Supporting information for

Cyclododecanone as a recyclable protecting group for the synthesis of highly functionalized 3-amino-2-thiohydantoins from conventional starting materials

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General Experimental procedure:

Analytical methods: Chemicals were purchased from Aldrich and they were used without further purification. TLC -Thin layer chromatography (Merck, Silica gel 60 F254) was performed on pre-coated silica gel on alumina plates. IR spectra were recorded in the range 4000-400cm-1 on Thermo Nicolet Avatar 330 FTIR spectrometer in KBr pellets. ^{1}H NMR and ^{13}C NMR spectra were recorded using a Bruker AMX 400 FT. HRMS analysis was obtained from JEOL GC Mate.

Synthesis of 2-cyclododecylidenehydrazine carbothiamide from CDD:

In an oven dried three necked RB flask mixture of CDD (2mmol) and thiosemicarbazide (2mmol) were taken and dissolved in ethanol (5ml). To this 0.2ml of acetic acid was added and refluxed for about 30 min in waterbath.The completion of the reaction was monitored from TLC and the formed precipitate was filtered, washed with water and dried.

2-cyclododecylidenehydrazine carbothiamide: White color solid (0.4853g, 95%) Mp 190-192°C; ^{1}H-NMR (400MHz, DMSO) δ (ppm) 10.090 (s, 1H), 8.057 (s, 1H), 7.375 (s, 1H), 3.178 (d, J=5.2, 1H), 2.424-2.392 (t, J=6.4, 1H), 2.292-2.260 (t, J=6.4, 2H), 1.666 (s, 2H), 1.549-1.498 (q, J=7.2, 2H), 1.480-1.277 (m, 14H); ^{13}CNMR (100MHz, DMSO) δ (ppm) 178.3, 155.4, 31.1, 27.8, 25.2, 23.6, 23.3, 22.8, 22.4, 21.7; IR (KBr) υ (cm^{-1}) 3406, 3226, 3145, 2933, 2902, 2852, 1595, 1500, 1462,1290,1240,1070,1055,719; HRMS calcd for $C_{13}H_{25}N_3S$ (M+) 255.1769,found 255.1767.

Synthesis 2-((E)-5-(2-fluorobenzylidine)-3-((E)-2-fluorobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl) acetic acid: Pale yellow color solid.

With 5ml of acetic acid 2mmol of (6) and 4mmol of chloroacetic acid were taken in a oven dried three necked RB flask and refluxed for about 1hr. The disappearance of (6) was monitored from TLC, when (6) had completely reacted 4mmol of 2-fluorobenzaldehyde was added and refluxed further for about 2 hrs. After the completion of the reaction, the reaction mass was poured in ice cooled water and the formed yellow precipitate was filtered, dried and washed with n-hexane. The obtained filtrate was dried in vacuum and the recovered CDD can be used for further reactions for a number of times.

2-((E) - 5-(2-fluorobenzylidine)-3-((E)-2-fluorobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7a (Table-2,Entry 1) Pale yellow color amorphous solid (0.7918g, 94%) Mp 220-223°C;^{1}H NMR (400 MHz, DMSO) δ (ppm) 12.08(s,1H), 8.51(s,2H), 7.93-7.89(t, J=8Hz,2H), 7.55-7.50(q, J=8Hz,2H), 7.33-7.29(t, J=8Hz,4H), 3.92 (s,2H); ^{13}C NMR(100MHz,DMSO) δ (ppm) 174.2, 162.0, 159.5, 148.9, 132.7, 132.6, 127.7, 127.6, 124.0, 121.6, 121.5, 116.2, 116.0, 33.0; IR (KBr) υ (cm^{-1}) 3572, 3192, 2949, 2762, 1732, 1649,1330,1247;HRMS calcd for $C_{19}H_{13}F_2N_3O_3S$ (M+) 401.0646, found 401.0649.

2-((E)-5-(2-chlorobenzylidine)-3-((E)-2-chlorobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7b (Table-2,Entry 2) Pale yellow color amorphous solid (0.8359g,92%) Mp 213-215°C; ^{1}H NMR (400 MHz, DMSO) δ (ppm) 12.212 (s,1H), 8.061(s,1H), 7.992-7.968(d, J=12,2H), 7.751-7.732(d, J=7.6,1H), 7.651-7.632 (d, J=7.6,1H) 7.562-7.539(d, J=9.2,2H), 7.508-7.397(m,3H), 3.896(s,2H) ^{13}C NMR (100 MHz,DMSO) δ (ppm) 174.0, 167.0, 151.8, 130.8, 130.2, 130.0, 128.9,128.0,127.6,127.5,33.1.; IR (KBr) υ (cm^{-1}) 3400, 2976, 2935, 2767, 1718, 1653, 1508, 1303, 1244; HRMS calcd for $C_{19}H_{13}Cl_2N_3O_3S$ (M+) 433.0055,found 433.0061

2-((E) - 5-(3-hydroxybenzylidine)-3-((E)-3-hydroxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid:7c (Table-2,Entry 3) Pale yellow color amorphous solid(0.7596g,91%) Mp 283-285°C;^{1}H NMR (400 MHz, DMSO) δ (ppm) 11.98(s,1H), 9.67(s,2H), 8.31(s,2H),7.28-7.24(t, J=8Hz,2H) 7.21(s, 2H), 7.16-7.14(d, J=8Hz,2H), 6.86-6.84(d, J=8Hz,2H), 3.854(s,2H); ^{13}CNMR (100MHz,DMSO) δ (ppm) 157.5, 156.3, 135.4, 129.8, 119.3, 117.9, 113.2, 33.0; IR (KBr) υ (cm^{-1}) 3415,3045,2941,2752,1710,1649,1327,1247.;HRMS calcd for $C_{19}H_{15}N_3O_5S$ (M+) 397. 0732,found 397.0738.

2-((E)-5-(3-nitrobenzylidine)-3-((E)-3-nitrobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7d (Table-2,Entry 4) Pale yellow color amorphous solid(0.9033g,95%) Mp 254-257°C;^{1}H NMR (400 MHz, DMSO) δ (ppm) 12.23 (s,1H), 8.58(s,4H), 8.31-8.29(t,J=4.0,2H), 8.21-8.194(d,J=4.0,2H), 7.79-7.75(t,J=8Hz,2H), 3.93(s,2H); ^{13}C NMR(100MHz,DMSO) δ (ppm) 174.0,166.9,154.2,148.1,135.9,135.4,135.3,133.3,130.8, 130.7,130.3,125.2, 124.7, 123.9, 122.4, 121.8, 33.0; IR (KBr) υ (cm^{-1}) 3410,3043,2939,2765,1963,1940,1716,1633,1170.9; HRMS calcd for $C_{19}H_{13}N_5O_7S$ (M+) 455.0536,found 455.0540.

2-((E)-5-(3,4-dihydroxybenzylidine)-3-((E)-3,4-dihydroxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7e (Table-2,Entry 5) Pale yellow color amorphous solid (0.8448g,94%)Mp 275-278°C.; ^{1}H NMR (400 MHz, DMSO) δ (ppm) 11.86(s,1H), 9.51(s,2H), 9.29(s,2H), 8.19(s,2H), 7.24(s,2H), 7.01-6.98(q, J=4,2H), 6.79-6.77(d, J=8Hz,2H), 3.87(s,2H); ^{13}CNMR (100MHz,DMSO) δ (ppm) 156.4, 148.5, 145.5, 125.6, 121.3, 115.4, 113.1, 32.9 IR(KBr) υ (cm^{-1}) 3466,3153,2765,1683,1589,1282.; HRMS calcd for $C_{19}H_{15}N_3O_7S$ (M+) 429.0631,found 429.0631

2-((E) - 5-(4-methoxybenzylidine)-3-((E)-4-methoxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid :7f (Table-2,Entry 6) Pale yellow color amorphous solid(0.7388g,83%) Mp 210-212°C.;^{1}H NMR (400 MHz, DMSO) δ (ppm)11.92(s,1H), 8.34(s,2H), 7.72-7.69(d, J=12,4H), 7.03-7.01(d, J=12,4H), 3.88(s,2H), 3.81(s,6H); ^{13}CNMR (100MHz,DMSO) δ (ppm) 174.4,161.8,156.3,129.8,127.3,114.8,55.8,33.4.; IR(KBr) υ (cm^{-1})3454, 3010, 2941, 2763, 1724, 1631,1327,1249.; HRMS calcd for $C_{21}H_{19}N_3O_5S$ (M+) 425.1045, found 425.1049.

2-((E)-5-(4-ethylbenzylidine)-3-((E)-4-ethylbenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7g (Table-2,Entry 7) Pale yellow color amorphous solid(0.7585g,86%); Mp 231-232°C; ^{1}H NMR (400 MHz, DMSO) δ (ppm)12.0(s,1H), 8.37(s,2H), 7.68-7.66(d, J=8,4H), 7.31-7.29(d, J=8,4H), 3.844(s,2H), 2.67-2.61(q, J=8Hz,4H), 1.21-1.17(d, J=8,6H); ^{13}CNMR (100MHz,DMSO) δ (ppm) 174.4, 156.1, 146.7, 131.7, 128.2, 127.7, 32.9, 28.1, 15.3; IR (KBr) υ (cm^{-1}) 3419, 3180, 3024, 2960, 2752, 1712, 1593, 1330, 1209; HRMS calcd for $C_{23}H_{23}N_3O_3S$ (M+) 421.1460, found 421.1463.

2-((E)-5-(4-fluorobenzylidine)-3-((E)-4-fluorobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7h (Table-2,Entry 8) Pale yellow color amorphous solid (0.7754g,92%); Mp 246-249°C; ^{1}H NMR (400 MHz, DMSO) δ(ppm) 11.997(s,1H), 8.418(s,1H), 7.840-7.804(q,J=5.6,4H), 7.335-7.291(t,J=8.8,5H), 3.906(s,2H) ^{13}CNMR (100MHz,DMSO) δ (ppm)174.0,165.2,164.6,162.1,155.0, 132.2,130.8,130.7,130.1, 129.8,129.7,116.1, 116.0, 115.8, 32.9; IR (KBr) υ (cm^{-1}) 3320,2958,2760,1714,1647, 12285; HRMS calcd for $C_{19}H_{13}F_2N_3O_3S$ (M+) 401.0646,found 401.0641

2-((E) - 5-(4-ethoxybenzylidine)-3-((E)-4-ethoxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7i (Table-2,Entry 9) Pale yellow color amorphous solid (0.7576g ,80%); Mp 240-243°C;^{1}H NMR (400 MHz, DMSO) δ (ppm) 11.920(s,1H),9.025(s,1H), 7.692-7.602 (q, J=8.8,4H), 7.012-6.975(t, J=8.0,5H), 4.110-4.067 (q, J=3.2,4H), 3.879(s,2H) 1.376-1.360(t, J=6.4,6H); ^{13}CNMR(100MHz,DMSO)δ(ppm) 174.0, 171.9, 160.5, 155.8, 130.1, 129.2, 126.6, 114.6, 63.2, 32.9,21.0,14.5; IR(KBr) υ (cm^{-1}) 3390,2976,2935,2767,1718,1631,1244; HRMS calcd for $C_{23}H_{23}N_3O_5S$ (M+) 453.1358,found 453.1351.

2-((E)-5-(4-methylbenzylidine)-3-((E)-4-methylbenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7j (Table-2,Entry 10) Pale yellow color amorphous solid(0.7029g,85%); Mp 221-223°C; ^{1}H NMR (400 MHz, DMSO) δ (ppm) 11.954(s,1H),8.361(s,1H),7.659-7.639(d, J=8.0,4H), 7.574-7.554(d, J=8Hz,1H),7.283-7.263(d, J=8.0,4H),3.889(s,2H), 2.363-2.347(t, J=5.2,6H) ^{13}CNMR(100MHz,DMSO) δ (ppm) 184.1,156.1,140.5,131.4,129.8,129.3,127.9,127.6,32.9,21.0; IR

(KBr) υ (cm^{-1}) 3390,2953,2762,1708,1649,1205; HRMS calcd for $C_{21}H_{19}N_3O_3S$ (M+) 393.1147,found 393.1142.

2-((E)-5-(4-bromobenzylidine)-3-((E)-4-bromobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7k (Table-2,Entry 11) Pale yellow color amorphous solid(0.9669g,89%); Mp 217-220°C;^{1}H NMR (400 MHz, DMSO) δ (ppm)12.145(s,1H),8.595(s,1H),7.974-7.950(d,J=9.6,2H),7.725-7.702(d,J=9.2,1H),7.487(s,1H), 7.458(s,1H), 7.428-7.424(d, J=1.6Hz, 1H)7.442-7.438 (d, J=5.6, 1H), 7.404-7.390 (d, J=5.6,2H) 3.934(s,2H); ^{13}CNMR (100MHz,DMSO) δ (ppm) 174.2, 173.2, 171.9, 167.0, 158.6, 155.9,154.2,133.5,133.3,132.7,131.4,129.1,128.5,127.8,126.4,125,124.1,123.8,33.1IR(KBr) υ (cm^{-1}) 3390, 2993, 2773, 11720,1637,1232; HRMS calcd for $C_{19}H_{13}Br_2N_3O_3S$ (M+) 520.9044,found 520.9036.

