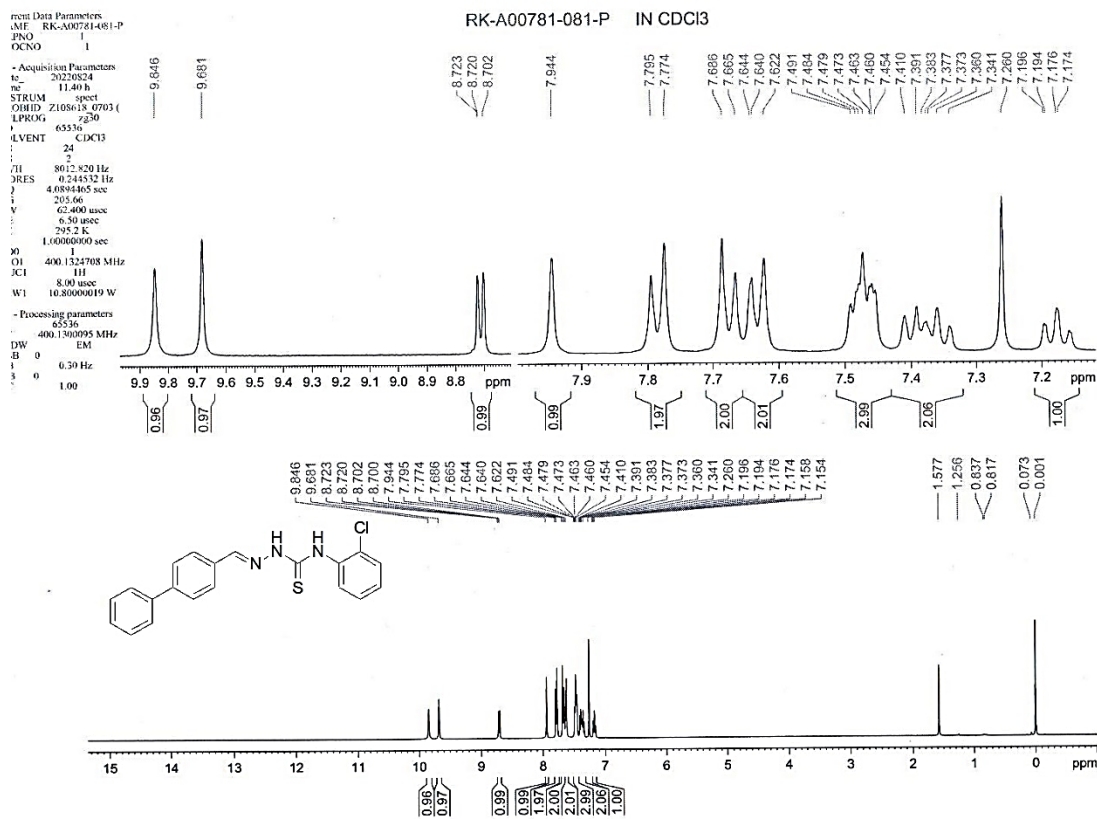
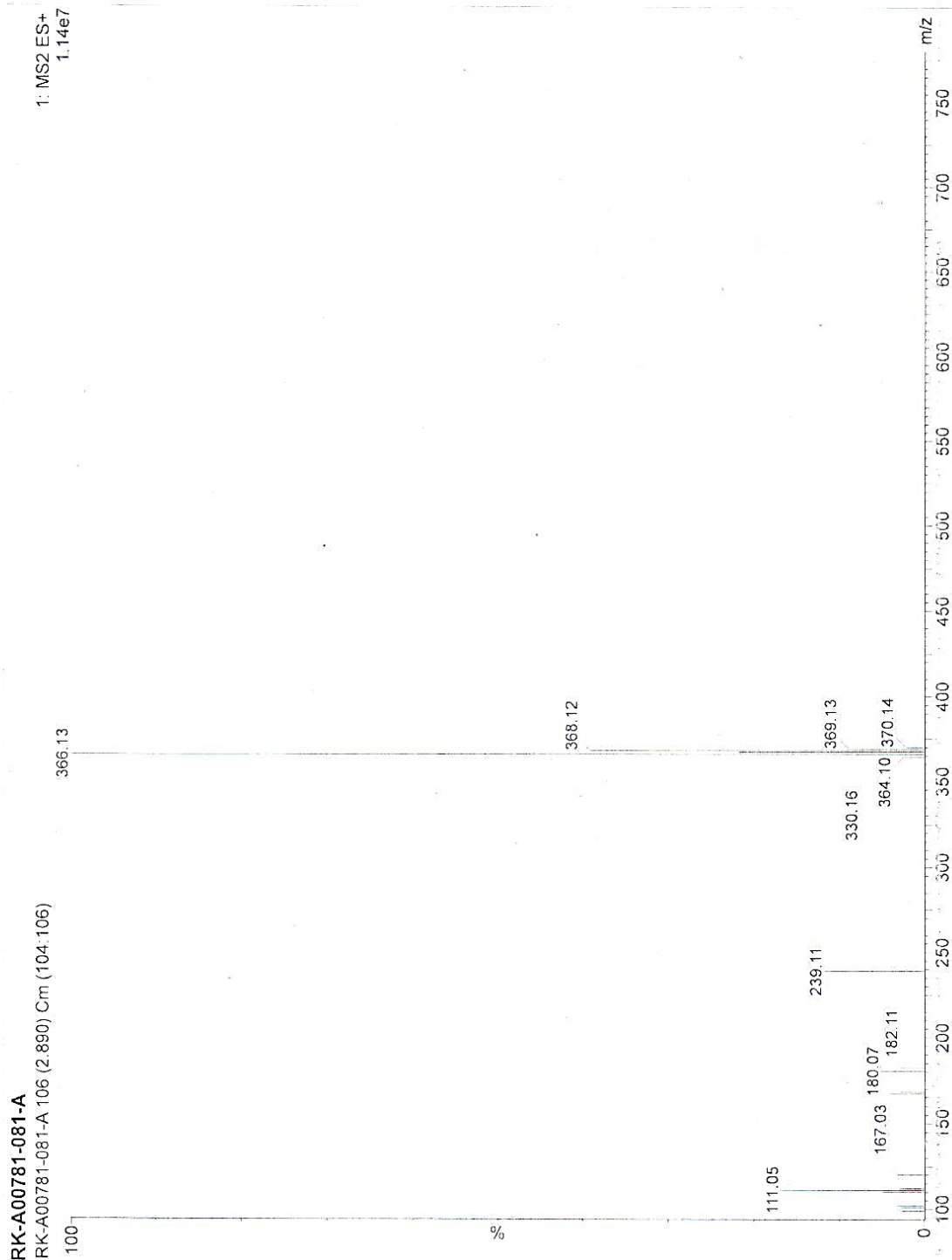


