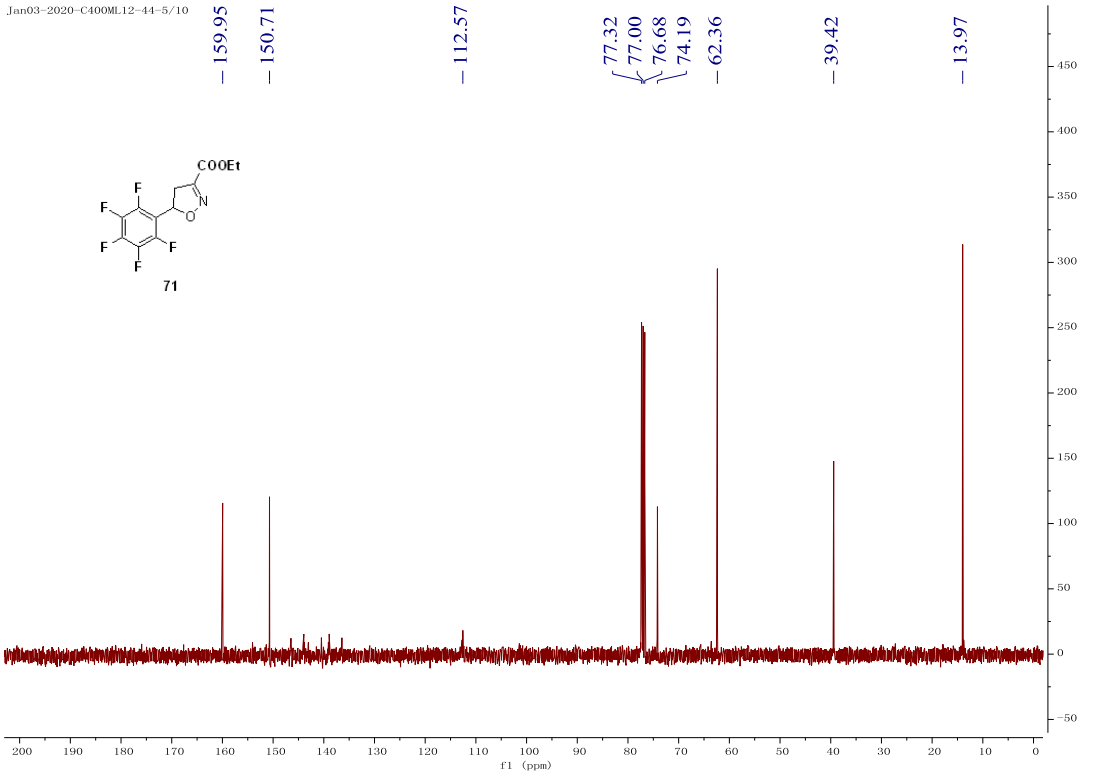

Jan03-2019-h400-ML10-1-8-1/10
7.26
4.34
4.33
4.31
4.29
4.20
4.17
4.16
4.13
3.36
3.32
3.31
3.28
2.97
2.93
2.93
2.89
1.36
1.34
1.32
0.11
COOEt
Si
O
N
69
1.99
0.94
1.00
1.00
3.01
9.01
f1 (ppm)

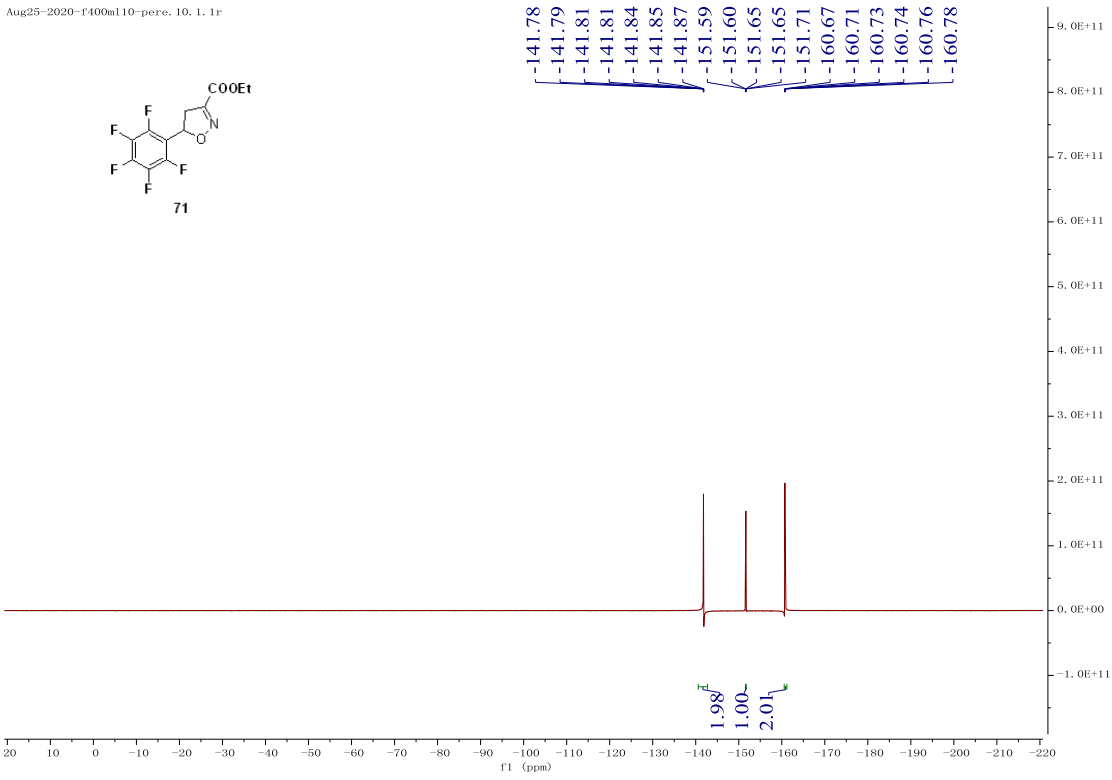

Jan03-2019-c400-ML10-1-8-1/10
160.99
151.30
77.32
77.30
77.00
76.68
61.86
36.15
14.06
-4.18
COOEt
Si
O
N
69
f1 (ppm)

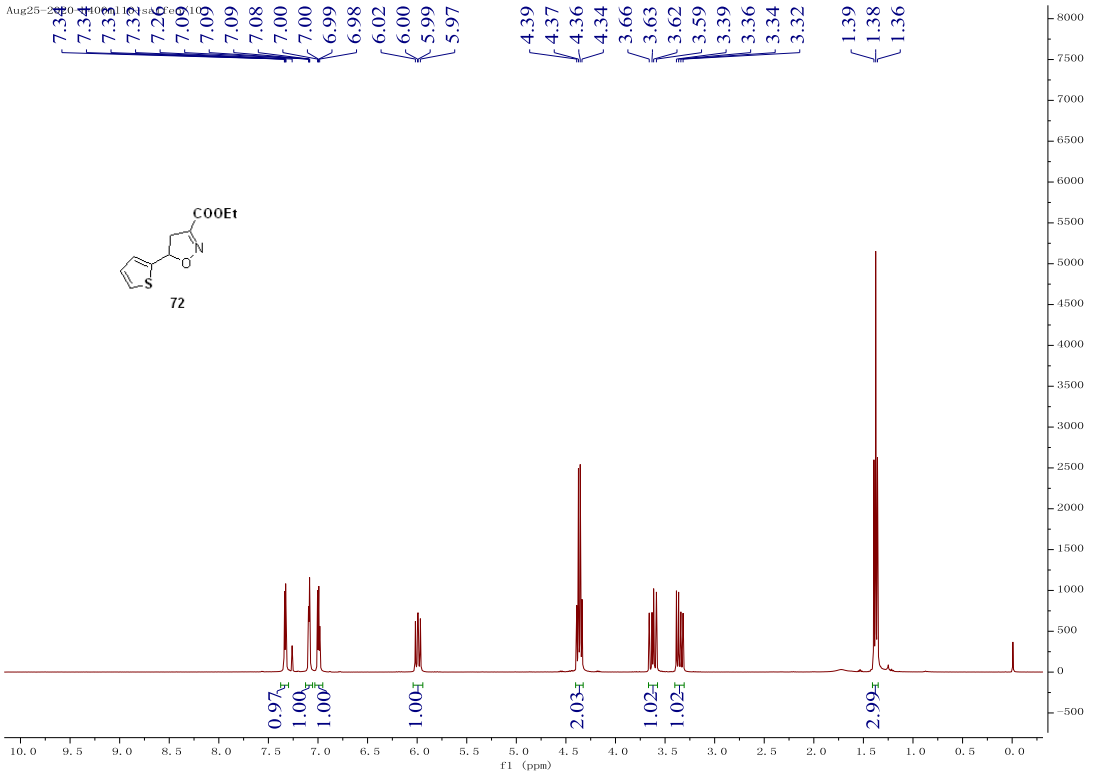

7.97
7.92
7.91
7.96
7.95
7.92
7.74
7.73
7.72
7.72
7.71
7.70
7.70
7.69
7.62
7.61
7.61
7.60
7.59
7.59
7.58
7.58
7.57
5.57
5.56
5.54
5.53
4.35
4.33
4.31
4.30
3.95
3.94
3.90
3.89
3.68
3.65
3.63
3.60
1.35
1.34
1.32
COOEt
O
S
O
O
N
70
2.00
1.00
2.00
1.00
2.00
1.02
1.03
3.05
f1 (ppm)

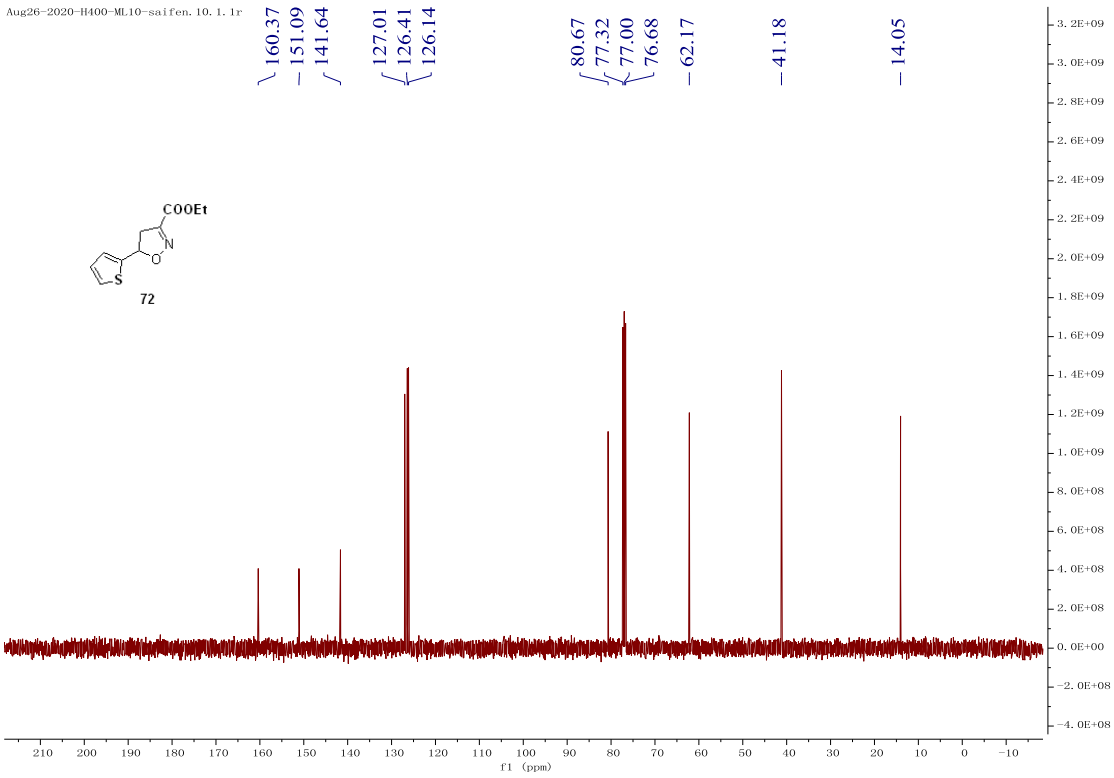

Nov27-2018-C400-ML09-1-85-4/10
158.72
151.93
134.83
134.68
129.72
129.36
93.96
77.32
77.00
76.68
62.68
35.63
13.94
COOEt
70
f1 (ppm)

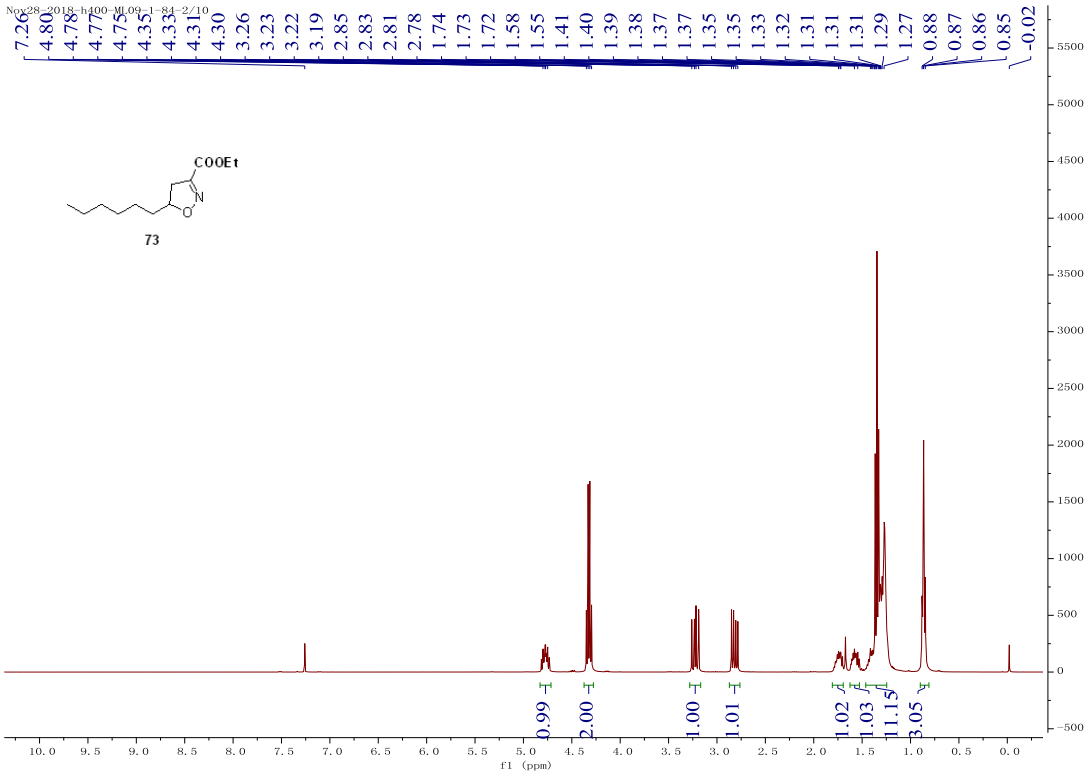

Jan03-2020-h400ML12-44-5/10
7.26
6.08
6.06
6.05
6.03
4.39
4.37
4.35
4.34
3.68
3.65
3.64
3.61
3.39
3.37
3.34
3.32
1.39
1.37
1.35
COOEt
F
71
f1 (ppm)

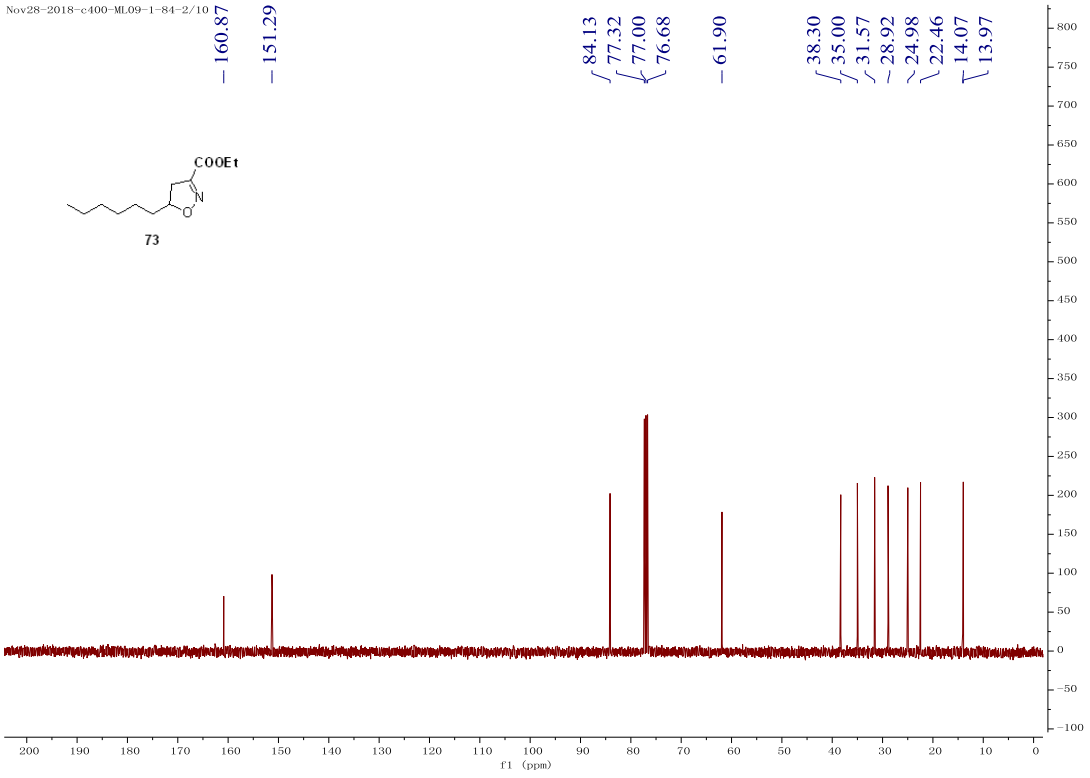

Jan03-2020-C400ML12-44-5/10
159.95
150.71
112.57
77.32
77.00
76.68
74.19
62.36
39.42
13.97
COOEt
F
F
F
F
F
N
O
71
f1 (ppm)

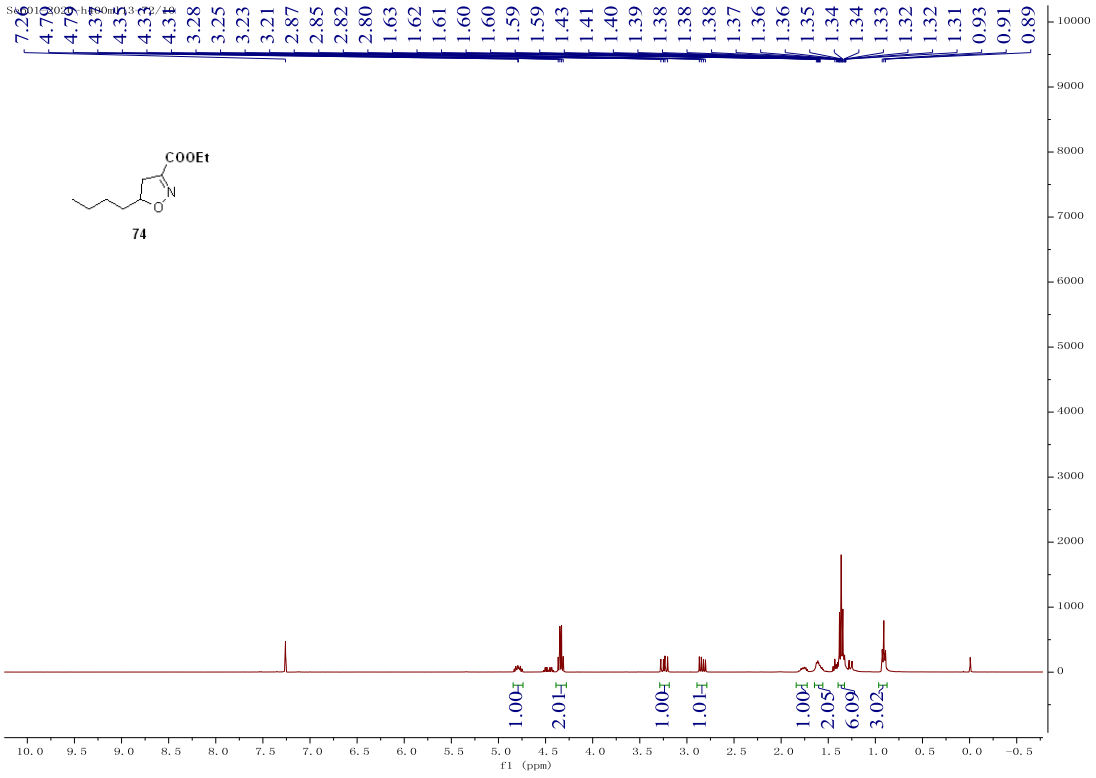

Aug25-2020-f400ml10-pere.10.1.1r
-141.78
-141.79
-141.81
-141.81
-141.84
-141.85
-141.87
-151.59
-151.60
-151.65
-151.65
-151.71
-160.67
-160.71
-160.73
-160.74
-160.76
-160.78
COOEt
F
F
F
F
F
N
O
71
1.98
1.00
2.01
f1 (ppm)