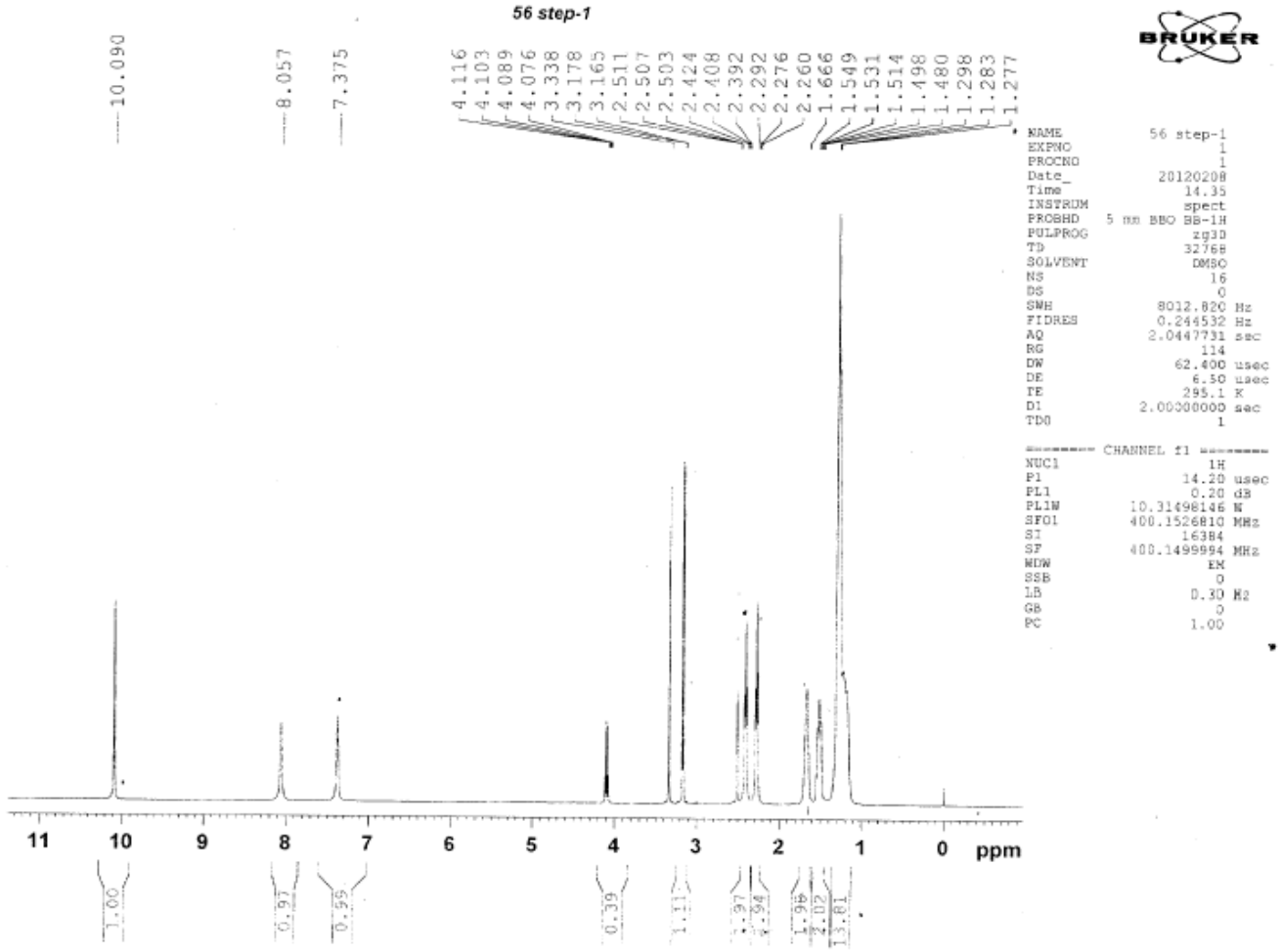
2-((E)-5-(4-hydroxybenzylidine)-3-((E)-4-hydroxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7l (Table-2,Entry 12) Pale yellow color amorphous solid (0.7597g,91%); Mp 292-295°C;^{1}H NMR (400 MHz, DMSO) δ (ppm) 11.88 (s, 1H), 10.02(s, 2H), 8.28(s, 2H), 7.60-7.58(d, J=8, 4H), 6.85-6.83(d, J=8, 4H), 3.87(s, 2H); ^{13}C NMR (100MHz, DMSO) δ (ppm) 173.2, 159.8, 158.6, 156.0, 129.4, 125.1, 115.6, 78.9, 33.021; IR(KBr) υ (cm^{-1})3496, 3223, 2929, 2850, 1705, 1639,1242; HRMS calcd for $C_{19}H_{15}N_3O_5S$ (M+) 397.0732,found 397.0735.

2-((E)-5-(4-benzyloxybenzylidine)-3-((E)-4-benzyloxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7m (Table-2, Entry13) Pale yellow color amorphous solid(1.0510g,88%) Mp 263-266°C;^{1}H NMR (400 MHz, DMSO) δ (ppm) 11.900(s,1H), 9.045(s,1H), 7.7167.694(d, J=8.8,4H), 7.4757.457(q, J=7.2,5H), 7.4167.411(t, J=2,4H), 7.334-7.323(d, J=4.4,2H), 7.167-7.114(t, J=9.2,4H), 5.230(s,2H), 4.052(t, J=2,2H), 3.880(s,2H); ^{13}C NMR (100MHz, DMSO) δ (ppm) 174.0,163.8,160.3,155.7,136.6,130.1,129.2128.4,127.8,127.7,126.9,115.3,1,69.3,32.8 IR (KBr) υ (cm^{-1}) 3490, 2958, 2937, 2765,1714,1639,1244; HRMS calcd for $C_{33}H_{27}N_3O_5S$ (M+) 577.1671,found 577.1677.

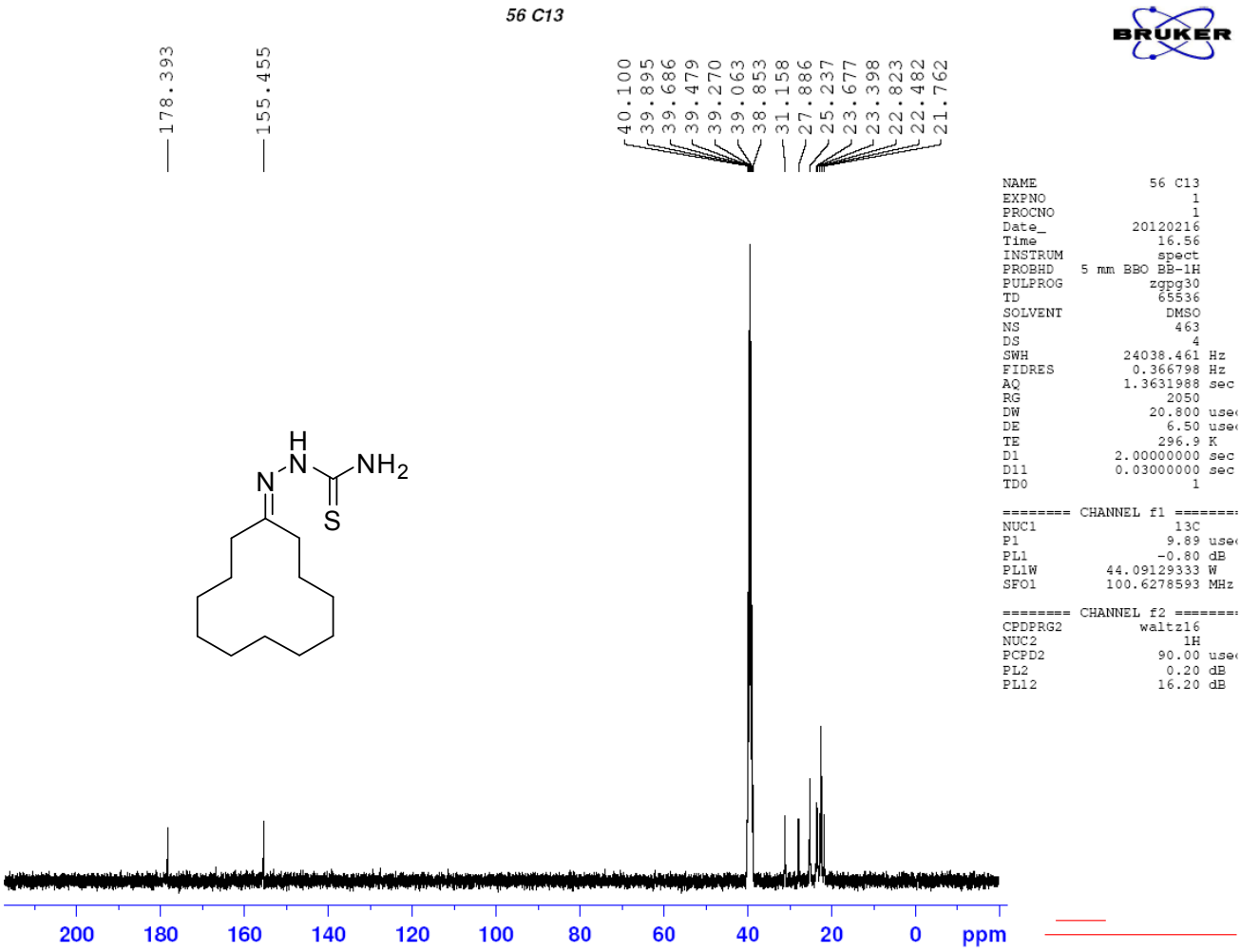
2-((E)-4-oxo-5-((E)-3-phenylallydene)-3-((E)-((E)-3-phenylallydene)amino)-2-thioxoimidazolidine-1-yl)acetic acid : 7n (Table-2,Entry14) Pale yellow color amorphous solid(0.6912g,79%) Mp 227-230°C;^{1}H NMR (400 MHz, DMSO) δ (ppm) 12.092(s,1H),8.004(s,1H), 8.023-7.989(t, J=7.6,2H), 7.724-7.686(m,1H),7.662(s,1H), 7.602-7.501(m,4H), 7.460-7.414(q, J=7.6,1H),7.387-7.309(m,6H),3.919(s,2H); ^{13}CNMR(100MHz,DMSO) δ (ppm) 174.1,162.0,159.5, 150.6,148.9, 132.6, 132.5,132.0,128.8,127.5,127.1,125.3,124.8,121.6,121.5,119.9,116.2,116.0,33.0; IR (KBr) υ (cm^{-1}) 3352, 3217, 3140, 3060, 2931,2860,2737,1707,1638,1238; HRMS calcd for $C_{23}H_{19}O_3N_3O_3S$ (M+) 417.1147, found 417.1148.

2-cyclododecylidenehydrazine carbothiamide:

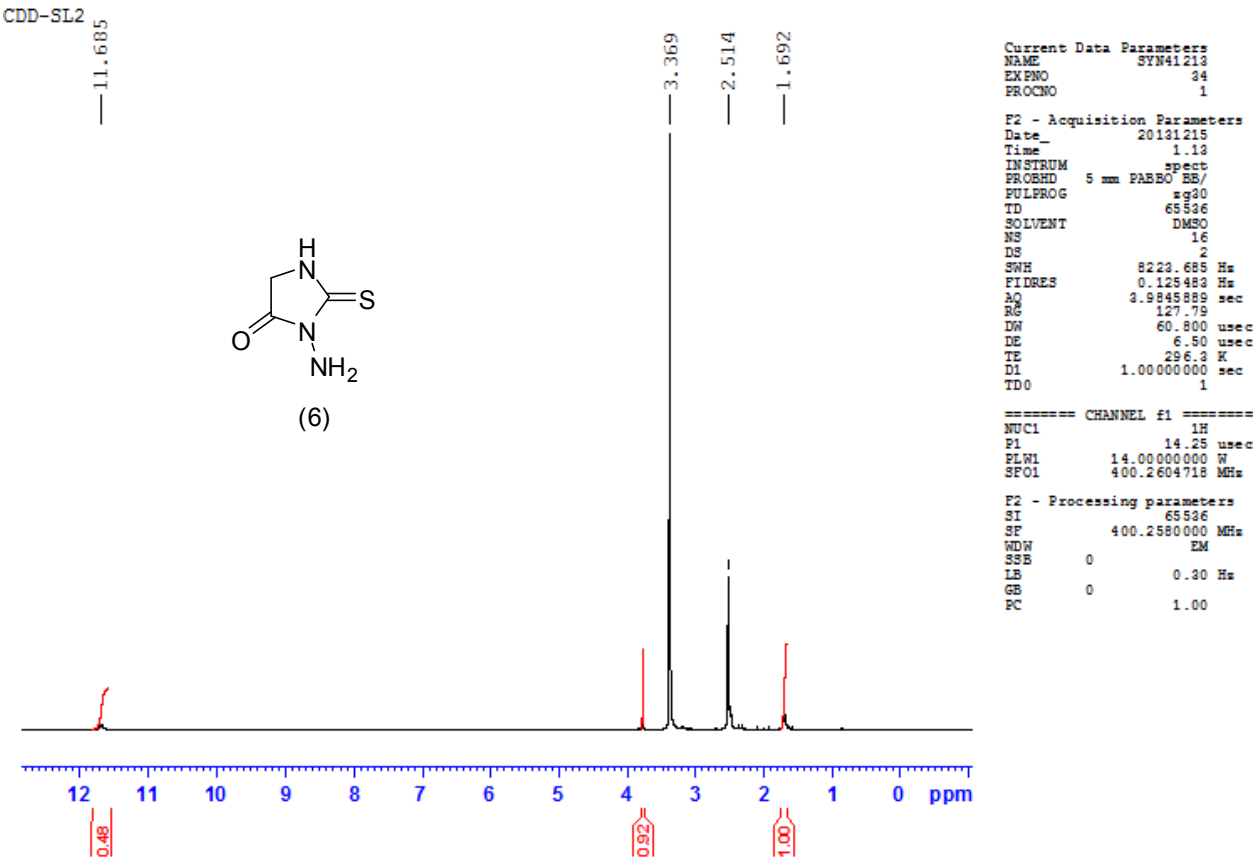
^{1}H NMR, DMSO, 400 MHz



^{13}C NMR, DMSO, 400 MHz



^{1}H NMR of 3-amino-2-thioxoimidazolidin-4-one (6)