Supplementary File

A Novel Thiosemicarbazone based sensor for Transition metals



¹H NMR of (E)-1-(4-phenylbenzylidene)-4-(2-chlorophenyl)thiosemicarbazide



Mass Spectra of (E)-1-(4-phenylbenzylidene)-4-(2-chlorophenyl)thiosemicarbazide

XEVO-TQD#QCA1591

24-Aug-2022 11:55:27

RK-A00781-081-A.Sm (Mn, 2x3)

Time	Height	Area	Area%
2.12	212871	5418.69	0.05
2.80	20790544	9977875.00	99.95

3: Diode Array

Range: 2.097e+2

Area

Area%

2.80

1.0e+2

0.0

-0.00

0.25

0.50

0.75

1.00

1.25

1.50

1.75

2.00

2.25

2.50

2.75

3.00

3.25

3.50

3.75

4.00

1.07

0.05

0.30

0.41

0.68

0.74

0.93

1.12

1.34

1.53

1.70

1.89

1.97

2.08

2.23

2.27

2.41

2.63

2.79

3.04

3.15

3.29

3.48

3.64

3.81

3.97

3.99

7.15e3

0.01

0.21

0.37

0.51

0.67

0.86

1.05

1.14

1.44

1.52

1.57

1.77

1.93

2.04

2.23

2.42

2.59

2.64

2.92

3.03

3.11

3.27

3.36

3.55

3.71

3.88

3.93

5.35e4

0.14

0.25

0.47

0.63

0.79

0.93

1.04

1.29

1.34

1.56

1.70

1.89

2.08

2.41

2.52

2.63

2.74

3.04

3.21

3.37

3.45

3.67

3.97

1.35e6

0.12

0.31

0.78

0.94

1.03

1.33

1.66

1.74

1.96

2.15

2.23

2.45

2.64

2.84

2.89

3.08

3.19

3.41

3.68

3.90

5.72e7

0.01

0.21

0.37

0.51

0.67

0.86

1.05

1.14

1.44

1.52

1.57

1.77

1.93

2.04

2.23

2.42

2.59

2.64

2.92

3.03

3.11

3.27

3.36

3.55

3.71

3.88

3.93

5.35e4

0.14

0.25

0.47

0.63

0.79

0.93

1.04

1.29

1.34

1.56

1.70

1.89

2.08

2.41

2.52

2.63

2.74

3.04

3.21

3.37

3.45

3.67

3.97

1.35e6

0.12

0.31

0.78

0.94