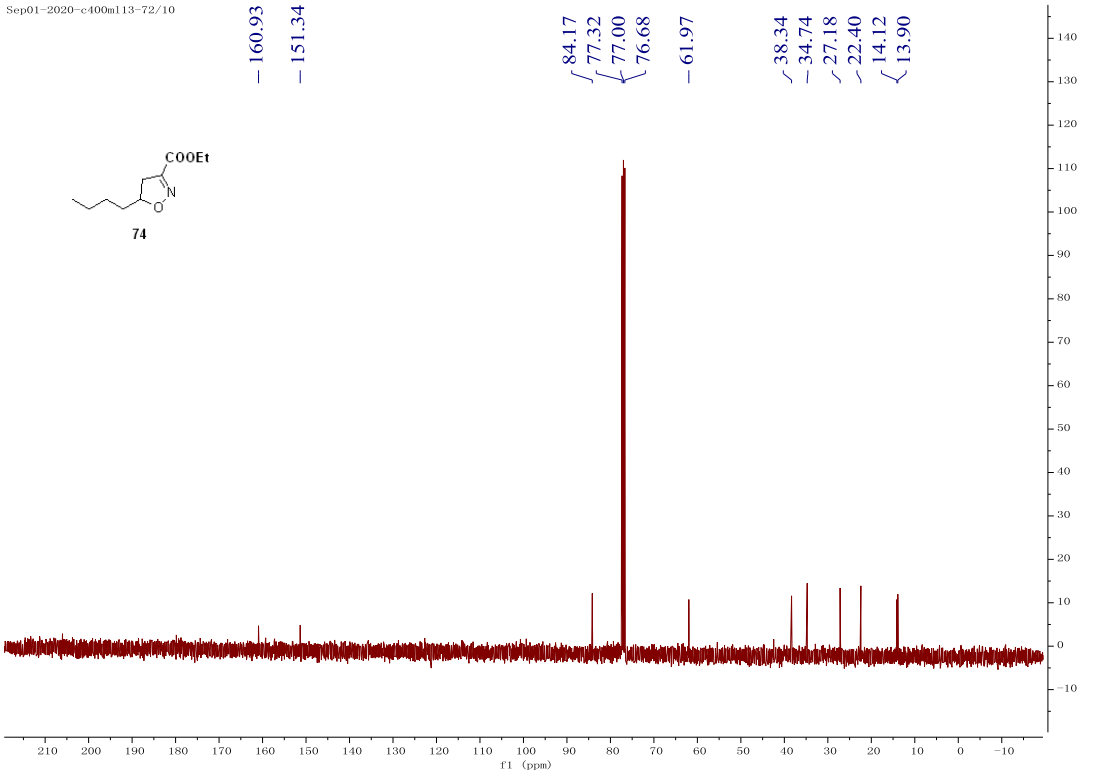

7.34
7.34
7.33
7.32
7.26
7.09
7.09
7.09
7.08
7.00
7.00
6.99
6.98
6.02
6.00
5.99
5.97
4.39
4.37
4.36
4.34
3.66
3.63
3.62
3.59
3.39
3.36
3.34
3.32
1.39
1.38
1.36
COOEt
72
0.97
1.00
1.00
1.00
2.03
1.02
1.02
2.99
f1 (ppm)

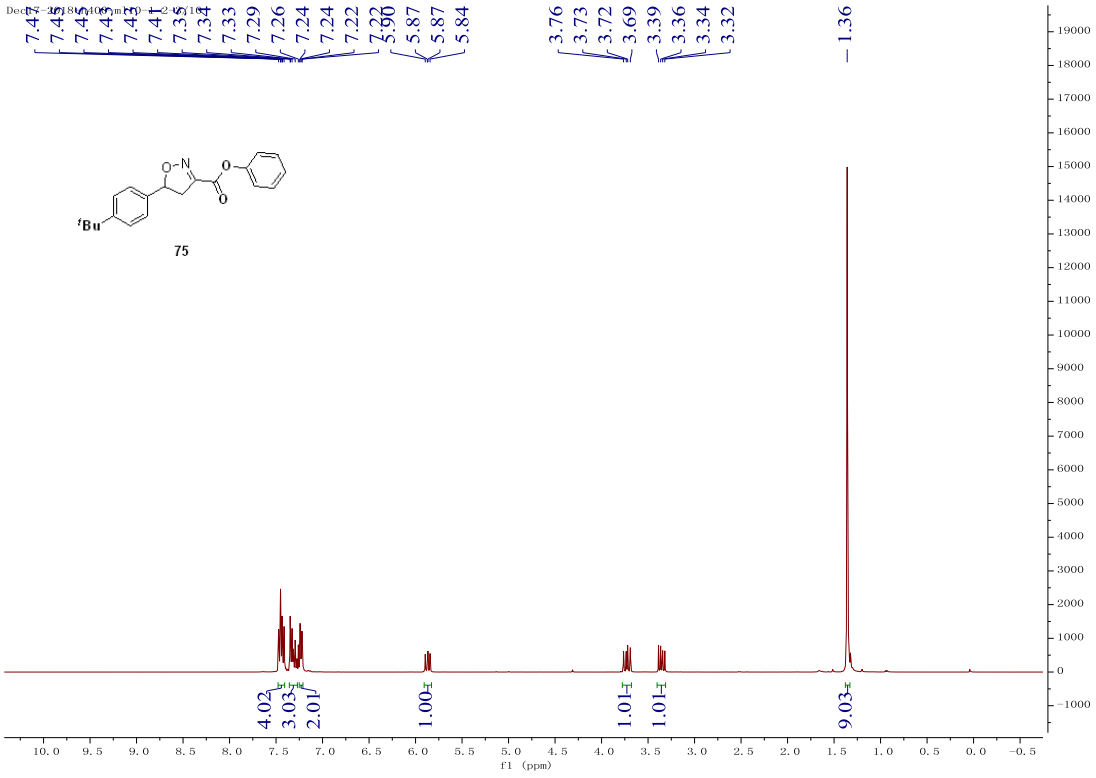

160.37
151.09
141.64
127.01
126.41
126.14
80.67
77.32
77.00
76.68
62.17
41.18
14.05
COOEt
72
f1 (ppm)


Nov28-2018-h400-ML09-1-84-2/10
7.26
4.80
4.78
4.77
4.75
4.35
4.33
4.31
4.30
3.26
3.23
3.22
3.19
2.85
2.83
2.81
2.78
1.74
1.73
1.72
1.58
1.55
1.41
1.40
1.39
1.38
1.37
1.37
1.35
1.35
1.33
1.32
1.31
1.31
1.29
1.27
0.88
0.87
0.86
0.85
-0.02
COOEt
73
0.99
2.00
1.00
1.01
1.02
1.03
11.15
3.05
f1 (ppm)


Nov28-2018-c400-ML09-1-84-2/10
160.87
151.29
84.13
77.32
77.00
76.68
61.90
38.30
35.00
31.57
28.92
24.98
22.46
14.07
13.97
COOEt
73
f1 (ppm)


7.26
4.70
4.79
4.35
4.33
4.31
3.28
3.25
3.23
3.21
2.87
2.85
2.82
2.80
1.63
1.62
1.61
1.60
1.60
1.59
1.59
1.43
1.41
1.40
1.39
1.38
1.38
1.38
1.37
1.36
1.36
1.35
1.34
1.34
1.33
1.32
1.32
1.31
0.93
0.91
0.89
COOEt
N
O
74
1.00
2.01
1.00
1.01
1.00
2.05
6.09
3.02
f1 (ppm)


Sep01-2020-c400m113-72/10
160.93
151.34
84.17
77.32
77.00
76.68
61.97
38.34
34.74
27.18
22.40
14.12
13.90
COOEt
N
O
74
f1 (ppm)


7.47
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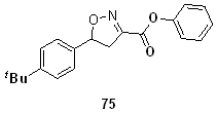
7.45
7.43
7.41
7.35
7.34
7.33
7.29
7.26
7.24
7.24
7.22
7.22
5.90
5.87
5.87
5.84
3.76
3.73
3.72
3.69
3.39
3.36
3.34
3.32
1.36
4.02
3.03
2.01
1.00
1.01
1.01
9.03
f1 (ppm)

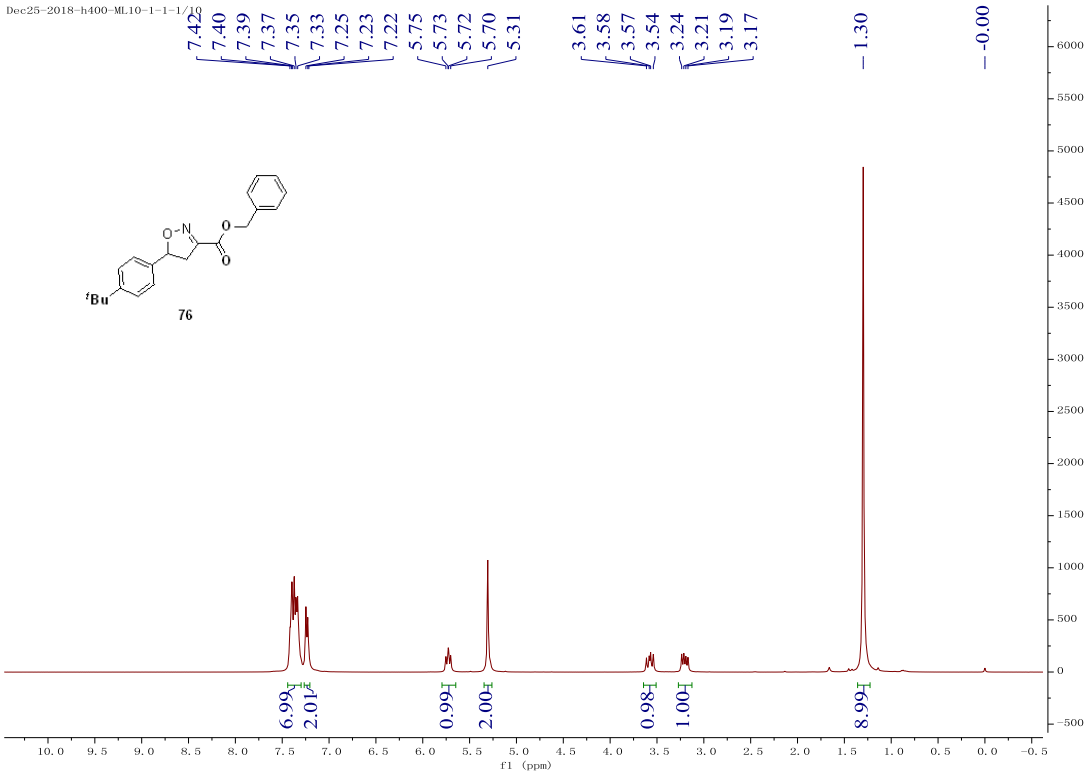

tBu

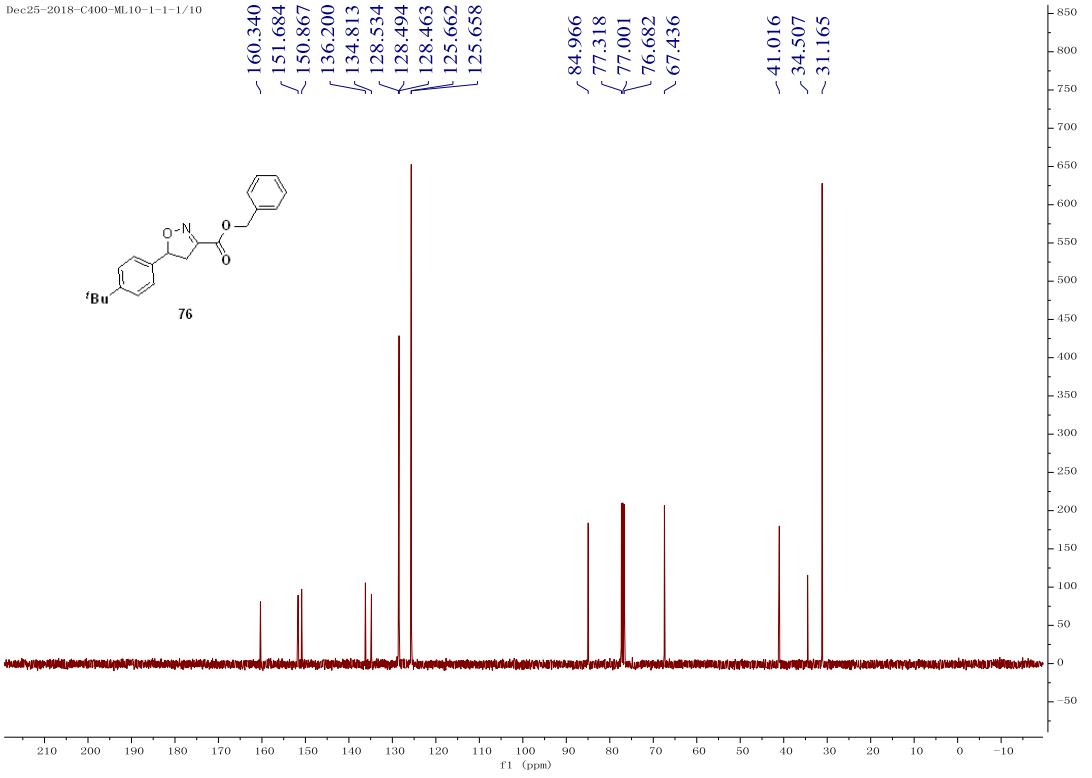
75

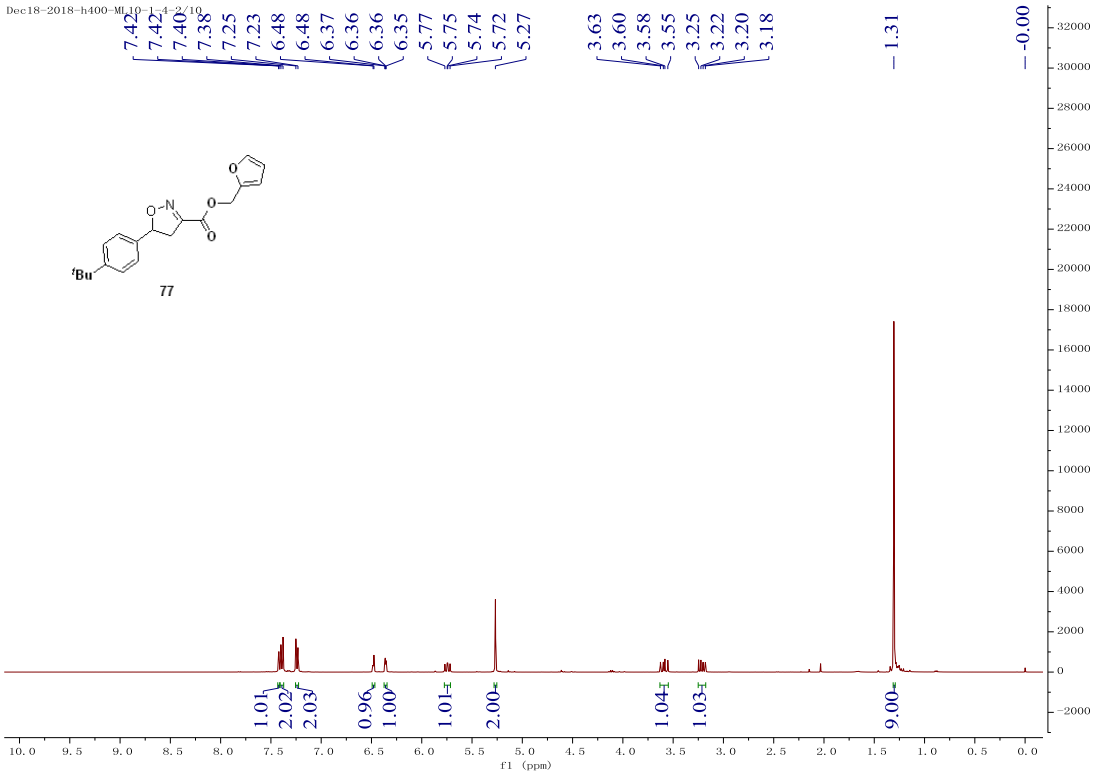
Dec17-2018-c400-ml10-1-2-3/10
159.02
151.84
150.72
150.02
136.06
129.47
126.30
125.75
125.71
121.25
85.39
77.32
77.00
76.68
40.88
34.55
31.18
f1 (ppm)

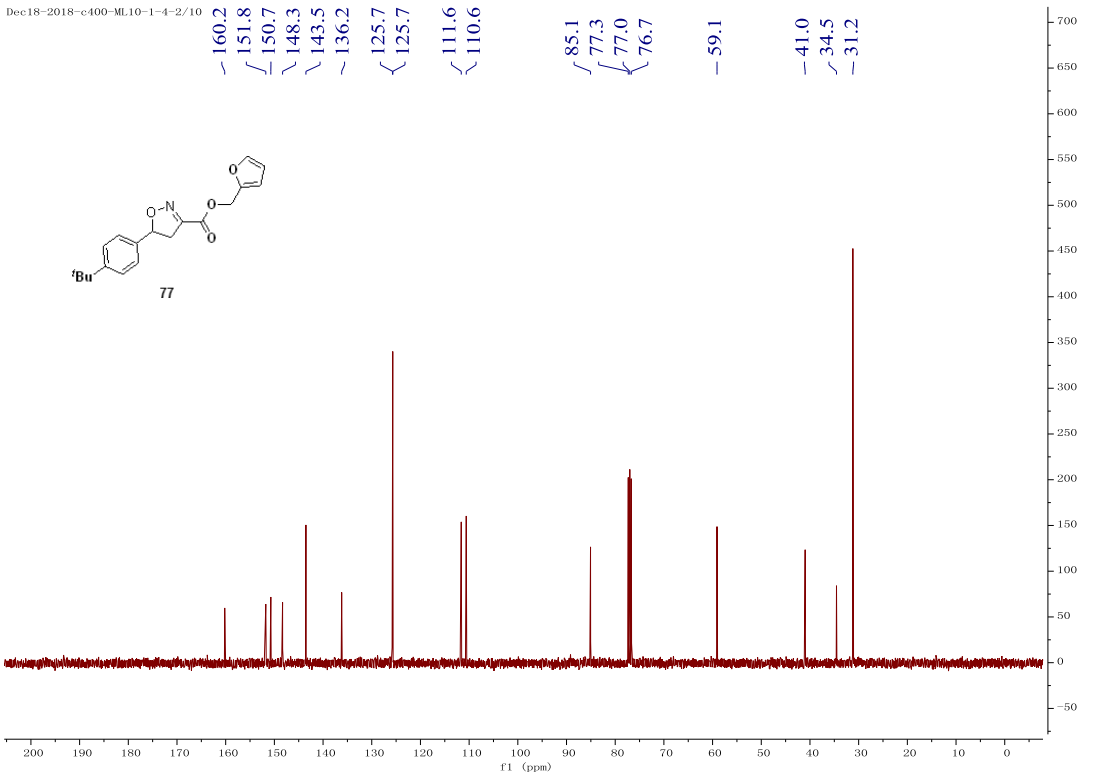
tBu

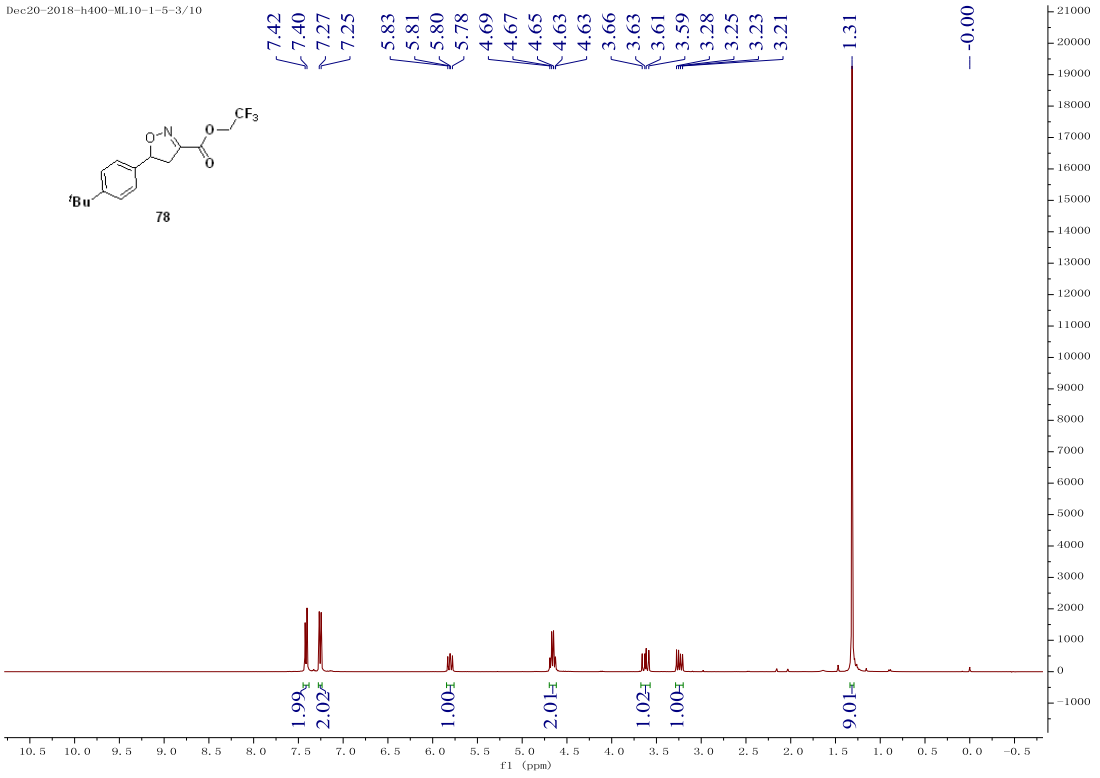
75

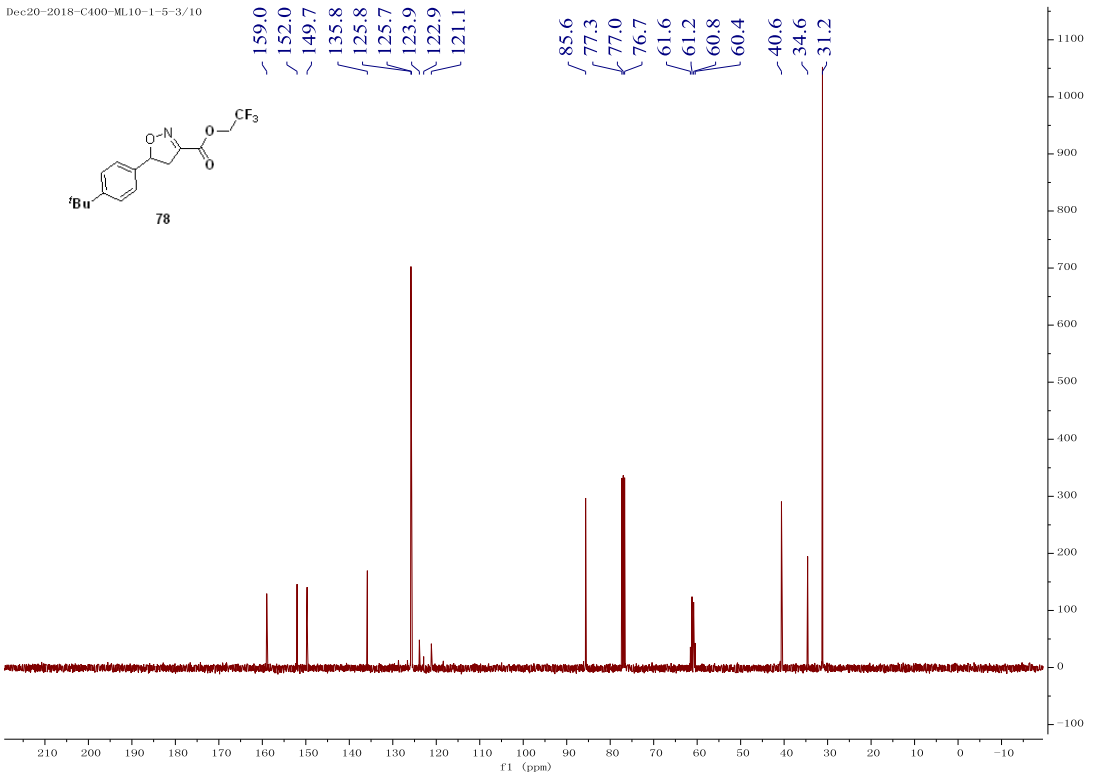

Dec25-2018-h400-ML10-1-1-1/10
7.42
7.40
7.39
7.37
7.35
7.33
7.25
7.23
7.22
5.75
5.73
5.72
5.70
5.31
3.61
3.58
3.57
3.54
3.24
3.21
3.19
3.17
1.30
-0.00
6.99
2.01
0.99
2.00
0.98
1.00
8.99
f1 (ppm)
76

