Novel ((3Z,5Z)-3,5-bis(phenylimino)-1,2-dithiolan-4-yl) and 3H-[1,2]dithiolo [3,4-*b*]quinolin-4(9H)-one heterocycles: an effective and facile green route

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Supporting information

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1.. General

The NMR spectra were recorded on 400M NMR spectrometer. In all cases $CDCl_3$ was used as solvent. Chemical Shifts are reported in *ppm* from tetramethylsilane with the solvent resonance as the internal standard (deuterochloroform: δ7.27 *ppm*). Data are reported as follows: chemical shifts, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz). The C and H elemental analyses were performed on a Perkin-Elmer elemental analyzer. Infrared spectra were recorded using pressed KBr plates in the 4000-400 cm^{-1} ranges. Crystals data were collected on four circle diffractometer with graphite monochromated Mo K_α radiation (λ = 0.71073Å). Intensities were corrected for Lorentz and polarization effects and empirical absorption, and the data reduction was carried out using SADABS program. The structure was solved by direct methods using SHELXS-97. All the non-hydrogen atoms were refined on F^2 anisotropically by full-matrix least squares method. The hydrogen atom positions were fixed geometrically at calculated distances and allowed to ride on the parent carbon atoms.

1-isothio-cyanatobenzene, a variety of 1-(substituted-phenyl)ethanone derivatives, organic solvent and other chemical reagents were obtained from commercial sources and used without further purification. The effects of reaction conditions introduced here were general method, not solvent-free synthesis route (**2** and **3**).

2. Study on the effects of reaction condition for ((3Z,5Z)-3,5-bis(phenylimino) -1,2-dithiolan-4-yl) derivatives 1

2-1 General Synthesis Process: To a 50 mL flask 0.01 mol of 1-(substituted-phenyl) ethanone derivatives in 20 mL of dioxane, 0.02 mol (1.12 g) of KOH was added with stirring at room temperature, then dropwise added 0.02 mol 1-isothio-cyanatobenzene dioxane solvent in three hours. The reaction was maintained six hours until the yellow precipitation was formed. The precipitation was filtered, washed with diethyl ether, dried in the air. The yellow single crystals suitable for X-ray measurements were obtained by recrystallized from mixture solvent (acetic ether **:** cyclohexane = 1 **:** 3). Compounds **(1)** are stable in the solid state and in any organic solvent. Compounds **1a** ~ **1j** were characterized by element analysis, IR, and ^{1}H NMR spectroscopy, and **1e**, **1h** and **1i** were also characterized by X-ray diffraction.

2-2 The effects of solvents.

Table S1 The effects of solvent to the reaction

Solvent	Yield（%）	Solvent	Yield（%）
1,4-dioxine	91.5	cyclohexane	40.0
tetrahydrofuran	71.0	petroleum ether	25.9
ethyl ether	65.5	pyridine	45.8
ethanol	0	benzene	42.4
methanol	0	toluene	40.7
water	0	n-hexane	35.5
DMF	12.7	ethyl acetate	0

2-3 The effects of the Base.

Table S2 The effects of base to the reaction

entry	base	solvent	Tem. (°)	Time (h)	Yield%
1	KOH	Dioxane	r.t.	6	91.5
2	K_2CO_3	Dioxane	r.t.	6	0
3	Na_2CO_3	Dioxane	r.t.	6	0
4	NaOH	Dioxane	r.t.	6	64.5
5	Na	Dioxane	r.t.	6	71.0
6	NaOEt	Dioxane	r.t.	5	0
7	$N(Et)_3$	Dioxane	r.t.	6	0

2-4 The effects of the temperature.

Table S3 The effection of temperature to the reaction

entry	base	solvent	Tem. (°)	Time (h)	Yield%
1	KOH	Dioxane	-10	6	81.4
2	KOH	Dioxane	0	6	85.7
3	KOH	Dioxane	25	6	91.5
4	KOH	Dioxane	40.	6	86.3
5	KOH	Dioxane	70.	6	77.4
6	KOH	Dioxane	100	5	56.9

2-5 The Element Analysis found for compounds (1)

Table S4 Element Analysis: Found (Calad) of compounds 1a-1j

Comp.	Formula	W	C/%	H/%	N/%	S/%
1 a	$C_{22}H_{15}ClN_2OS_2$	422.95	62.406(2.48)	3.55 (3.57)	6.59(6.62)	15.16(15.13)
1 b	$C_{22}H_{15}ClN_2OS_2$	422.95	62.55(62.55)	3.45 (3.58)	6.59(6.64)	15.19(15.13）
1c	$C_{22}H_{15}BrN_2OS_2$	467.40	56.44(56.65)	3.21 (3.24)	6.22(6.01)	13.65 (13.69)
1d	$C_{22}H_{15}FN_2OS_2$	406.49	65.15(65.01)	3.70 (3.72)	6.88(6.90)	15.72 (15.74)
1e	$C_{22}H_{14}Cl_2N_2OS_2$	457.39	57.80(57.90)	3.00 (3.09)	6.14(6.12)	13.89 (13.99)
1f	$C_{22}H_{14}Cl_2N_2OS_2$	457.39	57.80(57.90)	3.00 (3.09)	6.15(6.12)	13.89 (13.99)
1g	$C_{22}H_{14}Cl_2N_2OS_2$	457.39	57.81(57.90)	2.99 (3.09)	6.15(6.12)	13.89 (13.99)
1h	$C_{22}H_{13}Cl_2FN_2OS_2$	475.38	55.65(55.70)	2.66 (2.76)	5.96(5.91)	13.40 (13.46)
1i	$C_{23}H_{17}BrN_2OS_2$	481.42	57.60(57.50)	3.55 (3.57)	5.94(5.83)	13.20 (13.29)
1j	$C_{21}H_{15}N_3OS_2$	389.45	64.66(64.77)	3.88 (3.89)	10.88(10.80)	16.40 (16.43)

3. Study on the effects of reaction condition for 3H-[1,2]dithiolo[3,4-*b*] quinolin-4(9H)-one 2

3-1 General Synthesis Process: As an example, the synthesis of (3Z)-7-chloro-9-phenyl-3-(phenylimino)-3H-[1,2]dithiolo [3,4-*b*]quinolin-4(9H)-one **2e** is given to illustrate the general procedure. To a 50 mL flask 0.01 mol of 1-(2,4-dichlorophenyl) ethanone in 20 mL of anhydrous dioxane, 0.04 mol (1.75 g) KOH and a little metal K was added with stirring, refluxing for 10 mins, then dropwise added 0.02 mol 1-isothio cyanatobenzene in three hours. The reaction was maintained six hours until the yellow precipitation was formed. The precipitation was filtered, washed with diethyl ether, dissolved in the water, added extra $Ce(NO_3)_3$ aquo with stirring. The yellow precipitation was formed, isolated by filteration. The yellow single crystals suitable for X-ray measurements were obtained by recrystallized from mixture solvent (acetic ether **:**

petroleum ether = 1 **:** 2). We have gotten five 3H-[1,2]dithiolo[3,4-*b*] quinolin-4(9H)-one. Five compounds **2a, 2e, 2f, 2h** and **2i** were characterized by element analysis (See Table S7), IR, and ^{1}H NMR spectroscopy, and **2e** were also characterized by X-ray diffraction.

3-2 The effects of solvent

Table S5 the effects of solvent to the reaction

solvent	Yield（%）	solvent	Yield（%）
1,4-dioxine	50.0	cyclohexane	13.1
tetrahydrofuran	41.2	petroleum ether	11.1
ethyl ether	35.6	pyridine	34.1
n-hexane	12.1	benzene	17.2
DMF	10.7	toluene	14.3

3-3 The effects of the catalyst

Table S6 the effects of catalyst to the reaction

catalyzer	Yield（%）	catalyst	Yield（%）
$Ce(NO_3)_3$	63.0	$CuCl_2$	0
$Ce(NO_3)_4$	0	$FeCl_3$	15
$CeCl_3$	59.0	H_2O_2	0
$GdCl_3$	56.3	$Pb(NO_3)_4$	0
$NaNO_3$	4.6	air	4.3

3-4 The Element Analysis found for compound (2)

Table S7 Element Analysis: Found (Calad) of compounds 2a~2e

Comp	Formula	W	C/%	H/%	N/%	S/%
2a	$C_{22}H_{14}N_2OS_2$	386.49	68.31(68.37)	3.70 (3.65)	7.30 (7.25)	16.50(16.55)
2e	$C_{22}H_{13}ClN_2OS_2$	420.93	62.75 (62.78)	3.10 (3.11)	6.68 (6.66)	15.23(15.20)
2f	$C_{22}H_{13}ClN_2OS_2$	420.93	62.67 (62.78)	3.10 (3.11)	6.68 (6.66)	15.25(15.20)
2h	$C_{22}FH_{12}ClN_2OS_2$	438.92	60.05 (60.20)	2.66 (2.76)	6.40 (6.38)	14.56(14.58)
2i	$C_{23}H_{16}N_2OS_2$	400.51	68.80 (68.97)	3.99 (4.03)	7.02 (6.99)	15.96(15.97)

4. The comparing result for solvent-free method and general method.

Table S8 The comparing result.

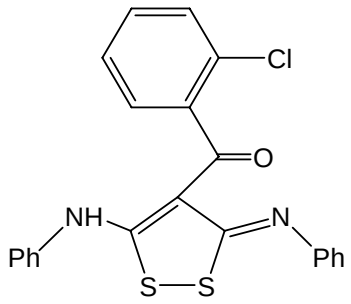
Entry	Condition	solvent	Temp. (°C)	React. Time	Yield%
1a	General	Dioxane	Room Temp.	6 hour	73.0
	Solvent-free	No	Room Temp.	10 minutes	96.0
1b	General	Dioxane	Room Temp.	6 hour	91.5
	Solvent-free	No	Room Temp.	10 minutes	88.0
1e	General	Dioxane	Room Temp.	6 hour	73.5
	Solvent-free	No	Room Temp.	15 minutes	68.0
1f	General	Dioxane	Room Temp.	6 hour	75.0
	Solvent-free	No	Room Temp.	15 minutes	65.0
1j	General	Dioxane	Room Temp.	6 hour	91.5
	Solvent-free	No	Room Temp.	15 minutes	86.0

5. Spectra data

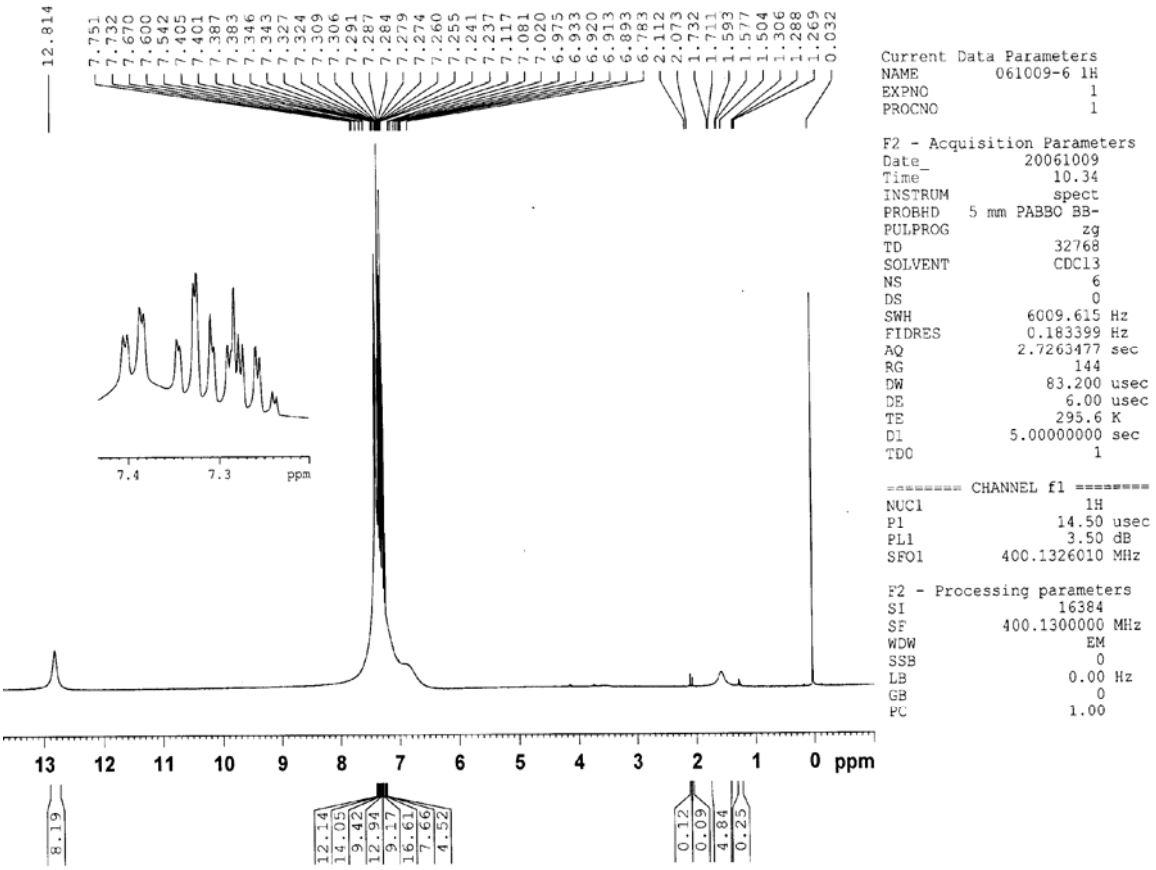
5-1 Spectra data for ((3Z,5Z)-3,5-bis(phenylimino)-1,2-dithiolan-4-yl) derivatives 1

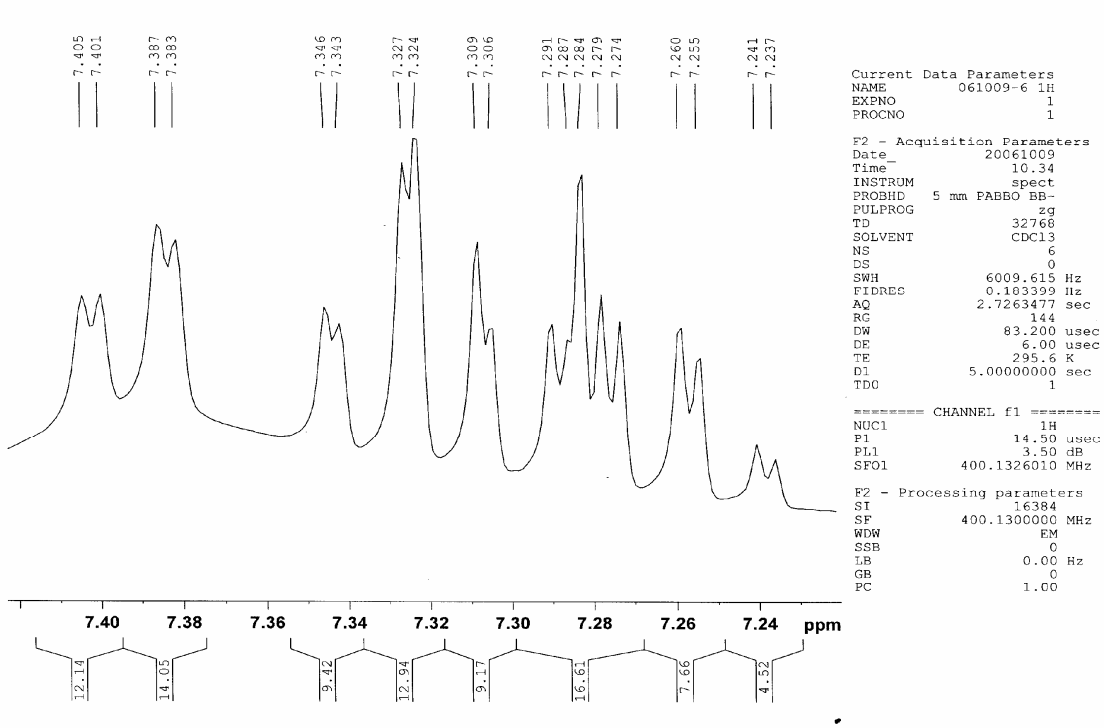
1a:

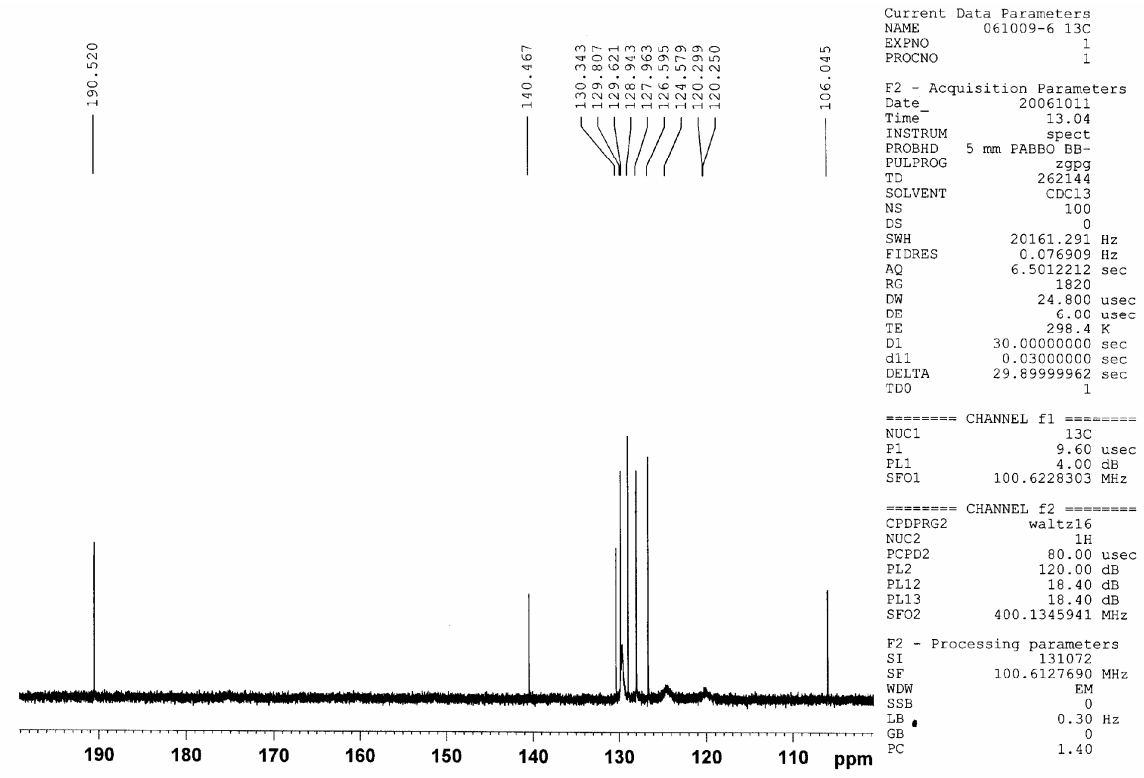
(2-chlorophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 73%. mp 170-172 ^{o}C; ^{1}H NMR (400Hz, $CDCl_3$): δ12.814(s, 1H N-H); 7.751-6.783(m,15H -C=C-H).; IR (ν_{max}, cm^{-1}): 3446*w*, N-H）; 1637s, -C=O）; 1583(s, -C=N-）; 1544 (s, N-H); 1191 (m, S-C).EA (Anal. Calc. (%) for $C_{22}H_{15}ClN_2OS_2$):C 62.48 H 3.57 N 6.62 S 15.13; Found (%):C 62.406, H 3.55,N 6.59 S 15.16.