1.03

1.33

1.66

1.74

1.96

2.15

2.23

2.45

2.64

2.84

2.89

3.08

3.19

3.41

3.68

3.90

5.72e7

0.01

0.21

0.37

0.51

0.67

0.86

1.05

1.14

1.44

1.52

1.57

1.77

1.93

2.04

2.23

2.42

2.59

2.64

2.92

3.03

3.11

3.27

3.36

3.55

3.71

3.88

3.93

5.35e4

0.14

0.25

0.47

0.63

0.79

0.93

1.04

1.29

1.34

1.56

1.70

1.89

2.08

2.41

2.52

2.63

2.74

3.04

3.21

3.37

3.45

3.67

3.97

1.35e6

0.12

0.31

0.78

0.94

1.03

1.33

1.66

1.74

1.96

2.15

2.23

2.45

2.64

2.84

2.89

3.08

3.19

3.41

3.68

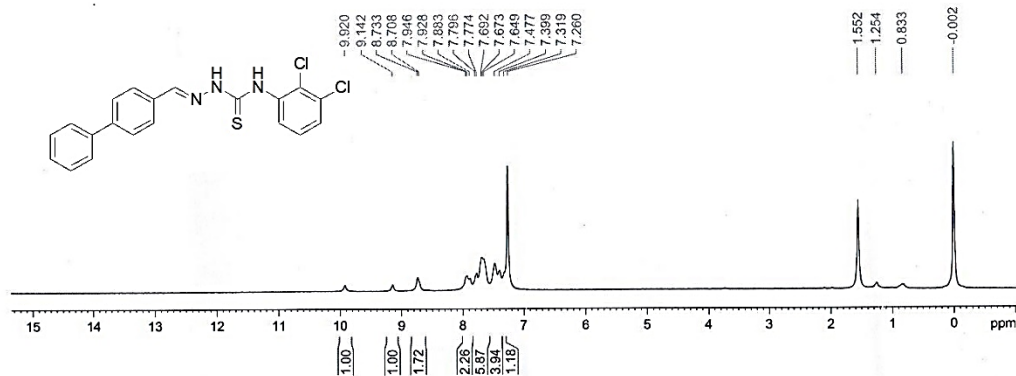
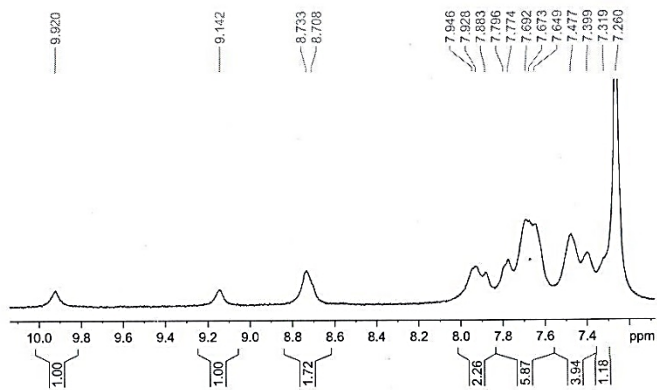
3.90

5.72e7

Mass Spectra of (E)-1-(4-phenylbenzylidene)-4-(2-chlorophenyl)thiosemicarbazide

Current Data Parameters
 NAME RK-A00781-109
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20220906
 Time_ 11:39 h
 INSTRUM spect
 RECIDID 2108618 0703 (C
 PULPROG zg30
 D 65536
 SOLVENT CDCl3
 NS 216
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 CG 205.66
 JW 62.400 uscc
 SE 6.50 uscc
 TE 295.3 K
 D1 1.0000009 sec
 TD0 1
 FID01 400.1324708 MHz
 NUC1 1H
 H 8.00 uscc
 PLW1 10.80000019 W
 F2 - Processing parameters
 SI 65536
 SF 400.1300095 MHz
 AWDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 C 1.00

RK-A00781-109(INSOLUBLE) IN CDCl3



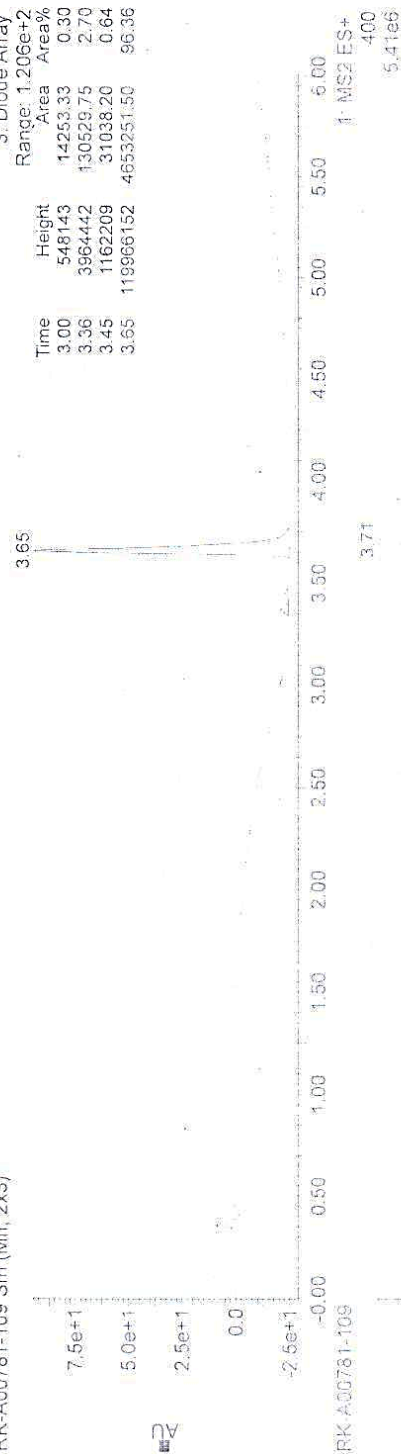
¹H NMR Spectra of (E)-1-(4-phenylbenzylidene)-4-(2,3-dichlorophenyl)thiosemicarbazide

XEVO-TQD#QCA1591

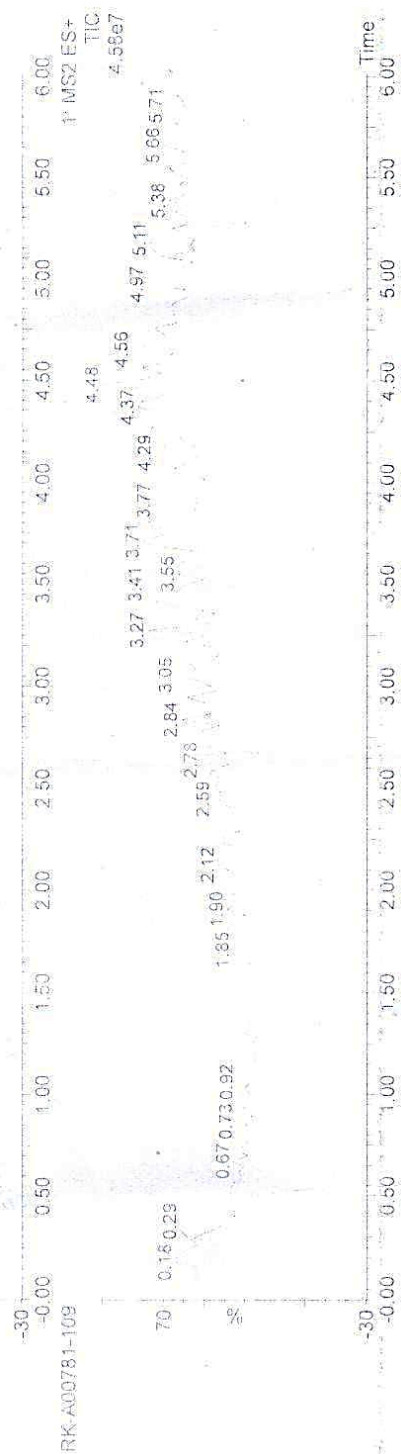
06-Sep-2022 11:16:25
 RK-A00781-109 Sm (Mn, 2x3)