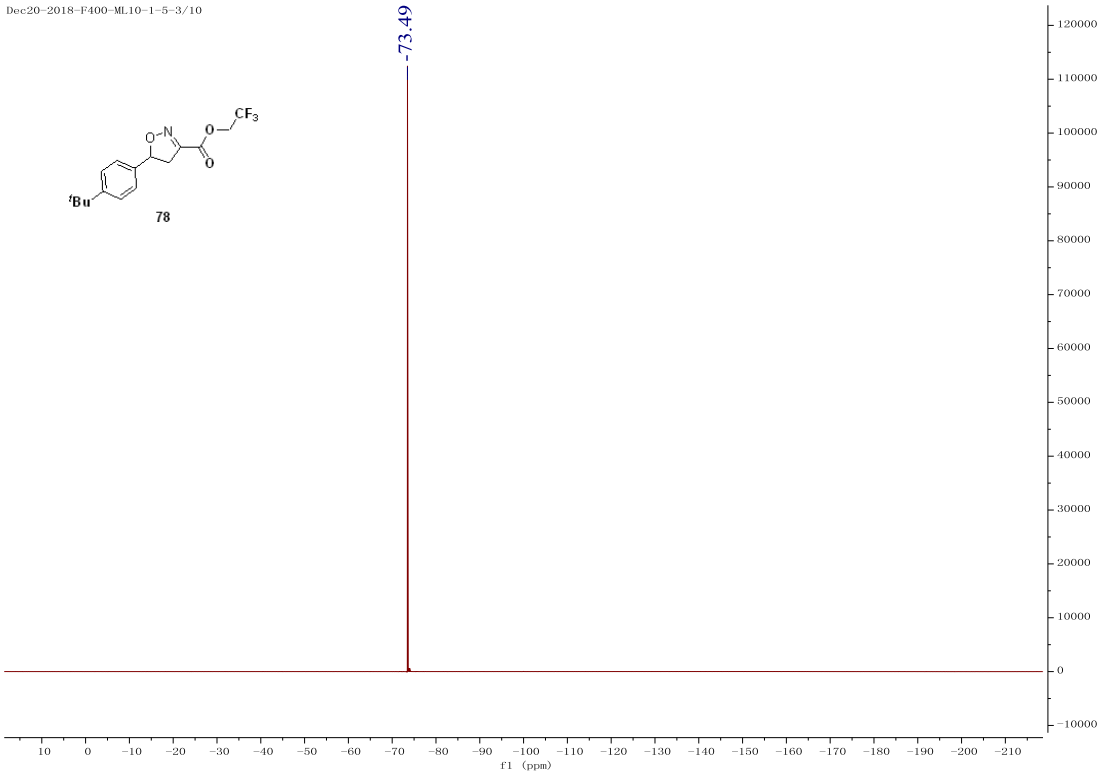

Dec25-2018-C400-ML10-1-1-1/10
160.340
151.684
150.867
136.200
134.813
128.534
128.494
128.463
125.662
125.658
84.966
77.318
77.001
76.682
67.436
41.016
34.507
31.165
f1 (ppm)
76

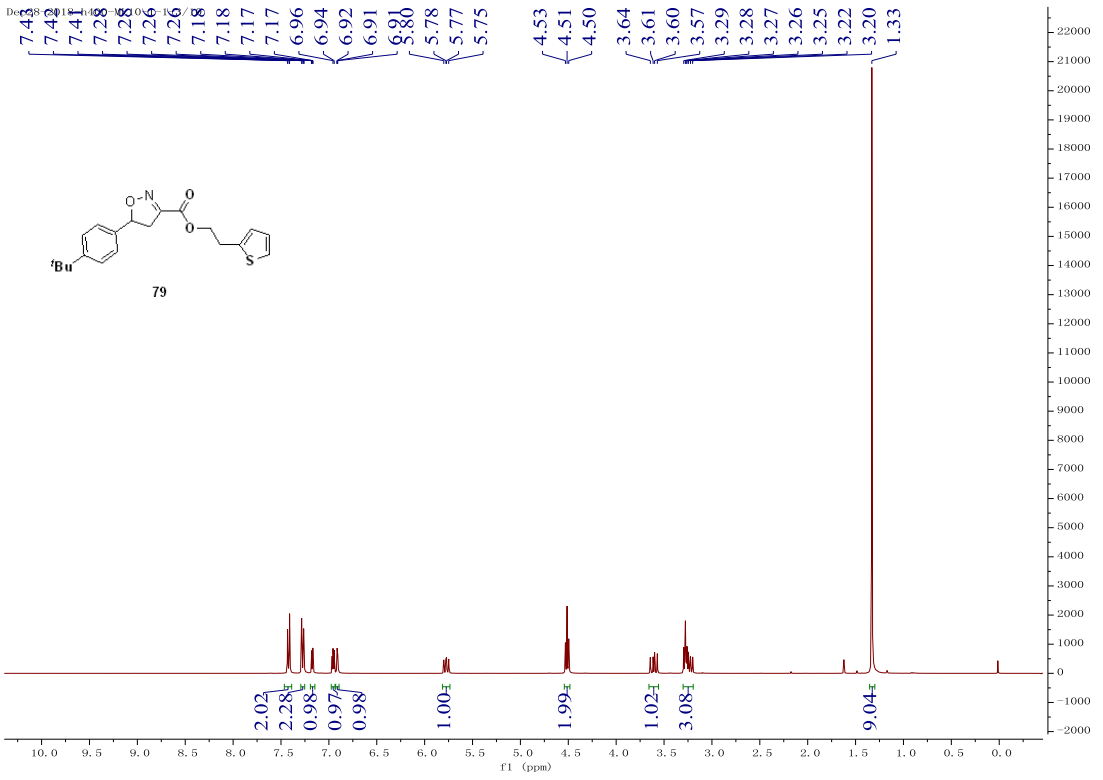

Dec18-2018-h400-ML10-1-4-2/10
7.42
7.42
7.40
7.38
7.25
7.23
6.48
6.48
6.37
6.36
6.36
6.35
5.77
5.75
5.74
5.72
5.27
3.63
3.60
3.58
3.55
3.25
3.22
3.20
3.18
1.31
-0.00
tBu
77
1.01
2.02
2.03
0.96
1.00
1.01
2.00
1.04
1.03
9.00
f1 (ppm)

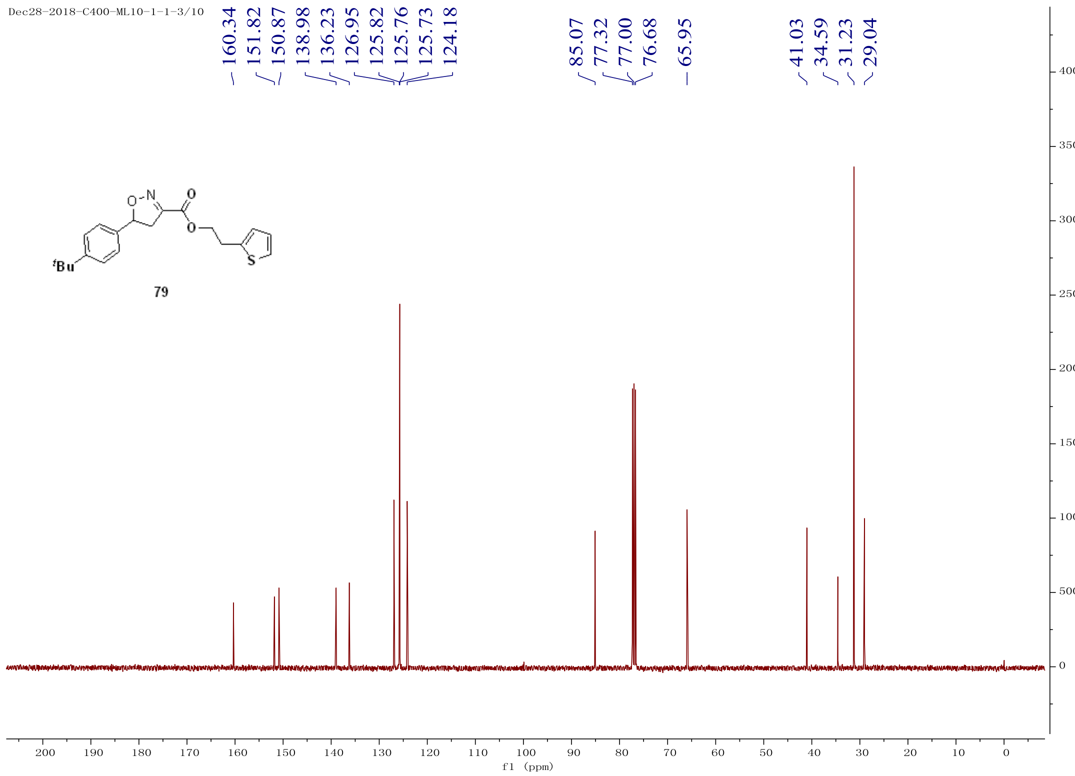

Dec18-2018-c400-ML10-1-4-2/10
160.2
151.8
150.7
148.3
143.5
136.2
125.7
125.7
111.6
110.6
85.1
77.3
77.0
76.7
59.1
41.0
34.5
31.2
tBu
77
f1 (ppm)

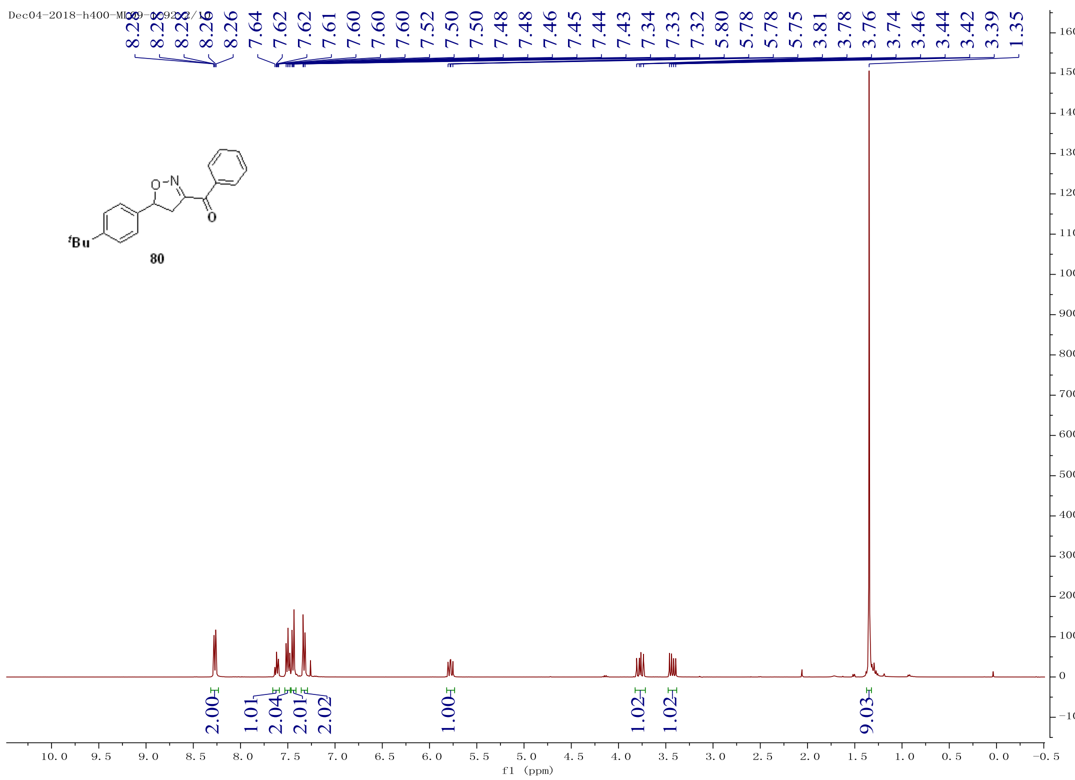

Dec20-2018-h400-ML10-1-5-3/10
7.42
7.40
7.27
7.25
5.83
5.81
5.80
5.78
4.69
4.67
4.65
4.63
4.63
3.66
3.63
3.61
3.59
3.28
3.25
3.23
3.21
1.31
-0.00
1.99
2.02
1.00
2.01
1.02
1.00
9.01
f1 (ppm)
78


Dec20-2018-C400-ML10-1-5-3/10
159.0
152.0
149.7
135.8
125.8
125.7
123.9
122.9
121.1
85.6
77.3
77.0
76.7
61.6
61.2
60.8
60.4
40.6
34.6
31.2
f1 (ppm)
78


Dec20-2018-F400-ML10-1-5-3/10
-73.49
78
f1 (ppm)


7.43
7.42
7.41
7.28
7.26
7.18
7.17
6.96
6.94
6.92
6.91
5.80
5.78
5.77
5.75
4.53
4.51
4.50
3.64
3.61
3.60
3.57
3.29
3.28
3.27
3.26
3.25
3.22
3.20
1.33
79
2.02
2.28
0.98
0.97
0.98
1.00
1.99
1.02
3.08
9.04
f1 (ppm)


Dec28-2018-C400-ML10-1-1-3/10
160.34
151.82
150.87
138.98
136.23
126.95
125.82
125.76
125.73
124.18
85.07
77.32
77.00
76.68
65.95
41.03
34.59
31.23
29.04
O–N
O
O
S
tBu
79
f1 (ppm)


8.26
8.26
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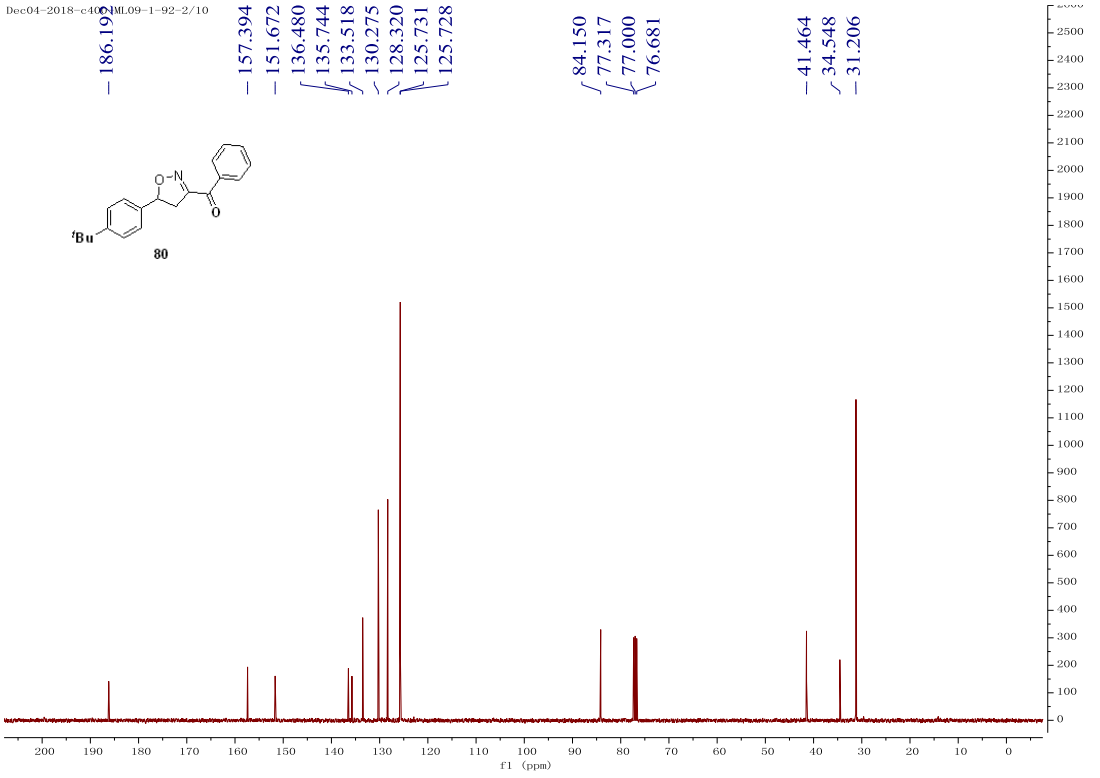
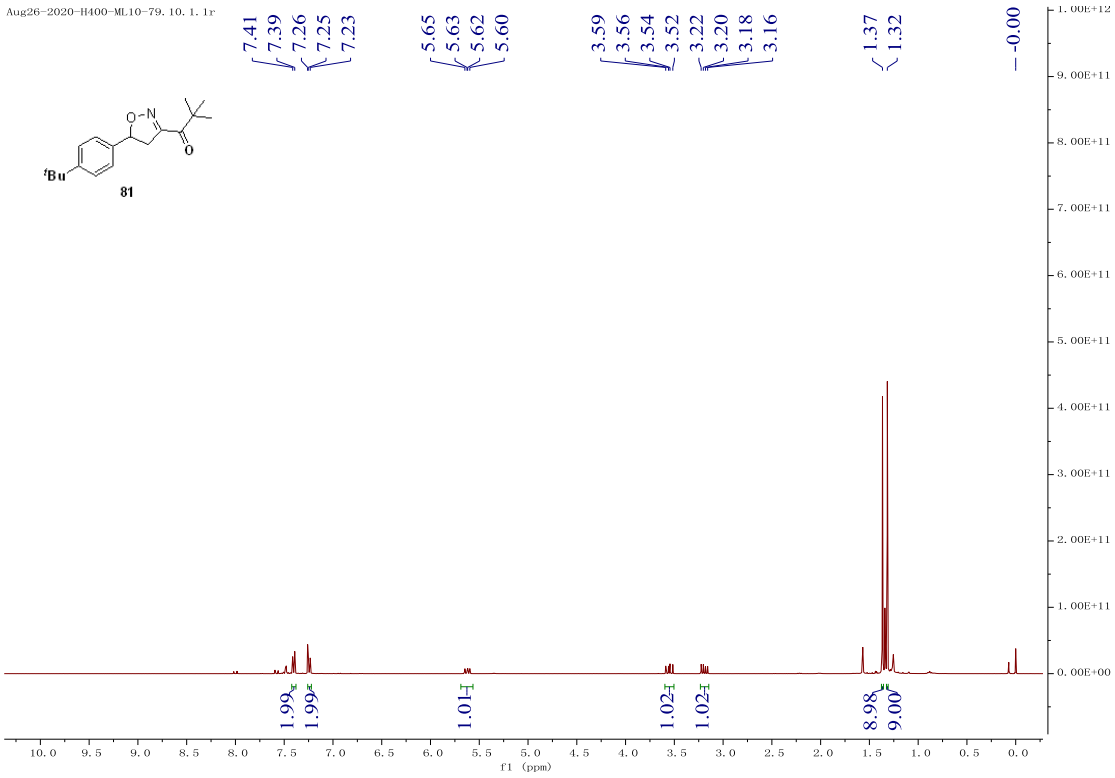
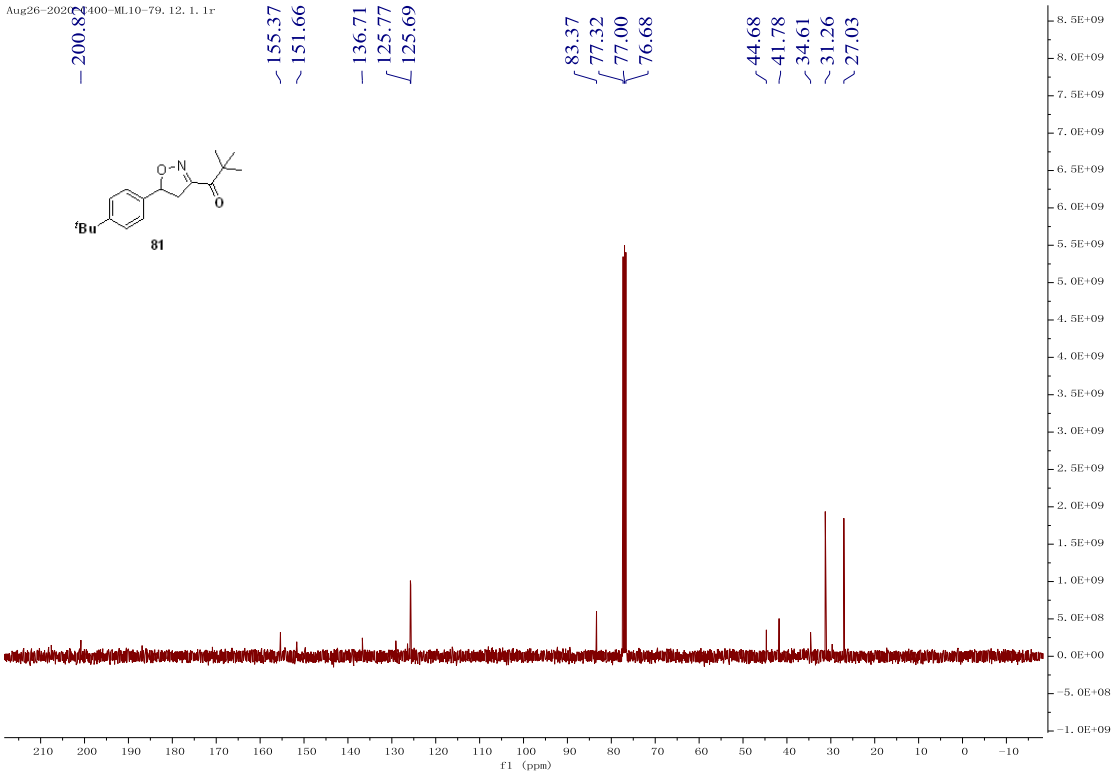
7.62
7.62
7.61
7.60
7.60
7.60
7.52
7.50
7.50
7.48
7.48
7.46
7.45
7.44
7.43
7.34
7.33
7.32
5.80
5.78
5.78
5.75
3.81
3.78
3.76
3.74
3.46
3.44
3.42
3.39
1.35
O–N
O
tBu
80
2.00
1.01
2.04
2.01
2.02
1.00
1.02
1.02
9.03
f1 (ppm)


