

Biological and catalytic potential of sustainable low and high valent metal-Schiff base sulfonate salicylidene pincer complexes

Mohamed Shaker S. Adam^{1,2*}, Omar M. El-Hady², Farman Ullah³

¹ Department of Chemistry, College of Science, King Faisal University, P.O. Box 380 Al Hufuf 31982 Al Hassa, Saudi Arabia.

² Chemistry Department, Faculty of Science, Sohag University, Sohag-82534, Egypt.

³ Department of Chemistry, Winnipeg University 515 Portage Avenue, Winnipeg, Manitoba, R3B 2E9 Canada

*corresponding author e-mail: madam@kfu.edu.sa; shakeradam61@yahoo.com (M.S.S. Adam).

TABLE S1

Activity index (%) of the antibacterial assay for HSaln ligand and MSaln complexes.

Compound	Activity index (%)		
	Serratia Marcescence (-ve)	Escherichia coli (-ve)	Staphylococcus aureus (+ve)
HSaln	25.00	21.62	30.43
VOSaln	90.00	91.89	91.30
VOSaln-Ph	75.00	78.38	78.26
MnSaln	85.00	89.19	86.96
MoO ₂ Saln	82.50	86.49	82.61
UO ₂ Saln	95.00	94.59	95.65

TABLE S2

Activity index (%) of antifungal assay for HSaln ligand and MSaln complexes.

Compound	Activity index (%)		
	Candida albicans	Aspergillus flavus	Trichophyton Rubrum
HSaln	18.92	32.00	35.48
VOSaln	78.38	76.00	80.65
VOSaln-Ph	91.89	92.00	93.55
MnSaln	89.19	88.00	90.32
MoO ₂ Saln	86.49	84.00	87.09
UO ₂ Saln	97.30	96.00	96.77

Table S3

Cytotoxic activity (IC₅₀) of HSaln ligand and its MSaln complexes various Colon carcinoma cells, (HCT-116 cell line), hepatic cellular carcinoma cells (HepG-2) and breast carcinoma cells (MCF-7).

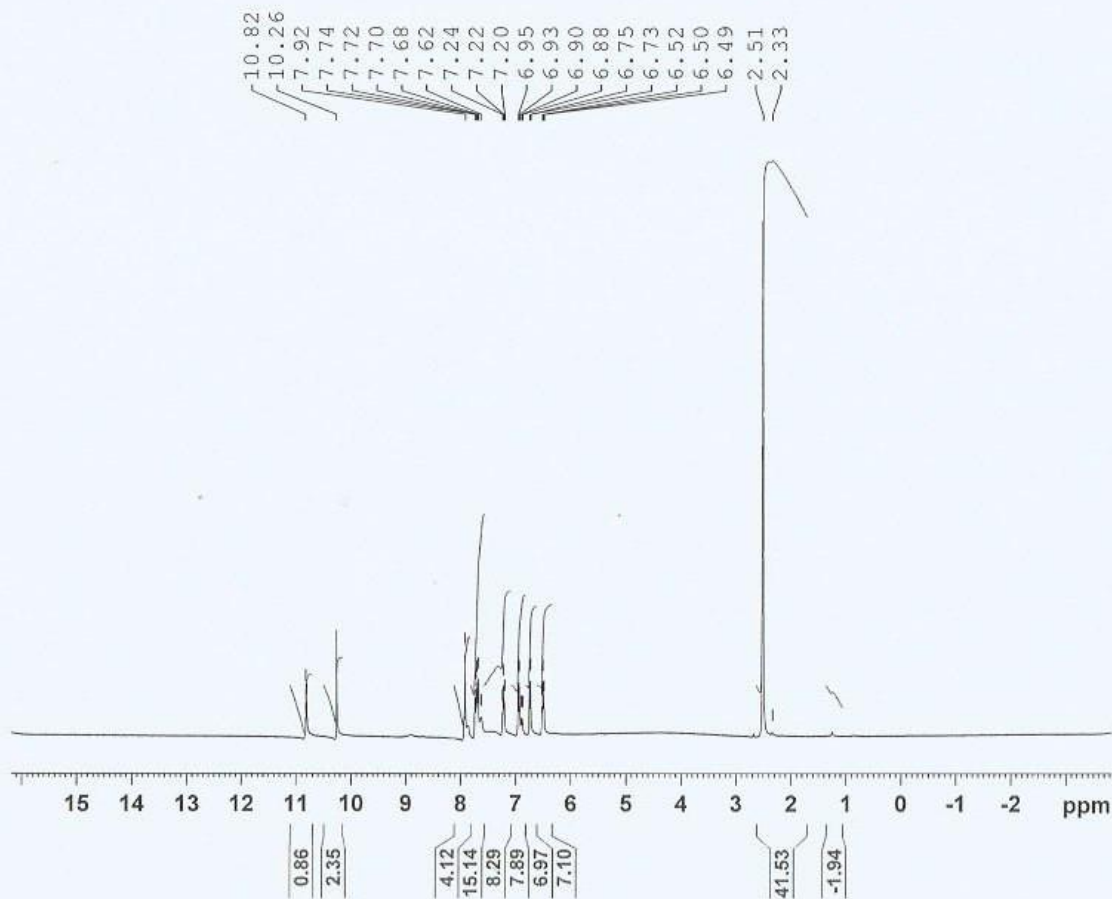
Compound	IC ₅₀ (μg μL ⁻¹)		
	HCT-116	MCF-7	HepG-2
HSaln ligand	111.50±0.14	85.70±0.23	93.20±0.15
MnSaln	23.50±0.12	14.20±0.12	17.50±0.17
VOSaln-Ph	35.60±0.21	24.90±0.13	28.90±0.15
VOSaln	29.20±0.13	18.50±0.11	21.30±0.12
MoO ₂ Saln	33.10±0.15	21.30±0.16	25.40±0.18
UO ₂ Saln	17.70±0.19	9.60±0.10	11.60±0.13
Vinblastine standard	13.30±0.11	4.12±0.14	7.50±0.10

NMR spectral data of HSaln ligand:

¹H NMR (DMSO-*d*₆, 400 MHz): δ 6.50 (t, ³*J* = 6.9 and 7.2 Hz, 1H), 6.74 (d, ³*J* = 8.2 Hz, 1H), 6.94 (dd, ³*J* = 8.0 and 8.3 Hz, 1H), 7.22 (t, ³*J* = 7.0 and 7.4 Hz, 1H), 7.70 (dd, ³*J* = 7.7 Hz, 2H), 7.92 (s, 1H), 10.26 (s, 1H, phenolic-OH), 10.82 ppm (s br, 1H, CH=N).

¹³C NMR (100 MHz, DMSO-*d*₆, dept-135): δ 110.18 (C_q), 115.05 (CH), 116.83 (CH), 116.96 (CH), 121.48 (CH), 126.92 (CH), 131.61 (CH), 134.20 (CH), 140.72 (C_q), 151.94 (C_q), 161.15 (C_q), 169.99 (C_q), 192.11 ppm (CH, CH=N).

