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Supporting Information

Synthesis of 2-Iminothiazolidin-4-ones via Copper-Catalyzed [2 + 1 + 2] Tandem Annulation

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Experimental Section

1. General information

Melting points were tested using a melting point instrument and are uncorrected. IR spectra were collected from an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets (Bruker Tensor 27). ^{1}H and $^{13}C\{1H\}$ NMR spectra were recorded on a Bruker AVANCE 400 (^{1}H: 400 MHz) or a Bruker AVANCE 500 (^{1}H: 500 MHz) instrument. HRMS were recorded on an Agilent Mass spectrometer using ESI-TOF (electrospray ionization-time of flight). TLC was performed using commercially available 100−400 mesh silica gel plates (GF254). Unless otherwise noted, chemicals purchased from the vendors were used without further purification.

2. General procedure for synthesis of 2-iminothiazolidin-4-ones derivatives

A mixture of alkyl amines (0.222 mmol, 1.2 equiv), isothiocyanates (0.185 mmol), ethyl 2-diazoacetate (0.278 mmol, 1.5 equiv), CuI (0.074 mmol, 0.4 equiv) was stirred in CH_3CN/THF (v/v = 1:1, 2.0 mL) at room temperature (25 °C) for 12 h. After completion of the reaction (monitored by TLC), water (10 mL) was added to the reaction mixture, and the resulting mixture was extracted with ethyl acetate. The combined organic layers were then dried over $MgSO_4$, filtered, and then concentrated in vacuum. The residue was purified by using flash chromatography on silica gel to give the desired product (eluted with a mixture of petroleum ether and ethyl acetate (v/v = 15:1)).

3. The gram-scale synthesis of 4a

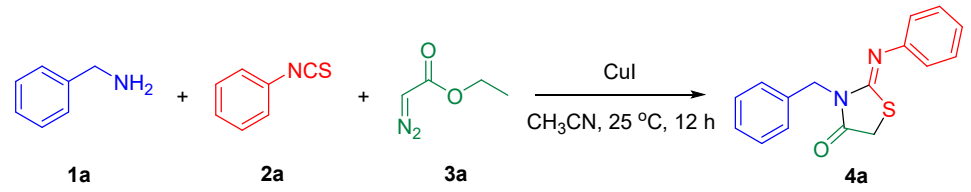
To a solution of phenylmethanamine **1a** (7.2 mmol, 0.778 g), phenyl isothiocyanate **2a** (6.0 mmol, 0.810 g), ethyl 2-diazoacetate **3a** (9.0 mmol, 1.141 g) in 60.0 mL of CH_3CN/THF (v/v = 1:1) was added CuI (2.4 mmol, 0.457 g, 0.4 equiv) under air atmosphere. The solution was stirred at room temperature (25 °C) for 12 h (monitored by TLC). Water (30 mL) was added, and the resulting mixture was extracted with ethyl acetate. The combined organic phase was dried over $MgSO_4$, filtered, and then concentrated under reduced pressure. The crude product was purified by using flash column chromatography on silica gel eluted with a mixture of petroleum ether/ethyl acetate (v/v = 15:1) to afford the desired compound **4a** (1.44 g, yield of 85%).

4. General procedure for synthesis of 2-iminothiazolidin-4-ones derivatives of bioactive molecules

Alkyl amines (0.222 mmol, 1.2 equiv), isothiocyanates (0.185 mmol), ethyl 2-diazoacetate (0.278 mmol, 1.5 equiv), and CuI (0.074 mmol, 0.4 equiv) were added to CH_3CN/THF (v/v = 1:1, 2.0 mL). The mixture was stirred at room temperature (25 °C) for 12 h. Then, 4-nitrobenzaldehyde (0.204 mmol, 1.1 equiv), hexahydropyridine (0.370 mmol, 2.0 equiv), and ethanol (1.0 mL) were added, followed by heating under reflux for 12 h. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and the solvent was concentrated under reduced pressure. The crude residue was purified by using silica gel chromatography eluted with a mixture of petroleum ether/ethyl acetate (v/v = 15:1) to provide the desired product.

Screening Reaction Conditions

Table S1. The effect of the amount of CuI[a]



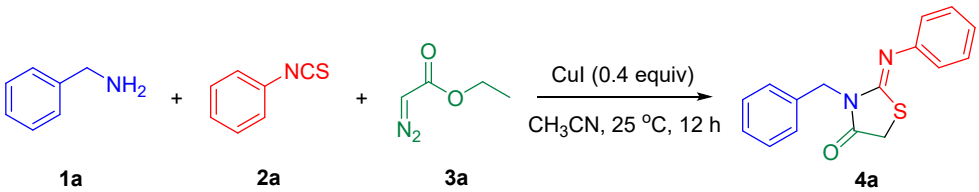
1a **2a** **3a** **4a**

Entry	CuI (equiv)	Yield (%)[b]
1	0.2	0
2	0.3	0
3	0.4	78
4	0.5	59
5	0.6	46
6	0.8	44
7	1.0	46

[a] Reaction conditions: **1a** (0.222 mmol), **2a** (0.185 mmol), **3a** (0.278 mmol) and CuI in CH_3CN (2 mL), open to air at room temperature (25 °C) for 12 h.

[b] Isolated yield.

Table S2. The ratio of reactants[a]



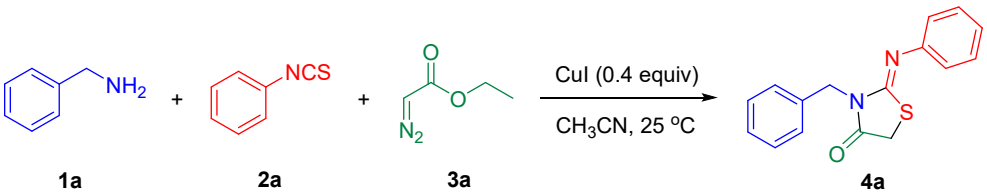
1a **2a** **3a** **4a**

Entry	**1a**:**2a**:**3a** (mole ratio)	Yield (%)[b]
1	1.2:1:1.5	78
2	1.2:1:2.3	57
3	1.2:2:2.3	26
4	2.4:1:1.5	43
5	2.4:1:2.3	56
6	2.4:1:3.0	75

[a] Reaction conditions: **1a**, **2a**, **3a** and CuI (0.4 equiv) in CH_3CN (2 mL), open to air at room temperature (25 °C) for 12 h.

[b] Isolated yield.

Table S3. The effect of reaction time[a]



1a **2a** **3a** **4a**

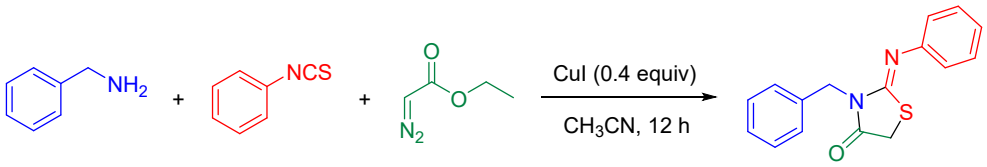
Entry	Time (h)	Yield (%)[b]
1	8	59
2	10	60
3	18	16

[a] Reaction conditions: **1a** (0.222 mmol), **2a** (0.185 mmol), **3a** (0.278 mmol) and CuI (0.4 equiv) in CH_3CN (2 mL), open to air

at room temperature (25 °C).

[b] Isolated yield.

Table S4. The effect of reaction temperature[a]



1a **2a** **3a** **4a**

Entry	T (°C)	Yield (%)[b]
1	rt	78
2	40	64
3	50	61
4	60	57
5	70	61
6	80	58

[a] Reaction conditions: **1a** (0.222 mmol), **2a** (0.185 mmol), **3a** (0.278 mmol) and CuI (0.4 equiv) in CH_3CN (2 mL), open to air for 12 h.

[b] Isolated yield.

X-ray Crystallographic Data for 5p

The crystal growth procedure: Compound **5p** (30 mg) was dissolved in 0.5 mL of CH_2Cl_2, and then the mixture was added into a solution of petroleum ether (5 mL)/ethyl acetate (5 mL). The mixed solution was evaporated slowly at room temperature (25 °C) to afford the crystals **5p**. Crystal data collection and refinement parameters of **5p** are summarized in Table S5.

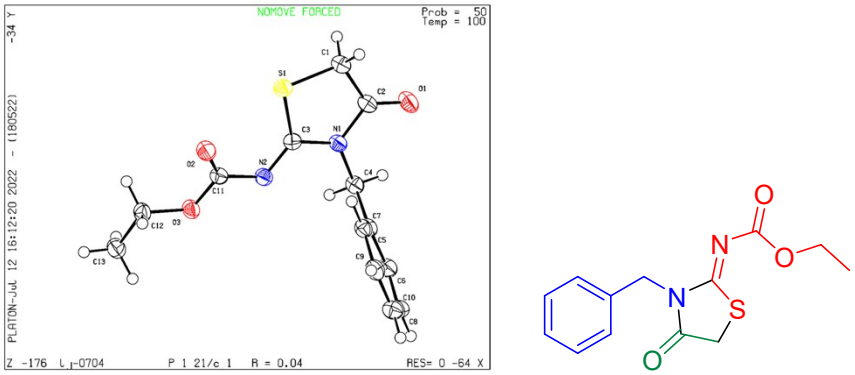


Figure S1. The Crystal Structure of 5p

The CCDC number of **5p** is 2190019, the detail information please see 5p.cif document.

Table S5. Crystal data and structure refinement for compound 5p

Identification code	2190019
Empirical formula	$C_{13}H_{14}N_2O_3S$
Formula weight	278.32

Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.5249(3)
b/Å	5.74470(10)
c/Å	12.9917(2)
α/°	90.00
β/°	108.935(2)
γ/°	90.00
Volume/Å^3	1307.76(4)
Z	4
ρ_{calc}g/cm^3	1.414
μ/mm^{-1}	2.265
F(000)	584.0
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.096 to 155.468
Index ranges	$-22 \leq h \leq 23$, $-6 \leq k \leq 6$, $-16 \leq l \leq 15$
Reflections collected	6834
Independent reflections	2654
Data/restraints/parameters	2654/0/173
Goodness-of-fit on F^2	1.110
Final R indexes [I>=2σ (I)]	R1 = 0.0351, wR_2 = 0.1016
Final R indexes [all data]	R1 = 0.0363, wR_2 = 0.1029
Largest diff. peak/hole / e Å^{-3}	0.32/-0.35

CIF files of 5p

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lj-0704

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: lj-0704

Bond precision: C-C = 0.0019 A Wavelength=1.54184

Cell: a=18.5249(3) b=5.7447(1) c=12.9917(2)
alpha=90 beta=108.935(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1307.76(4)	1307.76(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H14 N2 O3 S	C13 H14 N2 O3 S
Sum formula	C13 H14 N2 O3 S	C13 H14 N2 O3 S
Mr	278.32	278.32
Dx,g cm-3	1.414	1.414
Z	4	4
Mu (mm-1)	2.265	2.265
F000	584.0	584.0
F000'	587.03	
h,k,lmax	23,7,16	23,6,16
Nref	2790	2654
Tmin,Tmax	0.873,0.893	0.459,1.000
Tmin'	0.797	

Correction method= # Reported T Limits: Tmin=0.459 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.951 Theta(max)= 77.734

R(reflections)= 0.0351(2488) wR2(reflections)= 0.1029(2654)

S = 1.110 Npar= 173

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree

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Alert level C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report

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Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 86 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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  0 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
  1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  4 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  1 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
  1 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

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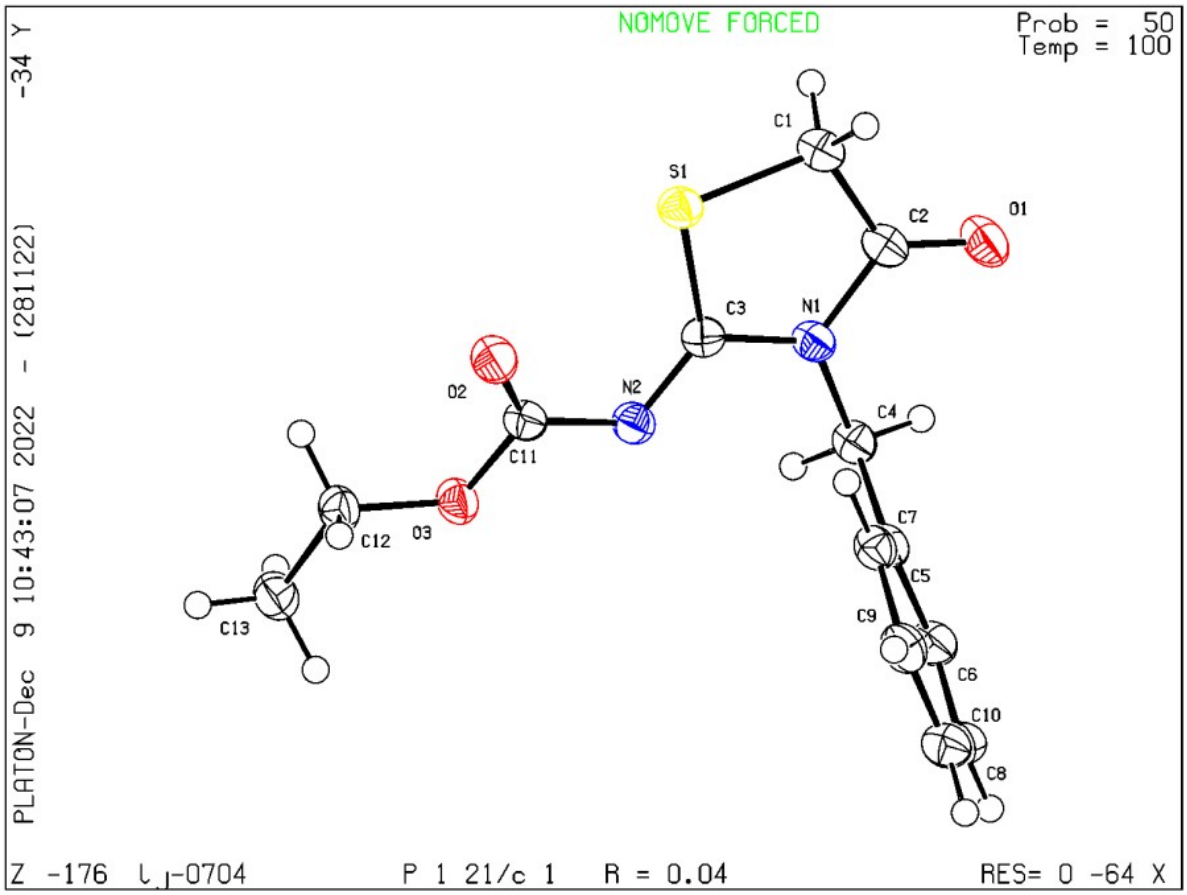
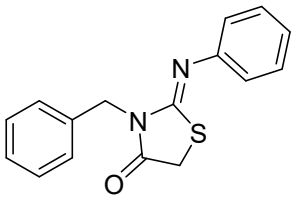
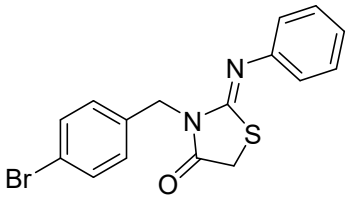


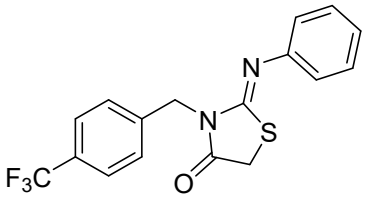
Compound Characterization



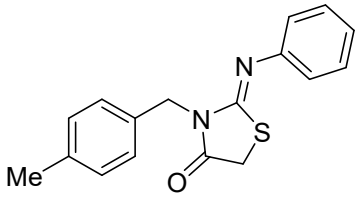
(*Z*)-3-Benzyl-2-(phenylimino)thiazolidin-4-one (4a).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 85% yield (44.3 mg, 0.16 mmol); IR (KBr, cm^{-1}) 3431, 2930, 1717, 1645, 1594, 1428, 1381, 1325, 1155, 1080, 772, 692; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.55 (d, J = 7.2 Hz, 2H), 7.38-7.30 (m, 5H), 7.16 (t, J = 7.4 Hz, 1H), 6.98 (d, J = 7.8 Hz, 2H), 5.05 (s, 2H), 3.79 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 153.9, 148.0, 136.0, 129.3, 129.1, 128.5, 127.9, 124.7, 121.0, 46.3, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{13}N_2OS$ 281.0754, found 281.0755.



(*Z*)-3-(4-Bromobenzyl)-2-(phenylimino)thiazolidin-4-one (4b).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 74% yield (49.3 mg, 0.14 mmol); mp 110-112 °C; IR (KBr, cm^{-1}) 3419, 3187, 3034, 2932, 1715, 1642, 1590, 1485, 1380, 1262, 1159, 1012, 800, 769, 693; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.46 (d, J = 8.3 Hz, 2H), 7.41 (d, J = 8.3 Hz, 2H), 7.35 (t, J = 7.7 Hz, 2H), 7.15 (t, J = 7.4 Hz, 1H), 6.94 (d, J = 7.8 Hz, 2H), 4.97 (s, 2H), 3.81 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 153.8, 147.8, 134.9, 131.6, 131.0, 129.3, 124.8, 122.1, 121.0, 45.6, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{12}BrN_2OS$ 358.9859, found 358.9858.

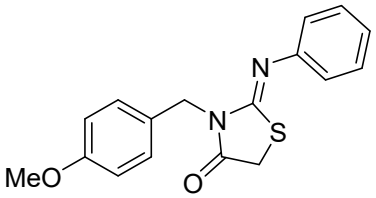


(*Z*)-2-(Phenylimino)-3-(4-(trifluoromethyl)benzyl)thiazolidin-4-one (4c). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 70% yield (45.3 mg, 0.13 mmol); mp 121-122 °C; IR (KBr, cm^{-1}) 3436, 3034, 2917, 2850, 1720, 1637, 1595, 1378, 1325, 1155, 1066, 871, 770; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.62 (q, J = 8.2 Hz, 4H), 7.36 (t, J = 7.7 Hz, 2H), 7.16 (t, J = 7.4 Hz, 1H), 6.95 (d, J = 7.6 Hz, 2H), 5.08 (s, 2H), 3.84 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 153.7, 147.7, 139.7 (d, J = 5.0 Hz), 130.2 (q, J = 130.0 Hz), 129.3 (d, J = 4.2 Hz), 125.5 (q, J = 3.7 Hz), 125.2, 124.8, 123.0, 120.9, 45.7, 32.7; ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -62.56; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{17}H_{12}F_3N_2OS$ 349.0628, found 349.0629.

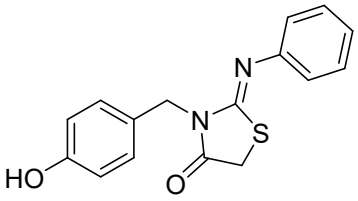


(*Z*)-3-(4-Methylbenzyl)-2-(phenylimino)thiazolidin-4-one (4d).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 80% yield (43.8 mg, 0.15 mmol); mp 92-94 °C; IR (KBr, cm^{-1}) 3435, 3028, 2949, 1722, 1642, 1594, 1425, 1380, 1262, 1155, 1022, 807, 769; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.44 (d, J = 7.7 Hz, 2H), 7.35 (t, J = 7.6 Hz, 2H), 7.15 (d, J = 7.1 Hz, 3H), 6.96 (d, J = 7.7 Hz, 2H), 4.99 (s, 2H), 3.79 (s, 2H), 2.35 (s, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.7, 154.0,

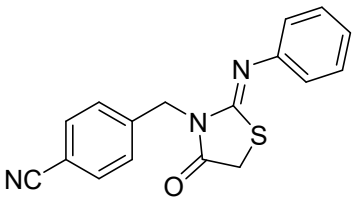
148.0, 137.7, 133.0, 129.3, 129.2, 129.2, 124.6, 121.0, 46.0, 32.7, 21.2; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{15}N_2OS$ 295.0911, found 295.0910.



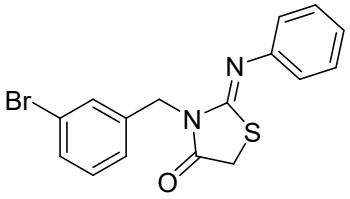
(*Z*)-3-(4-Methoxybenzyl)-2-(phenylimino)thiazolidin-4-one (4e).[1] Eluent: petroleum ether/ethyl acetate (v/v = 10:1). Yellow solid: 91% yield (52.5 mg, 0.17 mmol); mp 135-137 °C; IR (KBr, cm^{-1}) 3430, 3033, 2952, 1713, 1643, 1591, 1506, 1381, 1246, 1159, 1028, 760, 689; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.50 (d, J = 8.5 Hz, 2H), 7.35 (t, J = 7.8 Hz, 2H), 7.15 (t, J = 7.4 Hz, 1H), 6.97 (d, J = 7.6 Hz, 2H), 6.87 (d, J = 8.5 Hz, 2H), 4.97 (s, 2H), 3.80 (s, 3H), 3.78 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 159.4, 154.0, 148.0, 130.7, 129.2, 128.3, 124.6, 121.0, 113.8, 55.3, 45.8, 32.7; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{15}N_2O_2S$ 311.0860, found 311.0860.



(*Z*)-3-(4-Hydroxybenzyl)-2-(phenylimino)thiazolidin-4-one (4f). Eluent: petroleum ether/ethyl acetate (v/v = 3:1). Yellow solid: 77% yield (42.5 mg, 0.14 mmol); mp 129-130 °C; IR (KBr, cm^{-1}) 3395, 3032, 2941, 1705, 1649, 1594, 1515, 1428, 1325, 1262, 1158, 1103, 764, 695; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.41 (d, J = 8.3 Hz, 2H), 7.35 (t, J = 7.8 Hz, 2H), 7.15 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 7.6 Hz, 2H), 6.76 (d, J = 8.4 Hz, 2H), 4.96 (s, 2H), 3.79 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 172.2, 155.7, 154.2, 147.9, 130.9, 129.3, 128.0, 124.7, 121.0, 115.3, 45.8, 32.8; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{16}H_{13}N_2O_2S$ 297.0703, found 297.0702.

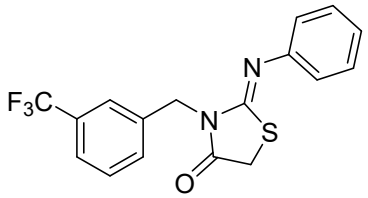


(*Z*)-4-((4-Oxo-2-(phenylimino)thiazolidin-3-yl)methyl)benzonitrile (4g).[1] Eluent: petroleum ether/ethyl acetate (v/v = 5:1). Yellow oil: 87% yield (49.4 mg, 0.16 mmol); IR (KBr, cm^{-1}) 3431, 3060, 2924, 2228, 1728, 1633, 1594, 1491, 1390, 1337, 1160, 1025, 768, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.60 (q, J = 8.2 Hz, 4H), 7.34 (t, J = 7.7 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 7.7 Hz, 2H), 5.05 (s, 2H), 3.84 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 153.7, 147.5, 141.0, 132.4, 129.6, 129.4, 124.9, 120.9, 118.6, 111.9, 45.8, 32.7; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{12}N_3OS$ 306.0707, found 306.0705.

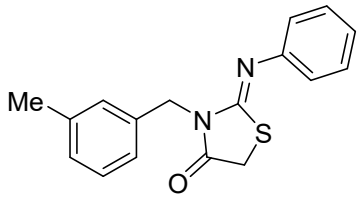


(*Z*)-3-(3-Bromobenzyl)-2-(phenylimino)thiazolidin-4-one (4h).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 95% yield (63.3 mg, 0.18 mmol); mp 91-93 °C; IR (KBr, cm^{-1}) 3431, 3060, 2930, 1717, 1633, 1594, 1378, 1155, 1071, 768, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.70 (s, 1H), 7.46-7.43 (m, 2H), 7.36 (t, J = 7.8 Hz, 2H), 7.21 (t, J = 7.8 Hz, 1H), 7.15 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 7.6 Hz, 2H), 4.99 (s, 2H), 3.83 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.5,

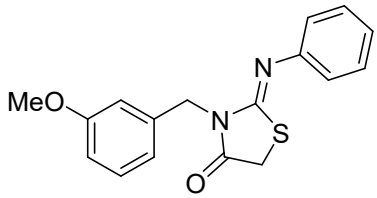
153.8, 147.7, 138.0, 132.1, 131.1, 130.1, 129.3, 127.8, 124.8, 122.5, 121.0, 45.6, 32.7; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{16}H_{12}BrN_2OS$ 358.9859, found 358.9857.



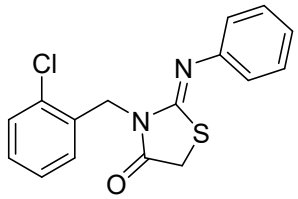
(*Z*)-2-(Phenylimino)-3-(3-(trifluoromethyl)benzyl)thiazolidin-4-one (4i). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 74% yield (47.9 mg, 0.14 mmol); IR (KBr, cm^{-1}) 3439, 3064, 2930, 1725, 1636, 1594, 1378, 1325, 1164, 1071, 768, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.85 (s, 1H), 7.72 (d, J = 7.6 Hz, 1H), 7.58 (d, J = 7.7 Hz, 1H), 7.47 (t, J = 7.7 Hz, 1H), 7.36 (t, J = 7.7 Hz, 2H), 7.16 (t, J = 7.4 Hz, 1H), 6.95 (d, J = 7.7 Hz, 2H), 5.08 (s, 2H), 3.83 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 153.8, 147.7, 136.8, 132.6, 130.9 (q, J = 125.0 Hz), 129.3, 129.0, 126.2 (q, J = 15.0 Hz), 125.1, 124.8, 123.0, 120.9, 45.8, 32.7; ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -62.55; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{12}F_3N_2OS$ 349.0628, found 349.0631.



(*Z*)-3-(3-Methylbenzyl)-2-(phenylimino)thiazolidin-4-one (4j).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 70% yield (38.3 mg, 0.13 mmol); IR (KBr, cm^{-1}) 3431, 3045, 2937, 1717, 1633, 1594, 1487, 1378, 1325, 1155, 768, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.36 (dd, J = 14.2, 7.4 Hz, 4H), 7.24 (t, J = 13.0 Hz, 1H), 7.15 (dd, J = 16.6, 7.7 Hz, 2H), 6.97 (d, J = 7.6 Hz, 2H), 5.01 (s, 2H), 3.81 (s, 2H), 2.37 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.7, 154.0, 148.0, 138.2, 135.9, 129.8, 129.3, 128.7, 128.4, 126.2, 124.6, 121.0, 46.3, 32.7, 21.5; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{15}N_2OS$ 295.0911, found 295.0913.

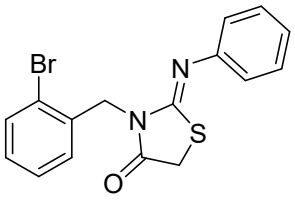


(*Z*)-3-(3-Methoxybenzyl)-2-(phenylimino)thiazolidin-4-one (4k).[1] Eluent: petroleum ether/ethyl acetate (v/v = 10:1). Yellow oil: 77% yield (44.4 mg, 0.14 mmol); IR (KBr, cm^{-1}) 3434, 3055, 2934, 1722, 1633, 1589, 1487, 1379, 1260, 1155, 1040, 768, 694; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.37 (t, J = 7.8 Hz, 2H), 7.28 (d, J = 8.1 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 7.13 (d, J = 7.4 Hz, 2H), 6.98 (d, J = 7.6 Hz, 2H), 6.88-6.87 (m, 1H), 5.03 (s, 2H), 3.82 (s, 3H), 3.81 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 159.7, 154.0, 148.0, 137.4, 129.5, 129.3, 124.6, 121.4, 121.0, 114.5, 113.6, 55.3, 46.2, 32.7; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{15}N_2O_2S$ 311.0860, found 311.0861.

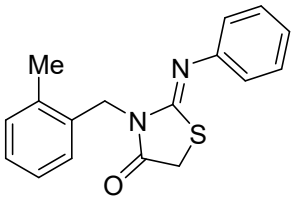


(*Z*)-3-(2-Chlorobenzyl)-2-(phenylimino)thiazolidin-4-one (4l).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 65% yield (38.0 mg, 0.12 mmol); IR (KBr, cm^{-1}) 3445, 3055, 2926, 1725, 1644, 1588, 1379, 1162, 1049, 764, 741, 690; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.39 (d, J = 7.0 Hz, 1H), 7.33 (t, J = 7.6 Hz, 2H), 7.23 (s, 2H), 7.18 (d, J = 6.7 Hz, 1H), 7.13 (t,

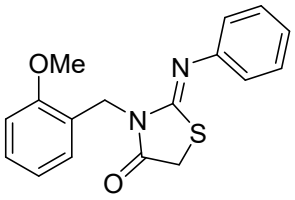
J = 7.3 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 2H), 5.18 (s, 2H), 3.91 (s, 2H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 153.3, 147.7, 133.1, 132.9, 129.7, 129.2, 128.8, 127.6, 126.8, 124.7, 121.0, 44.2, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{12}ClN_2OS$ 315.0364, found 315.0367.



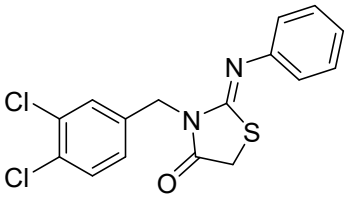
(*Z*)-3-(2-Bromobenzyl)-2-(phenylimino)thiazolidin-4-one (4m). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 73% yield (48.6 mg, 0.14 mmol); mp 85-87 °C; IR (KBr, cm^{-1}) 3444, 3055, 2920, 1722, 1643, 1591, 1376, 1159, 1028, 760, 739, 693; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.58 (d, *J* = 7.9 Hz, 1H), 7.35-7.28 (m, 3H), 7.14 (dd, *J* = 14.4, 7.1 Hz, 3H), 6.92 (d, *J* = 7.7 Hz, 2H), 5.14 (s, 2H), 3.92 (s, 2H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 153.3, 147.6, 134.4, 133.0, 129.2, 128.9, 127.4, 127.2, 124.8, 122.9, 121.0, 46.6, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{12}BrN_2OS$ 358.9859, found 358.9861.



(*Z*)-3-(2-Methylbenzyl)-2-(phenylimino)thiazolidin-4-one (4n). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 85% yield (46.5 mg, 0.16 mmol); mp 85-86 °C; IR (KBr, cm^{-1}) 3444, 3055, 2921, 1722, 1643, 1591, 1488, 1376, 1345, 1159, 744, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.34 (t, *J* = 7.7 Hz, 2H), 7.27-7.26 (m, 1H), 7.19 (d, *J* = 3.2 Hz, 3H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 2H), 5.06 (s, 2H), 3.86 (s, 2H), 2.48 (s, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.8, 153.9, 147.9, 136.2, 133.8, 130.5, 129.3, 127.5, 127.1, 126.1, 124.7, 121.0, 43.9, 32.7, 19.6; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{17}H_{15}N_2OS$ 295.0911, found 295.0914.

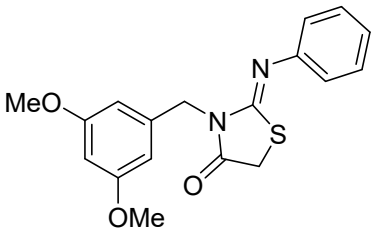


(*Z*)-3-(2-Methoxybenzyl)-2-(phenylimino)thiazolidin-4-one (4o).[1] Eluent: petroleum ether/ethyl acetate (v/v = 10:1). Yellow solid: 61% yield (35.2 mg, 0.11 mmol); mp 96-98 °C; IR (KBr, cm^{-1}) 3427, 3034, 2921, 1732, 1632, 1589, 1488, 1380, 1244, 1160, 1025, 748, 692; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.34 (t, *J* = 7.7 Hz, 2H), 7.28 (d, *J* = 6.9 Hz, 1H), 7.14 (t, *J* = 8.3 Hz, 2H), 6.95 (t, *J* = 8.5 Hz, 3H), 6.90 (d, *J* = 8.2 Hz, 1H), 5.12 (s, 2H), 3.89 (s, 2H), 3.88 (s, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 157.2, 153.8, 148.1, 129.2, 128.5, 127.4, 124.5, 123.6, 121.0, 120.3, 110.5, 55.5, 41.9, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{17}H_{15}N_2O_2S$ 311.0860, found 311.0863.

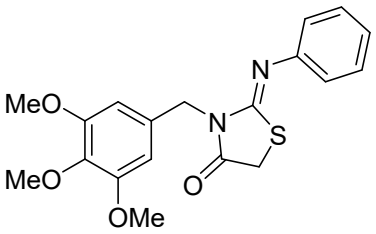


(*Z*)-3-(3,4-Dichlorobenzyl)-2-(phenylimino)thiazolidin-4-one (4p). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 81% yield (52.4 mg, 0.15 mmol); mp 127-129 °C; IR (KBr, cm^{-1}) 3427, 3033, 2928, 1715, 1634, 1589, 1472, 1376, 1328, 1159, 1029, 894, 764, 687; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.65 (s, 1H), 7.41-7.34 (m, 4H), 7.16 (t, *J* = 7.3 Hz, 1H), 6.95

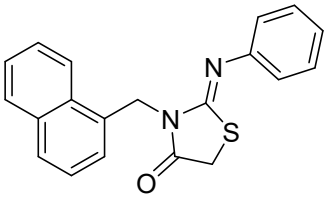
(d, J = 7.7 Hz, 2H), 4.96 (s, 2H), 3.82 (s, 2H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 153.7, 147.6, 136.0, 132.5, 132.2, 131.2, 130.5, 129.4, 128.7, 124.9, 121.0, 45.1, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{11}Cl_2N_2OS$ 348.9975, found 348.9976.



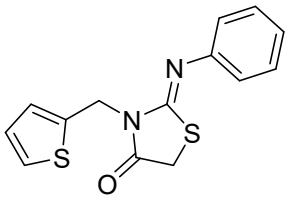
(*Z*)-3-(3,5-Dimethoxybenzyl)-2-(phenylimino)thiazolidin-4-one (4q). Eluent: petroleum ether/ethyl acetate (v/v = 5:1). Yellow oil: 63% yield (39.9 mg, 0.12 mmol); IR (KBr, cm^{-1}) 3437, 3032, 2937, 1723, 1632, 1589, 1434, 1380, 1322, 1160, 1067, 768, 692; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.35 (t, J = 7.8 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 7.4 Hz, 2H), 6.69 (d, J = 2.2 Hz, 2H), 6.41 (t, J = 2.1 Hz, 1H), 4.97 (s, 2H), 3.80 (s, 2H), 3.78 (s, 6H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 160.8, 154.1, 148.0, 138.1, 129.3, 124.6, 121.0, 106.9, 100.1, 55.4, 46.3, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{18}H_{17}N_2O_3S$ 341.0965, found 341.0965.



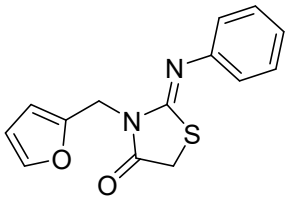
(*Z*)-2-(Phenylimino)-3-(3,4,5-trimethoxybenzyl)thiazolidin-4-one (4r).[1] Eluent: petroleum ether/ethyl acetate (v/v = 3:1). Yellow solid: 53% yield (36.5 mg, 0.10 mmol); mp 124-125 °C; IR (KBr, cm^{-1}) 3427, 3035, 2928, 1715, 1620, 1589, 1457, 1333, 1328, 1126, 771, 692; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.35 (t, J = 7.6 Hz, 2H), 7.14 (t, J = 7.3 Hz, 1H), 6.94 (d, J = 7.8 Hz, 2H), 6.84 (s, 2H), 4.94 (s, 2H), 3.84 (s, 9H), 3.80 (s, 2H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.7, 154.4, 153.1, 148.1, 137.8, 131.6, 129.4, 124.7, 120.9, 106.8, 60.8, 56.2, 46.5, 32.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{19}H_{19}N_2O_4S$ 371.1071, found 371.1075.



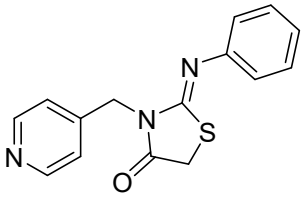
(*Z*)-3-(Naphthalen-1-ylmethyl)-2-(phenylimino)thiazolidin-4-one (4s).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 60% yield (36.9 mg, 0.11 mmol); IR (KBr, cm^{-1}) 3435, 3055, 2925, 1727, 1633, 1594, 1487, 1375, 1325, 1155, 1022, 766, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.41 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.83 (d, J = 8.2 Hz, 1H), 7.58 (t, J = 7.9 Hz, 2H), 7.52 (t, J = 7.3 Hz, 1H), 7.46 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 7.7 Hz, 2H), 7.15 (t, J = 7.4 Hz, 1H), 6.95 (d, J = 7.7 Hz, 2H), 5.54 (s, 2H), 3.86 (s, 2H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.8, 153.9, 147.9, 133.8, 131.5, 130.9, 129.3, 128.7, 128.5, 126.7, 126.4, 125.8, 125.2, 124.7, 123.9, 121.0, 44.3, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{20}H_{15}N_2OS$ 331.0911, found 331.0912.



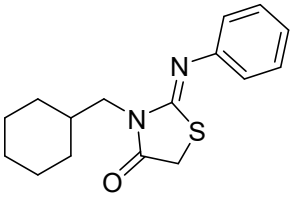
(*Z*)-2-(Phenylimino)-3-(thiophen-2-ylmethyl)thiazolidin-4-one (4t).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 73% yield (38.9 mg, 0.14 mmol); IR (KBr, cm^{-1}) 3428, 3034, 2922, 1723, 1632, 1589, 1420, 1380, 1322, 1140, 1022, 772, 692; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.37 (t, J = 7.7 Hz, 2H), 7.26 (d, J = 4.8 Hz, 1H), 7.23 (d, J = 2.8 Hz, 1H), 7.16 (t, J = 7.4 Hz, 1H), 7.02 (d, J = 7.6 Hz, 2H), 6.98-6.96 (m, 1H), 5.18 (s, 2H), 3.79 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.1, 153.4, 147.8, 137.1, 129.3, 128.6, 126.5, 126.3, 124.7, 121.0, 40.6, 32.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{14}H_{11}N_2OS_2$ 287.0318, found 287.0321.



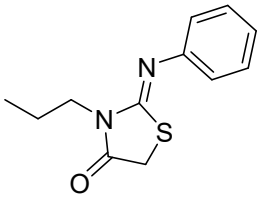
(*Z*)-3-(Furan-2-ylmethyl)-2-(phenylimino)thiazolidin-4-one (4u).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 65% yield (32.7 mg, 0.12 mmol); IR (KBr, cm^{-1}) 3437, 3035, 2923, 1723, 1632, 1589, 1380, 1322, 1157, 1066, 768, 697; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.37-7.33 (m, 3H), 7.14 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 7.5 Hz, 2H), 6.42 (d, J = 3.1 Hz, 1H), 6.34-6.33 (m, 1H), 5.03 (s, 2H), 3.82 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.3, 153.4, 149.1, 147.9, 142.3, 129.3, 124.7, 121.0, 110.5, 109.6, 39.1, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{14}H_{11}N_2O_2S$ 271.0547, found 271.0545.



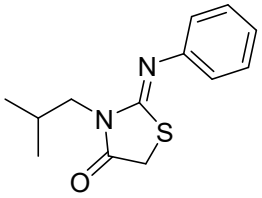
(*Z*)-2-(Phenylimino)-3-(pyridin-4-ylmethyl)thiazolidin-4-one (4v).[2] Eluent: petroleum ether/ethyl acetate (v/v = 1:1). Yellow solid: 60% yield (31.4 mg, 0.11 mmol); mp 116-118 °C; IR (KBr, cm^{-1}) 3439, 3075, 3050, 2963, 2912, 1722, 1642, 1592, 1416, 1375, 1357, 1261, 1166, 1026, 801, 774, 706; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.60 (s, 2H), 7.36-7.32 (m, 4H), 7.15 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 7.7 Hz, 2H), 5.02 (s, 2H), 3.88 (s, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 171.5, 153.5, 150.0, 147.5, 144.5, 129.3, 124.9, 123.5, 120.9, 45.2, 32.7; HRMS (ESI) *m/z* $[M + H]^+$ calcd for $C_{15}H_{14}N_3OS$ 284.0852, found 284.0853.



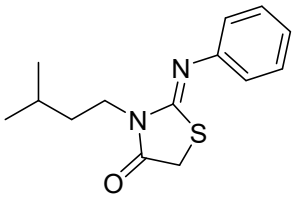
(*Z*)-3-(Cyclohexylmethyl)-2-(phenylimino)thiazolidin-4-one (4w).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 73% yield (38.9 mg, 0.14 mmol); mp 91-92 °C; IR (KBr, cm^{-1}) 3435, 3050, 2931, 1723, 1640, 1590, 1380, 1351, 1136, 1024, 772, 700; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.34 (t, J = 7.5 Hz, 2H), 7.13 (t, J = 7.2 Hz, 1H), 6.94 (d, J = 7.6 Hz, 2H), 3.80 (s, 2H), 3.72 (d, J = 7.3 Hz, 2H), 1.95-1.92 (m, 1H), 1.70 (d, J = 16.7 Hz, 4H), 1.34-1.16 (m, 4H), 1.06 (dd, J = 22.6, 11.0 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 172.1, 154.7, 148.2, 129.3, 124.6, 121.0, 49.1, 35.9, 32.6, 30.7, 26.3, 25.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{19}N_2OS$ 287.1224, found 287.1226.



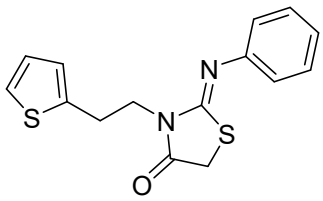
(*Z*)-2-(Phenylimino)-3-propylthiazolidin-4-one (4x). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 89% yield (38.5 mg, 0.16 mmol); IR (KBr, cm^{-1}) 3435, 3055, 2925, 1727, 1633, 1594, 1487, 1375, 1325, 1191, 1124, 766, 697; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.35 (t, J = 7.8 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 6.95 (d, J = 7.6 Hz, 2H), 3.82 (t, J = 7.5 Hz, 2H), 3.80 (s, 2H), 1.77 (dt, J = 14.9, 7.5 Hz, 2H), 0.98 (t, J = 7.4 Hz, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.9, 154.4, 148.2, 129.3, 124.6, 121.0, 44.8, 32.7, 20.6, 11.3; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{12}H_{13}N_2OS$ 233.0754, found 233.0756.



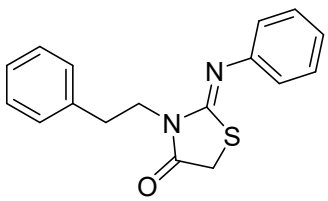
(*Z*)-3-Isobutyl-2-(phenylimino)thiazolidin-4-one (4y).[3] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 70% yield (32.1 mg, 0.13 mmol); IR (KBr, cm^{-1}) 3437, 3054, 2961, 2938, 1729, 1633, 1593, 1454, 1381, 1262, 1129, 1025, 798, 767, 696; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.34 (t, J = 7.7 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 6.94 (d, J = 7.6 Hz, 2H), 3.81 (s, 2H), 3.70 (d, J = 7.5 Hz, 2H), 2.32-2.24 (m, 1H), 0.97 (d, J = 6.7 Hz, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 172.1, 154.6, 148.2, 129.2, 124.5, 120.9, 50.2, 32.6, 26.7, 20.1; HRMS (ESI) *m/z* $[M + H]^+$ calcd for $C_{13}H_{17}N_2OS$ 249.1056, found 249.1058.



(*Z*)-3-Isopentyl-2-(phenylimino)thiazolidin-4-one (4za). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 80% yield (38.8 mg, 0.15 mmol); IR (KBr, cm^{-1}) 3435, 3055, 2925, 1727, 1633, 1504, 1375, 1325, 1243, 1155, 1022, 766, 697; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.35 (t, J = 7.5 Hz, 2H), 7.14 (t, J = 7.3 Hz, 1H), 6.96 (d, J = 7.6 Hz, 2H), 3.87 (t, J = 7.2 Hz, 2H), 3.78 (s, 2H), 1.66-1.58 (m, 3H), 0.98 (d, J = 5.9 Hz, 6H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, ppm) δ 171.7, 154.2, 148.2, 129.3, 124.6, 121.0, 41.9, 35.9, 32.7, 26.1, 22.5; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{14}H_{17}N_2OS$ 261.1067, found 261.1067.

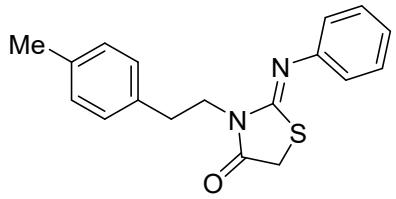


(*Z*)-2-(Phenylimino)-3-(2-(thiophen-2-yl)ethyl)thiazolidin-4-one (4zb). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 59% yield (33.0 mg, 0.11 mmol); IR (KBr, cm^{-1}) 3435, 3055, 2925, 1720, 1633, 1594, 1487, 1375, 1175, 1075, 770, 695; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.36 (t, J = 7.7 Hz, 2H), 7.16 (dd, J = 15.7, 6.4 Hz, 2H), 6.97-6.91 (m, 4H), 4.14 (t, J = 7.3 Hz, 2H), 3.77 (s, 2H), 3.29 (t, J = 7.2 Hz, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 154.0, 148.0, 140.0, 129.3, 127.0, 125.7, 124.7, 124.1, 121.0, 44.1, 32.7, 27.1; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{15}H_{13}N_2OS_2$ 301.0475, found 301.0473.