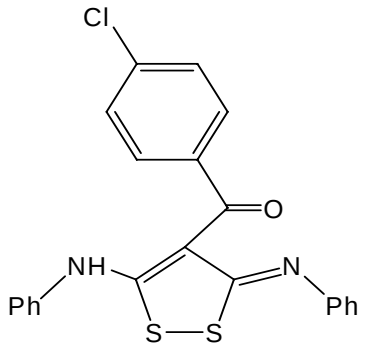




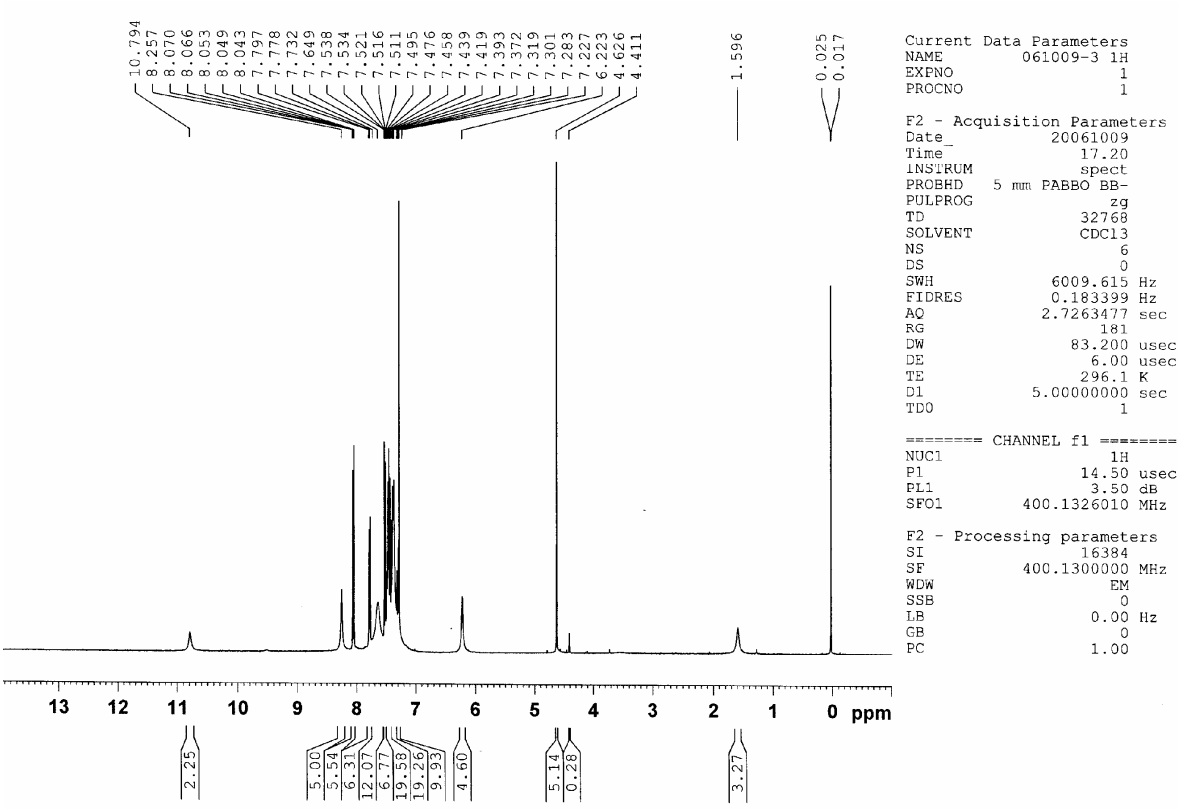


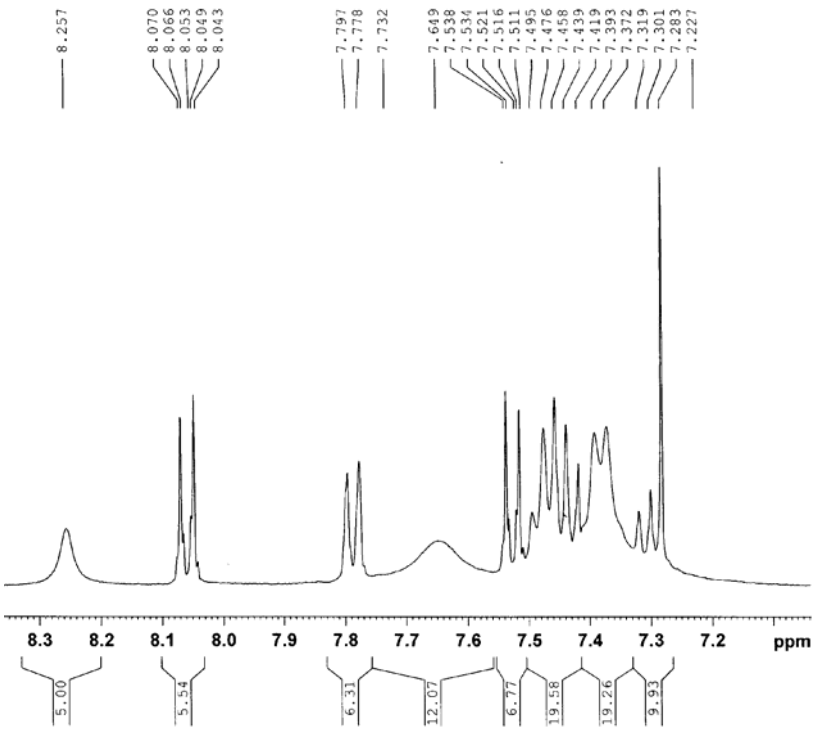
1b:

(4-chlorophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 91.5%. mp 148-150 ^{o}C; ^{1}H NMR (400Hz, $CDCl_3$): δ10.794(s, 1H N-H); 8.257-6.223(m, 15H -C=C-H).; IR (ν_{max}, cm^{-1}): 3443（*w*, N-H）; 1608（s, -C=O）; 1591(S, -C=N-); 1517 (s, N-H); 1212(m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{15}ClN_2OS_2$):C 62.55 H 3.58 N 6.64 S 15.13; Found (%):C 62.55, H 3.45, N 6.59 S 15.19.



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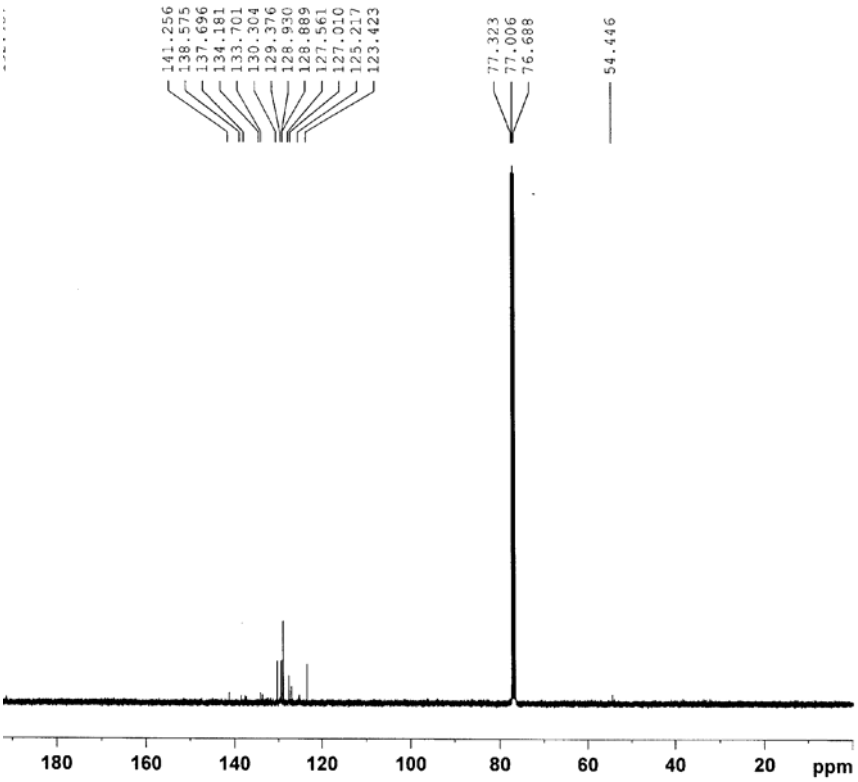


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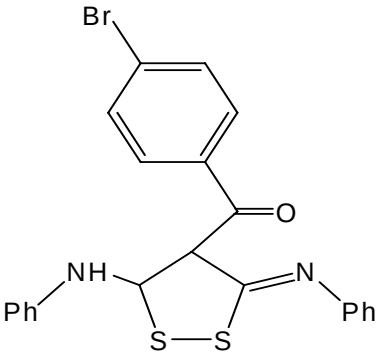
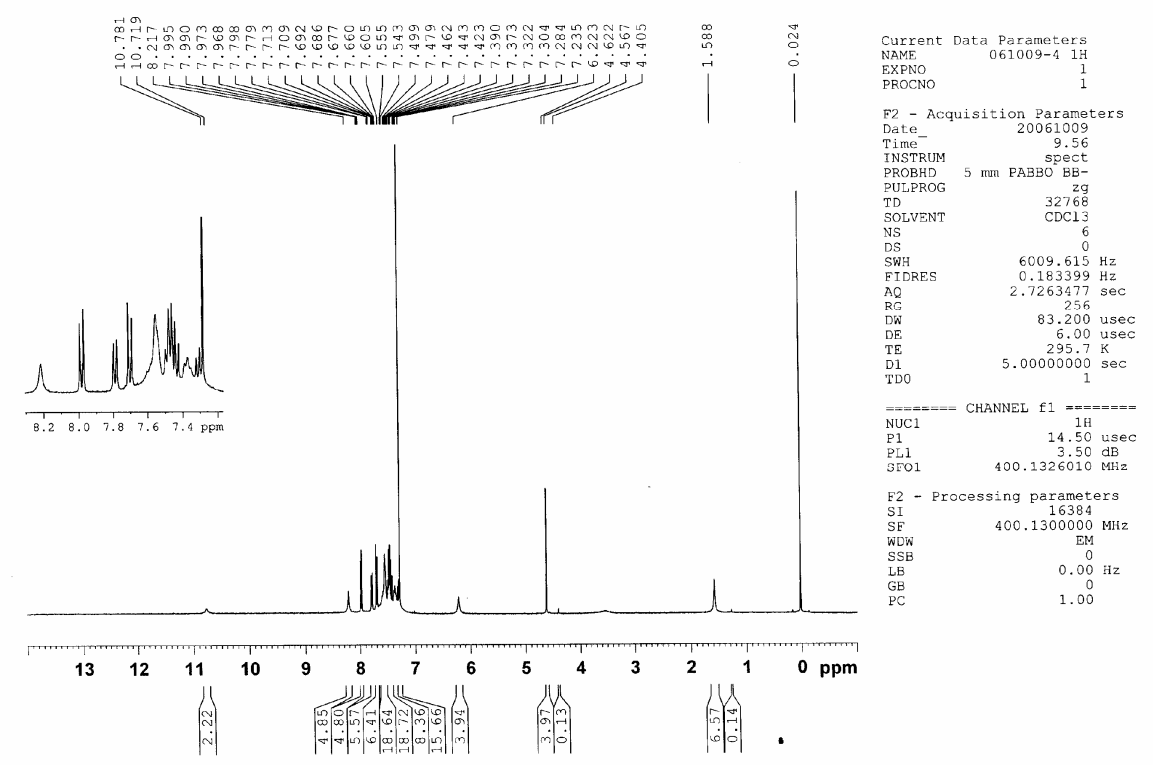
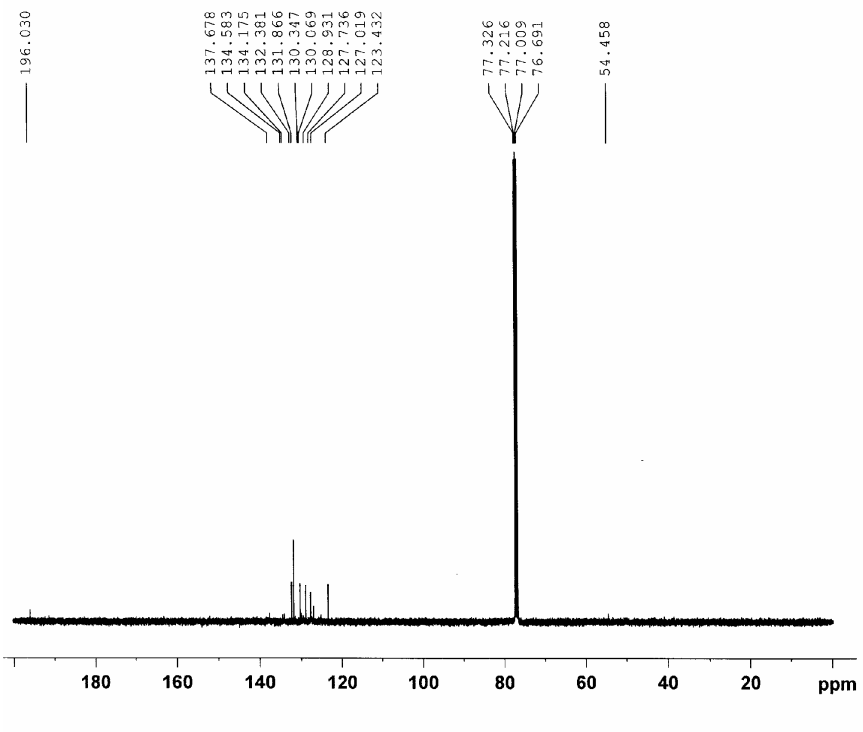
1c:

(4-bromophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 93%. mp 154-156°C; ^{1}H NMR (400Hz, $CDCl_3$): δ10.781(s, 1H N-H); 8.217-6.223(m, 15H -C=C-H).IR(ν_{max}, cm^{-1}): 3441(w, N-H); 1608(s, -C=O）; 1590(S, -C=N-）; 1515 (s, N-H); 1212(m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{15}BrN_2OS_2$):C 56.65 H 3.24 N 6.01 S 13.69; Found (%):C 56.44, H 3.21,N 6.22 S 13.65.