SSA-3
proton_su DMSO (C:\nmr-data) Student 16



Current Data Parameters
NAME Jul29-2017
EXPNO 250
PROCNO 1

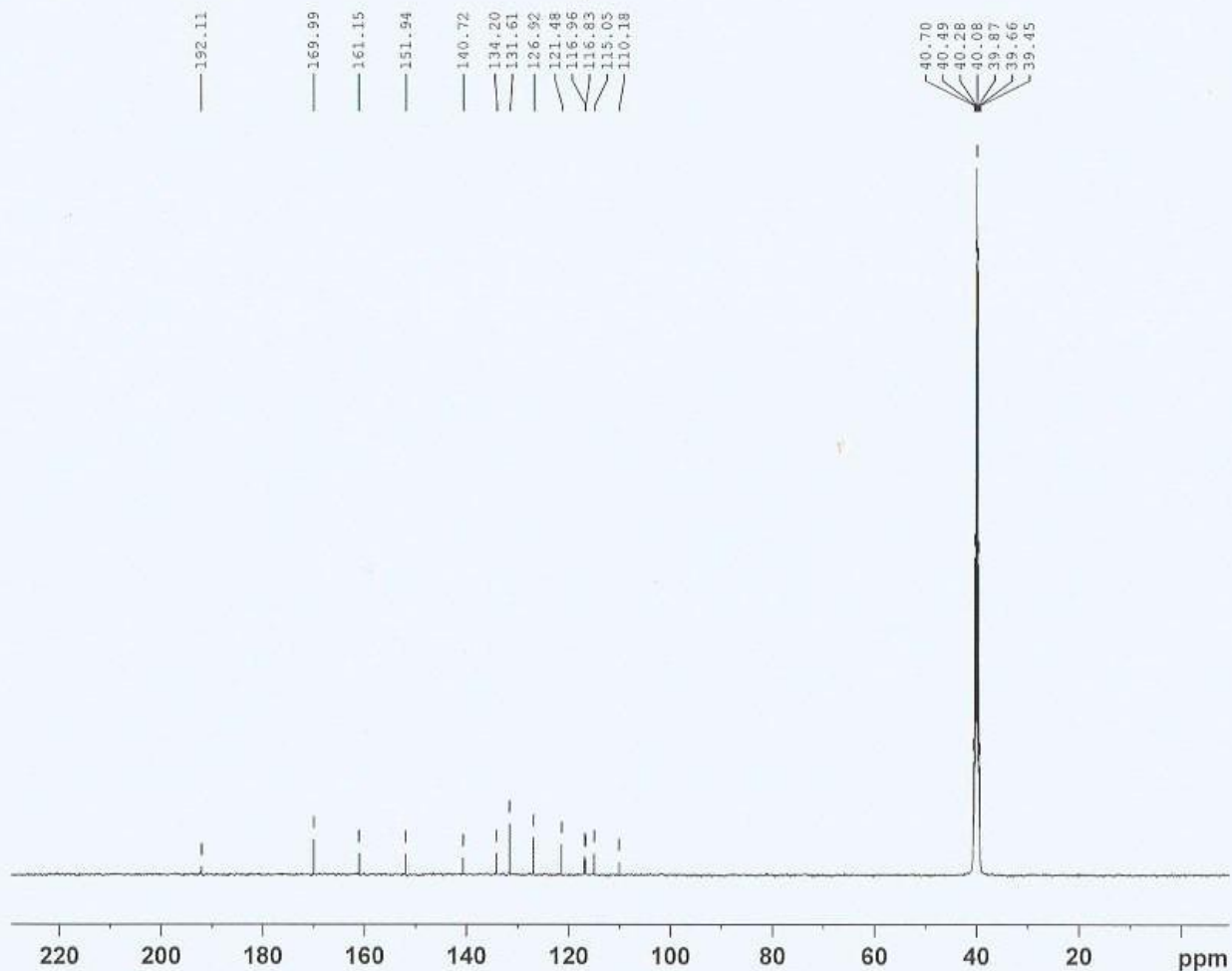
F2 - Acquisition Parameters
Date_ 20170729
Time 11.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 314.2 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SF01 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig. S1: ¹H NMR of HSAln ligand.

SSA-3
c13_su DMSO {C:\nmr-data} Student 17



Current Data Parameters
NAME Jul31-2017
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date 20170731
Time 10.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.04
DW 20.800 usec
DE 6.50 usec
TE 308.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6238364 MHz
NUC1 13C
P1 9.50 usec
PLW1 56.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41091001 W
PLW13 0.33284000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

Fig. S2: ^{13}C NMR of HSaln ligand.

SSA-3
c13_su DMSO {C:\nmr-data} Student 17



Current Data Parameters
NAME Jul131-2017
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time_ 10.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.04
DW 20.800 usec
DE 6.50 usec
TE 308.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6238364 MHz
NUC1 13C
P1 9.50 usec
PLW1 56.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41091001 W
PLW13 0.33284000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

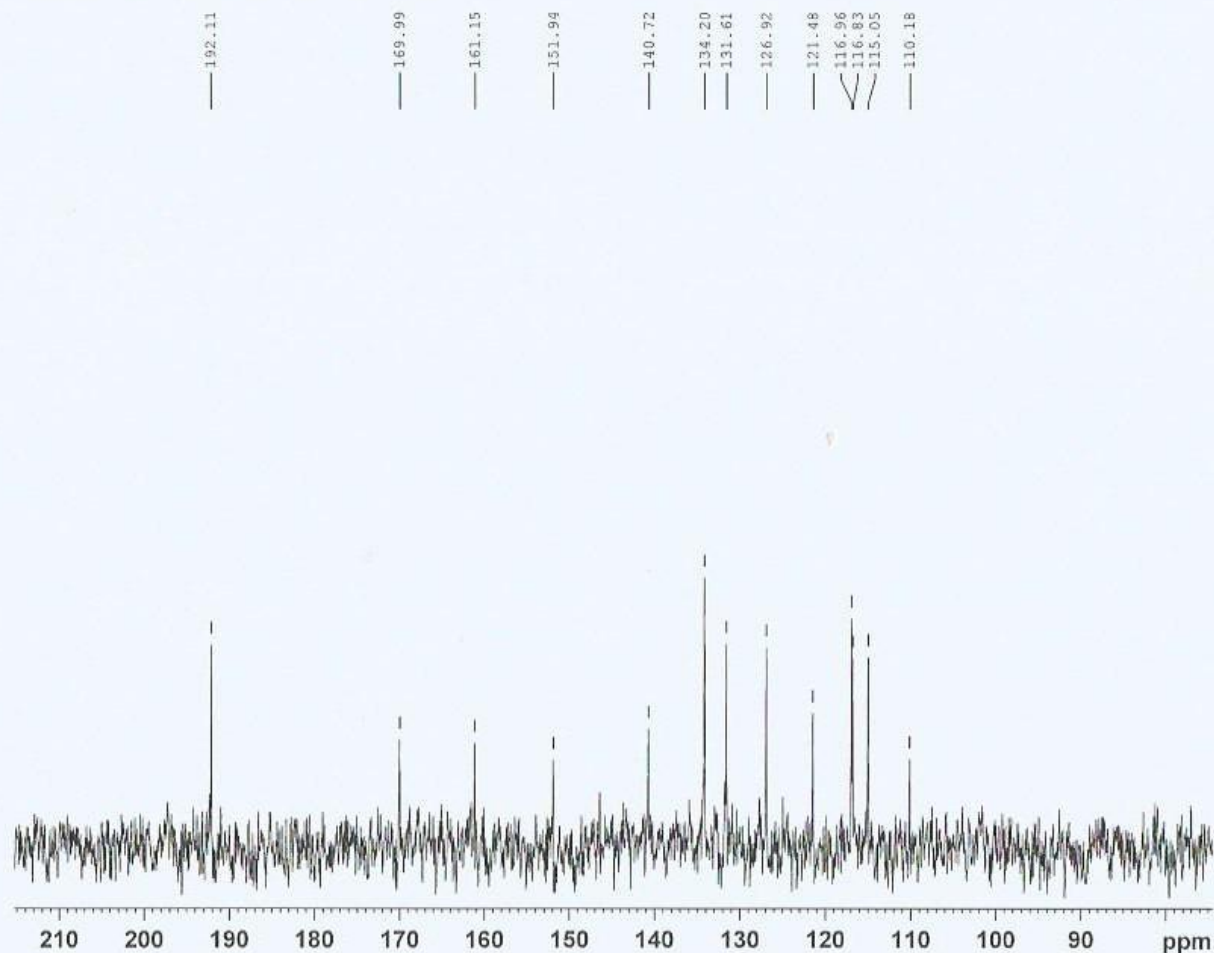
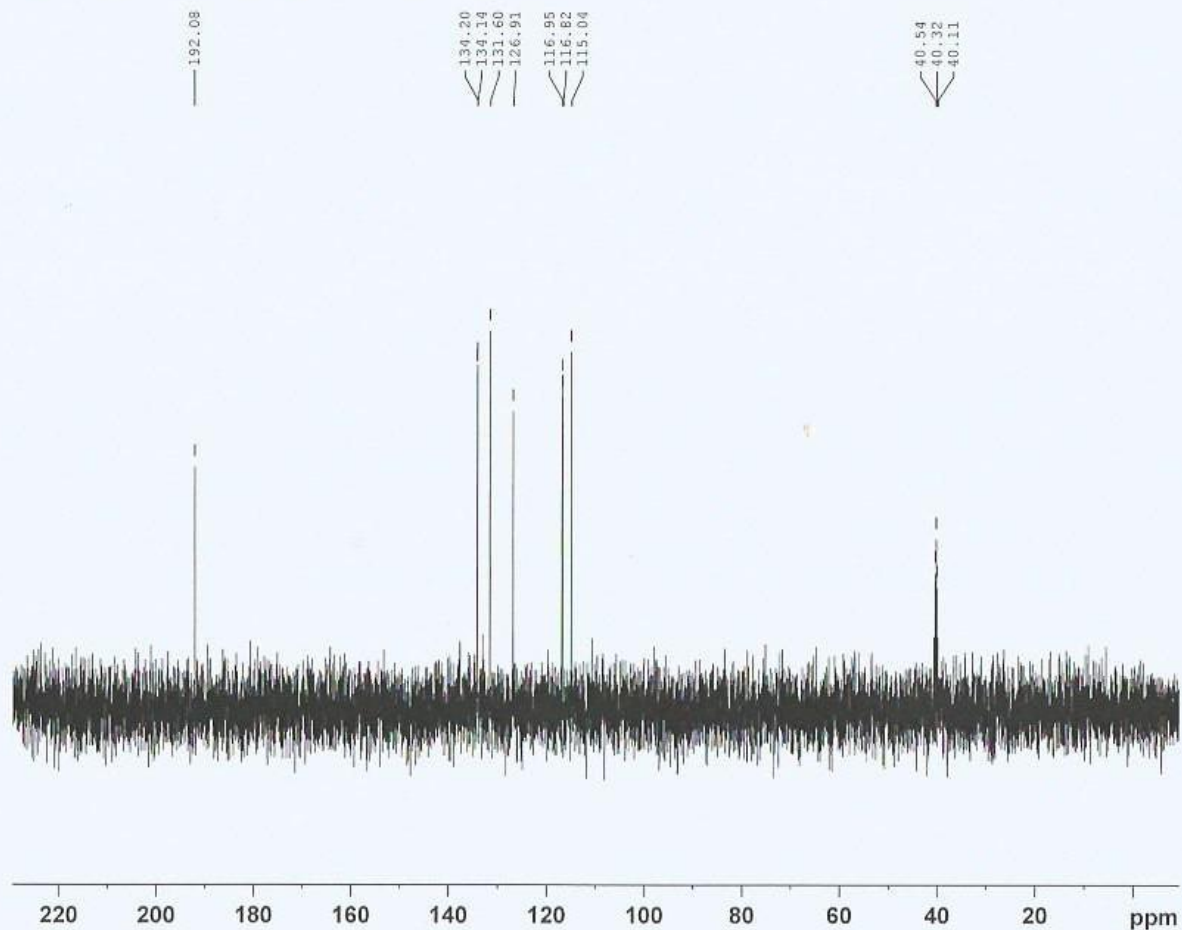