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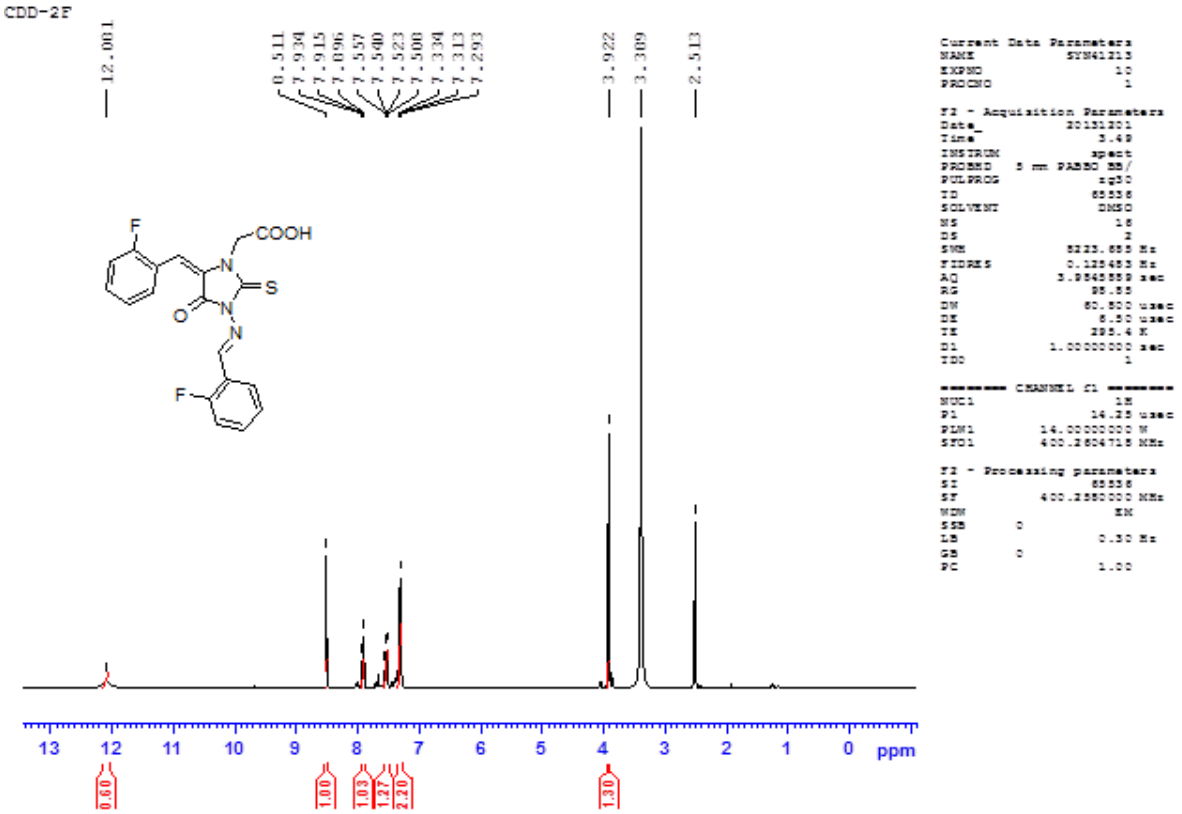
2-((E) - 5-(2-fluorobenzylidine)-3-((E)-2-fluorobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid (7a)

^{1}H NMR, DMSO, 400 MHz



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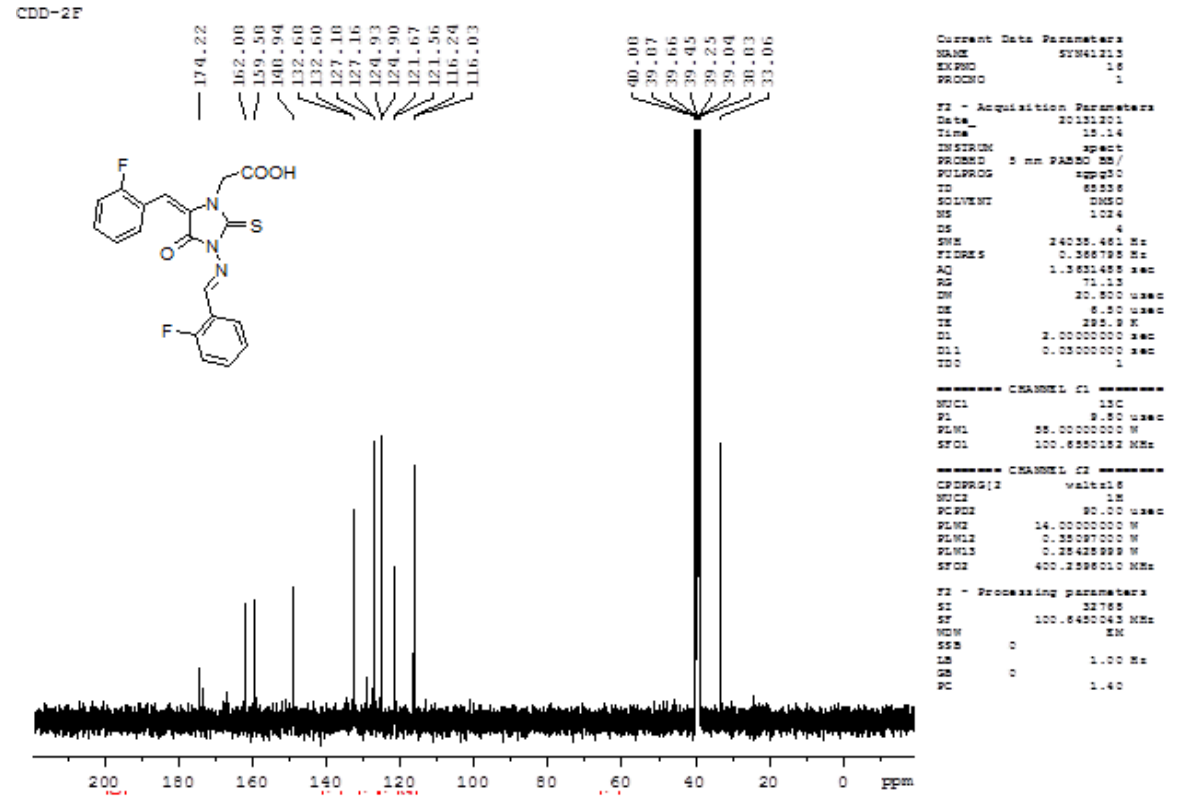
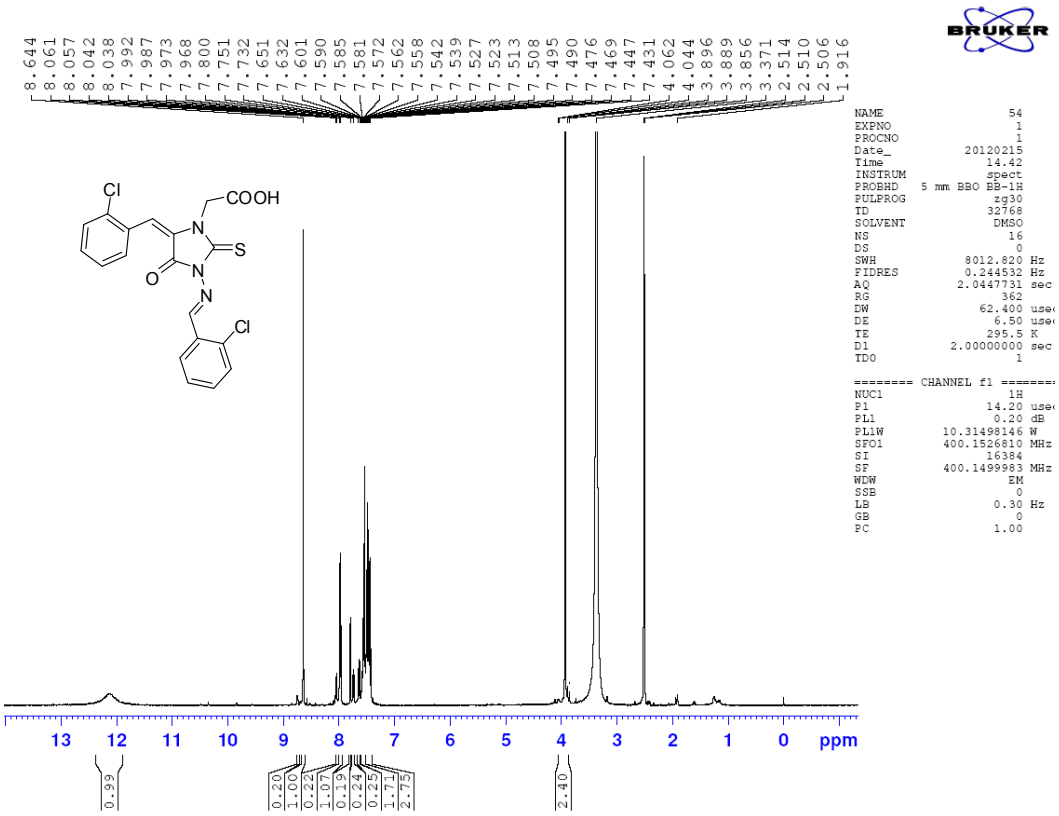
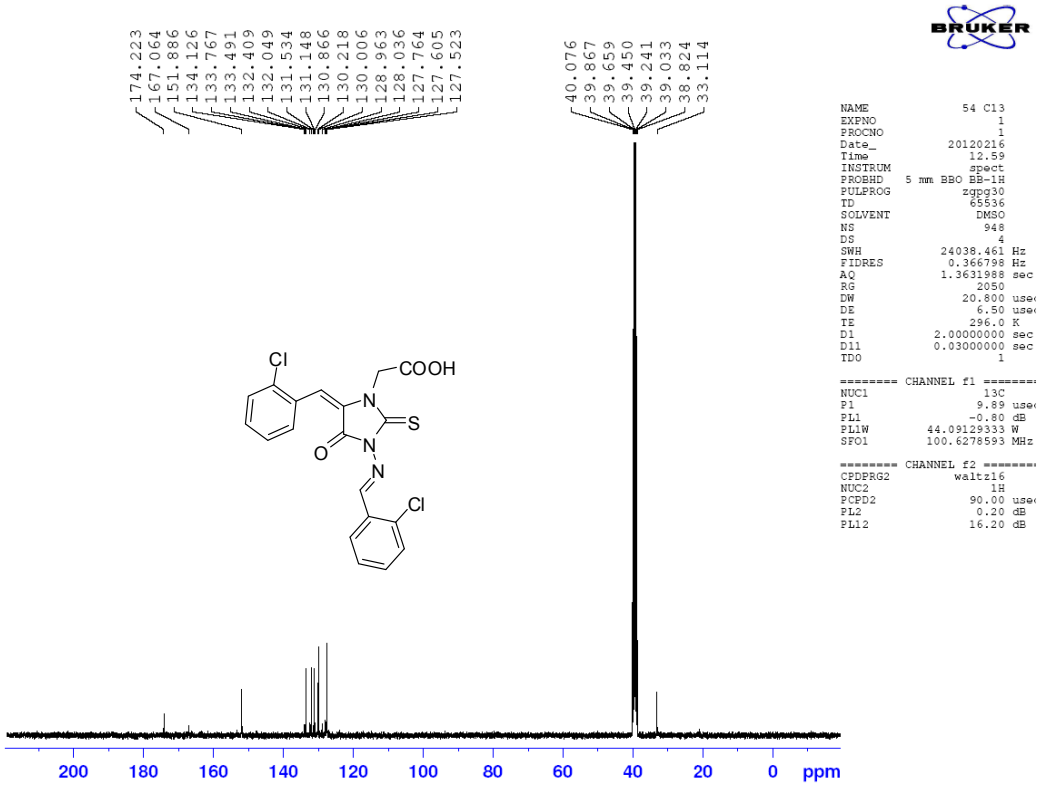


2-((E) - 5-(2-chlorobenzylidine)-3-((E)-2-chlorobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7b