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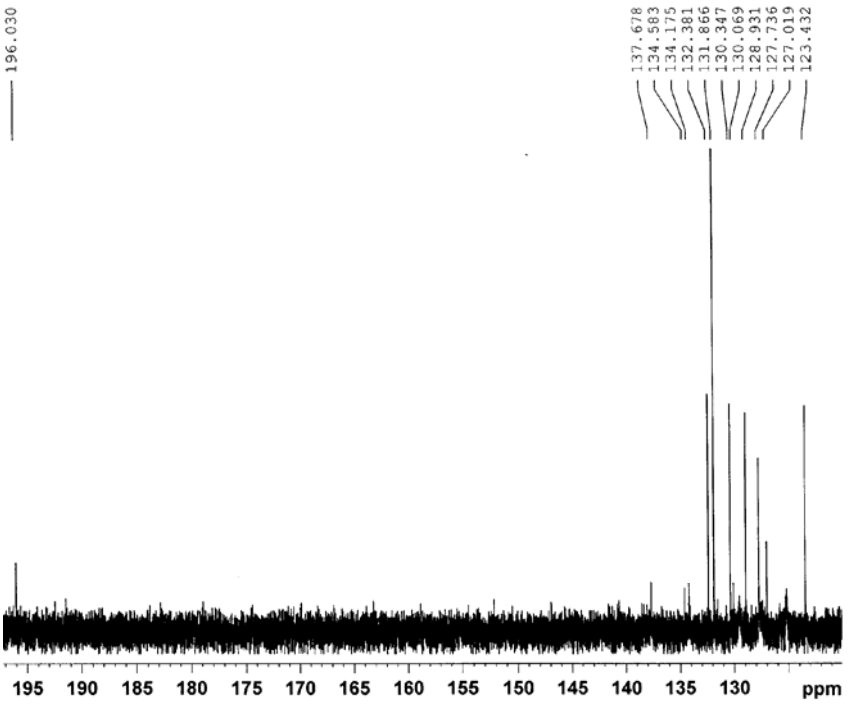


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DELTA        29.89999962 sec
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PL1                 4.00 dB
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PL13               18.40 dB
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SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
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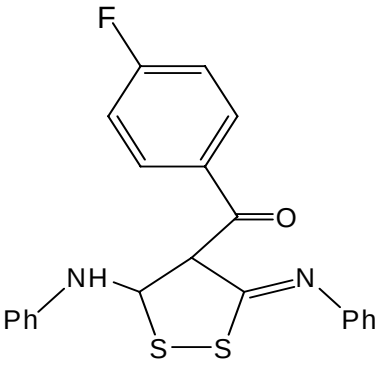
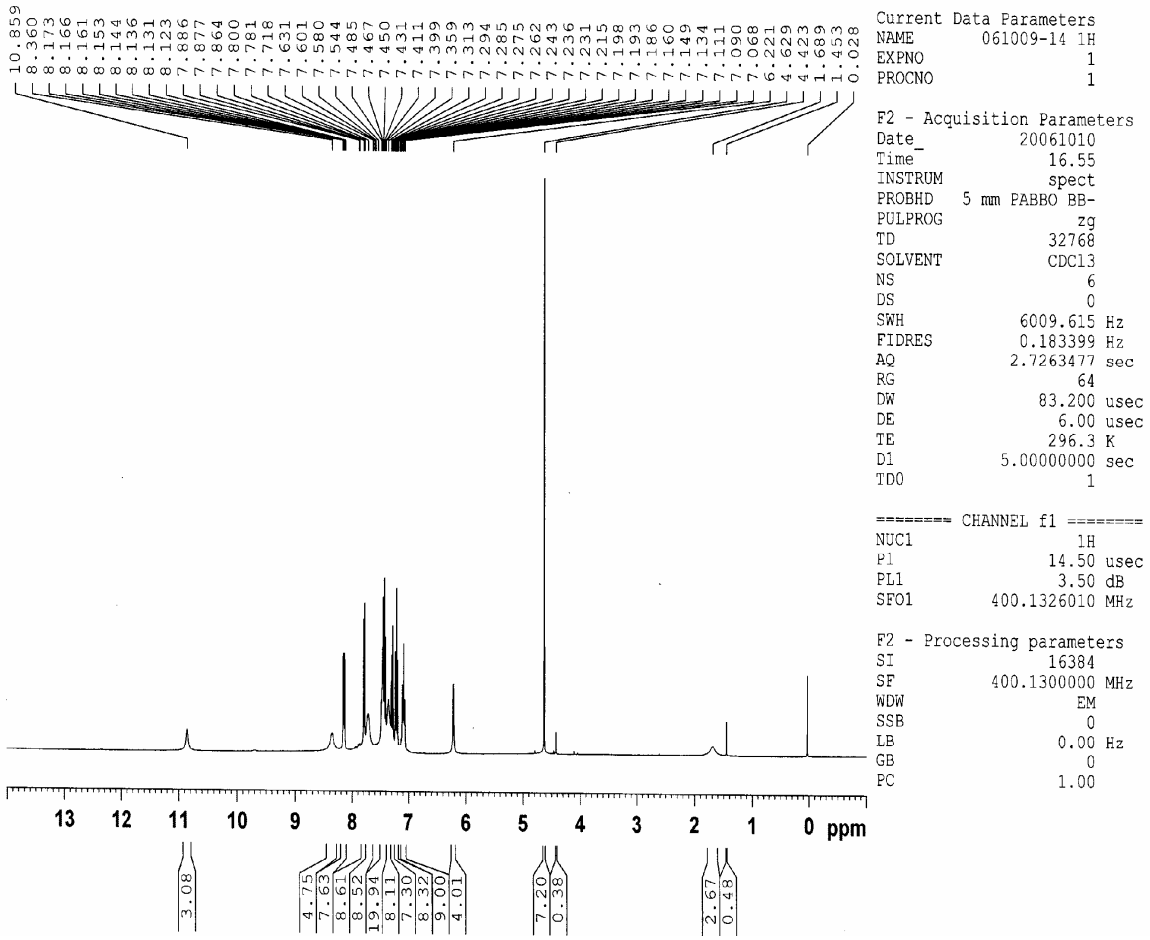
1d:

(4-fluorophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 56%. mp 144-146°C; ^{1}H NMR (400Hz, $CDCl_3$): δ10.829(s, 1H, N-H); 8.36-6.221(m,15H, -C=C-H). IR(ν_{max}, cm^{-1}): 3448(w, N-H）；1615 (s, -C=O); 1592 (S, -C=N-); 1509 (s, N-H); 1205(m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{15}FN_2OS_2$):C 65.01 H 3.72 N 6.90 S 15.74; Found (%):C 65.15, H 3.70, N 6.88 S 15.72.

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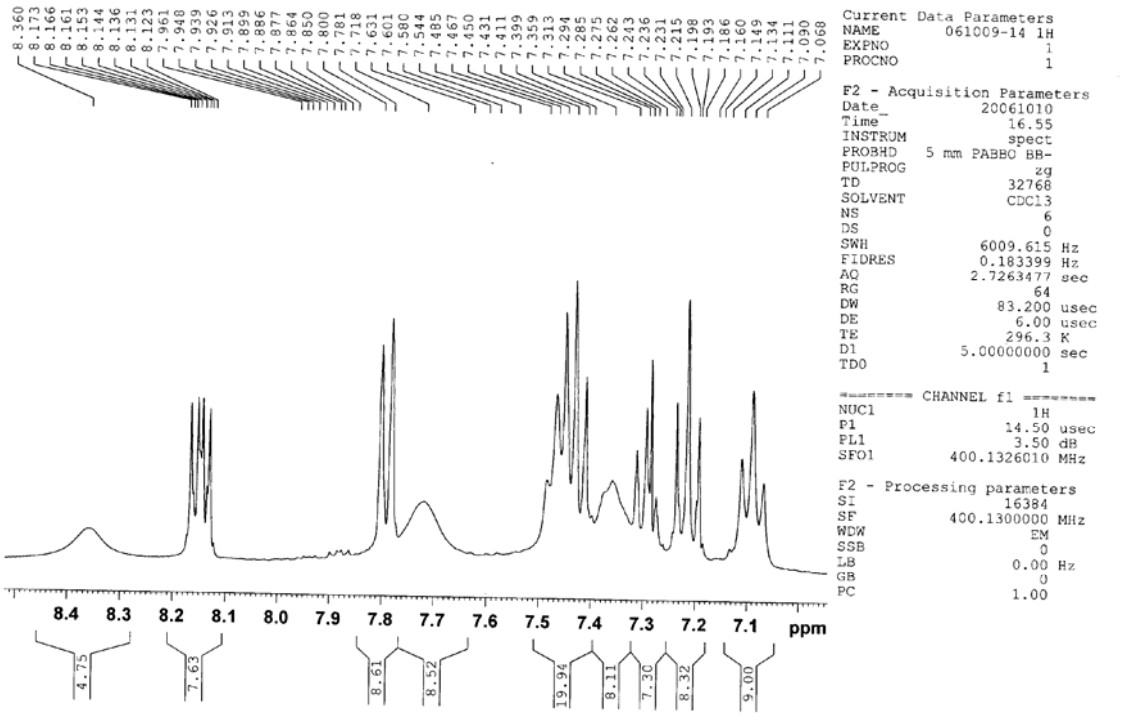
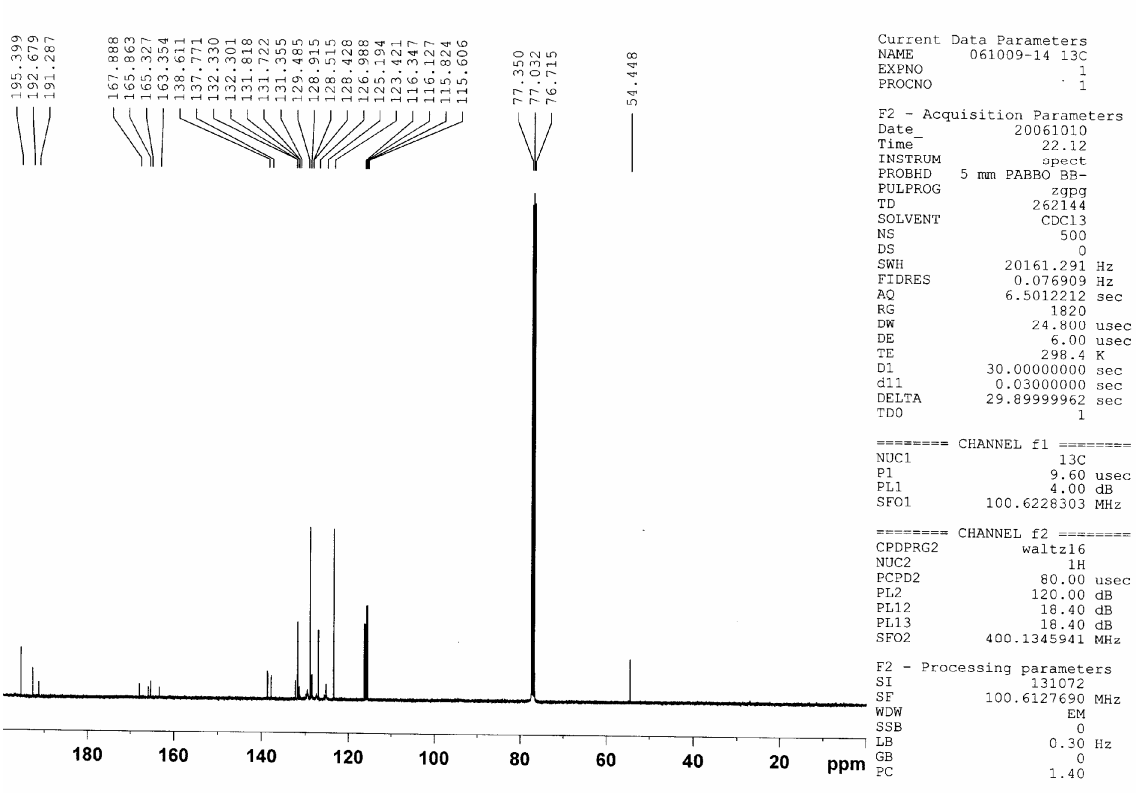
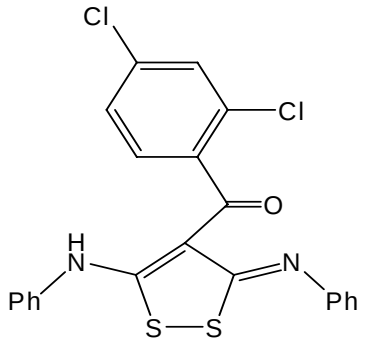


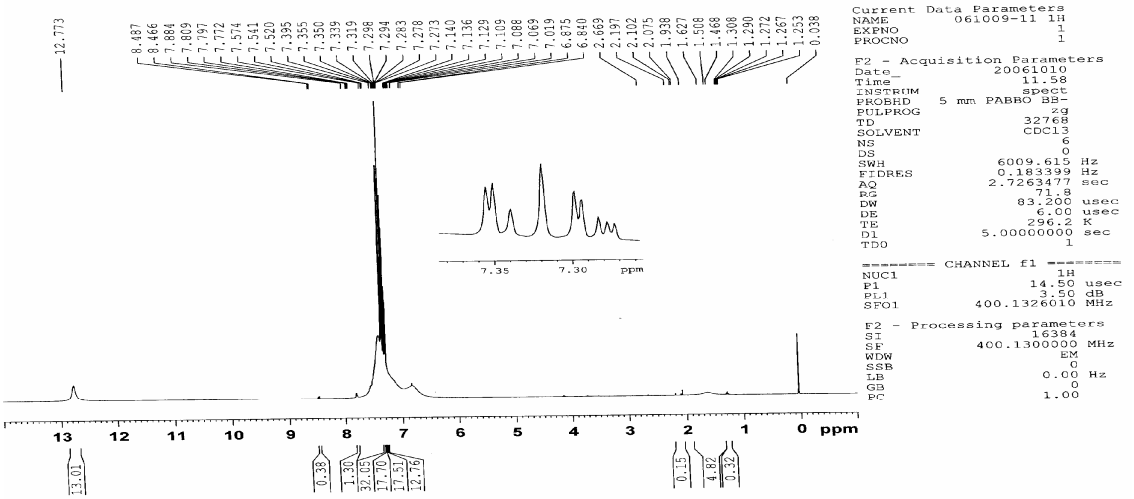


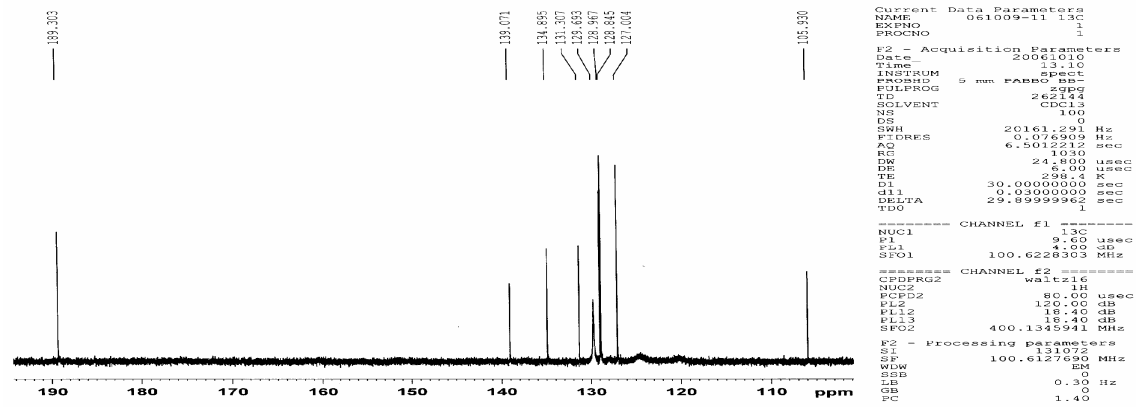
1e:

(2,4-dichlorophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



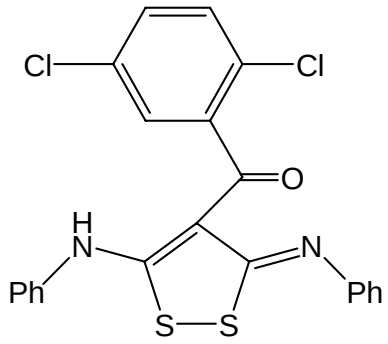
Yield: 73.5%. mp 164-166°C; ^{1}H NMR (400Hz, $CDCl_3$): δ12.773(s, 1H N-H); 8.487-6.840(m, 14H -C=C-H).IR(ν_{max}, cm^{-1}): 3430(w, N-H); 1606(s, -C=O); 1585(S, -C=N-); 1533(s, N-H); 1192(m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{14}Cl_2N_2OS_2$):C 57.90 H 3.09 N 6.12 S 13.99; Found (%):C 57.80, H 3.00,N 6.14 S 13.89.