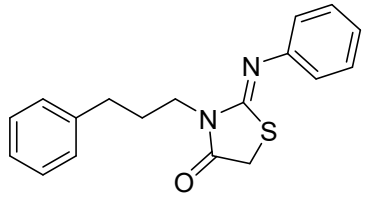


(*Z*)-3-Phenethyl-2-(phenylimino)thiazolidin-4-one (4zc). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 92% yield (50.4 mg, 0.17 mmol); mp 118-120 °C; IR (KBr, cm^{-1}) 3429, 3036, 2923, 1720, 1637, 1589, 1380, 1322, 1151, 1066, 768,

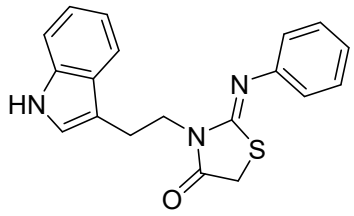
697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.36 (t, J = 7.8 Hz, 2H), 7.30 (dd, J = 12.8, 6.9 Hz, 4H), 7.26-7.23 (m, 1H), 7.15 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 7.6 Hz, 2H), 4.11 (t, J = 7.5 Hz, 2H), 3.75 (s, 2H), 3.05 (t, J = 7.5 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 154.0, 148.1, 138.1, 129.3, 129.1, 128.5, 126.6, 124.6, 121.0, 44.2, 33.2, 32.6; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{15}N_2OS$ 295.0911, found 295.0908.



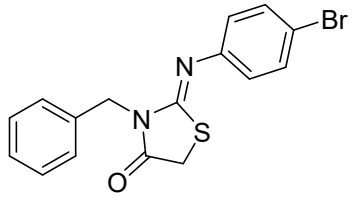
(*Z*)-3-(4-Methylphenethyl)-2-(phenylimino)thiazolidin-4-one (4zd). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 85% yield (48.7 mg, 0.16 mmol); IR (KBr, cm^{-1}) 3434, 3045, 2934, 1725, 1630, 1592, 1383, 1344, 1211, 1155, 1025, 768, 696; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.35 (t, J = 7.6 Hz, 2H), 7.16 (t, J = 7.5 Hz, 3H), 7.12 (d, J = 7.6 Hz, 2H), 6.92 (d, J = 7.7 Hz, 2H), 4.07 (t, J = 8.0 Hz, 2H), 3.75 (s, 2H), 3.00 (t, J = 7.5 Hz, 2H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 154.0, 148.1, 136.1, 135.0, 129.2, 129.2, 128.9, 124.6, 121.0, 44.3, 32.7, 32.7, 21.1; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{18}H_{17}N_2OS$ 309.1067, found 309.1067.



(*Z*)-2-(Phenylimino)-3-(3-phenylpropyl)thiazolidin-4-one (4ze).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 60% yield (34.4 mg, 0.11 mmol); IR (KBr, cm^{-1}) 3431, 3024, 2930, 1717, 1643, 1594, 1428, 1389, 1207, 1145, 768, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.36 (t, J = 7.8 Hz, 2H), 7.30 (t, J = 7.5 Hz, 2H), 7.24 (d, J = 7.3 Hz, 2H), 7.20 (t, J = 7.2 Hz, 1H), 7.16 (t, J = 7.4 Hz, 1H), 6.97 (d, J = 7.6 Hz, 2H), 3.94 (t, J = 7.3 Hz, 2H), 3.72 (s, 2H), 2.73 (t, J = 7.5 Hz, 2H), 2.14-2.08 (m, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.8, 154.3, 148.1, 141.2, 129.3, 128.4, 128.3, 126.0, 124.6, 121.0, 43.1, 33.2, 32.7, 28.3; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{18}H_{17}N_2OS$ 309.1067, found 309.1067.

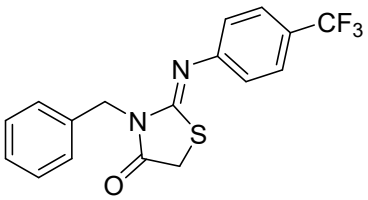


(*Z*)-3-(2-(1H-Indol-3-yl)ethyl)-2-(phenylimino)thiazolidin-4-one (4zf). Eluent: petroleum ether/ethyl acetate (v/v = 5:1). Yellow solid: 77% yield (47.7 mg, 0.14 mmol); mp 155-156 °C; IR (KBr, cm^{-1}) 3348, 3050, 2968, 1723, 1619, 1586, 1372, 1157, 1098, 1011, 744, 697; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.08 (s, 1H), 7.78 (d, J = 7.8 Hz, 1H), 7.36 (dd, J = 13.0, 5.4 Hz, 3H), 7.17 (ddd, J = 21.6, 14.9, 7.2 Hz, 3H), 7.10 (s, 1H), 6.95 (d, J = 7.6 Hz, 2H), 4.18 (t, J = 8.0 Hz, 2H), 3.74 (s, 2H), 3.22 (t, J = 7.5 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.8, 154.2, 148.2, 136.2, 129.3, 127.7, 124.6, 122.3, 122.1, 121.1, 119.6, 118.9, 112.5, 111.1, 43.8, 32.8, 23.0; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{19}H_{16}N_3OS$ 334.1020, found 334.1017.

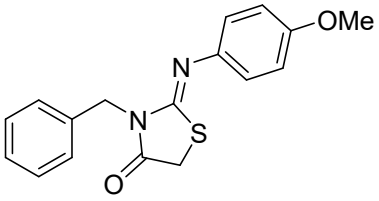


(*Z*)-3-Benzyl-2-((4-bromophenyl)imino)thiazolidin-4-one (5a).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow

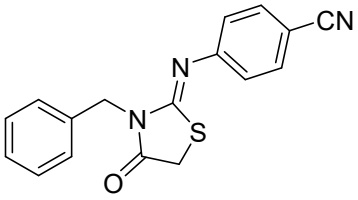
solid: 72% yield (48.0 mg, 0.13 mmol); mp 103-105 °C; IR (KBr, cm^{-1}) 3330, 3069, 3030, 2963, 2929, 1723, 1627, 1580, 1483, 1385, 1335, 1151, 1007, 831, 701, 676; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.50 (d, J = 7.0 Hz, 2H), 7.45 (d, J = 8.4 Hz, 2H), 7.35-7.29 (m, 3H), 6.83 (d, J = 8.4 Hz, 2H), 5.01 (s, 2H), 3.83 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 154.6, 146.9, 135.8, 132.3, 129.1, 128.5, 128.0, 122.8, 117.7, 46.3, 32.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{12}BrN_2OS$ 358.9859, found 358.9858.



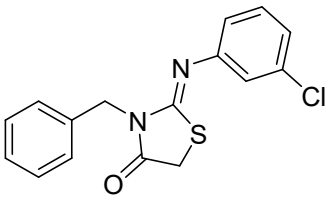
(*Z*)-3-Benzyl-2-((4-(trifluoromethyl)phenyl)imino)thiazolidin-4-one (5b).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 91% yield (58.9 mg, 0.17 mmol); mp 95-96 °C; IR (KBr, cm^{-1}) 3331, 3068, 3034, 2982, 2939, 1734, 1633, 1607, 1384, 1371, 1161, 1065, 847, 702, 671; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.60 (d, J = 8.2 Hz, 2H), 7.51 (d, J = 6.7 Hz, 2H), 7.36-7.32 (m, 3H), 7.03 (d, J = 8.2 Hz, 2H), 5.02 (s, 2H), 3.85 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.4, 155.0, 151.0, 135.7, 129.1, 128.6, 128.1, 126.5 (q, J = 3.7 Hz), 126.1 (d, J = 179.6 Hz), 123.4 (d, J = 46.5 Hz), 121.3, 46.4, 32.8; ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -61.94; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{17}H_{12}F_3N_2OS$ 349.0628, found 349.0629.



(*Z*)-3-Benzyl-2-((4-methoxyphenyl)imino)thiazolidin-4-one (5c).[1] Eluent: petroleum ether/ethyl acetate (v/v = 10:1). Yellow oil: 90% yield (51.9 mg, 0.17 mmol); IR (KBr, cm^{-1}) 3435, 3055, 2925, 1727, 1633, 1504, 1375, 1325, 1243, 1155, 1022, 828, 766, 697; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.52 (d, J = 7.0 Hz, 2H), 7.32 (dq, J = 13.9, 6.8 Hz, 3H), 6.90 (q, J = 8.9 Hz, 4H), 5.03 (s, 2H), 3.81 (s, 5H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.7, 156.8, 153.6, 141.1, 136.0, 129.1, 128.5, 127.9, 122.1, 114.5, 55.5, 46.3, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{17}H_{15}N_2O_2S$ 311.0860, found 311.0859.

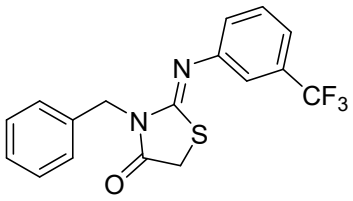


(*Z*)-4-((3-Benzyl-4-oxothiazolidin-2-ylidene)amino)benzonitrile (5d).[1] Eluent: petroleum ether/ethyl acetate (v/v = 5:1). Yellow oil: 71% yield (40.3 mg, 0.13 mmol); IR (KBr, cm^{-1}) 3425, 3034, 2965, 2223, 1727, 1630, 1592, 1494, 1380, 1155, 1080, 843, 696; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.63 (d, J = 8.3 Hz, 2H), 7.48 (d, J = 6.7 Hz, 2H), 7.36-7.32 (m, 3H), 7.02 (d, J = 8.3 Hz, 2H), 5.01 (s, 2H), 3.87 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.3, 155.4, 152.0, 135.5, 133.5, 129.1, 128.6, 128.1, 122.0, 119.0, 108.0, 46.4, 32.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{17}H_{12}N_3OS$ 306.0707, found 306.0710.

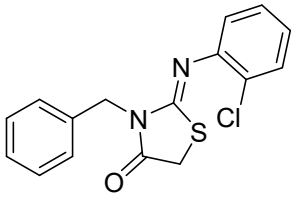


(*Z*)-3-Benzyl-2-((3-chlorophenyl)imino)thiazolidin-4-one (5e).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 98% yield (57.3 mg, 0.18 mmol); IR (KBr, cm^{-1}) 3436, 3038, 2933, 1727, 1631, 1585, 1380, 1339, 1164, 1083, 784, 694;

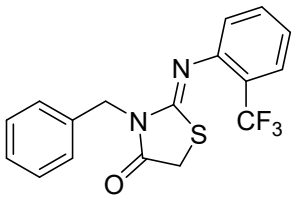
^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.51 (d, J = 7.0 Hz, 2H), 7.37-7.31 (m, 3H), 7.28 (t, J = 7.9 Hz, 1H), 7.13 (d, J = 7.9 Hz, 1H), 6.97 (s, 1H), 6.85 (d, J = 7.8 Hz, 1H), 5.02 (s, 2H), 3.84 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 155.0, 149.2, 135.8, 134.7, 130.3, 129.1, 128.6, 128.0, 124.7, 121.4, 119.3, 46.3, 32.8; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{16}H_{12}ClN_2OS$ 315.0364, found 315.0361.



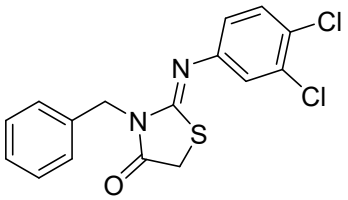
(*Z*)-3-Benzyl-2-((3-(trifluoromethyl)phenyl)imino)thiazolidin-4-one (5f). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 97% yield (62.8 mg, 0.18 mmol); IR (KBr, cm^{-1}) 3425, 3033, 2925, 1630, 1592, 1494, 1380, 1335, 1155, 1025, 803, 696; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.52 (d, J = 7.0 Hz, 2H), 7.46 (t, J = 7.8 Hz, 1H), 7.40 (d, J = 7.7 Hz, 1H), 7.34 (dq, J = 14.1, 6.9 Hz, 3H), 7.23 (s, 1H), 7.14 (d, J = 7.7 Hz, 1H), 5.04 (s, 2H), 3.84 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 155.4, 148.4, 135.7, 131.7 (q, J = 32.4 Hz), 129.8, 129.1, 128.6, 128.1, 124.5, 124.0 (d, J = 273.0 Hz), 121.3 (q, J = 3.8 Hz), 118.2 (q, J = 3.8 Hz), 46.4, 32.7; ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -62.64; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{12}F_3N_2OS$ 349.0628, found 349.0627.



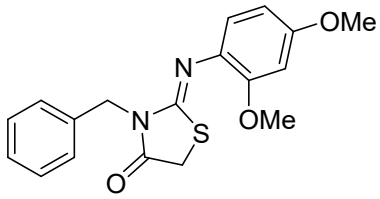
(*Z*)-3-Benzyl-2-((2-chlorophenyl)imino)thiazolidin-4-one (5g).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 69% yield (40.3 mg, 0.13 mmol); IR (KBr, cm^{-1}) 3438, 3063, 2931, 1727, 1630, 1584, 1380, 1335, 1165, 1057, 754, 701; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.58 (d, J = 7.1 Hz, 2H), 7.43 (d, J = 7.9 Hz, 1H), 7.32 (dq, J = 14.0, 6.9 Hz, 3H), 7.23 (t, J = 7.6 Hz, 1H), 7.09 (t, J = 7.6 Hz, 1H), 6.95 (d, J = 7.8 Hz, 1H), 5.07 (s, 2H), 3.83 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 156.0, 145.1, 135.7, 130.2, 129.3, 128.5, 128.0, 127.5, 126.5, 125.6, 121.8, 46.4, 32.9; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{16}H_{12}ClN_2OS$ 315.0364, found 315.0366.



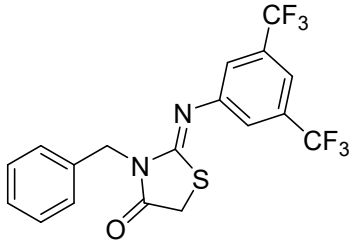
(*Z*)-3-Benzyl-2-((2-(trifluoromethyl)phenyl)imino)thiazolidin-4-one (5h).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 97% yield (62.8 mg, 0.18 mmol); IR (KBr, cm^{-1}) 3439, 3036, 2937, 1731, 1634, 1380, 1317, 1166, 1032, 763, 699; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.68 (d, J = 7.8 Hz, 1H), 7.53 (d, J = 7.1 Hz, 2H), 7.49 (t, J = 7.8 Hz, 1H), 7.36-7.31 (m, 3H), 7.22 (t, J = 7.6 Hz, 1H), 7.01 (d, J = 7.9 Hz, 1H), 5.04 (s, 2H), 3.83 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 155.6, 146.2, 135.6, 132.7, 129.2, 128.5, 128.0, 126.9 (q, J = 5.1 Hz), 124.3, 123.6 (d, J = 316.8 Hz), 122.6 (d, J = 11.7 Hz), 121.4, 46.6, 32.8; ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -61.63; HRMS (ESI) *m/z* [M – H]$^-$ calcd for $C_{17}H_{12}F_3N_2OS$ 349.0628, found 349.0631.



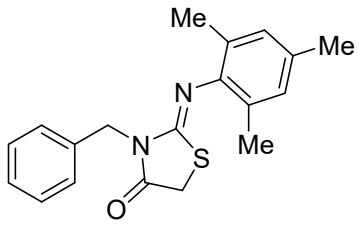
(*Z*)-3-Benzyl-2-((3,4-dichlorophenyl)imino)thiazolidin-4-one (5i). Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 90% yield (58.3 mg, 0.17 mmol); IR (KBr, cm^{-1}) 3439, 3040, 2933, 1727, 1629, 1582, 1467, 1377, 1167, 1026, 817, 697; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.48 (d, J = 6.9 Hz, 2H), 7.39 (d, J = 8.5 Hz, 1H), 7.34-7.31 (m, 3H), 7.07 (d, J = 1.9 Hz, 1H), 6.81 (dd, J = 8.4, 2.0 Hz, 1H), 5.00 (s, 2H), 3.84 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.4, 155.6, 147.4, 135.6, 132.9, 130.9, 129.0, 128.6, 128.1, 128.1, 123.1, 120.7, 46.4, 32.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{16}H_{11}Cl_2N_2OS$ 348.9975, found 348.9972.



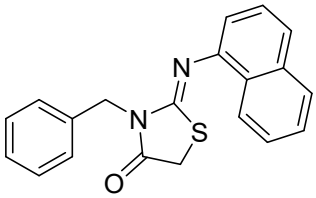
(*Z*)-3-Benzyl-2-((2,4-dimethoxyphenyl)imino)thiazolidin-4-one (5j).[1] Eluent: petroleum ether/ethyl acetate (v/v = 5:1). Yellow oil: 57% yield (36.1 mg, 0.11 mmol); IR (KBr, cm^{-1}) 3431, 3032, 2958, 1722, 1637, 1504, 1381, 1209, 1166, 1033, 802, 701; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.59 (d, J = 7.1 Hz, 2H), 7.31 (dq, J = 14.2, 7.0 Hz, 3H), 6.79 (d, J = 8.5 Hz, 1H), 6.55 (d, J = 2.2 Hz, 1H), 6.46 (dd, J = 8.5, 2.3 Hz, 1H), 5.06 (s, 2H), 3.80 (d, J = 6.0 Hz, 6H), 3.77 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.8, 157.9, 155.1, 151.9, 136.1, 130.7, 129.2, 128.4, 127.8, 121.5, 104.2, 100.2, 55.9, 55.5, 46.3, 32.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{18}H_{17}N_2O_3S$ 341.0965, found 341.0964.



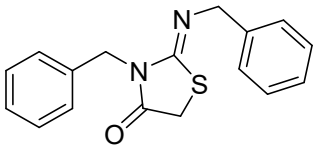
(*Z*)-3-Benzyl-2-((3,5-bis(trifluoromethyl)phenyl)imino)thiazolidin-4-one (5k).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 81% yield (62.6 mg, 0.15 mmol); mp 123-125 °C; IR (KBr, cm^{-1}) 3448, 3069, 3030, 2957, 1722, 1634, 1388, 1281, 1168, 1126, 979, 884, 794, 697; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.64 (s, 1H), 7.49 (d, J = 6.8 Hz, 2H), 7.39-7.33 (m, 5H), 5.03 (s, 2H), 3.89 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.3, 156.8, 149.3, 135.4, 132.7 (q, J = 97.0 Hz), 129.0, 128.7, 128.2, 123.1 (q, J = 260.7 Hz), 121.7 (d, J = 2.9 Hz), 118.1 (dt, J = 7.7, 3.8 Hz), 46.5, 32.8; ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -62.94; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{18}H_{11}F_6N_2OS$ 417.0502, found 417.0499.



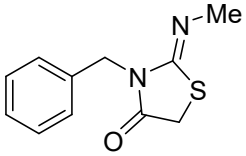
(*Z*)-3-Benzyl-2-(mesitylimino)thiazolidin-4-one (5l).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 55% yield (33.0 mg, 0.10 mmol); IR (KBr, cm^{-1}) 3436, 3035, 2959, 1727, 1641, 1380, 1339, 1170, 1032, 800, 701; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.53 (d, J = 7.0 Hz, 2H), 7.35-7.30 (m, 3H), 6.85 (s, 2H), 5.08 (s, 2H), 3.82 (s, 2H), 2.27 (s, 3H), 1.97 (s, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.8, 153.6, 143.1, 136.0, 133.5, 129.0, 128.9, 128.4, 127.9, 127.9, 46.3, 32.9, 20.8, 17.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{19}H_{19}N_2OS$ 323.1224, found 323.1224.



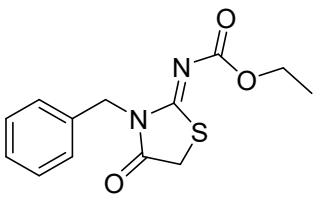
(*Z*)-3-Benzyl-2-(naphthalen-1-ylimino)thiazolidin-4-one (5m).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow oil: 77% yield (47.3 mg, 0.14 mmol); IR (KBr, cm^{-1}) 3439, 3055, 2965, 1725, 1632, 1571, 1380, 1261, 1080, 1026, 804, 703; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.83 (d, J = 8.1 Hz, 1H), 7.65 (d, J = 8.3 Hz, 1H), 7.61 (dd, J = 14.7, 7.8 Hz, 3H), 7.48 (t, J = 7.4 Hz, 1H), 7.44-7.34 (m, 5H), 7.02 (d, J = 7.2 Hz, 1H), 5.18 (s, 2H), 3.84 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.8, 154.4, 144.4, 136.0, 134.4, 129.1, 128.6, 128.0, 127.9, 127.4, 126.4, 125.7, 125.6, 124.8, 123.4, 115.0, 46.6, 32.8; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{20}H_{15}N_2OS$ 331.0911, found 331.0913.



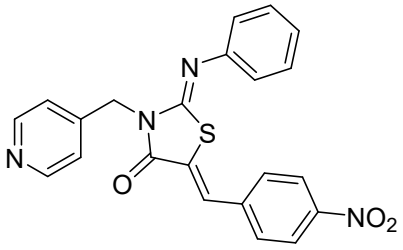
(*Z*)-3-Benzyl-2-(benzylimino)thiazolidin-4-one (5n).[1] Eluent: petroleum ether/ethyl acetate (v/v = 15:1). Yellow solid: 70% yield (38.3 mg, 0.13 mmol); mp 67-69 °C; IR (KBr, cm^{-1}) 3341, 3066, 3027, 2960, 2927, 1715, 1646, 1495, 1422, 1377, 1328, 1261, 1157, 1027, 801, 704; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.47 (d, J = 6.5 Hz, 2H), 7.35-7.27 (m, 8H), 4.97 (s, 2H), 4.54 (s, 2H), 3.85 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.5, 152.7, 139.3, 136.3, 129.0, 128.4, 128.4, 127.8, 127.4, 126.9, 55.4, 46.2, 32.7; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{17}H_{15}N_2OS$ 295.0911, found 295.0909.



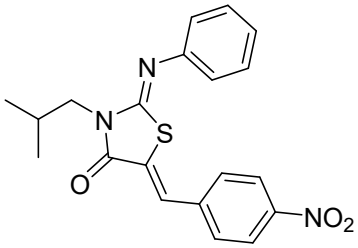
(*Z*)-3-Benzyl-2-(methylimino)thiazolidin-4-one (5o).[1] Eluent: petroleum ether/ethyl acetate (v/v = 10:1). Yellow solid: 70% yield (28.5 mg, 0.13 mmol); mp 157-159 °C; IR (KBr, cm^{-1}) 3335, 3081, 3019, 2973, 2938, 1720, 1639, 1409, 1375, 1293, 1112, 1033, 790, 734; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.36-7.33 (m, 4H), 7.28-7.26 (m, 1H), 4.52 (s, 2H), 3.84 (s, 2H), 3.23 (s, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 171.6, 153.7, 139.2, 128.5, 127.6, 127.0, 55.5, 32.8, 29.6; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{11}H_{11}N_2OS$ 219.0598, found 219.0599.



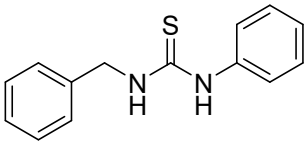
Ethyl (*Z*)-(3-benzyl-4-oxothiazolidin-2-ylidene)carbamate (5p).[1] Eluent: petroleum ether/ethyl acetate (v/v = 5:1). Yellow solid: 42% yield (21.6 mg, 0.08 mmol); mp 140-142 °C; IR (KBr, cm^{-1}) 3473, 3072, 3041, 2963, 2940, 1743, 1674, 1541, 1379, 1261, 1168, 1019, 799, 731; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.44 (d, J = 6.6 Hz, 2H), 7.32-7.28 (m, 3H), 5.02 (s, 2H), 4.28 (q, J = 7.1 Hz, 2H), 3.78 (s, 2H), 1.37 (t, J = 7.1 Hz, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, ppm) δ 173.5, 172.7, 162.3, 135.1, 129.0, 128.6, 128.2, 62.8, 47.0, 32.8, 14.3; HRMS (ESI) *m/z* $[M - H]^-$ calcd for $C_{13}H_{13}N_2O_3S$ 277.0652, found 277.0650.



(*Z*)-5-((*Z*)-4-Nitrobenzylidene)-2-(phenylimino)-3-(pyridin-4-ylmethyl)thiazolidin-4-one (7).[2] Eluent: petroleum ether/ethyl acetate (v/v = 2:1). Orange solid: 40% yield (30.7 mg, 0.07 mmol); mp 142-144 °C; IR (KBr, cm^{-1}) 3450, 3036, 2960, 2922, 1644, 1591, 1455, 1379, 1338, 1262, 1018, 801, 709; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.63 (s, 2H), 8.26 (d, J = 8.4 Hz, 2H), 7.80 (s, 1H), 7.59 (d, J = 8.3 Hz, 2H), 7.40 (d, J = 7.4 Hz, 4H), 7.23 (d, J = 7.3 Hz, 1H), 6.96 (d, J = 7.7 Hz, 2H), 5.19 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 165.9, 150.2, 148.4, 147.7, 147.2, 144.3, 139.6, 130.4, 129.6, 128.5, 125.9, 125.6, 124.3, 123.4, 120.9, 45.5; HRMS (ESI) *m/z* $[M + H]^+$ calcd for $C_{22}H_{17}N_4O_3S$ 417.1016, found 417.1013.



(*Z*)-3-Isobutyl-5-((*Z*)-4-nitrobenzylidene)-2-(phenylimino)thiazolidin-4-one (8).[3] Eluent: petroleum ether/ethyl acetate (v/v = 20:1). Yellow solid: 61% yield (43.0 mg, 0.11 mmol); mp 116-118 °C; IR (KBr, cm^{-1}) 3438, 3032, 2961, 2940, 1705, 1644, 1592, 1381, 1342, 1126, 848, 767, 696; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.24 (d, J = 8.5 Hz, 2H), 7.75 (s, 1H), 7.59 (d, J = 8.5 Hz, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.22 (t, J = 7.4 Hz, 1H), 6.99 (d, J = 7.6 Hz, 2H), 3.86 (d, J = 7.4 Hz, 2H), 2.35 (td, J = 13.6, 6.9 Hz, 1H), 1.01 (d, J = 6.6 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) δ 166.5, 149.4, 147.9, 147.5, 140.0, 130.3, 129.5, 127.4, 126.6, 125.2, 124.2, 121.0, 50.6, 27.0, 20.1; HRMS (ESI) *m/z* $[M + H]^+$ calcd for $C_{20}H_{20}N_3O_3S$ 382.1220, found 382.1217.



1-Benzyl-3-phenylthiourea (9).[4] Eluent: petroleum ether/ethyl acetate (v/v = 5:1). White solid; mp 152-154 °C; IR (KBr, cm^{-1}) 3363, 3149, 2972, 2921, 1538, 1504, 1294, 1242, 1065, 970, 741, 693; ^{1}H NMR (500 MHz, DMSO-d_6, ppm) δ 9.63 (s, 1H), 8.17 (s, 1H), 7.43 (d, J = 7.8 Hz, 2H), 7.33 (dd, J = 11.2, 6.3 Hz, 6H), 7.26 (td, J = 8.5, 4.2 Hz, 1H), 7.12 (t, J = 7.3 Hz, 1H), 4.75 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6, ppm) δ 181.3, 139.6, 139.5, 129.1, 128.8, 127.9, 127.4, 124.8, 123.8, 47.7.

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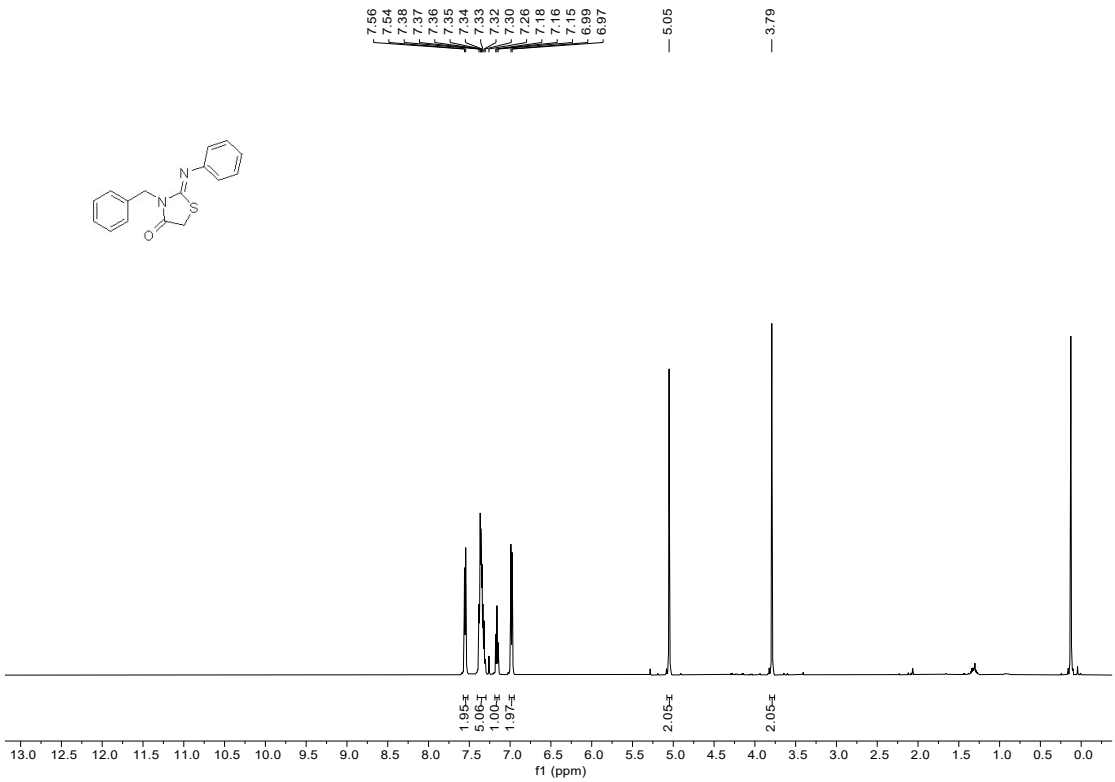
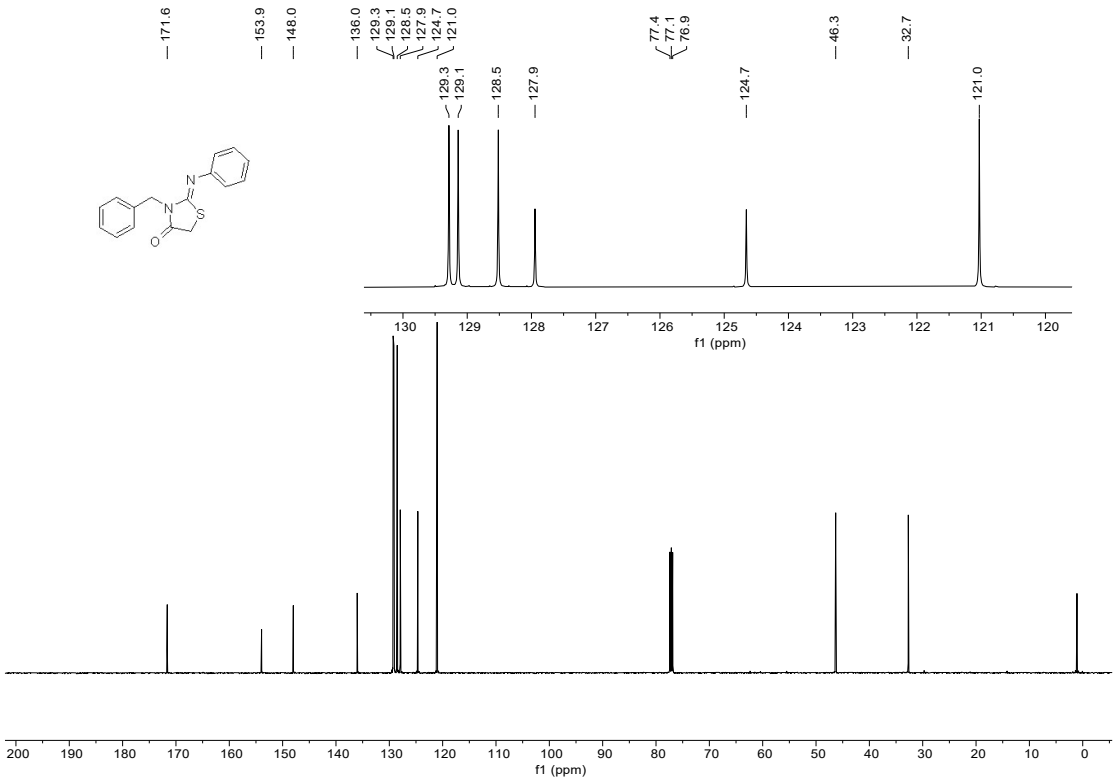
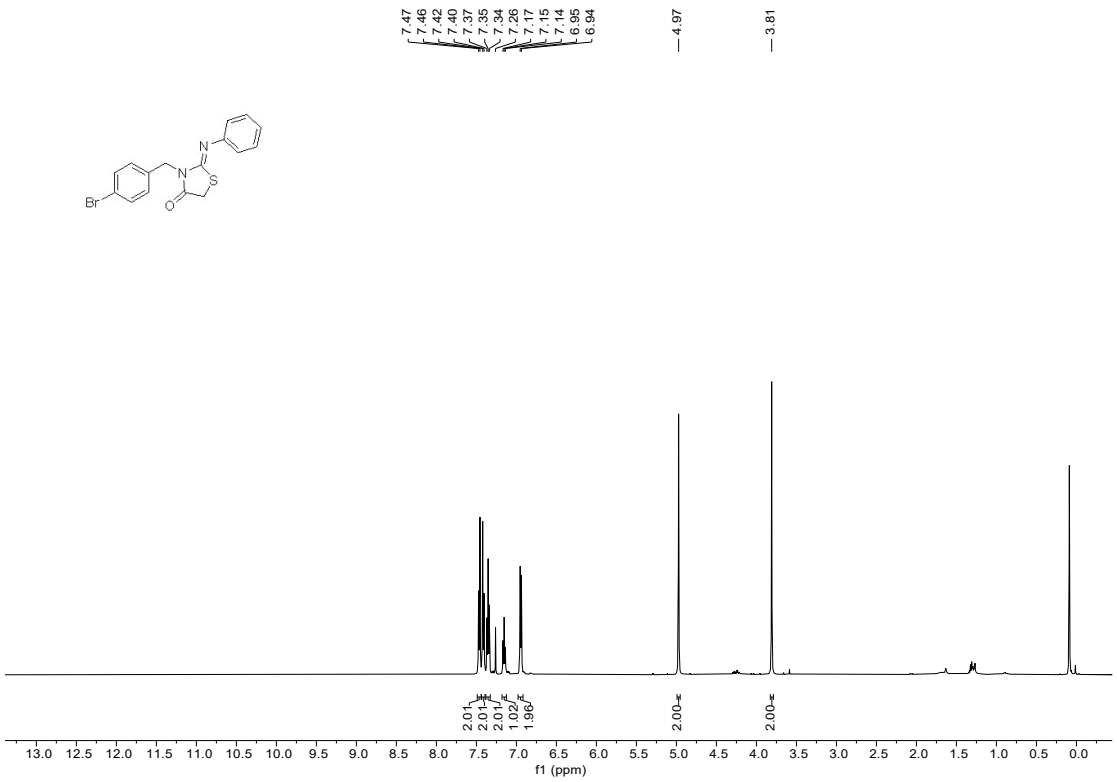
NMR Spectra



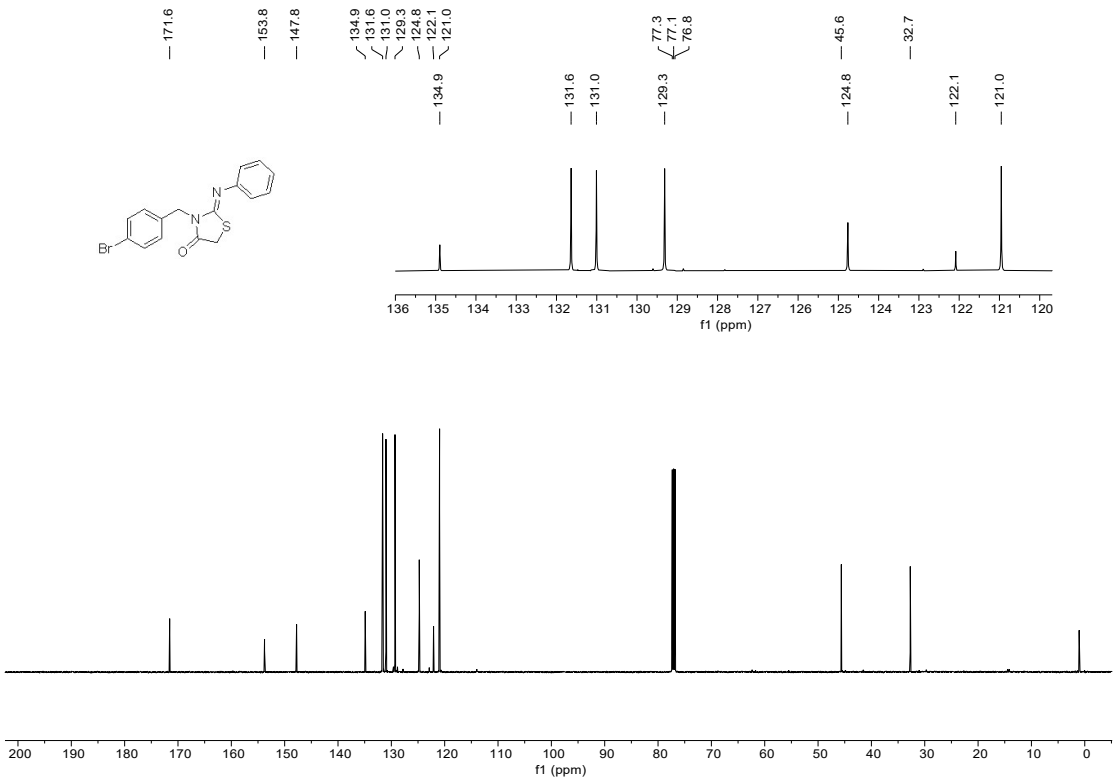
^{1}H NMR of **4a** in $CDCl_3$ (500 MHz)



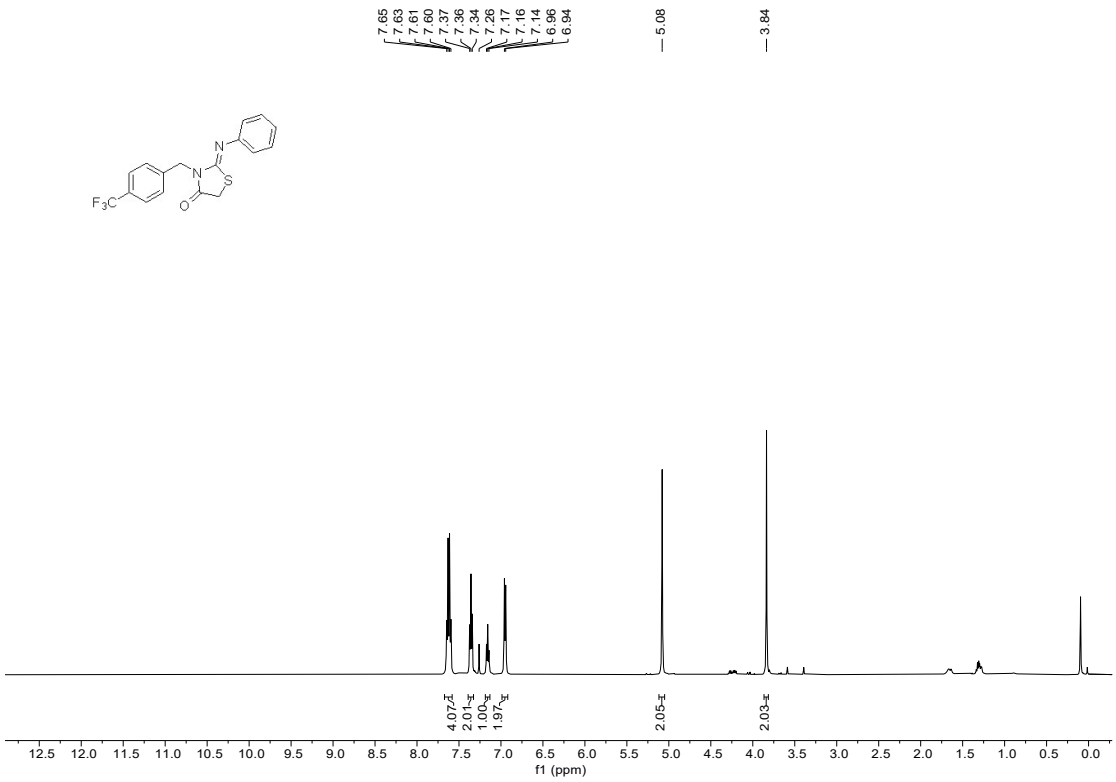
^{13}C{^{1}H} NMR of **4a** in $CDCl_3$ (126 MHz)



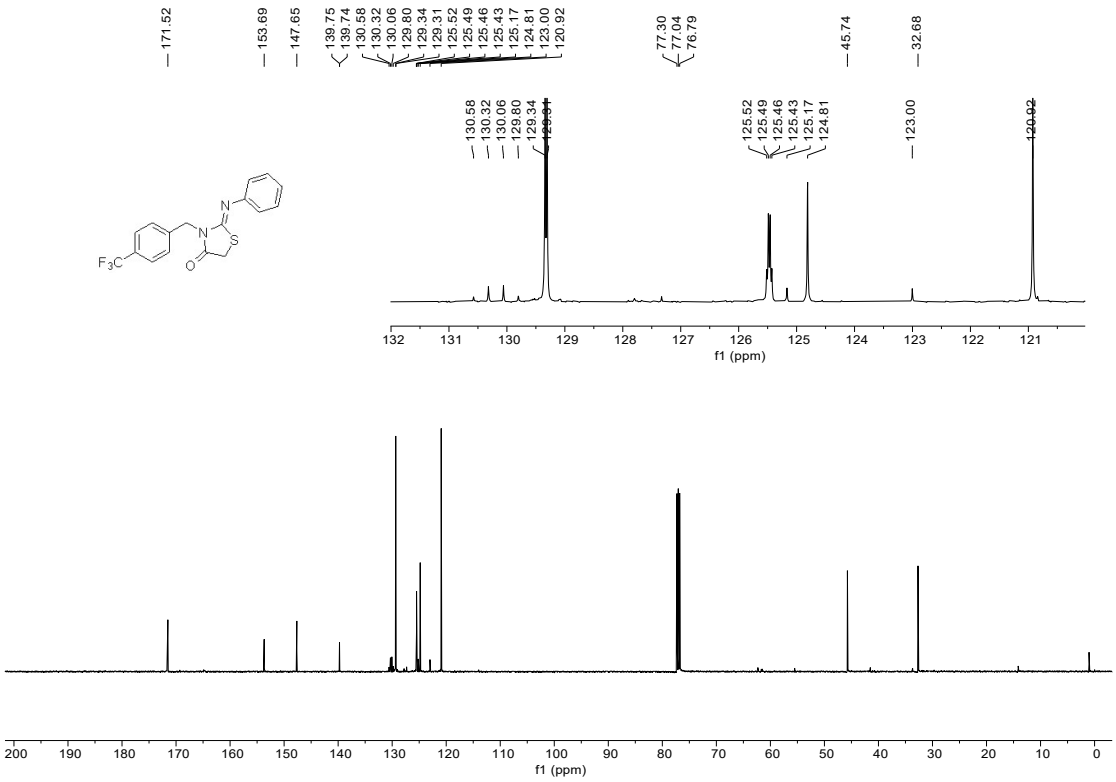
^{1}H NMR of **4b** in $CDCl_3$ (500 MHz)



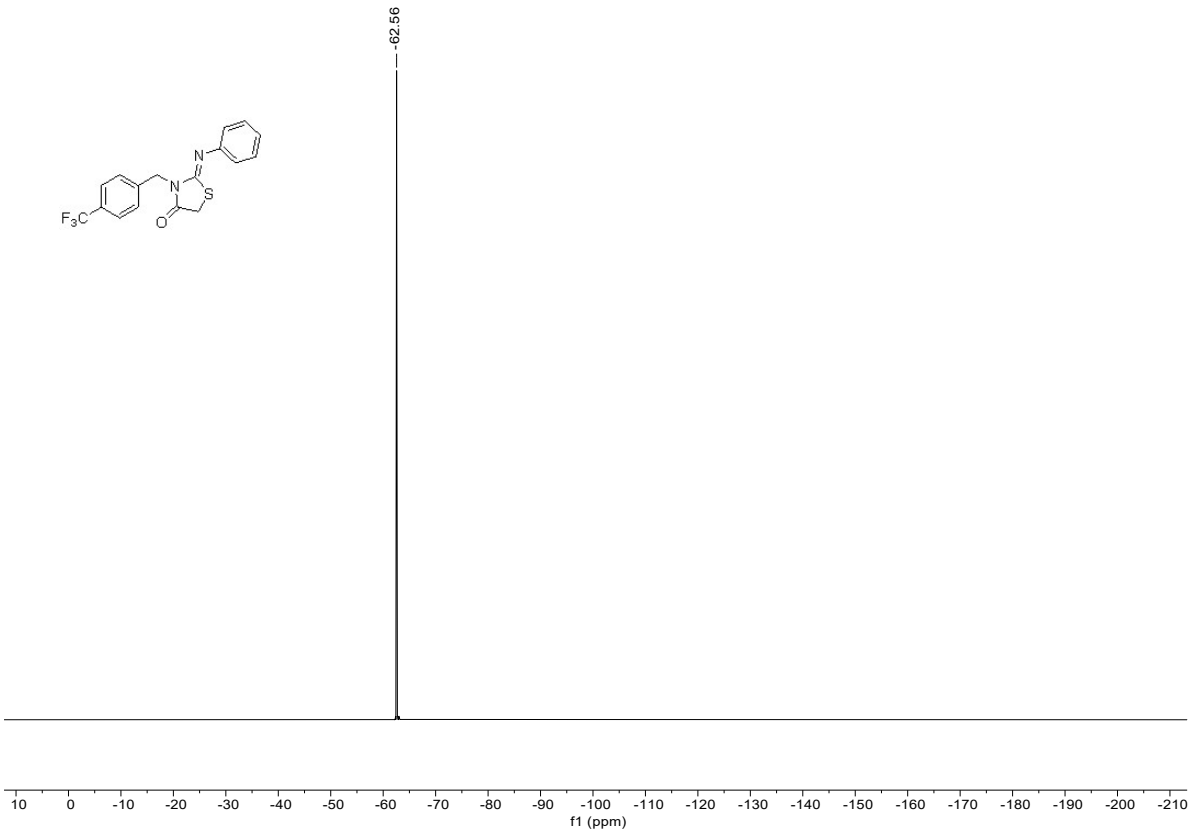
^{13}C{^{1}H} NMR of **4b** in $CDCl_3$ (126 MHz)