^{1}H NMR, DMSO, 400 MHz

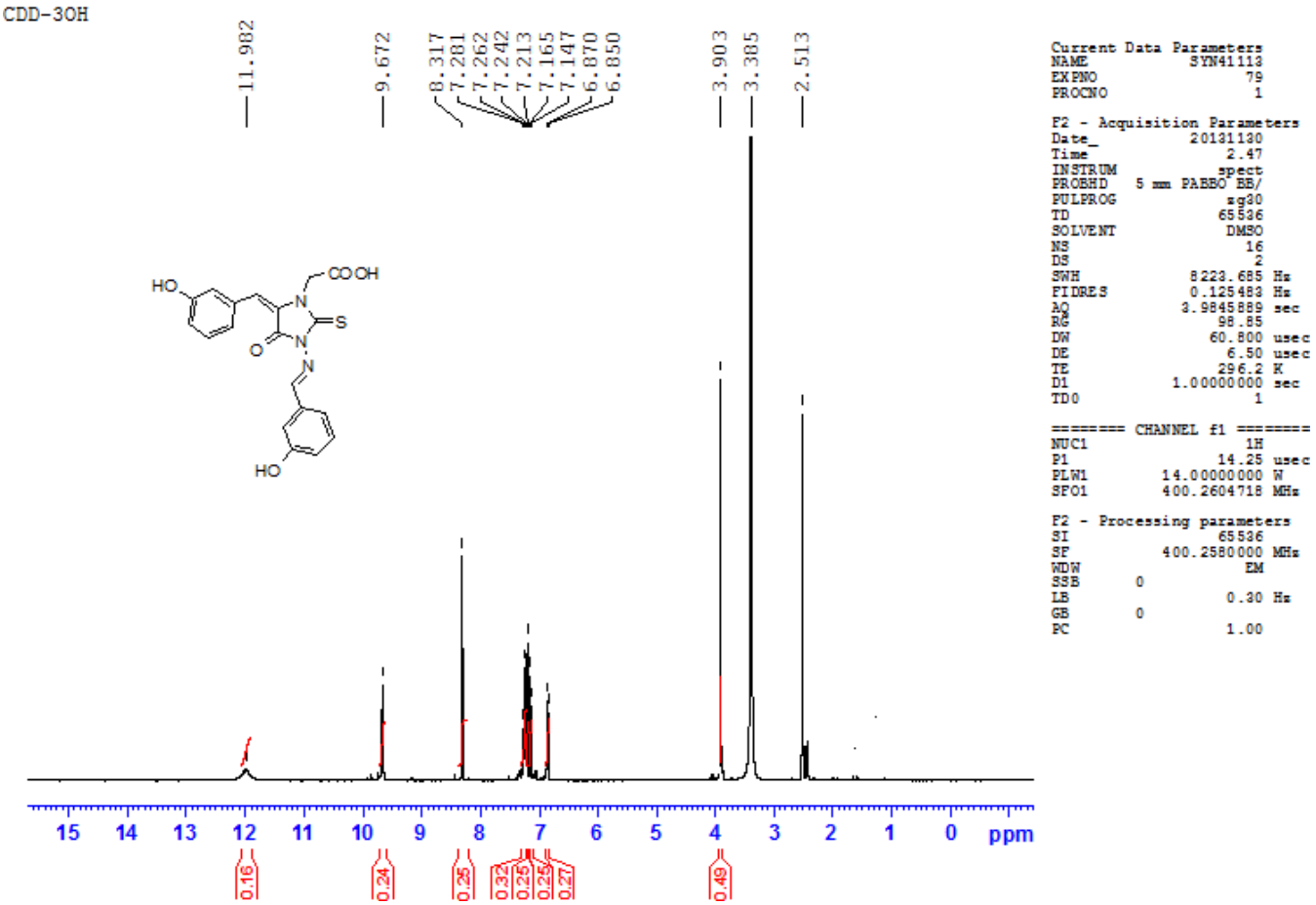


^{13}C NMR, DMSO, 400 MHz

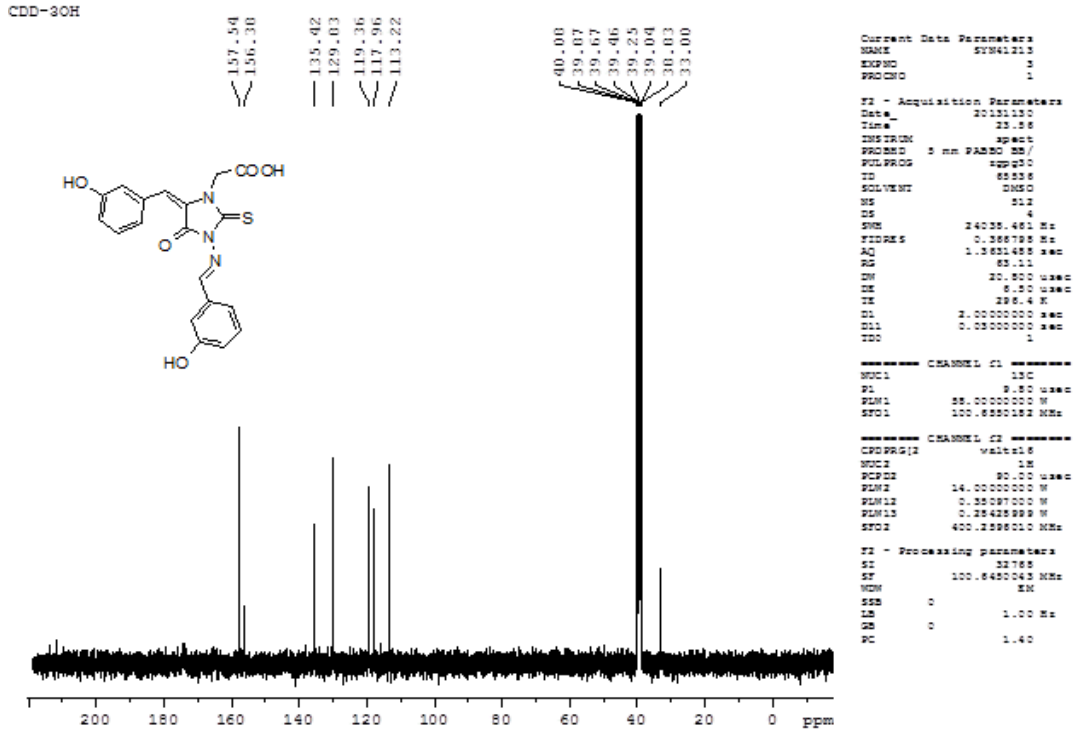


2-((E) - 5-(3-hydroxybenzylidine)-3-((E)-3-hydroxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7c

^{1}H NMR, DMSO, 400 MHz

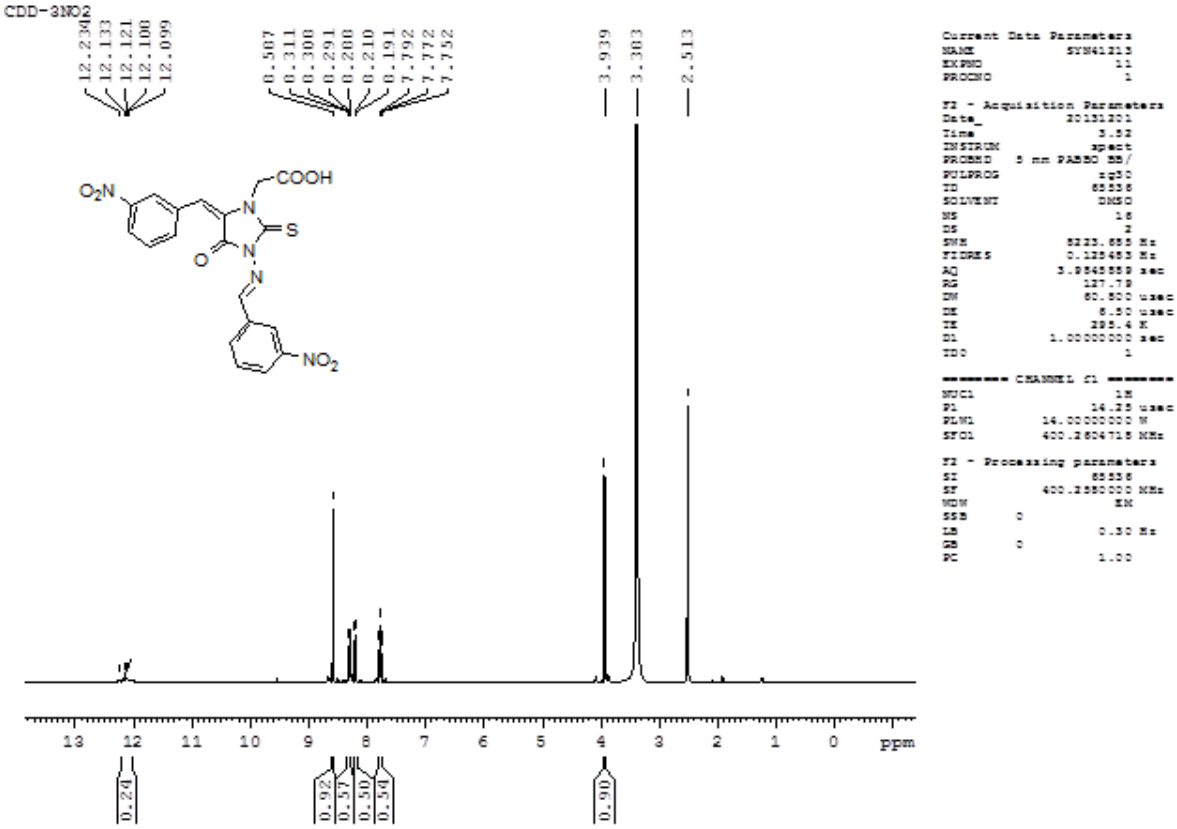


^{13}C NMR, DMSO, 400 MHz

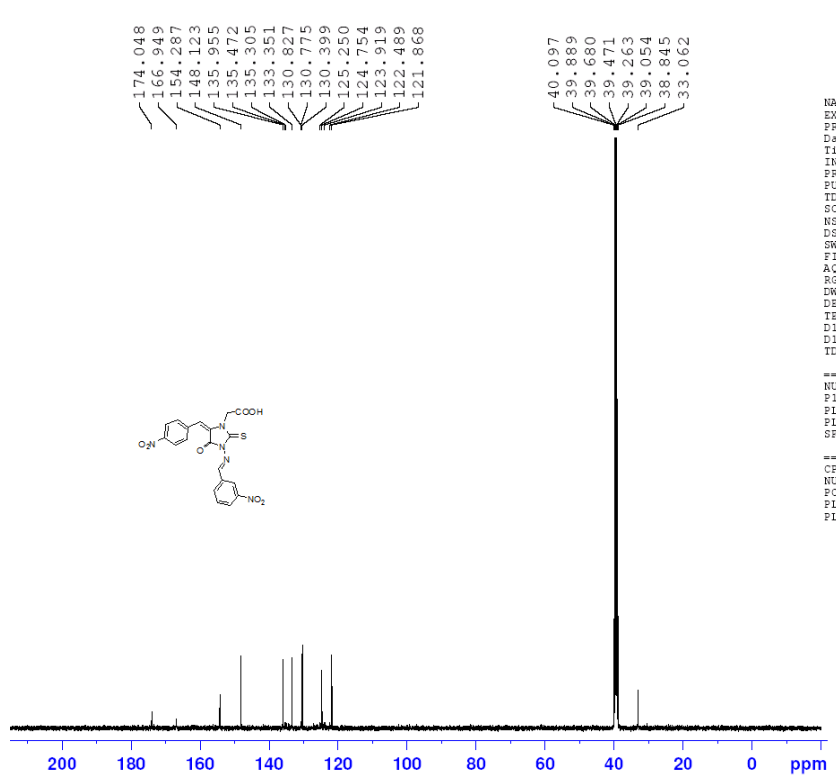


2-((E) - 5-(3-nitrobenzylidine)-3-((E)-3-nitrobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7d