Fig. S3: ^{13}C NMR of HSAln zoom in the aromatic region.

SSA-3
dept135_su DMSO (C:\nmr-data) Student 17



Current Data Parameters
NAME Jul131-2017
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time 11.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.04
DW 20.800 usec
DE 6.50 usec
TE 308.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

----- CHANNEL f1 -----
SF01 100.6238364 MHz
NUC1 13C
P1 9.50 usec
P13 2000.00 usec
PLW0 0 W
PLW1 56.00000000 W
SPNAM[5] Crp60comp.4
SPOALS 0.500
SPOFFS5 0 Hz
SFWS 7.72189999 W

----- CHANNEL f2 -----
SF02 400.1312797 MHz
NUC2 1H
CFDPRG[2] waltz16
P3 12.30 usec
P4 24.60 usec
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41091001 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig. S4: ^{135}C Dept CNMR of HSaln ligand.

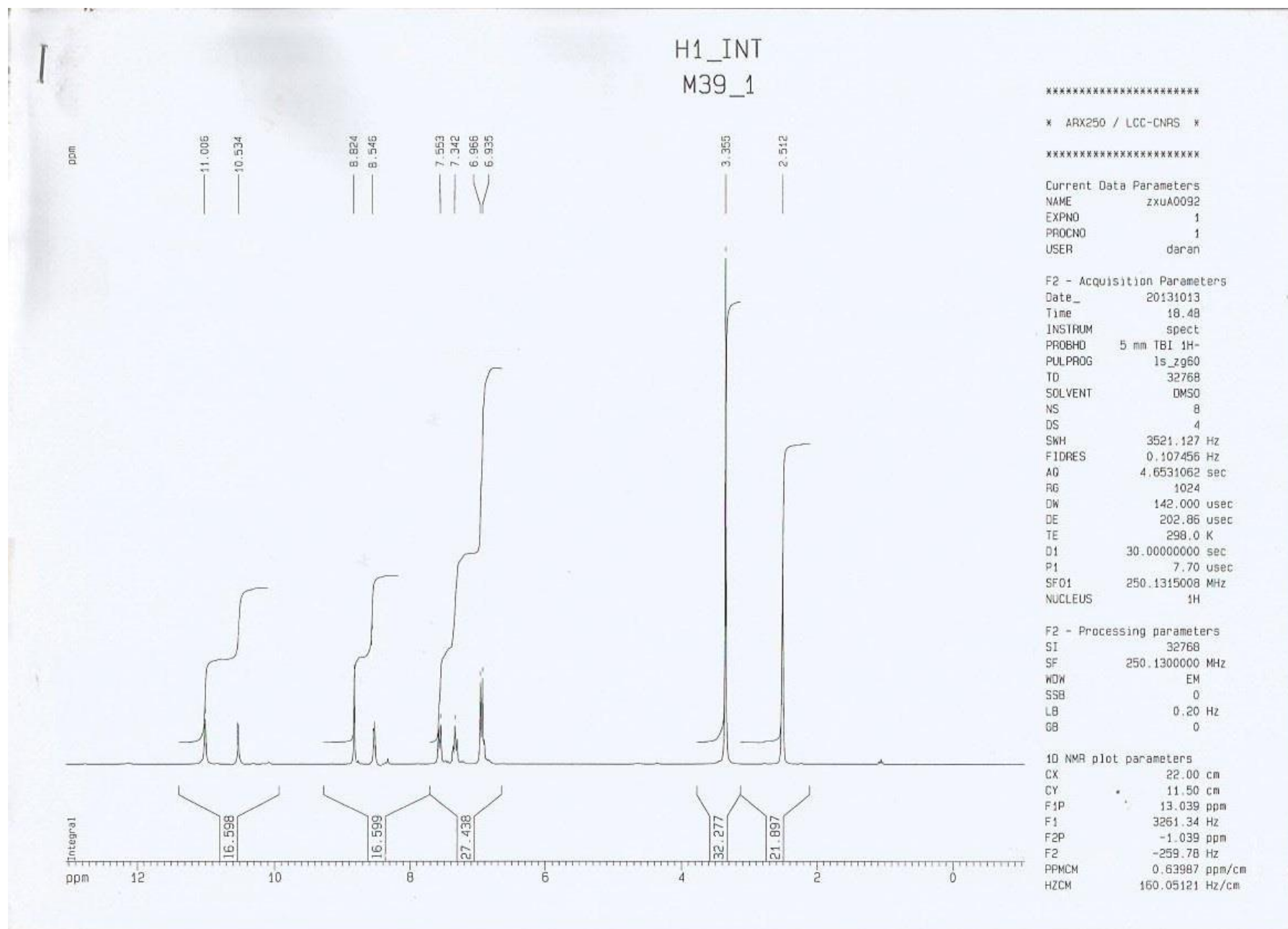


Fig. S5: ^1H NMR of MoO_2Saln complex.