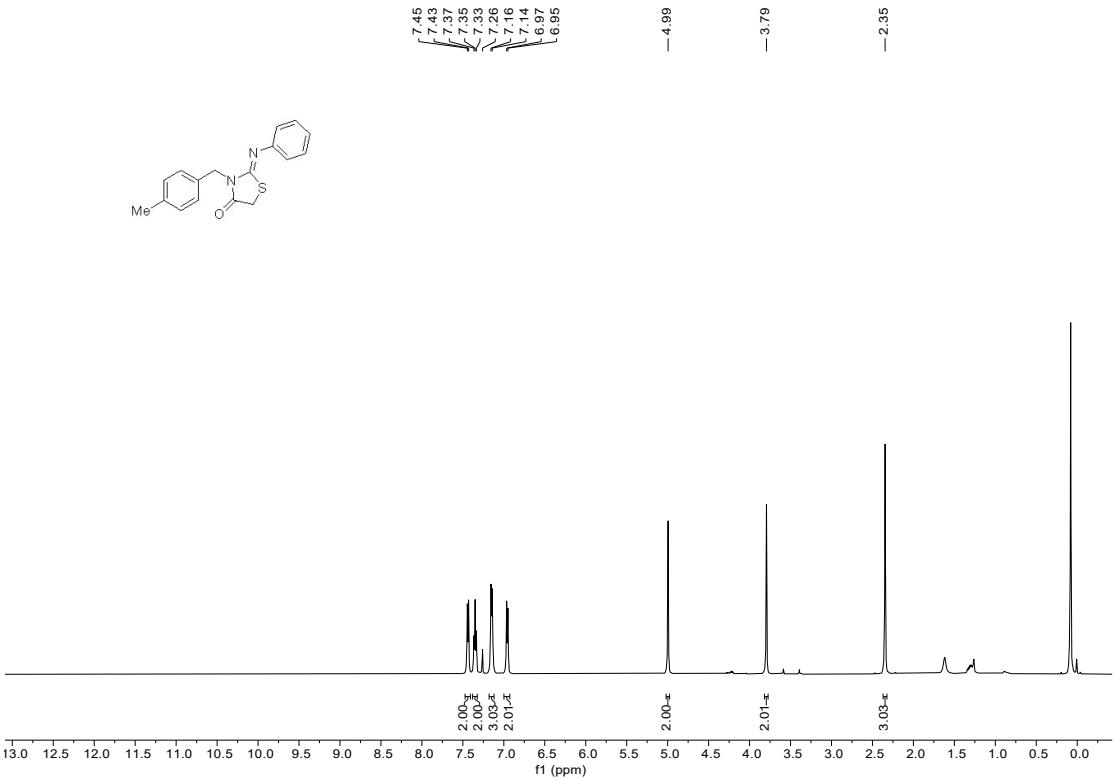
^{1}H NMR of **4c** in $CDCl_3$ (500 MHz)



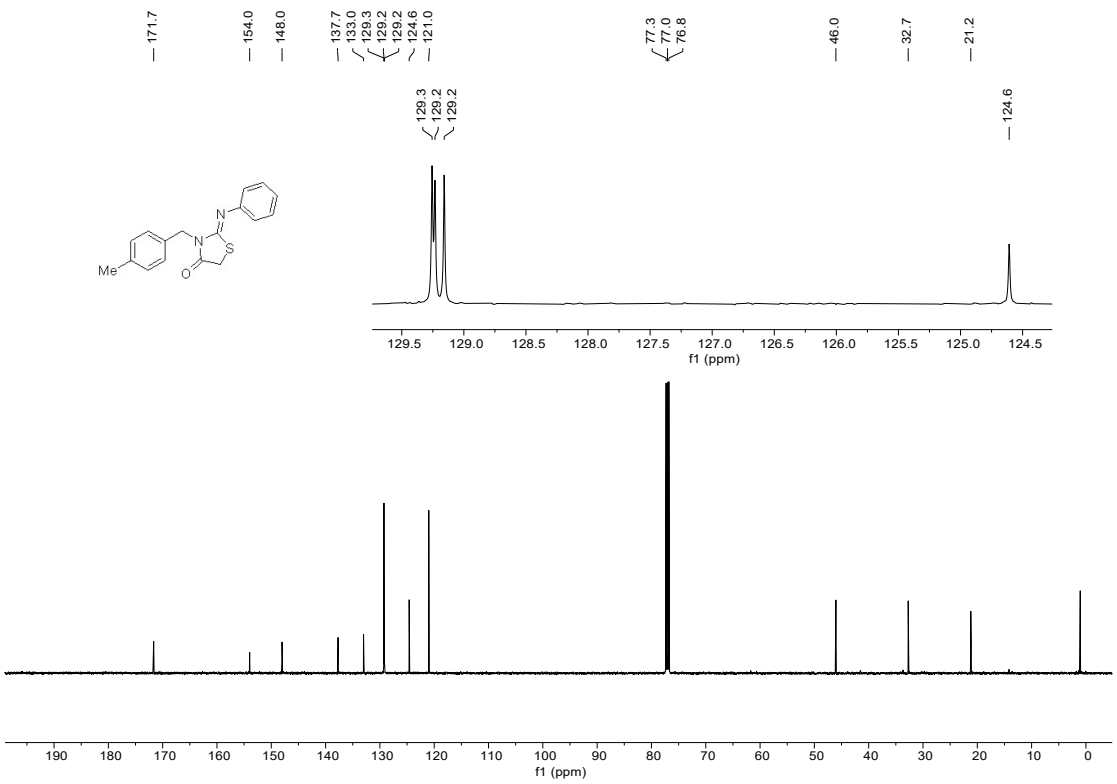
^{13}C{^{1}H} NMR of **4c** in $CDCl_3$ (126 MHz)



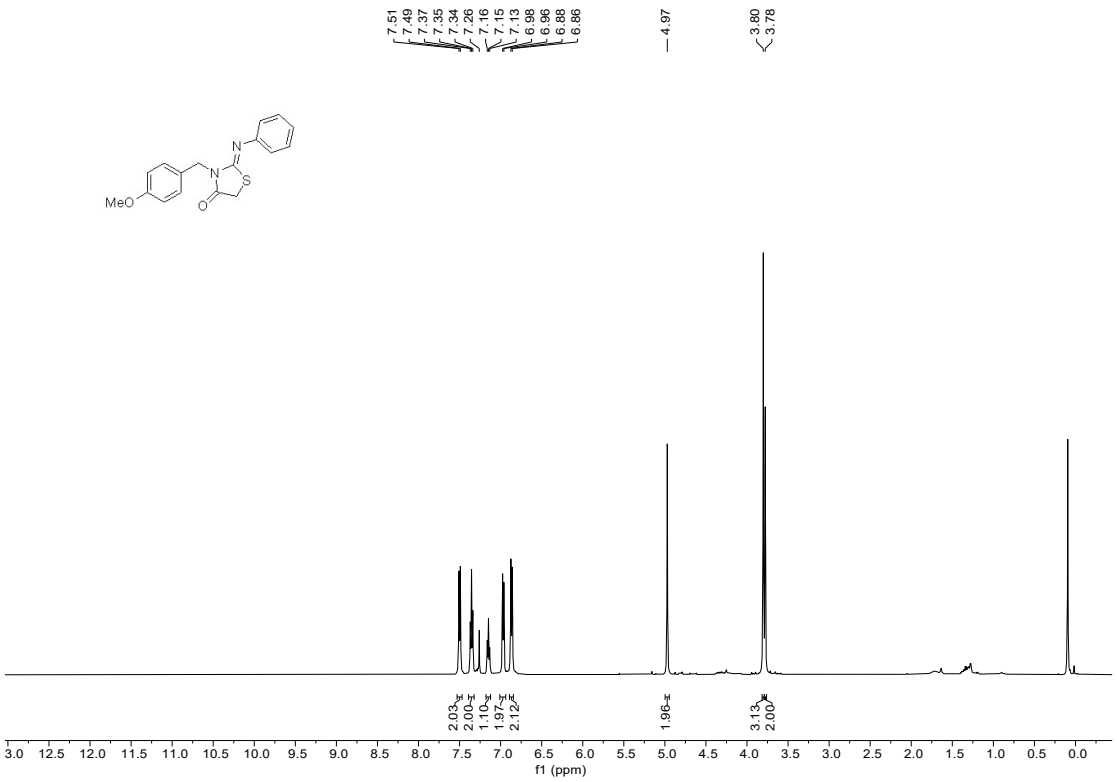
^{19}F NMR of **4c** in $CDCl_3$ (471 MHz)



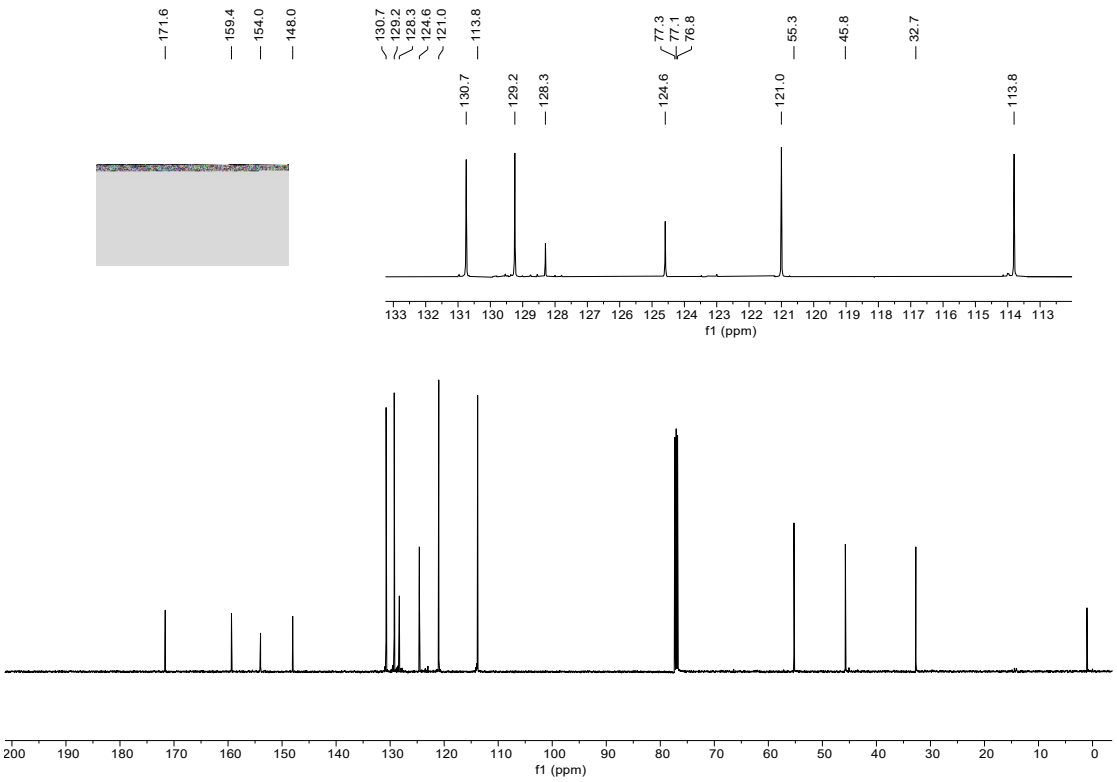
^{1}H NMR of **4d** in $CDCl_3$ (500 MHz)



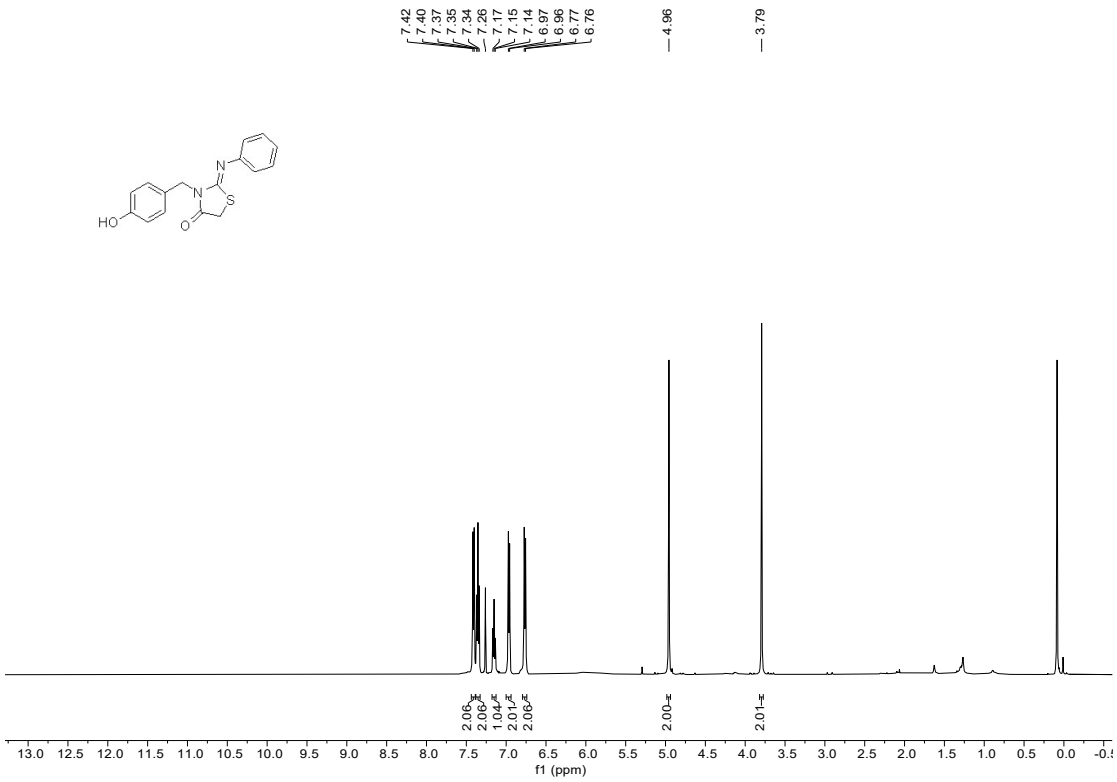
$^{13}C\{^{1}H\}$ NMR of **4d** in $CDCl_3$ (126 MHz)



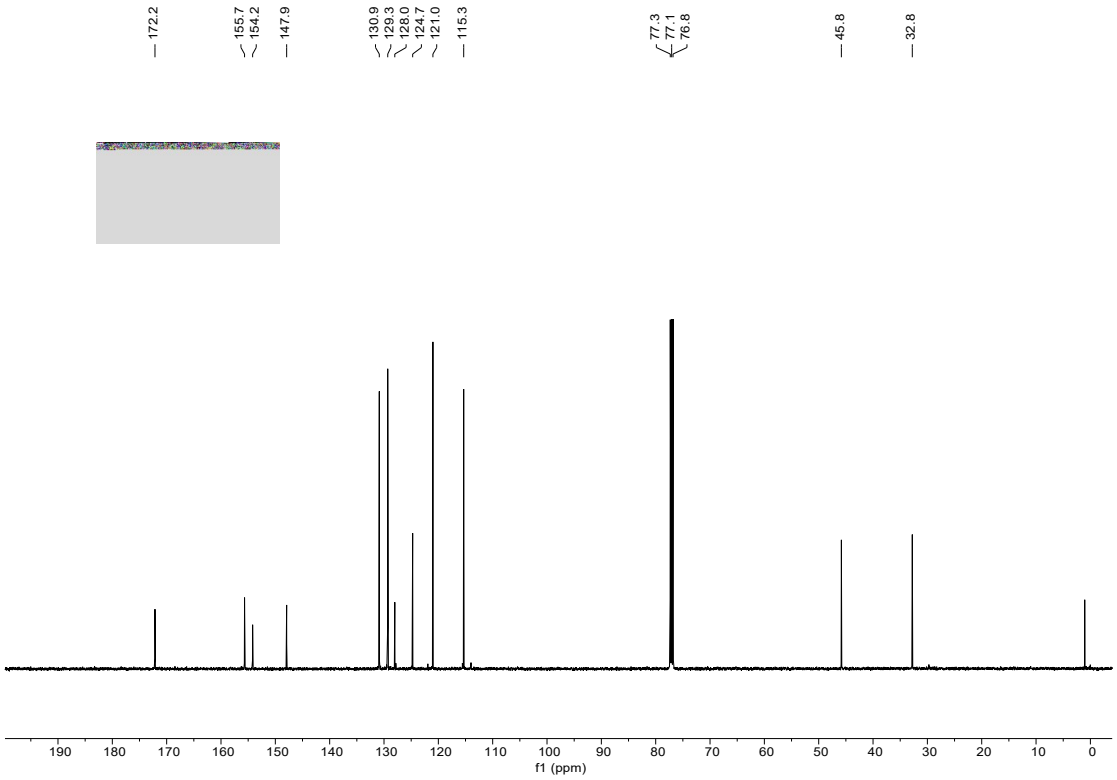
^{1}H NMR of **4e** in $CDCl_3$ (500 MHz)



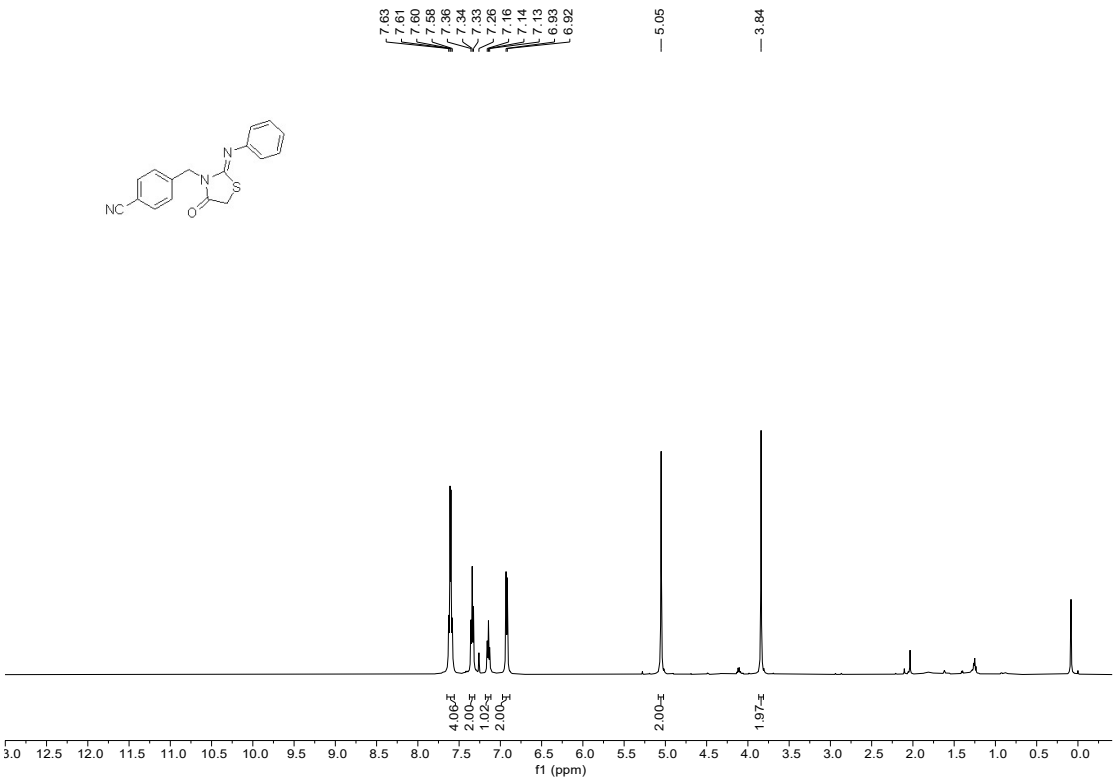
$^{13}C\{^{1}H\}$ NMR of **4e** in $CDCl_3$ (126 MHz)



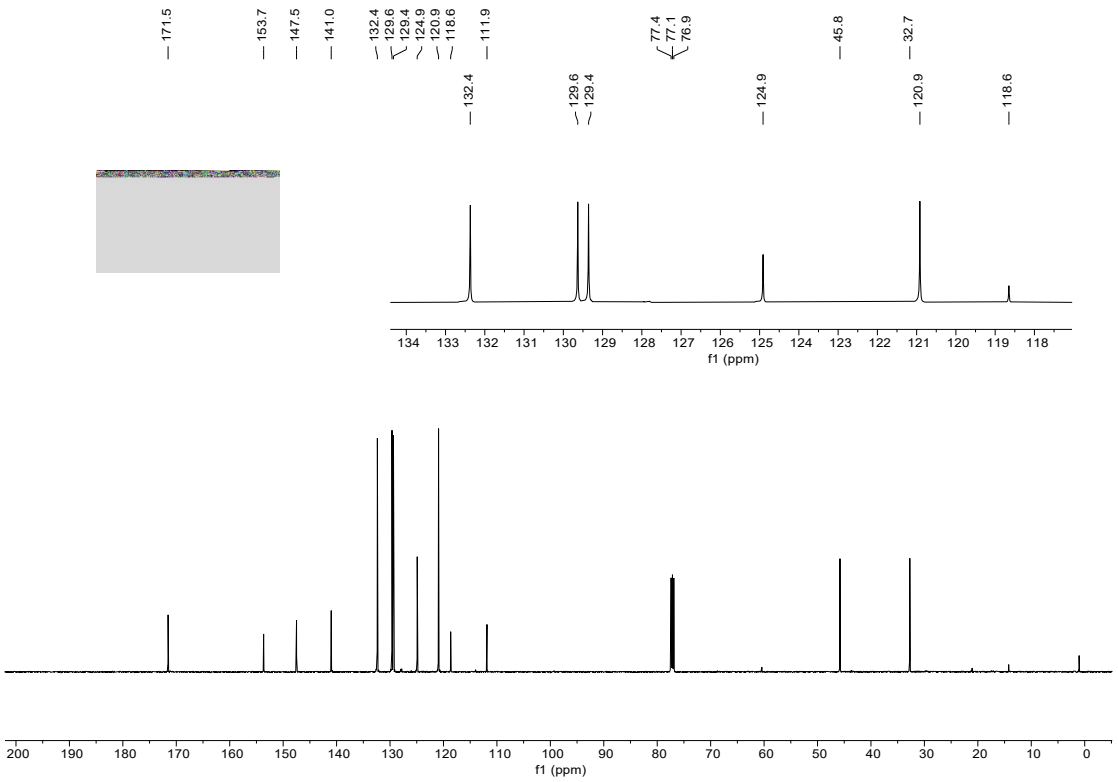
^{1}H NMR of **4f** in $CDCl_3$ (500 MHz)



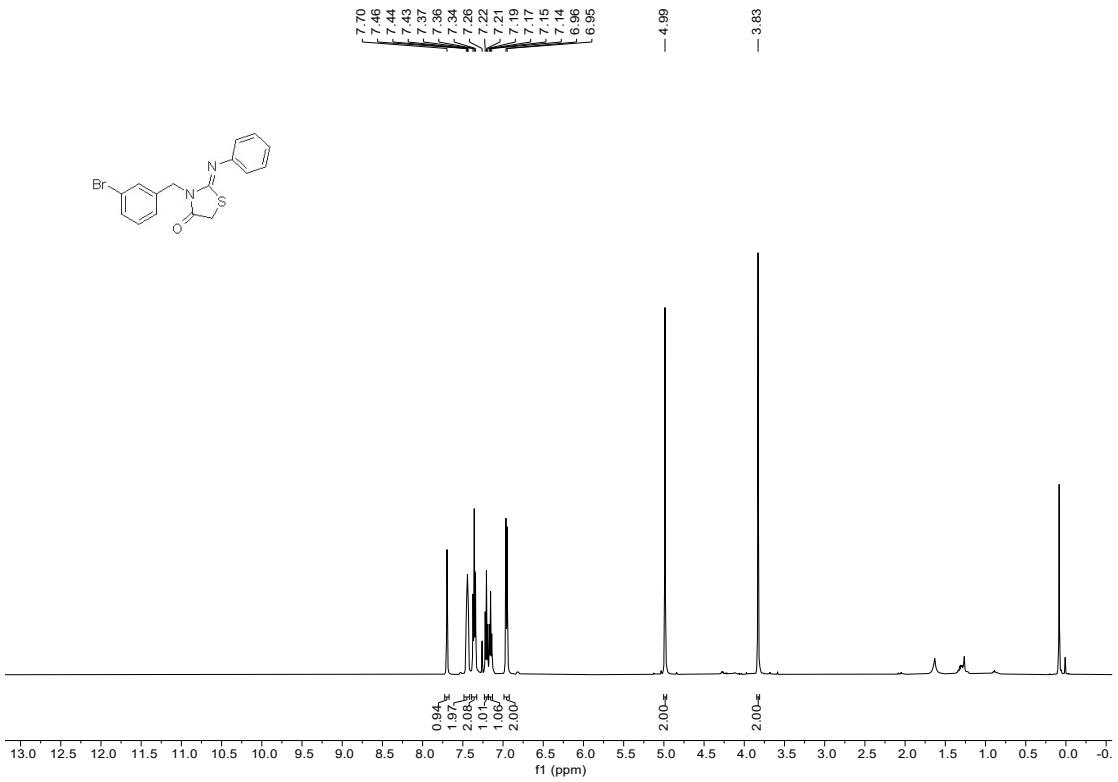
$^{13}C\{^{1}H\}$ NMR of **4f** in $CDCl_3$ (126 MHz)



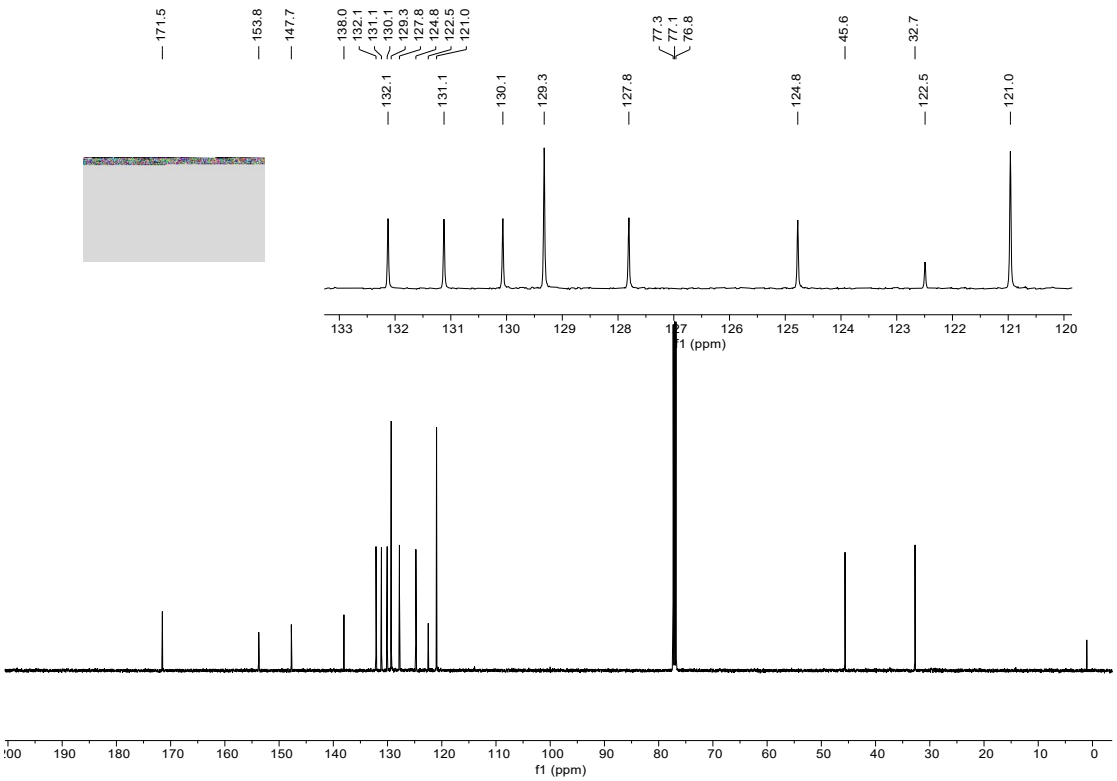
^{1}H NMR of **4g** in $CDCl_3$ (500 MHz)



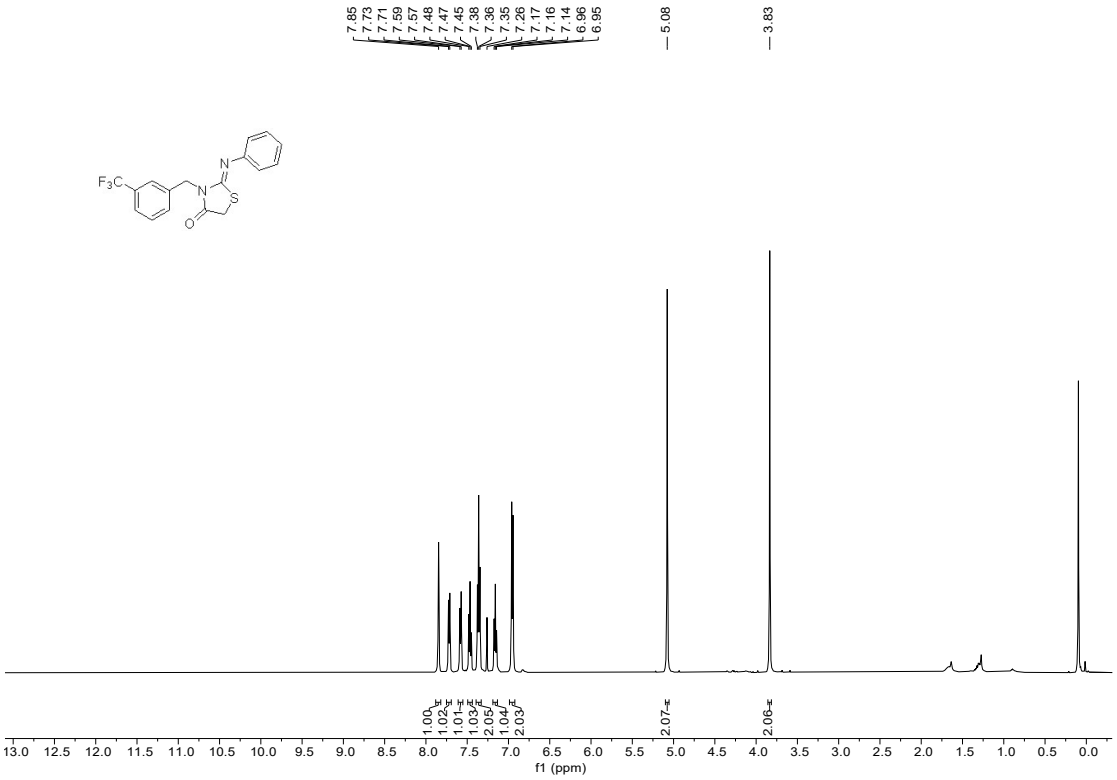
$^{13}C\{^{1}H\}$ NMR of **4g** in $CDCl_3$ (126 MHz)



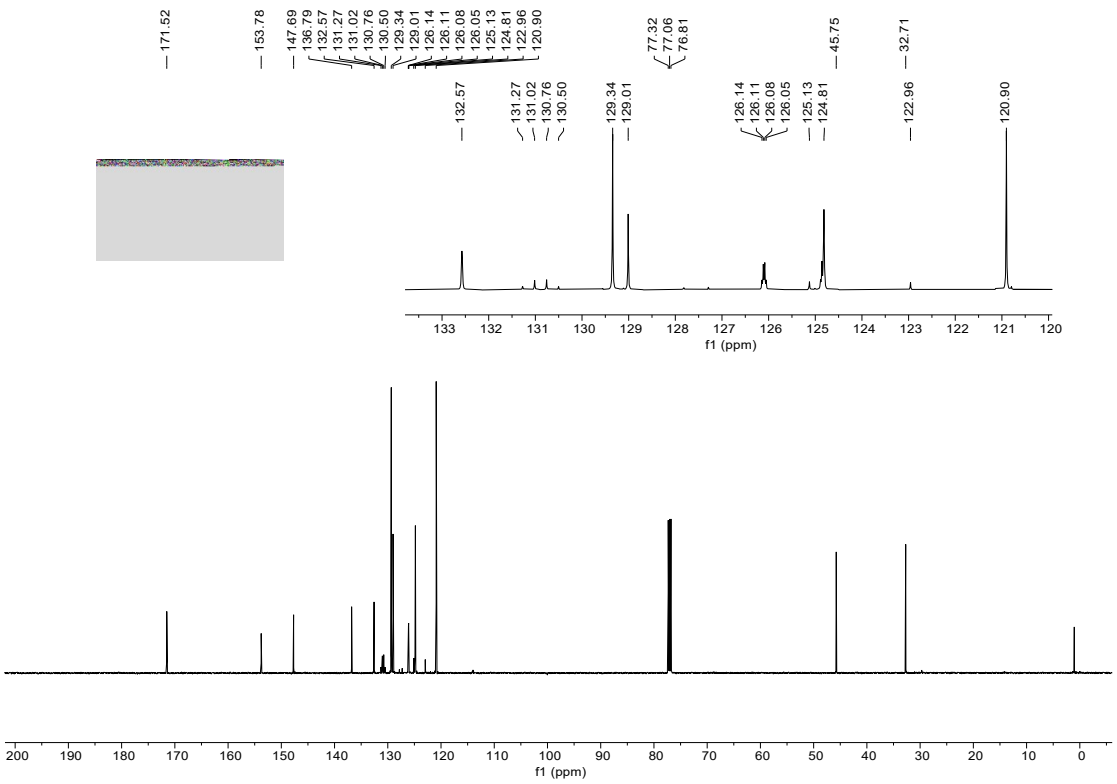
^{1}H NMR of **4h** in $CDCl_3$ (500 MHz)



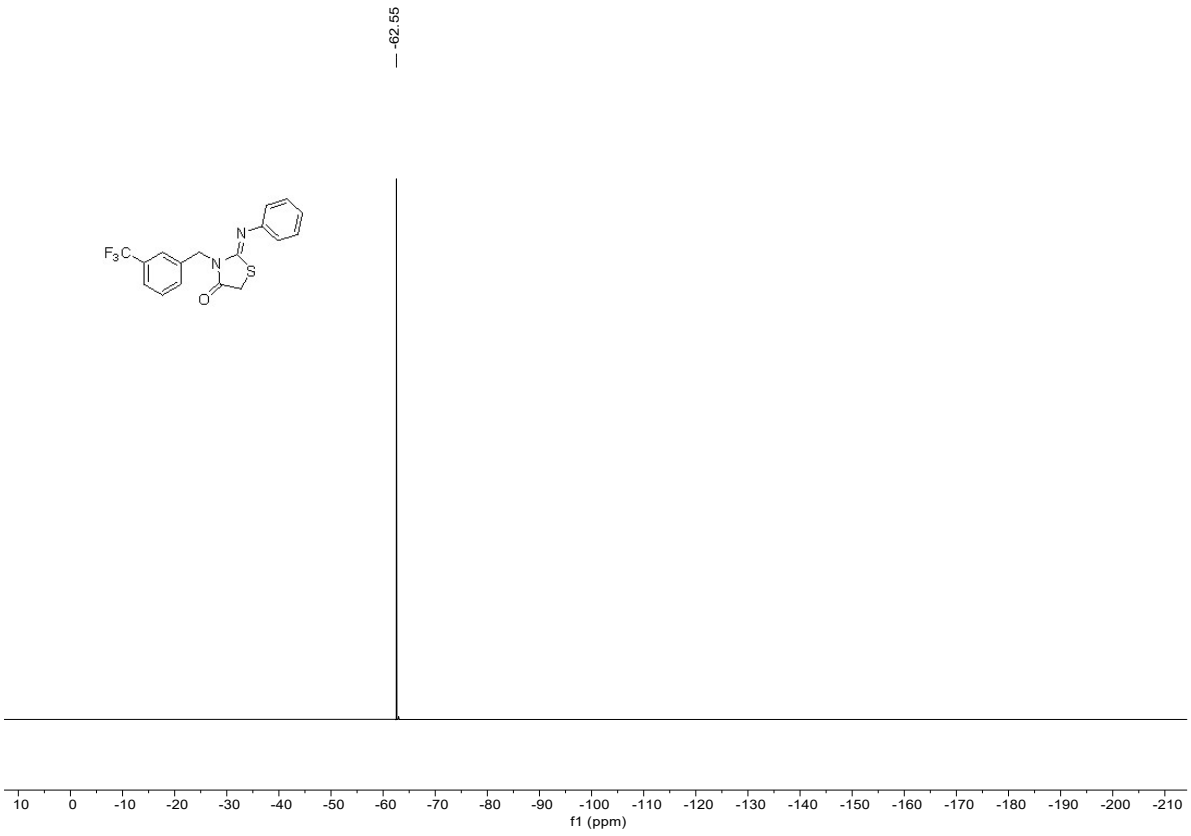
$^{13}C\{^{1}H\}$ NMR of **4h** in $CDCl_3$ (126 MHz)



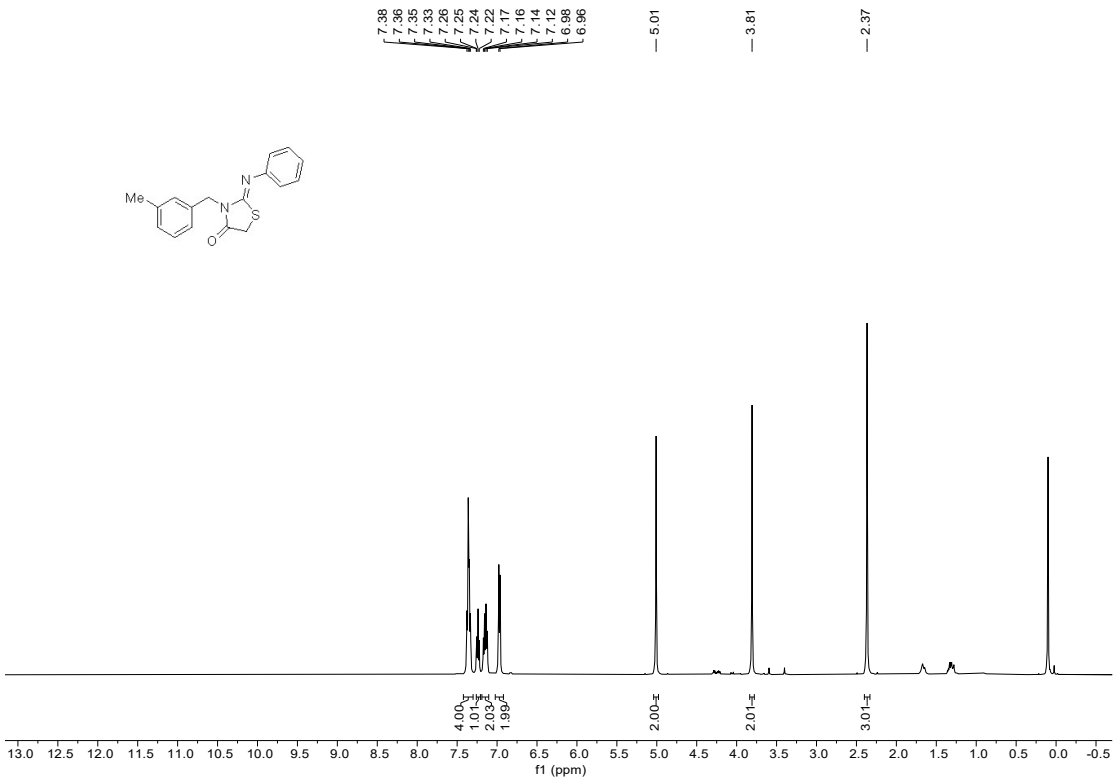
^{1}H NMR of **4i** in $CDCl_3$ (500 MHz)



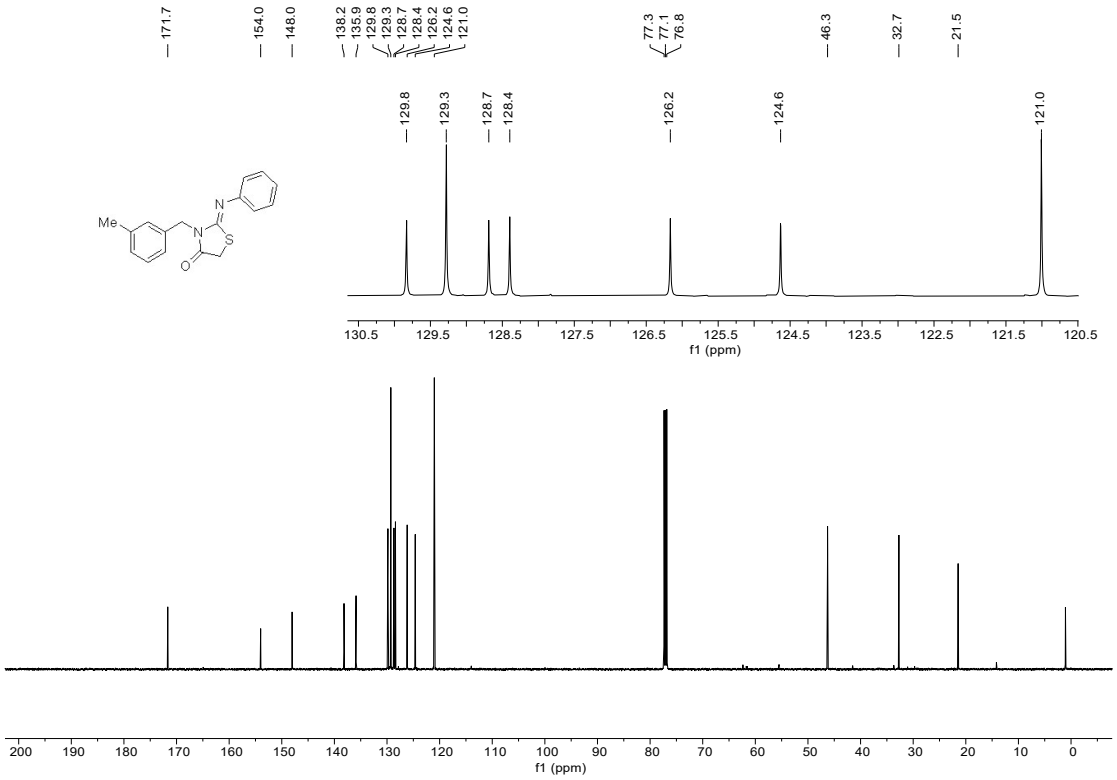
$^{13}C\{^{1}H\}$ NMR of **4i** in $CDCl_3$ (126 MHz)



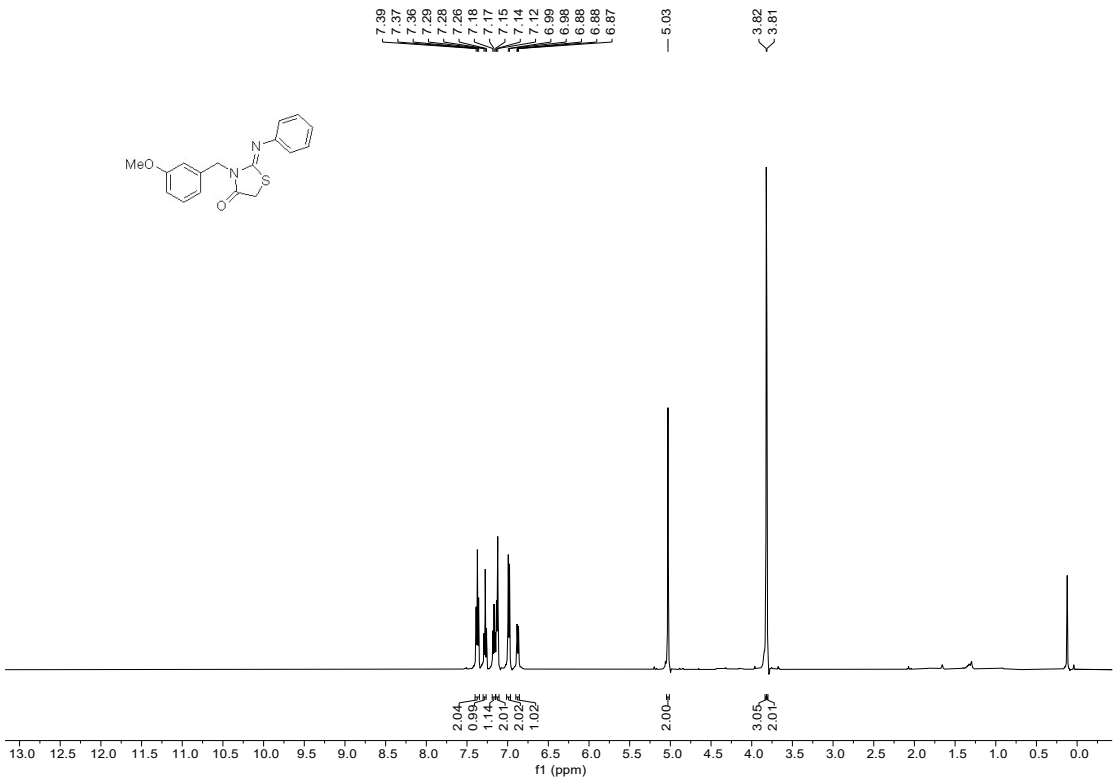
^{19}F NMR of **4i** in $CDCl_3$ (471 MHz)