^{1}H NMR, DMSO, 400 MHz

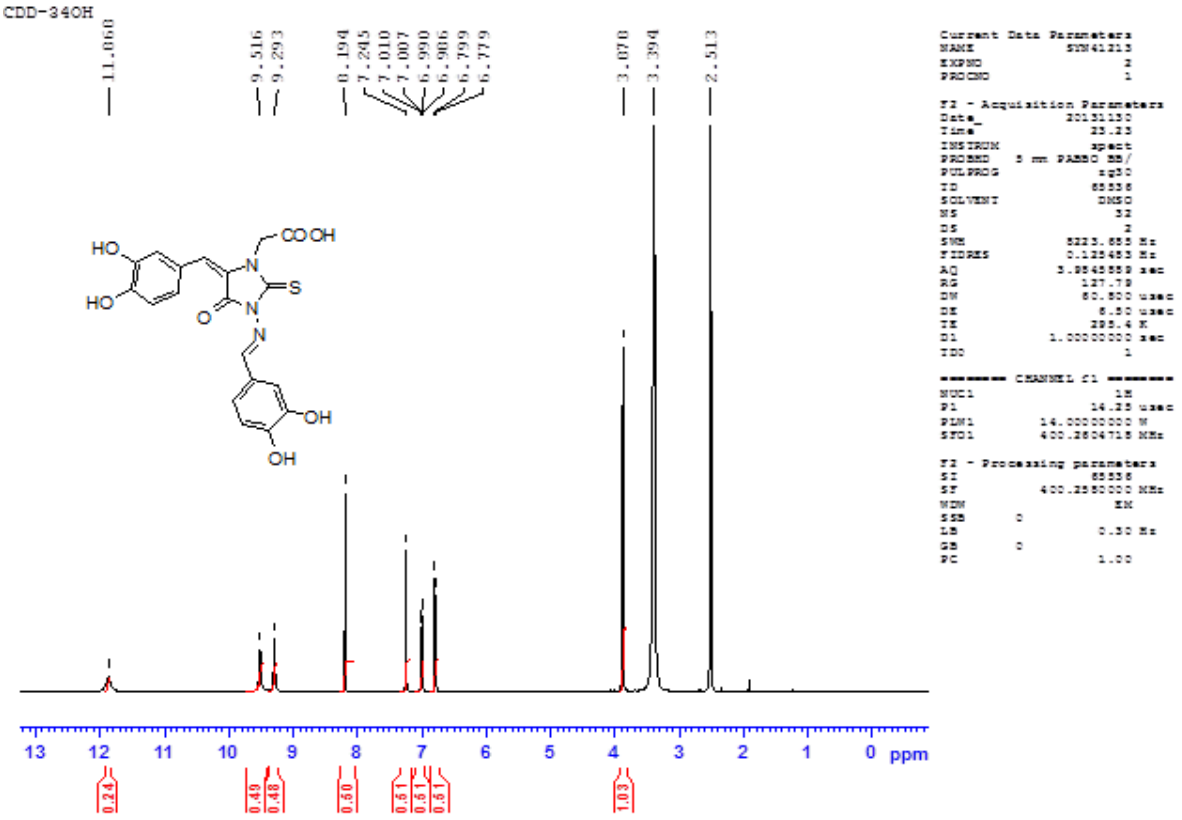


^{13}C NMR, DMSO, 400 MHz

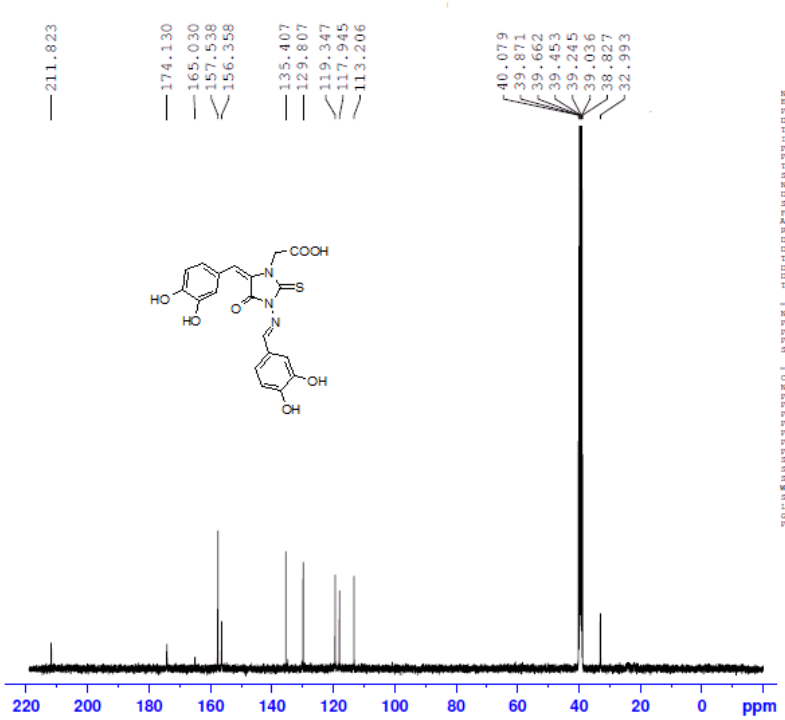


2-((E) - 5-(3,4-dihydroxybenzylidine)-3-((E)-3,4-dihydroxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid (7e)

^{1}H NMR, DMSO, 400 MHz

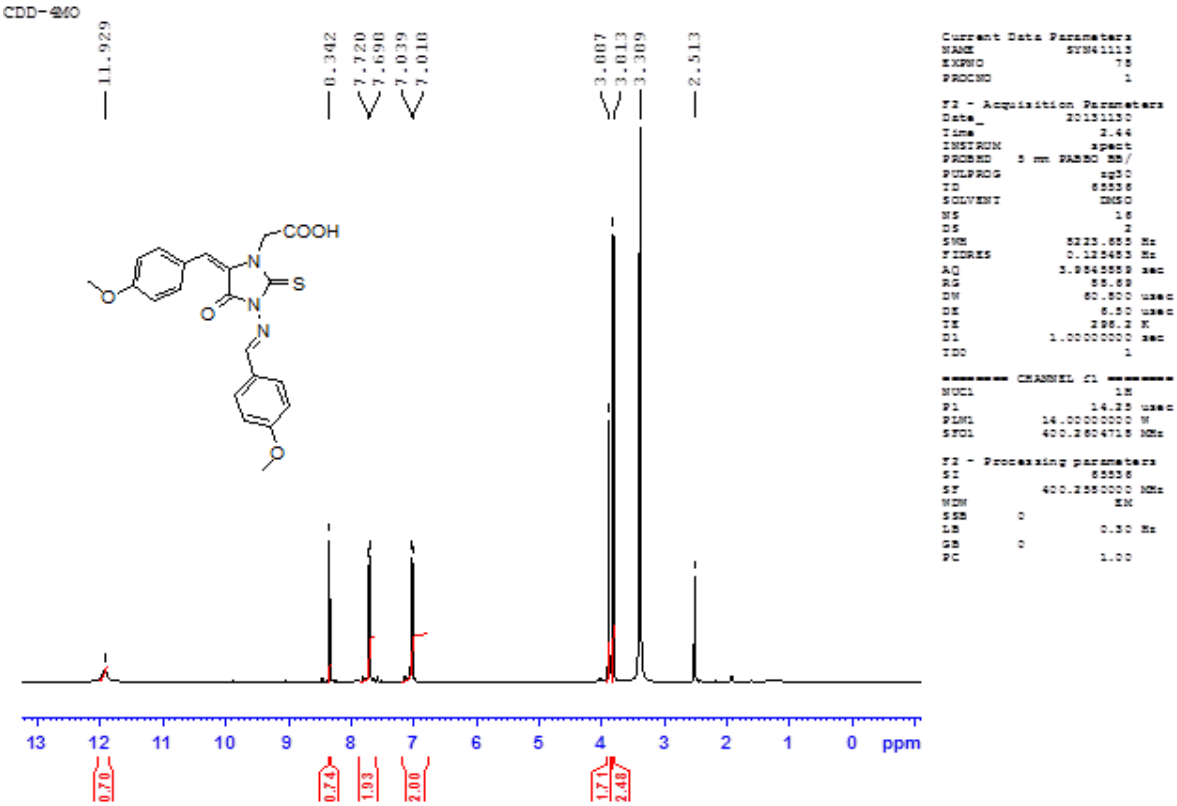


^{13}C NMR, DMSO, 400 MHz

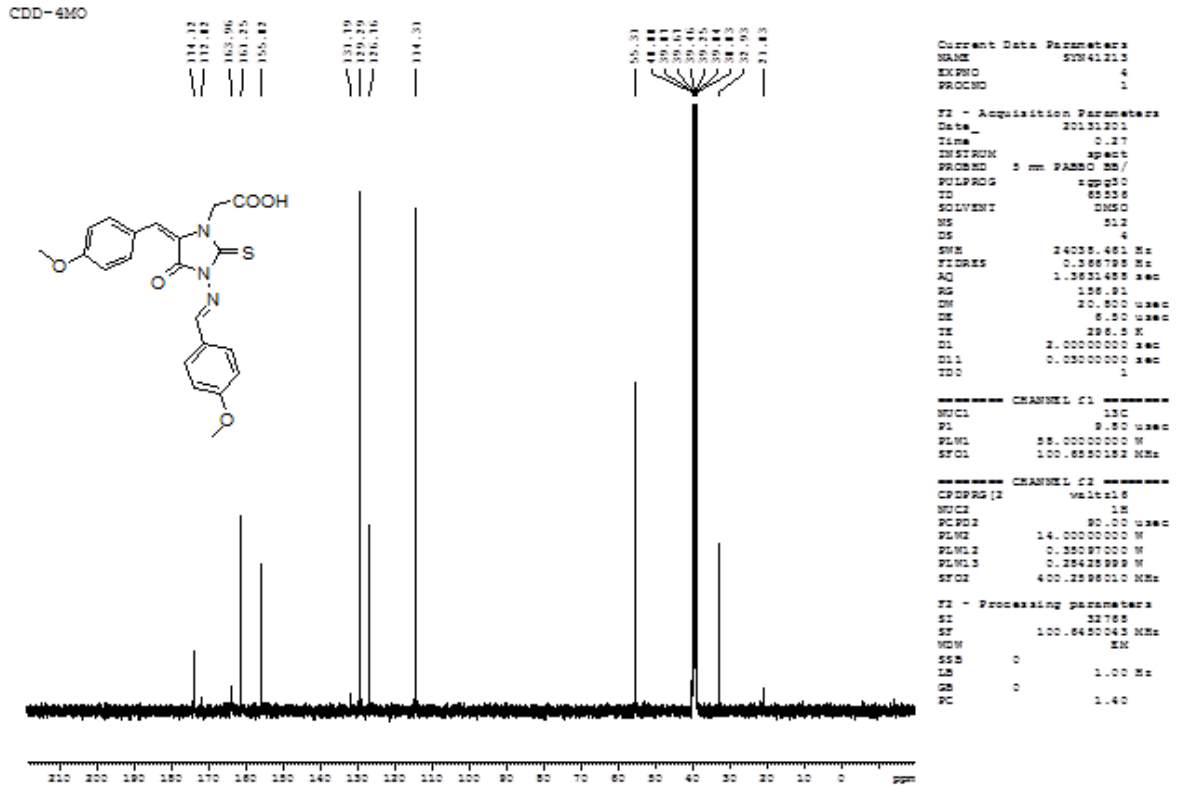


2-((E) - 5-(4-methoxybenzylidine)-3-((E)-4-methoxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid :7f

^{1}H NMR, DMSO, 400 MHz

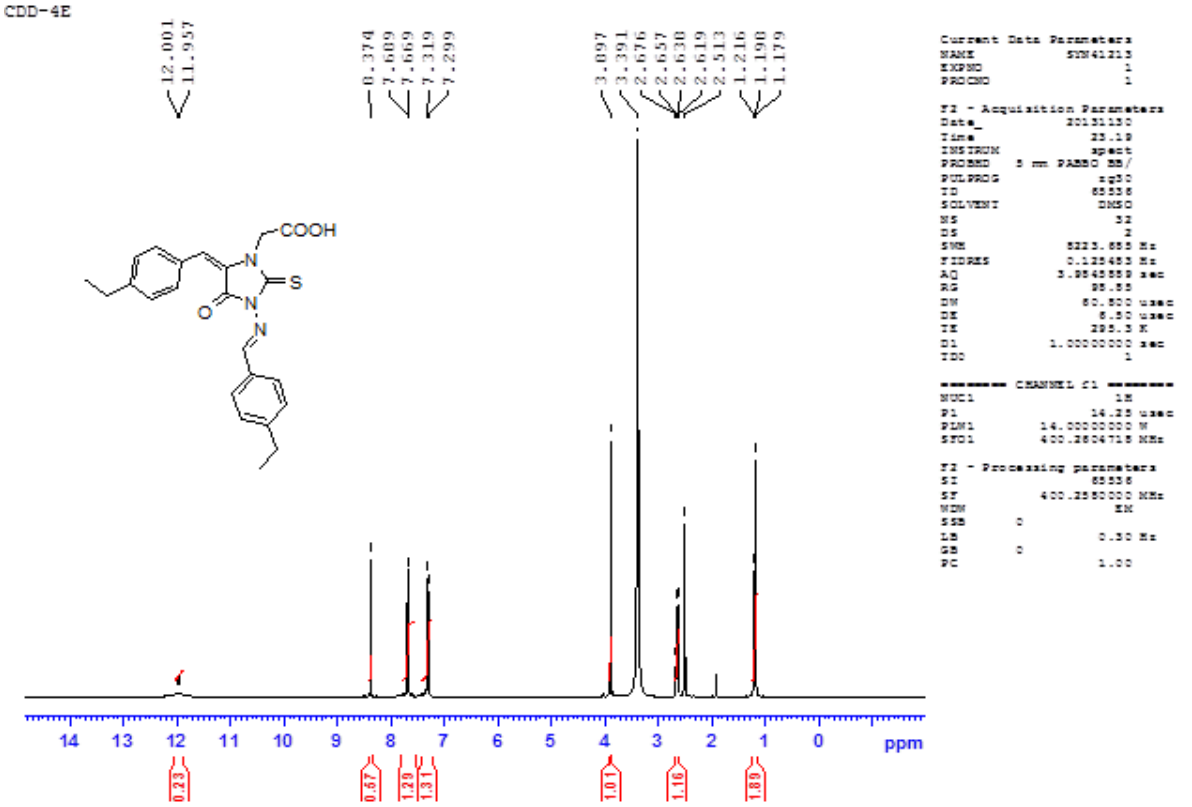


^{13}C NMR, DMSO, 400 MHz



2-((E) - 5-(4-ethylbenzylidine)-3-((E)-4-ethylbenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7g