Dec04-2018-c400-NMR09-1-92-2/10
186.192
157.394
151.672
136.480
135.744
133.518
130.275
128.320
125.731
125.728
84.150
77.317
77.000
76.681
41.464
34.548
31.206
tBu
80
f1 (ppm)


Aug26-2020-H400-ML10-79. 10. 1. 1r
7.41
7.39
7.26
7.25
7.23
5.65
5.63
5.62
5.60
3.59
3.56
3.54
3.52
3.22
3.20
3.18
3.16
1.37
1.32
-0.00
tBu
81
1.99
1.99
1.01
1.02
1.02
8.98
9.00
f1 (ppm)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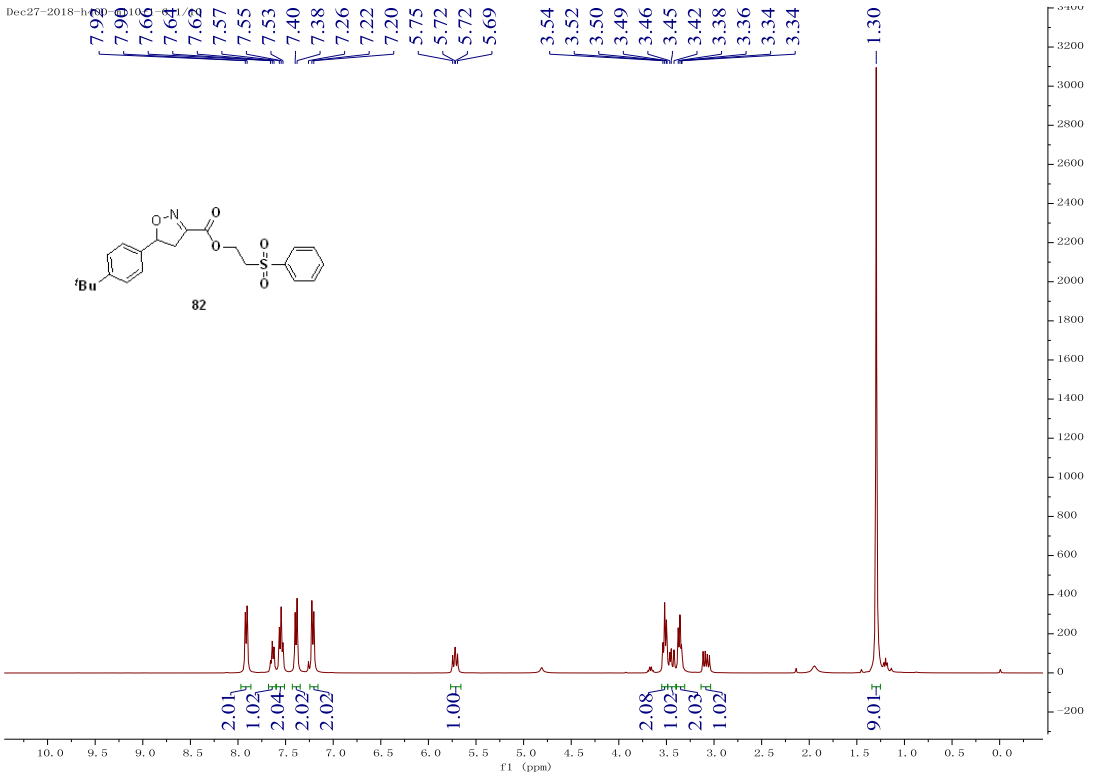
151.66
136.71
125.77
125.69
83.37
77.32
77.00
76.68
44.68
41.78
34.61
31.26
27.03
81
f1 (ppm)


7.92
7.90
7.66
7.64
7.62
7.57
7.55
7.53
7.40
7.38
7.26
7.22
7.20
5.75
5.72
5.72
5.69
3.54
3.52
3.50
3.49
3.46
3.45
3.42
3.38
3.36
3.34
3.34
1.30
2.01
1.02
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2.02
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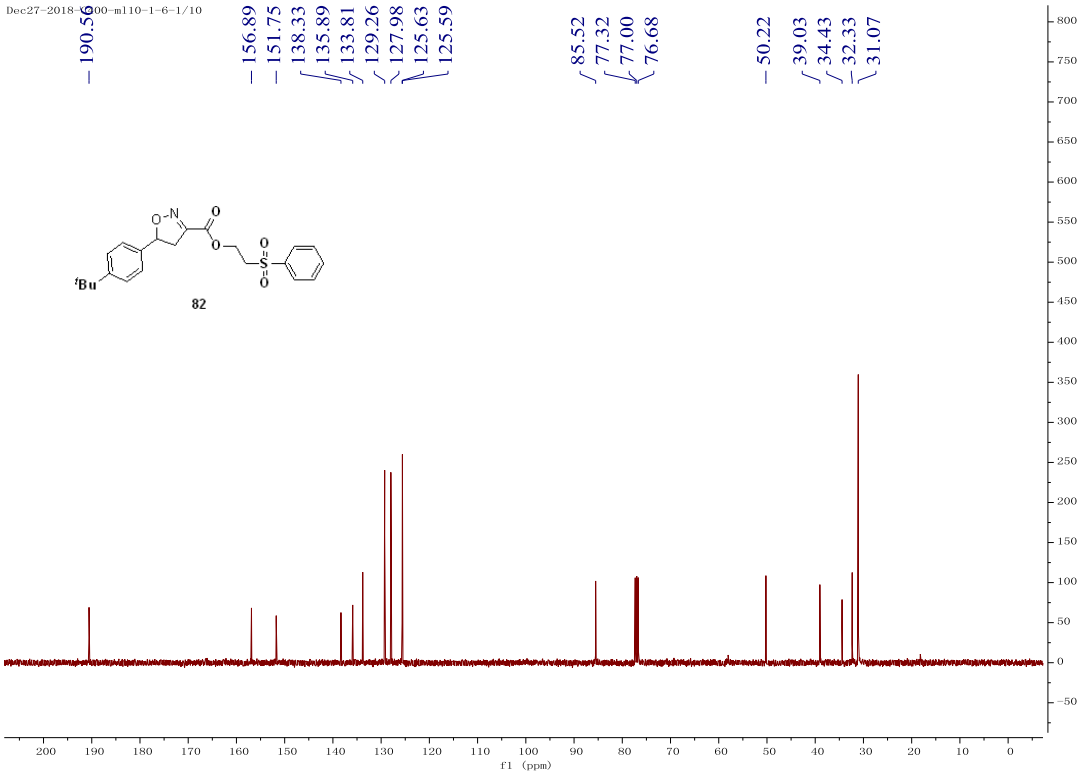
1.02
2.03
1.02
9.01
82
f1 (ppm)



Cartesian Coordinates and Energies

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.911917	-0.688096	-0.627765
2	6	0	-3.963318	-1.619167	-0.163713
3	6	0	-2.696821	-1.193346	0.255622
4	6	0	-2.344455	0.179642	0.218826
5	6	0	-3.311538	1.103376	-0.248644
6	6	0	-4.580039	0.676210	-0.668192
7	1	0	-5.902379	-1.025934	-0.953019
8	1	0	-4.215248	-2.685340	-0.126245
9	1	0	-1.975223	-1.933228	0.619594
10	1	0	-3.056225	2.169751	-0.281002
11	1	0	-5.310396	1.410659	-1.026745
12	6	0	-1.029936	0.690876	0.641461
13	1	0	-0.926377	1.785349	0.597507
14	6	0	0.034252	-0.027255	1.071957
15	1	0	-0.001550	-1.123749	1.129192
16	6	0	1.309791	0.611006	1.533017
17	1	0	1.545491	0.334665	2.575429
18	1	0	1.276802	1.708391	1.443527
19	8	0	2.465961	0.096647	0.781466
20	6	0	2.782152	0.772821	-0.364865
21	8	0	2.229323	1.793590	-0.769703

22	6	0	3.898121	0.137185	-1.069170
23	1	0	4.307823	0.544336	-1.994543
24	7	0	4.448226	-0.958435	-0.606288
25	7	0	4.919953	-1.922467	-0.186427

Zero-point correction= 0.185901 (Hartree/Particle)
Thermal correction to Energy= 0.200001
Thermal correction to Enthalpy= 0.200946
Thermal correction to Gibbs Free Energy= 0.141885
Sum of electronic and zero-point Energies= -684.912606
Sum of electronic and thermal Energies= -684.898506
Sum of electronic and thermal Enthalpies= -684.897562
Sum of electronic and thermal Free Energies= -684.956622
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -685.28939507

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.768197	0.010437	0.000041
2	6	0	0.911224	0.853130	-1.274068
3	1	0	1.931300	1.272868	-1.329533
4	1	0	0.744059	0.233688	-2.173020
5	1	0	0.193589	1.691287	-1.284266
6	6	0	1.732651	-1.180413	-0.002590
7	1	0	2.773578	-0.812278	-0.001943
8	1	0	1.587220	-1.809227	0.893171
9	1	0	1.587000	-1.805560	-0.900877
10	6	0	0.911949	0.848181	1.277284
11	1	0	0.193672	1.685726	1.291347
12	1	0	0.746082	0.225146	2.173989
13	1	0	1.931753	1.268484	1.333412
14	8	0	-0.572338	-0.654439	-0.000771
15	7	0	-1.634959	0.304174	0.000332
16	8	0	-2.701120	-0.253981	-0.000305

Zero-point correction= 0.128308 (Hartree/Particle)
Thermal correction to Energy= 0.137021
Thermal correction to Enthalpy= 0.137965
Thermal correction to Gibbs Free Energy= 0.095841
Sum of electronic and zero-point Energies= -362.844215
Sum of electronic and thermal Energies= -362.835502
Sum of electronic and thermal Enthalpies= -362.834558
Sum of electronic and thermal Free Energies= -362.876682
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -363.08456328

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.901655	-1.975805	0.674954
2	6	0	-5.275612	-1.099304	1.581591
3	6	0	-4.332745	-0.166973	1.131354
4	6	0	-3.988785	-0.090922	-0.242206
5	6	0	-4.632196	-0.976026	-1.141912
6	6	0	-5.576591	-1.909314	-0.690021
7	1	0	-6.639990	-2.702390	1.032426
8	1	0	-5.527891	-1.141767	2.647409
9	1	0	-3.863223	0.512247	1.851675
10	1	0	-4.378874	-0.926925	-2.208091
11	1	0	-6.059345	-2.584983	-1.405341
12	6	0	-2.997669	0.855434	-0.778871
13	1	0	-2.894175	0.840461	-1.873915
14	6	0	-2.222746	1.720329	-0.081733

15	1	0	-2.268653	1.776726	1.013847
16	6	0	-1.285852	2.676160	-0.749847
17	1	0	-1.494601	3.722844	-0.473179
18	1	0	-1.291934	2.572943	-1.846086
19	8	0	0.105010	2.488253	-0.260121
20	6	0	0.843059	1.566586	-0.909158
21	8	0	0.506334	0.897038	-1.876420
22	6	0	2.196014	1.369823	-0.261086
23	1	0	3.028286	1.236054	-0.958233
24	7	0	2.488791	2.219640	0.787036
25	7	0	2.538991	2.217907	1.951904
26	6	0	3.892644	-1.711449	-0.236896
27	6	0	3.045910	-2.950977	0.104620
28	1	0	3.338514	-3.809245	-0.527079
29	1	0	3.186730	-3.235672	1.162598
30	1	0	1.971637	-2.756556	-0.062060
31	6	0	5.385528	-1.990151	0.007692
32	1	0	5.733913	-2.802558	-0.655184
33	1	0	5.992387	-1.090551	-0.198669
34	1	0	5.562040	-2.296629	1.053975
35	6	0	3.662510	-1.269900	-1.693874
36	1	0	2.607298	-1.004295	-1.880007
37	1	0	4.298689	-0.403131	-1.951732
38	1	0	3.924945	-2.092872	-2.383570
39	8	0	3.607634	-0.638099	0.714123
40	7	0	2.108203	-0.225275	0.689991
41	8	0	1.774954	0.054724	1.843800

Zero-point correction= 0.315847 (Hartree/Particle)
Thermal correction to Energy= 0.338748
Thermal correction to Enthalpy= 0.339692
Thermal correction to Gibbs Free Energy= 0.260565
Sum of electronic and zero-point Energies= -1047.725894
Sum of electronic and thermal Energies= -1047.702993
Sum of electronic and thermal Enthalpies= -1047.702049
Sum of electronic and thermal Free Energies= -1047.781176
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1048.34064969

TS1’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.803370	0.309611	-0.881426
2	6	0	-6.144933	-0.899480	-0.586962
3	6	0	-4.839756	-0.891729	-0.079825
4	6	0	-4.156483	0.330749	0.143574
5	6	0	-4.833304	1.538061	-0.158467
6	6	0	-6.141392	1.529357	-0.664551
7	1	0	-7.825525	0.298161	-1.276219
8	1	0	-6.655071	-1.855320	-0.753382
9	1	0	-4.345742	-1.843834	0.143818
10	1	0	-4.318278	2.492220	0.008104
11	1	0	-6.644301	2.476844	-0.889699
12	6	0	-2.782220	0.407365	0.665641
13	1	0	-2.383742	1.428063	0.766568
14	6	0	-1.983448	-0.621950	1.034583
15	1	0	-2.321081	-1.664191	0.961539
16	6	0	-0.621238	-0.412277	1.610091
17	1	0	-0.524929	-0.842169	2.623541
18	1	0	-0.342757	0.654289	1.649238
19	8	0	0.347620	-1.113117	0.739722
20	6	0	1.588001	-1.247231	1.248621
21	8	0	1.970814	-0.883852	2.352366
22	6	0	2.507761	-1.951206	0.280483
23	1	0	3.216832	-2.654250	0.736750

24	7	0	1.936084	-2.475637	-0.848860
25	7	0	1.957248	-2.455400	-2.008870
26	6	0	3.314327	1.790005	-0.167458
27	6	0	2.191352	2.837893	-0.057599
28	1	0	2.616911	3.830954	0.175281
29	1	0	1.631247	2.915368	-1.006494
30	1	0	1.482063	2.568560	0.744882
31	6	0	4.294379	2.179598	-1.293554
32	1	0	4.747550	3.168049	-1.093223
33	1	0	5.115703	1.447153	-1.386511
34	1	0	3.767746	2.230036	-2.263368
35	6	0	4.049919	1.651775	1.179216
36	1	0	3.347907	1.347140	1.973874
37	1	0	4.851339	0.894535	1.121965
38	1	0	4.512085	2.613712	1.467900
39	8	0	2.600504	0.573613	-0.518798
40	7	0	3.630226	-0.675230	-0.574400
41	8	0	3.777256	-1.022229	-1.737522

Zero-point correction= 0.315288 (Hartree/Particle)
Thermal correction to Energy= 0.338426
Thermal correction to Enthalpy= 0.339370
Thermal correction to Gibbs Free Energy= 0.260499
Sum of electronic and zero-point Energies= -1047.724311
Sum of electronic and thermal Energies= -1047.701173
Sum of electronic and thermal Enthalpies= -1047.700229
Sum of electronic and thermal Free Energies= -1047.779100
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1048.33836280

N_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.558483
2	7	0	0.000000	0.000000	-0.558483

Zero-point correction= 0.005364 (Hartree/Particle)
Thermal correction to Energy= 0.007724
Thermal correction to Enthalpy= 0.008668
Thermal correction to Gibbs Free Energy= -0.013106
Sum of electronic and zero-point Energies= -109.515585
Sum of electronic and thermal Energies= -109.513224
Sum of electronic and thermal Enthalpies= -109.512280
Sum of electronic and thermal Free Energies= -109.534054
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -109.55571545

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.666147	-1.670539	0.278469
2	6	0	-5.891735	-1.252731	1.377500
3	6	0	-4.787089	-0.412810	1.189470
4	6	0	-4.424835	0.030143	-0.108173
5	6	0	-5.215270	-0.399212	-1.202741
6	6	0	-6.322342	-1.239693	-1.013533
7	1	0	-7.531197	-2.325735	0.431035
8	1	0	-6.154023	-1.582630	2.389424
9	1	0	-4.200689	-0.096663	2.059428
10	1	0	-4.949937	-0.065144	-2.213437
11	1	0	-6.917713	-1.557439	-1.877265
12	6	0	-3.275927	0.912674	-0.372987
13	1	0	-3.138851	1.184600	-1.430186
14	6	0	-2.401887	1.418029	0.528950

15	1	0	-2.484246	1.179141	1.597961
16	6	0	-1.303595	2.369584	0.157048
17	1	0	-1.423193	3.338367	0.673354
18	1	0	-1.257002	2.537414	-0.931125
19	8	0	0.000651	1.894785	0.634629
20	6	0	0.688190	1.073915	-0.227005
21	8	0	0.308911	0.762091	-1.352976
22	6	0	1.931850	0.679955	0.440153
23	1	0	2.169582	0.999166	1.452272
24	6	0	5.240221	-0.693737	0.179918
25	6	0	5.294849	-2.069347	-0.501145
26	1	0	6.345738	-2.315114	-0.738142
27	1	0	4.906315	-2.849577	0.176974
28	1	0	4.713156	-2.091693	-1.434473
29	6	0	6.098881	-0.691234	1.454637
30	1	0	7.150327	-0.890149	1.183404
31	1	0	6.047264	0.284759	1.967070
32	1	0	5.769988	-1.477562	2.156323
33	6	0	5.641315	0.458214	-0.749815
34	1	0	5.029323	0.482076	-1.665941
35	1	0	5.548970	1.428931	-0.231463
36	1	0	6.696250	0.329343	-1.049820
37	8	0	3.889848	-0.447460	0.774229
38	7	0	2.827309	-0.104500	-0.158969
39	8	0	2.831827	-0.566899	-1.304268

Zero-point correction= 0.309918 (Hartree/Particle)
Thermal correction to Energy= 0.330900
Thermal correction to Enthalpy= 0.331844
Thermal correction to Gibbs Free Energy= 0.257393
Sum of electronic and zero-point Energies= -938.285448
Sum of electronic and thermal Energies= -938.264466
Sum of electronic and thermal Enthalpies= -938.263522
Sum of electronic and thermal Free Energies= -938.337973
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -938.86263097

INT1’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.984748	1.217122	0.198876
2	6	0	5.025492	1.135947	1.226251
3	6	0	3.867776	0.366131	1.058017
4	6	0	3.637803	-0.342993	-0.148296
5	6	0	4.612796	-0.249889	-1.172017
6	6	0	5.772942	0.520049	-1.002095
7	1	0	6.890249	1.818678	0.336922
8	1	0	5.183801	1.676246	2.166819
9	1	0	3.135521	0.313530	1.871470
10	1	0	4.450810	-0.793785	-2.110916
11	1	0	6.512832	0.574221	-1.808988
12	6	0	2.441485	-1.166485	-0.390021
13	1	0	2.423830	-1.675378	-1.365517
14	6	0	1.395407	-1.367991	0.446200
15	1	0	1.351067	-0.885455	1.431677
16	6	0	0.266845	-2.291290	0.115528
17	1	0	0.175589	-3.109238	0.853849
18	1	0	0.381627	-2.743238	-0.885570
19	8	0	-0.978981	-1.510468	0.150032
20	6	0	-2.109487	-2.260705	0.093140
21	8	0	-2.114485	-3.495395	0.021207
22	6	0	-3.385617	-1.538855	0.094050
23	1	0	-4.280765	-2.153653	-0.002930
24	6	0	-2.553744	1.976081	-0.157338
25	6	0	-1.101468	2.393866	0.115467

26	1	0	-0.937808	3.410162	-0.282907
27	1	0	-0.890426	2.410063	1.198977
28	1	0	-0.391717	1.705248	-0.372479
29	6	0	-3.528424	2.898027	0.588029
30	1	0	-3.323401	3.944832	0.299365
31	1	0	-4.577578	2.667936	0.352379
32	1	0	-3.381521	2.812962	1.679082
33	6	0	-2.830014	1.889241	-1.661658
34	1	0	-2.121827	1.197837	-2.150796
35	1	0	-3.860023	1.557912	-1.871332
36	1	0	-2.698903	2.889822	-2.110268
37	8	0	-2.544872	0.599403	0.450861
38	7	0	-3.655523	-0.230309	0.153933
39	8	0	-4.790652	0.271950	0.036505