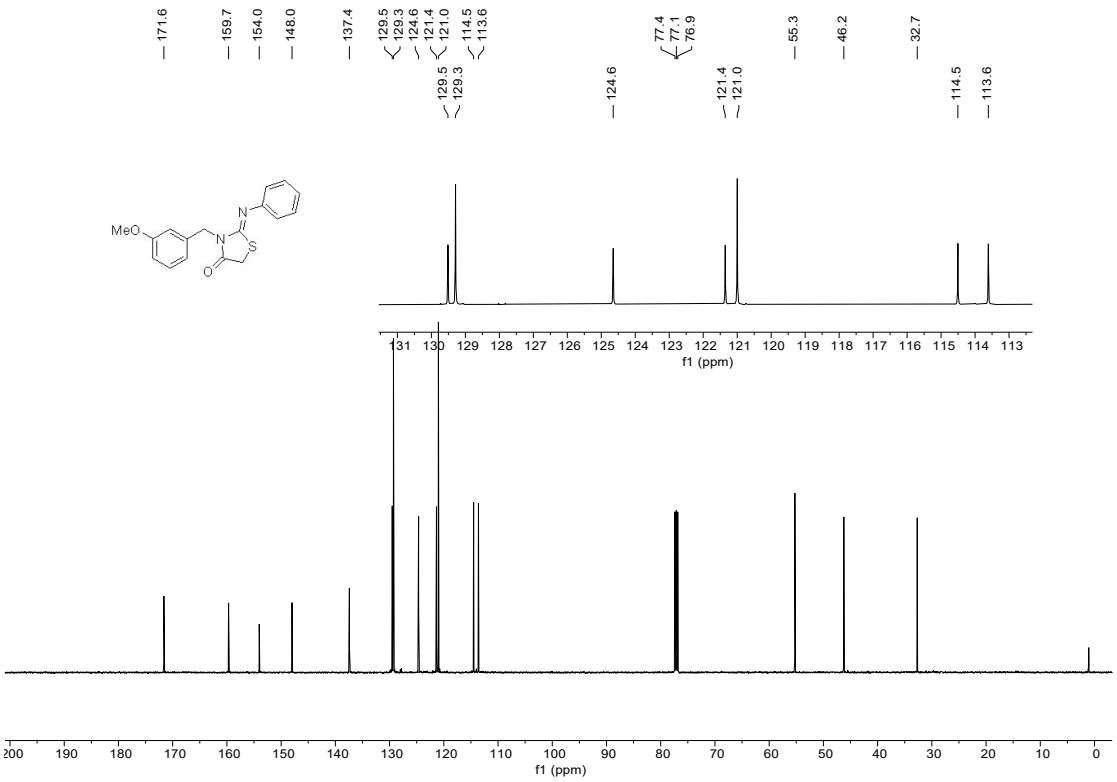
^{1}H NMR of **4j** in $CDCl_3$ (500 MHz)



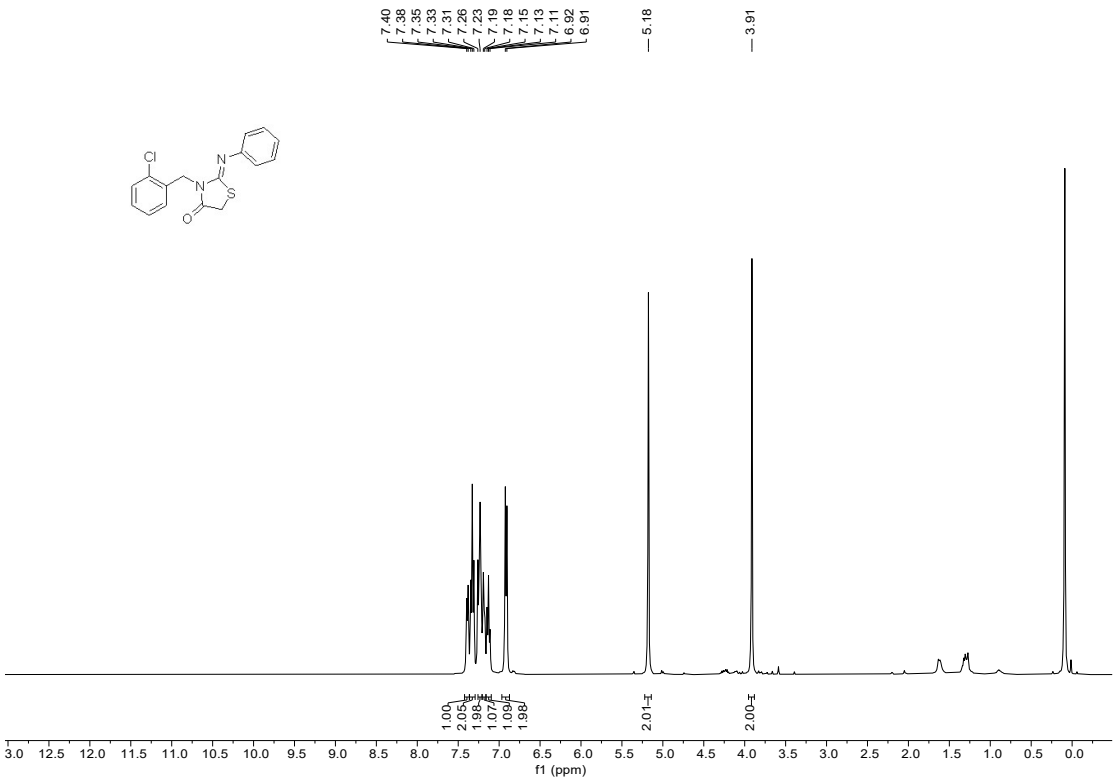
^{13}C{^{1}H} NMR of **4j** in $CDCl_3$ (126 MHz)



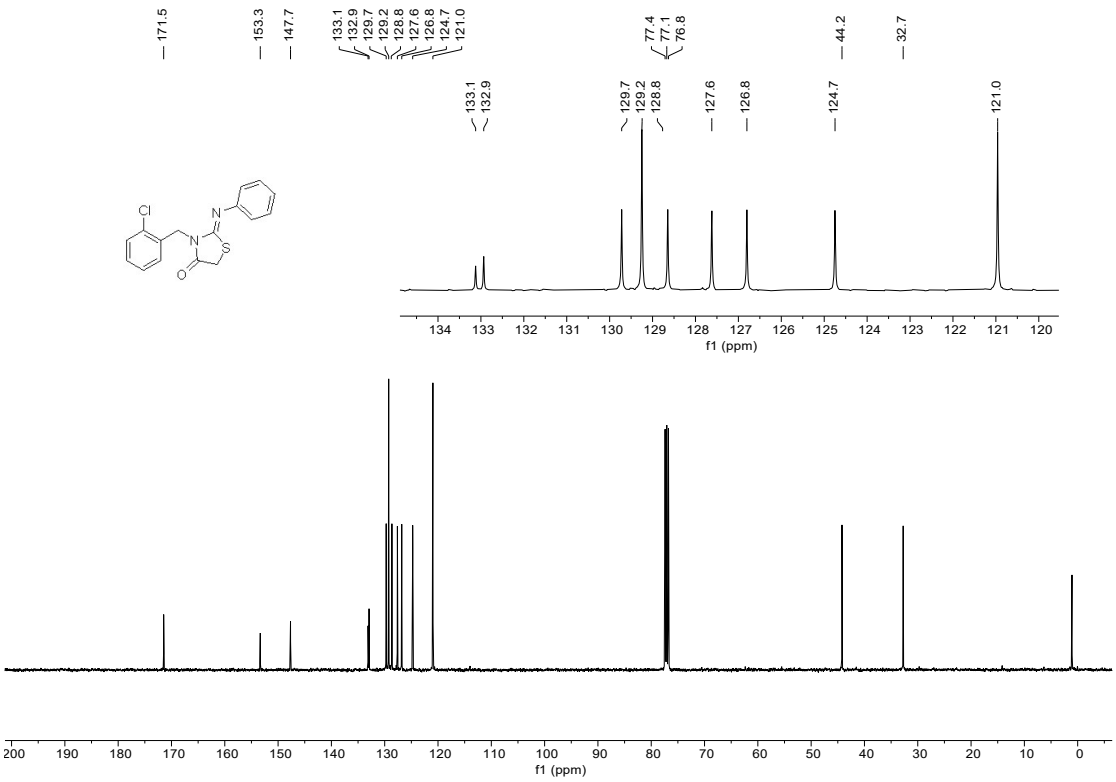
^{1}H NMR of **4k** in $CDCl_3$ (500 MHz)



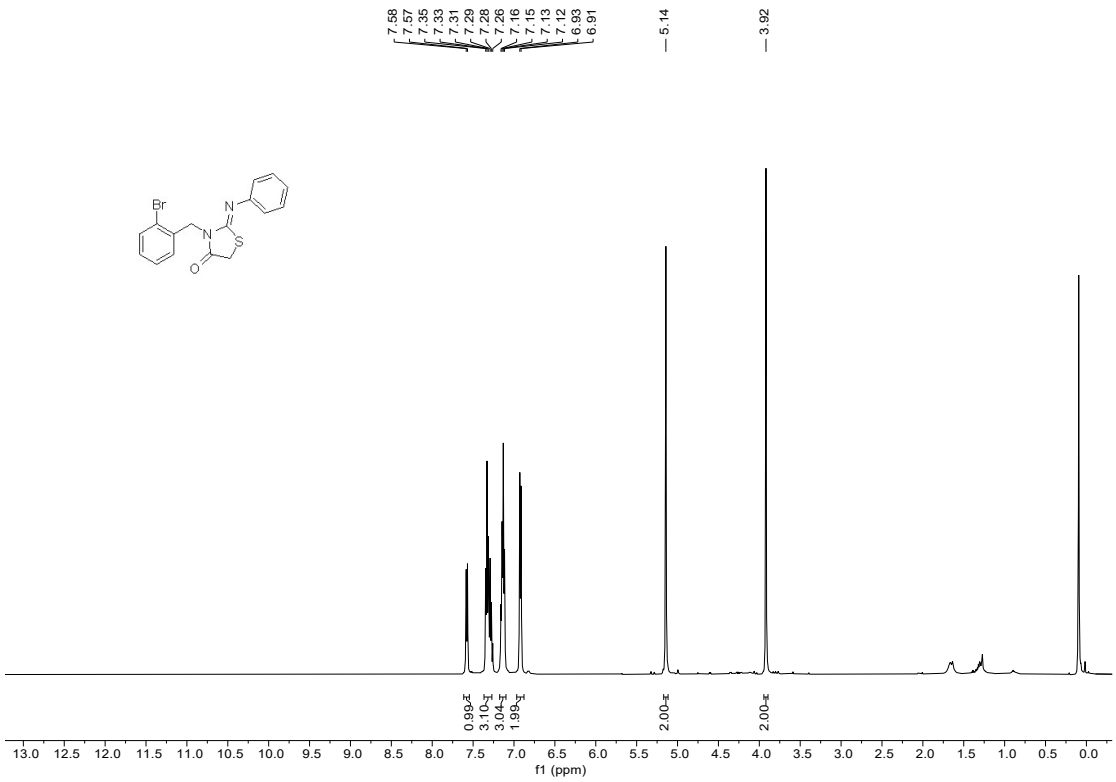
^{13}C{^{1}H} NMR of **4k** in $CDCl_3$ (126 MHz)



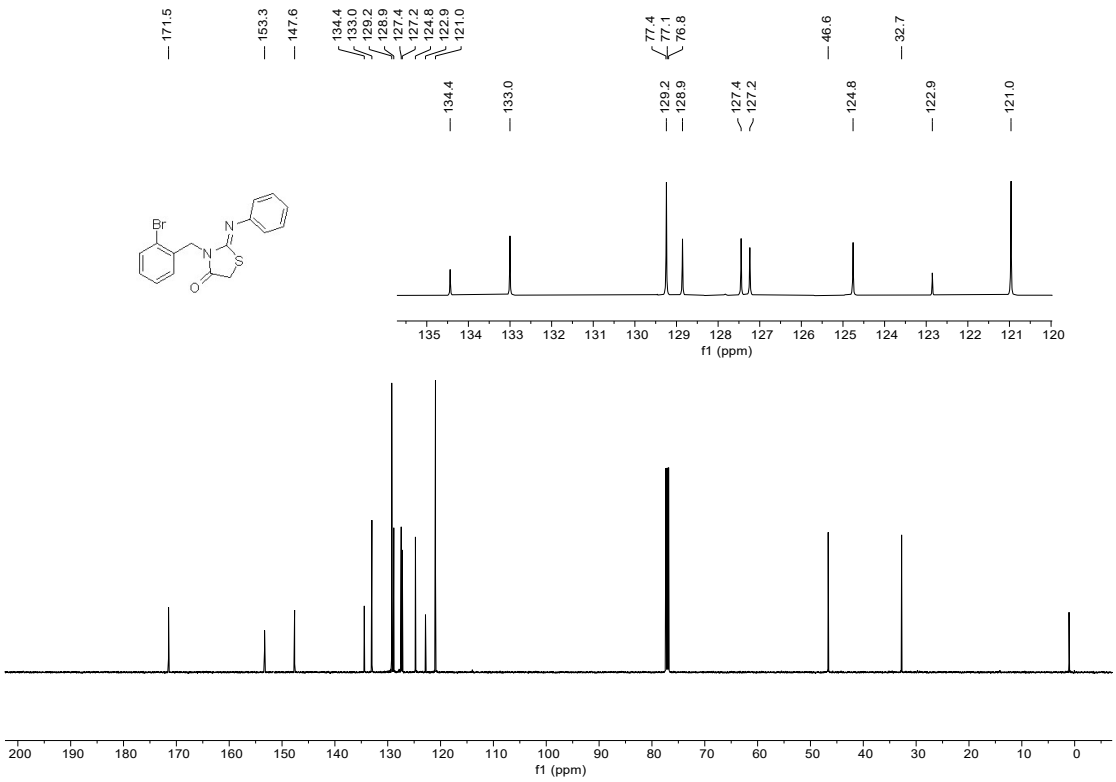
^{1}H NMR of **4l** in $CDCl_3$ (500 MHz)



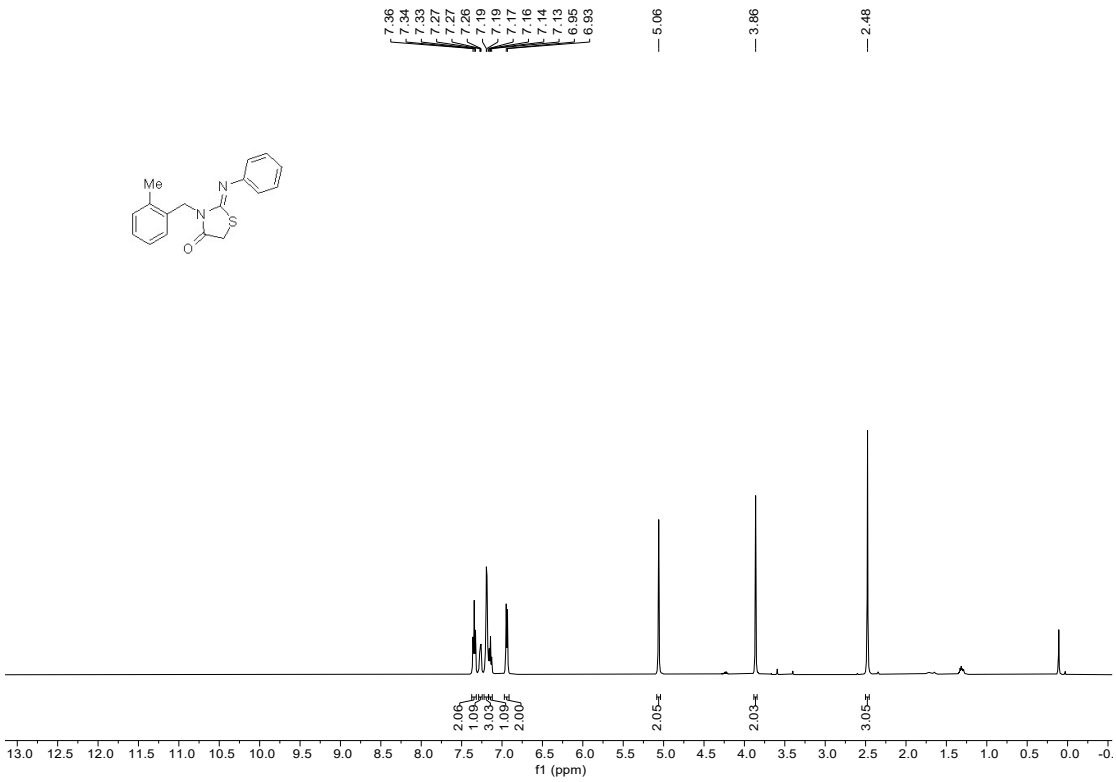
^{13}C{^{1}H} NMR of **4l** in $CDCl_3$ (126 MHz)



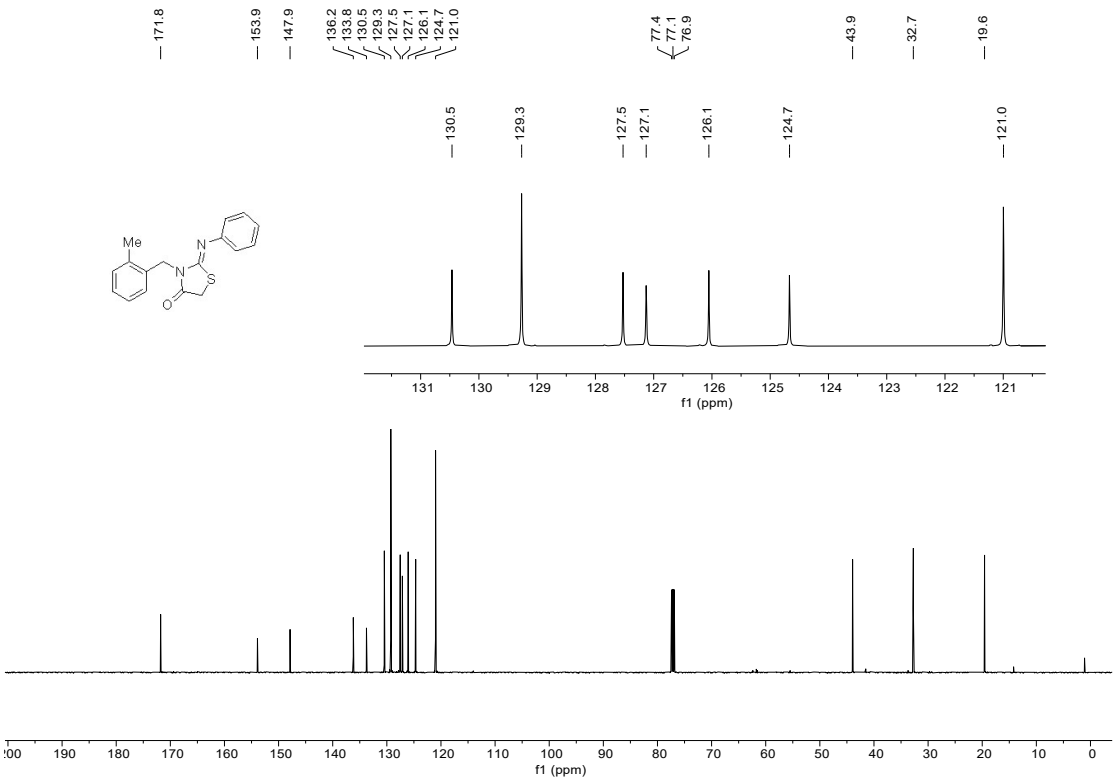
^{1}H NMR of **4m** in $CDCl_3$ (500 MHz)



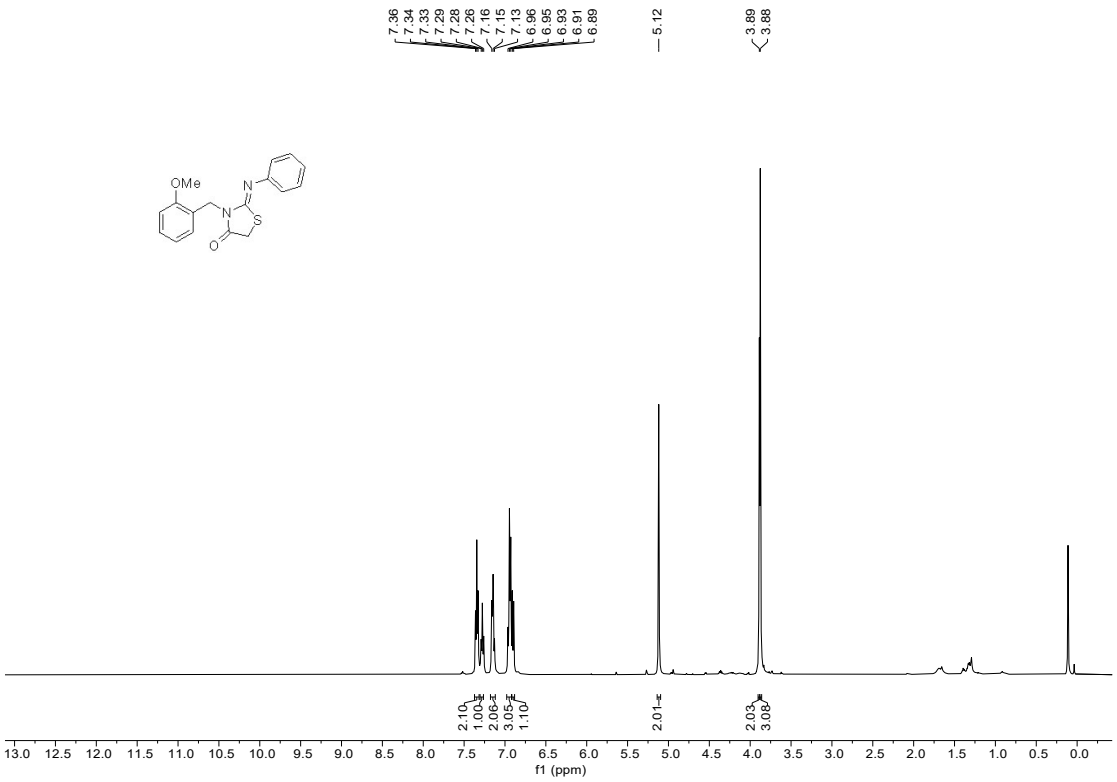
^{13}C{^{1}H} NMR of **4m** in $CDCl_3$ (126 MHz)



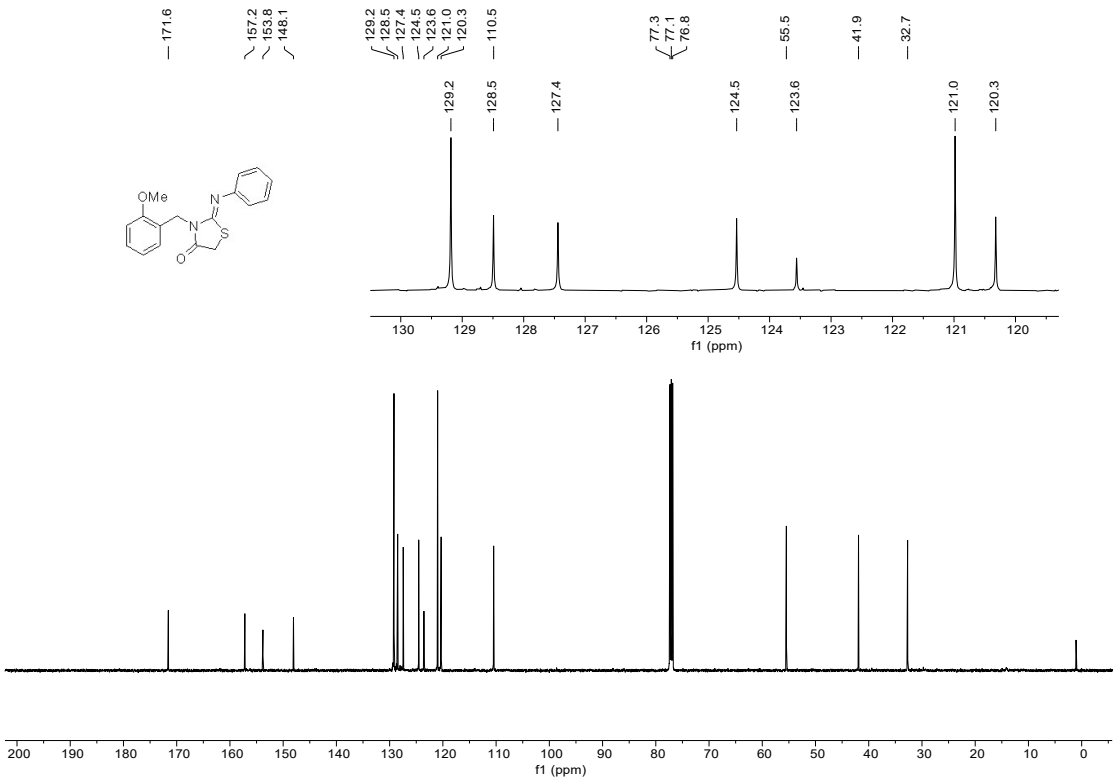
^{1}H NMR of **4n** in $CDCl_3$ (500 MHz)



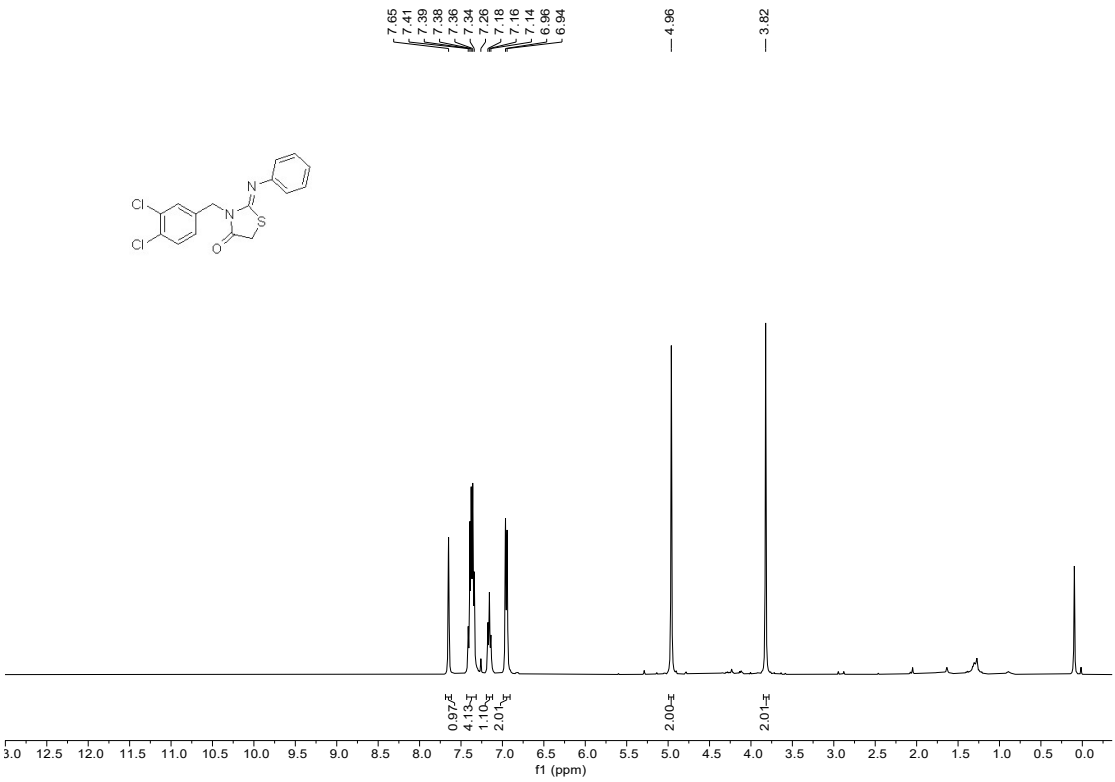
^{13}C{^{1}H} NMR of **4n** in $CDCl_3$ (126 MHz)



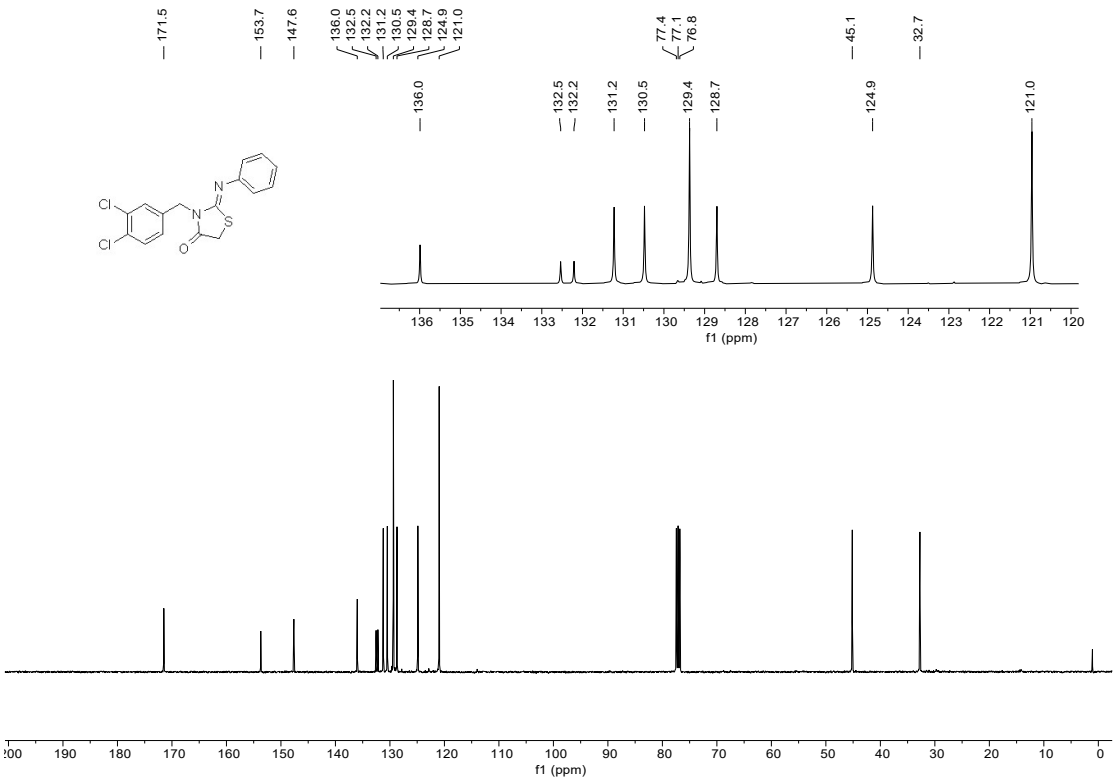
^{1}H NMR of **4o** in $CDCl_3$ (500 MHz)



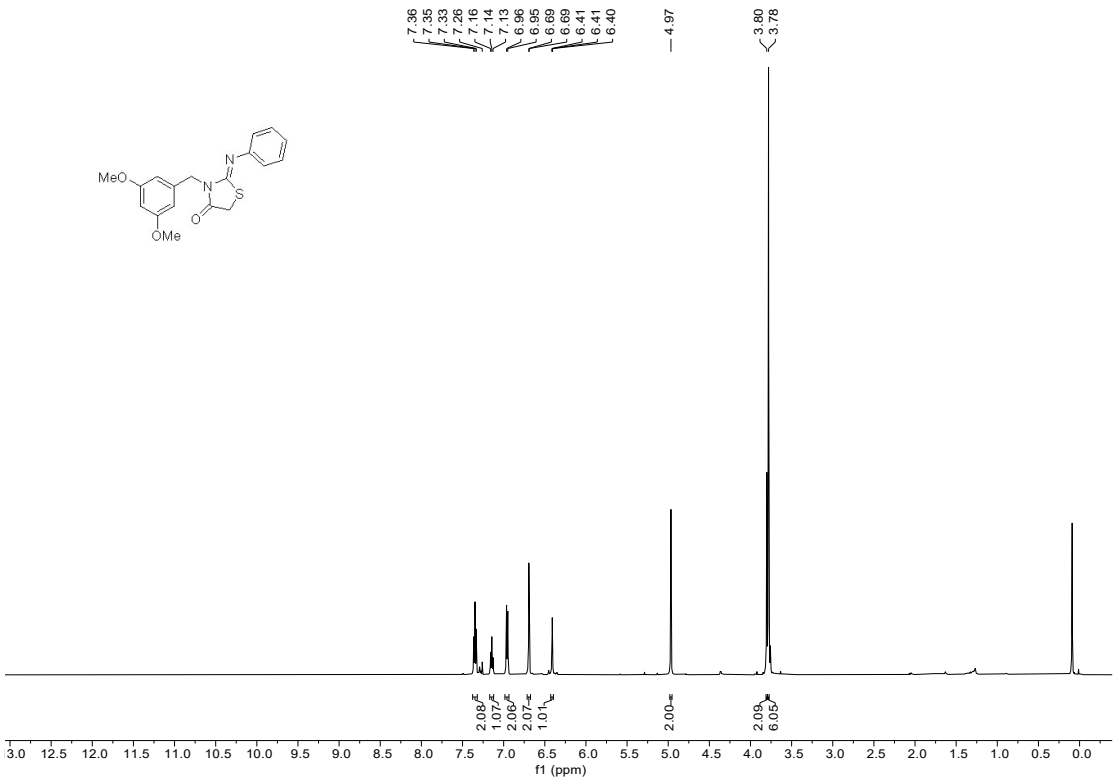
$^{13}C\{^{1}H\}$ NMR of **4o** in $CDCl_3$ (126 MHz)



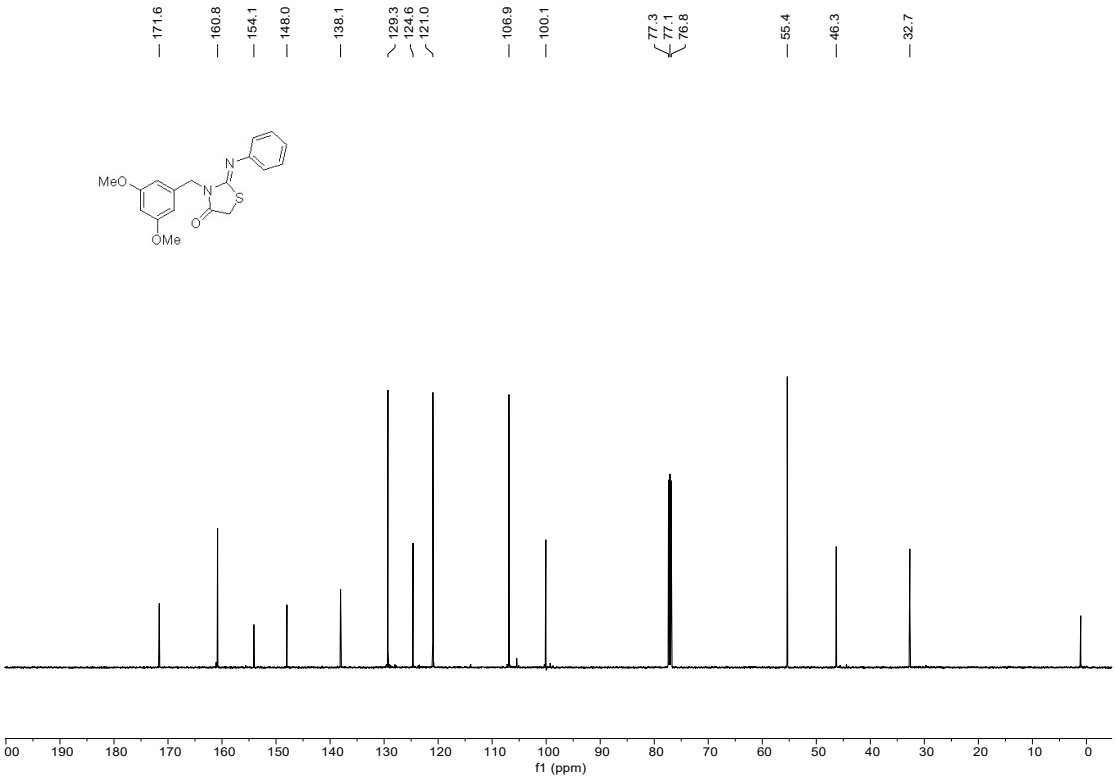
^{1}H NMR of **4p** in $CDCl_3$ (500 MHz)



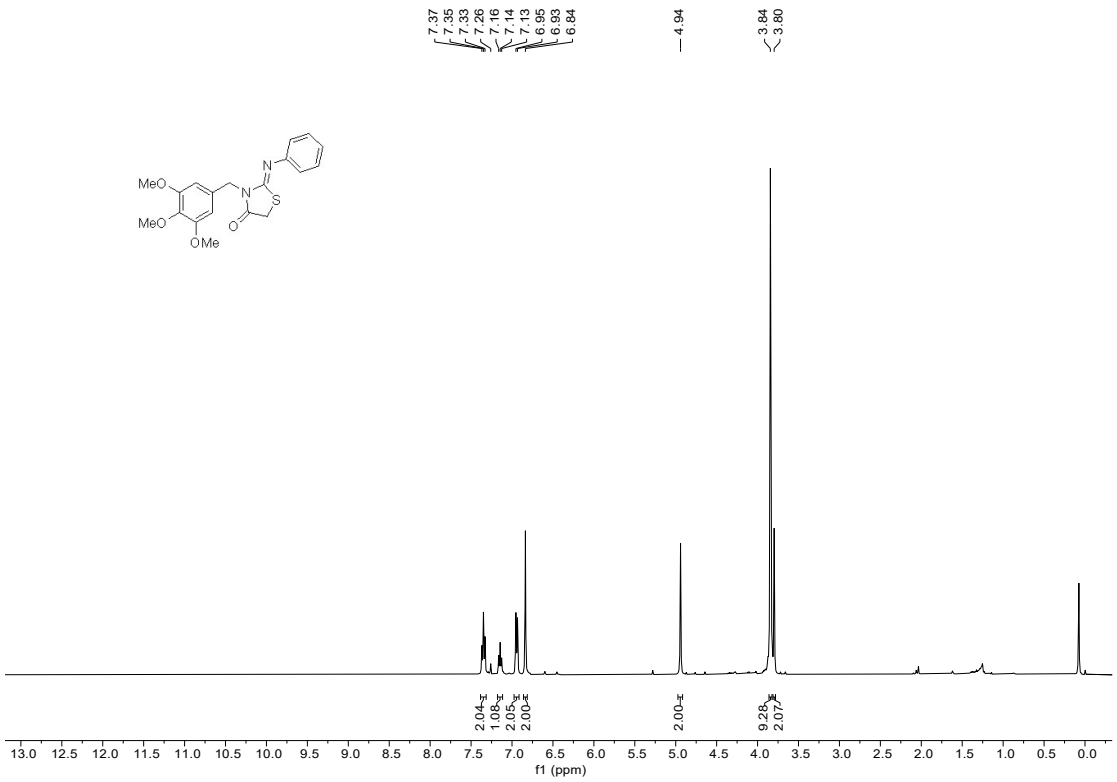
^{13}C{^{1}H} NMR of **4p** in $CDCl_3$ (126 MHz)



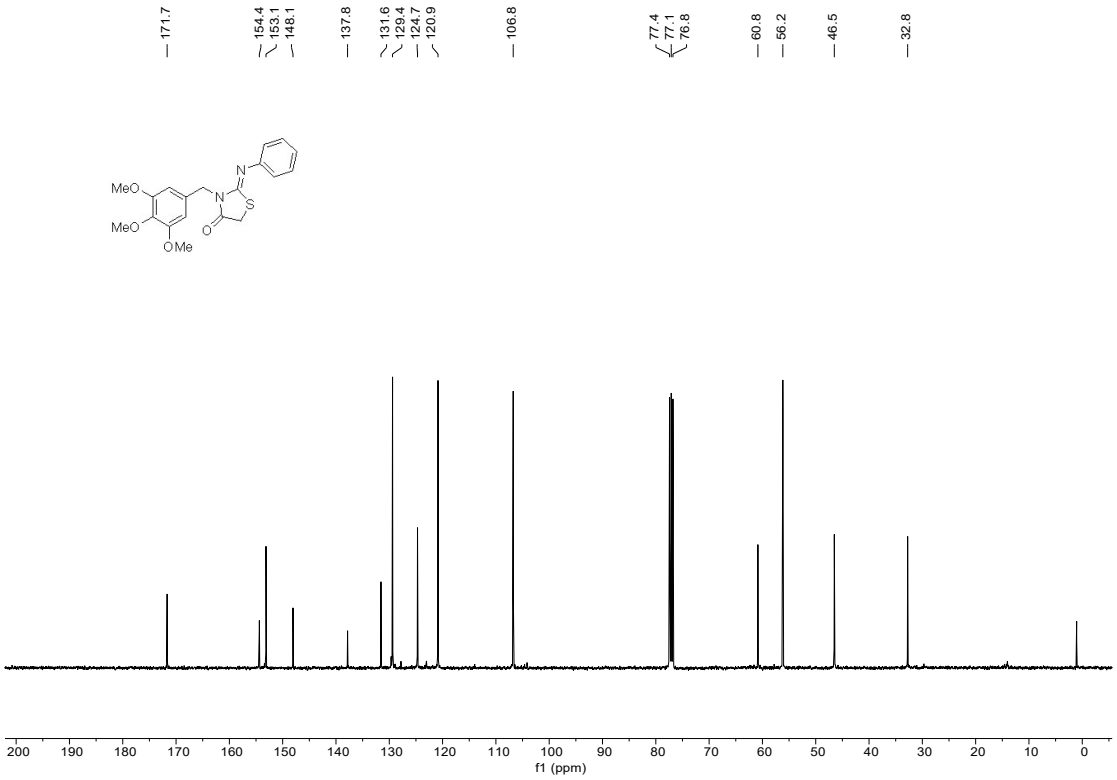
^{1}H NMR of **4q** in $CDCl_3$ (500 MHz)



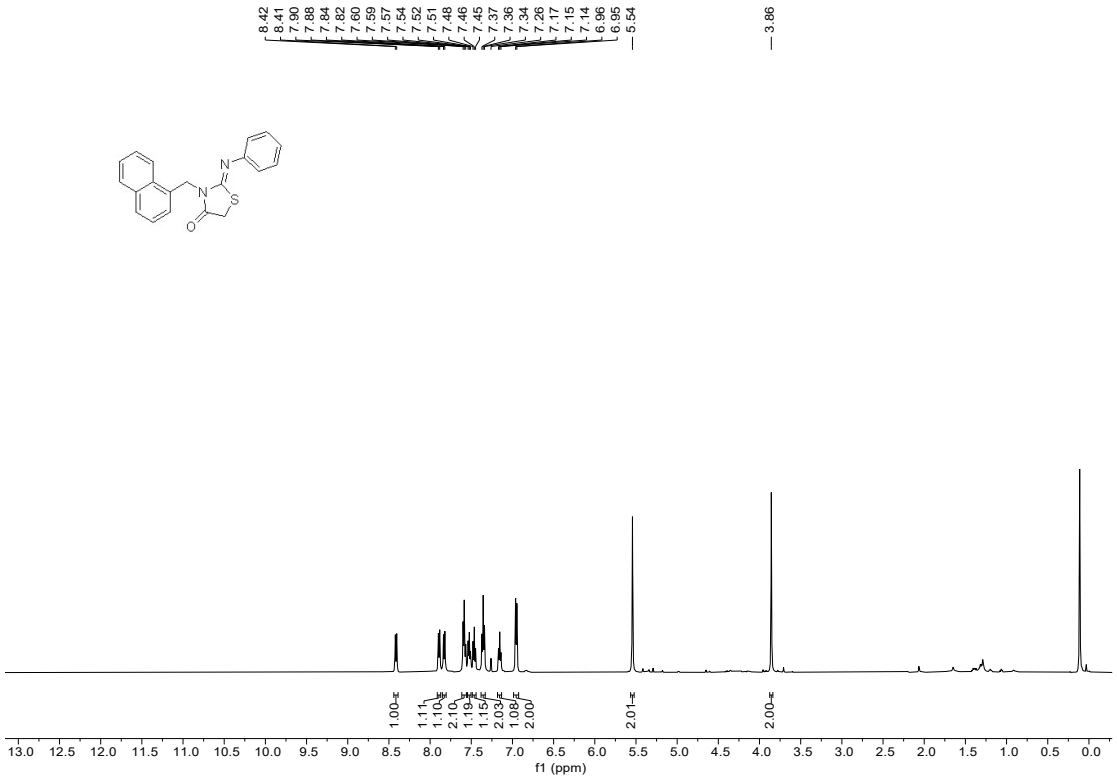
^{13}C{^{1}H} NMR of **4q** in $CDCl_3$ (126 MHz)



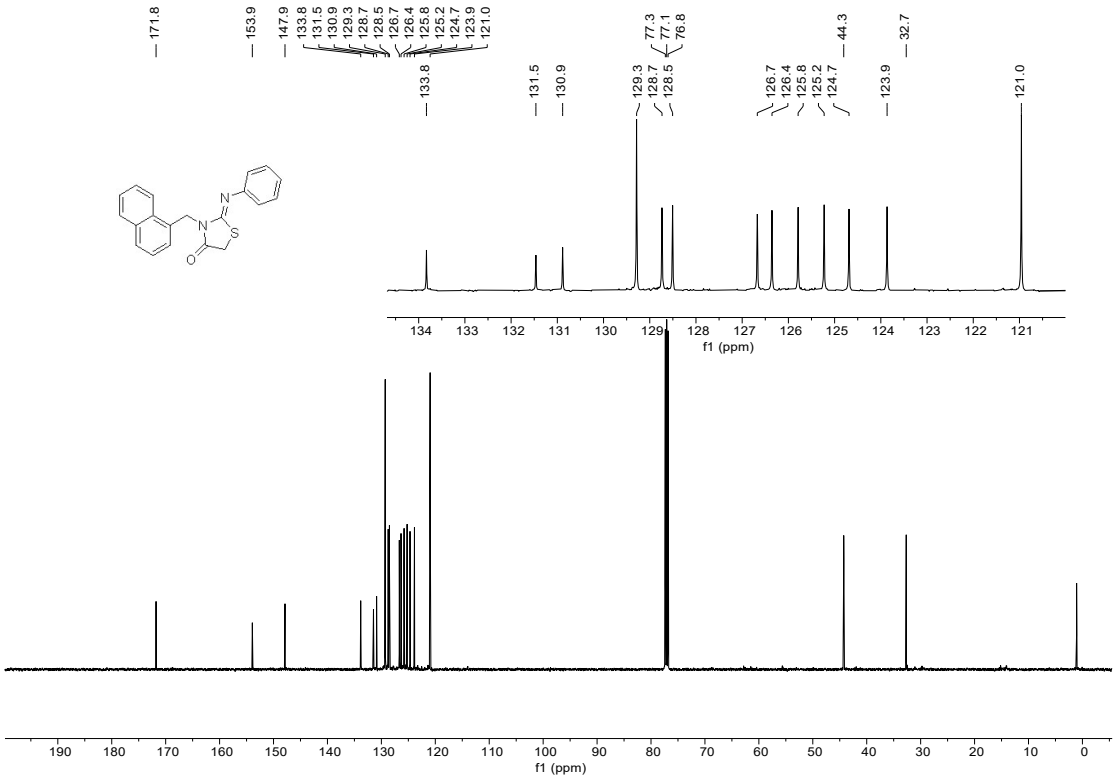
^{1}H NMR of **4r** in $CDCl_3$ (500 MHz)