^{1}H NMR, DMSO, 400 MHz

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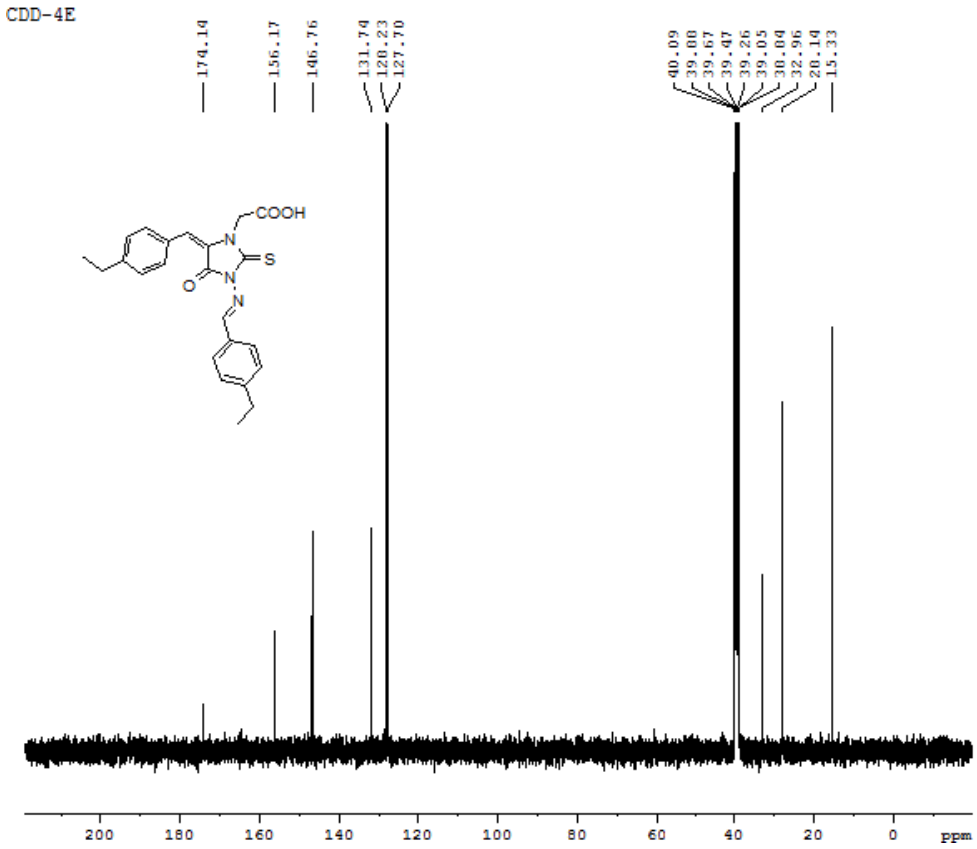
Current Data Parameters
NAME                  SYN41213
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20131130
Time                    23.19
INSTRUM                 spect
PROBHD     5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        32
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125453 Hz
AQ                  3.9845550 sec
RG                      98.55
DW                     60.800 usec
DE                      6.50 usec
TE                     295.3 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      14.25 usec
PLW1            14.00000000 W
SFO1            400.2604758 MHz

F2 - Processing parameters
SI                         65536
SF              400.2550000 MHz
WDW                           EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

^{13}C NMR, DMSO, 400 MHz

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Current Data Parameters
NAME                  SYN41213
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_               20131201
Time                    1.34
INSTRUM                 spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                     65536
SOLVENT                 DMSO
NS                        512
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     156.91
DW                     20.800 usec
DE                      6.50 usec
TE                     296.6 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

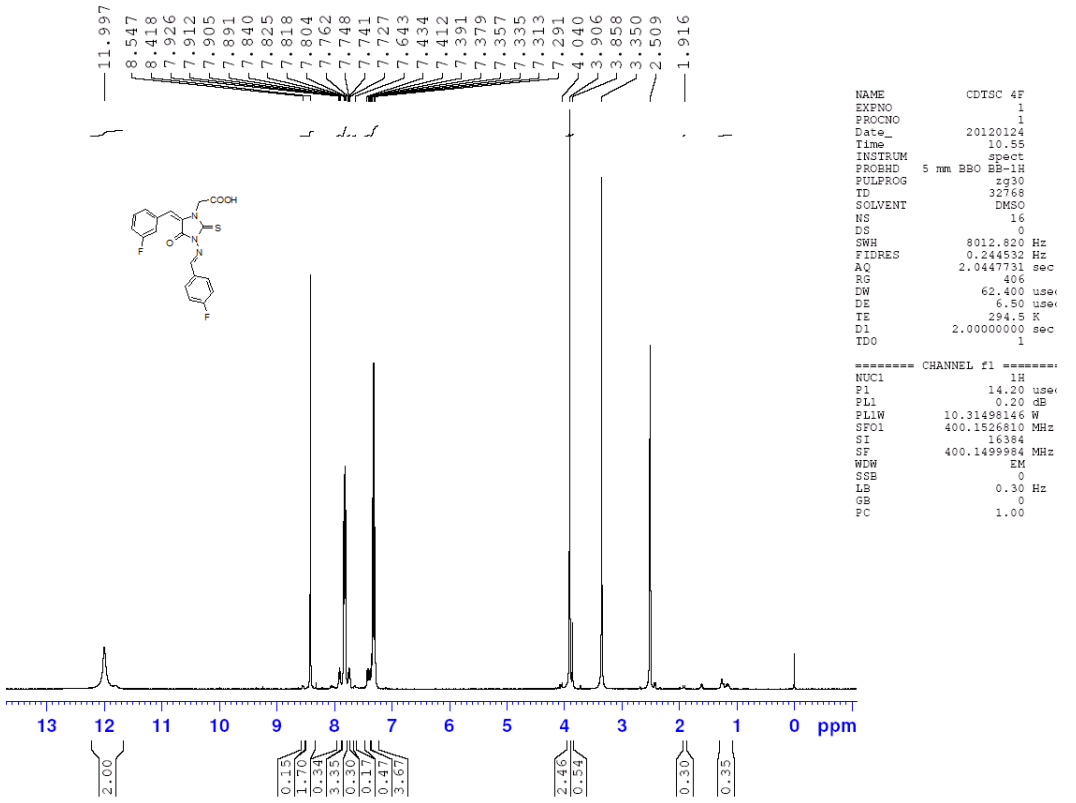
======== CHANNEL f1 ========
NUC1                       13C
P1                       9.80 usec
PLW1            58.00000000 W
SFO1            100.6550182 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                   90.00 usec
PLW2            14.00000000 W
PLW12            0.35097000 W
PLW13            0.28428999 W
SFO2            400.2596010 MHz

F2 - Processing parameters
SI                         32768
SF              100.6450043 MHz
WDW                           EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

2-((E) - 5-(4-fluorobenzylidine)-3-((E)-4-fluorobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7h

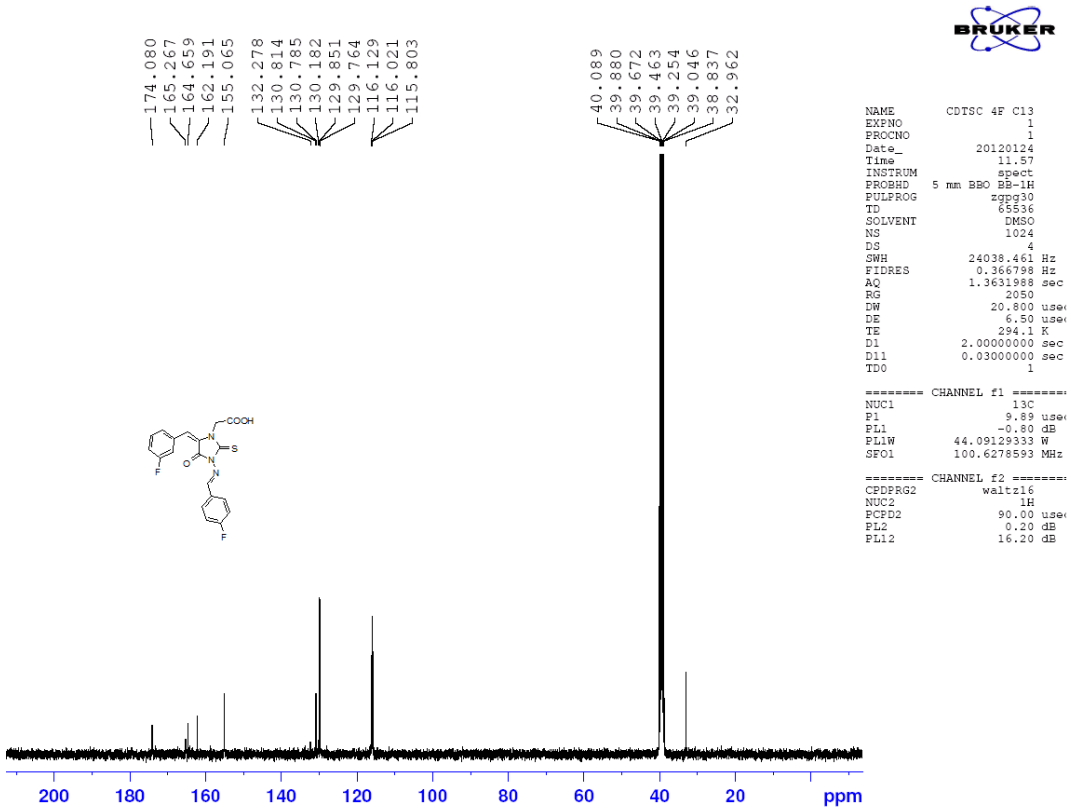
^{1}H NMR, DMSO, 400 MHz




```
NAME            CDTSC 4F
EXPNO                  1
PROCNO                 1
Date_           20120124
Time               10.55
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              2.0447731 sec
RG                   406
DW                62.400 use
DE                 6.50 use
TE                294.5 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.20 use
PL1                0.20 dB
PL1W         10.31498146 W
SFO1         400.1526810 MHz
SI                 16384
SF           400.1499984 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

^{13}C NMR, DMSO, 400 MHz



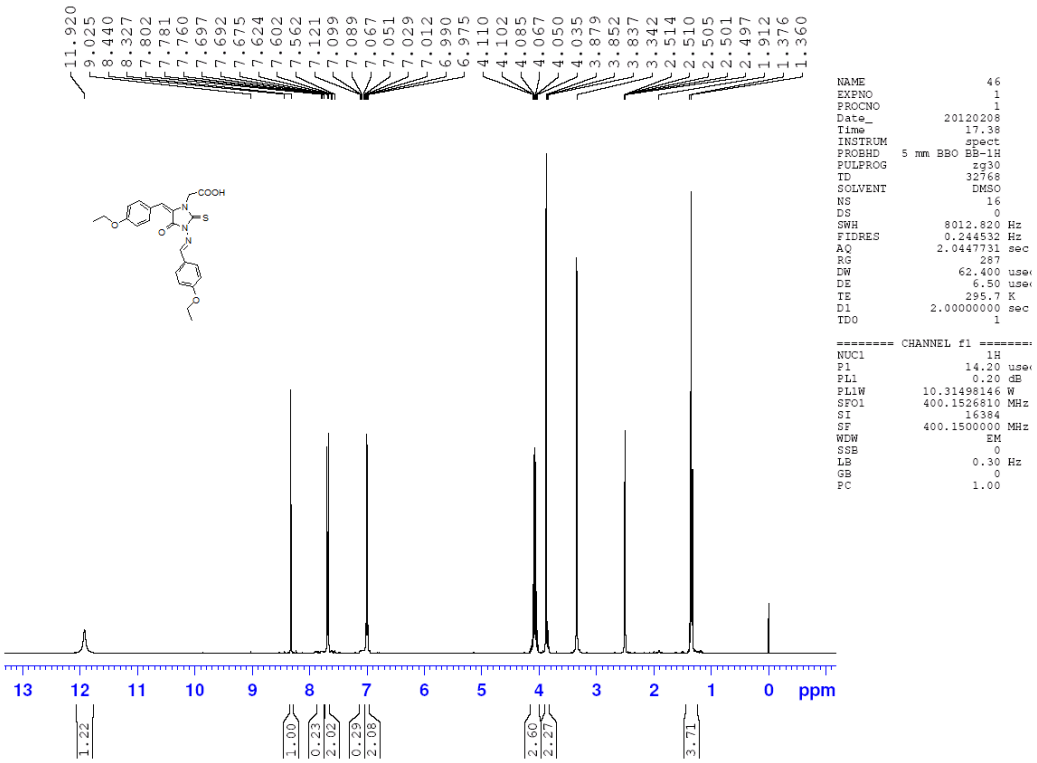

```
NAME        CDTSC 4F C13
EXPNO                  1
PROCNO                 1
Date_           20120124
Time               11.57
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                  2050
DW                20.800 use
DE                 6.50 use
TE                294.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.89 use
PL1               -0.80 dB
PL1W         44.09129333 W
SFO1         100.6278593 MHz