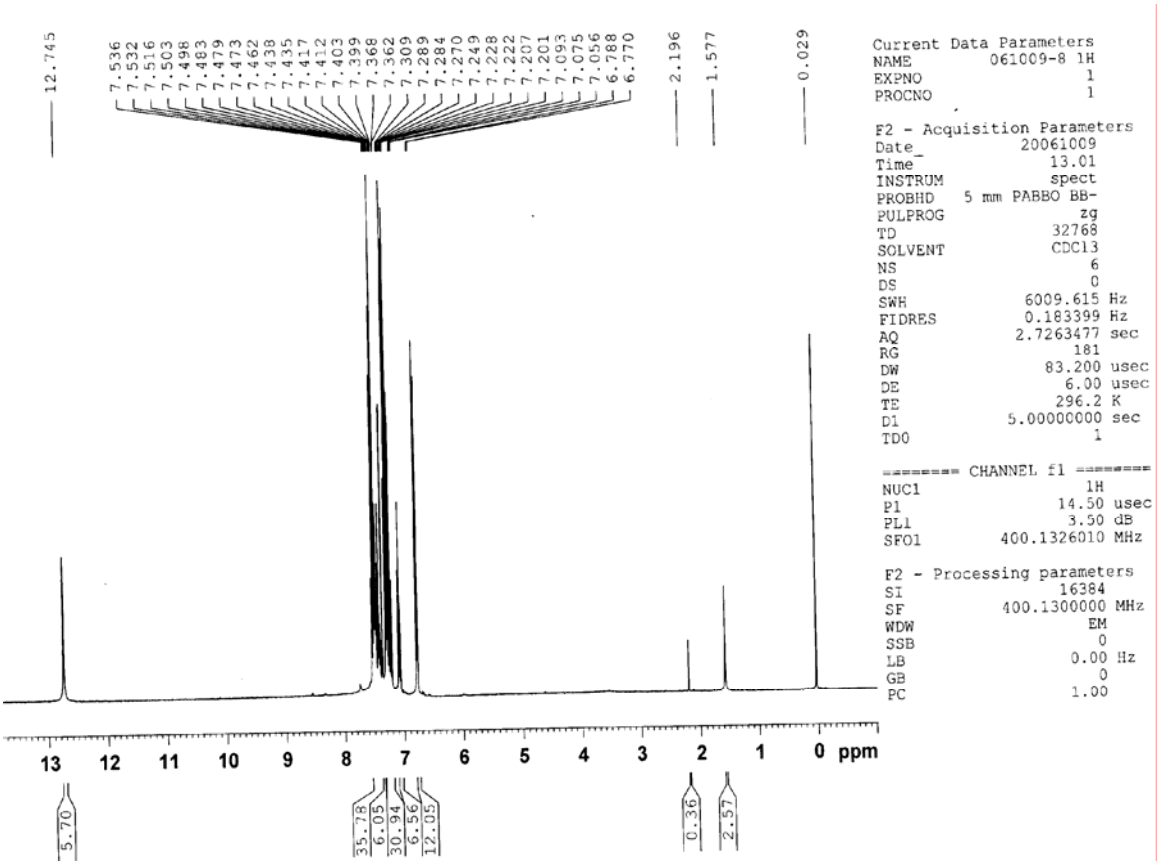


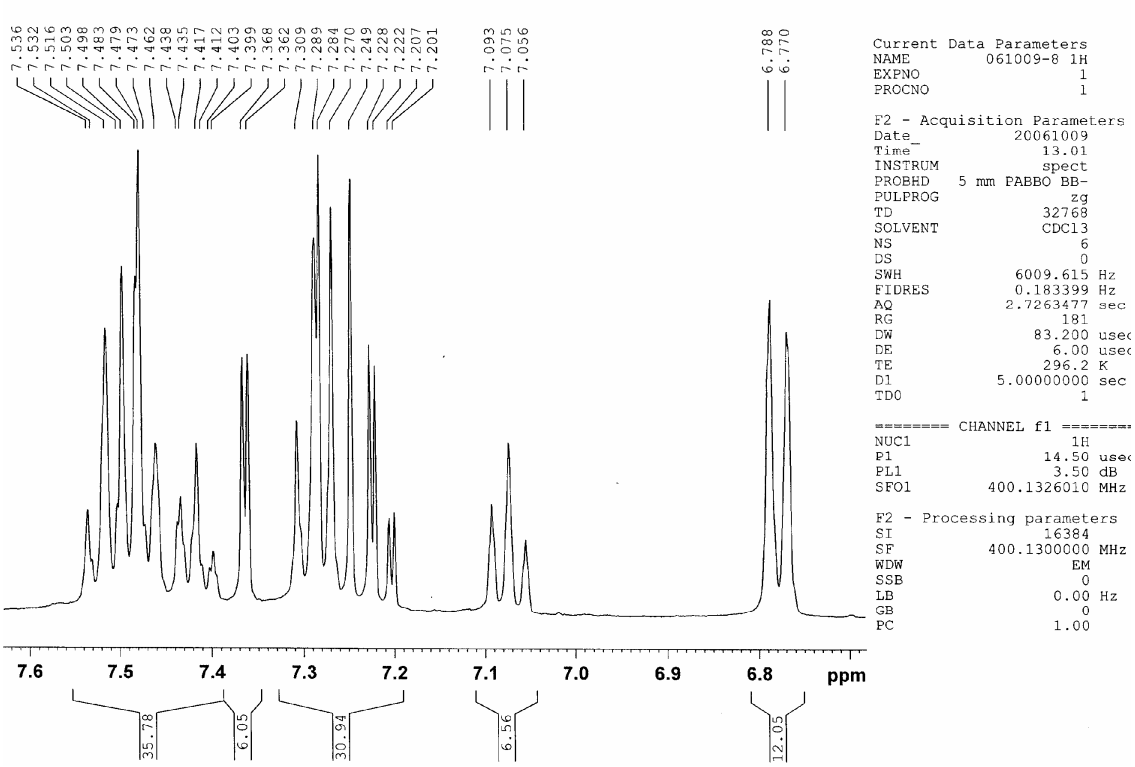
1f:

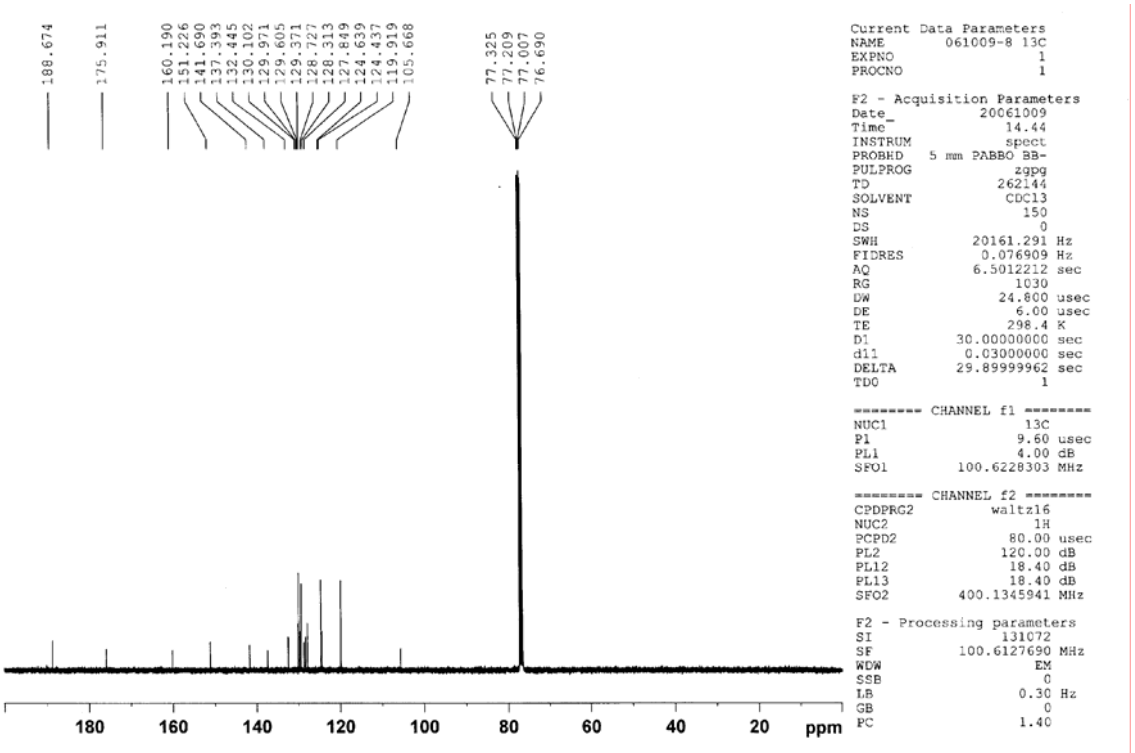
(2,5-dichlorophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 75%. mp 173-175°C; ^{1}H NMR (400MHz, $CDCl_3$): δ12.745(s, 1H N-H); 7.536-6.77(m, 14H -C=C-H).IR(ν_{max}, cm^{-1}): 3432, 3129(w, N-H); 1616(s, -C=O); 1581 (S, -C=N-); 1533(s, N-H); 1184 (m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{14}Cl_2N_2OS_2$):C 57.90 H 3.09 N 6.12 S 13.99; Found (%):C 57.80, H 3.00, N 6.15 S 13.89.

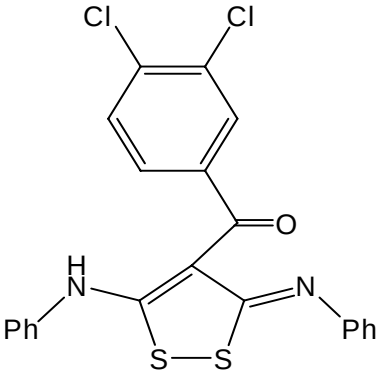




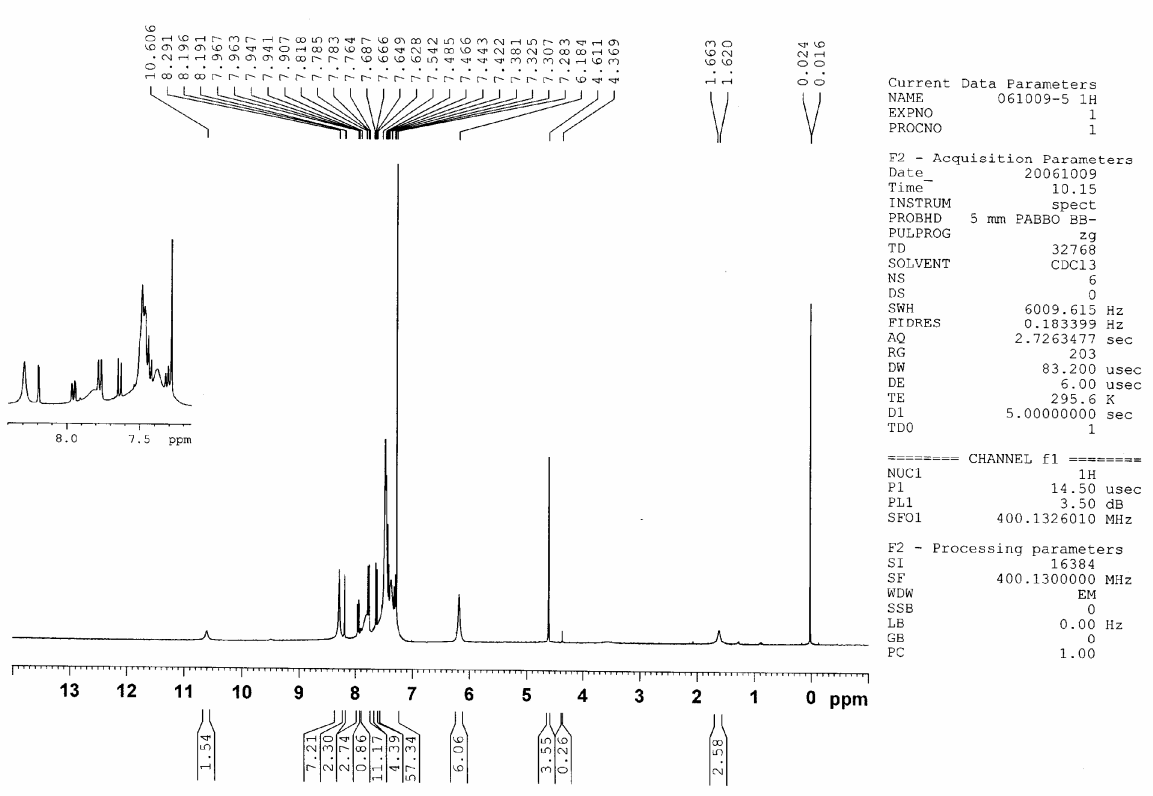


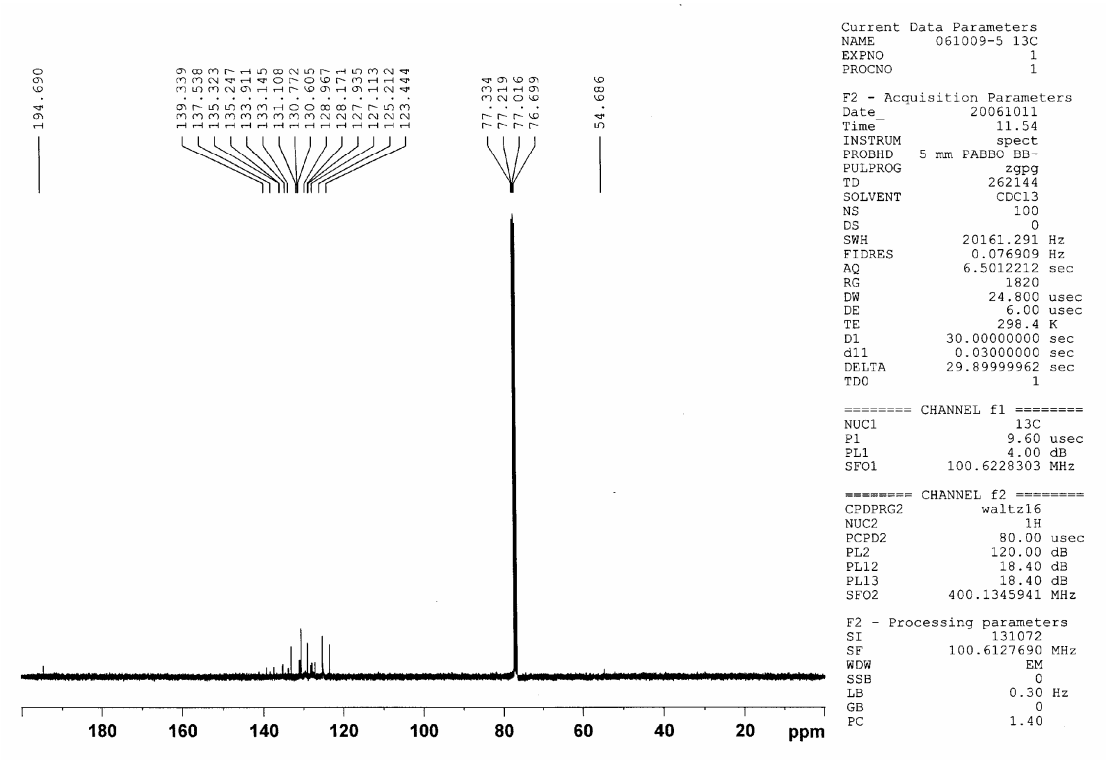
1g:

(3,4-dichlorophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 95%. mp 170-172°C; ^{1}H NMR (400MHz, $CDCl_3$): δ10.606(s, 1H N-H); 8.291-6.184(m, 14H -C=C-H). IR(ν_{max}, cm^{-1}): 3434(w, N-H); 1611 (s, -C=O); 1593 (S, -C=N-); 1521(s, N-H); 1211(m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{14}Cl_2N_2OS_2$):C 57.90H 3.09 N 6.12 S 13.99; Found (%):C 57.81, H 2.99,N 6.15 S 13.89.



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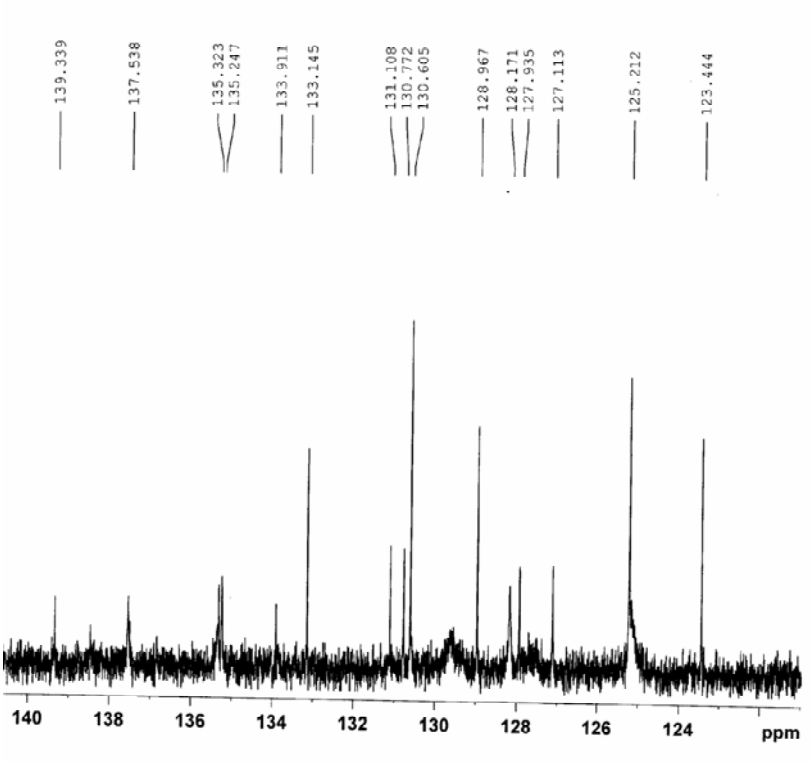
Current Data Parameters
NAME        061009-5 13C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20061011
Time              11.54
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                262144
SOLVENT             CDCl3
NS                    100
DS                      0
SWH           20161.291 Hz
FIDRES         0.076909 Hz
AQ             6.5012212 sec
RG                 1820
DW                24.800 usec
DE                 6.00 usec
TE                298.4 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.60 usec
PL1                 4.00 dB
SFO1         100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2               120.00 dB
PL12               18.40 dB
PL13               18.40 dB
SFO2         400.1345941 MHz

F2 - Processing parameters
SI                 131072
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME        061009-5 13C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20061011
Time              11.54
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                262144
SOLVENT             CDCl3
NS                    100
DS                      0
SWH           20161.291 Hz
FIDRES         0.076909 Hz
AQ             6.5012212 sec
RG                 1820
DW                24.800 usec
DE                 6.00 usec
TE                298.4 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                   1

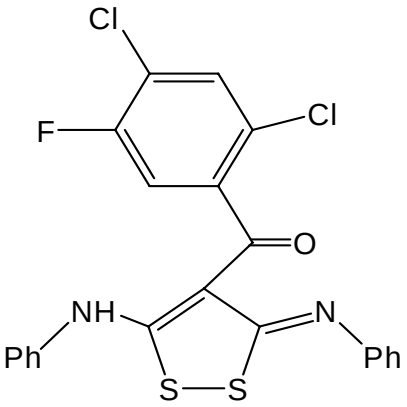
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.60 usec
PL1                 4.00 dB
SFO1         100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2               120.00 dB
PL12               18.40 dB
PL13               18.40 dB
SFO2         400.1345941 MHz