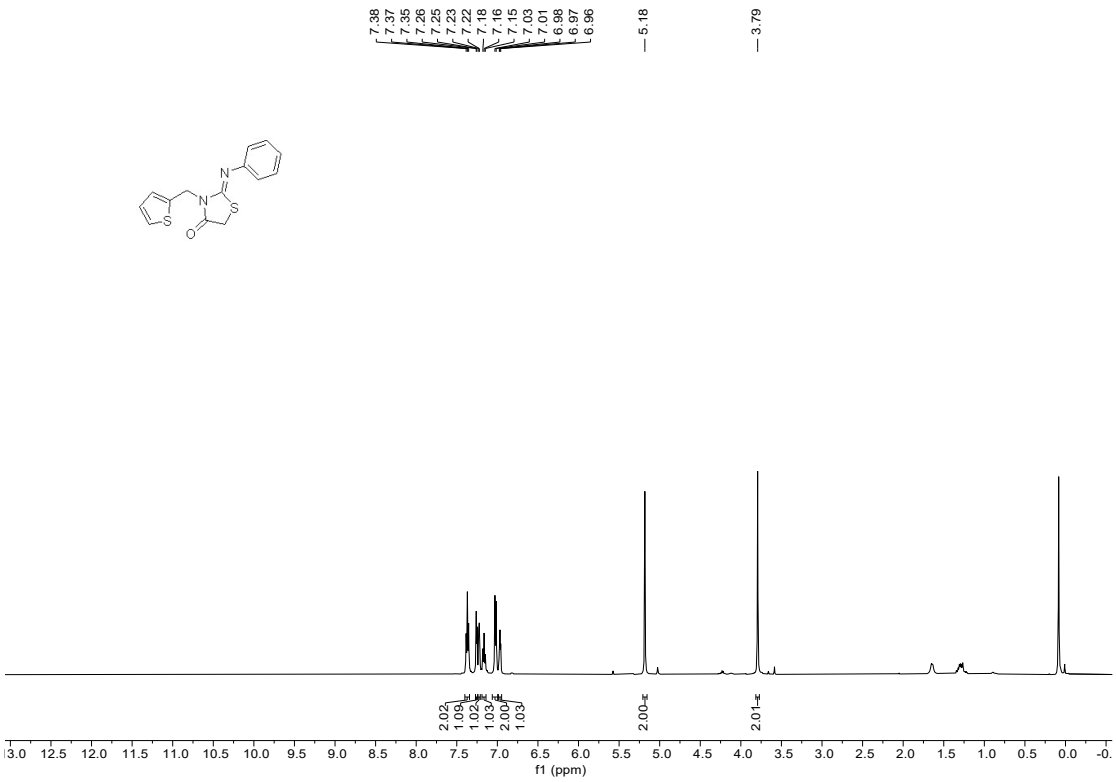
^{13}C{^{1}H} NMR of **4r** in $CDCl_3$ (126 MHz)



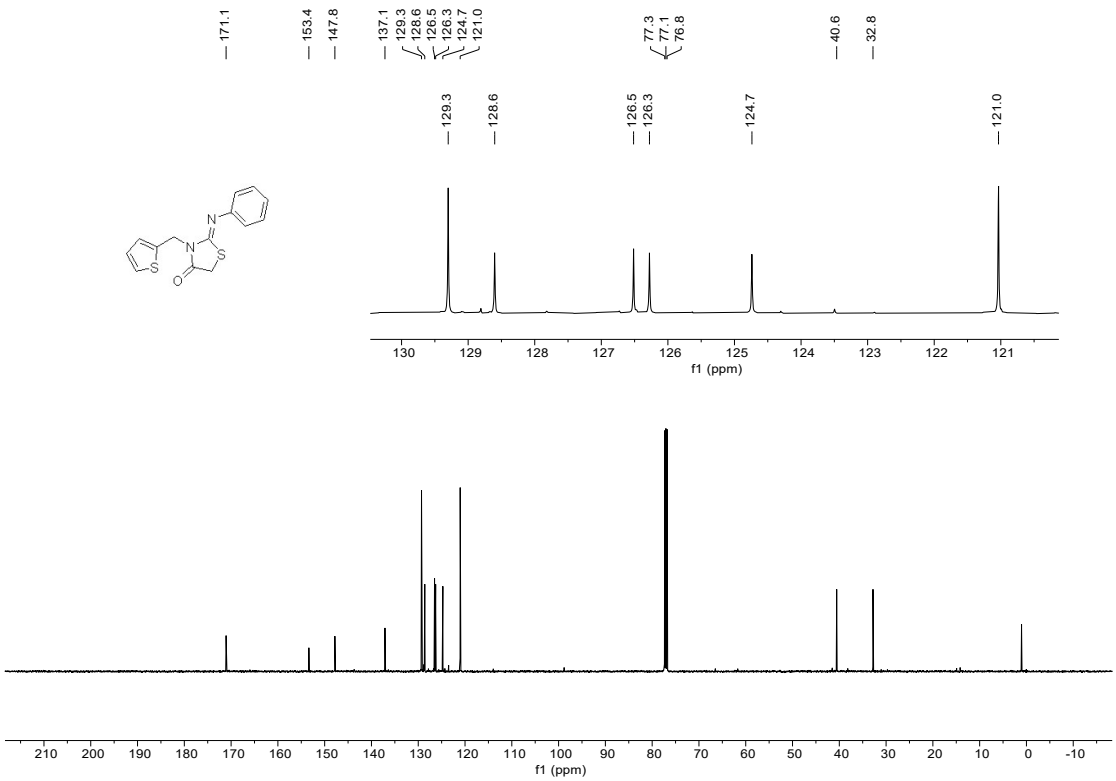
^{1}H NMR of **4s** in $CDCl_3$ (500 MHz)



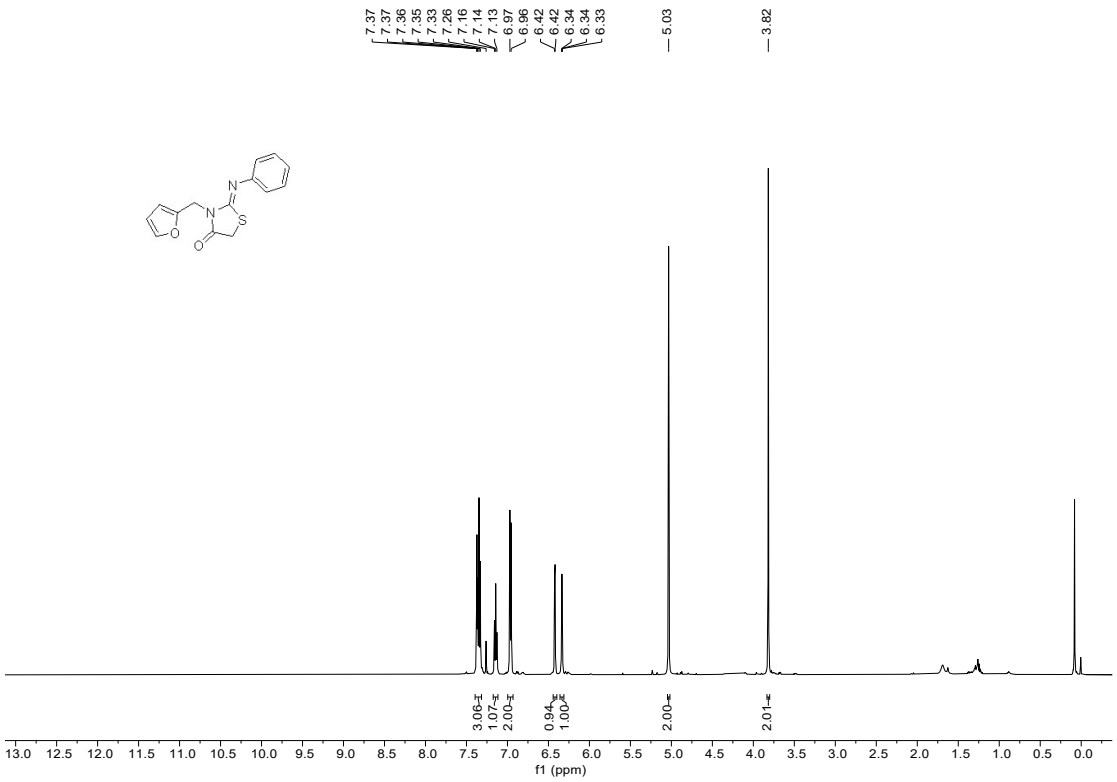
^{13}C{^{1}H} NMR of **4s** in $CDCl_3$ (126 MHz)



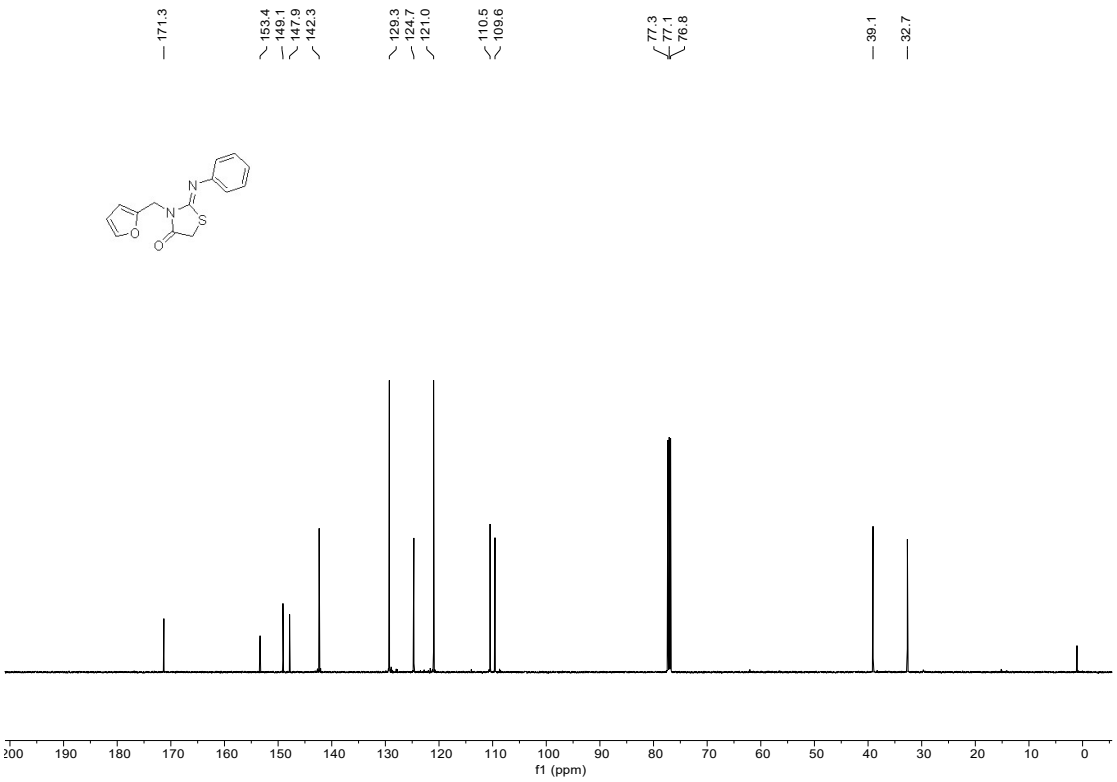
^{1}H NMR of **4t** in $CDCl_3$ (500 MHz)



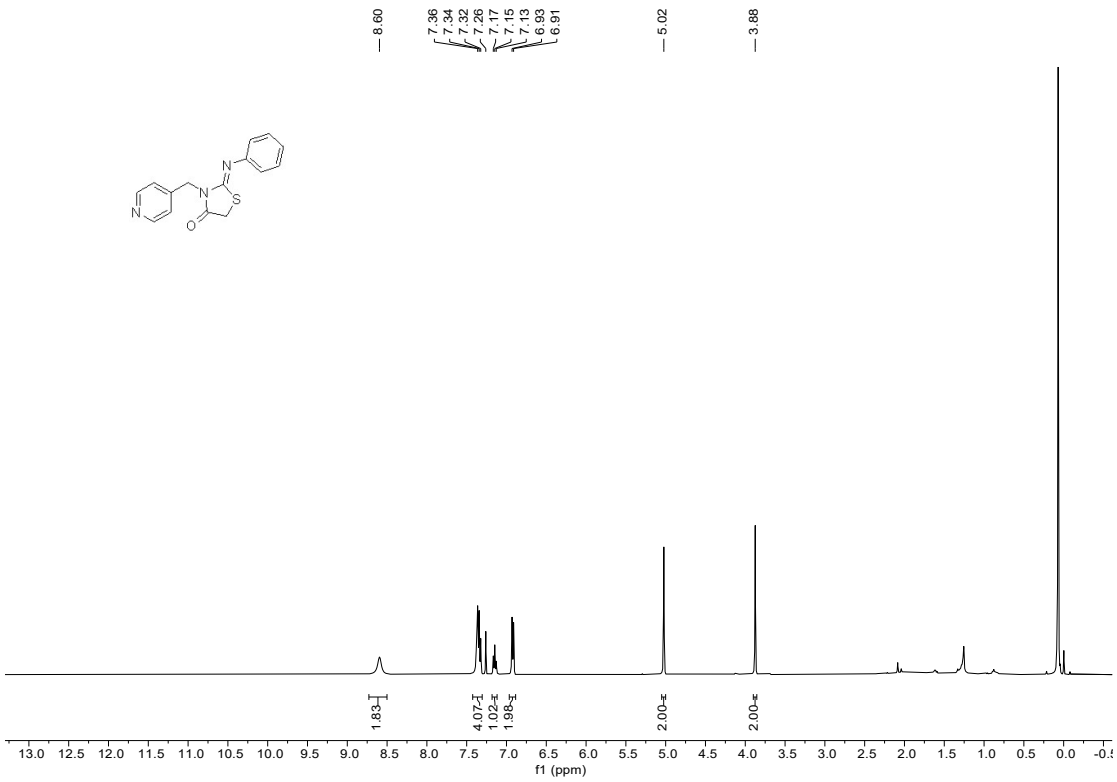
^{13}C{^{1}H} NMR of **4t** in $CDCl_3$ (126 MHz)



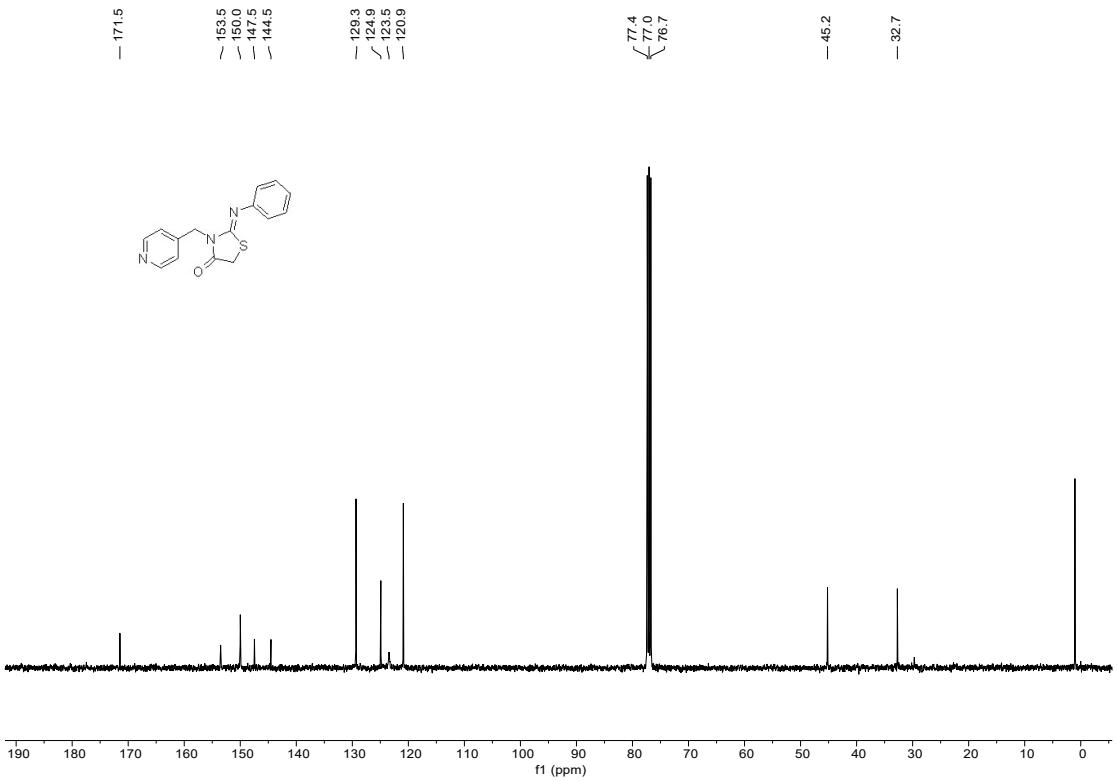
^{1}H NMR of **4u** in $CDCl_3$ (500 MHz)



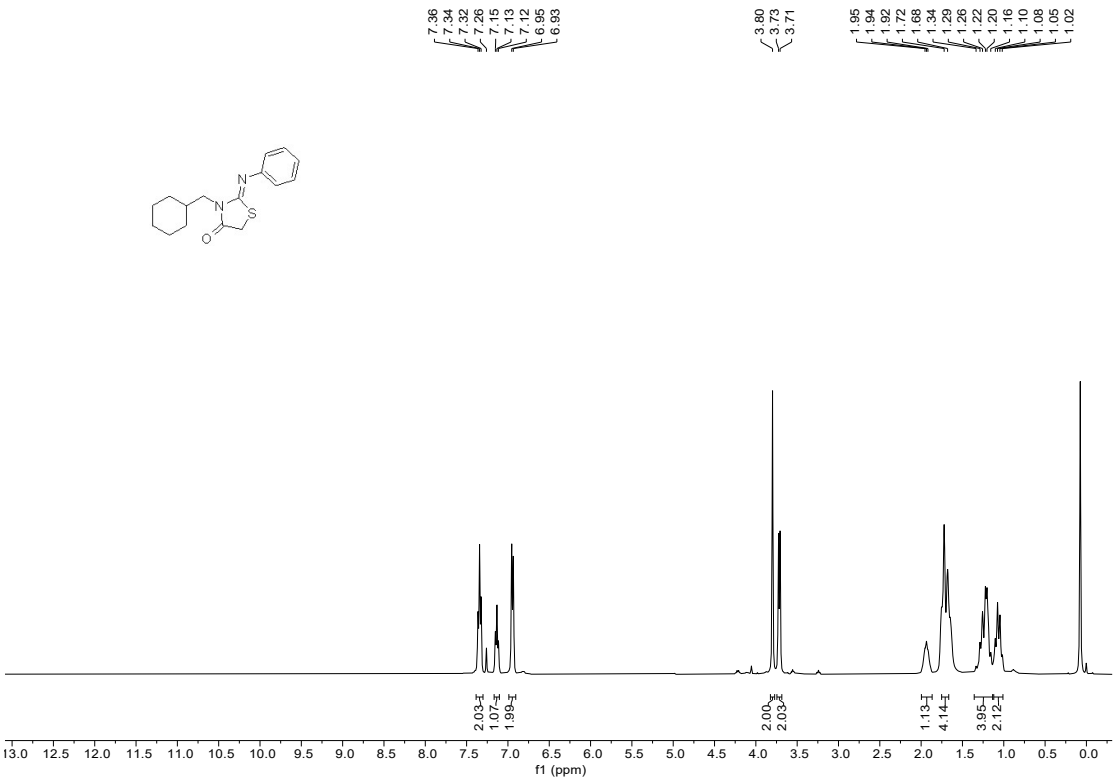
^{13}C{^{1}H} NMR of **4u** in $CDCl_3$ (126 MHz)



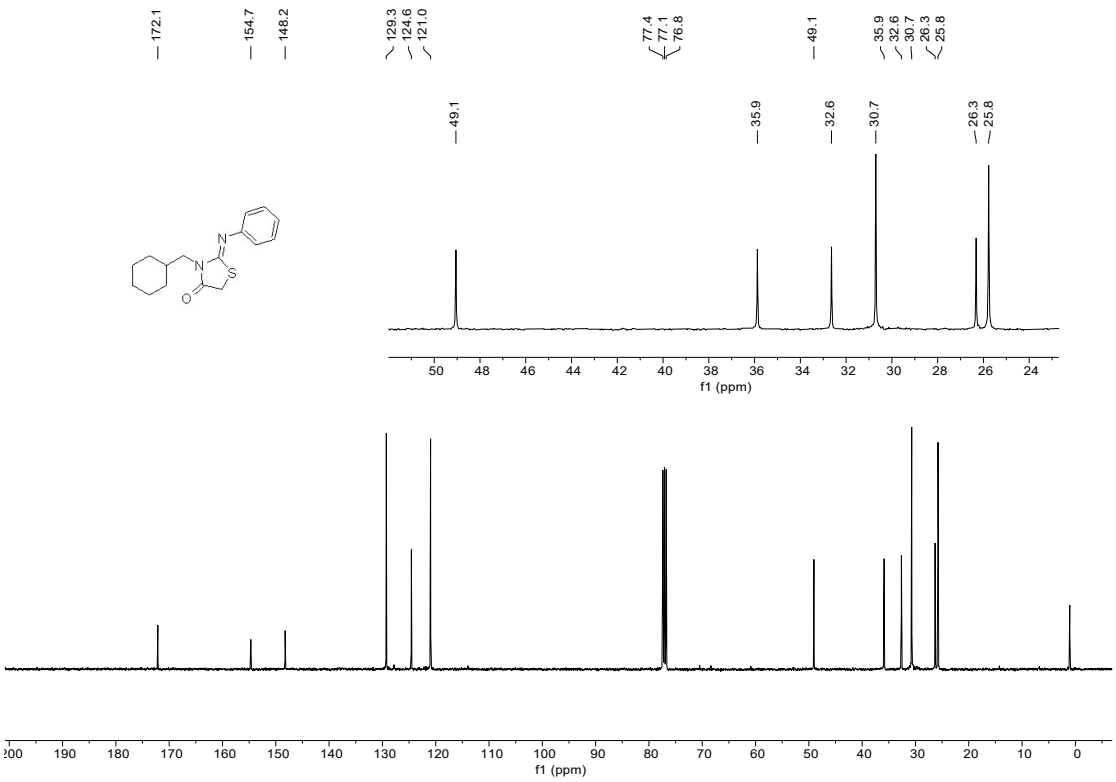
^{1}H NMR of **4v** in $CDCl_3$ (400 MHz)



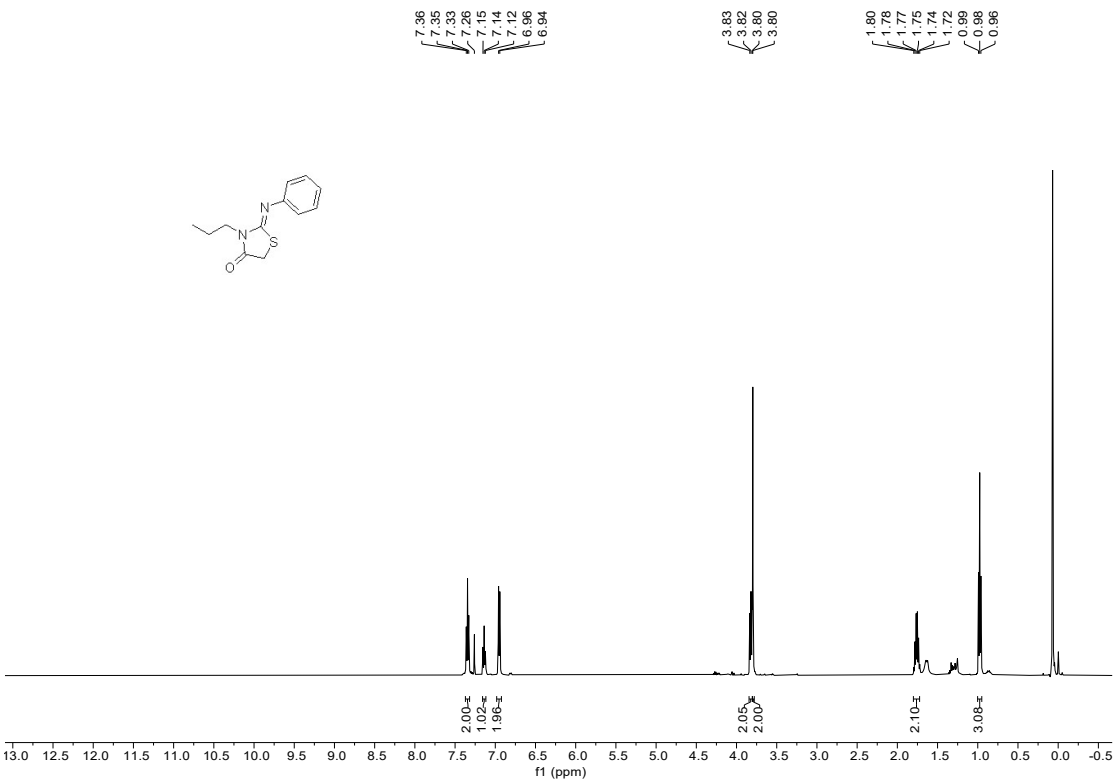
^{13}C{^{1}H} NMR of **4v** in $CDCl_3$ (100 MHz)



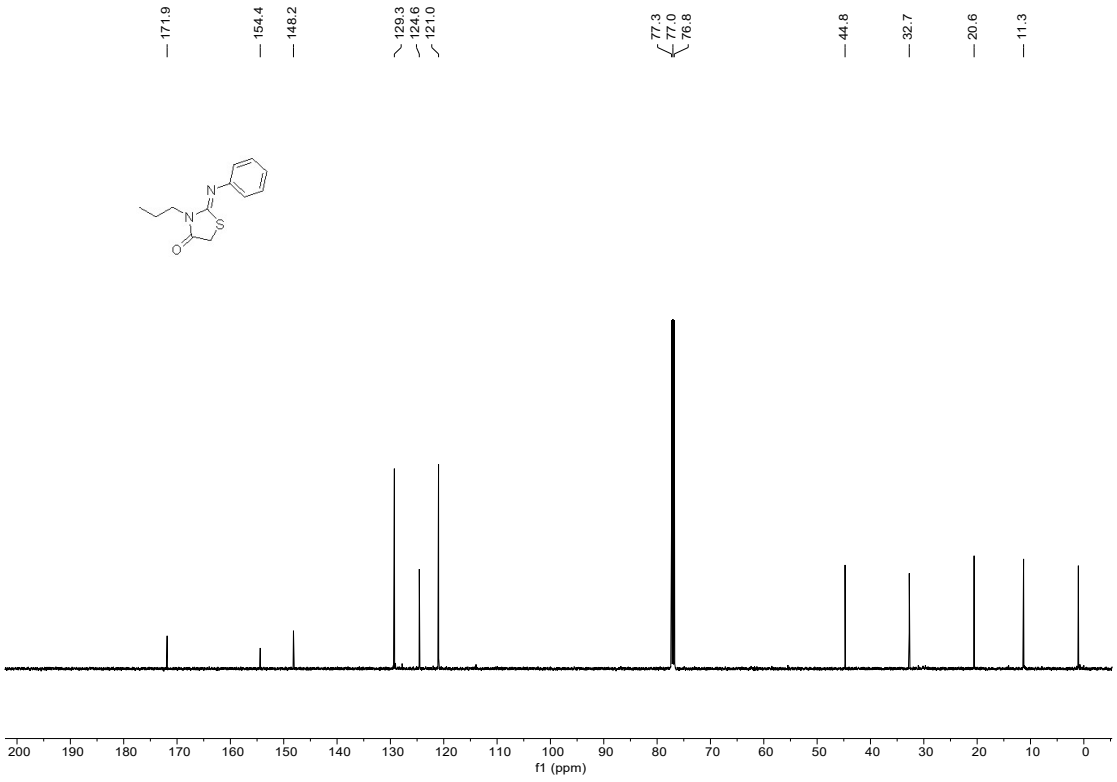
^{1}H NMR of **4w** in $CDCl_3$ (400 MHz)



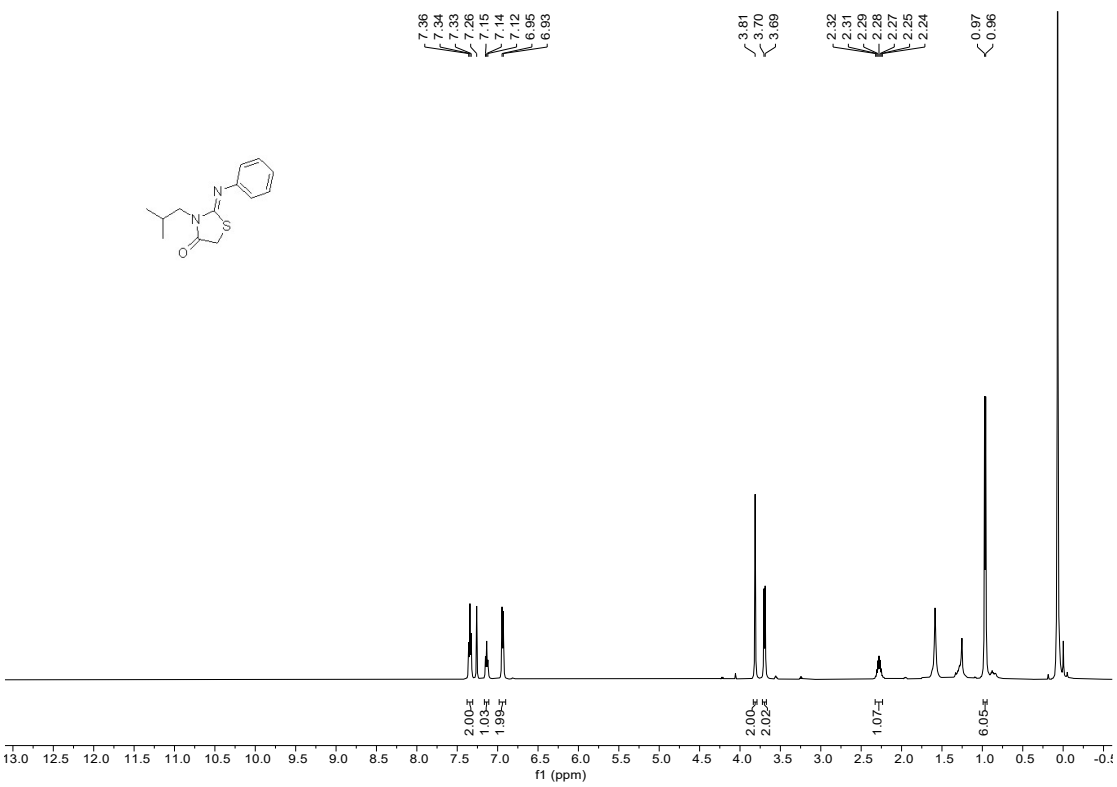
^{13}C{^{1}H} NMR of **4w** in $CDCl_3$ (100 MHz)



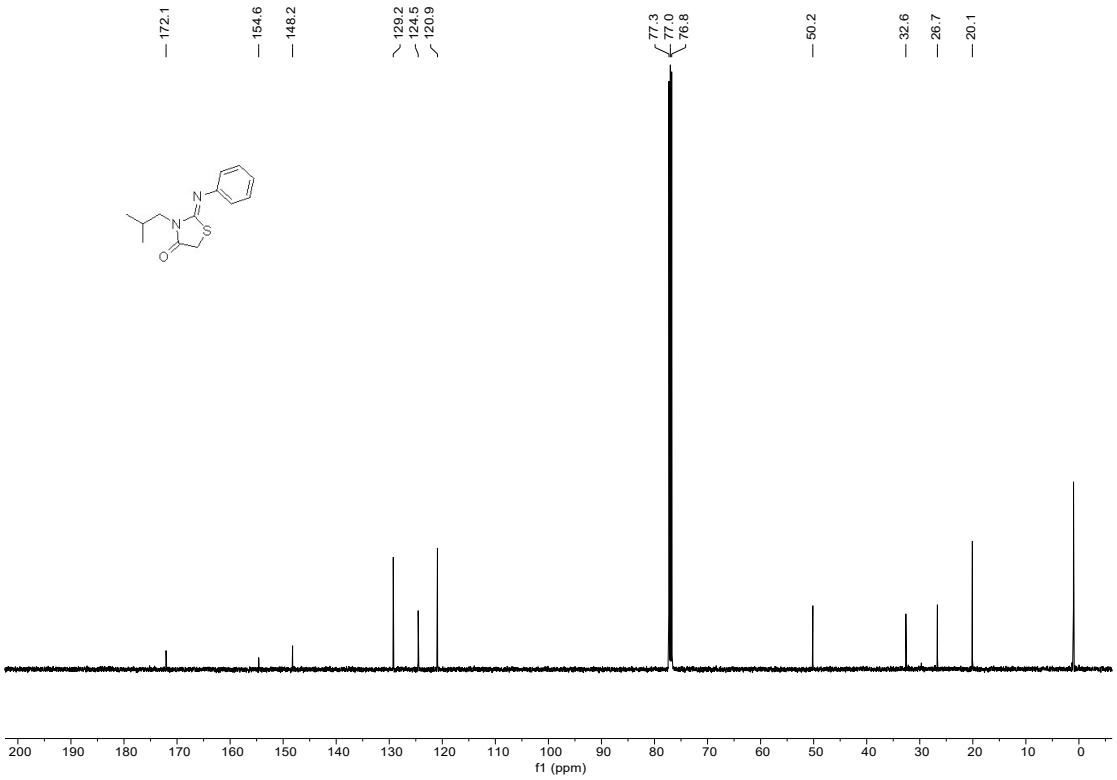
^{1}H NMR of **4x** in $CDCl_3$ (500 MHz)



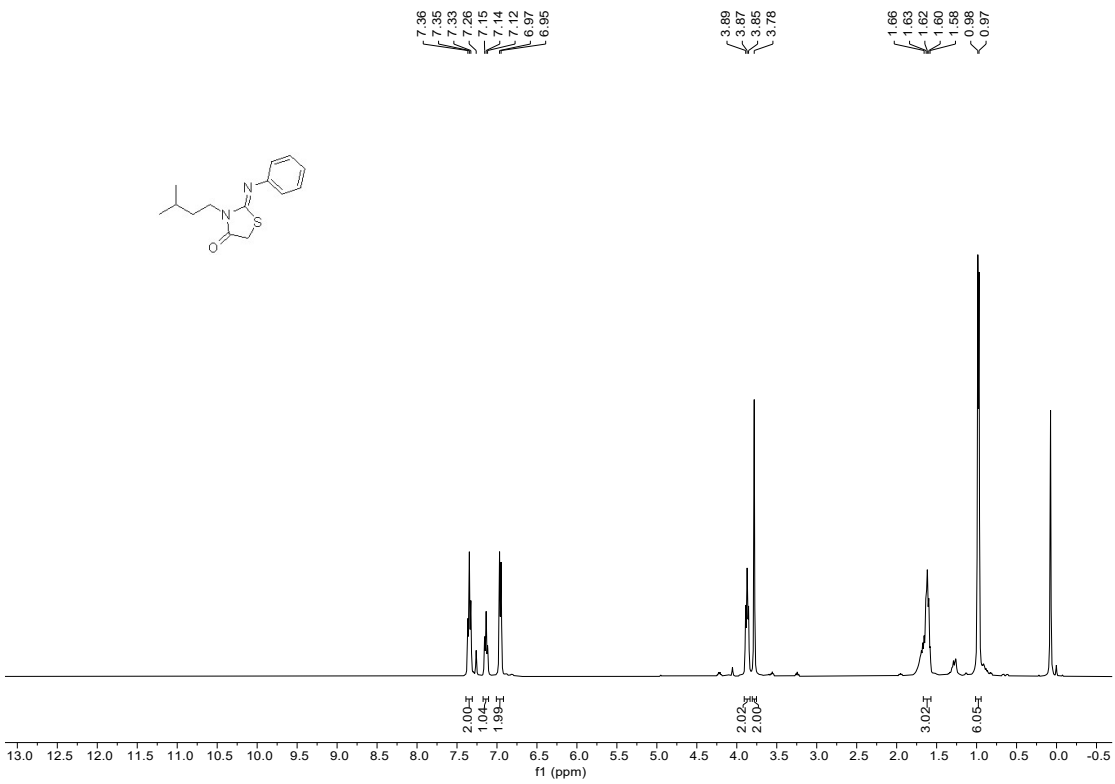
^{13}C{^{1}H} NMR of **4x** in $CDCl_3$ (126 MHz)



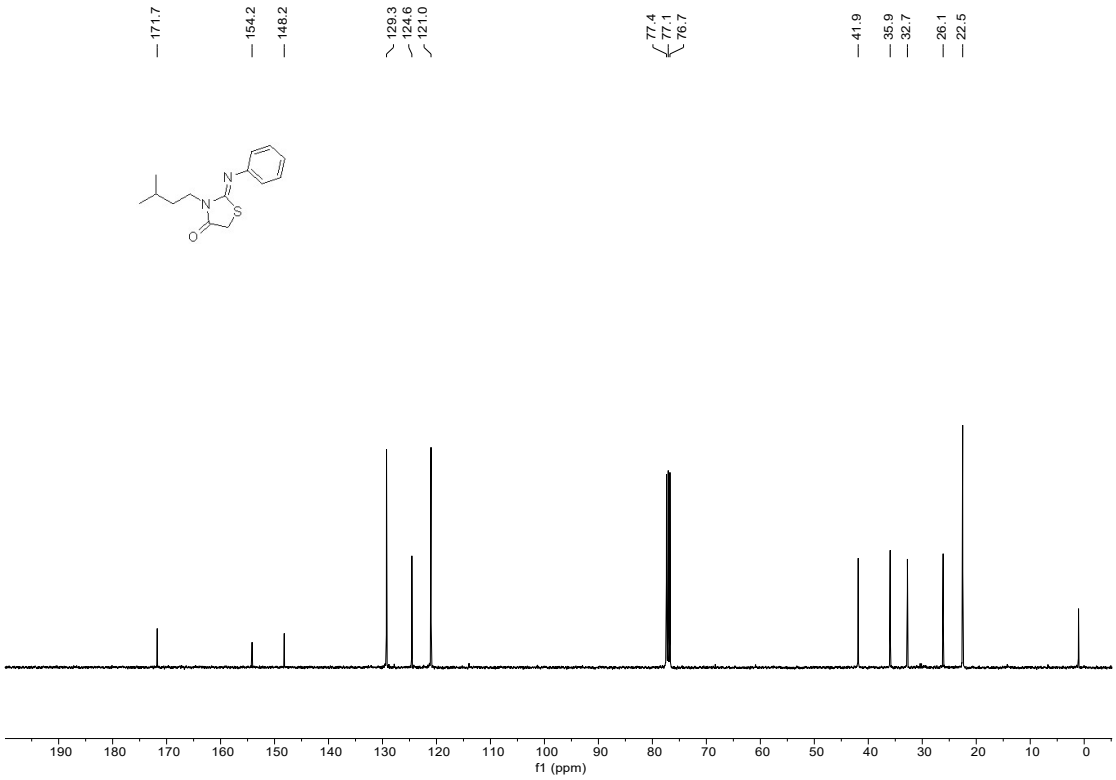
^{1}H NMR of **4y** in $CDCl_3$ (500 MHz)



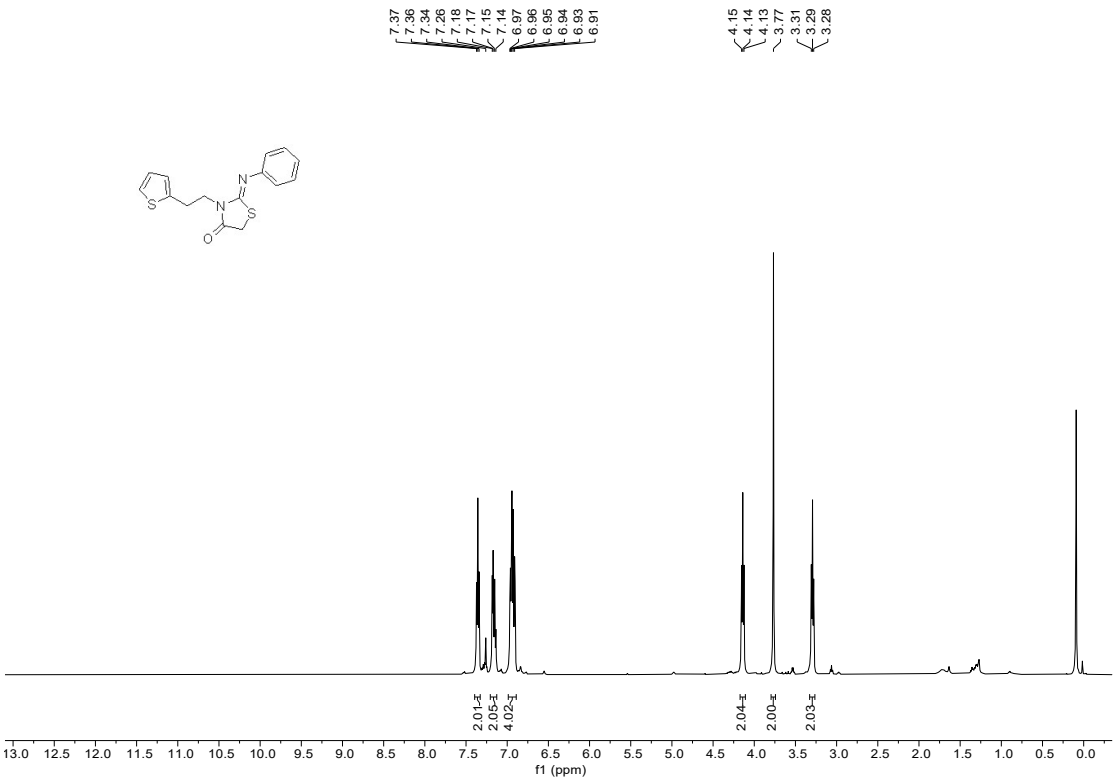
^{13}C{^{1}H} NMR of **4y** in $CDCl_3$ (126 MHz)



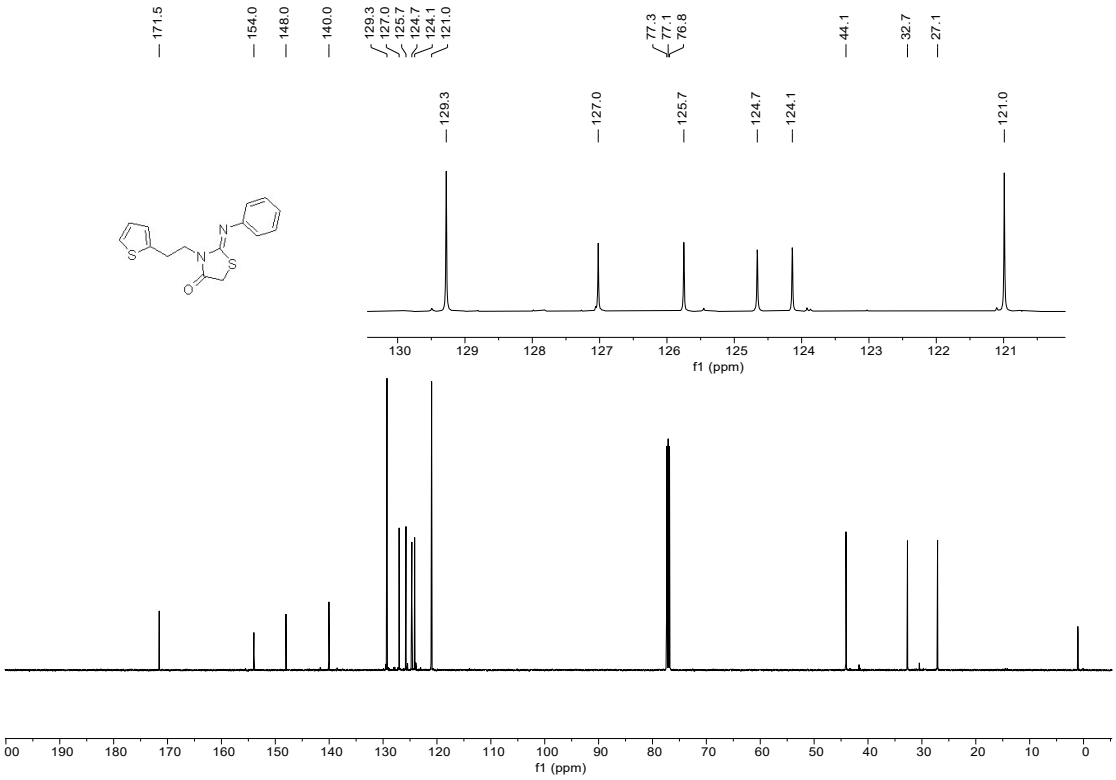
^{1}H NMR of **4za** in $CDCl_3$ (400 MHz)