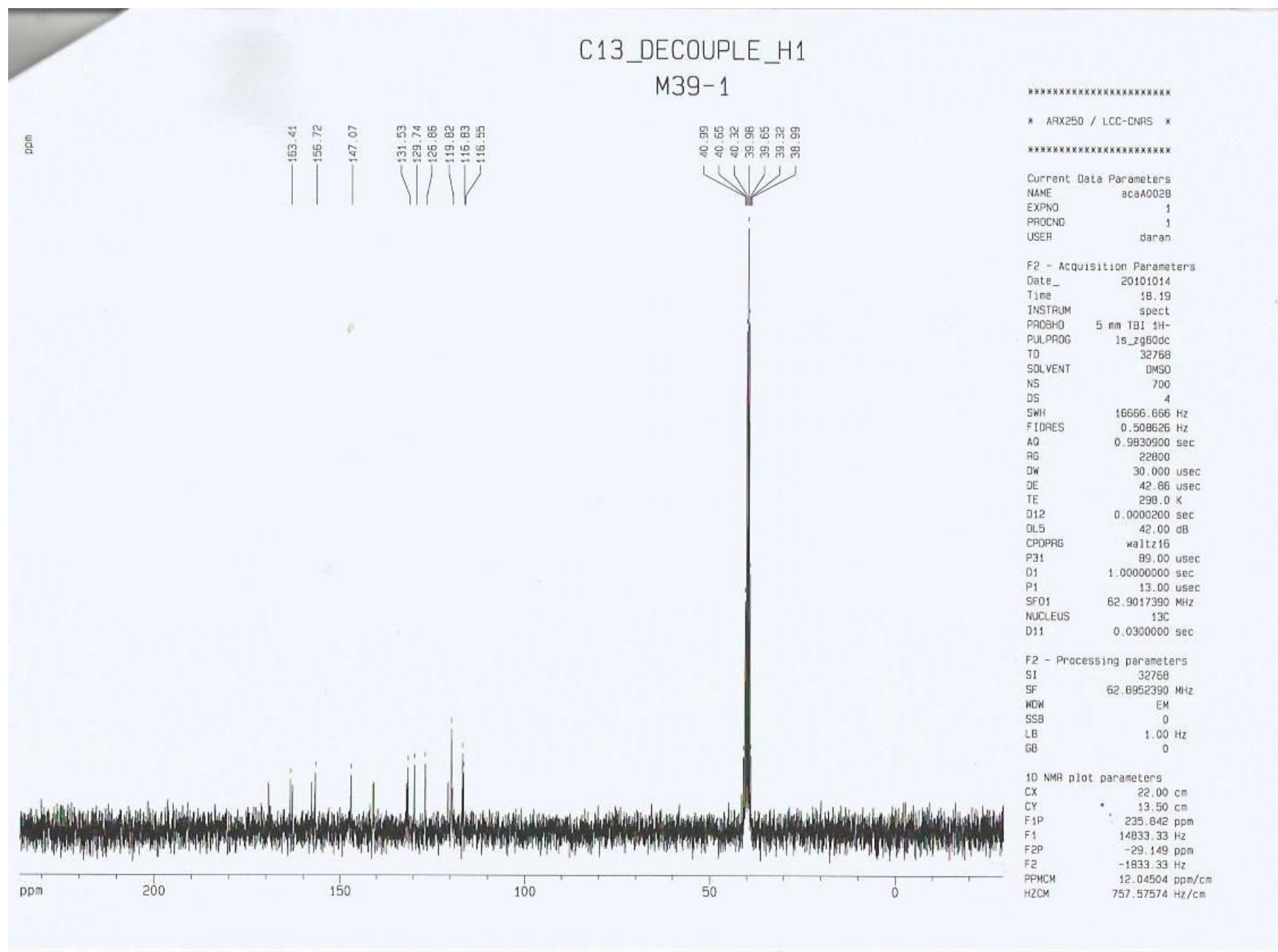
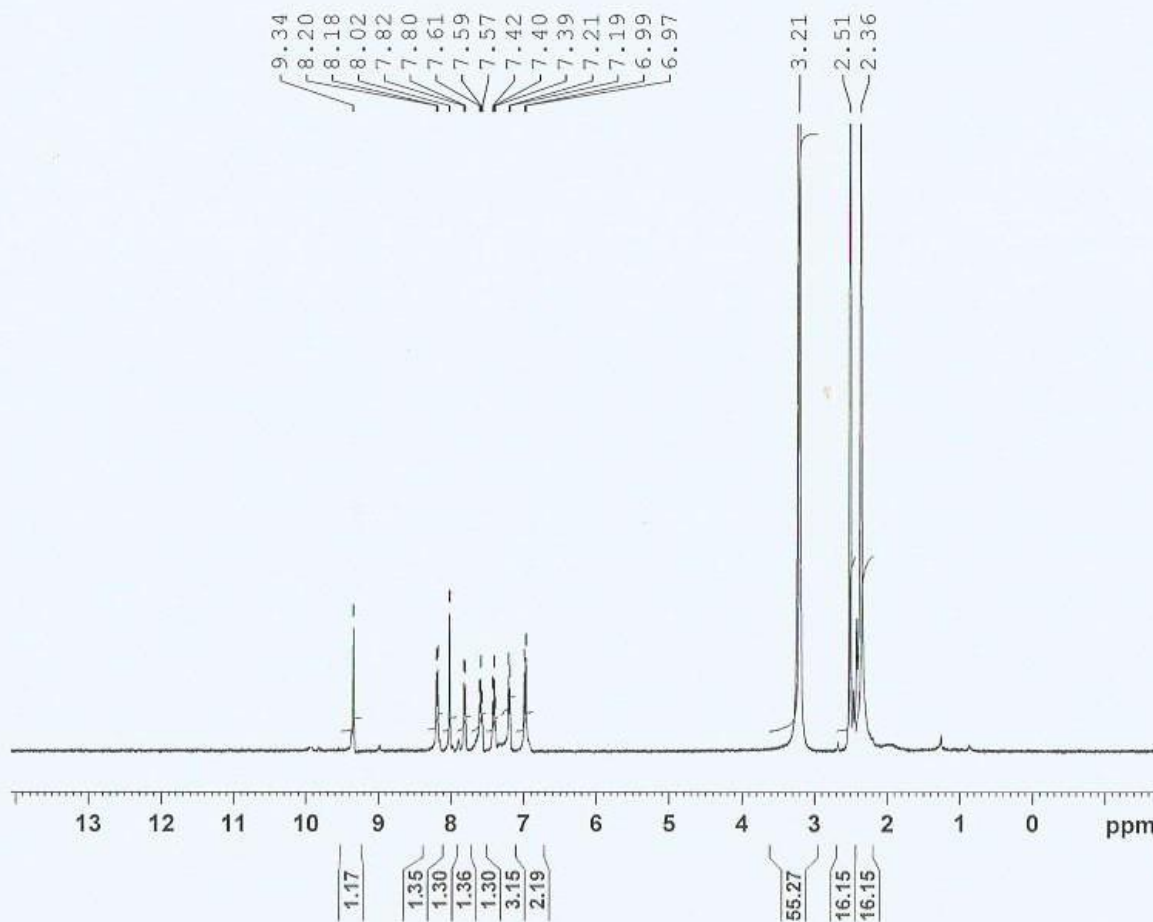


Fig. S6: ^{13}C NMR of MoO_2Saln complex.