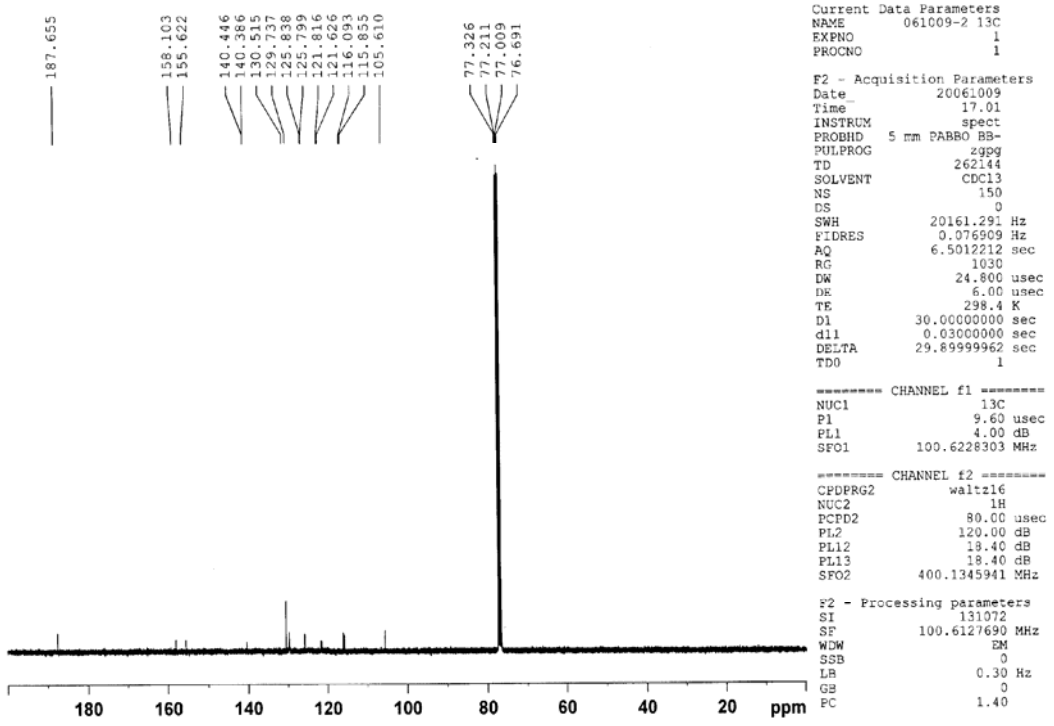
F2 - Processing parameters
SI                 131072
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.40
```

1h:

(2,4-dichloro-5-fluorophenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 78.5%. mp 168-170°C; ^{1}H NMR (400Hz, $CDCl_3$): δ12.781(s, 1H N-H); 7.699-6.70(m,13H -C=C-H).IR(ν_{max}, cm^{-1}): 3448(w, NH); 1625(s, -C=O); 1584(S, -C=N-); 1537(s, N-H); 1167(m, S—C). EA (Anal. Calc. (%) for $C_{22}H_{13}Cl_2FN_2OS_2$):C 55.70H 2.76 N 5.91 S 13.46; Found (%):C 55.65, H 2.66, N 5.96 S 13.40.



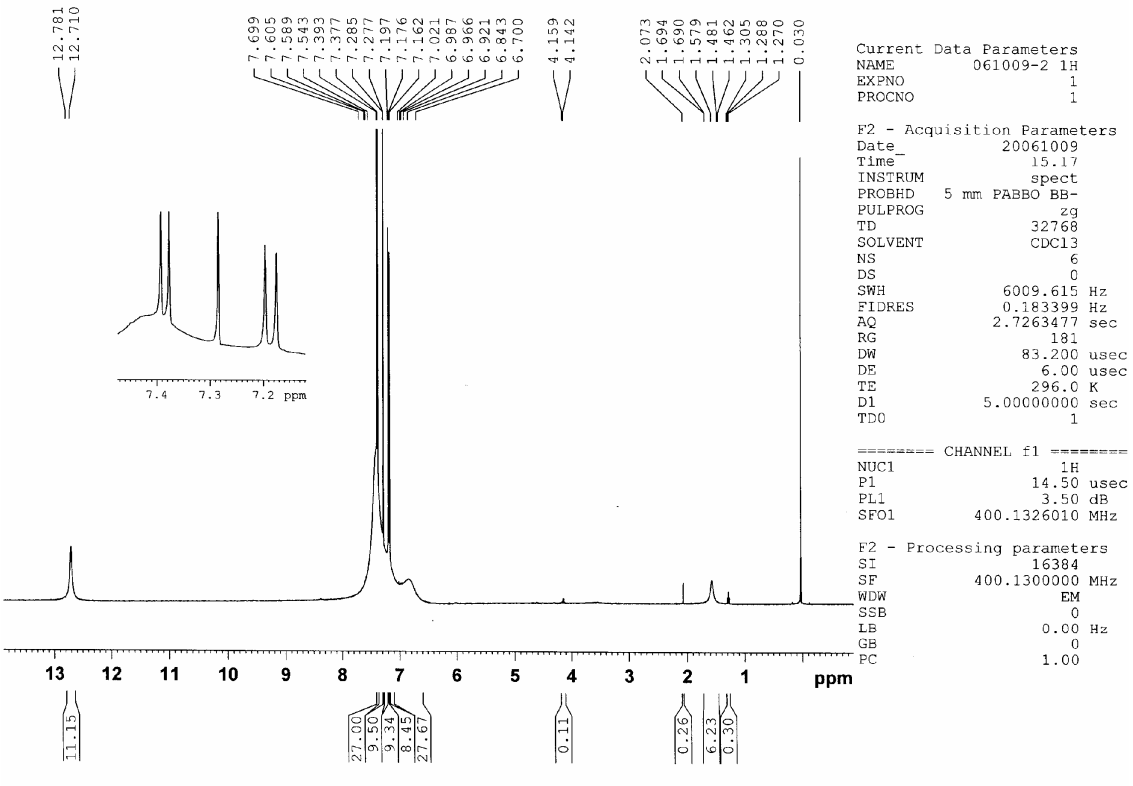

```
Current Data Parameters
NAME          061009-2 13C
EXPNO                   1
PROCNO                  1

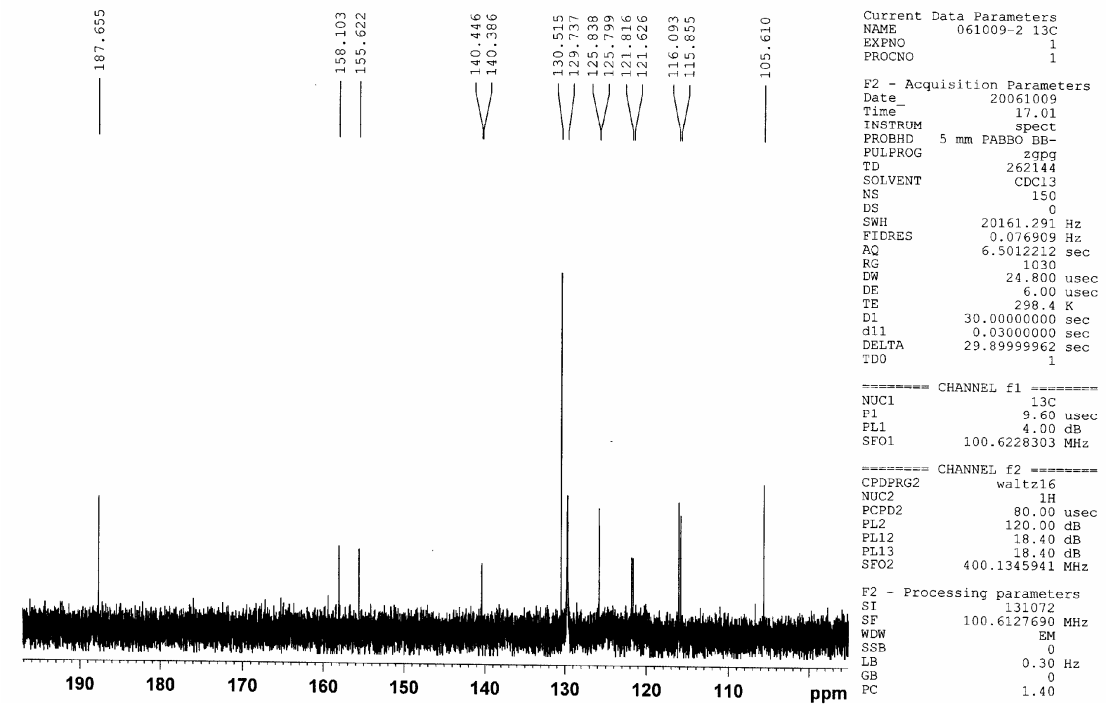
F2 - Acquisition Parameters
Date_           20061009
Time              17.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD              262144
SOLVENT           CDCl3
NS                  150
DS                    0
SWH           20161.291 Hz
FIDRES        0.076909 Hz
AQ            6.5012212 sec
RG                 1030
DW               24.800 usec
DE                6.00 usec
TE               298.4 K
D1           30.00000000 sec
d11           0.03000000 sec
DELTA        29.89999962 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                9.60 usec
PL1               4.00 dB
SFO1        100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              120.00 dB
PL12              18.40 dB
PL13              18.40 dB
SFO2        400.1345941 MHz

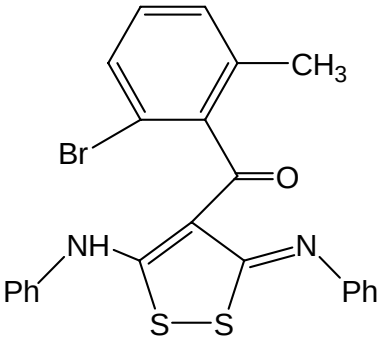
F2 - Processing parameters
SI                131072
SF          100.6127690 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.40
```



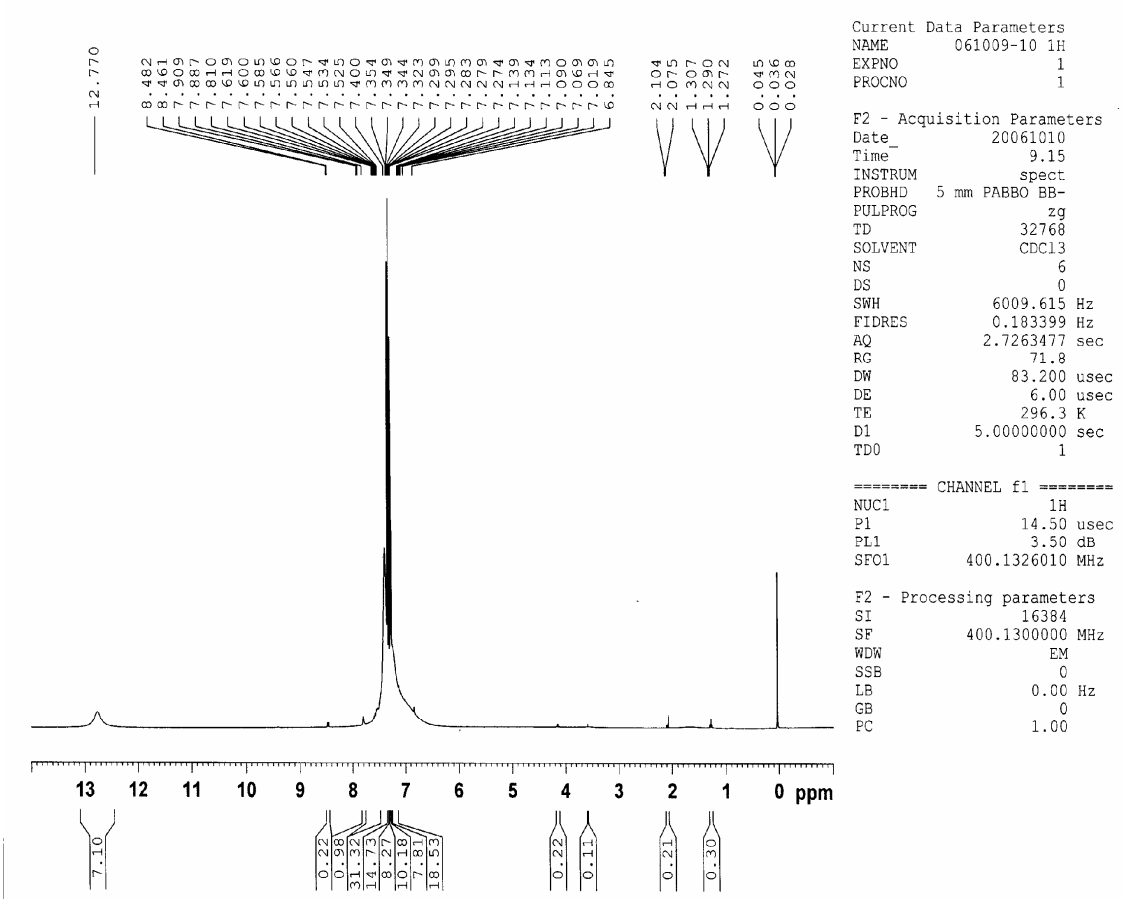


1i:

(2-bromo-6-methylphenyl)((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)methanone



Yield: 71%. mp 172-174°C; ^{1}H NMR (400Hz, $CDCl_3$): δ12.770(s, 1H N-H); 8.482-6.845(m, 14H -C=C-H).IR(ν_{max}, cm^{-1}): 3433(w, N-H); 1609(s, -C=O); 1584 (S, -C=N-); 1545 (s, N-H); 1191(m, S-C). EA (Anal. Calc. (%) for $C_{23}H_{17}BrN_2OS_2$):C 57.50H3.57 N 5.83 S 13.29; Found (%):C 57.60, H 3.55,N 5.94 S 13.20.

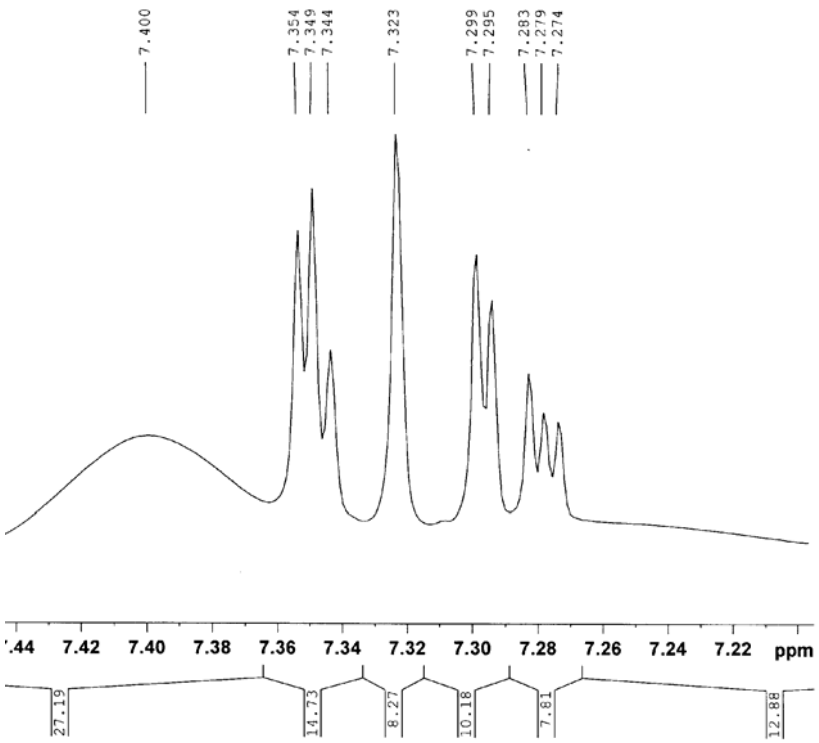



```
Current Data Parameters
NAME        061009-10 1H
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20061010
Time               9.15
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                    6
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7263477 sec
RG                 71.8
DW               83.200 usec
DE                6.00 usec
TE               296.3 K
D1           5.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.50 usec
PL1                3.50 dB
SFO1        400.1326010 MHz

F2 - Processing parameters
SI                16384
SF        400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```