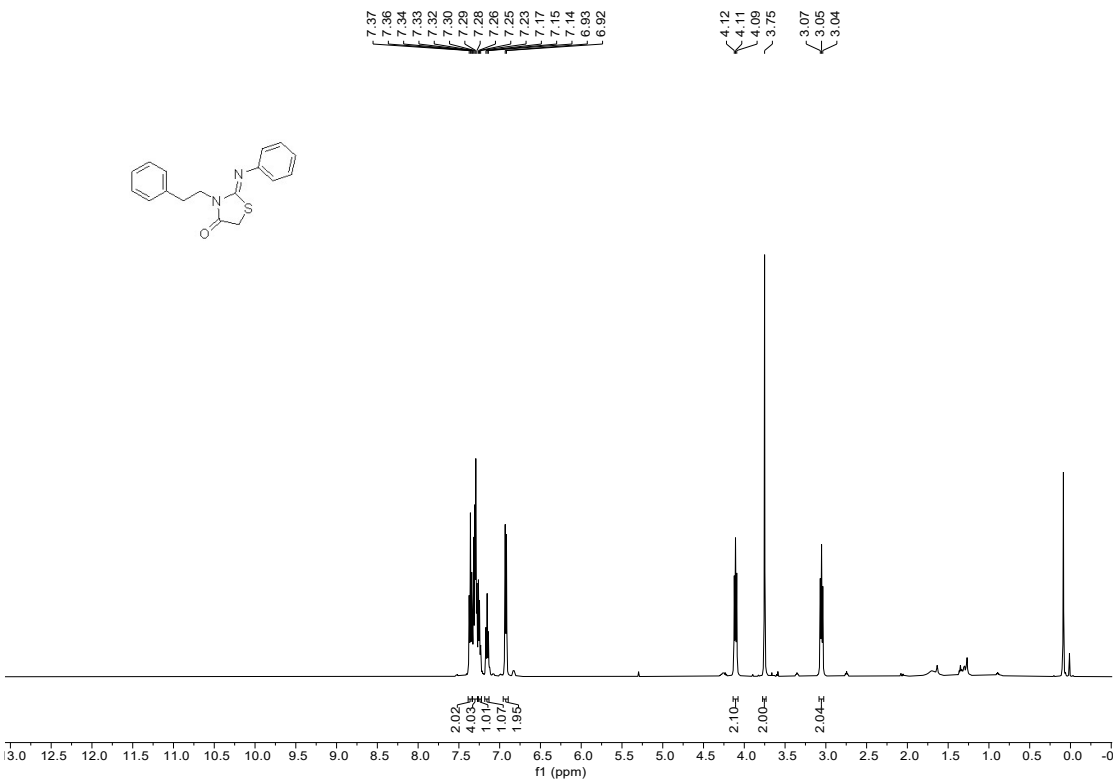
^{13}C{^{1}H} NMR of **4za** in $CDCl_3$ (100 MHz)



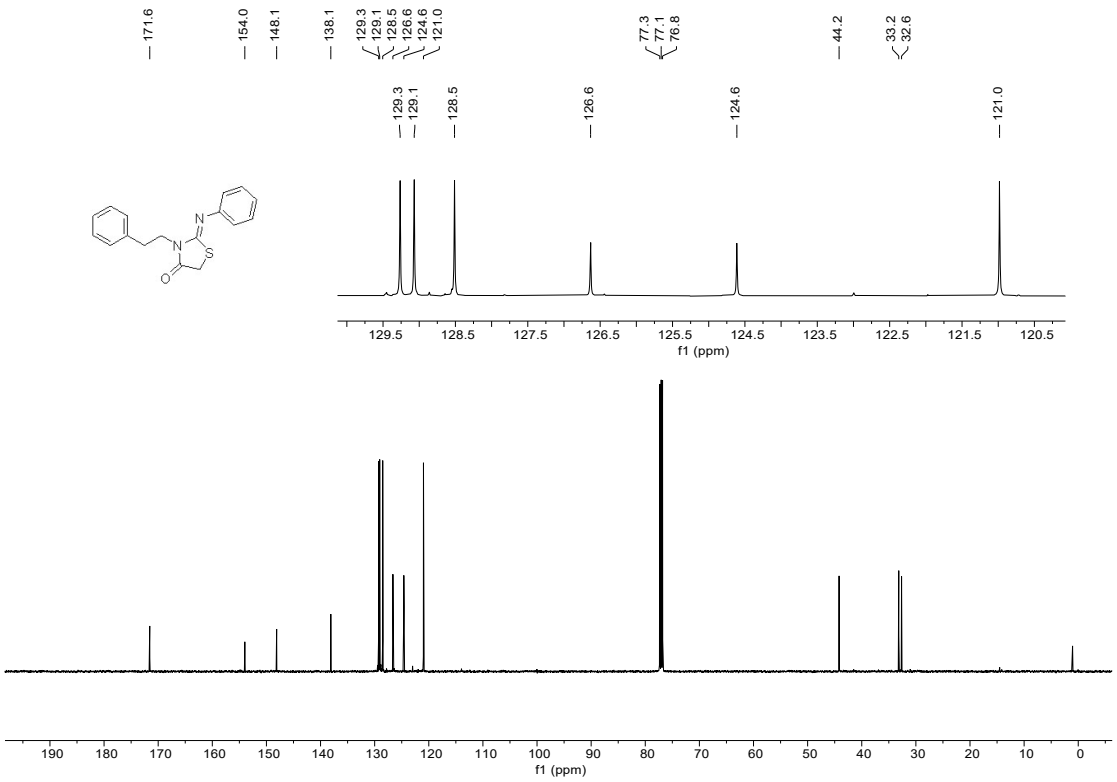
^{1}H NMR of **4zb** in $CDCl_3$ (500 MHz)



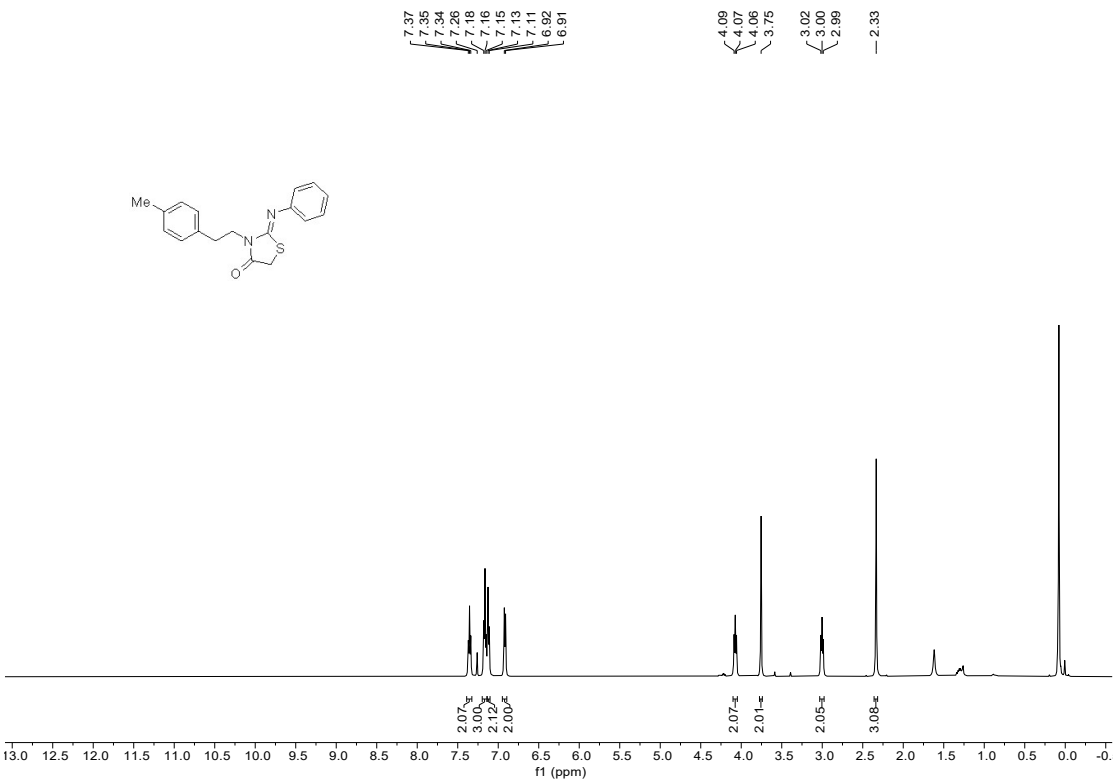
^{13}C{^{1}H} NMR of **4zb** in $CDCl_3$ (126 MHz)



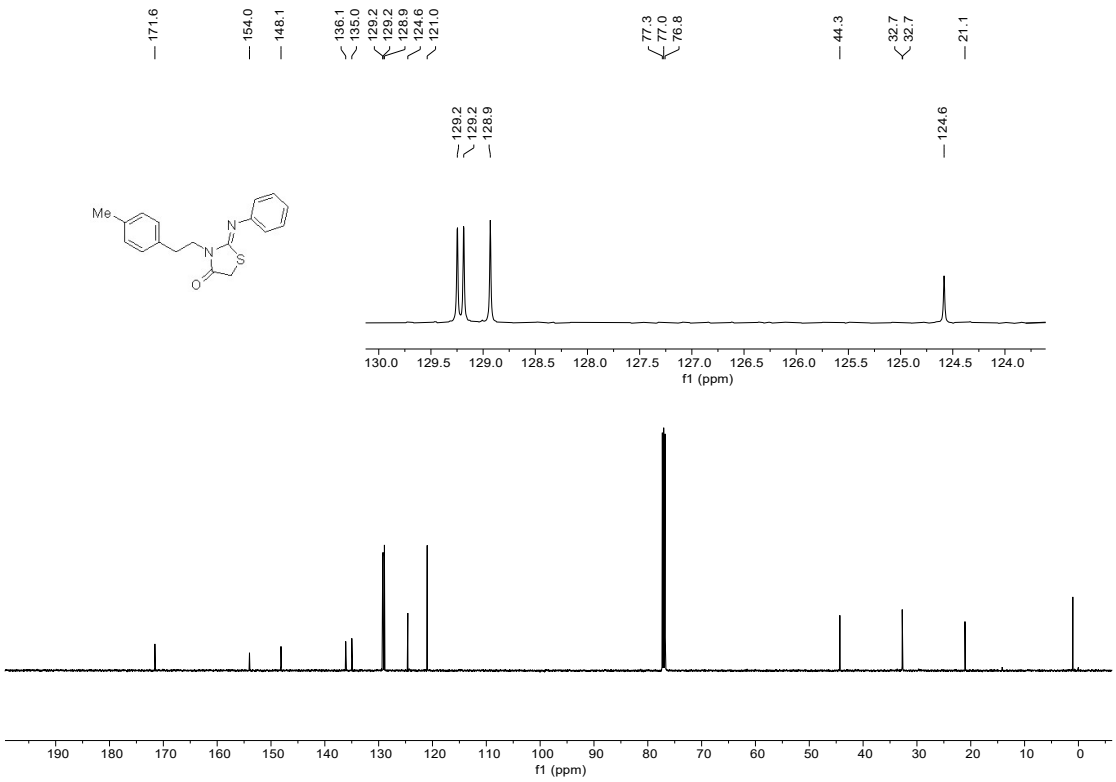
^{1}H NMR of **4zc** in $CDCl_3$ (500 MHz)



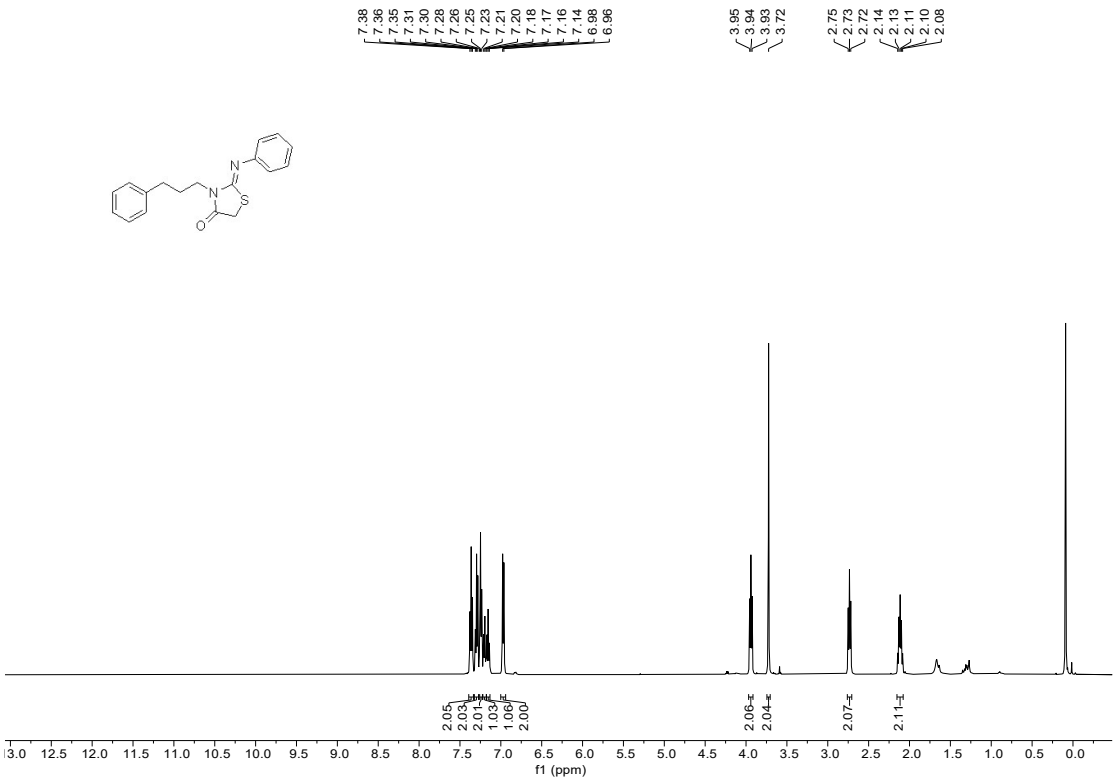
^{13}C{^{1}H} NMR of **4zc** in $CDCl_3$ (126 MHz)



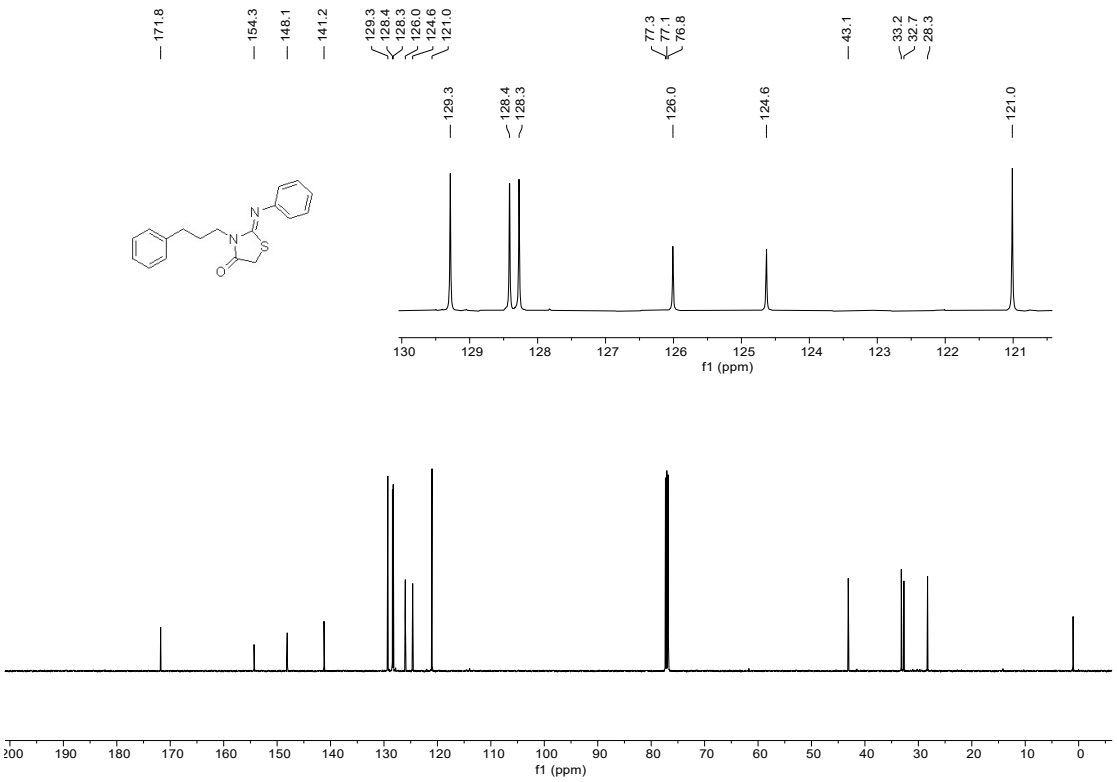
^{1}H NMR of **4zd** in $CDCl_3$ (500 MHz)



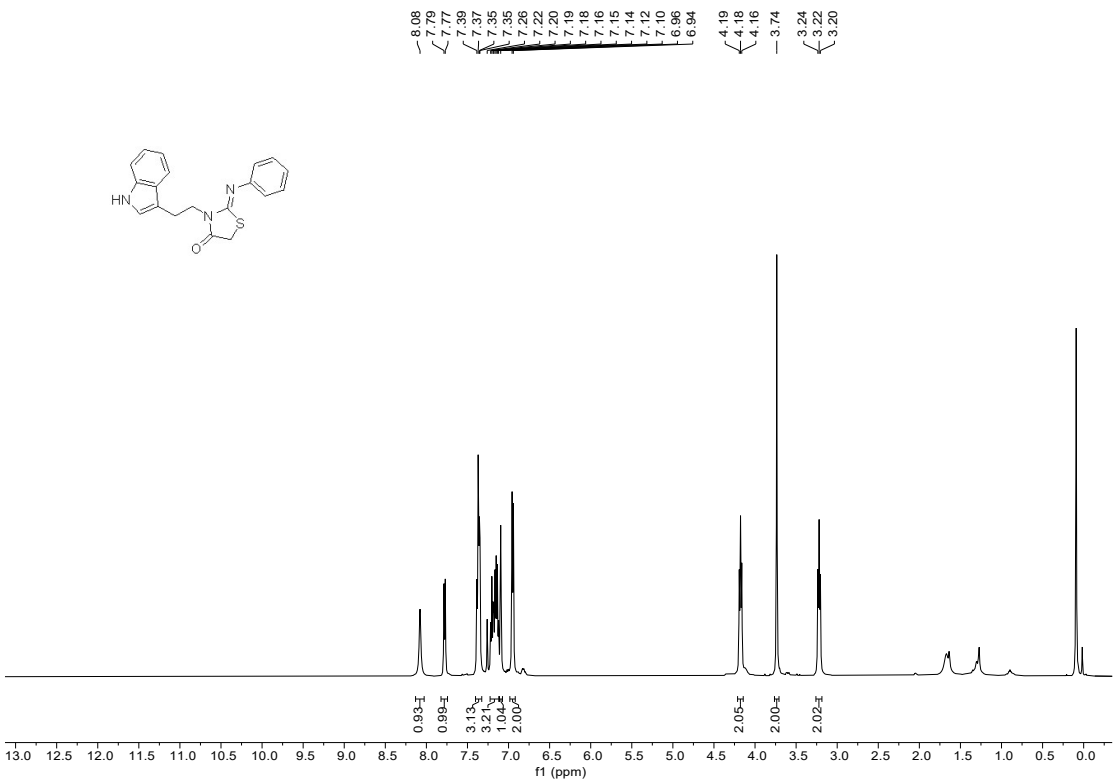
^{13}C{^{1}H} NMR of **4zd** in $CDCl_3$ (126 MHz)



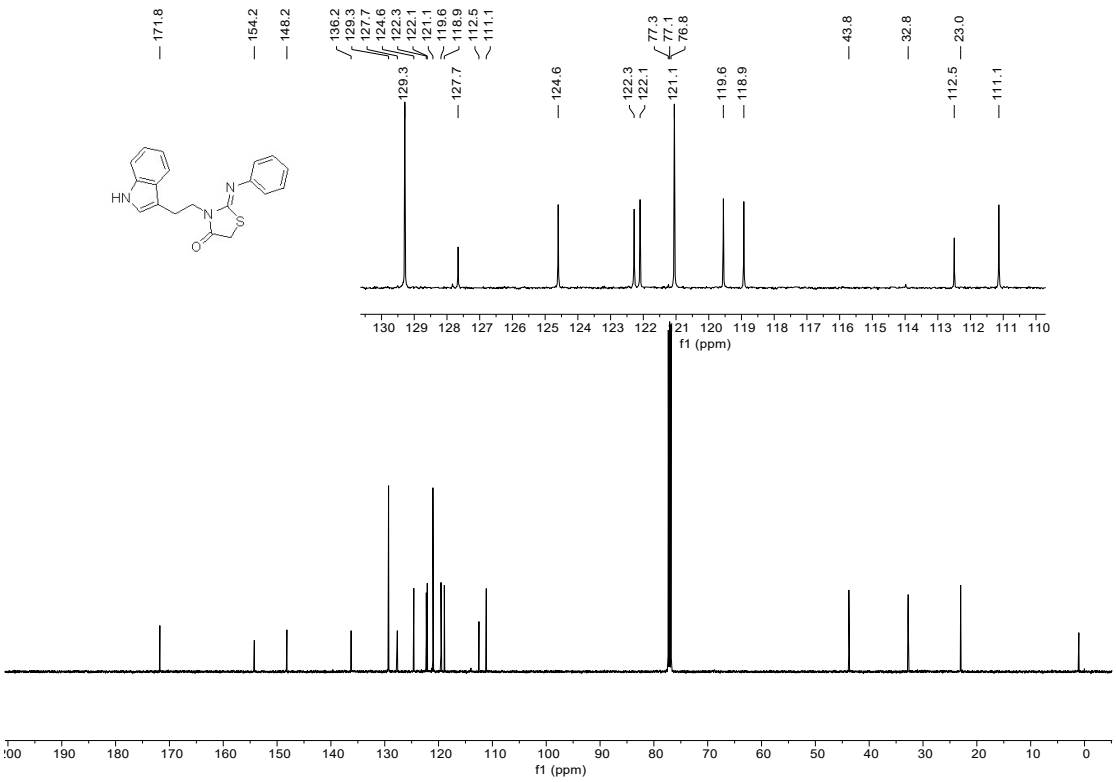
^{1}H NMR of **4ze** in $CDCl_3$ (500 MHz)



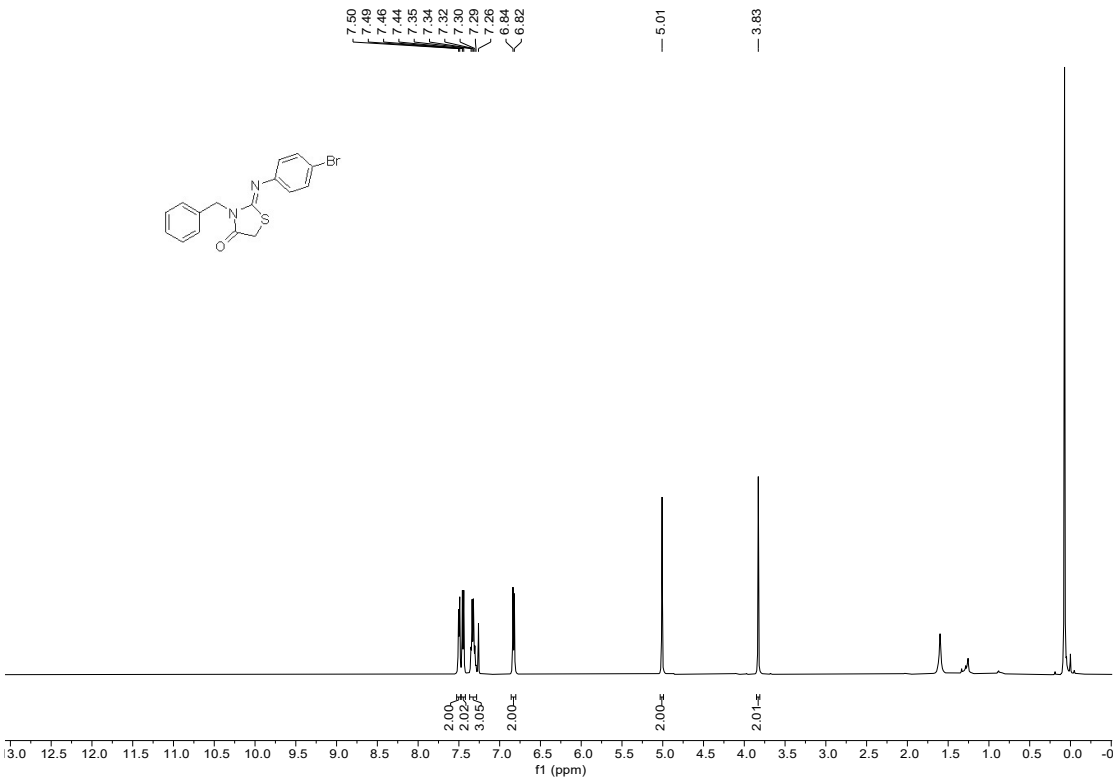
$^{13}C\{^{1}H\}$ NMR of **4ze** in $CDCl_3$ (126 MHz)



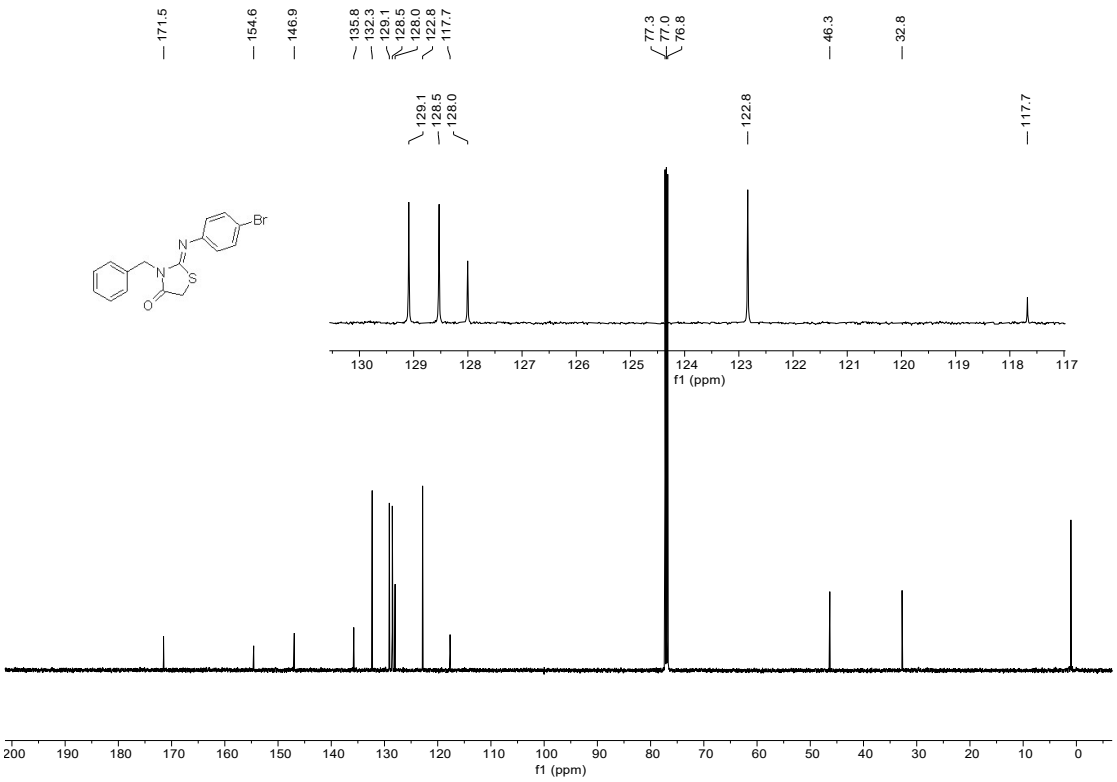
^{1}H NMR of **4zf** in $CDCl_3$ (500 MHz)



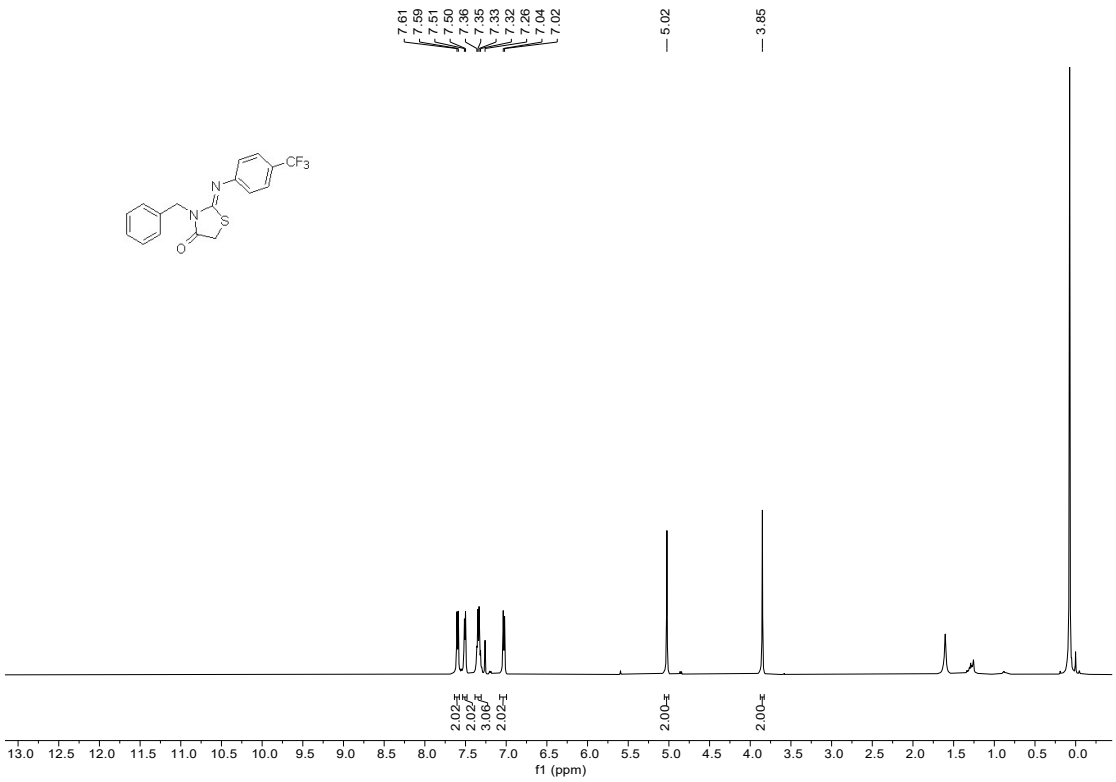
^{13}C{^{1}H} NMR of **4zf** in $CDCl_3$ (126 MHz)



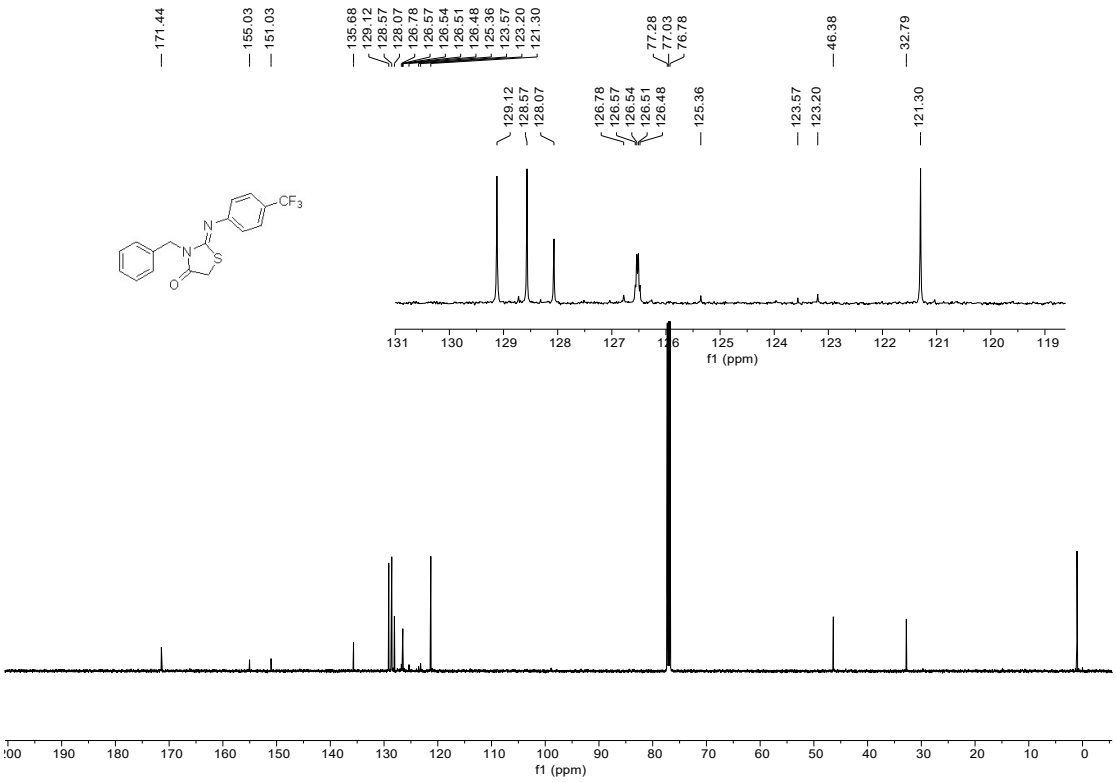
^{1}H NMR of **5a** in $CDCl_3$ (500 MHz)



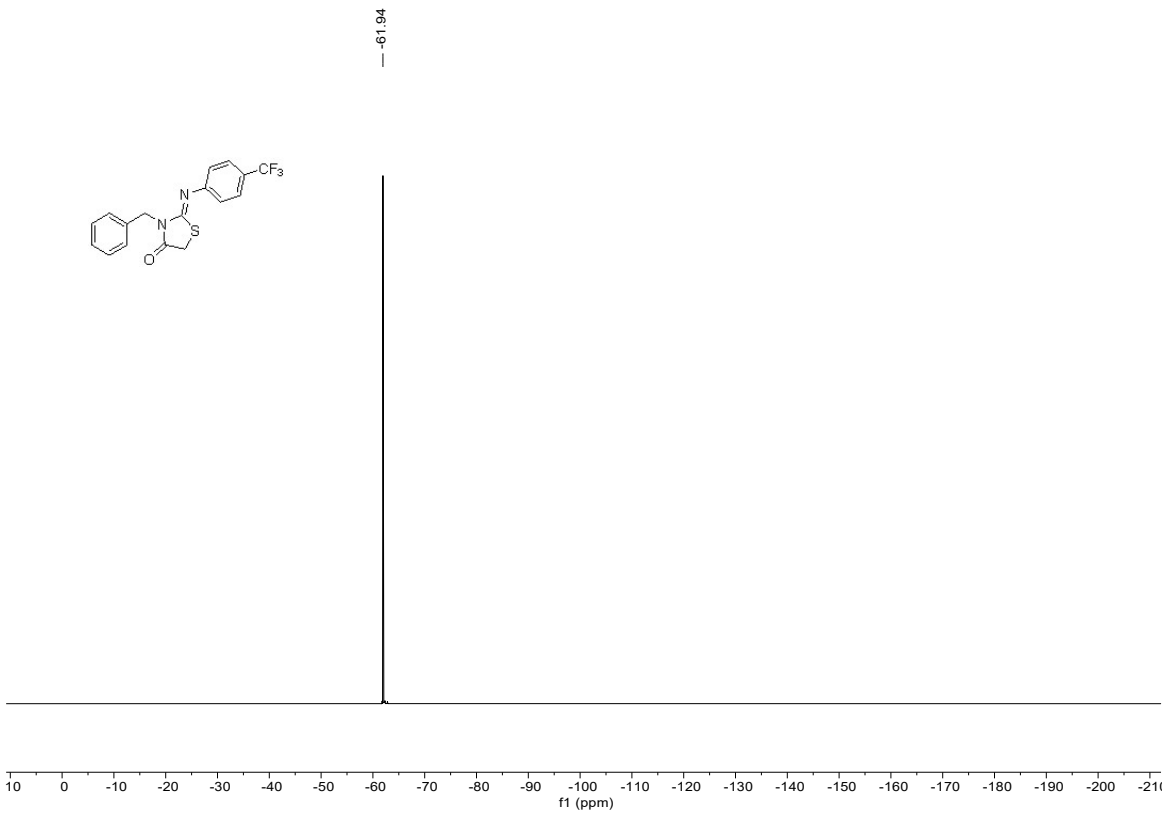
^{13}C{^{1}H} NMR of **5a** in $CDCl_3$ (126 MHz)



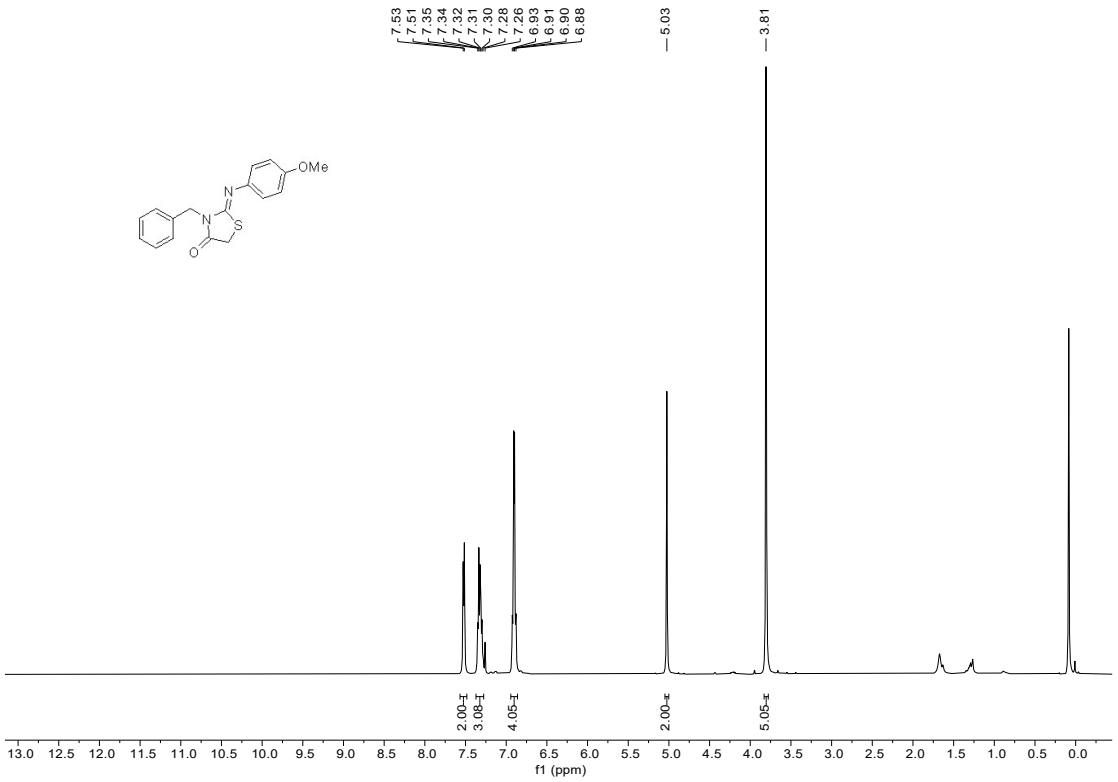
^{1}H NMR of **5b** in $CDCl_3$ (500 MHz)



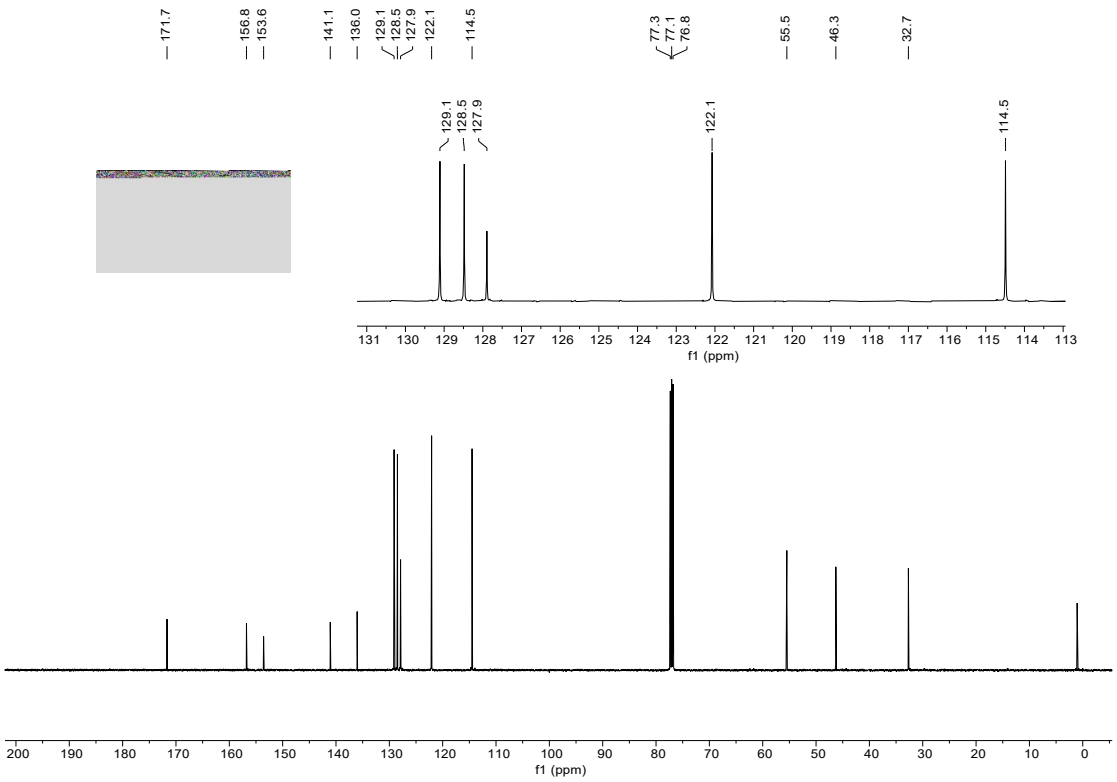
$^{13}C\{^{1}H\}$ NMR of **5b** in $CDCl_3$ (126 MHz)



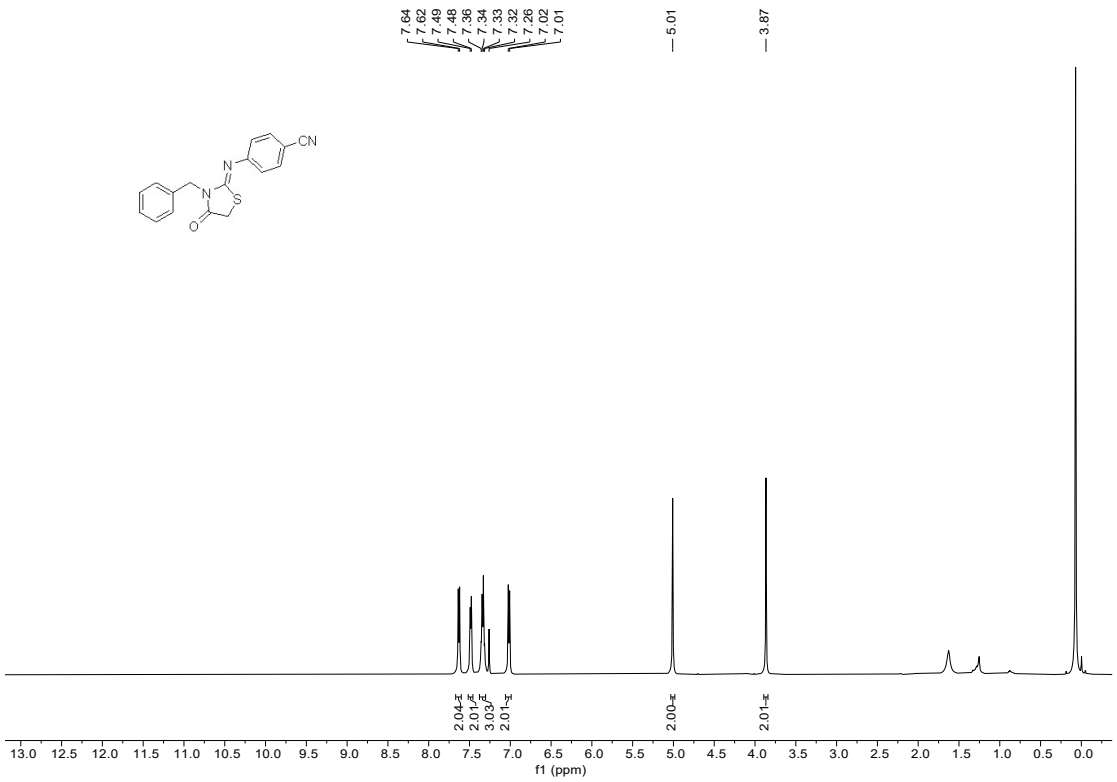
^{19}F NMR of **5b** in $CDCl_3$ (471 MHz)