3: Diode Array
 Range: 1.206e+2

Time	Height	Area	Area%
3.00	548143	14253.33	0.30
3.36	3864442	130529.75	2.70
3.45	1162209	31038.20	0.64
3.65	118966152	4853251.50	96.36



RK-A00781-109
 1: MS2 ES+
 400
 5.41e6

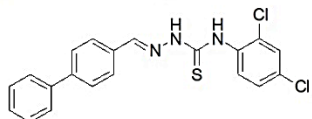
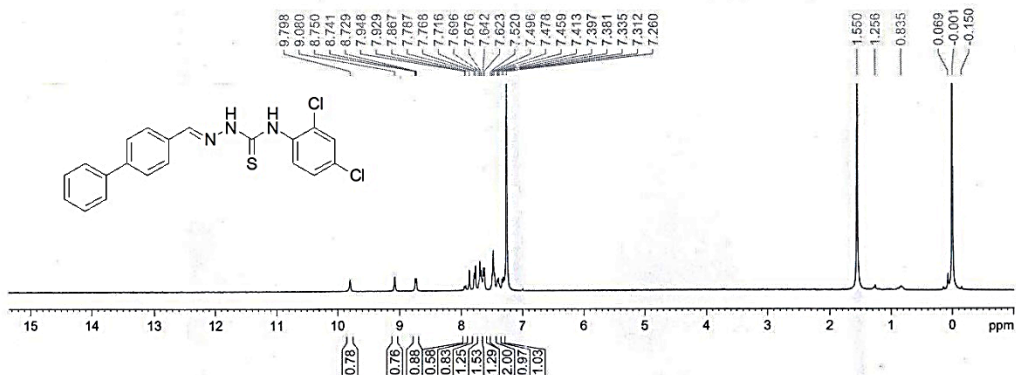
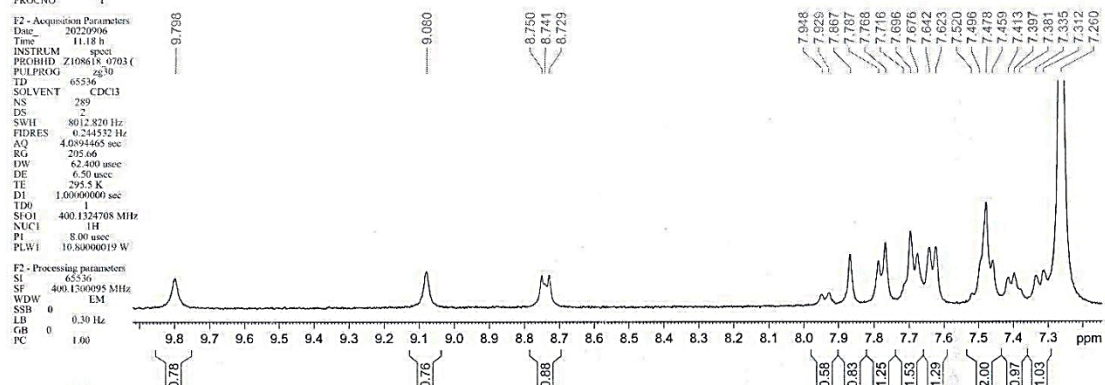


RK-A00781-109
 1: MS2 ES+
 TIC
 4.58e7

Mass Spectra of (E)-1-(4-phenylbenzylidene)-4-(2,3-dichlorophenyl)thiosemicarbazide

Current Data Parameters
 NAME RK-A00781-107
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20220906
 Time 11:18 h
 INSTRUM spect
 PROBHD Z108618-0703 C
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 289
 DS 2
 SWH 9612.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0394465 sec
 RG 205.66
 DW 62.400 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.0000000 sec
 TD0 400.1324708 MHz
 SFO1 400.1324708 MHz
 NUC1 1H
 PI 8.00 usec
 PLW1 10.80000019 W

RK-A00781-107 IN CDCl3

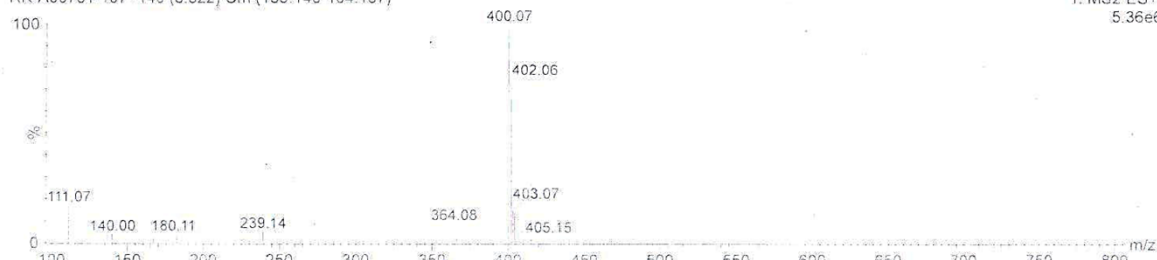


¹H NMR Spectra of (E)-1-(4-phenylbenzylidene)-4-(2,4-dichlorophenyl)thiosemicarbazide