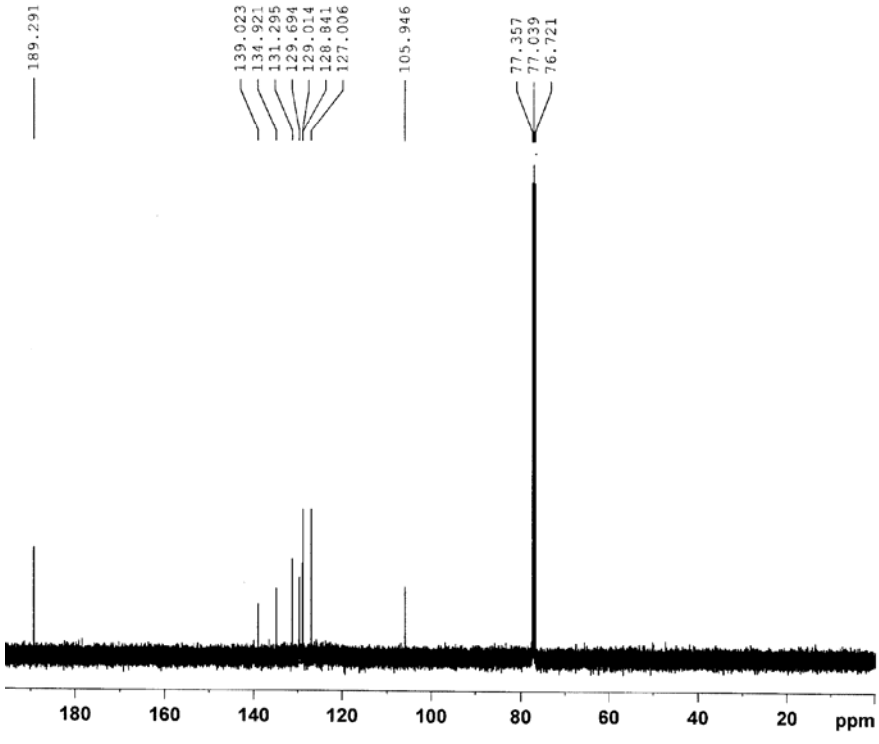



```
Current Data Parameters
NAME         061009-10 1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20061010
Time                9.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7263477 sec
RG                  71.8
DW                83.200 usec
DE                 6.00 usec
TE                296.3 K
D1             5.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.50 usec
PL1                 3.50 dB
SFO1          400.1326010 MHz

F2 - Processing parameters
SI                 16384
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME         061009-10 13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20061010
Time               11.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                262144
SOLVENT            CDCl3
NS                   100
DS                     0
SWH            20161.291 Hz
FIDRES          0.076909 Hz
AQ             6.5012212 sec
RG                  1030
DW                24.800 usec
DE                 6.00 usec
TE                298.5 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                    1

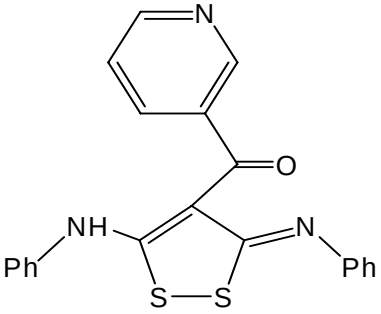
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.60 usec
PL1                4.00 dB
SFO1          100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2               120.00 dB
PL12               18.40 dB
PL13               18.40 dB
SFO2          400.1345941 MHz

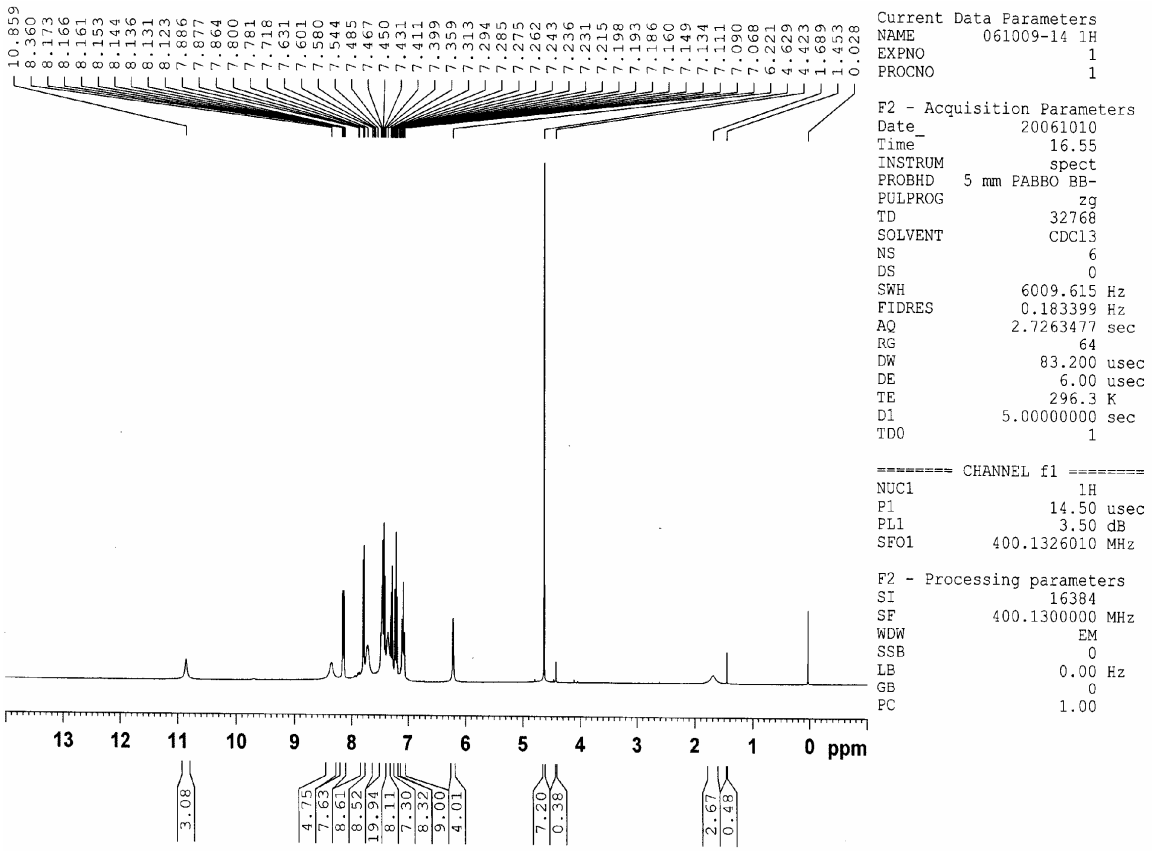
F2 - Processing parameters
SI                131072
SF            100.6127690 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.40
```

1j:

((3Z)-5-(phenylamino)-3-(phenylimino)-3H-1,2-dithiol-4-yl)(pyridin-3-yl)methanone



Yield: 91.5%. mp 145-147°C; ^{1}H NMR (400Hz, $CDCl_3$): δ10.859(s, 1H, N-H); 8.360-7.068(m, 15H, -C=C-H). IR(ν_{max}, cm^{-1}): 3427(w, N-H); 1618(s, -C=O); 1581 (S, -C=N-); 1496 (s, N-H); 1205(m, S-C). EA (Anal. Calc. (%) for $C_{21}H_{15}N_3OS_2$):C 64.77H3.89 N 10.80 S 16.43; Found (%):C 64.66, H 3.88,N 10.88 S 16.40.

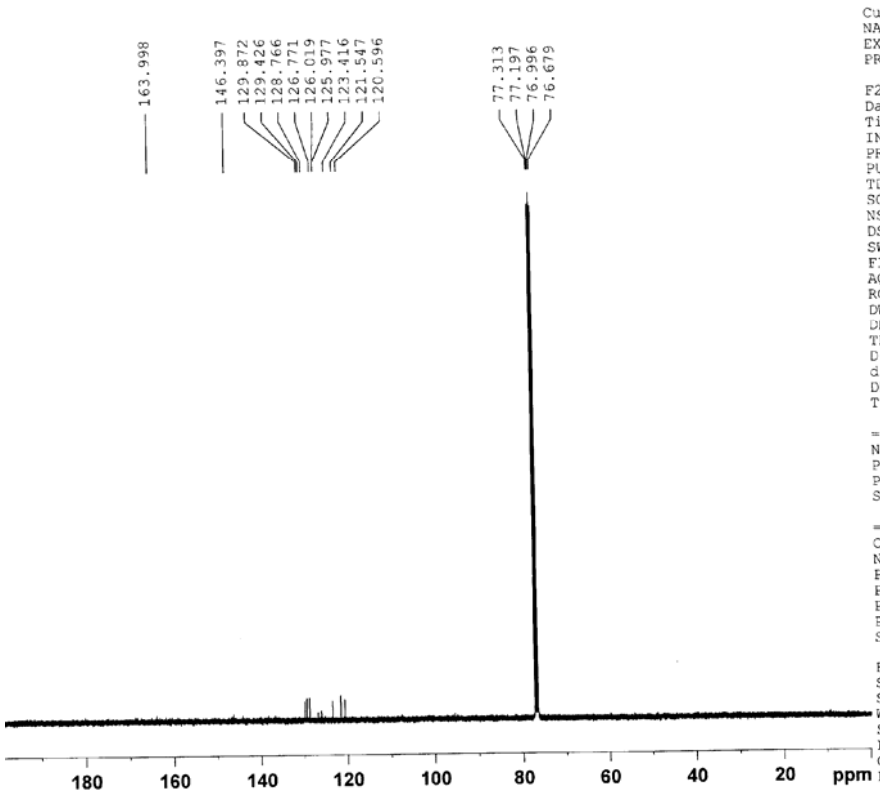



```
Current Data Parameters
NAME        061009-14 1H
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20061010
Time              16.55
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                    6
DS                    0
SWH            6009.615 Hz
FIDRES         0.183399 Hz
AQ             2.7263477 sec
RG                   64
DW               83.200 usec
DE                6.00 usec
TE               296.3 K
D1            5.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.50 usec
PL1                3.50 dB
SFO1         400.1326010 MHz

F2 - Processing parameters
SI                16384
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```



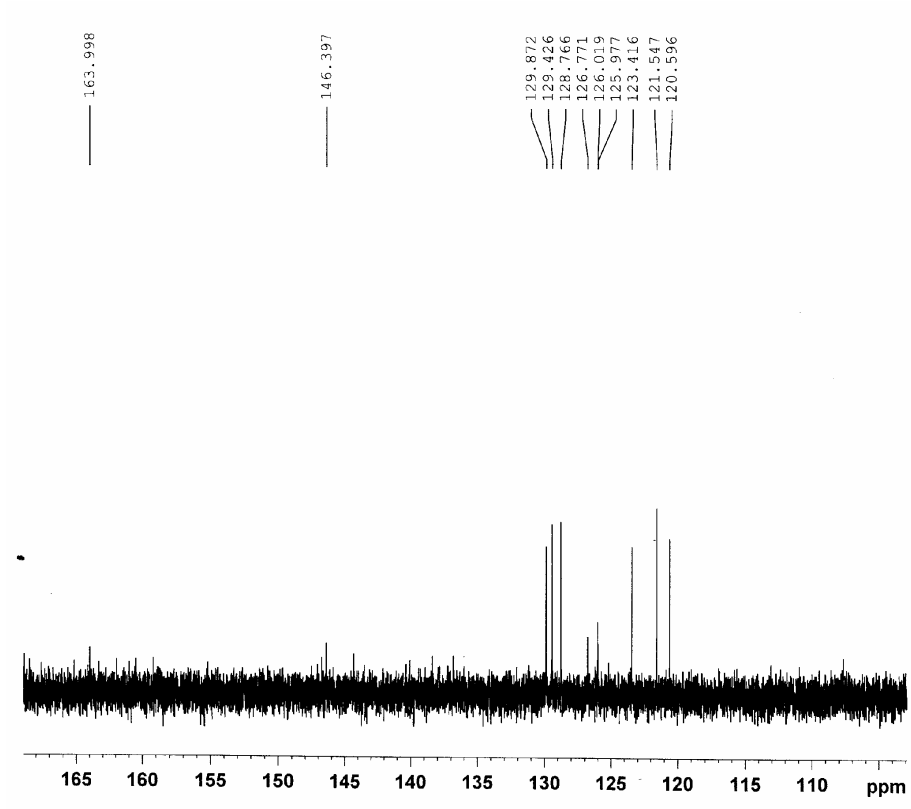

```
Current Data Parameters
NAME          061009-7 13C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20061009
Time                  12.46
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zgpg
TD                  262144
SOLVENT              CDCl3
NS                     150
DS                       0
SWH            20161.291 Hz
FIDRES          0.076909 Hz
AQ             6.5012212 sec
RG                    1030
DW                24.800 usec
DE                 6.00 usec
TE                 298.3 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.60 usec
PL1                4.00 dB
SFO1         100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2              120.00 dB
PL12              18.40 dB
PL13              18.40 dB
SFO2         400.1345941 MHz

F2 - Processing parameters
SI                  131072
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.40
```




```
Current Data Parameters
NAME          061009-7 13C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20061009
Time                  12.46
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zgpg
TD                  262144
SOLVENT              CDCl3
NS                     150
DS                       0
SWH            20161.291 Hz
FIDRES          0.076909 Hz
AQ             6.5012212 sec
RG                    1030
DW                24.800 usec
DE                 6.00 usec
TE                 298.3 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                     1

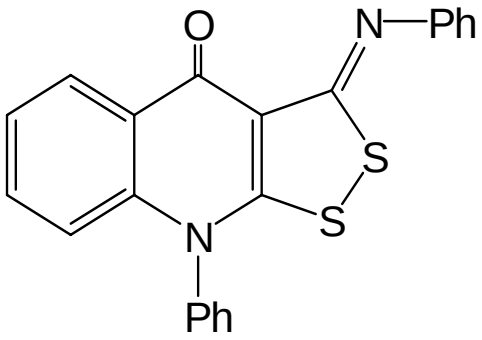
======== CHANNEL f1 ========
NUC1                  13C
P1                 9.60 usec
PL1                4.00 dB
SFO1         100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2              120.00 dB
PL12              18.40 dB
PL13              18.40 dB
SFO2         400.1345941 MHz