UO2-SSA
proton_su DMSO {C:\nmr-data} Student 8



Current Data Parameters
NAME Feb04-2018
EXPNO 250
PROCNO 1

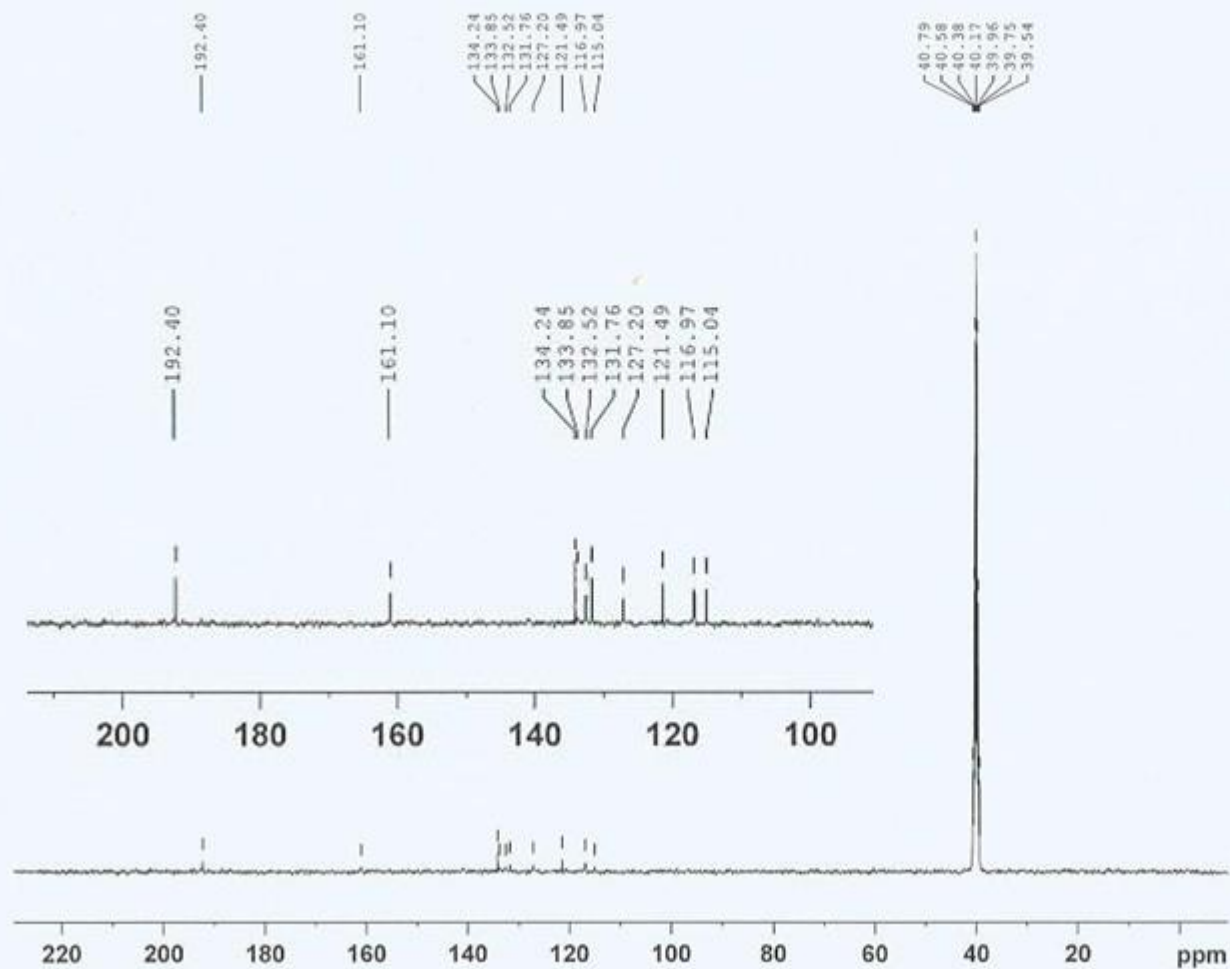
F2 - Acquisition Parameters
Date_ 20180205
Time 9.25
INSTRUM spect
PROBHD 5 mm PABBO BS/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 50
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 199.04
DW 62.400 usec
DE 6.50 usec
TE 323.2 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig. S7: ¹H NMR of UO₂Saln complex.

Zn-ssA
 c13_su DMSO (C:\nmr-data) Student 10



40.79
 40.58
 40.38
 40.17
 39.96
 39.75
 39.54

Current Data Parameters
 NAME Jul10-2017
 EXPNO 80
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170710
 Time 12.12
 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 199.04
 DW 20.800 usec
 DE 6.50 usec
 TE 323.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

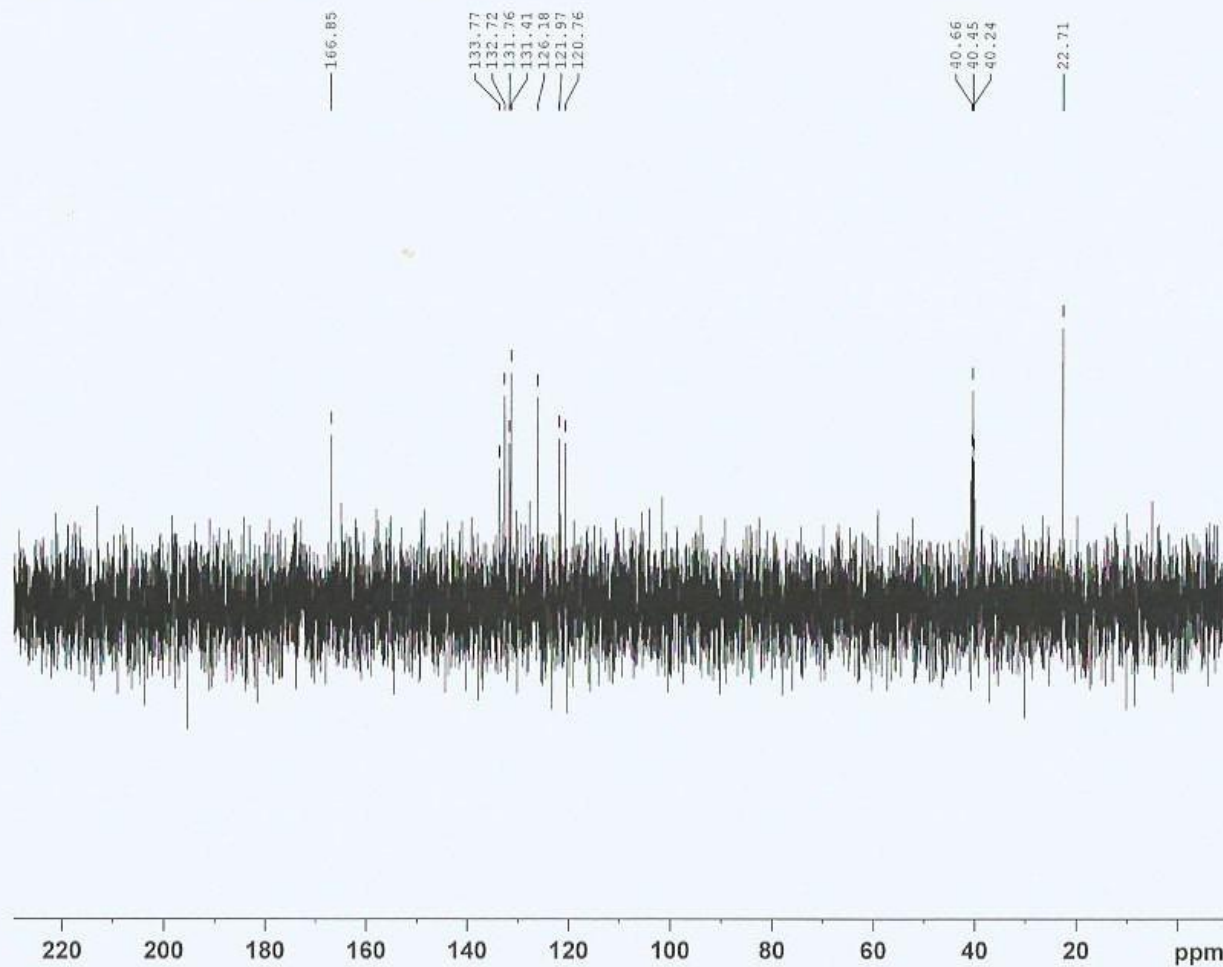
===== CHANNEL f1 =====
 SFO1 100.6238364 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 56.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 22.00000000 W
 PLW12 0.41091001 W
 PLW13 0.33284000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 6.00 Hz
 GB 0
 PC 1.40

Fig. S8: ¹³CNMR of UO₂Saln complex.

ZN-SSA
dept135_su DMSO {C:\nmr-data} Student 4



Current Data Parameters
NAME Sep10-2017
EXPNO 150
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170910
Time_ 23.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.04
DW 20.800 usec
DE 6.50 usec
TE 323.2 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6238364 MHz
NUC1 13C
P1 9.50 usec
P13 2000.00 usec
PLW0 0 W
PLW1 56.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFF5 0 Hz
SPW5 7.72189999 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P3 12.30 usec
P4 24.60 usec
PCPD2 90.00 usec
PLW2 22.00000000 W
PLW12 0.41091001 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig. S9: ^{135}C Dept CNMR of UO_2Saln complex.