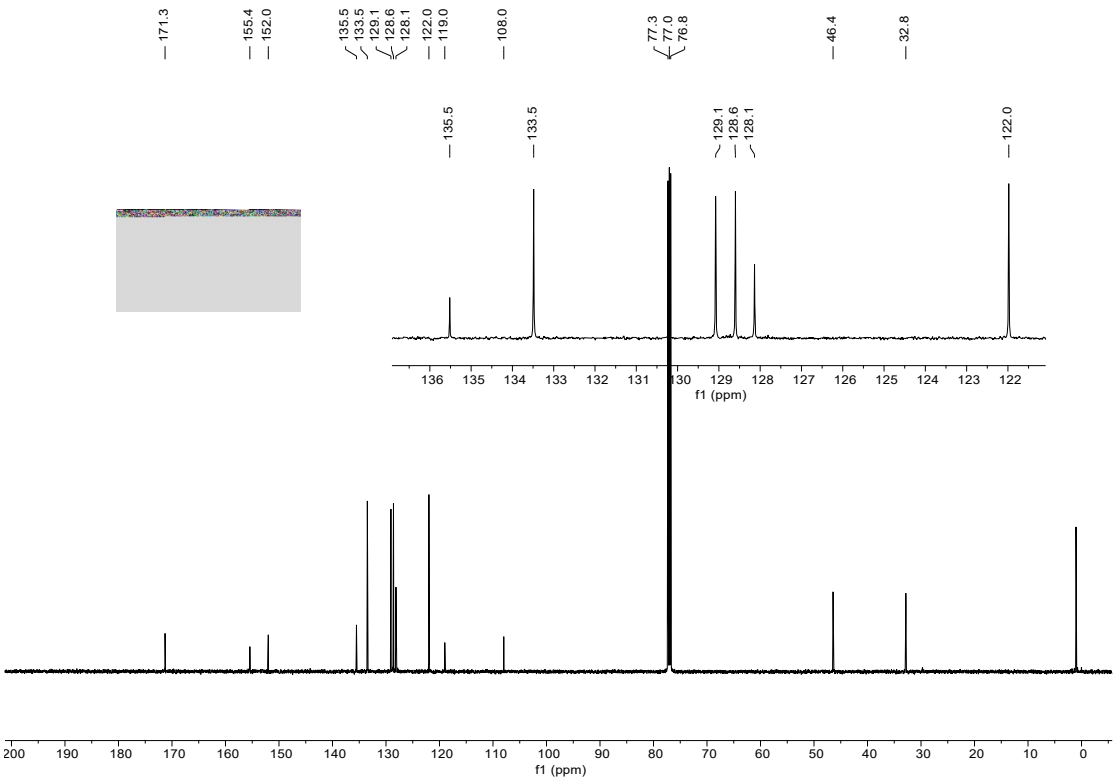
^{1}H NMR of **5c** in $CDCl_3$ (500 MHz)



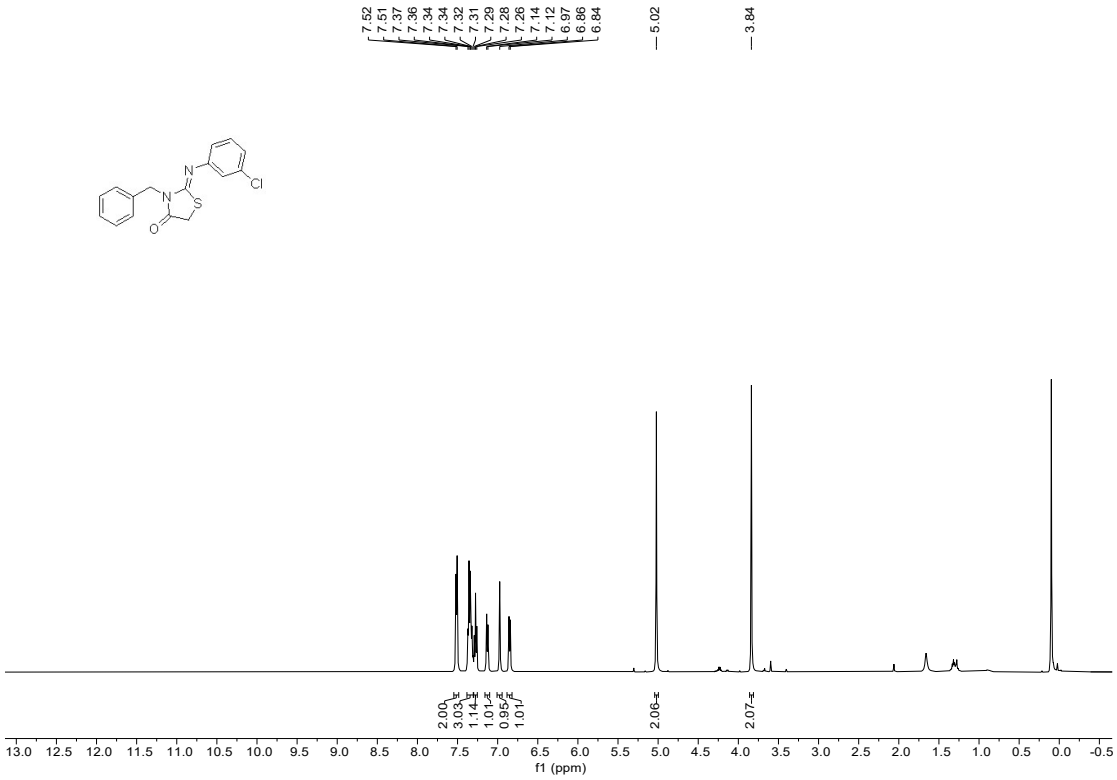
$^{13}C\{^{1}H\}$ NMR of **5c** in $CDCl_3$ (126 MHz)



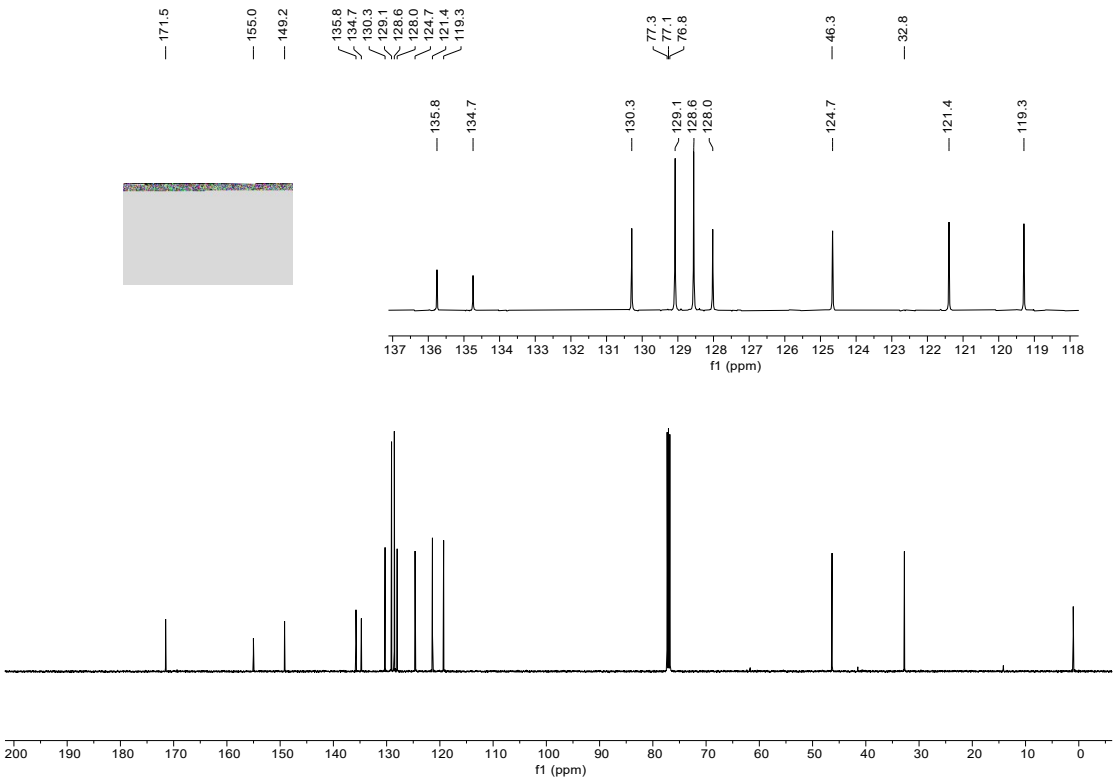
^{1}H NMR of **5d** in $CDCl_3$ (500 MHz)



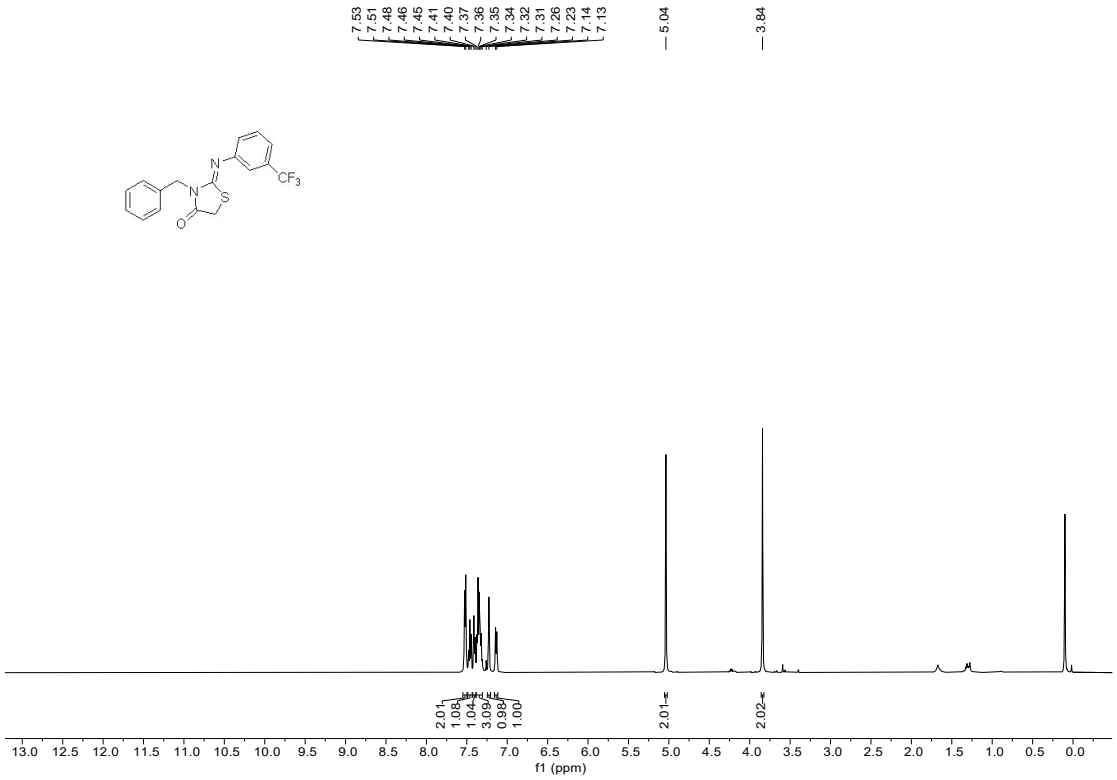
$^{13}C\{^{1}H\}$ NMR of **5d** in $CDCl_3$ (126 MHz)



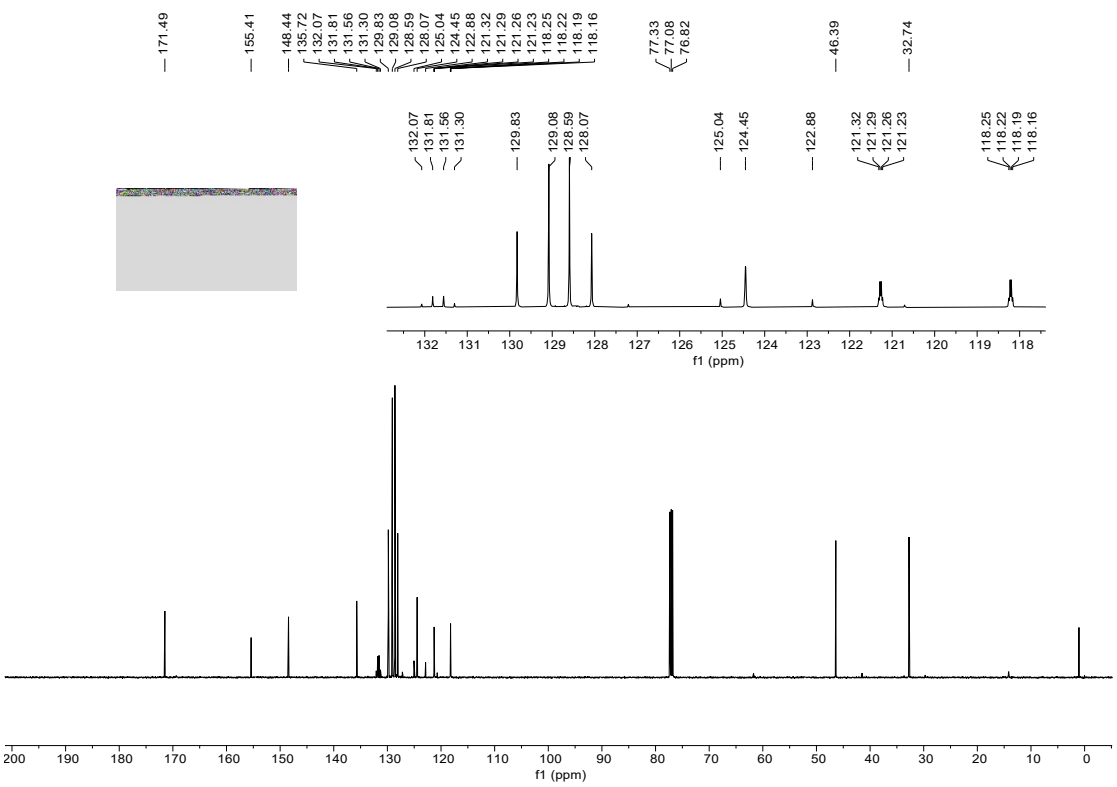
^{1}H NMR of **5e** in $CDCl_3$ (500 MHz)



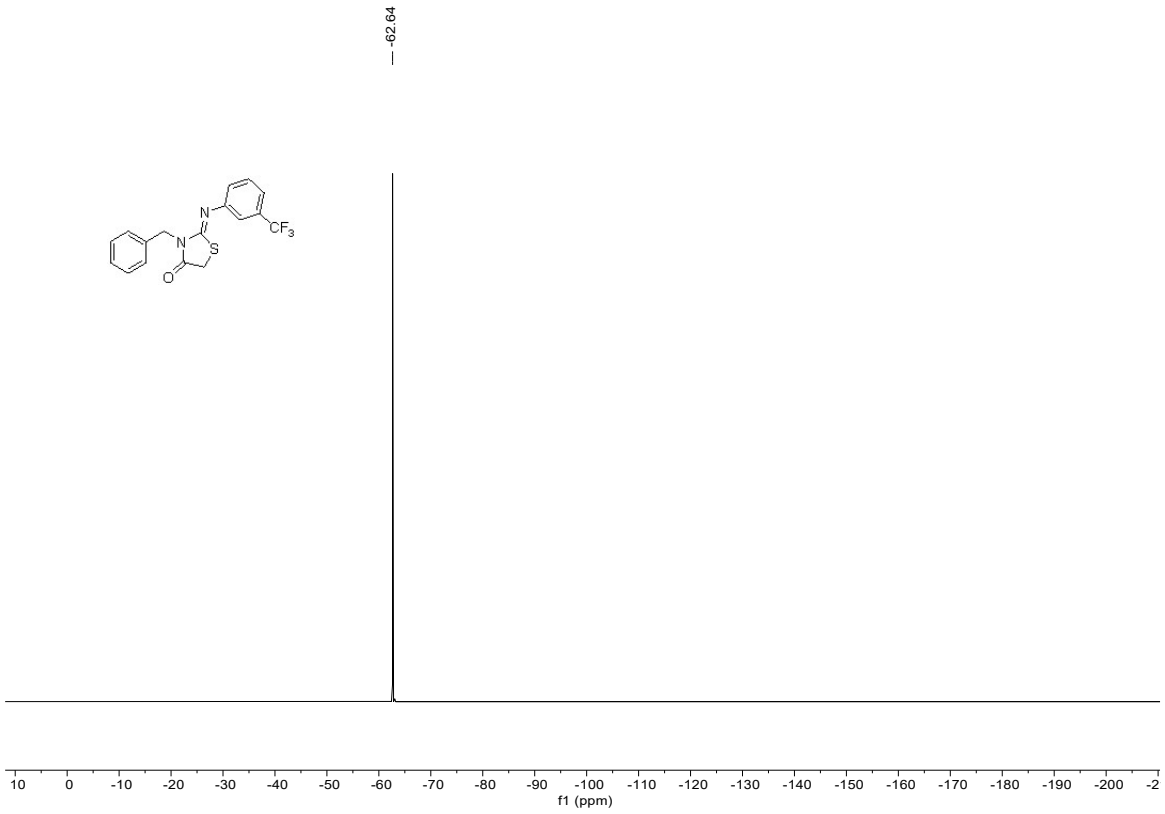
$^{13}C\{^{1}H\}$ NMR of **5e** in $CDCl_3$ (126 MHz)



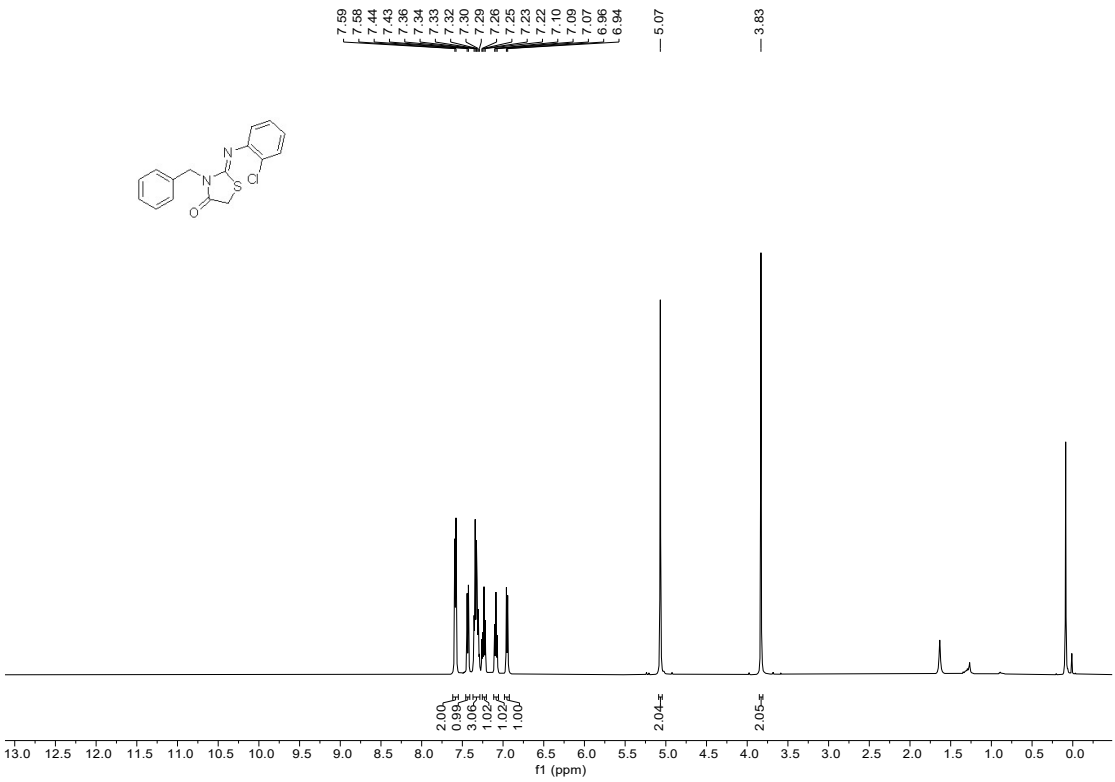
^{1}H NMR of **5f** in $CDCl_3$ (500 MHz)



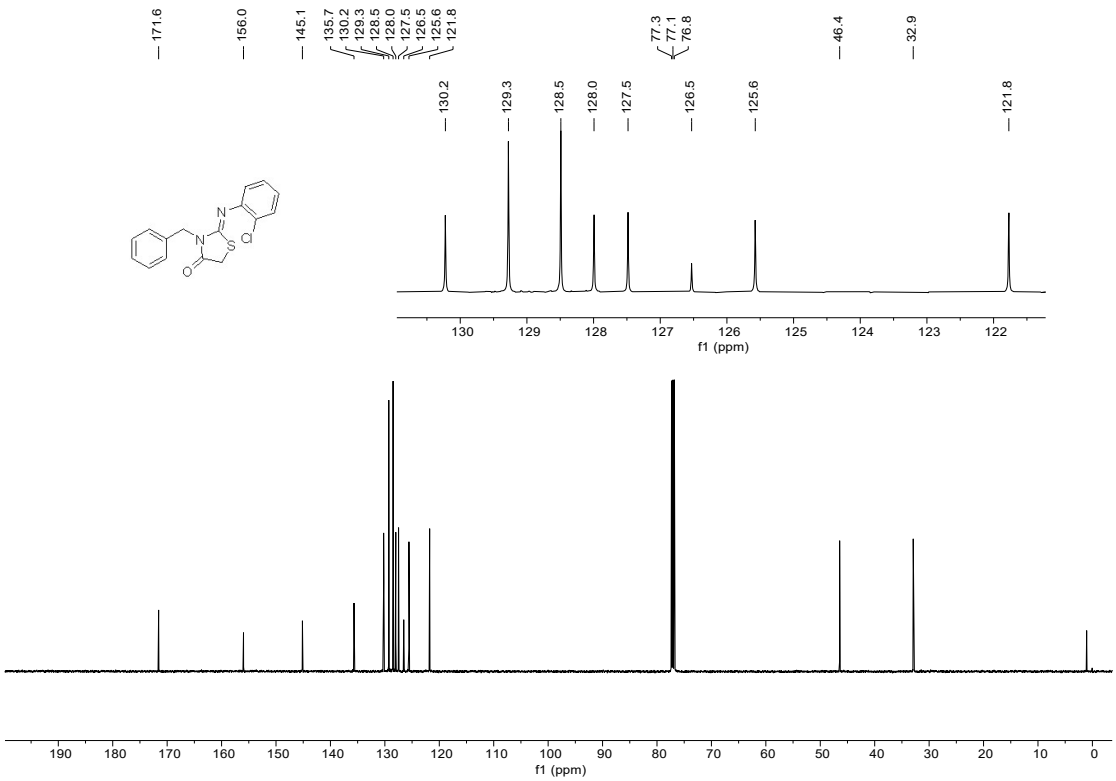
$^{13}C\{^{1}H\}$ NMR of **5f** in $CDCl_3$ (126 MHz)



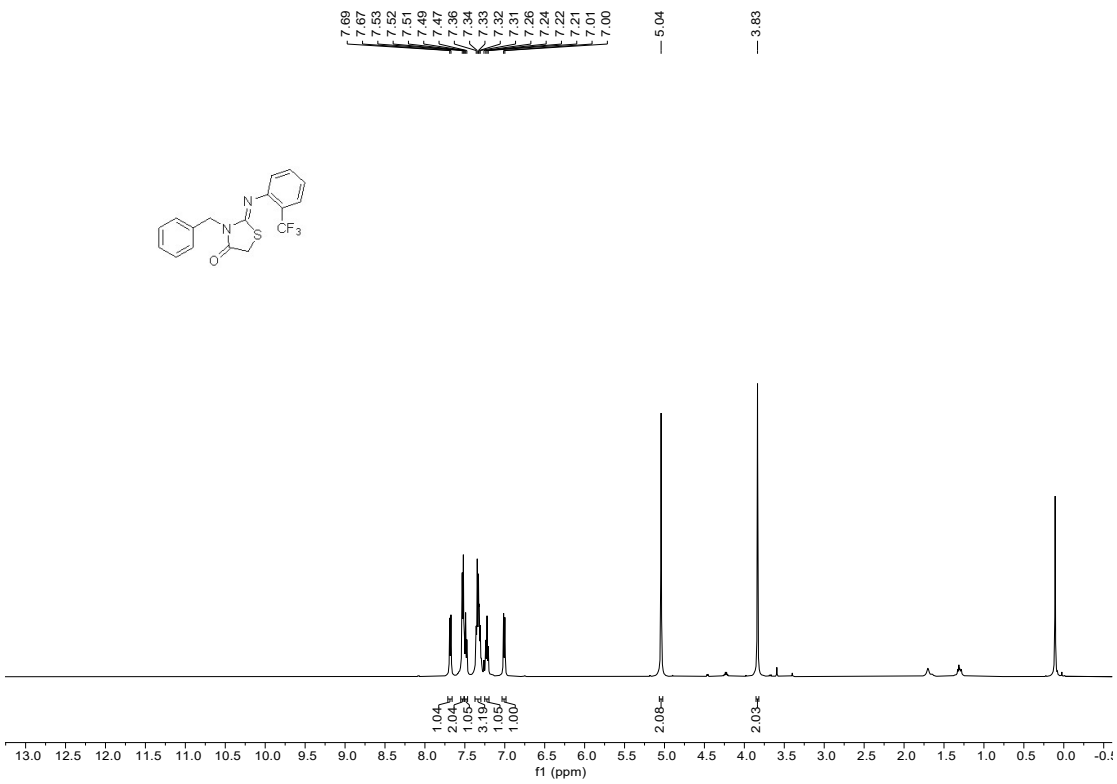
^{19}F NMR of **5f** in $CDCl_3$ (471 MHz)



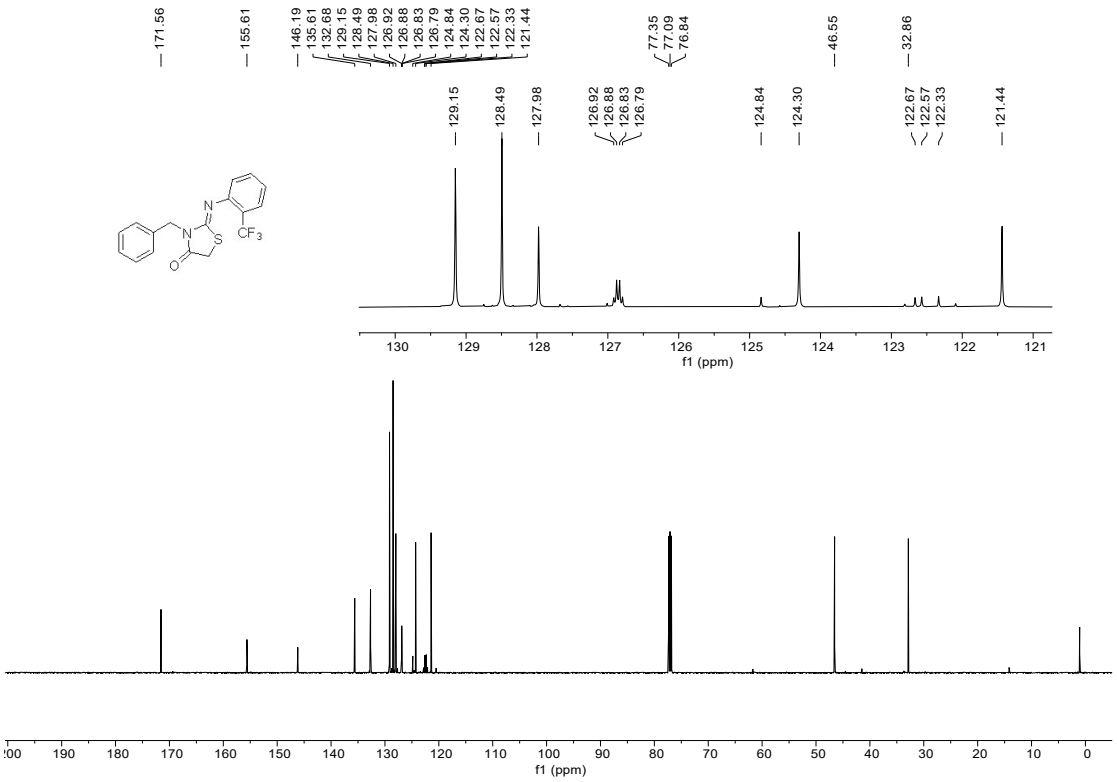
^{1}H NMR of **5g** in $CDCl_3$ (500 MHz)



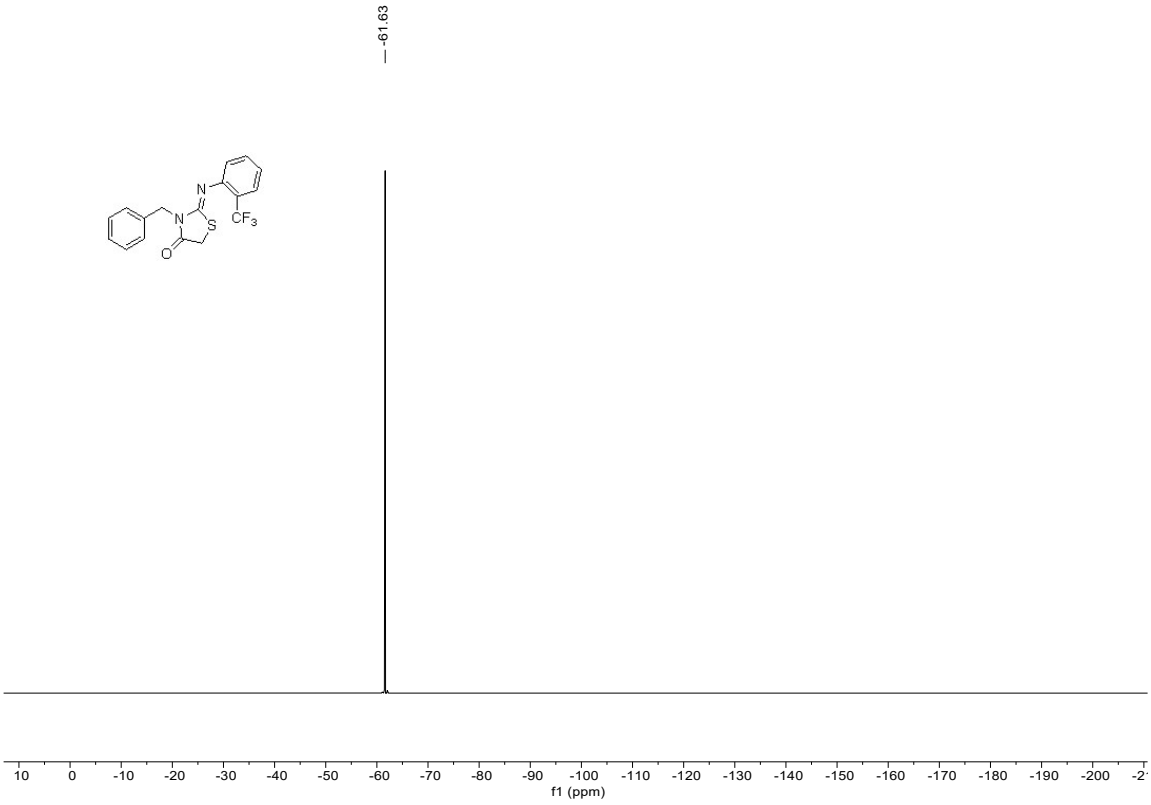
^{13}C{^{1}H} NMR of **5g** in $CDCl_3$ (126 MHz)



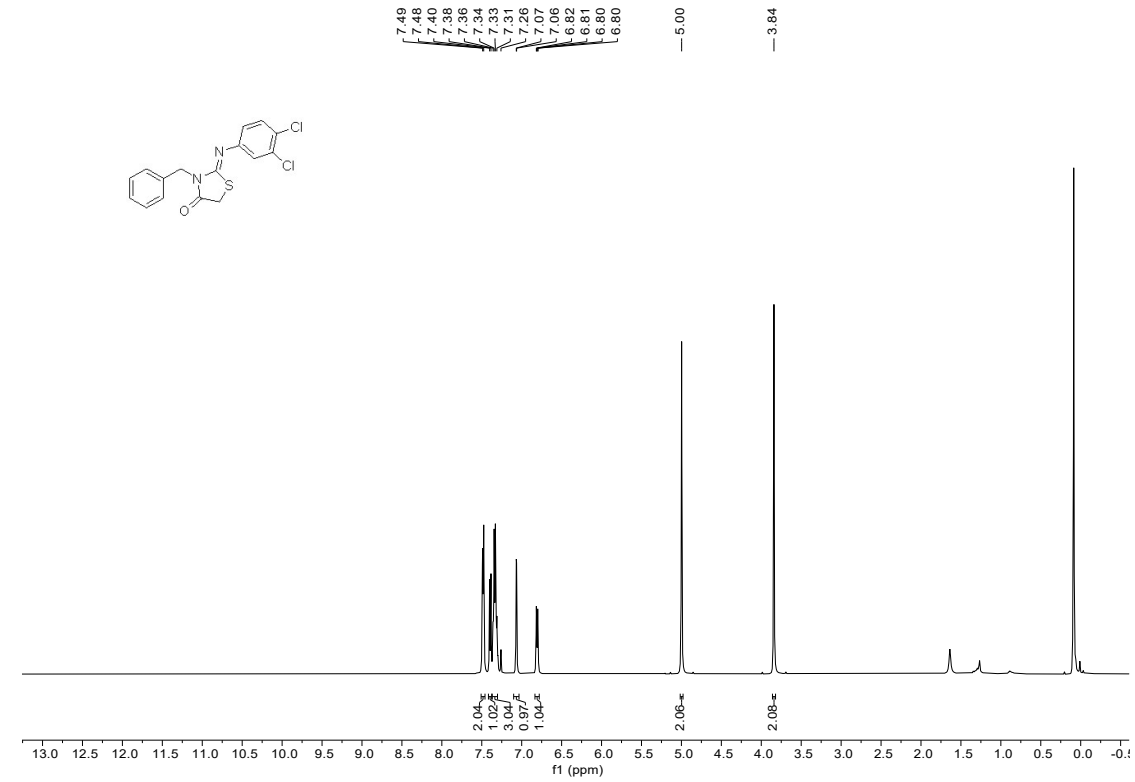
^{1}H NMR of **5h** in $CDCl_3$ (500 MHz)



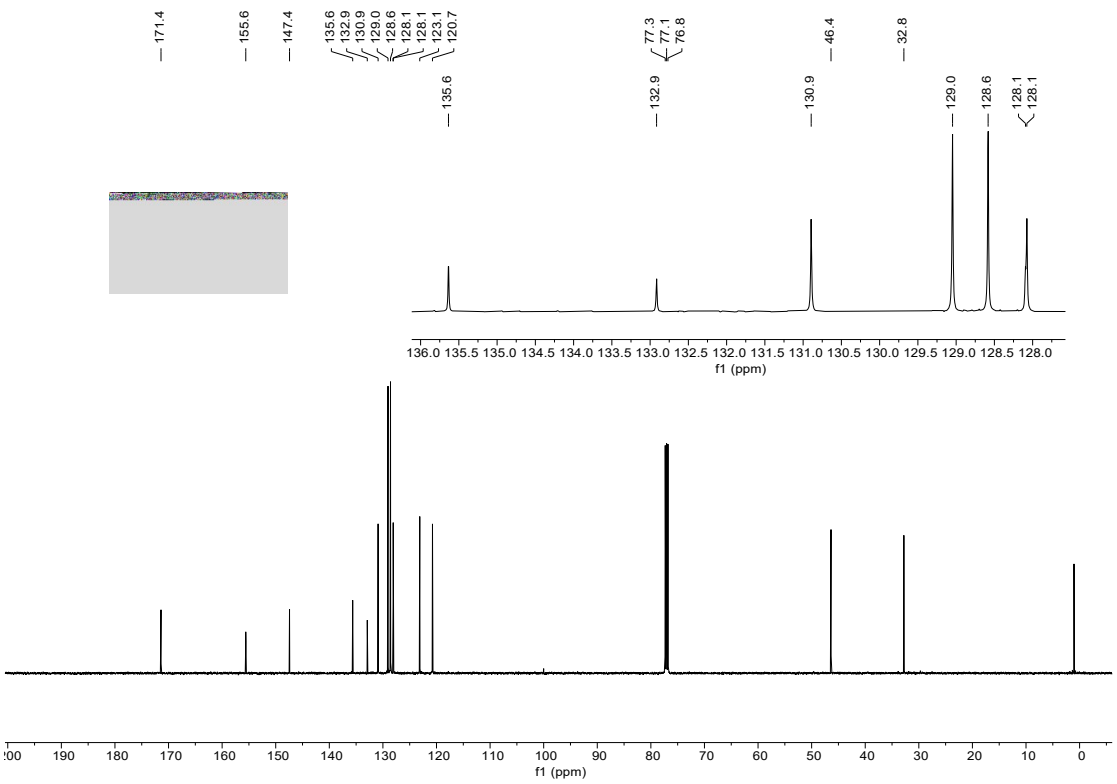
^{13}C{^{1}H} NMR of **5h** in $CDCl_3$ (126 MHz)



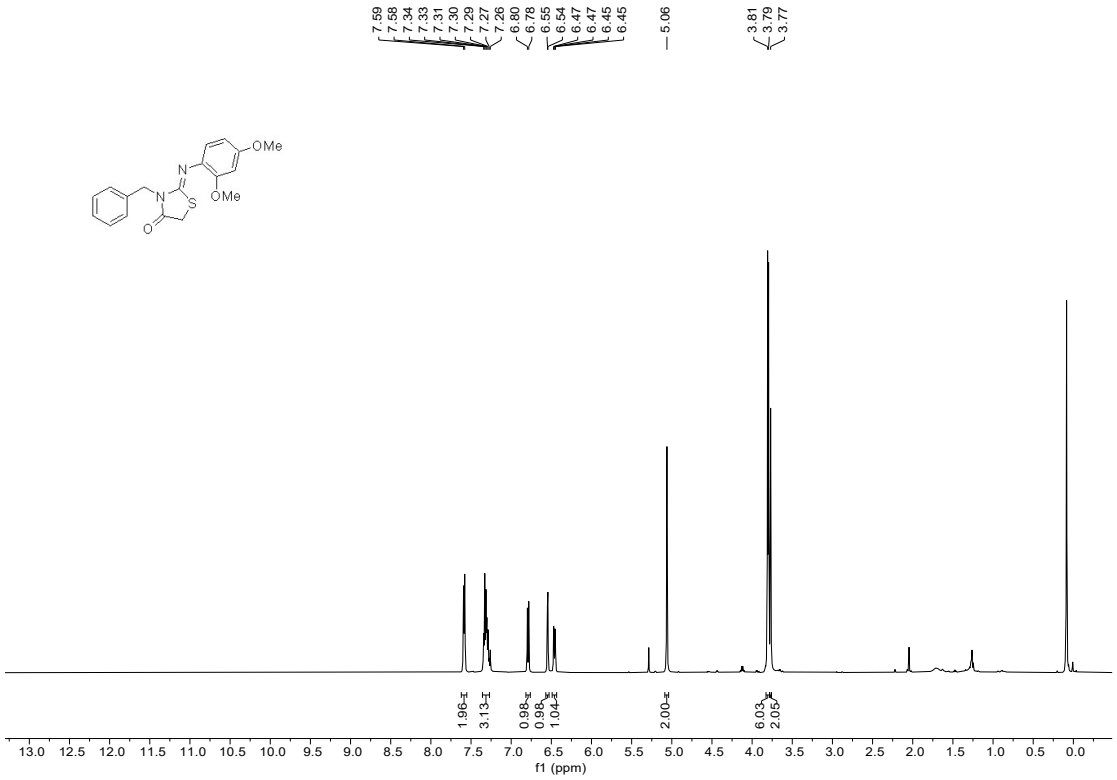
^{19}F NMR of **5h** in $CDCl_3$ (471 MHz)



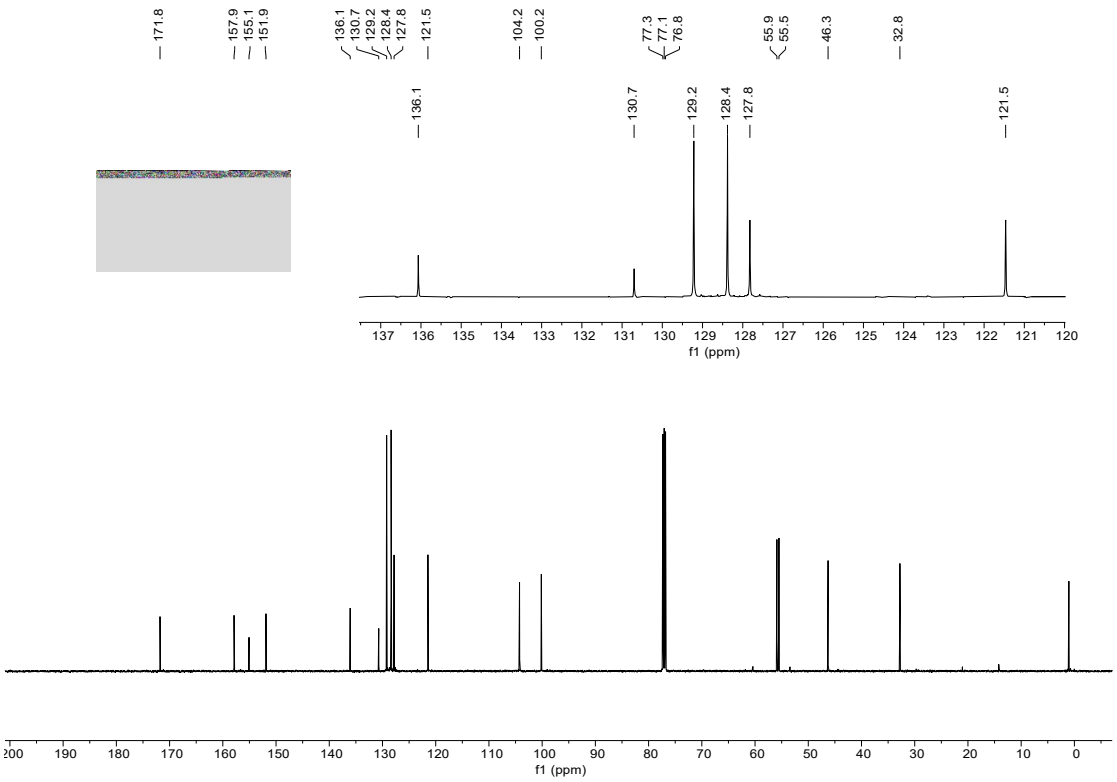
^{1}H NMR of **5i** in $CDCl_3$ (500 MHz)



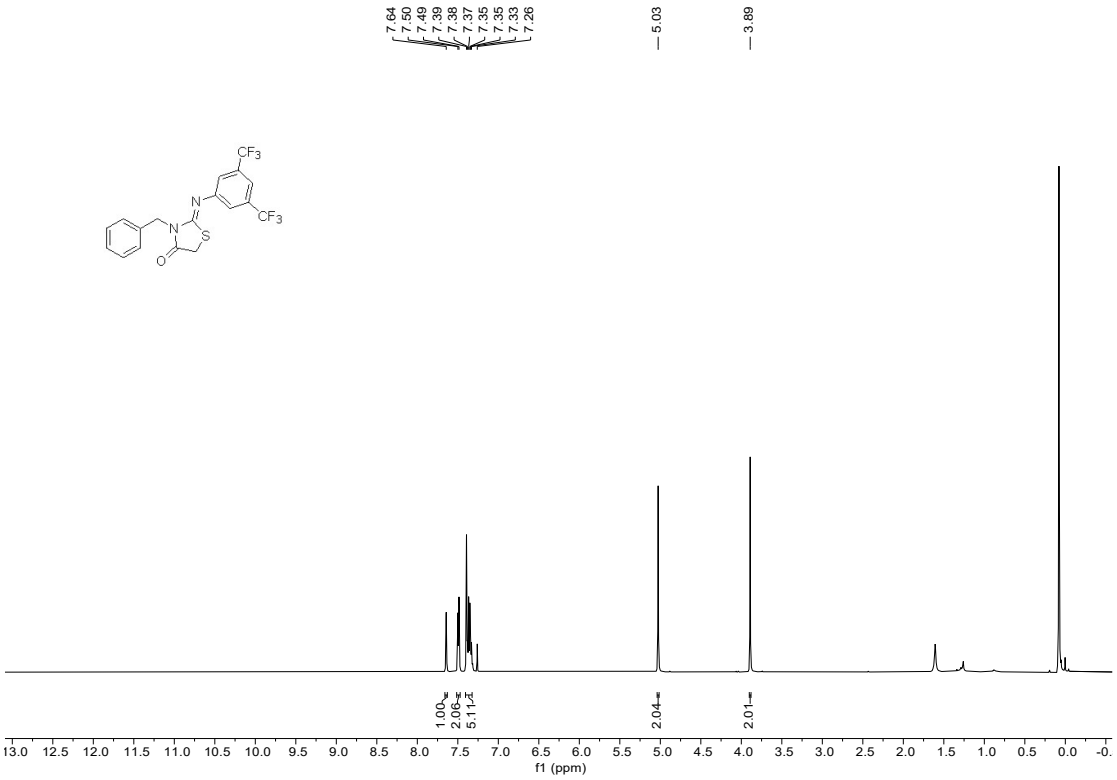
$^{13}C\{^{1}H\}$ NMR of **5i** in $CDCl_3$ (126 MHz)



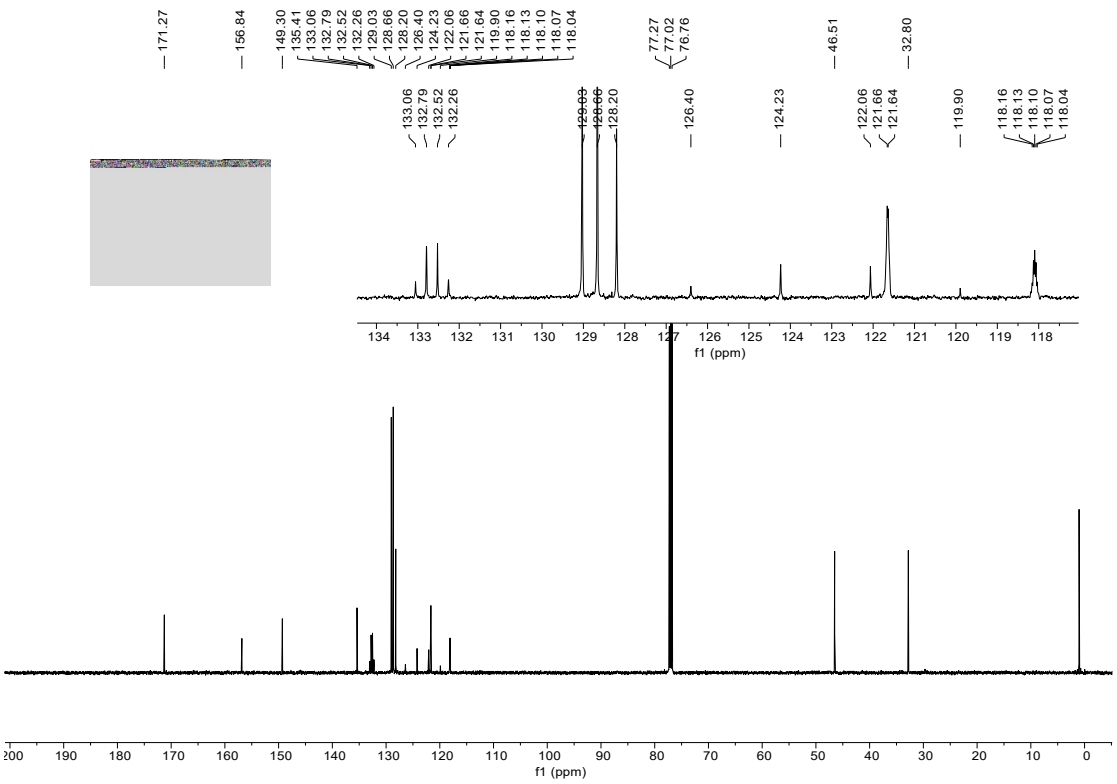
^{1}H NMR of **5j** in $CDCl_3$ (500 MHz)