RK-A00781-107

RK-A00781-107- 140 (3.822) Cm (139-140-104-137)

1. MS2 ES+
5.36e6



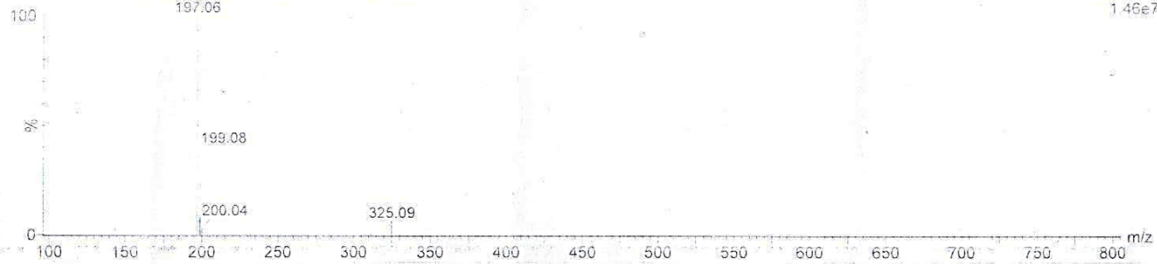
RK-A00781-107- 129 (3.520) Cm (128-129-89-126)

1. MS2 ES+
4.42e6



RK-A00781-107- 92 (2.506) Cm (91-92-(76-89+102-139))

1. MS2 ES+
1.46e7



Mass Spectra of (E)-1-(4-phenylbenzylidene)-4-(2,4-dichlorophenyl)thiosemicarbazide

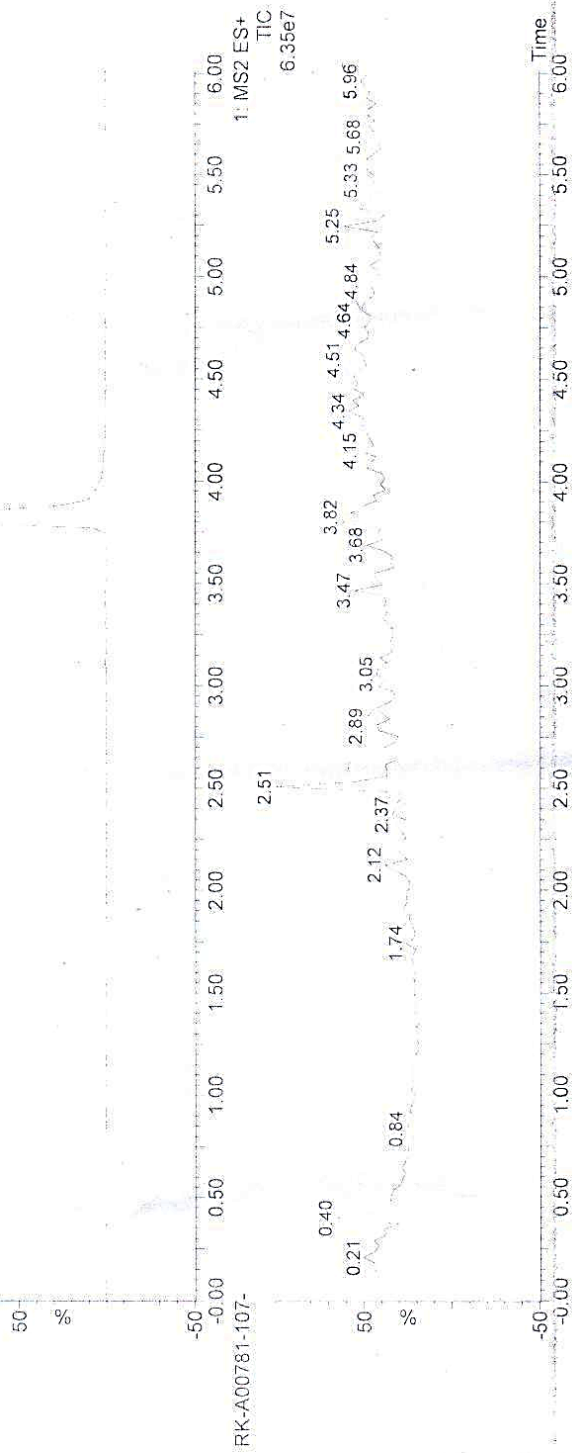
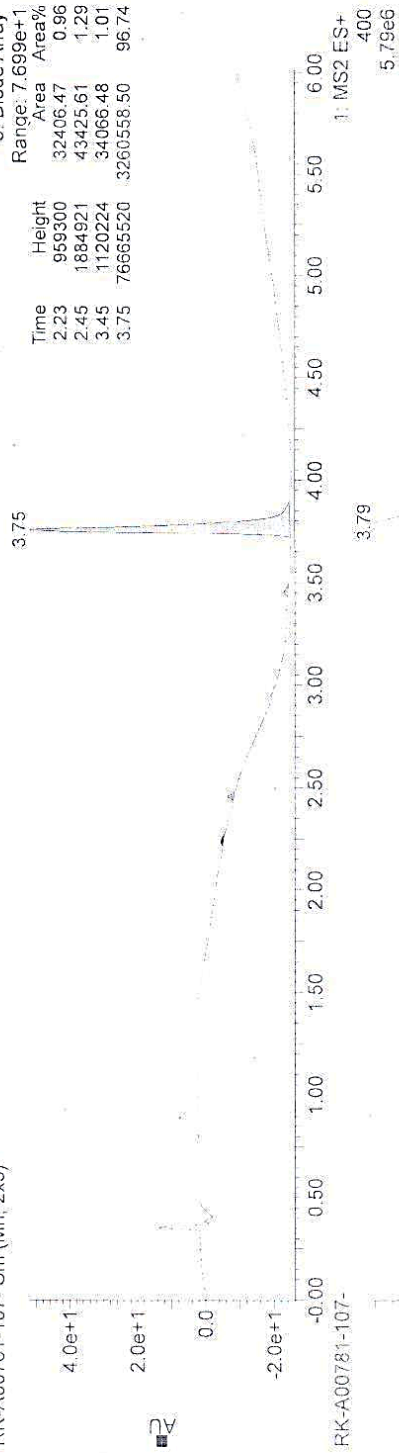
XEVO-TQD#QCA1591