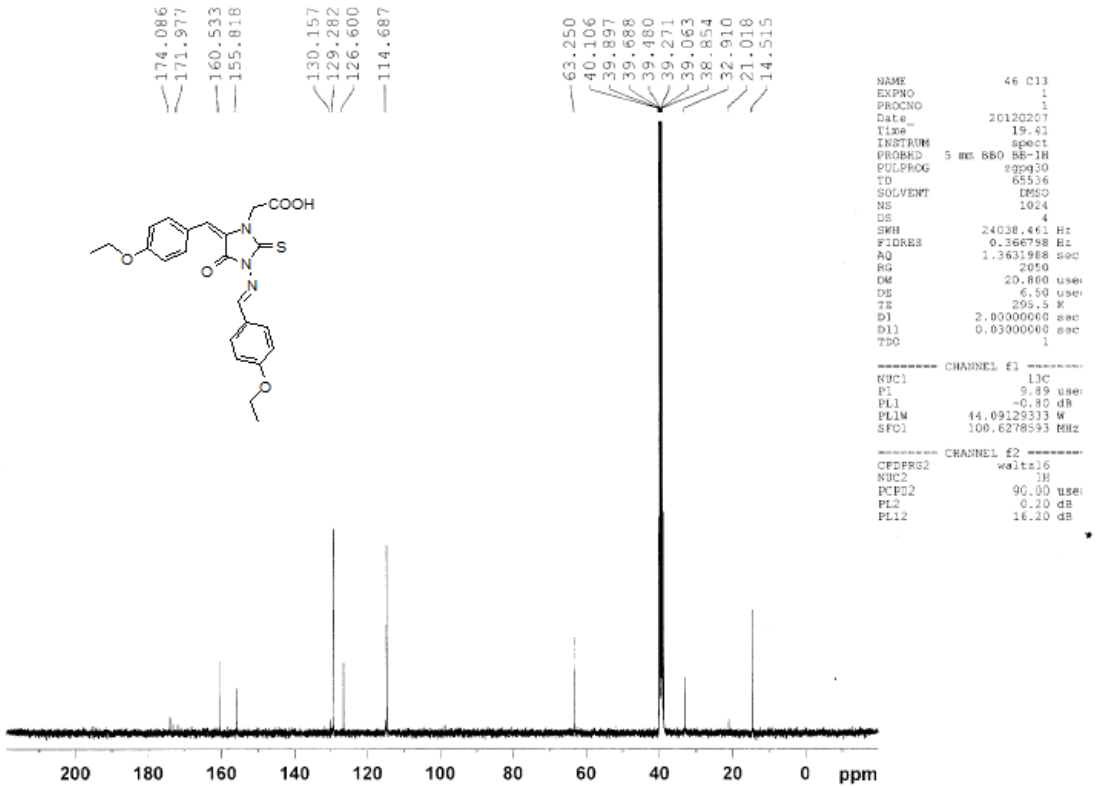
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 use
PL2                0.20 dB
PL12              16.20 dB
```

2-((E) - 5-(4-ethoxybenzylidine)-3-((E)-4-ethoxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7i

^{1}H NMR, DMSO, 400 MHz

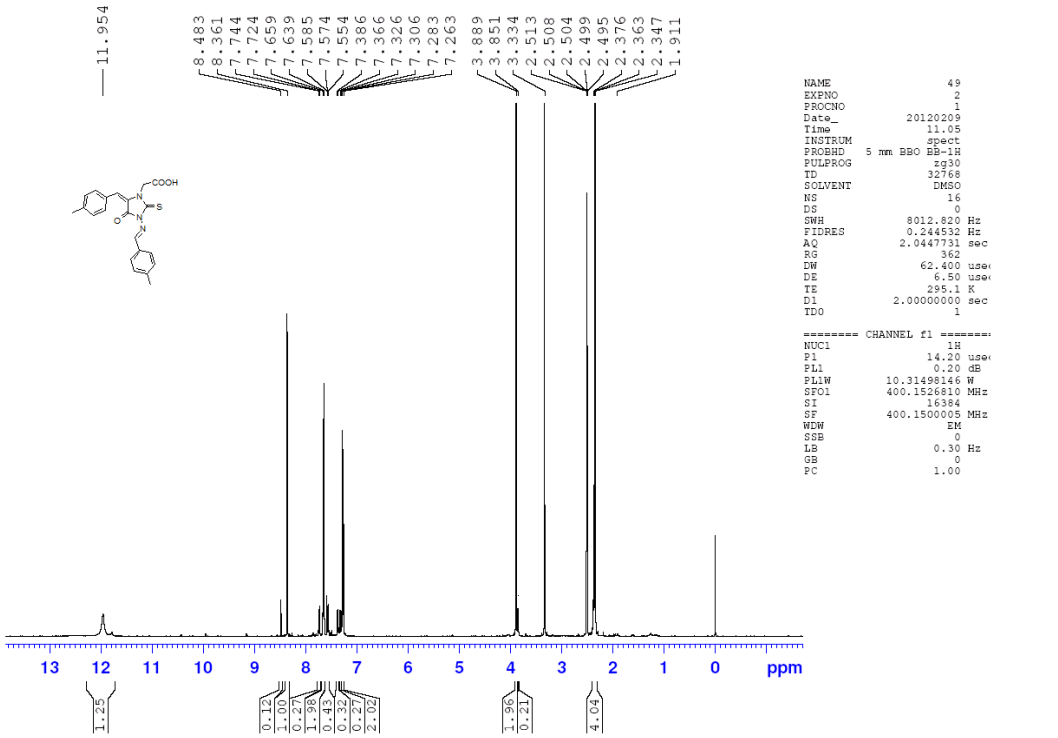


^{13}C NMR, DMSO, 400 MHz

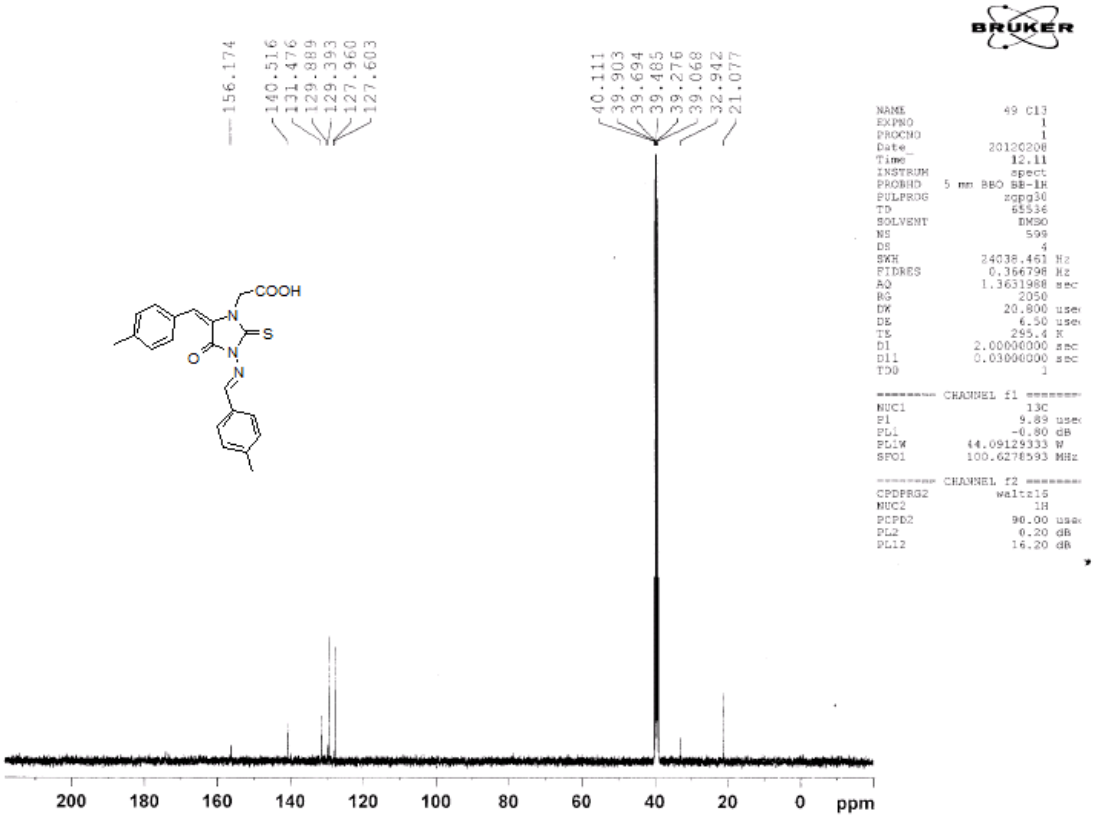


2-((E) - 5-(4-methylbenzylidine)-3-((E)-4-methylbenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7j

^{1}H NMR, DMSO, 400 MHz

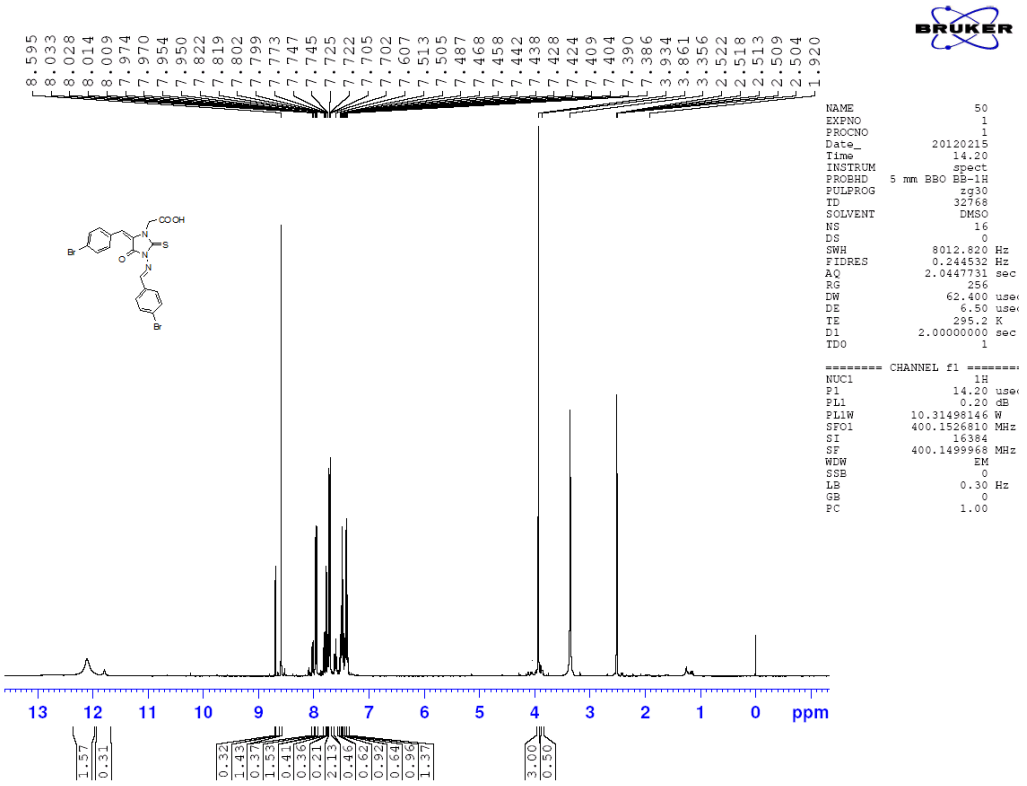


^{13}C NMR, DMSO, 400 MHz

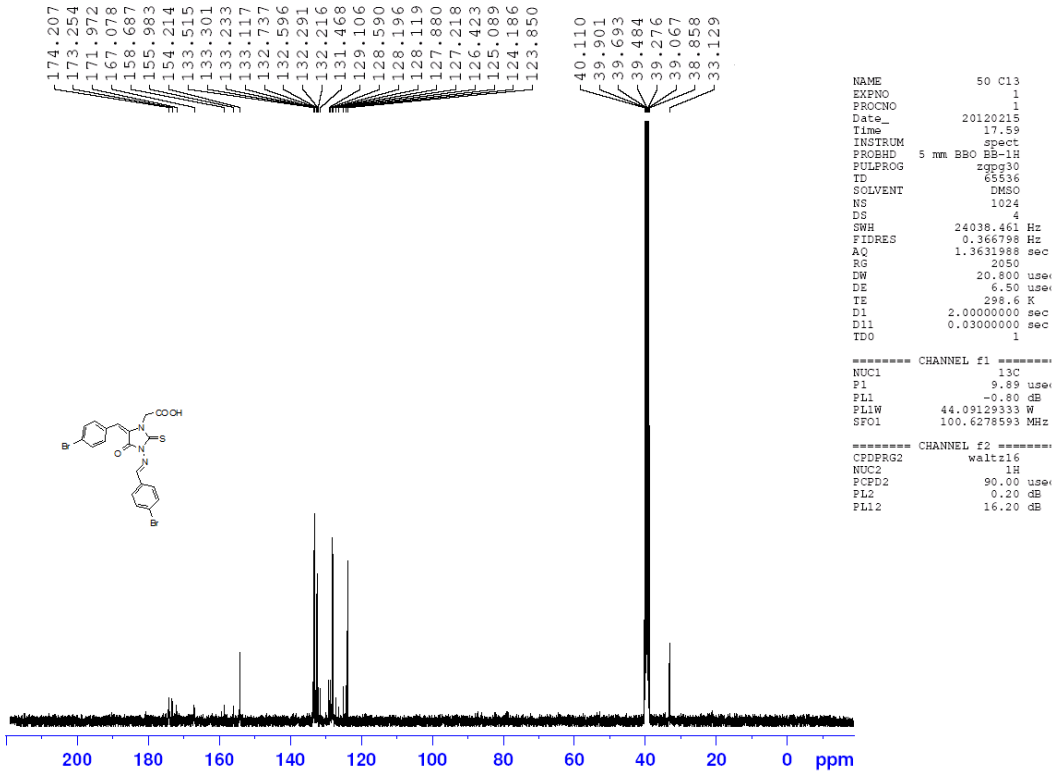


2-((E) - 5-(4-bromobenzylidine)-3-((E)-4-bromobenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7k

^{1}H NMR, DMSO, 400 MHz

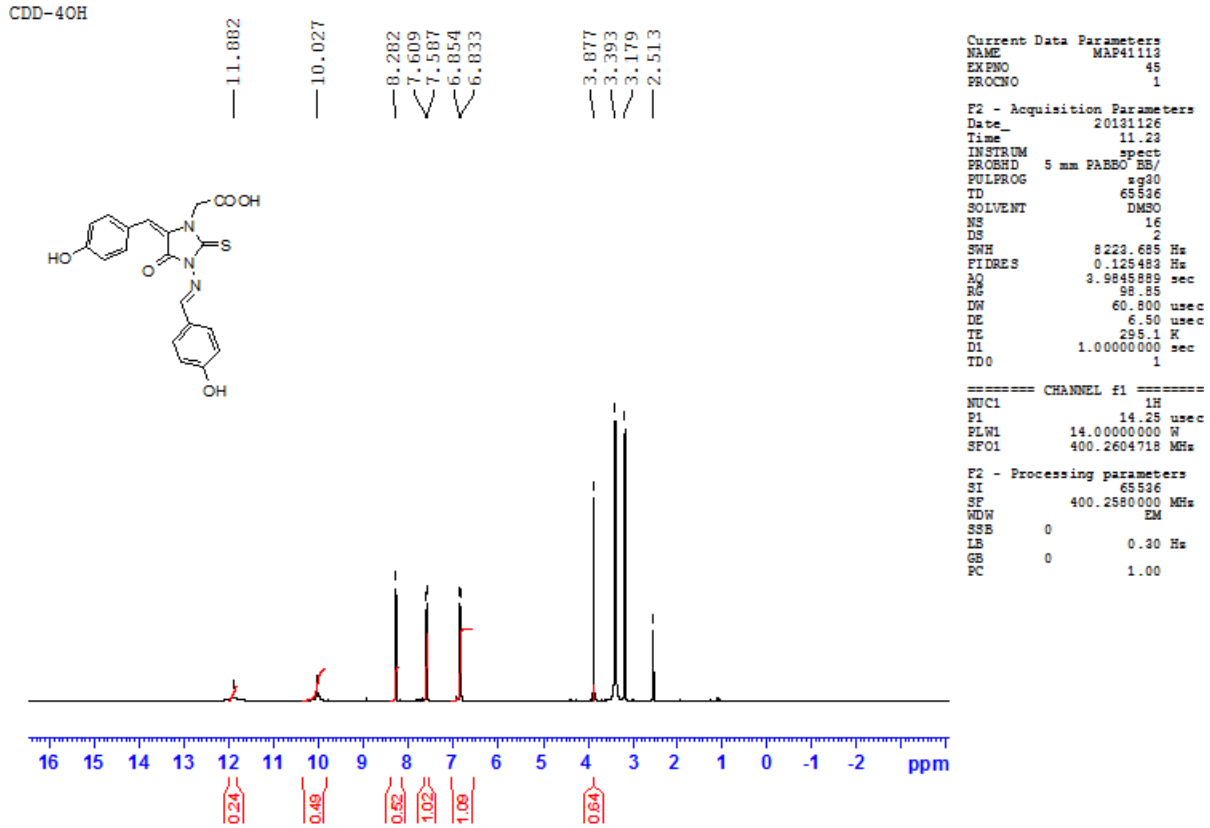


^{13}C NMR, DMSO, 400 MHz



2-((E) - 5-(4-hydroxybenzylidine)-3-((E)-4-hydroxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7l

^{1}H NMR, DMSO, 400 MHz

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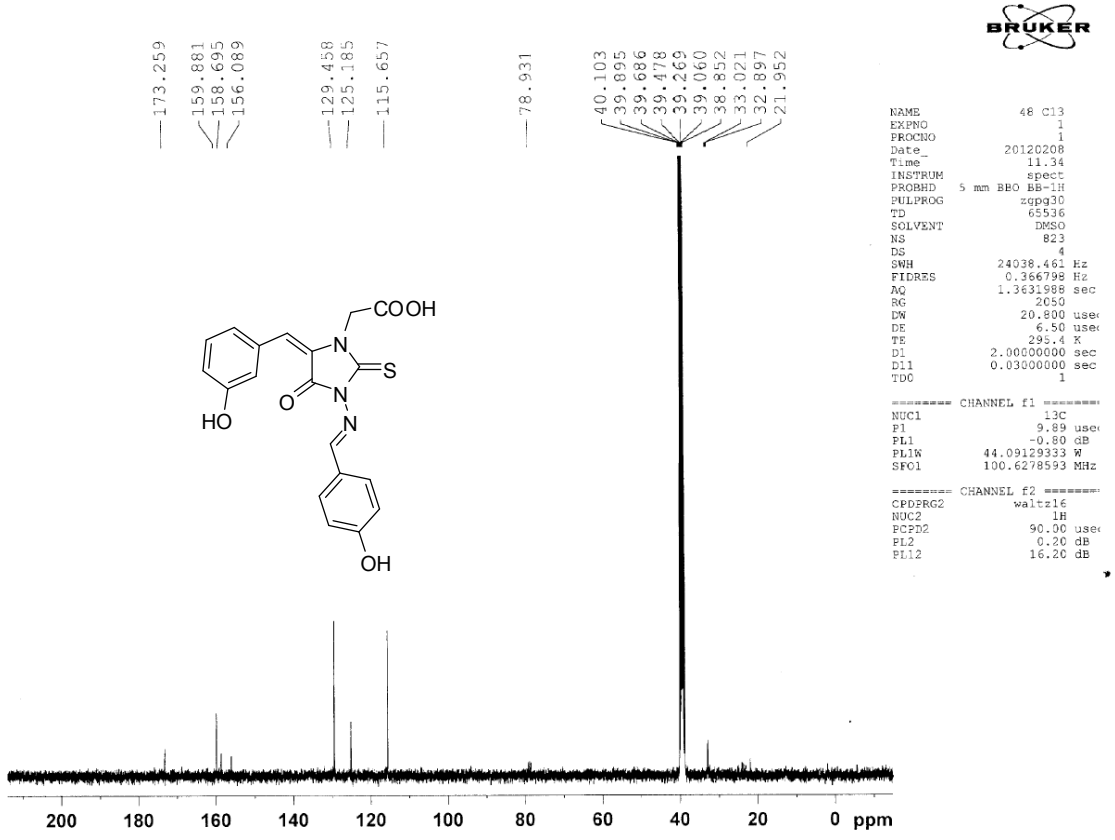
Current Data Parameters
NAME                  MAP41113
EXPNO                       45
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20131126
Time                     11.23
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9845889 sec
RG                       98.85
DW                      60.800 usec
DE                       6.50 usec
TE                      295.1 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.25 usec
PLW1                14.00000000 W
SFO1                400.2604718 MHz

F2 - Processing parameters
SI                      65536
SF                  400.2580000 MHz
WDW                         EM
SSB                  0
LB                       0.30 Hz
GB                   0
PC                       1.00
```