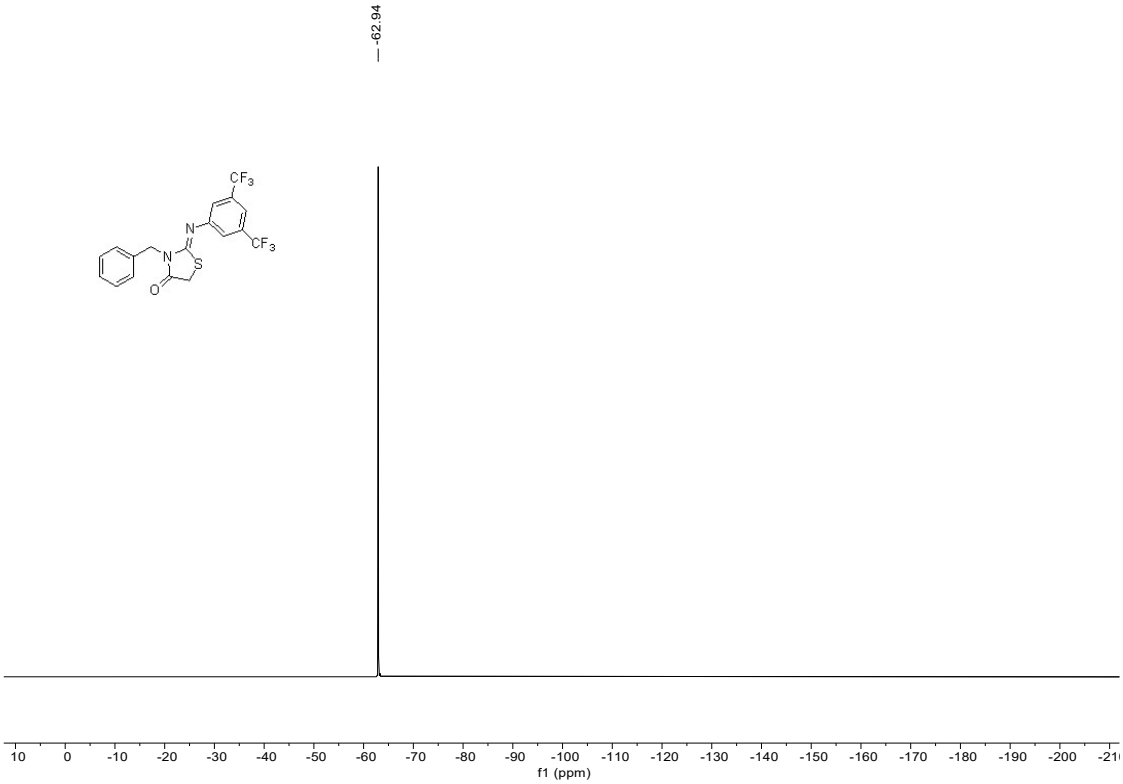
$^{13}C\{^{1}H\}$ NMR of **5j** in $CDCl_3$ (126 MHz)



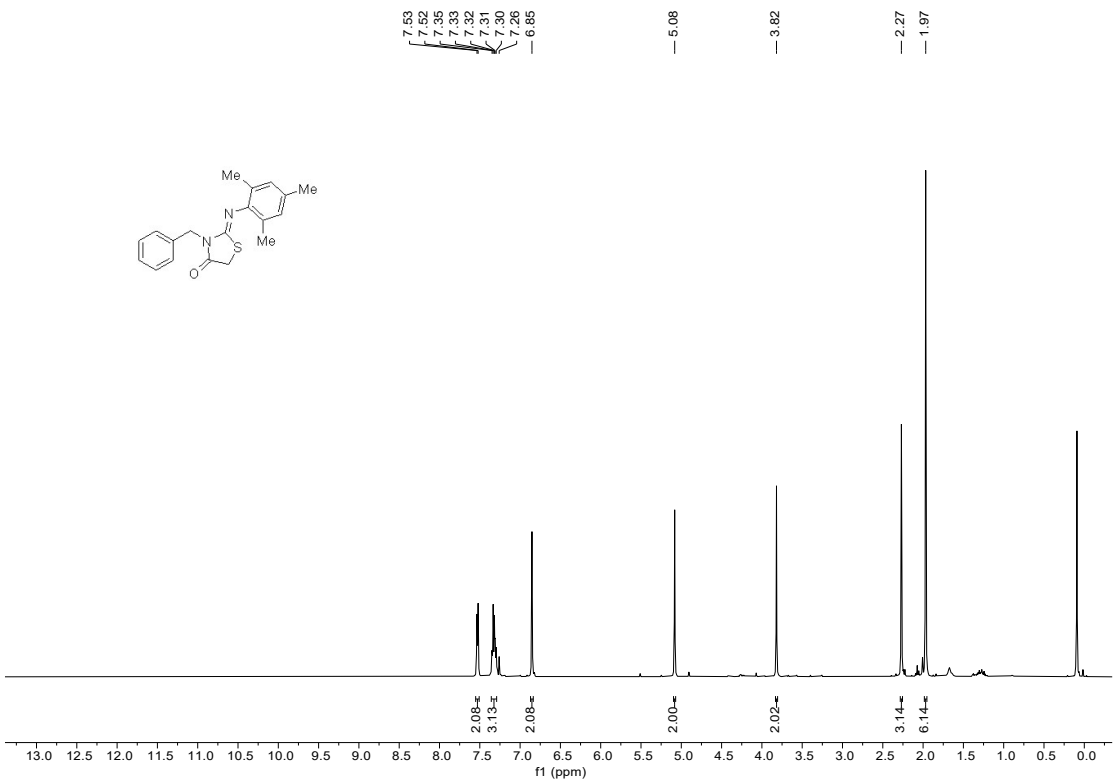
^{1}H NMR of **5k** in $CDCl_3$ (500 MHz)



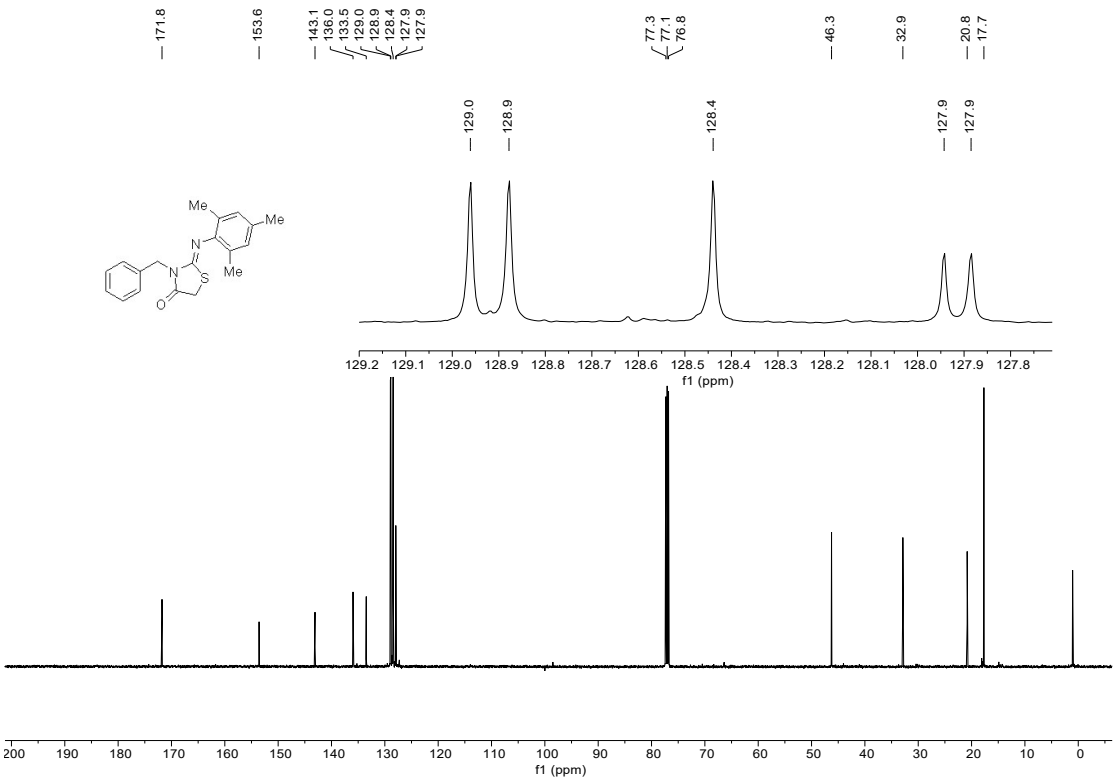
$^{13}C\{^{1}H\}$ NMR of **5k** in $CDCl_3$ (126 MHz)



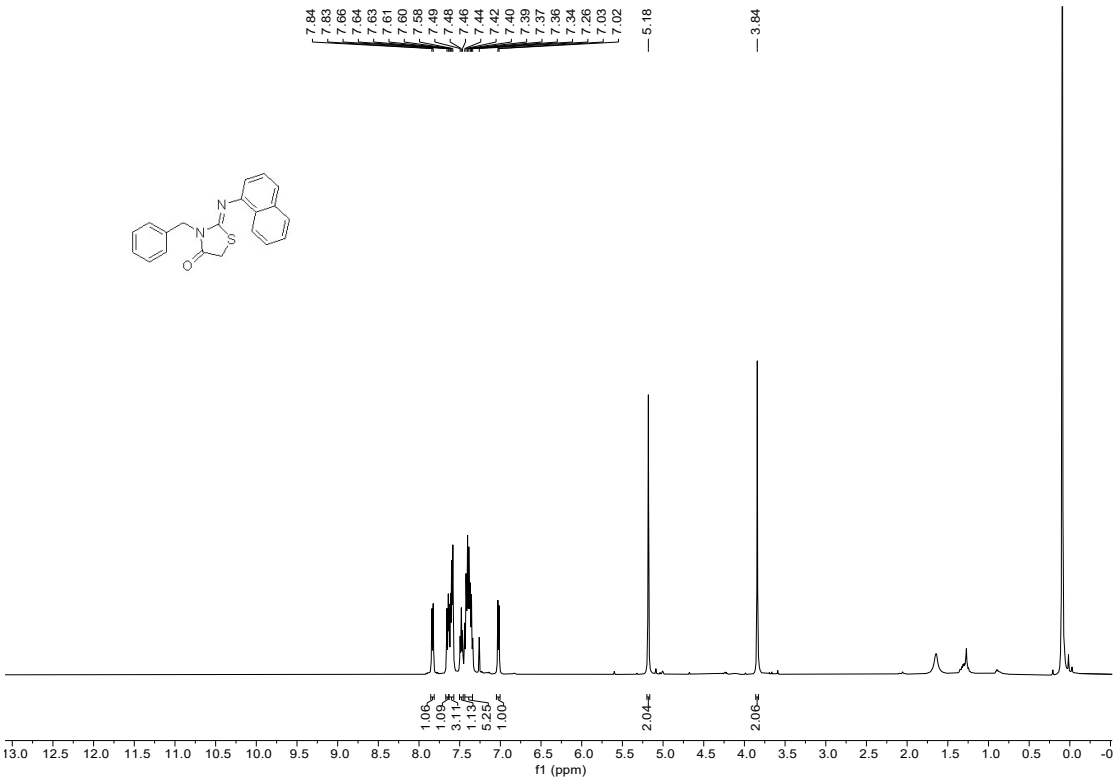
^{19}F NMR of **5k** in $CDCl_3$ (471 MHz)



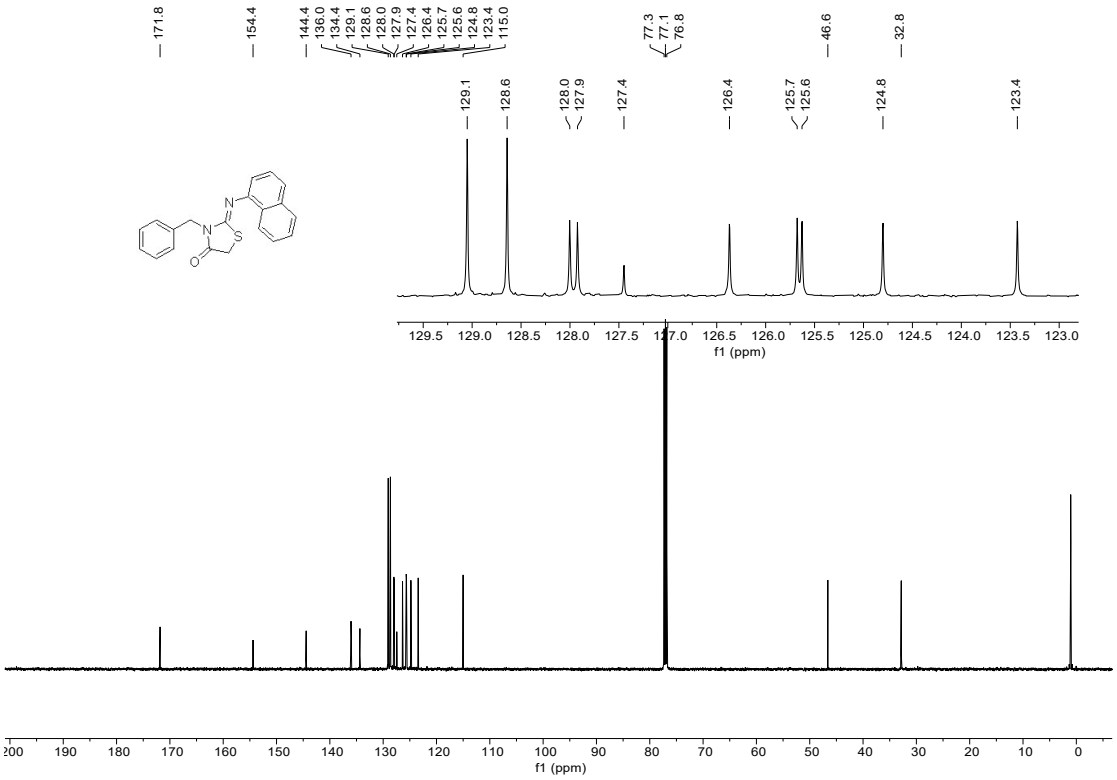
^{1}H NMR of **5l** in $CDCl_3$ (500 MHz)



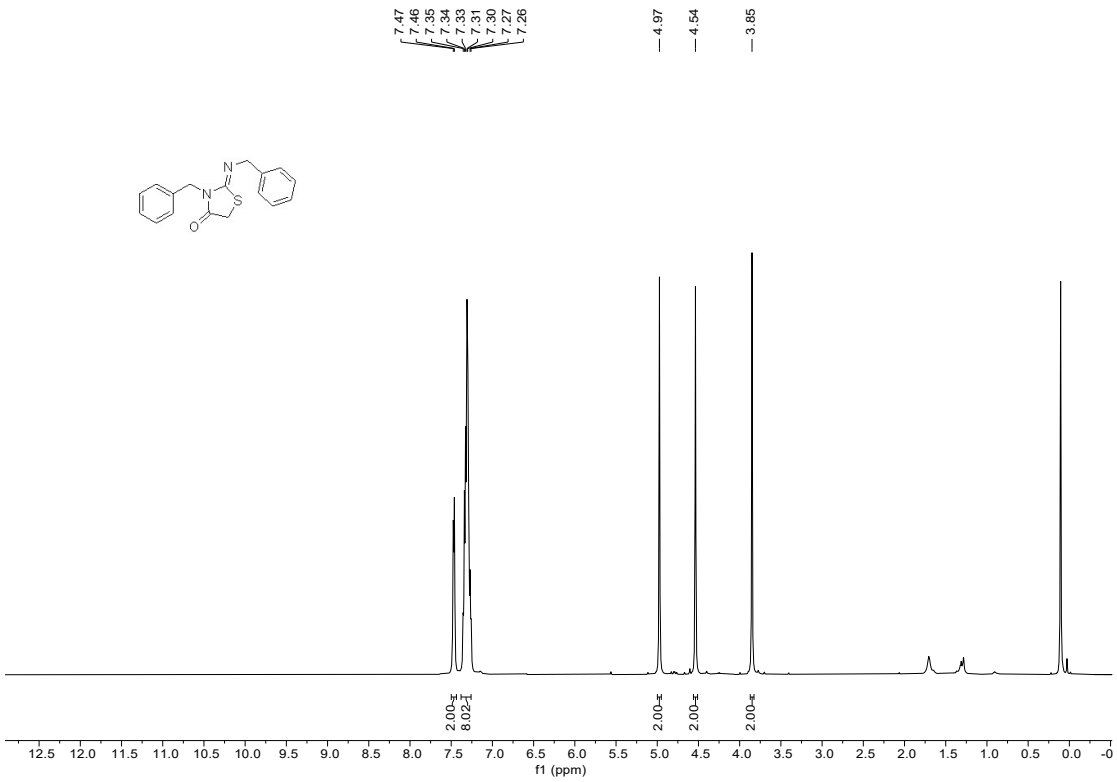
^{13}C{^{1}H} NMR of **5l** in $CDCl_3$ (126 MHz)



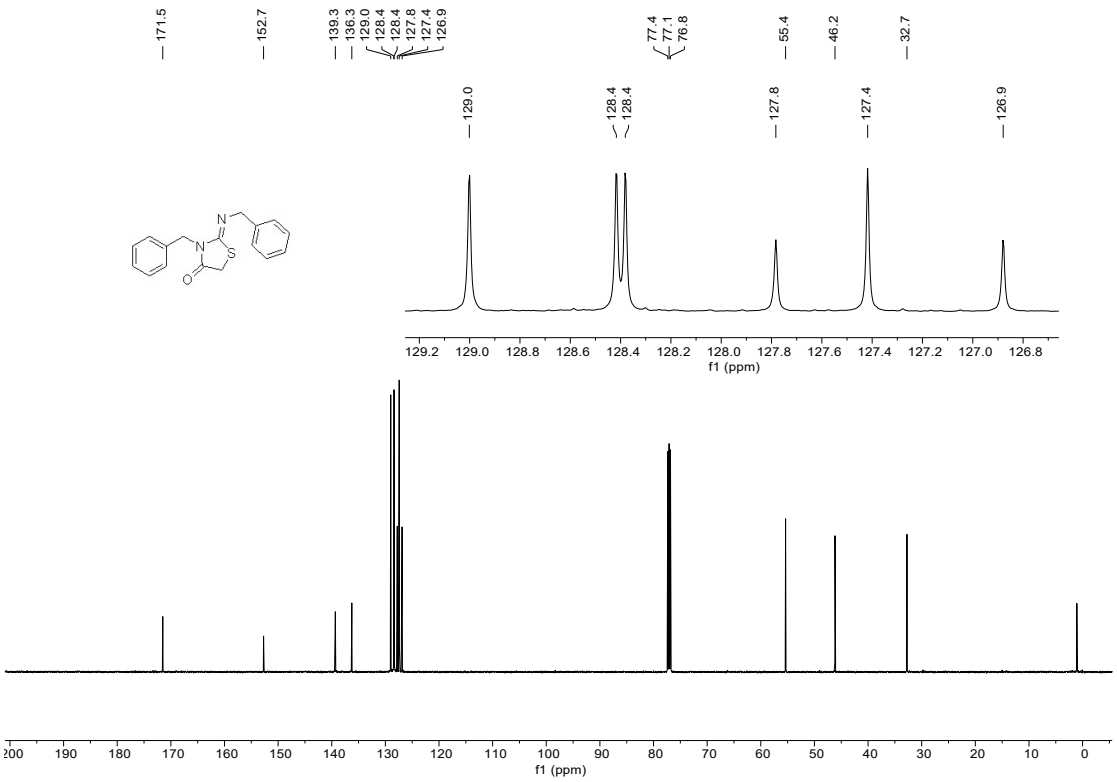
^{1}H NMR of **5m** in $CDCl_3$ (500 MHz)



^{13}C{^{1}H} NMR of **5m** in $CDCl_3$ (126 MHz)

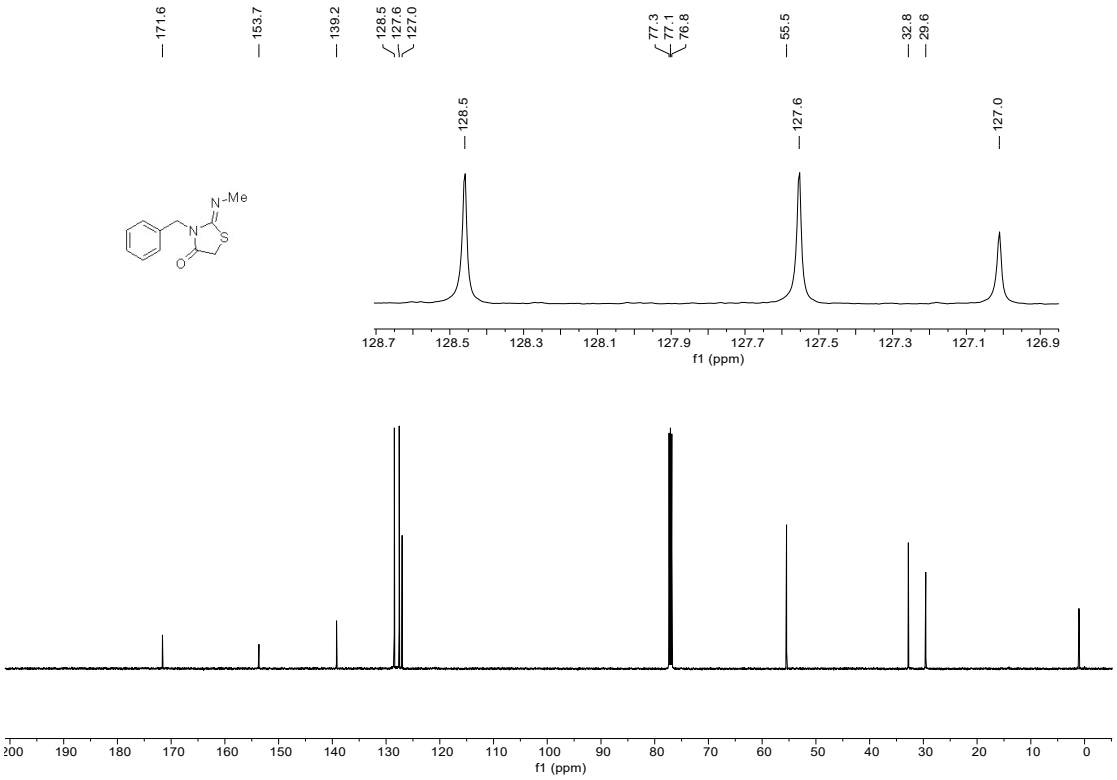


^{1}H NMR of **5n** in $CDCl_3$ (500 MHz)

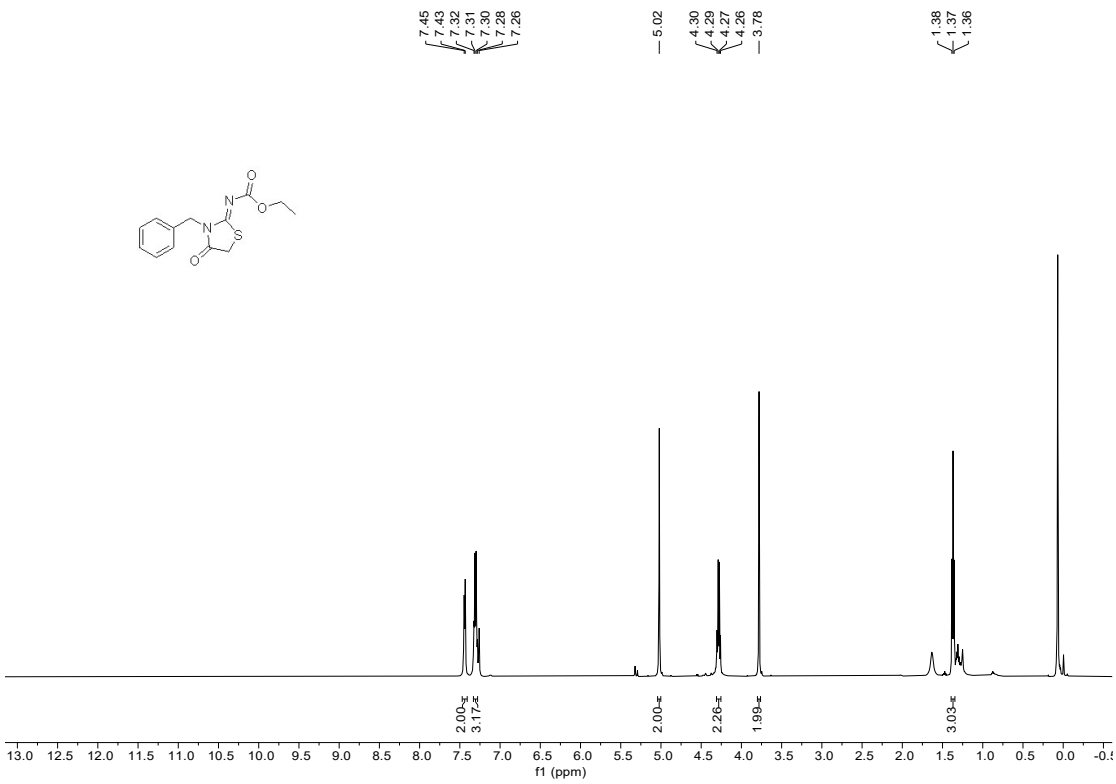


^{13}C{^{1}H} NMR of **5n** in $CDCl_3$ (126 MHz)

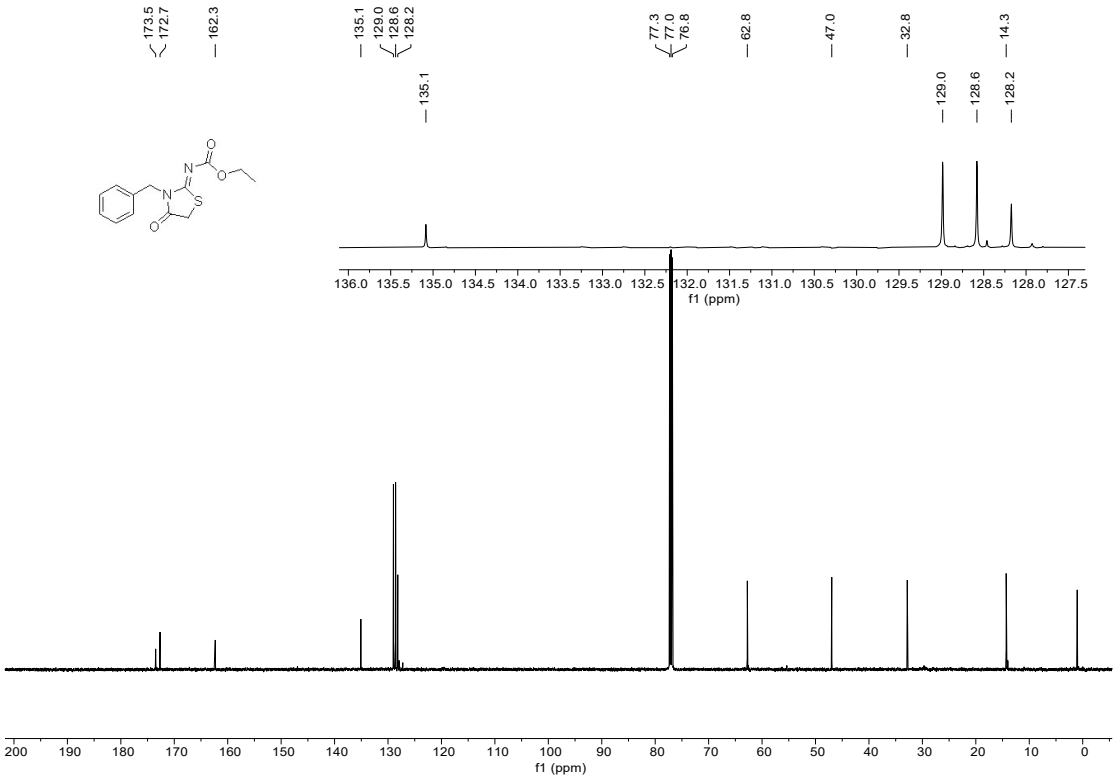
^{1}H NMR of **5o** in $CDCl_3$ (500 MHz)



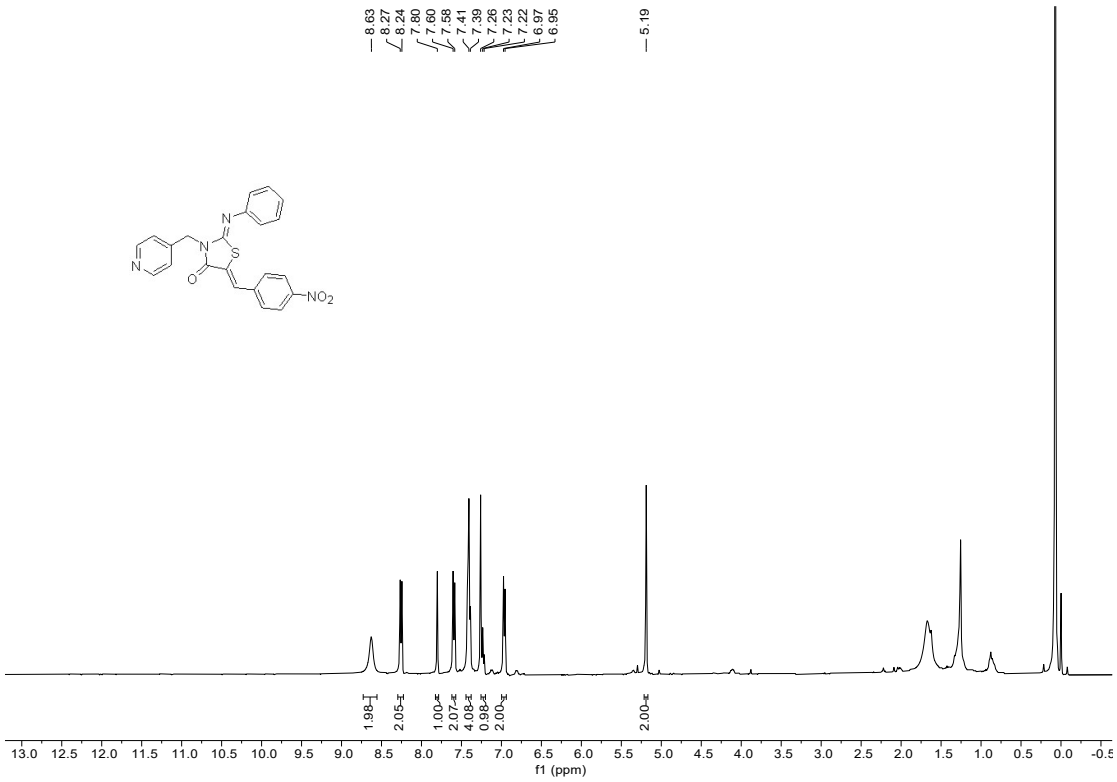
^{13}C{^{1}H} NMR of **5o** in $CDCl_3$ (126 MHz)



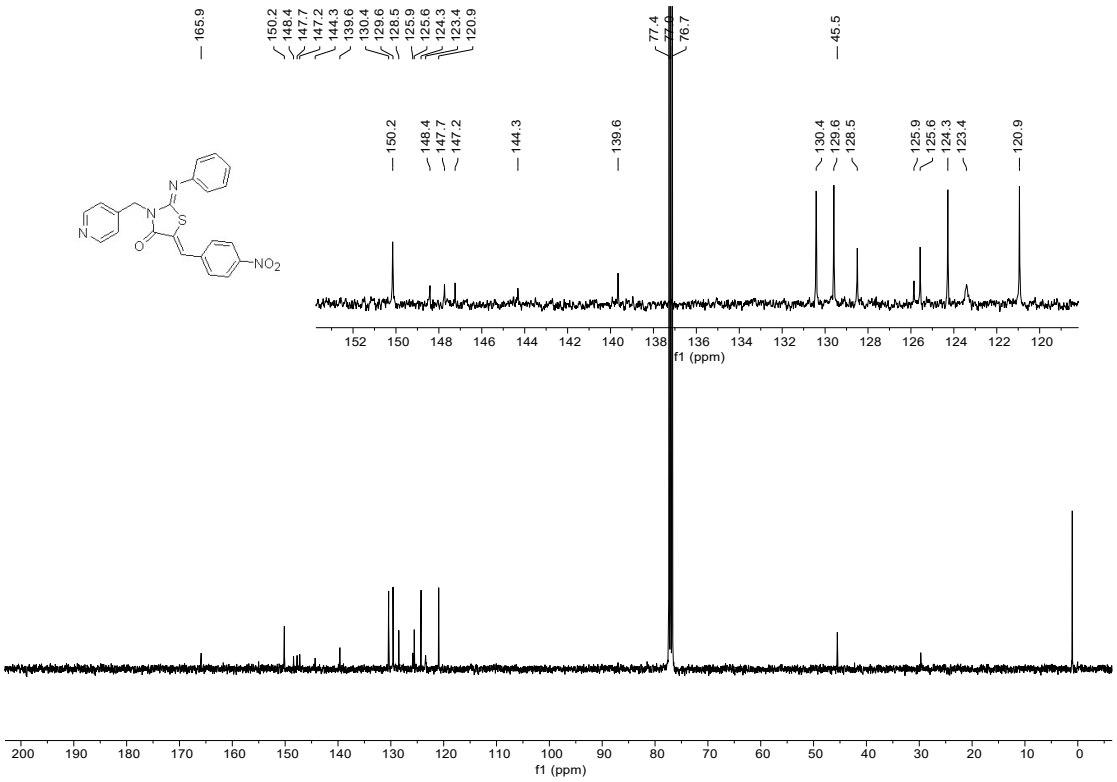
^{1}H NMR of **5p** in $CDCl_3$ (500 MHz)



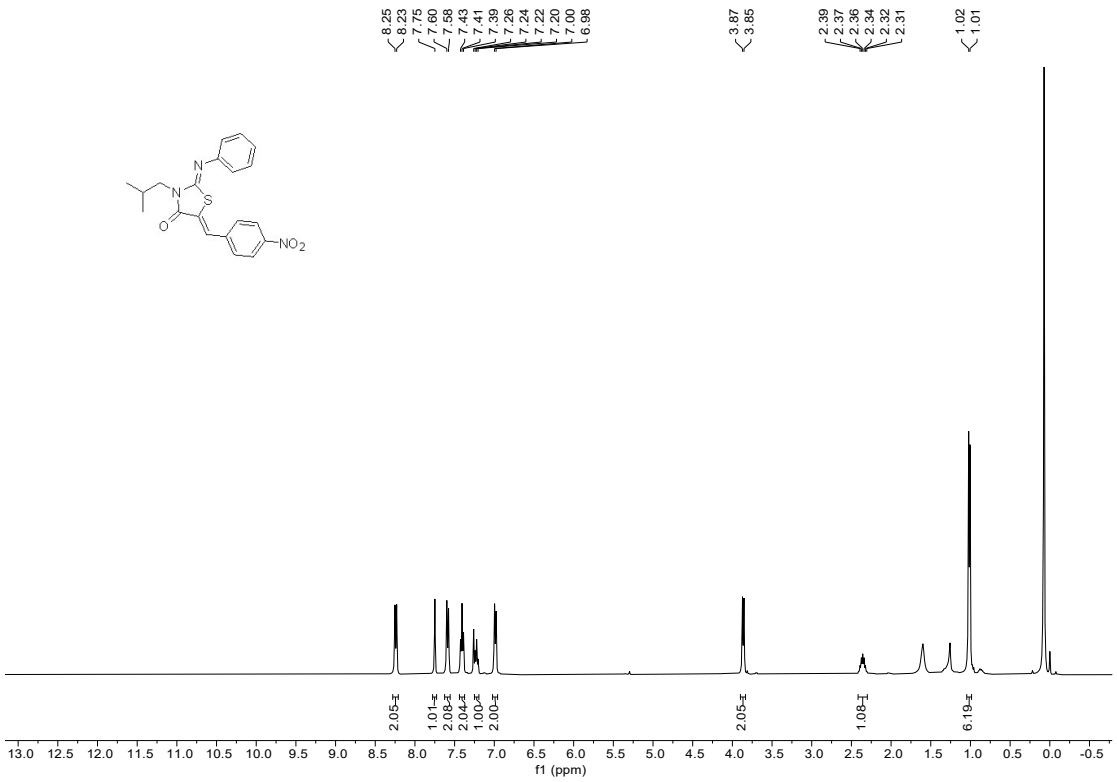
^{13}C{^{1}H} NMR of **5p** in $CDCl_3$ (126 MHz)



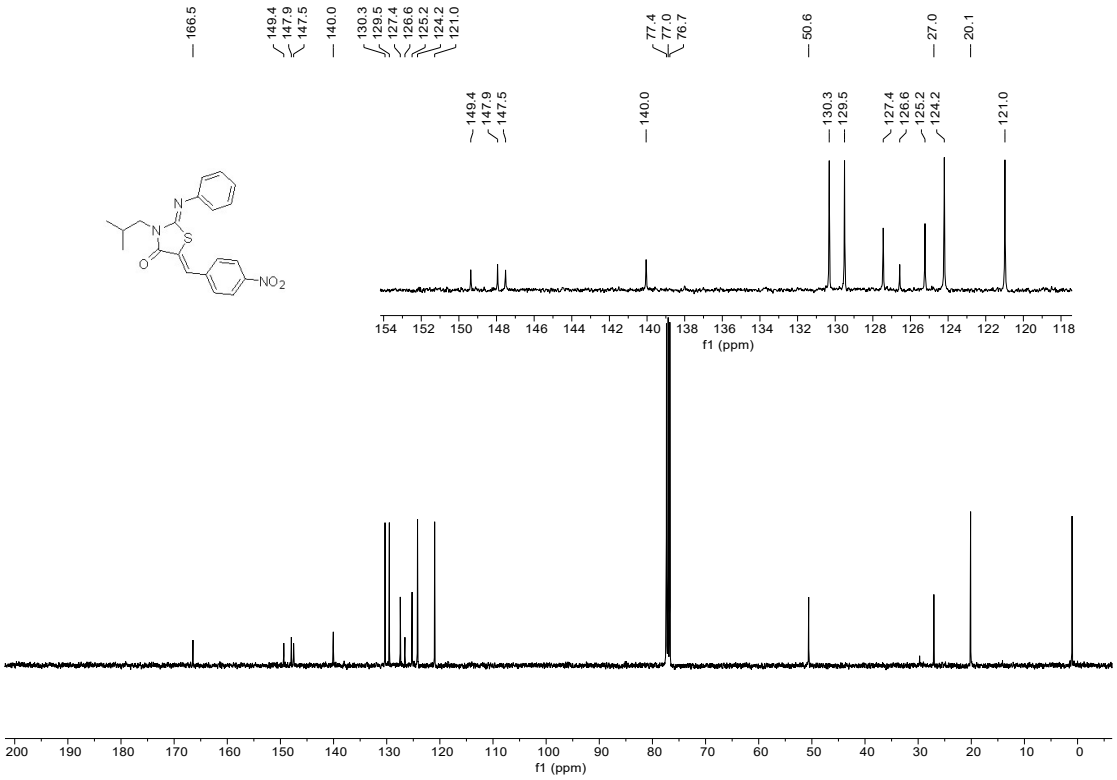
^{1}H NMR of **7** in $CDCl_3$ (400 MHz)



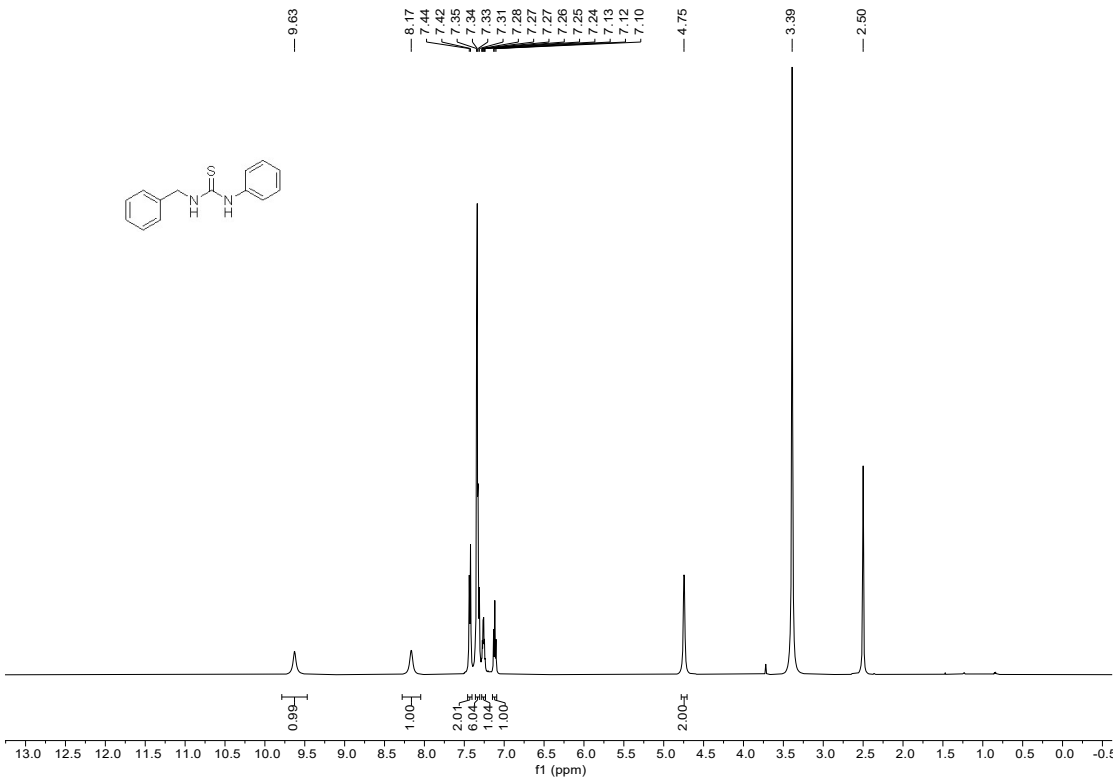
^{13}C{^{1}H} NMR of **7** in $CDCl_3$ (100 MHz)



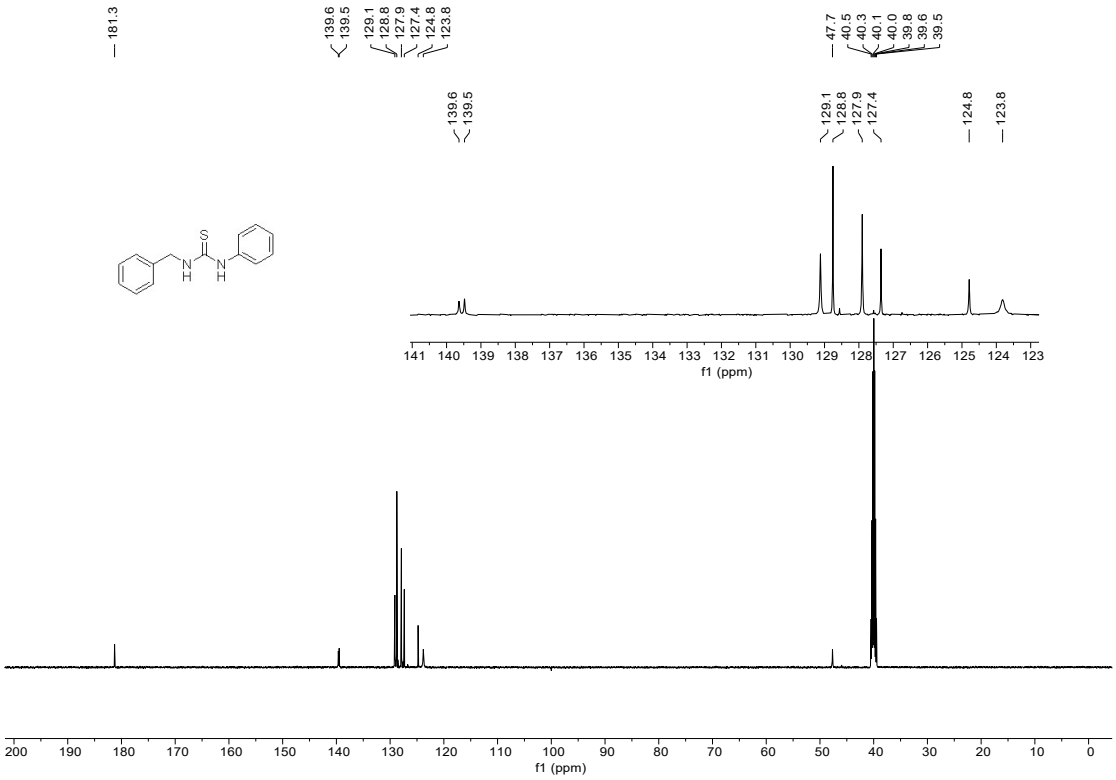
^{1}H NMR of **8** in $CDCl_3$ (400 MHz)



^{13}C{^{1}H} NMR of **8** in $CDCl_3$ (100 MHz)



^{1}H NMR of **9** in DMSO-d_6 (500 MHz)



^{13}C{^{1}H} NMR of **9** in DMSO-d_6 (126 MHz)