06-Sep-2022 11:09:42

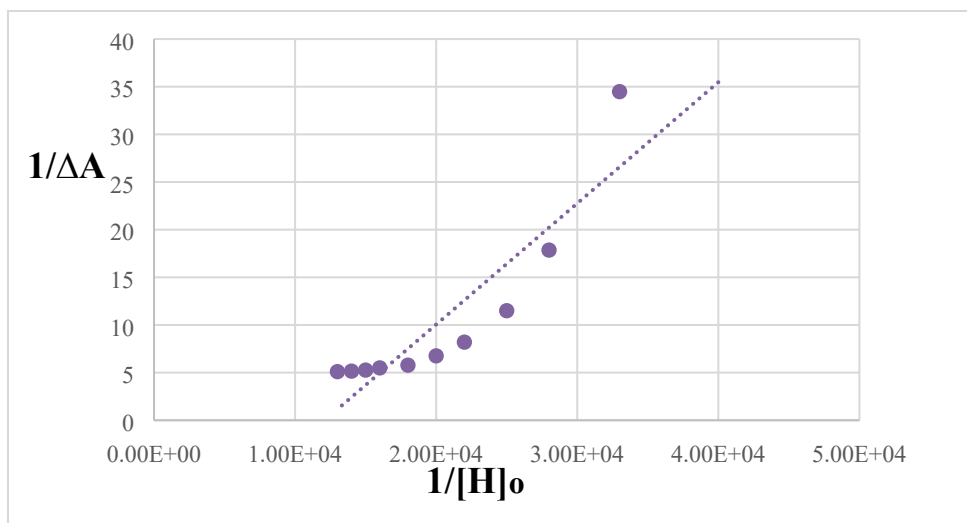
RK-A00781-107 - Sm (Mn, 2x3)

3: Diode Array
Range: 7.699e+1

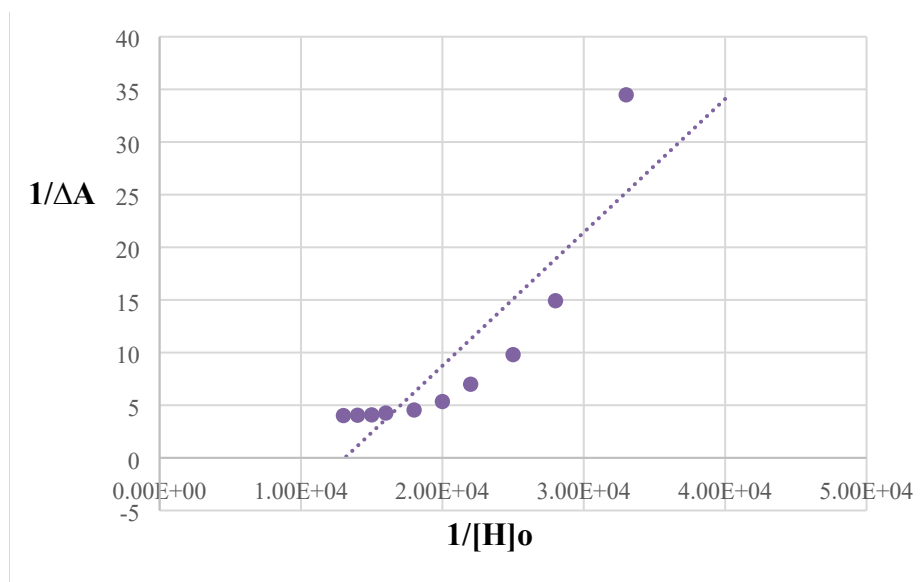
Time	Height	Area	Area%
2.23	959300	32406.47	0.96
2.45	1884921	43425.61	1.29
3.45	1120224	34066.48	1.01
3.75	7665520	3260538.50	96.74