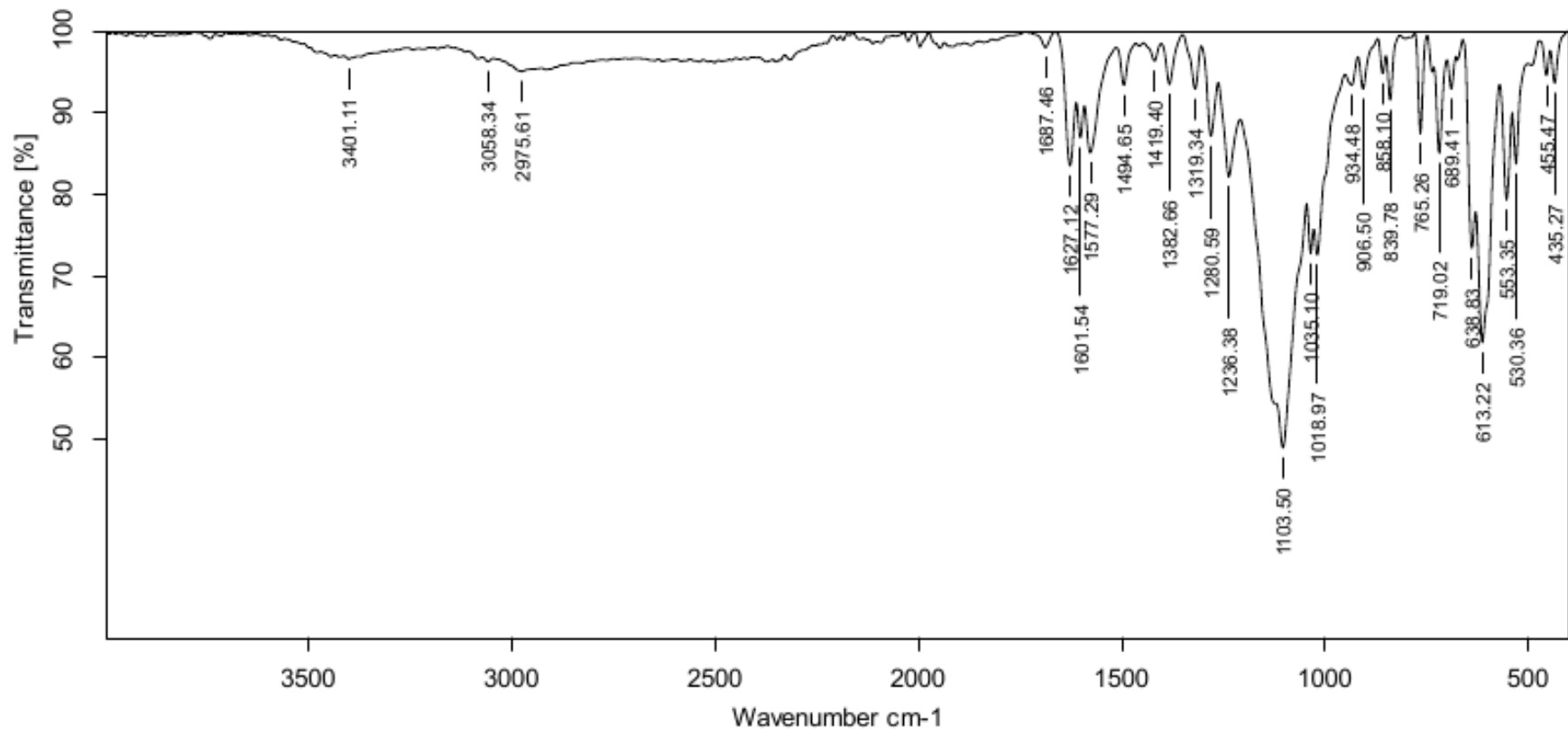


Fig. S10: IR spectra of HSaln ligand.

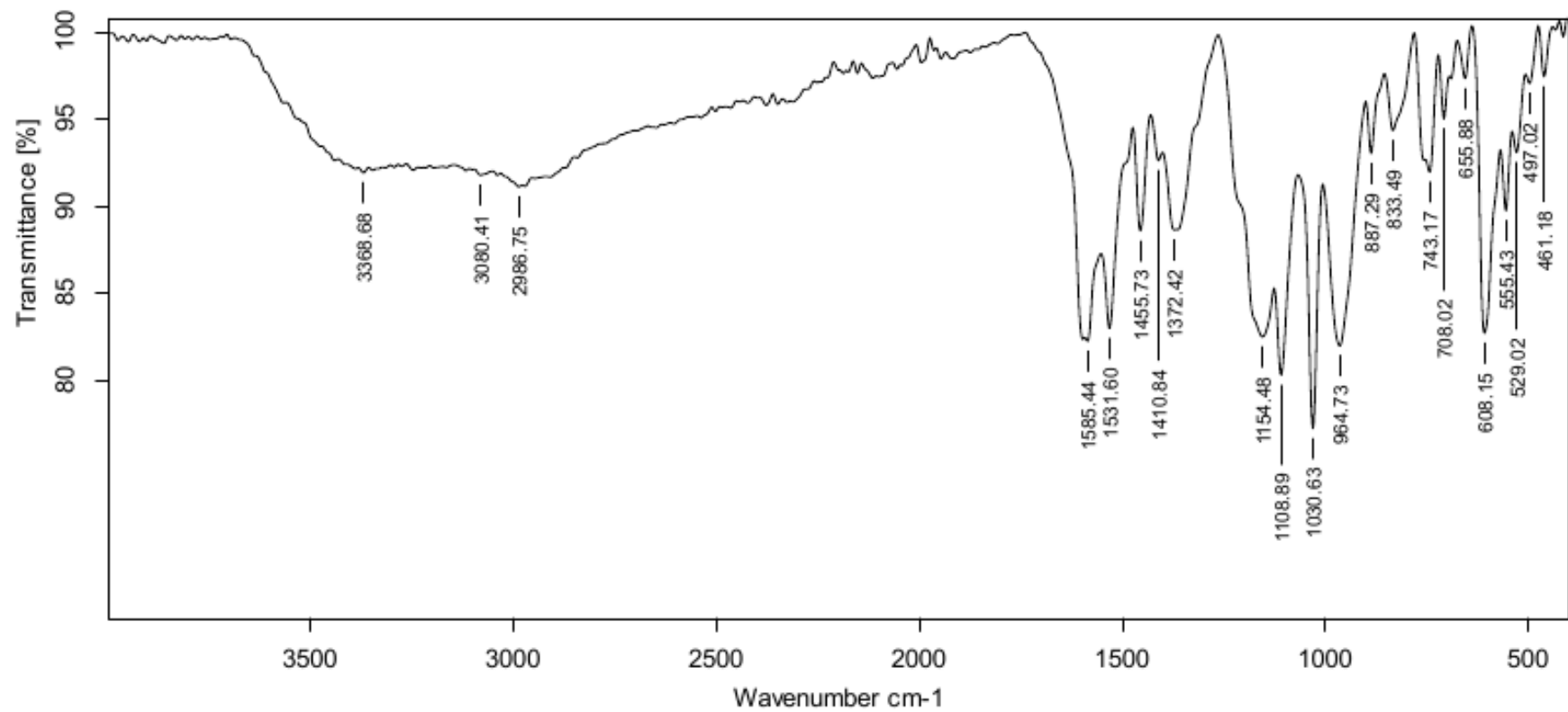


Fig. S11: IR spectra of VOSalN complex.