Zero-point correction= 0.310222 (Hartree/Particle)
Thermal correction to Energy= 0.331039
Thermal correction to Enthalpy= 0.331983
Thermal correction to Gibbs Free Energy= 0.258277
Sum of electronic and zero-point Energies= -938.280519
Sum of electronic and thermal Energies= -938.259702
Sum of electronic and thermal Enthalpies= -938.258758
Sum of electronic and thermal Free Energies= -938.332464
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -938.85754856

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.346696	-3.253492	-1.003554
2	8	0	1.450877	-3.354659	-0.037274
3	6	0	-0.342922	-1.900248	-0.954439
4	1	0	0.761452	-3.446249	-2.007332
5	1	0	-0.324089	-4.084121	-0.733508
6	6	0	2.058656	-2.183803	0.244265
7	8	0	2.989108	-2.124585	1.034969
8	6	0	1.532373	-0.986331	-0.528490
9	7	0	1.156508	0.070549	0.214499
10	8	0	0.481733	-0.073684	1.270197
11	6	0	-1.214289	-1.576660	0.085351
12	1	0	-1.206406	-2.213658	0.979421
13	6	0	-2.290618	-0.584937	0.038501
14	6	0	-2.476073	0.322293	-1.038488
15	6	0	-3.230045	-0.546197	1.102906
16	6	0	-3.549326	1.221704	-1.044249
17	1	0	-1.766212	0.332190	-1.872426
18	6	0	-4.304703	0.352752	1.093551
19	1	0	-3.106128	-1.239229	1.944389
20	6	0	-4.472053	1.243852	0.018930
21	1	0	-3.667882	1.914021	-1.886161
22	1	0	-5.015516	0.357897	1.928276
23	1	0	-5.310217	1.949746	0.008873
24	1	0	-0.492274	-1.426031	-1.932063
25	1	0	2.011828	-0.759688	-1.486145
26	8	0	1.013351	1.297553	-0.547472
27	6	0	1.899181	2.388328	-0.048690
28	6	0	3.362644	1.930812	-0.079589
29	1	0	4.021377	2.762874	0.226759
30	1	0	3.537763	1.089236	0.613418
31	1	0	3.658218	1.615900	-1.096233
32	6	0	1.467878	2.835272	1.355585
33	1	0	2.039966	3.734216	1.648424
34	1	0	0.393515	3.087249	1.372222
35	1	0	1.652737	2.050585	2.107219
36	6	0	1.633158	3.488489	-1.084351

37	1	0	2.232823	4.381802	-0.837024
38	1	0	1.911857	3.153394	-2.098752
39	1	0	0.567743	3.778010	-1.087641

Zero-point correction= 0.309343 (Hartree/Particle)
Thermal correction to Energy= 0.329173
Thermal correction to Enthalpy= 0.330117
Thermal correction to Gibbs Free Energy= 0.260222
Sum of electronic and zero-point Energies= -938.256853
Sum of electronic and thermal Energies= -938.237023
Sum of electronic and thermal Enthalpies= -938.236079
Sum of electronic and thermal Free Energies= -938.305974
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -938.83292745

TS2’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.019724	3.054931	-0.680730
2	8	0	1.444674	3.083300	-0.732644
3	6	0	-0.488231	1.630531	-0.391816
4	1	0	-0.354455	3.762652	0.098564
5	1	0	-0.361258	3.407454	-1.666505
6	6	0	2.000382	2.084363	-0.003061
7	8	0	3.207874	1.935949	0.072813
8	6	0	0.921435	1.275445	0.711882
9	7	0	1.154528	-0.070661	0.894719
10	8	0	0.580716	-0.759463	1.780784
11	6	0	-1.760515	1.491913	0.218453
12	1	0	-0.277892	0.949154	-1.231290
13	1	0	0.614947	1.729275	1.664334
14	8	0	1.609250	-0.677017	-0.334509
15	6	0	2.492047	-1.870269	-0.154442
16	6	0	1.629237	-3.118646	0.081200
17	1	0	2.270380	-4.018722	0.097054
18	1	0	1.090668	-3.052105	1.038822
19	1	0	0.890646	-3.238900	-0.731170
20	6	0	3.499200	-1.624675	0.974796
21	1	0	4.260999	-2.423887	0.964274
22	1	0	4.003987	-0.653419	0.834876
23	1	0	3.010377	-1.631778	1.963267
24	6	0	3.191580	-1.934784	-1.519536
25	1	0	3.837055	-2.829681	-1.560956
26	1	0	2.453105	-2.007949	-2.337497
27	1	0	3.817899	-1.042126	-1.688478
28	1	0	-2.051593	2.272000	0.936581
29	6	0	-2.720165	0.432129	0.024012
30	6	0	-2.547335	-0.643418	-0.899428
31	6	0	-3.940690	0.467333	0.764759
32	6	0	-3.533449	-1.620737	-1.058624
33	1	0	-1.625877	-0.714361	-1.487517
34	6	0	-4.924329	-0.512882	0.598244
35	1	0	-4.100234	1.286557	1.476867
36	6	0	-4.729504	-1.566515	-0.314251
37	1	0	-3.372239	-2.436800	-1.772876
38	1	0	-5.849865	-0.456871	1.183270
39	1	0	-5.498087	-2.336336	-0.444956

Zero-point correction= 0.309470 (Hartree/Particle)
Thermal correction to Energy= 0.329173
Thermal correction to Enthalpy= 0.330117
Thermal correction to Gibbs Free Energy= 0.260958
Sum of electronic and zero-point Energies= -938.254175
Sum of electronic and thermal Energies= -938.234472
Sum of electronic and thermal Enthalpies= -938.233528

Sum of electronic and thermal Free Energies= -938.302687
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -938.82999393

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.113454	3.039250	-0.987725
2	8	0	-1.008675	3.490793	-0.157568
3	6	0	0.134952	1.510067	-0.860415
4	1	0	-0.077984	3.364222	-2.024486
5	1	0	1.019473	3.537242	-0.609589
6	6	0	-1.879347	2.463225	0.073547
7	8	0	-2.911668	2.610274	0.700889
8	6	0	-1.341956	1.179151	-0.592938
9	7	0	-1.400660	0.041569	0.345056
10	8	0	-0.219925	0.217913	1.154244
11	6	0	0.819149	1.000460	0.438151
12	1	0	1.033855	1.852916	1.108964
13	6	0	2.096934	0.210003	0.235191
14	6	0	2.100234	-1.034184	-0.430931
15	6	0	3.316551	0.734796	0.707507
16	6	0	3.302184	-1.729649	-0.628475
17	1	0	1.148866	-1.451919	-0.779663
18	6	0	4.521920	0.040568	0.505777
19	1	0	3.321309	1.696487	1.235695
20	6	0	4.517413	-1.194070	-0.163101
21	1	0	3.291983	-2.695952	-1.146189
22	1	0	5.462469	0.463170	0.877550
23	1	0	5.454892	-1.740374	-0.318156
24	1	0	0.542508	1.026905	-1.760232
25	1	0	-1.943899	0.944870	-1.484330
26	8	0	-1.200464	-1.127947	-0.501636
27	6	0	-1.998845	-2.271614	-0.008792
28	6	0	-3.493694	-1.932147	-0.110332
29	1	0	-4.107389	-2.793733	0.208881
30	1	0	-3.745588	-1.072575	0.534094
31	1	0	-3.767605	-1.681887	-1.151183
32	6	0	-1.595808	-2.636996	1.426781
33	1	0	-2.139939	-3.543094	1.749316
34	1	0	-0.513121	-2.840871	1.492948
35	1	0	-1.841699	-1.822319	2.128673
36	6	0	-1.617775	-3.385934	-0.992210
37	1	0	-2.193299	-4.300138	-0.763100
38	1	0	-1.843690	-3.089718	-2.031992
39	1	0	-0.542875	-3.630026	-0.922247

Zero-point correction= 0.313404 (Hartree/Particle)
Thermal correction to Energy= 0.332185
Thermal correction to Enthalpy= 0.333129
Thermal correction to Gibbs Free Energy= 0.265969
Sum of electronic and zero-point Energies= -938.306288
Sum of electronic and thermal Energies= -938.287507
Sum of electronic and thermal Enthalpies= -938.286563
Sum of electronic and thermal Free Energies= -938.353723
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -938.88147940

INT2’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.137676	2.987420	-0.466261
2	8	0	1.289644	3.151245	-0.858577

3	6	0	-0.196785	1.506413	-0.116147
4	1	0	-0.339919	3.649161	0.394437
5	1	0	-0.736233	3.297597	-1.334763
6	6	0	2.071361	2.155631	-0.306521
7	8	0	3.261781	2.065670	-0.537052
8	6	0	1.140078	1.373628	0.608250
9	7	0	1.242337	-0.043357	0.983182
10	8	0	-0.157124	-0.264565	1.437092
11	6	0	-1.093016	0.782902	0.882299
12	1	0	-0.146359	0.923350	-1.053558
13	1	0	1.091603	1.933206	1.566256
14	8	0	1.415825	-0.756033	-0.259749
15	6	0	2.237624	-1.972303	-0.060628
16	6	0	1.542070	-2.935569	0.910252
17	1	0	2.134182	-3.863900	1.005112
18	1	0	1.445144	-2.488273	1.913845
19	1	0	0.534381	-3.204234	0.548596
20	6	0	3.635678	-1.576428	0.434950
21	1	0	4.290451	-2.465342	0.480435
22	1	0	4.093096	-0.837694	-0.245514
23	1	0	3.586173	-1.134908	1.444934
24	6	0	2.296847	-2.555507	-1.478361
25	1	0	2.900690	-3.479851	-1.479326
26	1	0	1.286315	-2.804776	-1.847602
27	1	0	2.759758	-1.839837	-2.180701
28	1	0	-1.356962	1.451807	1.723642
29	6	0	-2.333363	0.112766	0.337007
30	6	0	-2.240086	-0.936906	-0.601210
31	6	0	-3.606098	0.549781	0.753767
32	6	0	-3.400824	-1.525916	-1.123027
33	1	0	-1.249901	-1.293132	-0.907394
34	6	0	-4.769488	-0.038541	0.228938
35	1	0	-3.684572	1.357748	1.491791
36	6	0	-4.669493	-1.077106	-0.711157
37	1	0	-3.317099	-2.341035	-1.851173
38	1	0	-5.753672	0.311959	0.560456
39	1	0	-5.575410	-1.540464	-1.118372

Zero-point correction=	0.312844 (Hartree/Particle)
Thermal correction to Energy=	0.331846
Thermal correction to Enthalpy=	0.332790
Thermal correction to Gibbs Free Energy=	0.265266
Sum of electronic and zero-point Energies=	-938.285372
Sum of electronic and thermal Energies=	-938.266370
Sum of electronic and thermal Enthalpies=	-938.265426
Sum of electronic and thermal Free Energies=	-938.332950
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d)	energy in DMF= -938.8600036

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.123111
2	1	0	0.000000	0.762663	-0.492445
3	1	0	0.000000	-0.762663	-0.492445

Zero-point correction=	0.020372 (Hartree/Particle)
Thermal correction to Energy=	0.023207
Thermal correction to Enthalpy=	0.024151
Thermal correction to Gibbs Free Energy=	0.002666
Sum of electronic and zero-point Energies=	-76.396519
Sum of electronic and thermal Energies=	-76.393684
Sum of electronic and thermal Enthalpies=	-76.392740
Sum of electronic and thermal Free Energies=	-76.414224
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d)	energy in DMF= -76.46694406

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.611015	3.298611	0.422321
2	8	0	0.728301	3.745925	0.031187
3	6	0	-0.593933	1.752076	0.476526
4	1	0	-0.823984	3.738669	1.408824
5	1	0	-1.318647	3.706187	-0.317619
6	6	0	1.613955	2.714261	-0.072242
7	8	0	2.783748	2.874840	-0.367808
8	6	0	0.884832	1.409501	0.255982
9	7	0	1.012752	0.473514	-0.797138
10	8	0	-0.174159	0.251450	-1.353921
11	6	0	-1.308329	1.005589	-0.667335
12	1	0	-1.665079	1.689253	-1.457095
13	6	0	-2.397295	0.034947	-0.281320
14	6	0	-2.108895	-1.144878	0.438158
15	6	0	-3.732525	0.334507	-0.617828
16	6	0	-3.150847	-2.003299	0.820622
17	1	0	-1.066252	-1.401134	0.665840
18	6	0	-4.773210	-0.521800	-0.222222
19	1	0	-3.956773	1.244639	-1.186928
20	6	0	-4.484211	-1.692077	0.498440
21	1	0	-2.920678	-2.922100	1.372267
22	1	0	-5.808469	-0.276549	-0.484726
23	1	0	-5.294370	-2.364479	0.802762
24	1	0	-0.956087	1.394744	1.452477
25	8	0	1.256459	-1.364070	0.353239
26	6	0	2.208845	-2.248927	-0.266926
27	6	0	3.600078	-1.588068	-0.356770
28	1	0	4.316628	-2.253954	-0.871329
29	1	0	3.546380	-0.638983	-0.917486
30	1	0	4.009916	-1.376333	0.648186
31	6	0	1.689734	-2.615113	-1.667904
32	1	0	2.343871	-3.369284	-2.142006
33	1	0	0.668748	-3.032308	-1.605269
34	1	0	1.658714	-1.726296	-2.321308
35	6	0	2.277620	-3.512739	0.622138
36	1	0	2.983481	-4.249759	0.195894
37	1	0	2.621078	-3.256414	1.640625
38	1	0	1.284165	-3.988901	0.702112
39	1	0	1.451558	0.923891	1.253221
40	8	0	1.969454	0.011502	2.212631
41	1	0	1.700115	-0.822558	1.318398
42	1	0	2.937188	0.174346	2.130666

Zero-point correction= 0.329971 (Hartree/Particle)
Thermal correction to Energy= 0.351081
Thermal correction to Enthalpy= 0.352025
Thermal correction to Gibbs Free Energy= 0.279330
Sum of electronic and zero-point Energies= -1014.676798
Sum of electronic and thermal Energies= -1014.655689
Sum of electronic and thermal Enthalpies= -1014.654745
Sum of electronic and thermal Free Energies= -1014.727439
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1015.31356220

TS3’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.139002	3.289351	-0.695688

2	8	0	-1.310185	3.503602	-0.632584
3	6	0	0.380674	1.764346	-0.572886
4	1	0	0.480148	3.702816	-1.655817
5	1	0	0.591267	3.861885	0.132352
6	6	0	-1.980342	2.392717	-0.217698
7	8	0	-3.178637	2.378363	-0.013100
8	6	0	-0.975910	1.237640	-0.090237
9	7	0	-0.851696	0.763878	1.247048
10	8	0	0.409832	0.804215	1.627299
11	6	0	1.359871	1.318686	0.524608
12	1	0	1.865867	2.163290	1.020450
13	6	0	2.344963	0.227804	0.194221
14	6	0	1.914398	-1.024814	-0.297178
15	6	0	3.721885	0.473808	0.369457
16	6	0	2.862303	-2.010042	-0.613010
17	1	0	0.838554	-1.234852	-0.400877
18	6	0	4.665312	-0.512585	0.040245
19	1	0	4.054015	1.444226	0.757529
20	6	0	4.236489	-1.756617	-0.451129
21	1	0	2.526121	-2.984074	-0.986851
22	1	0	5.733873	-0.309330	0.172881
23	1	0	4.970783	-2.530084	-0.703406
24	1	0	0.658533	1.330422	-1.544594
25	1	0	-1.393392	0.249683	-0.587147
26	8	0	-1.343115	-1.209097	-0.045314
27	6	0	-2.240232	-2.288683	-0.041670
28	6	0	-3.644364	-1.832411	0.420586
29	1	0	-4.373529	-2.664597	0.426025
30	1	0	-3.591687	-1.414574	1.442694
31	1	0	-4.031898	-1.042147	-0.248564
32	6	0	-1.691473	-3.379053	0.914959
33	1	0	-2.375080	-4.246965	0.965131
34	1	0	-0.701958	-3.733115	0.574530
35	1	0	-1.578206	-2.968734	1.934805
36	6	0	-2.314906	-2.862828	-1.482420
37	1	0	-2.999140	-3.730921	-1.526790
38	1	0	-2.686436	-2.093164	-2.183228
39	1	0	-1.315145	-3.187488	-1.821822

Zero-point correction= 0.307731 (Hartree/Particle)
Thermal correction to Energy= 0.327024
Thermal correction to Enthalpy= 0.327968
Thermal correction to Gibbs Free Energy= 0.259012
Sum of electronic and zero-point Energies= -938.259084
Sum of electronic and thermal Energies= -938.239790
Sum of electronic and thermal Enthalpies= -938.238846
Sum of electronic and thermal Free Energies= -938.307802
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -938.83142330

^{t}BuOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.992050	0.003144	1.701272
2	8	0	0.037455	0.000534	1.465972
3	6	0	-0.007297	-0.000089	0.013320
4	6	0	0.682299	1.268806	-0.522615
5	1	0	0.637651	1.320086	-1.626150
6	1	0	0.199022	2.174228	-0.113439
7	1	0	1.749943	1.286693	-0.230333
8	6	0	-1.501236	-0.002621	-0.338165
9	1	0	-1.647469	-0.003257	-1.432551
10	1	0	-1.996900	-0.898112	0.078189
11	1	0	-1.999780	0.891571	0.077533
12	6	0	0.686659	-1.266916	-0.521775

13	1	0	0.643008	-1.318613	-1.625345
14	1	0	1.754162	-1.281234	-0.228727
15	1	0	0.206124	-2.173869	-0.112810

Zero-point correction= 0.131560 (Hartree/Particle)
Thermal correction to Energy= 0.138492
Thermal correction to Enthalpy= 0.139436
Thermal correction to Gibbs Free Energy= 0.102395
Sum of electronic and zero-point Energies= -233.533814
Sum of electronic and thermal Energies= -233.526882
Sum of electronic and thermal Enthalpies= -233.525938
Sum of electronic and thermal Free Energies= -233.562980
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -233.74820976

^{t}BuOH-H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.199634	-0.000041	-1.143890
2	6	0	0.683137	-0.000005	-0.003386
3	6	0	0.448238	1.268309	0.844205
4	1	0	1.138339	1.322570	1.706942
5	1	0	0.592088	2.174814	0.228544
6	1	0	-0.584709	1.286908	1.241059
7	6	0	2.105625	-0.001077	-0.583983
8	1	0	2.865514	-0.000870	0.217859
9	1	0	2.265200	-0.895644	-1.213104
10	1	0	2.265954	0.892517	-1.214299
11	6	0	0.446882	-1.267186	0.845469
12	1	0	1.137249	-1.321436	1.707987
13	1	0	-0.585934	-1.284158	1.242774
14	1	0	0.589474	-2.174418	0.230603
15	1	0	-2.974239	0.769545	0.400936
16	8	0	-2.888861	-0.000079	-0.203288
17	1	0	-1.129514	-0.000215	-0.787563
18	1	0	-2.974753	-0.768894	0.401858

Zero-point correction= 0.155347 (Hartree/Particle)
Thermal correction to Energy= 0.165474
Thermal correction to Enthalpy= 0.166418
Thermal correction to Gibbs Free Energy= 0.121086
Sum of electronic and zero-point Energies= -309.936941
Sum of electronic and thermal Energies= -309.926814
Sum of electronic and thermal Enthalpies= -309.925869
Sum of electronic and thermal Free Energies= -309.971202
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -310.21886077

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.732371	1.725870	-0.131055
2	8	0	-3.125197	1.329264	-0.449297
3	6	0	-0.905324	0.438507	-0.294415
4	1	0	-1.469464	2.531028	-0.830807
5	1	0	-1.717401	2.101453	0.906835
6	6	0	-3.310681	-0.028862	-0.296596
7	8	0	-4.401500	-0.564467	-0.395548
8	6	0	-1.966023	-0.578522	0.004891
9	7	0	-1.599161	-1.593040	0.720399
10	8	0	-0.246165	-1.432663	1.026332
11	6	0	0.166681	0.007066	0.715825
12	1	0	0.054053	0.549584	1.673242
13	6	0	1.603987	0.012026	0.264423

14	6	0	2.556842	0.758090	0.985473
15	6	0	2.015181	-0.715568	-0.873306
16	6	0	3.898046	0.792947	0.568678
17	1	0	2.243210	1.317508	1.874976
18	6	0	3.355996	-0.687732	-1.282885
19	1	0	1.286656	-1.311969	-1.434483
20	6	0	4.300340	0.069195	-0.565245
21	1	0	4.628336	1.381944	1.134889
22	1	0	3.665905	-1.259672	-2.164803
23	1	0	5.347090	0.090424	-0.888818
24	1	0	-0.557407	0.335817	-1.340453

Zero-point correction= 0.178073 (Hartree/Particle)
Thermal correction to Energy= 0.189820
Thermal correction to Enthalpy= 0.190764
Thermal correction to Gibbs Free Energy= 0.138809
Sum of electronic and zero-point Energies= -704.792314
Sum of electronic and thermal Energies= -704.780566
Sum of electronic and thermal Enthalpies= -704.779622
Sum of electronic and thermal Free Energies= -704.831578
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -705.16436205