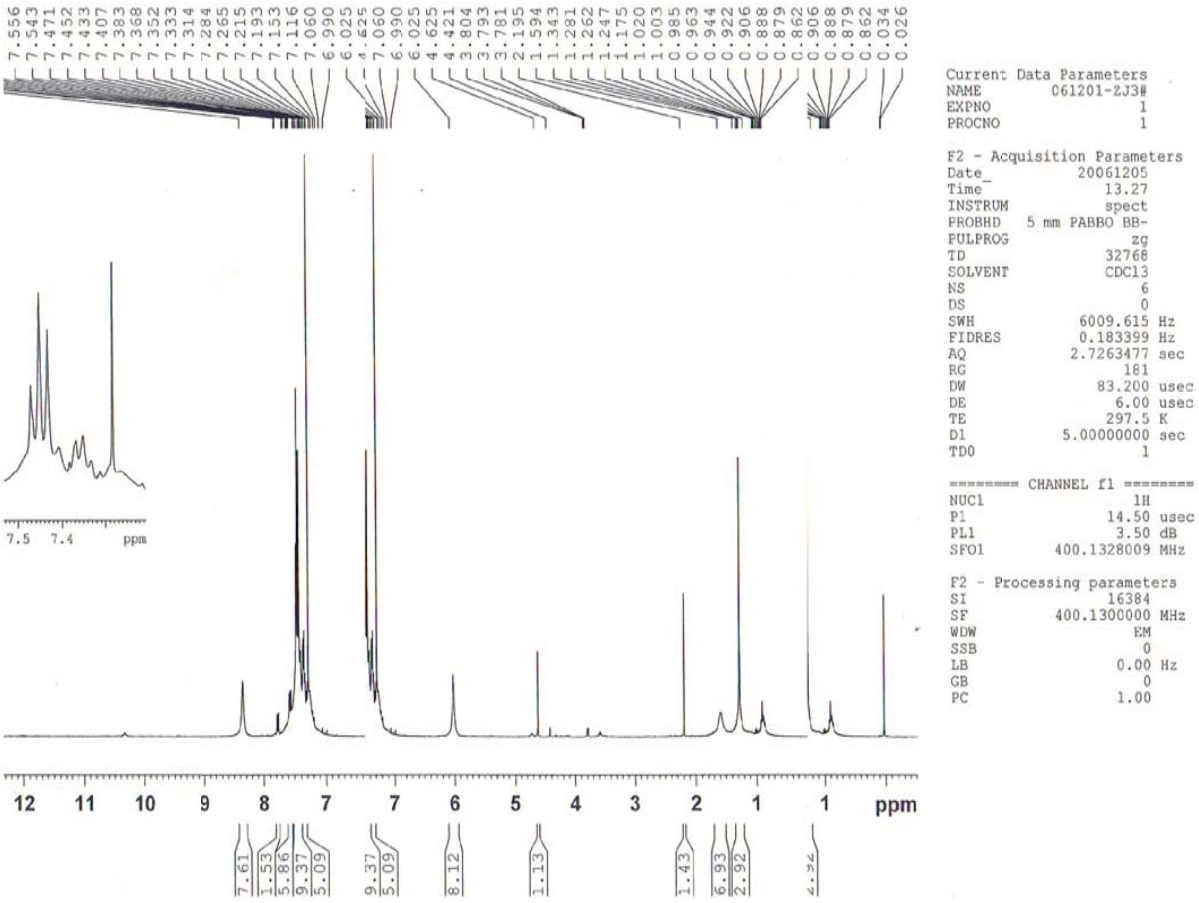
F2 - Processing parameters
SI                  131072
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.40
```

5-2. Spectra data for 3H-[1,2]dithiolo[3,4-*b*]quinolin-4(9H)-one (2)

2a: (3Z)-9-phenyl-3-(phenylimino)-3H-[1,2]dithiolo[3,4-b]quinolin-4(9H)-one

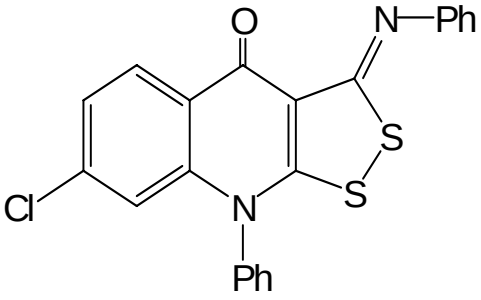


Yield: 50%. mp 253-255C; ^{1}H NMR (400Hz, $CDCl_3$): δ8.35-6.99 (m, 14H –C=C-H).IR(ν_{max}, cm^{-1}): 3437(w, N-H); 1643(s, -C=O); 1576 (s, -C=N-); 1193 (m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{14}N_2OS_2$):C 68.37H 3.65 N 7.25 S 16.55; Found (%):C 68.31, H 3.70,N 7.30 S 16.50.

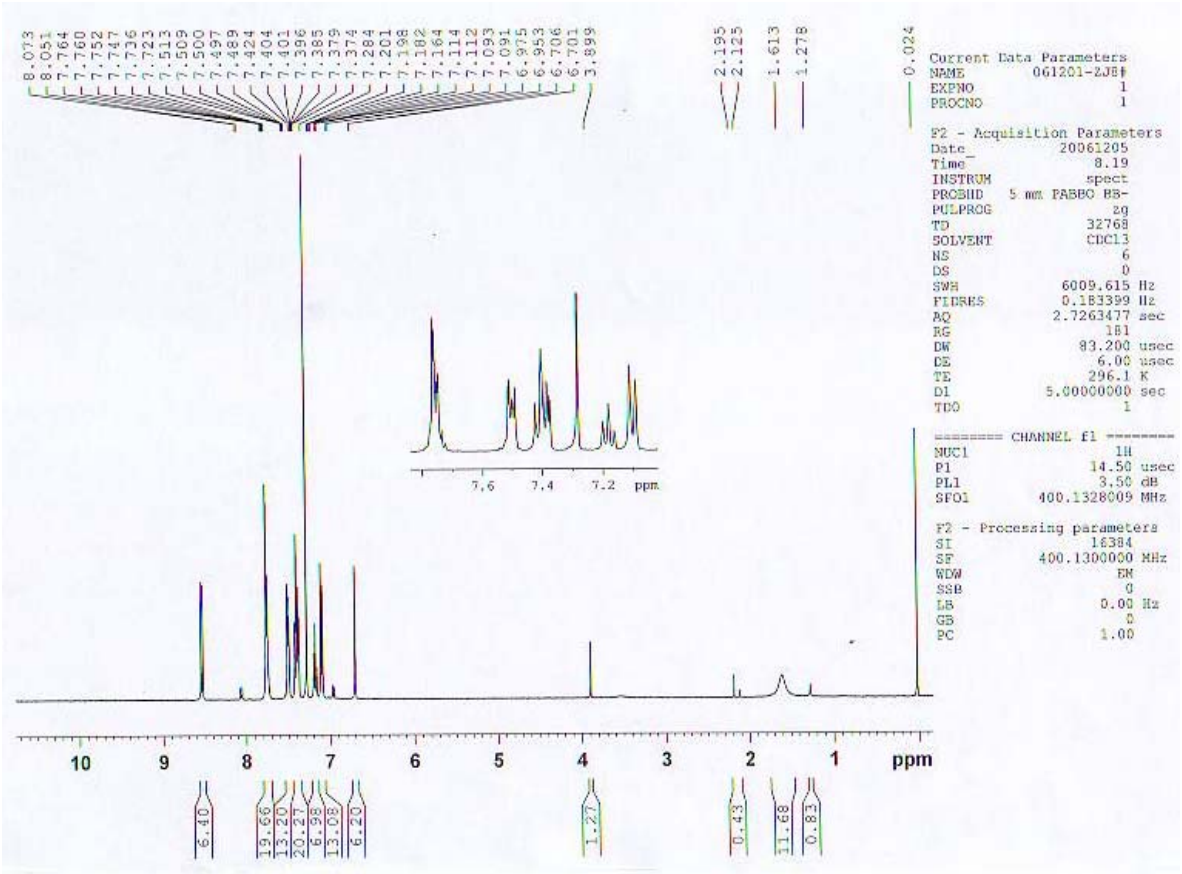


2e:

(3Z)-7-chloro-9-phenyl-3-(phenylimino)-3H-[1,2]dithiolo[3,4-b]quinolin-4(9H)-one

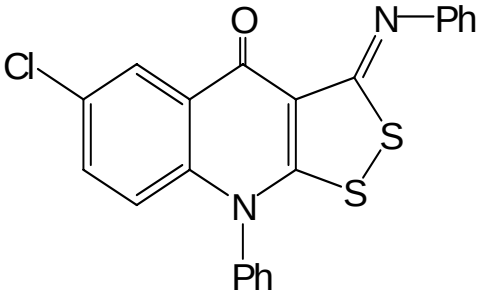


Yield: 63%. mp 274-276ºC; ^{1}H NMR (400Hz, $CDCl_3$): δ8.77-7.02 (m, 13H-C=C-H).IR(ν_{max}, cm^{-1}): 3435 (w, N-H); 1644 (s, -C=O); 1587 (s, -C=N-); 1194 (m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{13}ClN_2OS_2$):C 62.78 H 6.66 N 7.25 S 15.20; Found (%):C 62.75, H 3.10,N 6.68 S 15.23.

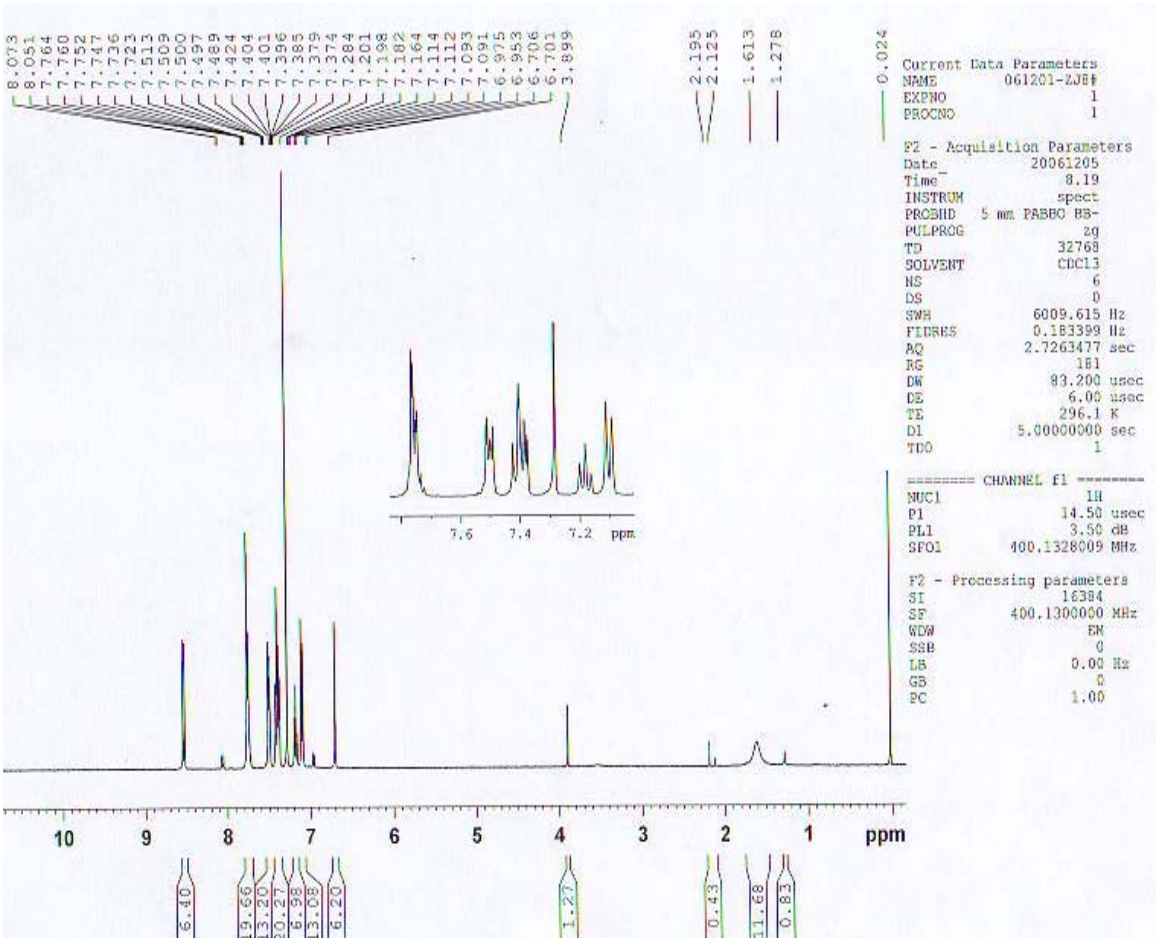


2f:

(3Z)-6-chloro-9-phenyl-3-(phenylimino)-3H-[1,2]dithiolo[3,4-b]quinolin-4(9H)-one

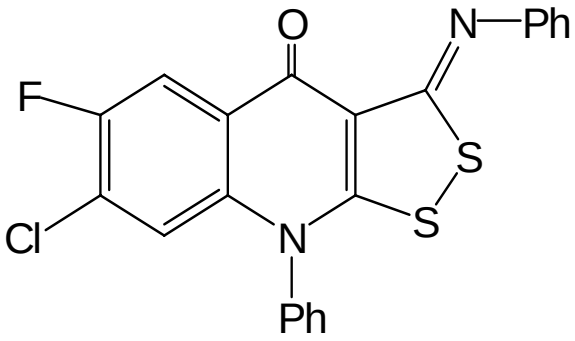


Yield: 60%. mp 270-272ºC; ^{1}H NMR (400Hz, $CDCl_3$): δ9.12-7.19 (m, 13H –C=C-H). IR(ν_{max}, cm^{-1}): 3417 (w, N-H); 1643 (s, -C=O); 1595 (s, -C=N-); 1214 (m, S-C). EA (Anal. Calc. (%) for $C_{22}H_{13}ClN_2OS_2$):C 62.78 H 6.66 N 7.25 S 15.20; Found (%):C 62.67, H 3.10,N 6.68 S 15.25.

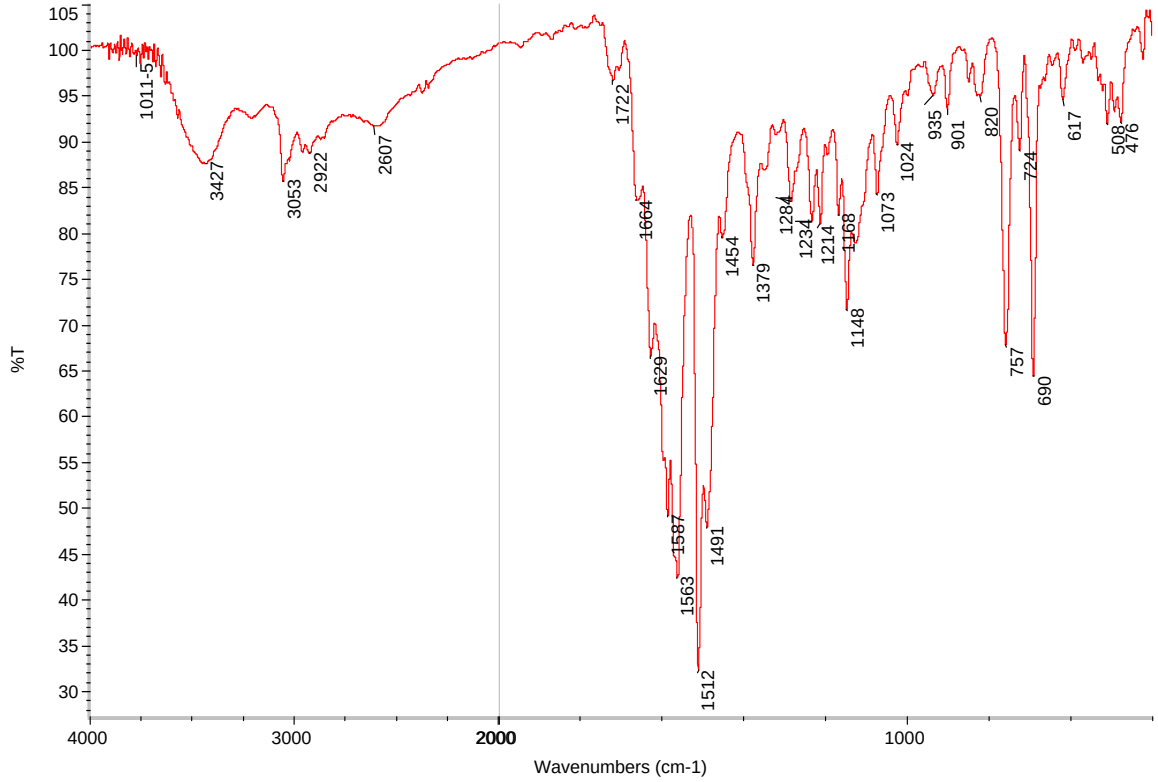


2h:

(3Z)-7-chloro-6-fluoro-9-phenyl-3-(phenylimino)-3H-[1,2]dithiolo[3,4-b]quinolin-4(9H)-one

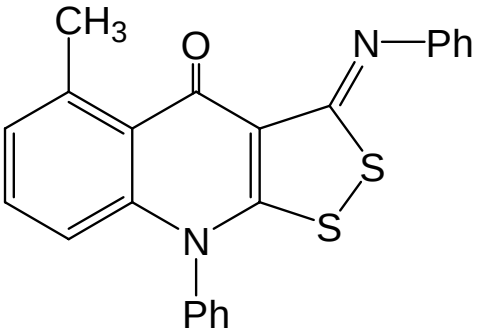


Yield: 70.5%. mp 288-290ºC; IR(ν_{max}, cm^{-1}): 3424 (w, N-H); 1634 (s, -C=O); 1579 (s, -C=N-); 1214 (m, S-C). EA (Anal. Calc. (%) for $C_{22}FH_{12}ClN_2OS_2$):C 62.78 H 6.66 N 7.25 S 15.20; Found (%):C 62.67, H 3.10,N 6.68 S 15.25.

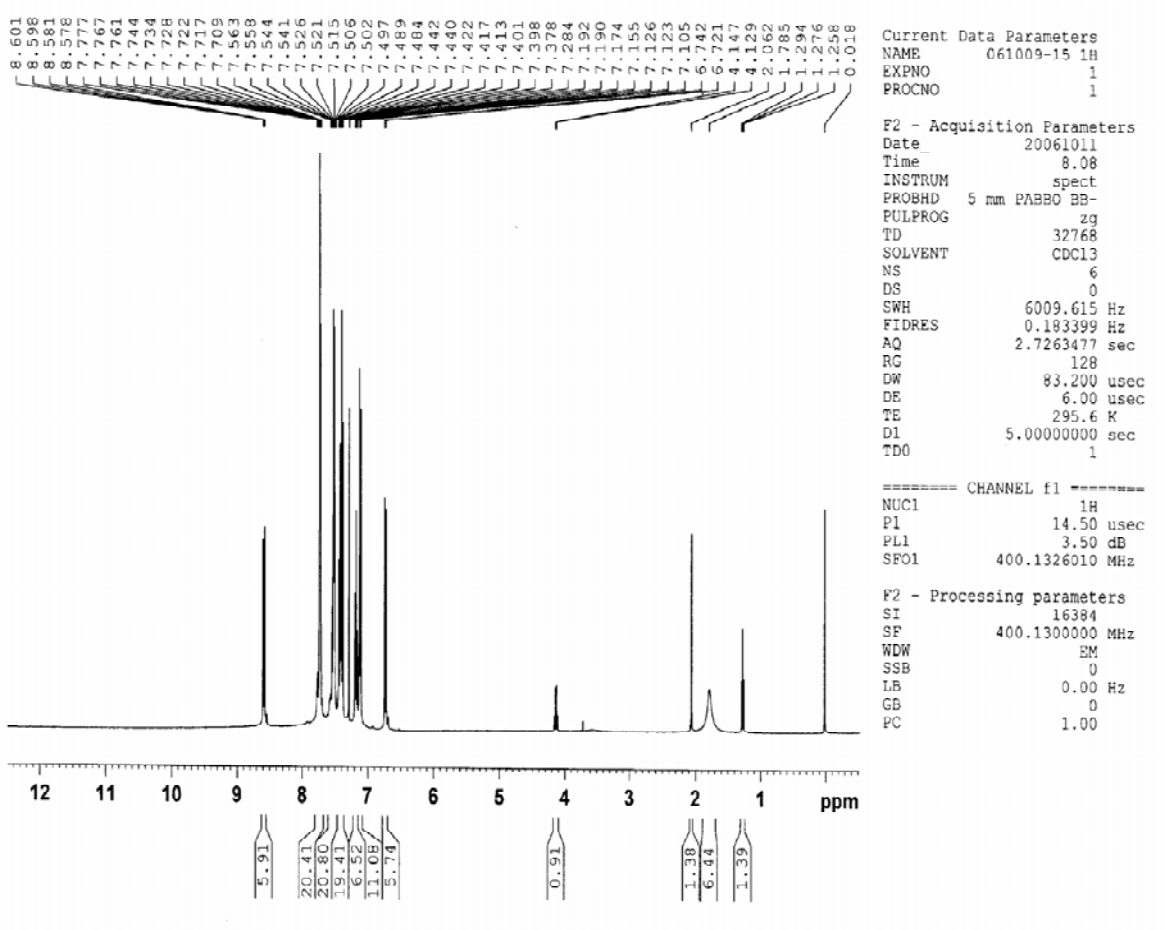


2i:

(3Z)-5-methyl-9-phenyl-3-(phenylimino)-3H-[1,2]dithiolo[3,4-b]quinolin-4(9H)-one



Yield: 85.5%. mp 260-262ºC; ^{1}H NMR (400Hz, $CDCl_3$): δ8.601-6.721 (m, 13H -C=C-H); IR(ν_{max}, cm^{-1}): 3427(w, N-H)；1629 (s, -C=O); 1587 (s, -C=N-); 1214 (m, S-C). EA (Anal. Calc. (%) for $C_{23}H_{16}N_2OS_2$):C 68.97 H 4.03 N 6.99 S 15.97; Found (%):C 68.80, H 3.99,N 7.02 S 15.96.



6. Crystallographic data for the compounds 1e

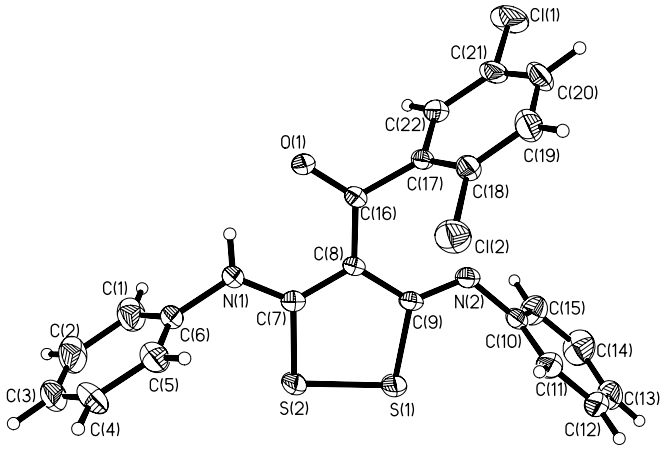


Table S8. Crystal data and structure refinement for **1e**.

Empirical formula	C22 H14 Cl2 N2 O S2
Formula weight	457.37
Temperature	293(2) K
Wavelength	0.71073 Å
Unit cell dimensions	a = 10.084(2)Å α= 87.60(3) deg. b = 10.331(2) Å β= 85.58(3) deg. c = 10.414(2) Å γ= 78.10(3) deg.
Volume	1058.1(4) $Å^3$
Z, Calculated density	2, 1.436 Mg/m^3
Absorption coefficient	0.520 mm^{-1}
F(000)	468
Theta range for data collection	1.96 to 26.97 deg.
Limiting indices	0<=h<=12,-12<=k<=13, -13<=l<=13
Reflections collected / unique	4872 / 4604 [R(int) = 0.0464]
Completeness to theta = 26.97	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4604 / 0 / 263
Goodness-of-fit on F^2	0.965
Final R indices [I>2sigma(I)]	R1 = 0.0668, wR2 = 0.1577
R indices (all data)	R1 = 0.1616, wR2 = 0.2053
Extinction coefficient	0.007(3)
Largest diff. peak and hole	0.438 and -0.490 e. $Å^{-3}$

Table S9. Bond lengths [A] and angles [deg] for **1e**.

S(1)-C(9)	1.804(4)	C(9)-S(1)-S(2)	96.46(2)
S(1)-S(2)	2.070(2)	C(7)-S(2)-S(1)	95.11(2)
S(2)-C(7)	1.747(4)	C(7)-N(1)-C(6)	124.0(4)
O(1)-C(16)	1.233(5)	C(9)-N(2)-C(10)	119.8(4)
N(1)-C(7)	1.323(5)	N(1)-C(7)-C(8)	126.3(4)
N(1)-C(6)	1.437(5)	N(1)-C(7)-S(2)	115.7(3)
N(2)-C(9)	1.270(5)	C(8)-C(7)-S(2)	118.0(3)
N(2)-C(10)	1.418(5)	C(7)-C(8)-C(9)	117.2(4)
C(7)-C(8)	1.399(6)	N(2)-C(9)-C(8)	127.0(4)
C(8)-C(9)	1.446(5)	N(2)-C(9)-S(1)	120.0(3)
		C(8)-C(9)-S(1)	113.0(3)

7.
Crystallographic data for the compounds 1h

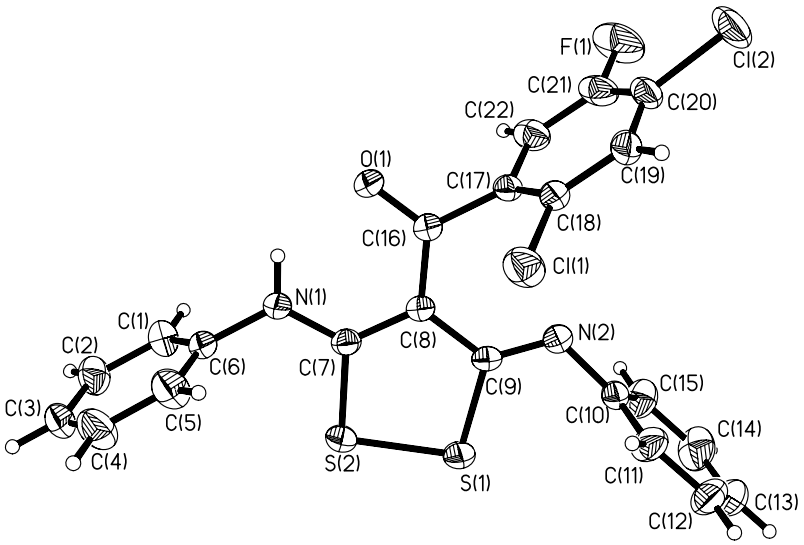


Table S10. Crystal data and structure refinement for **1h**.

Empirical formula	C22 H13 Cl2 F N2 O S2
Formula weight	475.36
Temperature	293(2) K
Wavelength	0.71073 Å
Unit cell dimensions	a = 9.896(2) Å alpha = 89.64(3) deg. b = 10.256(2) Å beta = 73.71(3) deg. c = 11.128(2) Å gamma = 82.42(3) deg.
Volume	1074.0(4) $Å^3$
Z, Calculated density	2, 1.470 Mg/m^3
Absorption coefficient	0.522 mm^{-1}
F(000)	484
Theta range for data collection	1.91 to 26.97 deg.
Limiting indices	0<=h<=11, -12<=k<=12, -13<=l<=13
Reflections collected / unique	4867 / 4592 [R(int) = 0.0286]
Completeness to theta = 26.97	98.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4592 / 0 / 271
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0482, wR2 = 0.1297
R indices (all data)	R1 = 0.0736, wR2 = 0.1461
Largest diff. peak and hole	0.505 and -0.325 e. $Å^{-3}$

Table S11. Bond lengths [A] and angles [deg] for **1h**.

S(1)-C(9)	1.798(2)	C(9)-S(1)-S(2)	96.36(8)
S(1)-S(2)	2.074(1)	C(7)-S(2)-S(1)	95.43(8)
S(2)-C(7)	1.751(2)	C(7)-N(1)-C(6)	123.74(2)
O(1)-C(16)	1.241(3)	C(9)-N(2)-C(10)	119.7(2)
N(1)-C(7)	1.336(3)	N(1)-C(7)-C(8)	126.0(2)
N(1)-C(6)	1.436(3)	N(1)-C(7)-S(2)	116.06(2)
N(2)-C(9)	1.269(3)	C(8)-C(7)-S(2)	117.92(2)
N(2)-C(10)	1.427(3)	C(7)-C(8)-C(9)	116.9(2)
C(7)-C(8)	1.401(3)	N(2)-C(9)-C(8)	126.4(2)
C(8)-C(9)	1.463(3)	N(2)-C(9)-S(1)	120.31(2)