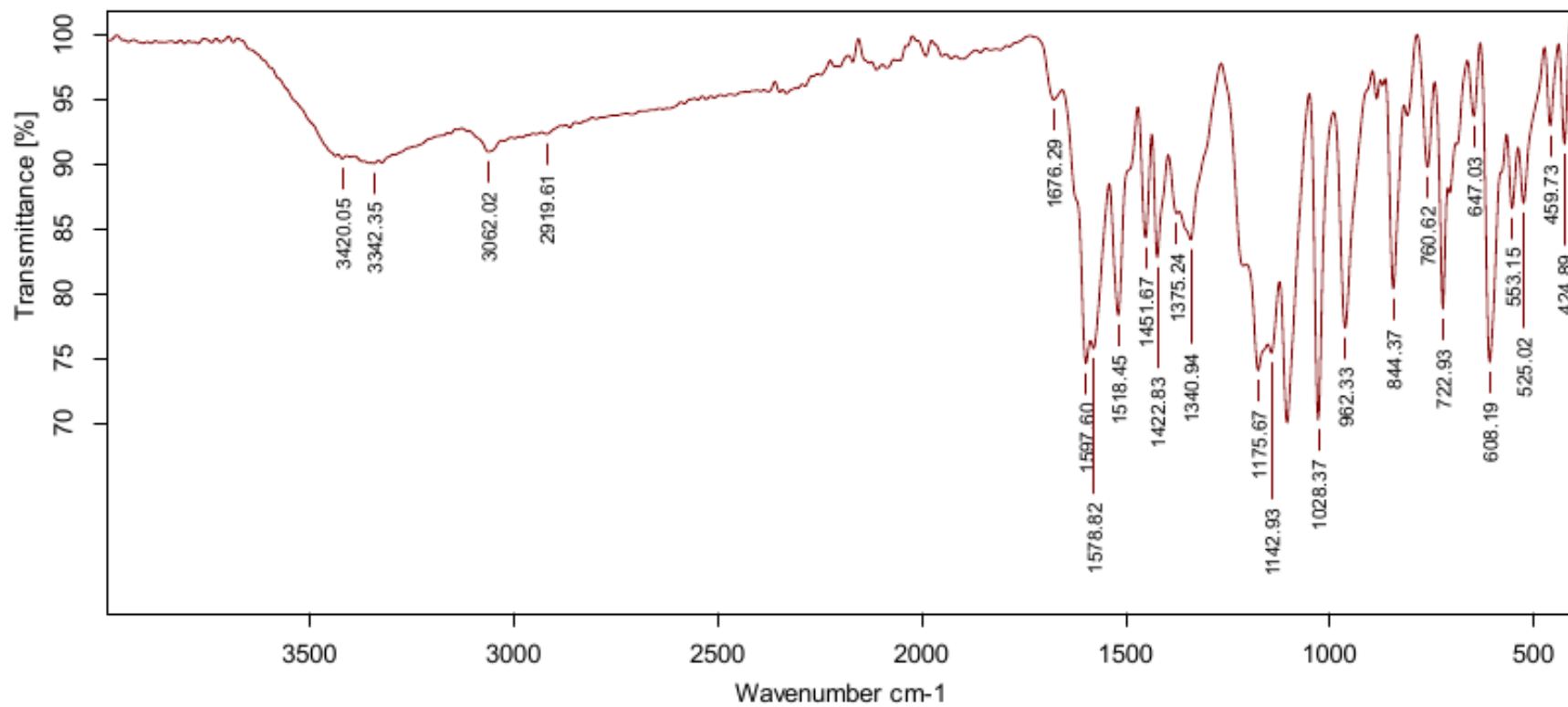


Fig. S12: IR spectra of VOSaln-Ph complex.

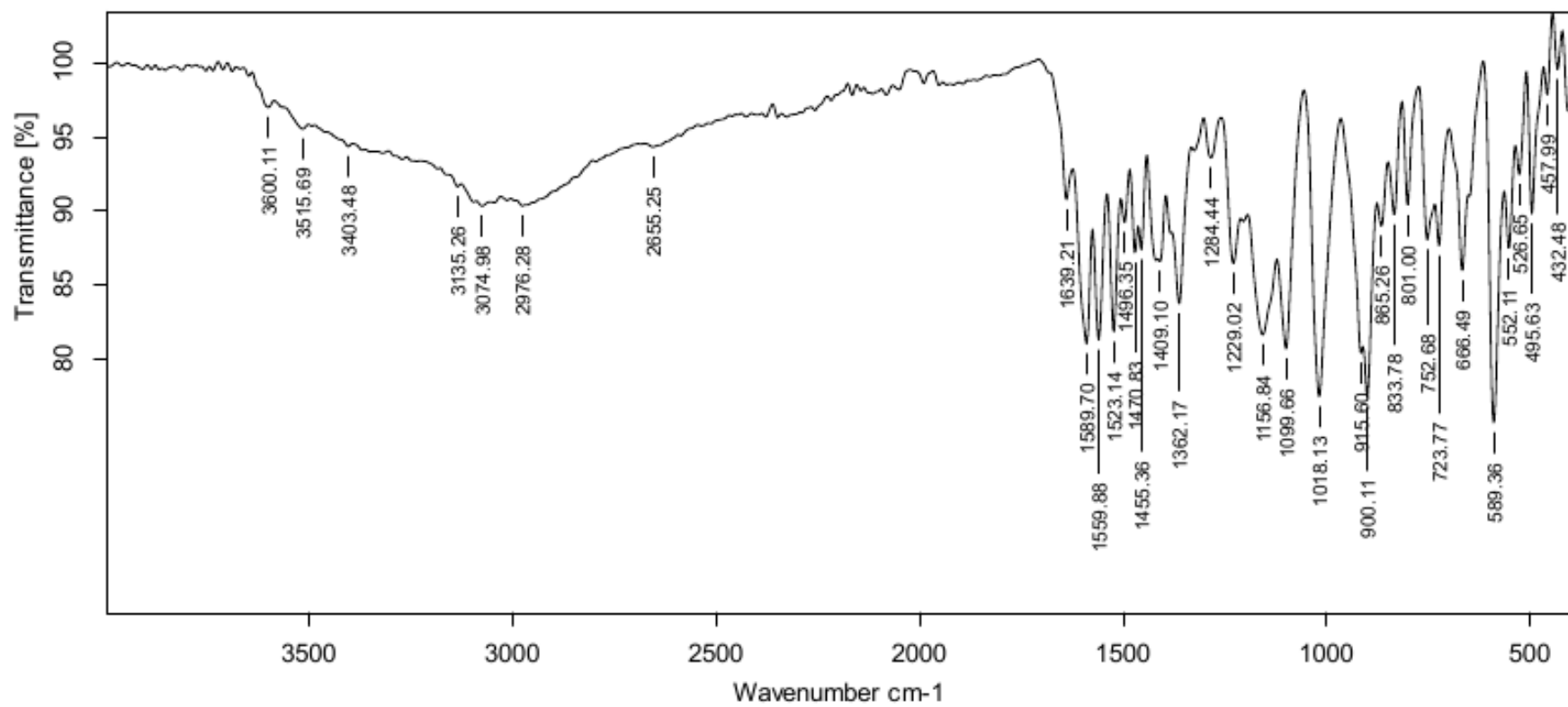


Fig. S13: IR spectra of UO₂Saln complex.

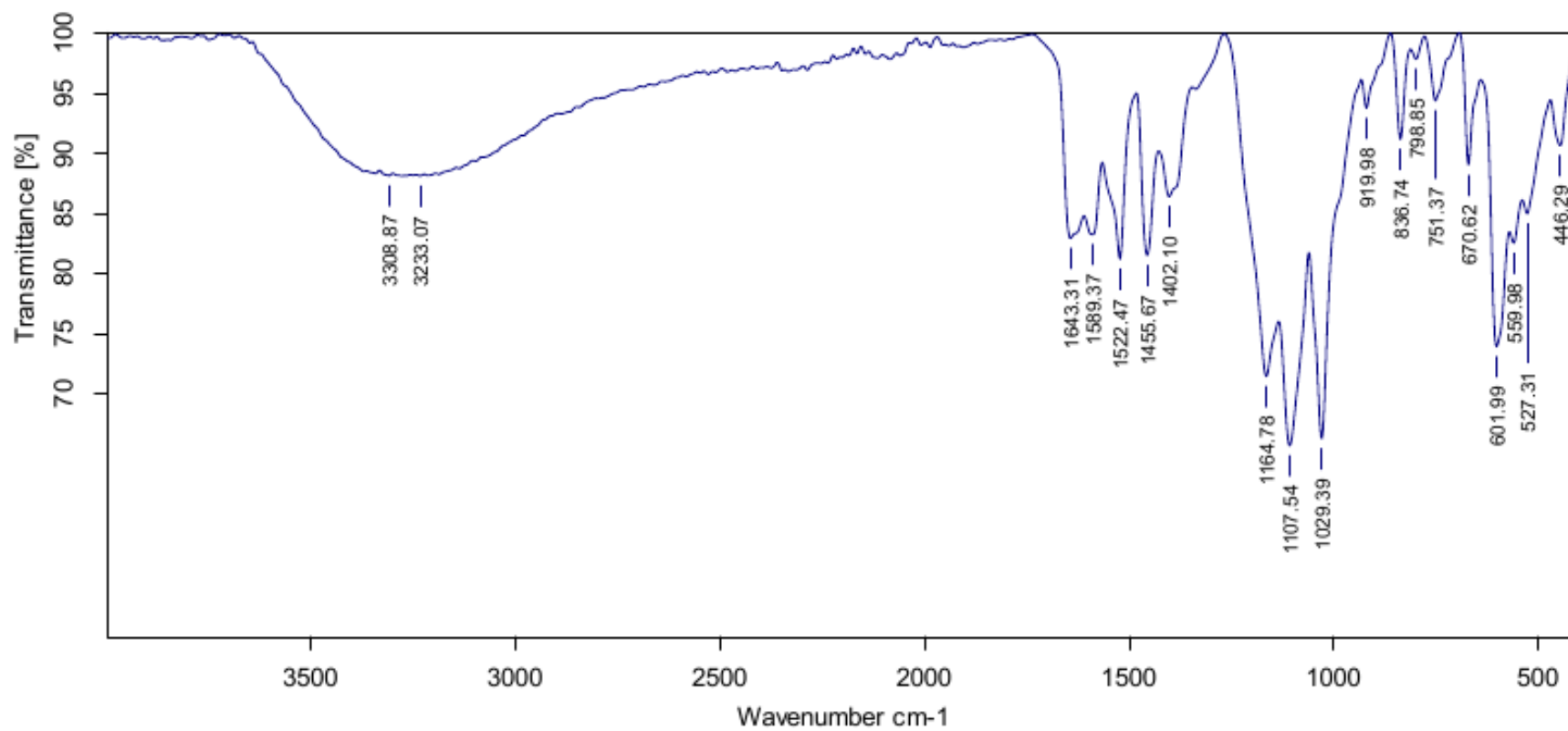


Fig. S14: IR spectra of MnSaln complex.