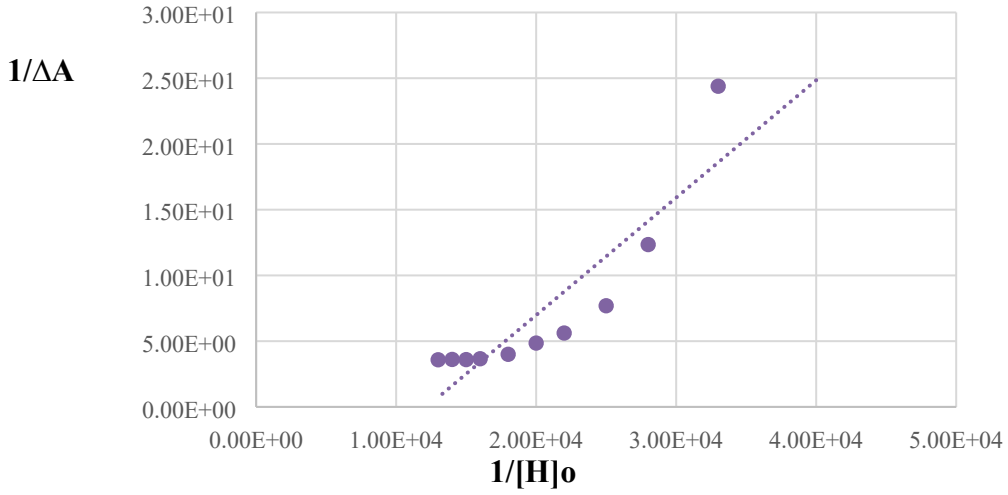
Mass Spectra of (E)-1-(4-phenylbenzylidene)-4-(2,4-dichlorophenyl)thiosemicarbazide