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.981440	0.285426	0.007024
2	6	0	-2.072868	-0.545245	-0.676755
3	1	0	-3.045260	-0.035264	-0.558739
4	1	0	-1.867708	-0.648667	-1.756717
5	1	0	-2.158698	-1.551506	-0.233555
6	6	0	-0.860037	1.684666	-0.606428
7	1	0	-1.760098	2.275648	-0.363002
8	1	0	0.026699	2.205697	-0.204603
9	1	0	-0.767999	1.628863	-1.705389
10	6	0	-1.150943	0.341708	1.529707
11	1	0	-1.172094	-0.672643	1.965031
12	1	0	-0.327755	0.910007	1.997061
13	1	0	-2.102368	0.843019	1.780640
14	8	0	0.363313	-0.315285	-0.290645
15	7	0	0.445139	-1.706291	0.087054
16	8	0	1.553797	-2.120941	-0.101793
17	8	0	2.561785	1.626568	0.114678
18	1	0	1.952510	0.868759	-0.043118
19	1	0	2.667359	1.998065	-0.786198

Zero-point correction= 0.151202 (Hartree/Particle)
Thermal correction to Energy= 0.163543
Thermal correction to Enthalpy= 0.164487
Thermal correction to Gibbs Free Energy= 0.113277
Sum of electronic and zero-point Energies= -439.244445
Sum of electronic and thermal Energies= -439.232104
Sum of electronic and thermal Enthalpies= -439.231160
Sum of electronic and thermal Free Energies= -439.282370
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -439.55302115

TS1-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.896106	-2.272883	0.498828
2	6	0	-5.206490	-1.589247	1.518256
3	6	0	-4.348359	-0.527753	1.206121
4	6	0	-4.155951	-0.123994	-0.139550

5	6	0	-4.859447	-0.820570	-1.153016
6	6	0	-5.719110	-1.883458	-0.839157
7	1	0	-6.567415	-3.102137	0.748861
8	1	0	-5.341416	-1.885613	2.564866
9	1	0	-3.825584	-0.005863	2.015151
10	1	0	-4.722915	-0.518567	-2.198778
11	1	0	-6.251446	-2.407675	-1.641017
12	6	0	-3.263610	0.976982	-0.535908
13	1	0	-3.250816	1.193716	-1.614138
14	6	0	-2.481856	1.734523	0.270279
15	1	0	-2.442099	1.567810	1.354635
16	6	0	-1.655035	2.867141	-0.249348
17	1	0	-1.872413	3.813968	0.271289
18	1	0	-1.763519	3.004952	-1.336185
19	8	0	-0.213723	2.656992	0.061994
20	6	0	0.484407	1.934693	-0.831510
21	8	0	0.084345	1.468805	-1.888661
22	6	0	1.896786	1.661613	-0.349018
23	1	0	2.659166	1.631514	-1.133447
24	7	0	2.289262	2.351888	0.776461
25	7	0	2.447172	2.208443	1.919406
26	6	0	3.498484	-1.482371	-0.939841
27	6	0	2.704381	-2.732368	-0.518588
28	1	0	2.891848	-3.569090	-1.215543
29	1	0	3.011985	-3.041750	0.496134
30	1	0	1.618034	-2.532323	-0.510957
31	6	0	5.005460	-1.790697	-0.986342
32	1	0	5.212576	-2.543353	-1.768360
33	1	0	5.587134	-0.880978	-1.218455
34	1	0	5.351100	-2.191309	-0.017383
35	6	0	3.016727	-0.934132	-2.293550
36	1	0	1.952648	-0.642189	-2.259153
37	1	0	3.612268	-0.054347	-2.599271
38	1	0	3.127272	-1.705947	-3.076875
39	8	0	3.403302	-0.457951	0.102680
40	7	0	1.862770	-0.043198	0.367127
41	8	0	1.700857	0.049538	1.579696
42	8	0	4.202450	-1.800223	2.525498
43	1	0	3.944729	-1.240642	1.747571
44	1	0	3.334883	-1.952271	2.954503

Zero-point correction= 0.339408 (Hartree/Particle)
Thermal correction to Energy= 0.365689
Thermal correction to Enthalpy= 0.366633
Thermal correction to Gibbs Free Energy= 0.279358
Sum of electronic and zero-point Energies= -1124.130188
Sum of electronic and thermal Energies= -1124.103907
Sum of electronic and thermal Enthalpies= -1124.102963
Sum of electronic and thermal Free Energies= -1124.190239
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1124.81263280

INT1-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.600780	-1.775929	0.177131
2	6	0	-5.576977	-1.817391	1.142706
3	6	0	-4.520305	-0.899499	1.097360
4	6	0	-4.458068	0.084256	0.077776
5	6	0	-5.499049	0.115181	-0.882796
6	6	0	-6.557559	-0.803971	-0.836087
7	1	0	-7.425728	-2.496184	0.217732
8	1	0	-5.605026	-2.570626	1.938647
9	1	0	-3.737091	-0.945494	1.862187
10	1	0	-5.467747	0.872119	-1.676231

11	1	0	-7.349618	-0.760684	-1.592531
12	6	0	-3.371536	1.071472	-0.033219
13	1	0	-3.490976	1.795136	-0.853048
14	6	0	-2.273387	1.180389	0.751360
15	1	0	-2.091562	0.484483	1.581241
16	6	0	-1.253892	2.264710	0.576622
17	1	0	-1.143988	2.869066	1.493298
18	1	0	-1.487091	2.922057	-0.275486
19	8	0	0.093305	1.688269	0.395462
20	6	0	0.469379	1.465888	-0.888067
21	8	0	-0.189347	1.751234	-1.889688
22	6	0	1.796094	0.840113	-1.031074
23	1	0	2.178419	0.669904	-2.034693
24	6	0	4.158075	-1.489855	-0.296135
25	6	0	4.400659	-1.759202	1.195802
26	1	0	4.842243	-2.765040	1.313218
27	1	0	5.101705	-1.015596	1.612459
28	1	0	3.465126	-1.725712	1.776307
29	6	0	5.446904	-1.676803	-1.108143
30	1	0	5.774837	-2.727949	-1.028648
31	1	0	5.283848	-1.441557	-2.173907
32	1	0	6.257743	-1.034821	-0.721378
33	6	0	3.007839	-2.326255	-0.860469
34	1	0	2.066705	-2.151676	-0.309290
35	1	0	2.841022	-2.113069	-1.930723
36	1	0	3.255061	-3.397711	-0.758587
37	8	0	3.888827	-0.028876	-0.553501
38	7	0	2.578532	0.448585	-0.033682
39	8	0	2.425871	0.484740	1.191704
40	8	0	5.509073	1.483980	1.427646
41	1	0	5.086316	1.042775	0.653962
42	1	0	4.769877	1.477075	2.071645

Zero-point correction= 0.333532 (Hartree/Particle)
Thermal correction to Energy= 0.357783
Thermal correction to Enthalpy= 0.358728
Thermal correction to Gibbs Free Energy= 0.276195
Sum of electronic and zero-point Energies= -1014.683481
Sum of electronic and thermal Energies= -1014.659229
Sum of electronic and thermal Enthalpies= -1014.658285
Sum of electronic and thermal Free Energies= -1014.740818
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1015.32948557

INT1-40

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.342238	0.694766	1.814177
2	8	0	0.916373	1.893938	1.083850
3	6	0	1.944379	-0.395897	0.944908
4	1	0	2.107162	1.097813	2.501014
5	1	0	0.508507	0.305229	2.424282
6	6	0	-0.324254	2.017785	0.499439
7	8	0	-0.614356	3.108768	0.013056
8	6	0	-1.180498	0.831425	0.496406
9	7	0	-2.445062	0.903070	0.064462
10	8	0	-3.089906	1.873707	-0.335427
11	6	0	1.435526	-1.652594	1.029600
12	1	0	0.569159	-1.797772	1.695506
13	1	0	-0.851731	-0.165677	0.775505
14	8	0	-3.055896	-0.415871	0.135401
15	6	0	-4.453988	-0.558097	-0.368296
16	6	0	-4.533099	-0.236371	-1.867277
17	1	0	-4.392110	0.836000	-2.069382
18	1	0	-3.771750	-0.809140	-2.425575

19	1	0	-5.528352	-0.531996	-2.244781
20	6	0	-5.435720	0.258046	0.485709
21	1	0	-5.332591	1.340496	0.319063
22	1	0	-6.467769	-0.036187	0.223439
23	1	0	-5.282430	0.044777	1.558326
24	6	0	-4.662142	-2.063380	-0.129777
25	1	0	-3.935953	-2.662178	-0.706079
26	1	0	-4.560546	-2.314516	0.940271
27	1	0	-5.679341	-2.340647	-0.456630
28	6	0	3.160418	-0.047915	0.142779
29	6	0	4.384586	-0.715040	0.388172
30	6	0	3.137119	0.959761	-0.850653
31	6	0	5.542344	-0.394766	-0.338655
32	1	0	4.427693	-1.482586	1.169385
33	6	0	4.295180	1.277875	-1.578449
34	1	0	2.205050	1.491152	-1.064055
35	6	0	5.501750	0.603397	-1.326508
36	1	0	6.478718	-0.924464	-0.127859
37	1	0	4.251584	2.056538	-2.348980
38	1	0	6.404368	0.854962	-1.895102
39	6	0	1.881729	-2.895291	0.304857
40	1	0	2.303955	-3.608774	1.042756
41	1	0	2.692891	-2.664649	-0.407840
42	6	0	0.711663	-3.584596	-0.427092
43	1	0	1.049599	-4.519042	-0.910120
44	1	0	-0.103533	-3.841274	0.274360
45	1	0	0.289739	-2.928532	-1.209835

Zero-point correction= 0.364600 (Hartree/Particle)
Thermal correction to Energy= 0.388649
Thermal correction to Enthalpy= 0.389593
Thermal correction to Gibbs Free Energy= 0.307002
Sum of electronic and zero-point Energies= -1016.840266
Sum of electronic and thermal Energies= -1016.816217
Sum of electronic and thermal Enthalpies= -1016.815273
Sum of electronic and thermal Free Energies= -1016.897865
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1017.49346457

TS2-40

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.616513	2.303408	0.644939
2	8	0	-0.444606	3.017973	1.161521
3	6	0	-1.257838	1.068610	-0.195195
4	1	0	-2.243093	2.033653	1.510135
5	1	0	-2.152752	3.063842	0.054192
6	6	0	0.638939	2.256219	1.415408
7	8	0	1.651865	2.739990	1.901294
8	6	0	0.501492	0.781058	1.081510
9	7	0	1.363601	0.336963	0.146773
10	8	0	1.509447	1.026802	-0.918446
11	6	0	-0.629330	1.343581	-1.434646
12	1	0	-0.379250	2.400840	-1.599217
13	1	0	0.287138	0.094506	1.905150
14	8	0	1.391949	-1.108719	0.017592
15	6	0	2.747560	-1.669098	0.261547
16	6	0	3.192816	-1.357273	1.696395
17	1	0	3.307379	-0.270642	1.853880
18	1	0	2.462909	-1.744982	2.429331
19	1	0	4.169135	-1.832976	1.898585
20	6	0	3.749618	-1.136202	-0.772007
21	1	0	3.915717	-0.052401	-0.653700
22	1	0	4.720561	-1.647488	-0.642284
23	1	0	3.392070	-1.325093	-1.798920

24	6	0	2.497576	-3.170344	0.068200
25	1	0	1.746201	-3.541257	0.787310
26	1	0	2.140934	-3.382022	-0.955167
27	1	0	3.437354	-3.726717	0.229736
28	6	0	-2.134592	-0.132586	0.081757
29	6	0	-2.832738	-0.817381	-0.941778
30	6	0	-2.370257	-0.562923	1.414268
31	6	0	-3.683983	-1.898661	-0.655281
32	1	0	-2.741933	-0.494150	-1.980055
33	6	0	-3.221439	-1.638003	1.703277
34	1	0	-1.881480	-0.050488	2.250225
35	6	0	-3.879812	-2.322419	0.667016
36	1	0	-4.204451	-2.401698	-1.478701
37	1	0	-3.368269	-1.942353	2.746156
38	1	0	-4.542758	-3.165905	0.890403
39	6	0	-0.600786	0.507201	-2.693446
40	1	0	-1.591716	0.596779	-3.190014
41	1	0	-0.479489	-0.563310	-2.447945
42	6	0	0.464496	0.945953	-3.710453
43	1	0	0.357168	0.378158	-4.652447
44	1	0	0.363589	2.020413	-3.953967
45	1	0	1.479332	0.779349	-3.314836

Zero-point correction= 0.364729 (Hartree/Particle)
Thermal correction to Energy= 0.387177
Thermal correction to Enthalpy= 0.388121
Thermal correction to Gibbs Free Energy= 0.312704
Sum of electronic and zero-point Energies= -1016.808161
Sum of electronic and thermal Energies= -1016.785713
Sum of electronic and thermal Enthalpies= -1016.784769
Sum of electronic and thermal Free Energies= -1016.860186
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1017.46009319

INT2-40

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.203531	1.129425	-1.889657
2	8	0	-0.766476	2.455556	-1.465950
3	6	0	-0.991791	0.170225	-0.669029
4	1	0	-2.256766	1.217260	-2.194346
5	1	0	-0.587202	0.833030	-2.755089
6	6	0	0.016516	2.372710	-0.350867
7	8	0	0.511963	3.354820	0.171987
8	6	0	0.140118	0.903540	0.080283
9	7	0	1.448397	0.368569	-0.448830
10	8	0	1.061973	-0.630968	-1.442544
11	6	0	-0.274019	-1.128372	-1.133191
12	1	0	-0.660311	-1.470934	-2.112089
13	1	0	0.143308	0.809211	1.173509
14	8	0	2.046672	-0.320479	0.675560
15	6	0	3.515782	-0.147550	0.683114
16	6	0	3.859386	1.336352	0.876449
17	1	0	3.493128	1.937468	0.027305
18	1	0	3.401253	1.725549	1.803371
19	1	0	4.953808	1.470065	0.948344
20	6	0	4.137123	-0.710009	-0.602412
21	1	0	3.799536	-0.145098	-1.487608
22	1	0	5.238612	-0.638493	-0.549062
23	1	0	3.865105	-1.771077	-0.740411
24	6	0	3.927990	-0.976248	1.907377
25	1	0	3.441108	-0.595442	2.822749
26	1	0	3.649901	-2.037160	1.778023
27	1	0	5.021515	-0.918978	2.048330
28	6	0	-2.301361	-0.027139	0.093493

29	6	0	-3.331899	-0.775496	-0.523157
30	6	0	-2.554893	0.539904	1.358713
31	6	0	-4.567199	-0.965847	0.112206
32	1	0	-3.162085	-1.214227	-1.513977
33	6	0	-3.795959	0.353926	1.994590
34	1	0	-1.793597	1.143716	1.863747
35	6	0	-4.804502	-0.400779	1.377785
36	1	0	-5.346536	-1.555541	-0.383908
37	1	0	-3.969547	0.807244	2.977264
38	1	0	-5.770033	-0.545553	1.875436
39	6	0	-0.277423	-2.295413	-0.135362
40	1	0	-1.325276	-2.623152	-0.002972
41	1	0	0.076987	-1.943318	0.849844
42	6	0	0.576650	-3.476976	-0.612700
43	1	0	1.633295	-3.179544	-0.725188
44	1	0	0.530153	-4.310974	0.110333
45	1	0	0.225878	-3.858985	-1.590033

Zero-point correction= 0.367810 (Hartree/Particle)
Thermal correction to Energy= 0.389726
Thermal correction to Enthalpy= 0.390671
Thermal correction to Gibbs Free Energy= 0.316993
Sum of electronic and zero-point Energies= -1016.867260
Sum of electronic and thermal Energies= -1016.845344
Sum of electronic and thermal Enthalpies= -1016.844399
Sum of electronic and thermal Free Energies= -1016.918077
BP86/6-311++G(d,p)/SMD//BP86/6-31G(d) energy in DMF= -1017.51820594

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.123761	-2.164507	0.260477
2	6	0	5.536078	-1.236555	1.138142
3	6	0	4.419201	-0.486393	0.744237
4	6	0	3.860413	-0.646478	-0.550032
5	6	0	4.476940	-1.578809	-1.427930
6	6	0	5.588043	-2.331703	-1.028294
7	1	0	6.995103	-2.748599	0.577135
8	1	0	5.951392	-1.091792	2.141969
9	1	0	3.987366	0.231757	1.443850
10	1	0	4.067231	-1.709730	-2.436686
11	1	0	6.038775	-3.046943	-1.725439
12	6	0	2.702839	0.080879	-1.086587
13	1	0	2.553364	-0.092867	-2.163860
14	6	0	1.758490	0.909983	-0.585230
15	6	0	0.699351	1.566013	-1.416817
16	1	0	0.884058	1.342207	-2.482239
17	1	0	0.674933	2.659641	-1.278105
18	8	0	-0.612766	1.023770	-1.078776
19	6	0	-1.604548	1.942525	-0.883521
20	8	0	-1.463483	3.164690	-0.981940
21	6	0	-2.901915	1.367215	-0.536043
22	1	0	-3.731911	2.044389	-0.347350
23	6	0	-5.042071	-1.413200	0.370035
24	6	0	-4.273451	-1.721176	1.661728
25	1	0	-4.729690	-2.600423	2.150414
26	1	0	-3.214187	-1.951862	1.467727
27	1	0	-4.331943	-0.871005	2.364215
28	6	0	-4.950968	-2.537044	-0.673782
29	1	0	-5.477273	-3.429410	-0.289494
30	1	0	-5.443243	-2.229800	-1.613401
31	1	0	-3.909653	-2.814680	-0.893847
32	6	0	-6.513595	-1.089003	0.677143
33	1	0	-6.597546	-0.262138	1.403330

34	1	0	-7.059051	-0.809793	-0.241343
35	1	0	-6.997218	-1.983378	1.107097
36	8	0	-4.608359	-0.107566	-0.211218
37	7	0	-3.185559	0.063641	-0.457604
38	8	0	-2.454236	-0.921309	-0.595104
39	35	0	1.613650	1.419194	1.342126

Zero-point correction= 0.300442 (Hartree/Particle)
Thermal correction to Energy= 0.322774
Thermal correction to Enthalpy= 0.323718
Thermal correction to Gibbs Free Energy= 0.244998
Sum of electronic and zero-point Energies= -950.866480
Sum of electronic and thermal Energies= -950.844148
Sum of electronic and thermal Enthalpies= -950.843204
Sum of electronic and thermal Free Energies= -950.921924
BP86/6-311++G(d,p)-SDD/SMD//BP86/6-31G(d)-LANL2DZ/SMD energy in DMF = -951.66444045

TS2-Br

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.216259	-3.047616	-0.314286
2	8	0	-0.796969	-3.085979	-1.365167
3	6	0	0.551673	-1.598456	0.027657
4	1	0	-0.173323	-3.585201	0.564904
5	1	0	1.079206	-3.596399	-0.722194
6	6	0	-1.736687	-2.113877	-1.262074
7	8	0	-2.690253	-2.072661	-2.020932
8	6	0	-1.504565	-1.123973	-0.129933
9	7	0	-1.424645	0.165442	-0.514331
10	8	0	-0.745074	0.477330	-1.533690
11	6	0	1.219761	-0.788105	-0.892154
12	1	0	1.230968	-1.219559	-1.903405
13	6	0	2.125146	0.353434	-0.720992
14	6	0	2.016255	1.322051	0.309538
15	6	0	3.176908	0.496507	-1.663526
16	6	0	2.943134	2.368498	0.405196
17	1	0	1.175188	1.277765	1.005951
18	6	0	4.106763	1.540757	-1.559207
19	1	0	3.266738	-0.233680	-2.476924
20	6	0	3.998371	2.480380	-0.519808
21	1	0	2.834508	3.111579	1.203799
22	1	0	4.915004	1.621495	-2.295175
23	1	0	4.720513	3.300532	-0.437912
24	1	0	-1.999768	-1.322343	0.825952
25	8	0	-1.550846	1.112999	0.563866
26	6	0	-2.652427	2.098438	0.334587
27	6	0	-3.974891	1.353536	0.117882
28	1	0	-4.801223	2.081197	0.031911
29	1	0	-3.955744	0.755785	-0.810351
30	1	0	-4.194982	0.680800	0.965807
31	6	0	-2.311605	3.022074	-0.843054
32	1	0	-3.066175	3.826692	-0.910059
33	1	0	-1.320750	3.487375	-0.701911
34	1	0	-2.307263	2.475349	-1.800223
35	6	0	-2.650027	2.865953	1.662114
36	1	0	-3.436684	3.640129	1.639277
37	1	0	-2.851278	2.189996	2.511416
38	1	0	-1.679461	3.365353	1.829053
39	35	0	0.961651	-1.424174	2.006176

Zero-point correction= 0.299509 (Hartree/Particle)
Thermal correction to Energy= 0.320709
Thermal correction to Enthalpy= 0.321654
Thermal correction to Gibbs Free Energy= 0.248115

Sum of electronic and zero-point Energies= -950.832678
Sum of electronic and thermal Energies= -950.811477
Sum of electronic and thermal Enthalpies= -950.810533
Sum of electronic and thermal Free Energies= -950.884072
BP86/6-311++G(d,p)-SDD/SMD//BP86/6-31G(d)-LANL2DZ/SMD energy in DMF = -951.62844627

INT2-Br

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.390892	-2.925994	-0.002369
2	8	0	-0.687499	-3.335435	-0.903286
3	6	0	0.189150	-1.411606	0.169733
4	1	0	0.270710	-3.473019	0.946160
5	1	0	1.346524	-3.197037	-0.475308
6	6	0	-1.717406	-2.437009	-0.858149
7	8	0	-2.760240	-2.607061	-1.455169
8	6	0	-1.329654	-1.240332	0.049819
9	7	0	-1.612678	0.021166	-0.651662
10	8	0	-0.476721	0.157116	-1.538516
11	6	0	0.705341	-0.572140	-1.041266
12	1	0	0.949832	-1.298478	-1.840402
13	6	0	1.896805	0.346055	-0.865117
14	6	0	1.759296	1.625818	-0.291521
15	6	0	3.162528	-0.078559	-1.315099
16	6	0	2.878332	2.461052	-0.156809
17	1	0	0.769394	1.951171	0.044258
18	6	0	4.284467	0.755125	-1.171252
19	1	0	3.270141	-1.064660	-1.783396
20	6	0	4.144169	2.027526	-0.592482
21	1	0	2.762712	3.455757	0.289120
22	1	0	5.264619	0.413950	-1.523454
23	1	0	5.015890	2.683695	-0.488394
24	1	0	-1.896289	-1.288846	0.991422
25	8	0	-1.530409	1.052613	0.357176
26	6	0	-2.571949	2.083705	0.127891
27	6	0	-3.961979	1.443048	0.254004
28	1	0	-4.748560	2.210374	0.138877
29	1	0	-4.114484	0.674709	-0.523071
30	1	0	-4.086327	0.969714	1.244752
31	6	0	-2.374774	2.753893	-1.238322
32	1	0	-3.107844	3.571119	-1.364104
33	1	0	-1.361488	3.183524	-1.325034
34	1	0	-2.522007	2.034882	-2.062172
35	6	0	-2.311916	3.068679	1.274979
36	1	0	-3.067670	3.873271	1.252083
37	1	0	-2.378584	2.560907	2.253371
38	1	0	-1.313072	3.531529	1.186511
39	35	0	0.943268	-0.870690	1.995844