		C(8)-C(9)-S(1)	113.35(2)

8. Crystallographic data for the compounds 1i

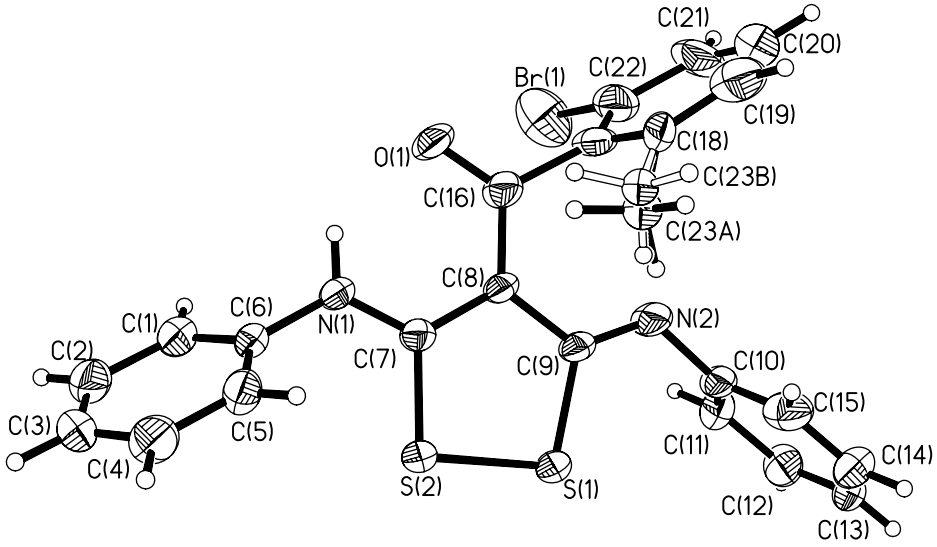


Table S12. Crystal data and structure refinement for **1i**.

Empirical formula	C23 H17 Br N2 O S2
Formula weight	481.42
Temperature	293(2) K
Wavelength	0.71073 Å
Unit cell dimensions	a = 6.3729(13) Å alpha = 108.64(3) deg. b = 12.941(3) Å beta = 96.27(3) deg. c = 13.413(3) Å gamma = 96.96(3) deg.
Volume	1027.5(4) Å ^{3}
Z, Calculated density	1, 1.556 Mg/m^3
Absorption coefficient	2.221 mm^-1
F(000)	488
Theta range for data collection	1.62 to 24.99 deg.
Limiting indices	-7<=h<=7, -14<=k<=15, -15<=l<=7
Reflections collected / unique	4243 / 3546 [R(int) = 0.0211]
Completeness to theta = 24.99	97.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3546 / 2 / 261
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0938, wR2 = 0.2734
R indices (all data)	R1 =0.1304, wR2 = 0.3077
Largest diff. peak and hole	0.969 and -1.032 e. Å $^{-3}$

Table S13. Bond lengths [A] and angles [deg] for **1i**

S(1)-C(9)	1.788(6)	C(9)-S(1)-S(2)	96.9(2)
S(1)-S(2)	2.066(3)	C(7)-S(2)-S(1)	95.4(2)
S(2)-C(7)	1.737(6)	C(7)-N(1)-C(6)	125.3(5)
O(1)-C(16)	1.231(9)	C(9)-N(2)-C(10)	120.1(6)
N(1)-C(7)	1.327(8)	N(1)-C(7)-C(8)	124.8(6)
N(1)-C(6)	1.428(9)	N(1)-C(7)-S(2)	116.8(5)
N(2)-C(9)	1.266(9)	C(8)-C(7)-S(2)	118.4(5)
N(2)-C(10)	1.419(9)	C(7)-C(8)-C(9)	115.3(5)
C(7)-C(8)	1.429(9)	N(2)-C(9)-C(8)	125.4(6)
C(8)-C(9)	1.464(9)	N(2)-C(9)-S(1)	120.7(5)
		C(8)-C(9)-S(1)	113.9(5)

9. Crystallographic data for the compounds 2e

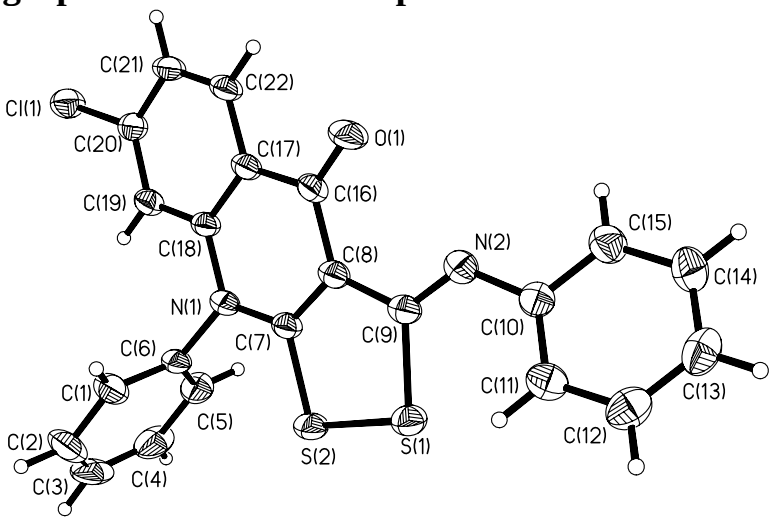


Table S14. Crystal data and structure refinement for **2e**

Empirical formula	C22 H13 Cl N2 O S2
Formula weight	420.91
Temperature	293(2) K
Wavelength	0.71073 Å
Unit cell dimensions	a = 11.497(2) Å alpha = 90 deg. b = 7.5370(15) Å beta = 103.64(3) deg. c = 22.384(5) Å gamma = 90 deg.
Volume	1884.9(7) $Å^3$
Z, Calculated density	4, 1.483 Mg/m^3
Absorption coefficient	0.440 mm^{-1}
F(000)	868
Theta range for data collection	1.82 to 26.96 deg.
Limiting indices	0<=h<=13, 0<=k<=8, -26<=l<=26
Reflections collected / unique	4160 / 3966 [R(int) = 0.0332]
Completeness to theta = 26.96	96.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3966 / 0 / 253
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1404
R indices (all data)	R1 = 0.1159, wR2 = 0.1700
Largest diff. peak and hole	0.603 and -0.365 e. $Å^{-3}$

Table S15. Bond lengths [Å] and angles [deg] for **2e**.

S(1)-C(9)	1.815(3)	C(9)-S(1)-S(2)	97.28(1)
S(1)-S(2)	2.062 (2)	C(7)-S(2)-S(1)	94.38(1)
S(2)-C(7)	1.745(3)	C(7)-N(1)-C(6)	118.8(2)
O(1)-C(16)	1.235(4)	C(9)-N(2)-C(10)	126.2(3)
N(1)-C(7)	1.358(4)	N(1)-C(7)-C(8)	124.6(3)
N(1)-C(6)	1.456(3)	N(1)-C(7)-S(2)	116.3(2)
N(2)-C(9)	1.277(4)	C(8)-C(7)-S(2)	119.1(3)
N(2)-C(10)	1.409(4)	C(7)-C(8)-C(9)	117.5(3)
C(7)-C(8)	1.384(4)	N(2)-C(9)-C(8)	124.5(3)
C(8)-C(9)	1.455(5)	N(2)-C(9)-S(1)	123.8(3)
		C(8)-C(9)-S(1)	111.6(2)

10. Drug screening report

Biology Principles. In the mitochondria of living cells, there are NADP-related dehydrogenases, which can reduce the ectogenic MTT (methyl thiazolyl tetrazolium) to undissoluvable amethyst crystal (formazan) and make it deposited in cells. Such phenomenon couldn't take place in dead cells. The MTT assay makes use of dimethyl sulfoxide (DMSO) or trigeminy reagent (10%SDS-5%isobutanol-0.01mol/L HCl) to dissolve the amethyst crystals and determine the OD value at 570nm wave by the Universal Microplate Reader ELx800 (BioTek) to reflect the amount of living cells indirectly. This assay is frequently used in the vitro research in antitomor drugs, especially as to the large-scale screening.

Methods and Highlights. Innoculate the tumor cells in exponential phase of growth to a 96-well plate quantitively and add drug solution to the medium after incubating for 24 hours. Incubate 48 hours continuously at 37 ℃ and 5% CO_2, add MTT solution and incubate for another 4 hours. Then, DMSO is added and the OD value at 570nm wave is determined by the Universal Microplate Reader ELx800 (BioTek) when the mixture is dissolved. Overnight incubation is needed before determining if the trigeminy reagent is used to dissolve precipitation.

Table S16 The Inhibition Effects of tested drugs on Vitro growth of **HepG-2**.

Entry	Concentration				**IC50**
	10^{-4}M	10^{-5}M	10^{-6}M	10^{-7}M	
1c	78.91%	62.72%	53.54%	2.22%	1.36×10^{-6}M
2a	48.19%	10.91%	3.65%	3.33%	3.11×10^{-4}M

Table S17 The Inhibition Effects of tested drugs on Vitro growth of **SMMC-7221**.

Entry	Concentration				**IC50**
	10^{-4}M	10^{-5}M	10^{-6}M	10^{-7}M	
1c	58.77%	15.57%	7.69%	6.41%	1.39×10^{-4}M
2a	11.88%	11.04%	5.30%	0.99%	7.34×10^{-3}M

Table S18. The Inhibition Effects of tested drugs on Vitro growth of HepG-2 at different time

Entry	Time (H)	Concentration			
		10^{-4}M	10^{-5}M	10^{-6}M	10^{-7}M
1b	12h	41.26%	29.14%	17.38%	14.36%
	24h	53.52%	35.06%	26.99%	16.46%
	48h	73.02%	50.54%	29.46%	18.85%
1h	12h	23.60%	16.77%	11.63%	10.36%
	24h	36.52%	20.67%	18.14%	13.70%
	48h	63.60%	25.62%	17.41%	15.75%
1d	12h	71.55%	59.21%	38.78%	10.37%
	24h	77.56%	66.82%	45.61%	11.02%
	48h	93.69%	83.65%	59.75%	16.04%
1j	12h	47.75%	35.41%	15.11%	12.80%
	24h	62.64%	41.33%	19.60%	10.22%
	48h	70.81%	50.72%	26.20%	18.04%
2d	12h	29.28%	18.33%	14.82%	12.36%
	24h	44.69%	24.89%	11.21%	8.24%
	48h	57.75%	15.02%	12.51%	0.02%