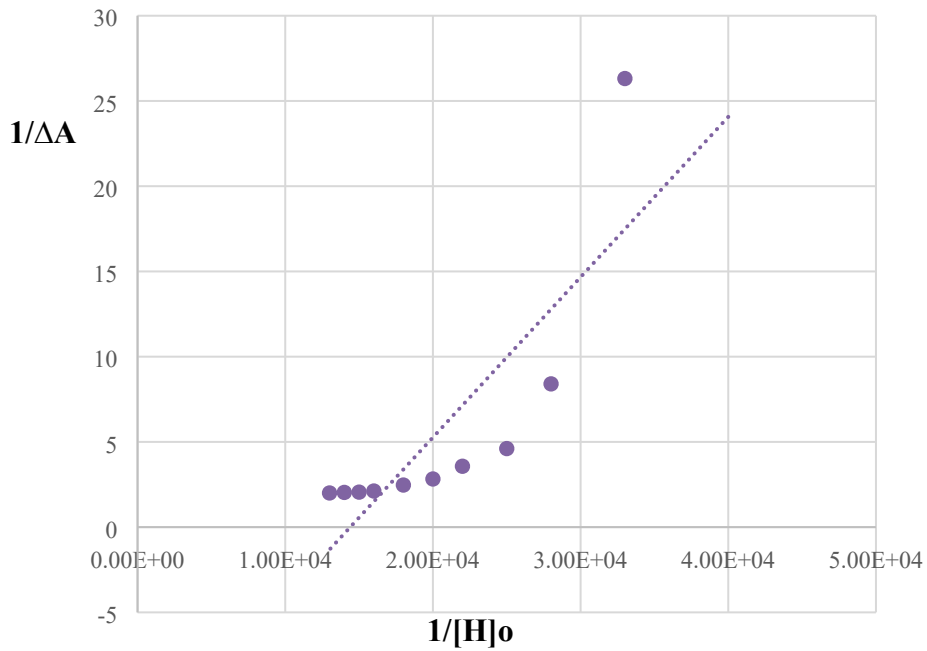
Binding constant of TSC1 with Co^{2+}



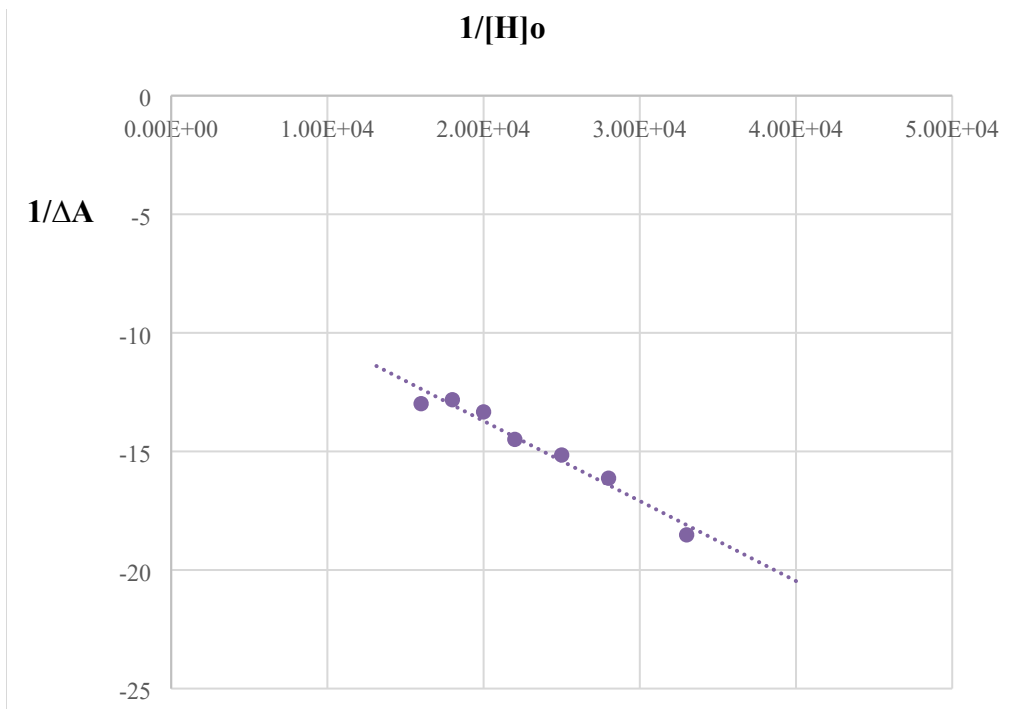
Binding constant TSC1 with Ni^{2+}



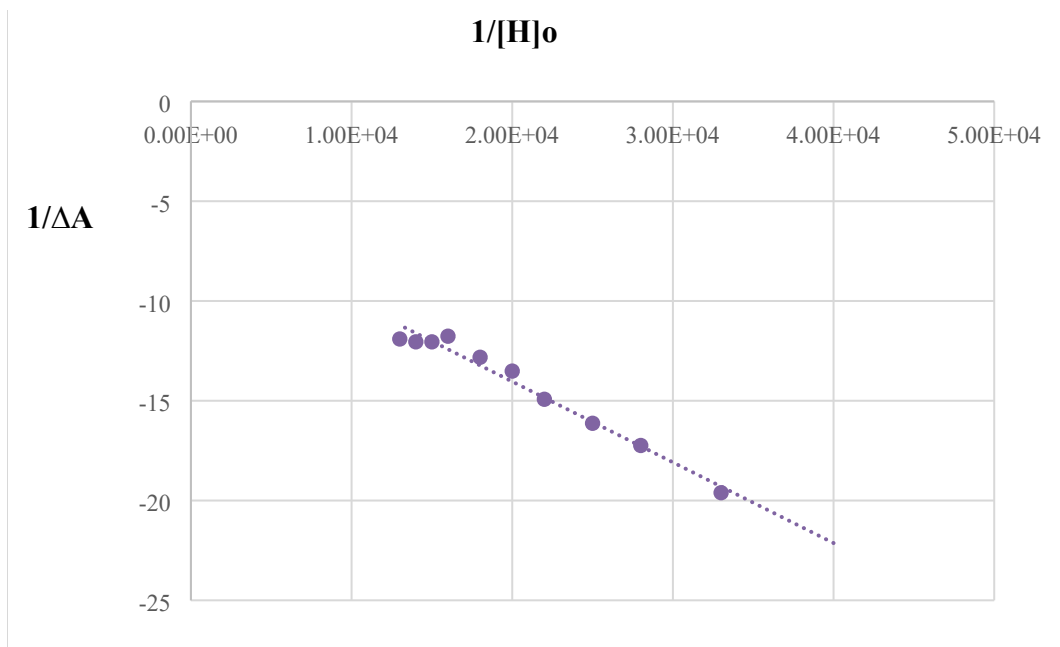
Binding constant TSC1 with Cu^{2+}



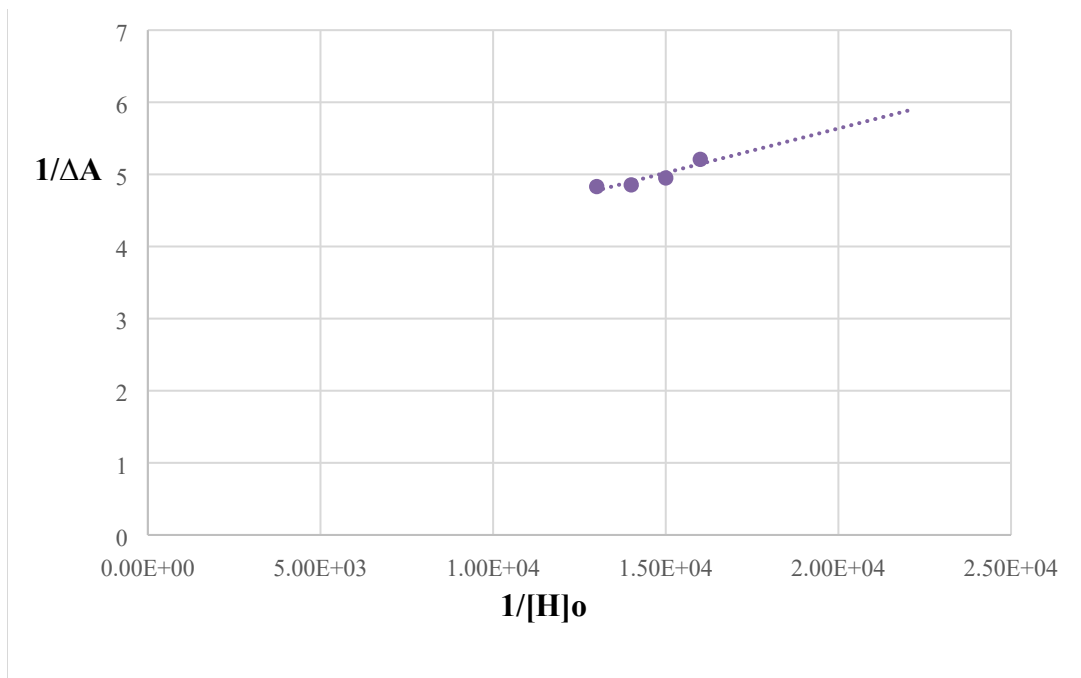
Binding constant TSC1 with Zn^{2+}



Binding constant of TSC2 with Hg²⁺



Binding constant of TSC2 with Sn²⁺



Binding constant of TSC3 with Mn^{2+}