Zero-point correction= 0.302686 (Hartree/Particle)
Thermal correction to Energy= 0.323199
Thermal correction to Enthalpy= 0.324143
Thermal correction to Gibbs Free Energy= 0.252681
Sum of electronic and zero-point Energies= -950.883250
Sum of electronic and thermal Energies= -950.862737
Sum of electronic and thermal Enthalpies= -950.861793
Sum of electronic and thermal Free Energies= -950.933255
BP86/6-311++G(d,p)-SDD/SMD//BP86/6-31G(d)-LANL2DZ/SMD energy in DMF = -951.67813003

TS3-Br

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.762101	2.892215	-0.830288
2	8	0	0.563230	3.484947	-0.976394
3	6	0	-0.558509	1.443560	-0.317868
4	1	0	-1.329741	3.528624	-0.138276
5	1	0	-1.249062	2.907813	-1.820294
6	6	0	1.559254	2.567662	-0.785204
7	8	0	2.734482	2.825896	-0.966198
8	6	0	0.939809	1.278111	-0.271816
9	7	0	1.334560	0.131673	-1.013519
10	8	0	0.254712	-0.396664	-1.611549
11	6	0	-1.032642	0.296153	-1.250000
12	1	0	-1.360029	0.736162	-2.208501
13	6	0	-2.044549	-0.731245	-0.802519
14	6	0	-1.677488	-1.817911	0.017814
15	6	0	-3.376541	-0.605712	-1.243169
16	6	0	-2.643896	-2.761125	0.398620
17	1	0	-0.636229	-1.921522	0.344920
18	6	0	-4.343261	-1.544039	-0.846637
19	1	0	-3.656727	0.229107	-1.896599
20	6	0	-3.977858	-2.624818	-0.026640
21	1	0	-2.353883	-3.607793	1.031321
22	1	0	-5.378212	-1.436689	-1.190339
23	1	0	-4.728609	-3.364119	0.274708
24	8	0	1.689202	-1.251304	0.427319
25	6	0	2.801712	-2.090959	0.038599
26	6	0	4.099950	-1.268546	-0.086309
27	1	0	4.933814	-1.910130	-0.424121
28	1	0	3.977016	-0.451806	-0.817808
29	1	0	4.396604	-0.829746	0.884568
30	6	0	2.469018	-2.791557	-1.290113
31	1	0	3.258320	-3.521868	-1.544557
32	1	0	1.508784	-3.331865	-1.216332
33	1	0	2.395465	-2.064799	-2.116723
34	6	0	2.937256	-3.136815	1.169312
35	1	0	3.773785	-3.825533	0.949335
36	1	0	3.140935	-2.646995	2.138542
37	1	0	2.012090	-3.731876	1.266217
38	1	0	1.479170	1.129856	0.910341
39	8	0	2.102345	0.581373	1.947000
40	1	0	2.007846	-0.420674	1.322856
41	1	0	3.034872	0.879531	1.824928
42	35	0	-1.418881	1.318537	1.591895

Zero-point correction= 0.319360 (Hartree/Particle)
Thermal correction to Energy= 0.342028
Thermal correction to Enthalpy= 0.342972
Thermal correction to Gibbs Free Energy= 0.265995
Sum of electronic and zero-point Energies= -1027.252327
Sum of electronic and thermal Energies= -1027.229659
Sum of electronic and thermal Enthalpies= -1027.228715
Sum of electronic and thermal Free Energies= -1027.305691
BP86/6-311++G(d,p)-SDD/SMD//BP86/6-31G(d)-LANL2DZ/SMD energy in DMF = -1028.10875398

INT3-Br

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.565066	-0.212195	1.733961
2	8	0	-2.986084	-0.097195	1.363273
3	6	0	-0.812213	-0.234031	0.404766
4	1	0	-1.329336	0.626772	2.401102
5	1	0	-1.422486	-1.170761	2.264949
6	6	0	-3.206229	-0.495078	0.060067
7	8	0	-4.315475	-0.591552	-0.430371
8	6	0	-1.856194	-0.759717	-0.503673

9	7	0	-1.427694	-1.528647	-1.461134
10	8	0	-0.054352	-1.657633	-1.314734
11	6	0	0.341774	-1.172774	0.055437
12	1	0	0.214083	-2.058595	0.711588
13	6	0	1.780930	-0.729218	0.059387
14	6	0	2.373484	-0.117647	-1.063619
15	6	0	2.546765	-0.942936	1.223370
16	6	0	3.717881	0.283284	-1.013982
17	1	0	1.789948	0.031932	-1.976898
18	6	0	3.886117	-0.526099	1.273583
19	1	0	2.091643	-1.436117	2.090331
20	6	0	4.474716	0.086534	0.154068
21	1	0	4.174408	0.752004	-1.892897
22	1	0	4.472148	-0.692481	2.184236
23	1	0	5.523348	0.402618	0.188553
24	35	0	-0.478983	1.769585	-0.199673

Zero-point correction= 0.167730 (Hartree/Particle)
Thermal correction to Energy= 0.181021
Thermal correction to Enthalpy= 0.181965
Thermal correction to Gibbs Free Energy= 0.125790
Sum of electronic and zero-point Energies= -717.379748
Sum of electronic and thermal Energies= -717.366457
Sum of electronic and thermal Enthalpies= -717.365513
Sum of electronic and thermal Free Energies= -717.421688
BP86/6-311++G(d,p)-SDD/SMD//BP86/6-31G(d)-LANL2DZ/SMD energy in DMF = -717.96690585

HBr

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.041122
2	1	0	0.000000	0.000000	-1.439275

Zero-point correction= 0.005280 (Hartree/Particle)
Thermal correction to Energy= 0.007640
Thermal correction to Enthalpy= 0.008585
Thermal correction to Gibbs Free Energy= -0.014019
Sum of electronic and zero-point Energies= -13.783005
Sum of electronic and thermal Energies= -13.780645
Sum of electronic and thermal Enthalpies= -13.779701
Sum of electronic and thermal Free Energies= -13.802304
BP86/6-311++G(d,p)-SDD/SMD//BP86/6-31G(d)-LANL2DZ/SMD energy in DMF = -14.01580048

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.592026	1.705156	0.000201
2	8	0	-3.045651	1.456119	0.000159
3	6	0	-1.001478	0.332100	0.000067
4	1	0	-1.356299	2.299633	-0.899026
5	1	0	-1.356344	2.299517	0.899511
6	6	0	-3.354171	0.108460	0.000017
7	8	0	-4.500106	-0.303758	-0.000052
8	6	0	-2.049821	-0.605476	-0.000009
9	7	0	-1.657223	-1.874125	-0.000148
10	8	0	-0.243807	-1.760059	-0.000171
11	6	0	0.147333	-0.435013	-0.000083
12	6	0	1.577723	-0.149515	-0.000040
13	6	0	2.535435	-1.192105	0.000200
14	6	0	2.015679	1.196806	-0.000252
15	6	0	3.902355	-0.887538	0.000245
16	1	0	2.207023	-2.235912	0.000370

17	6	0	3.384777	1.490356	-0.000214
18	1	0	1.284171	2.012212	-0.000453
19	6	0	4.332001	0.451209	0.000038
20	1	0	4.635979	-1.701095	0.000453
21	1	0	3.713224	2.535297	-0.000392
22	1	0	5.402470	0.684163	0.000070

Zero-point correction= 0.155989 (Hartree/Particle)
Thermal correction to Energy= 0.167198
Thermal correction to Enthalpy= 0.168142
Thermal correction to Gibbs Free Energy= 0.117901
Sum of electronic and zero-point Energies= -703.628810
Sum of electronic and thermal Energies= -703.617601
Sum of electronic and thermal Enthalpies= -703.616656
Sum of electronic and thermal Free Energies= -703.666898
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in DMF = -703.97290212

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.277311	0.266338	-0.000029
2	6	0	1.792455	-1.051837	0.000015
3	6	0	0.409683	-1.292221	0.000004
4	6	0	-0.520172	-0.224166	-0.000042
5	6	0	-0.013467	1.099858	-0.000103
6	6	0	1.366327	1.340150	-0.000092
7	1	0	2.491315	-1.896306	0.000055
8	1	0	0.035453	-2.323576	0.000038
9	1	0	-0.706523	1.948652	-0.000179
10	1	0	1.735891	2.372163	-0.000142
11	6	0	-1.962137	-0.537104	-0.000022
12	1	0	-2.194763	-1.612140	-0.000216
13	6	0	-2.990446	0.339200	0.000233
14	1	0	-2.848042	1.426683	0.000466
15	1	0	-4.026892	-0.016004	0.000220
16	1	0	3.356235	0.459222	-0.000024

Zero-point correction= 0.129677 (Hartree/Particle)
Thermal correction to Energy= 0.136635
Thermal correction to Enthalpy= 0.137579
Thermal correction to Gibbs Free Energy= 0.098258
Sum of electronic and zero-point Energies= -309.515140
Sum of electronic and thermal Energies= -309.508182
Sum of electronic and thermal Enthalpies= -309.507238
Sum of electronic and thermal Free Energies= -309.546559
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -309.72686406

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.223252	0.200160	-0.000046
2	6	0	1.299712	-0.796195	0.000055
3	1	0	1.152128	-1.877812	0.000118
4	8	0	0.373340	1.422490	0.000045
5	7	0	2.536235	-0.366230	0.000064
6	7	0	3.615994	0.034447	-0.000025
7	8	0	-0.978252	-0.443342	-0.000195
8	6	0	-2.151019	0.430842	-0.000014
9	1	0	-2.110492	1.077562	-0.893981
10	1	0	-2.110244	1.077704	0.893850
11	6	0	-3.380657	-0.460374	0.000093
12	1	0	-4.286665	0.171453	-0.000008

13	1	0	-3.409342	-1.103262	-0.896999
14	1	0	-3.409414	-1.102949	0.897418

Zero-point correction= 0.101745 (Hartree/Particle)
Thermal correction to Energy= 0.110496
Thermal correction to Enthalpy= 0.111441
Thermal correction to Gibbs Free Energy= 0.067688
Sum of electronic and zero-point Energies= -415.859196
Sum of electronic and thermal Energies= -415.850444
Sum of electronic and thermal Enthalpies= -415.849500
Sum of electronic and thermal Free Energies= -415.893253
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -416.08721364

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.769344	-0.011204	0.000003
2	6	0	-0.914305	-0.850396	-1.276472
3	1	0	-1.934810	-1.268759	-1.333056
4	1	0	-0.746537	-0.228689	-2.173585
5	1	0	-0.197328	-1.689006	-1.288913
6	6	0	-1.727921	1.184447	-0.000132
7	1	0	-2.770864	0.822234	-0.000426
8	1	0	-1.579111	1.810299	0.896936
9	1	0	-1.578670	1.810446	-0.897027
10	6	0	-0.914495	-0.850192	1.276614
11	1	0	-0.197555	-1.688823	1.289390
12	1	0	-0.746877	-0.228287	2.173619
13	1	0	-1.935028	-1.268497	1.333116
14	8	0	0.573680	0.650036	-0.000064
15	7	0	1.635420	-0.305956	-0.000108
16	8	0	2.700724	0.254318	0.000140

Zero-point correction= 0.128202 (Hartree/Particle)
Thermal correction to Energy= 0.136929
Thermal correction to Enthalpy= 0.137874
Thermal correction to Gibbs Free Energy= 0.095655
Sum of electronic and zero-point Energies= -362.844670
Sum of electronic and thermal Energies= -362.835942
Sum of electronic and thermal Enthalpies= -362.834998
Sum of electronic and thermal Free Energies= -362.877217
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -363.08499192

BF_3•OEt_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.281619	-1.048543	-0.008361
2	9	0	-0.898302	-1.773022	-0.048388
3	9	0	1.056936	-1.209028	-1.146938
4	9	0	0.985680	-1.227717	1.168412
5	8	0	-0.185601	0.520307	0.012287
6	6	0	-1.538133	0.798167	-0.560432
7	1	0	-1.478705	1.802371	-1.005222
8	1	0	-1.714910	0.065387	-1.361591
9	6	0	0.839789	1.515251	-0.412946
10	1	0	0.354410	2.493549	-0.276056
11	1	0	1.039915	1.351339	-1.484907
12	6	0	2.094208	1.419655	0.433222
13	1	0	2.651420	0.486668	0.261386
14	1	0	2.745521	2.264710	0.145072
15	1	0	1.862450	1.515706	1.506937
16	6	0	-2.581033	0.735783	0.538039

17	1	0	-3.567596	0.969772	0.098334
18	1	0	-2.631809	-0.269814	0.984543
19	1	0	-2.371792	1.475339	1.329937

Zero-point correction= 0.148492 (Hartree/Particle)
Thermal correction to Energy= 0.159224
Thermal correction to Enthalpy= 0.160168
Thermal correction to Gibbs Free Energy= 0.112440
Sum of electronic and zero-point Energies= -558.068560
Sum of electronic and thermal Energies= -558.057828
Sum of electronic and thermal Enthalpies= -558.056884
Sum of electronic and thermal Free Energies= -558.104611
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -558.40382238

OEt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	-0.286765	-0.000094
2	6	0	-1.183973	0.515604	0.000066
3	1	0	-1.196772	1.180384	-0.893869
4	1	0	-1.196654	1.180204	0.894135
5	6	0	1.183973	0.515604	-0.000006
6	1	0	1.196687	1.180221	0.894051
7	1	0	1.196739	1.180367	-0.893953
8	6	0	-2.399924	-0.401538	0.000053
9	1	0	-3.327580	0.198414	0.000166
10	1	0	-2.406356	-1.048082	-0.895740
11	1	0	-2.406243	-1.048251	0.895724
12	6	0	2.399924	-0.401538	-0.000044
13	1	0	2.406302	-1.048117	-0.895812
14	1	0	3.327580	0.198414	-0.000013
15	1	0	2.406297	-1.048216	0.895652

Zero-point correction= 0.133023 (Hartree/Particle)
Thermal correction to Energy= 0.139903
Thermal correction to Enthalpy= 0.140847
Thermal correction to Gibbs Free Energy= 0.102899
Sum of electronic and zero-point Energies= -233.522208
Sum of electronic and thermal Energies= -233.515328
Sum of electronic and thermal Enthalpies= -233.514384
Sum of electronic and thermal Free Energies= -233.552331
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -233.72980872

N_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.558495
2	7	0	0.000000	0.000000	-0.558495

Zero-point correction= 0.005363 (Hartree/Particle)
Thermal correction to Energy= 0.007724
Thermal correction to Enthalpy= 0.008668
Thermal correction to Gibbs Free Energy= -0.013106
Sum of electronic and zero-point Energies= -109.516145
Sum of electronic and thermal Energies= -109.513784
Sum of electronic and thermal Enthalpies= -109.512840
Sum of electronic and thermal Free Energies= -109.534614
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -109.55627391

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.123114
2	1	0	0.000000	0.762969	-0.492455
3	1	0	0.000000	-0.762969	-0.492455

Zero-point correction= 0.020370 (Hartree/Particle)
Thermal correction to Energy= 0.023205
Thermal correction to Enthalpy= 0.024149
Thermal correction to Gibbs Free Energy= 0.002664
Sum of electronic and zero-point Energies= -76.396752
Sum of electronic and thermal Energies= -76.393917
Sum of electronic and thermal Enthalpies= -76.392972
Sum of electronic and thermal Free Energies= -76.414457
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -76.46736563

^{t}BuOH-H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.194636	0.000116	-1.150349
2	6	0	0.679863	-0.000005	-0.002889
3	6	0	0.435125	1.267850	0.842629
4	1	0	1.114960	1.321099	1.713452
5	1	0	0.586542	2.174478	0.228879
6	1	0	-0.603093	1.284114	1.225218
7	6	0	2.107102	-0.000179	-0.571697
8	1	0	2.859927	-0.000303	0.236730
9	1	0	2.272140	-0.894561	-1.199755
10	1	0	2.272388	0.894193	-1.199707
11	6	0	0.434794	-1.267789	0.842656
12	1	0	1.114640	-1.321236	1.713459
13	1	0	-0.603416	-1.283746	1.225281
14	1	0	0.585919	-2.174466	0.228908
15	1	0	-2.966455	0.770104	0.397671
16	8	0	-2.865573	0.000010	-0.203951
17	1	0	-1.126852	0.000126	-0.797632
18	1	0	-2.966329	-0.770074	0.397703

Zero-point correction= 0.155168 (Hartree/Particle)
Thermal correction to Energy= 0.165386
Thermal correction to Enthalpy= 0.166330
Thermal correction to Gibbs Free Energy= 0.120584
Sum of electronic and zero-point Energies= -309.938240
Sum of electronic and thermal Energies= -309.928021
Sum of electronic and thermal Enthalpies= -309.927077
Sum of electronic and thermal Free Energies= -309.972823
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -310.22010719

INT1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.426588	-0.136716	-0.009726
2	6	0	-1.733306	-0.012238	1.487927
3	1	0	-2.772614	-0.336052	1.672593
4	1	0	-1.057651	-0.648992	2.080187
5	1	0	-1.636746	1.032006	1.832161
6	6	0	-1.554878	-1.585501	-0.501530
7	1	0	-2.616013	-1.877608	-0.410389
8	1	0	-1.259714	-1.678320	-1.559128
9	1	0	-0.953503	-2.277252	0.107359
10	6	0	-2.301776	0.790727	-0.864749

11	1	0	-2.249595	1.839420	-0.524280
12	1	0	-2.002253	0.744177	-1.926052
13	1	0	-3.354086	0.466586	-0.787693
14	8	0	-0.000617	0.288911	-0.262033
15	7	0	0.141806	1.979516	0.153667
16	8	0	1.152928	2.408766	-0.166500
17	5	0	1.299771	-0.667450	-0.006876
18	9	0	1.064400	-1.389447	1.154263
19	9	0	2.359845	0.214931	0.120189
20	9	0	1.385919	-1.459081	-1.137710

Zero-point correction= 0.141651 (Hartree/Particle)
Thermal correction to Energy= 0.154897
Thermal correction to Enthalpy= 0.155841
Thermal correction to Gibbs Free Energy= 0.102542
Sum of electronic and zero-point Energies= -687.375345
Sum of electronic and thermal Energies= -687.362099
Sum of electronic and thermal Enthalpies= -687.361154
Sum of electronic and thermal Free Energies= -687.414454
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -687.74228958

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.383150	-0.510283	-0.272091
2	6	0	0.866913	-0.845087	-0.155801
3	1	0	0.331317	-0.733141	-1.114102
4	8	0	3.131747	-1.265643	-0.864455
5	7	0	0.876027	-2.473153	0.246109
6	7	0	0.607989	-2.827590	1.307319
7	8	0	2.652272	0.651512	0.318801
8	6	0	4.064263	1.116561	0.247937
9	1	0	4.716225	0.232669	0.319351
10	1	0	4.165440	1.727054	1.157099
11	6	0	4.300618	1.920843	-1.017332
12	6	0	-1.929528	1.582130	0.310454
13	8	0	-1.721438	0.118493	0.363032
14	7	0	0.203797	-0.229719	0.911754
15	8	0	0.163307	-0.720688	2.024417
16	6	0	-1.184022	2.216592	-0.873103
17	1	0	-1.344603	3.309361	-0.859362
18	1	0	-0.097669	2.035323	-0.801836
19	1	0	-1.544733	1.824314	-1.836449
20	6	0	-3.450125	1.830210	0.200230
21	1	0	-3.994213	1.309259	1.006201
22	1	0	-3.627911	2.915106	0.306957
23	1	0	-3.852403	1.503376	-0.769511
24	6	0	-1.423257	2.144664	1.648080
25	1	0	-1.686479	3.214352	1.716099
26	1	0	-1.888899	1.617405	2.498774
27	1	0	-0.326876	2.063849	1.737233
28	5	0	-2.146089	-0.860313	-0.739607
29	9	0	-3.525195	-0.800650	-0.925436
30	9	0	-1.752573	-2.117987	-0.257554
31	9	0	-1.460157	-0.569579	-1.948812
32	1	0	3.615741	2.783644	-1.076732
33	1	0	5.336903	2.303275	-0.999423
34	1	0	4.180064	1.299740	-1.920922

Zero-point correction= 0.246153 (Hartree/Particle)
Thermal correction to Energy= 0.267759
Thermal correction to Enthalpy= 0.268703
Thermal correction to Gibbs Free Energy= 0.195893
Sum of electronic and zero-point Energies= -1103.232653

Sum of electronic and thermal Energies= -1103.211047
Sum of electronic and thermal Enthalpies= -1103.210102
Sum of electronic and thermal Free Energies= -1103.282912
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -1103.82314095