^{13}C NMR, DMSO, 400 MHz



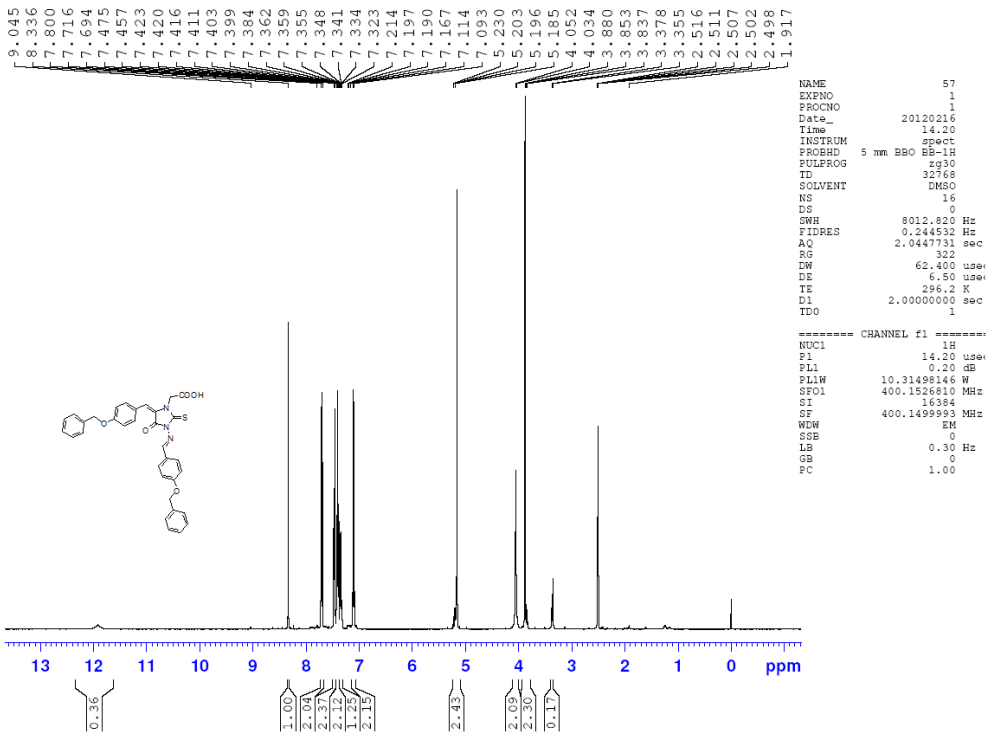

```
NAME                  48 C13
EXPNO                      1
PROCNO                     1
Date_                20120208
Time                    11.34
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                   DMSO
NS                          823
DS                            4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                        2050
DW                      20.800 use
DE                       6.50 use
TE                      295.4 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       9.89 use
PL1                     -0.80 dB
PL1W                44.09129333 W
SFO1                100.6278593 MHz

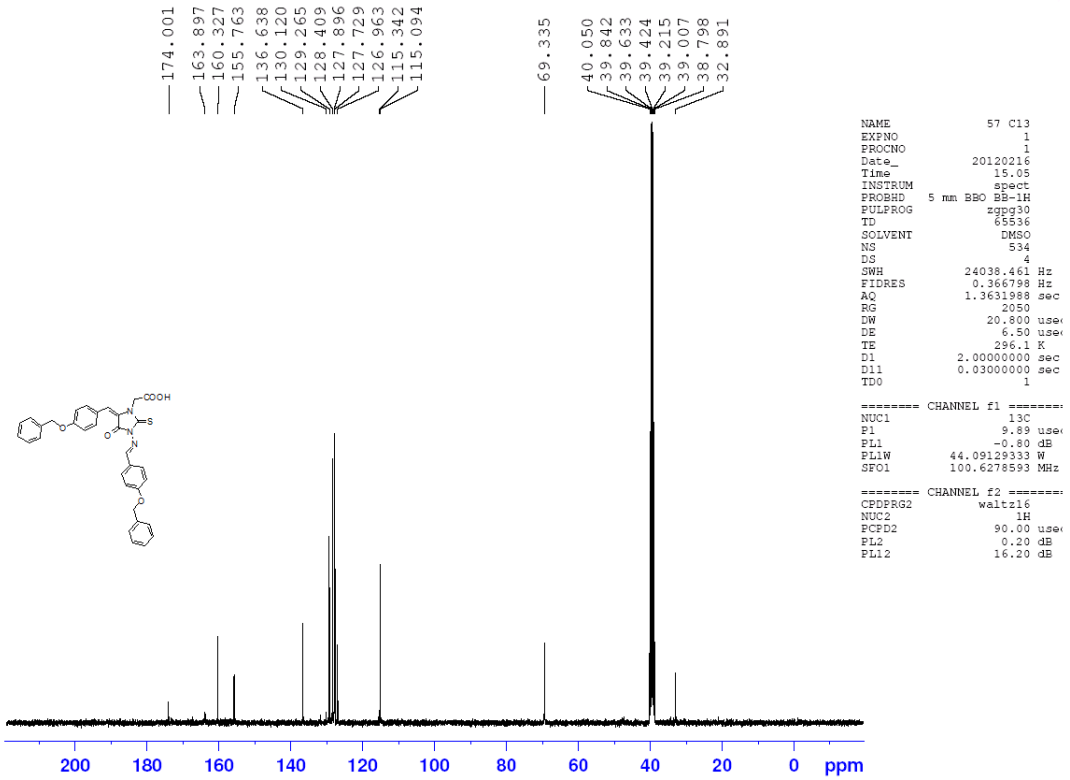
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    90.00 use
PL2                       0.20 dB
PL12                     16.20 dB
```

2-((E) - 5-(4-benzyloxybenzylidine)-3-((E)-4-benzyloxybenzylidineamino)-4-oxo-2-thioxoimidazolidine-1-yl)acetic acid: 7m

^{1}H NMR, DMSO, 400 MHz

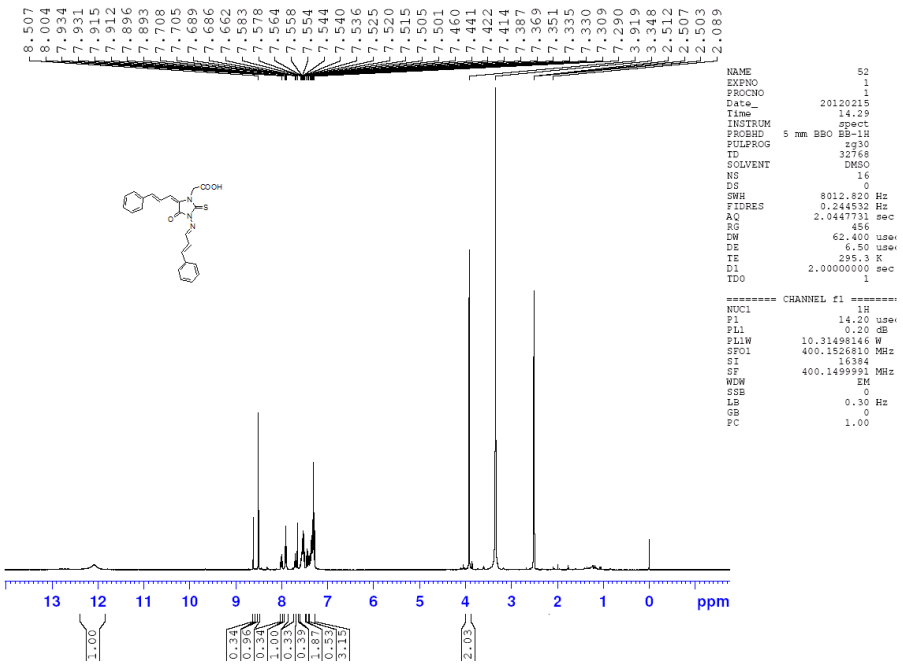


^{13}C NMR, DMSO, 400 MHz



2-((E)-4-oxo-5-(3-styrylbenzylidine)-3-((E)-styrylbenzylidineamino)-2-thioxoimidazolidine-1-yl)acetic acid : 7n (Table-2,Entry15)

^{1}H NMR, DMSO, 400 MHz



^{13}C NMR, DMSO, 400 MHz