INT2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.303169	-0.516398	0.568154
2	6	0	-0.821507	-0.373871	0.455852
3	1	0	-0.187680	-0.693181	1.279364
4	8	0	-2.788420	-0.958979	1.605853
5	8	0	-2.961156	-0.127579	-0.535476
6	6	0	-4.432052	-0.228105	-0.489214
7	1	0	-4.700620	-1.109057	0.114790
8	1	0	-4.709822	-0.403156	-1.539591
9	6	0	-5.044461	1.052639	0.055179
10	6	0	2.047358	1.361508	0.235358
11	8	0	1.516657	0.108624	-0.435165
12	7	0	-0.238289	0.070179	-0.624222
13	8	0	-0.545232	0.451270	-1.721955
14	6	0	1.995148	1.252279	1.761368
15	1	0	2.426457	2.174628	2.189012
16	1	0	0.959229	1.169206	2.131279
17	1	0	2.578517	0.395316	2.131011
18	6	0	3.493825	1.482903	-0.278061
19	1	0	3.524828	1.464414	-1.380340
20	1	0	3.888845	2.455539	0.064916
21	1	0	4.137496	0.683510	0.114921
22	6	0	1.210249	2.538008	-0.278228
23	1	0	1.659802	3.471290	0.101231
24	1	0	1.204612	2.581383	-1.380005
25	1	0	0.171043	2.499291	0.091767
26	5	0	2.021978	-1.399480	-0.155213
27	9	0	3.367055	-1.415379	-0.480719
28	9	0	1.244717	-2.154304	-1.019422
29	9	0	1.788160	-1.708190	1.185583
30	1	0	-4.736307	1.926775	-0.543775
31	1	0	-6.145155	0.970822	0.005671
32	1	0	-4.759634	1.219754	1.107863

Zero-point correction= 0.239389 (Hartree/Particle)
Thermal correction to Energy= 0.259450
Thermal correction to Enthalpy= 0.260395
Thermal correction to Gibbs Free Energy= 0.189336
Sum of electronic and zero-point Energies= -993.764525
Sum of electronic and thermal Energies= -993.744464
Sum of electronic and thermal Enthalpies= -993.743519
Sum of electronic and thermal Free Energies= -993.814578
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -994.31889702

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.619950	-0.403908	-0.746353
2	6	0	-0.432386	0.520485	-0.888010
3	1	0	0.265693	0.257608	-1.688037
4	8	0	-1.494790	-1.614342	-0.885863
5	7	0	-0.708266	1.871024	-0.823730
6	7	0	-0.612614	2.770204	-0.087742
7	8	0	-2.736740	0.261074	-0.398941
8	6	0	-3.935691	-0.561009	-0.147065

9	1	0	-3.938119	-1.395577	-0.866049
10	1	0	-4.766942	0.122754	-0.376056
11	6	0	-3.975739	-1.043465	1.294379
12	6	0	2.814974	-0.481982	0.039436
13	8	0	1.977657	0.711145	0.174419
14	7	0	0.554654	0.357835	0.680587
15	8	0	0.185802	1.257389	1.440654
16	6	0	2.270485	-1.451015	-1.025990
17	1	0	2.947107	-2.318961	-1.128056
18	1	0	1.271010	-1.835025	-0.757122
19	1	0	2.206964	-0.957912	-2.013483
20	6	0	4.164379	0.104673	-0.409317
21	1	0	4.557701	0.809808	0.344222
22	1	0	4.903145	-0.705296	-0.545804
23	1	0	4.058198	0.641839	-1.368532
24	6	0	2.952812	-1.177343	1.406299
25	1	0	3.690010	-1.998765	1.353195
26	1	0	3.291997	-0.456072	2.171251
27	1	0	1.988711	-1.603925	1.734795
28	1	0	-3.943147	-0.195360	1.999744
29	1	0	-4.919844	-1.593165	1.459543
30	1	0	-3.137638	-1.726137	1.514160

Zero-point correction= 0.231998 (Hartree/Particle)
Thermal correction to Energy= 0.249404
Thermal correction to Enthalpy= 0.250348
Thermal correction to Gibbs Free Energy= 0.186430
Sum of electronic and zero-point Energies= -778.673345
Sum of electronic and thermal Energies= -778.655939
Sum of electronic and thermal Enthalpies= -778.654995
Sum of electronic and thermal Free Energies= -778.718913
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -779.13877134

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.840971	-1.555598	-0.435959
2	6	0	-0.365498	-1.414549	-0.604875
3	1	0	0.153198	-2.238728	-1.094803
4	8	0	-2.387485	-2.567350	-0.872628
5	8	0	-2.442926	-0.533437	0.186024
6	6	0	-3.905813	-0.654390	0.320385
7	1	0	-4.120854	-1.574102	0.890704
8	1	0	-4.332344	-0.762185	-0.691341
9	6	0	-4.395962	0.594226	1.027614
10	6	0	2.755798	-0.814193	0.365619
11	8	0	1.700088	-0.405138	-0.691148
12	7	0	0.386549	-0.398909	-0.260060
13	8	0	-0.026285	0.650225	0.406967
14	6	0	2.582017	-0.026465	1.661420
15	1	0	3.447533	-0.249683	2.310434
16	1	0	2.554035	1.056628	1.469178
17	1	0	1.670338	-0.322360	2.207288
18	6	0	2.633739	-2.321928	0.570976
19	1	0	2.741389	-2.867058	-0.382275
20	1	0	3.439049	-2.653556	1.250390
21	1	0	1.673631	-2.596282	1.042671
22	6	0	4.026922	-0.419736	-0.385425
23	1	0	4.902083	-0.695286	0.227902
24	1	0	4.100758	-0.948830	-1.350957
25	1	0	4.053123	0.668075	-0.565759
26	5	0	0.192374	2.093016	-0.324614
27	9	0	-0.079965	1.878475	-1.665176
28	9	0	-0.750050	2.864329	0.329161

29	9	0	1.492528	2.513754	-0.090902
30	1	0	-5.494391	0.540948	1.126917
31	1	0	-3.962045	0.679099	2.038764
32	1	0	-4.144353	1.502973	0.454395

Zero-point correction= 0.239568 (Hartree/Particle)
Thermal correction to Energy= 0.259453
Thermal correction to Enthalpy= 0.260397
Thermal correction to Gibbs Free Energy= 0.188859
Sum of electronic and zero-point Energies= -993.771119
Sum of electronic and thermal Energies= -993.751235
Sum of electronic and thermal Enthalpies= -993.750290
Sum of electronic and thermal Free Energies= -993.821829
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -994.32569461

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.506347	-1.836825	-0.005580
2	6	0	0.584118	-1.093834	-0.751017
3	1	0	1.074527	-1.740877	-1.483346
4	8	0	-0.995167	-2.849823	-0.500673
5	8	0	-0.846594	-1.302284	1.174270
6	6	0	-1.880968	-2.040396	1.920042
7	1	0	-1.491876	-3.050965	2.131655
8	1	0	-2.769049	-2.136119	1.273730
9	6	0	-2.170682	-1.256687	3.185695
10	6	0	3.880834	-0.729021	-0.337837
11	8	0	2.637165	0.013440	-0.824656
12	7	0	1.482896	-0.293747	-0.122953
13	8	0	1.077364	0.595685	0.802552
14	6	0	3.934900	-0.741977	1.189255
15	1	0	4.883771	-1.210066	1.505435
16	1	0	3.887390	0.279981	1.594314
17	1	0	3.108955	-1.337546	1.615868
18	6	0	3.856756	-2.140630	-0.928173
19	1	0	3.755368	-2.110364	-2.027134
20	1	0	4.802366	-2.657380	-0.684460
21	1	0	3.032854	-2.742783	-0.506264
22	6	0	4.983456	0.136172	-0.950183
23	1	0	5.968228	-0.304288	-0.716999
24	1	0	4.881691	0.189461	-2.048438
25	1	0	4.944569	1.158154	-0.537744
26	6	0	-5.411611	0.450659	-0.302500
27	6	0	-4.682166	1.605048	0.037185
28	6	0	-3.341666	1.719938	-0.343711
29	6	0	-2.695740	0.682274	-1.075136
30	6	0	-3.452629	-0.475881	-1.415179
31	6	0	-4.791591	-0.586322	-1.028050
32	1	0	-5.162008	2.413625	0.599232
33	1	0	-2.766601	2.614584	-0.077612
34	1	0	-2.990549	-1.284380	-1.990015
35	1	0	-5.362790	-1.481234	-1.298443
36	6	0	-1.311453	0.875736	-1.453058
37	6	0	-0.471150	-0.028213	-2.107524
38	1	0	-0.896371	-0.901719	-2.618117
39	1	0	0.433604	0.381816	-2.571442
40	1	0	-0.873395	1.838977	-1.166630
41	5	0	1.499042	2.097880	0.648243
42	9	0	1.261214	2.513824	-0.667820
43	9	0	0.649476	2.721554	1.562011
44	9	0	2.840748	2.274674	1.003898
45	1	0	-6.462926	0.359385	-0.007926
46	1	0	-2.942699	-1.790032	3.768000

47	1	0	-1.268770	-1.160440	3.814365
48	1	0	-2.551250	-0.247824	2.951315

Zero-point correction= 0.371225 (Hartree/Particle)
Thermal correction to Energy= 0.398567
Thermal correction to Enthalpy= 0.399511
Thermal correction to Gibbs Free Energy= 0.310783
Sum of electronic and zero-point Energies= -1303.274012
Sum of electronic and thermal Energies= -1303.246670
Sum of electronic and thermal Enthalpies= -1303.245726
Sum of electronic and thermal Free Energies= -1303.334454
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -1304.03800492

INT4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.966643	0.876661	-0.125187
2	6	0	0.518934	1.081728	-0.047882
3	1	0	0.151401	2.083156	0.164991
4	8	0	2.741730	1.820143	0.065704
5	8	0	2.346776	-0.392935	-0.423914
6	6	0	3.791880	-0.622264	-0.492461
7	1	0	4.273350	0.270662	-0.922950
8	1	0	3.892499	-1.465038	-1.194676
9	6	0	4.361695	-0.964417	0.877645
10	6	0	-2.892766	-0.120214	0.112663
11	8	0	-1.733922	0.765513	-0.207532
12	7	0	-0.415419	0.146966	-0.233507
13	8	0	-0.301508	-1.065816	-0.441416
14	6	0	-2.662252	-0.865200	1.433926
15	1	0	-3.594731	-1.380953	1.724276
16	1	0	-1.866391	-1.622059	1.350795
17	1	0	-2.399760	-0.155136	2.237842
18	6	0	-3.995563	0.939632	0.274426
19	1	0	-4.124788	1.523055	-0.653714
20	1	0	-4.950292	0.434695	0.502317
21	1	0	-3.760705	1.632672	1.100459
22	6	0	-3.214303	-1.052180	-1.065884
23	1	0	-4.196392	-1.528252	-0.893328
24	1	0	-3.276085	-0.475040	-2.005422
25	1	0	-2.460653	-1.844295	-1.186038
26	1	0	3.856687	-1.846222	1.309281
27	1	0	5.437546	-1.197282	0.778963
28	1	0	4.256036	-0.116439	1.575544

Zero-point correction= 0.226018 (Hartree/Particle)
Thermal correction to Energy= 0.241508
Thermal correction to Enthalpy= 0.242452
Thermal correction to Gibbs Free Energy= 0.182767
Sum of electronic and zero-point Energies= -669.231355
Sum of electronic and thermal Energies= -669.215865
Sum of electronic and thermal Enthalpies= -669.214921
Sum of electronic and thermal Free Energies= -669.274606
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -669.65881562

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.014759	1.749687	0.974948
2	6	0	0.982499	0.649873	1.164107
3	1	0	1.730405	0.866465	1.929933
4	8	0	-0.382439	2.439658	1.926455

5	8	0	-0.416736	1.921441	-0.301840
6	6	0	-1.358236	3.024457	-0.518041
7	1	0	-0.886347	3.959876	-0.170282
8	1	0	-2.256984	2.843260	0.096012
9	6	0	-1.679325	3.062336	-2.001462
10	6	0	3.800910	-0.565748	-0.444157
11	8	0	2.675605	-0.804164	0.493560
12	7	0	1.453799	-0.079761	0.113723
13	8	0	0.690365	-0.630237	-0.717531
14	6	0	4.092855	0.936879	-0.549379
15	1	0	4.988055	1.100427	-1.175363
16	1	0	3.251247	1.478807	-1.015940
17	1	0	4.283536	1.373279	0.447157
18	6	0	4.946022	-1.307438	0.259613
19	1	0	4.706730	-2.378605	0.380398
20	1	0	5.867819	-1.224922	-0.342378
21	1	0	5.141508	-0.875324	1.256660
22	6	0	3.503582	-1.185892	-1.818427
23	1	0	4.401398	-1.117019	-2.458920
24	1	0	3.232144	-2.250998	-1.714922
25	1	0	2.676597	-0.664540	-2.327465
26	6	0	-4.691572	-1.224118	-0.714776
27	6	0	-3.845589	-2.290367	-1.069019
28	6	0	-2.570753	-2.398287	-0.497164
29	6	0	-2.101843	-1.446501	0.446382
30	6	0	-2.971294	-0.378145	0.793178
31	6	0	-4.244939	-0.270390	0.219184
32	1	0	-4.181169	-3.041043	-1.794105
33	1	0	-1.914489	-3.231115	-0.779284
34	1	0	-2.648389	0.374233	1.521067
35	1	0	-4.896806	0.563609	0.504625
36	6	0	-0.768845	-1.622177	1.028297
37	6	0	-0.210067	-0.861516	2.058215
38	1	0	-0.828267	-0.167781	2.639700
39	1	0	0.638066	-1.287345	2.606113
40	1	0	-0.232350	-2.519668	0.700693
41	1	0	-5.689106	-1.137024	-1.159927
42	1	0	-2.385127	3.888759	-2.198055
43	1	0	-0.770763	3.234892	-2.604224
44	1	0	-2.150554	2.120603	-2.331693

Zero-point correction= 0.356826 (Hartree/Particle)
Thermal correction to Energy= 0.379790
Thermal correction to Enthalpy= 0.380735
Thermal correction to Gibbs Free Energy= 0.302413
Sum of electronic and zero-point Energies= -978.725769
Sum of electronic and thermal Energies= -978.702805
Sum of electronic and thermal Enthalpies= -978.701861
Sum of electronic and thermal Free Energies= -978.780183
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -979.36367289

INT5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.866653	1.904003	-0.685361
2	6	0	-0.760800	0.446264	-1.174757
3	1	0	-1.582508	0.268028	-1.885490
4	8	0	0.009836	2.755021	-0.802802
5	8	0	-2.078065	2.132985	-0.137267
6	6	0	-2.306199	3.495956	0.358363
7	1	0	-2.181108	4.197304	-0.484637
8	1	0	-1.535196	3.723838	1.114329
9	6	0	-3.708026	3.541990	0.938670
10	6	0	-2.286564	-2.474352	0.261157

11	8	0	-1.338864	-1.732186	-0.590989
12	7	0	-0.981238	-0.451073	0.007058
13	8	0	0.346045	-0.578240	0.540849
14	6	0	-3.613085	-1.704745	0.350061
15	1	0	-4.351199	-2.274877	0.942424
16	1	0	-3.465745	-0.724939	0.834889
17	1	0	-4.034581	-1.536935	-0.657487
18	6	0	-2.458241	-3.786338	-0.517985
19	1	0	-1.496458	-4.322211	-0.605713
20	1	0	-3.175413	-4.443938	0.003809
21	1	0	-2.844064	-3.592577	-1.534604
22	6	0	-1.688047	-2.732107	1.651921
23	1	0	-2.376076	-3.360563	2.246028
24	1	0	-0.719769	-3.256518	1.573680
25	1	0	-1.529847	-1.787345	2.198692
26	6	0	5.246687	0.398706	0.733303
27	6	0	5.005718	-0.900468	0.257551
28	6	0	3.716405	-1.265625	-0.166747
29	6	0	2.658043	-0.336468	-0.131890
30	6	0	2.908836	0.967303	0.348710
31	6	0	4.193340	1.330714	0.779794
32	1	0	5.819457	-1.633892	0.220015
33	1	0	3.527020	-2.282883	-0.531250
34	1	0	2.093247	1.698684	0.376335
35	1	0	4.375114	2.345982	1.151198
36	6	0	1.277604	-0.745648	-0.597194
37	6	0	0.635688	0.097149	-1.731382
38	1	0	1.204351	1.017776	-1.934005
39	1	0	0.560687	-0.485673	-2.661927
40	1	0	1.283790	-1.813581	-0.876123
41	1	0	6.250207	0.685924	1.067622
42	1	0	-3.909282	4.559750	1.317214
43	1	0	-4.466676	3.303157	0.173159
44	1	0	-3.817145	2.834352	1.778833

Zero-point correction= 0.361209 (Hartree/Particle)
Thermal correction to Energy= 0.383187
Thermal correction to Enthalpy= 0.384132
Thermal correction to Gibbs Free Energy= 0.308856
Sum of electronic and zero-point Energies= -978.775663
Sum of electronic and thermal Energies= -978.753685
Sum of electronic and thermal Enthalpies= -978.752740
Sum of electronic and thermal Free Energies= -978.828016
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -979.41176432

TS5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213408	-2.096767	0.468514
2	6	0	-0.447183	-0.814764	0.743997
3	1	0	-1.129454	-0.245456	1.608647
4	8	0	-0.835645	-3.191196	0.875919
5	8	0	-2.363980	-1.877432	-0.204789
6	6	0	-3.170278	-3.074750	-0.479804
7	1	0	-3.405806	-3.562974	0.481327
8	1	0	-2.561684	-3.770878	-1.082184
9	6	0	-4.419820	-2.625797	-1.214836
10	6	0	-2.098856	2.561105	-0.404760
11	8	0	-1.131302	1.916963	0.433475
12	7	0	-0.422347	0.055520	-0.388045
13	8	0	0.827264	0.467534	-0.602160
14	6	0	-3.400116	1.737107	-0.497912
15	1	0	-4.125750	2.215140	-1.181463
16	1	0	-3.186804	0.721230	-0.872459

17	1	0	-3.885984	1.645404	0.491582
18	6	0	-2.385858	3.937444	0.245138
19	1	0	-1.455017	4.526476	0.329479
20	1	0	-3.109839	4.514361	-0.360262
21	1	0	-2.807478	3.811249	1.258968
22	6	0	-1.486482	2.763283	-1.804331
23	1	0	-2.163106	3.354218	-2.448612
24	1	0	-0.523522	3.299526	-1.729099
25	1	0	-1.302709	1.792141	-2.295171
26	6	0	5.800229	-0.271034	-0.699456
27	6	0	5.459408	0.746090	0.207402
28	6	0	4.125581	0.901484	0.619298
29	6	0	3.125063	0.031818	0.141699
30	6	0	3.474121	-0.988614	-0.769077
31	6	0	4.804058	-1.134913	-1.190070
32	1	0	6.230054	1.424056	0.590998
33	1	0	3.855771	1.699849	1.320955
34	1	0	2.702271	-1.665364	-1.153226
35	1	0	5.065303	-1.926854	-1.900963
36	6	0	1.703905	0.201222	0.609291
37	6	0	0.996246	-0.995182	1.247463
38	1	0	1.413697	-1.954878	0.898525
39	1	0	1.067219	-0.959108	2.345571
40	1	0	1.595761	1.110630	1.224236
41	8	0	-1.838963	0.733081	2.412851
42	1	0	-2.774238	0.446822	2.297436
43	1	0	-1.610881	1.440912	1.469255
44	1	0	6.839604	-0.390984	-1.025470
45	1	0	-4.167897	-2.128447	-2.167533
46	1	0	-5.041252	-3.510085	-1.442269
47	1	0	-5.020483	-1.933620	-0.599665

Zero-point correction= 0.377511 (Hartree/Particle)
Thermal correction to Energy= 0.401756
Thermal correction to Enthalpy= 0.402700
Thermal correction to Gibbs Free Energy= 0.322389
Sum of electronic and zero-point Energies= -1055.150800
Sum of electronic and thermal Energies= -1055.126555
Sum of electronic and thermal Enthalpies= -1055.125611
Sum of electronic and thermal Free Energies= -1055.205922
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -1055.84990378

43

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.434422	-0.356765	0.598887
2	6	0	1.108819	-0.481071	-0.057385
3	8	0	2.630560	-0.740552	1.752516
4	8	0	3.370016	0.207493	-0.200729
5	6	0	4.699328	0.352745	0.399370
6	1	0	5.062834	-0.648410	0.690110
7	1	0	4.605687	0.963050	1.314328
8	6	0	5.596319	1.007595	-0.635897
9	7	0	0.879119	-0.028863	-1.256531
10	8	0	-0.438328	-0.255483	-1.606462
11	6	0	-4.853368	1.035320	0.444643
12	6	0	-4.866751	-0.321903	0.083740
13	6	0	-3.664855	-0.976678	-0.235395
14	6	0	-2.439219	-0.284895	-0.183933
15	6	0	-2.433130	1.079565	0.177447
16	6	0	-3.633611	1.735510	0.487042
17	1	0	-5.813580	-0.872318	0.043826
18	1	0	-3.675461	-2.034520	-0.524916
19	1	0	-1.486132	1.631060	0.207357

20	1	0	-3.618473	2.796213	0.762356
21	6	0	-1.149687	-1.004590	-0.504943
22	6	0	-0.096236	-1.082011	0.623882
23	1	0	-0.377746	-0.494302	1.516289
24	1	0	0.089065	-2.118033	0.952532
25	1	0	-1.363599	-2.001748	-0.924610
26	1	0	-5.790062	1.549332	0.688540
27	1	0	5.220566	2.006836	-0.916936
28	1	0	6.609602	1.126784	-0.213165
29	1	0	5.673288	0.389490	-1.547338

Zero-point correction= 0.226103 (Hartree/Particle)
Thermal correction to Energy= 0.241031
Thermal correction to Enthalpy= 0.241975
Thermal correction to Gibbs Free Energy= 0.180903
Sum of electronic and zero-point Energies= -745.278707
Sum of electronic and thermal Energies= -745.263780
Sum of electronic and thermal Enthalpies= -745.262835
Sum of electronic and thermal Free Energies= -745.323907
BP86/6-311++G(d,p) /SMD//BP86/6-31G(d) /SMD energy in acetonitrile = -745.71251133