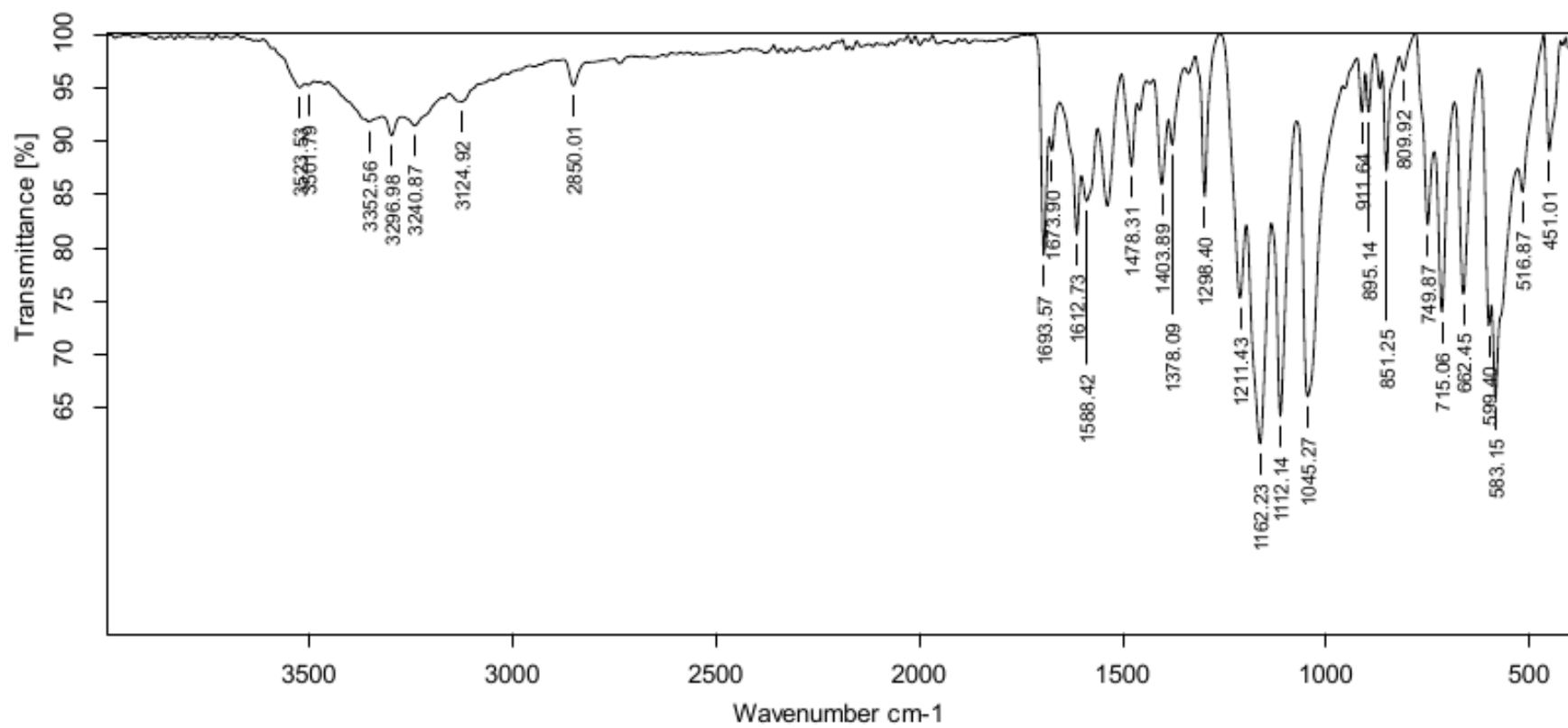


Fig. S15: IR spectra of MoO₂Saln complex.

MS (EI, 70 eV)

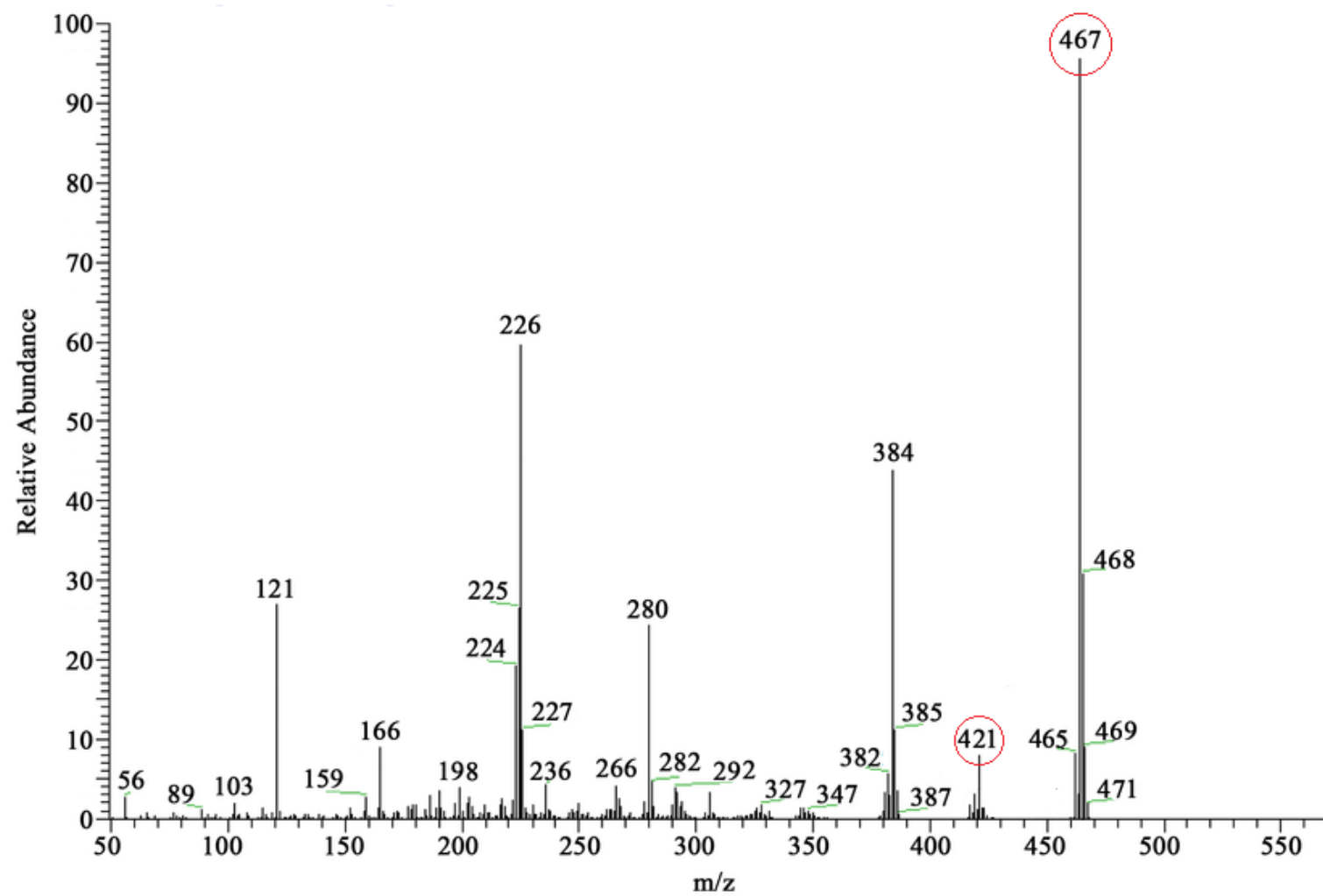


Fig. S16: MS of VOSaln complex.

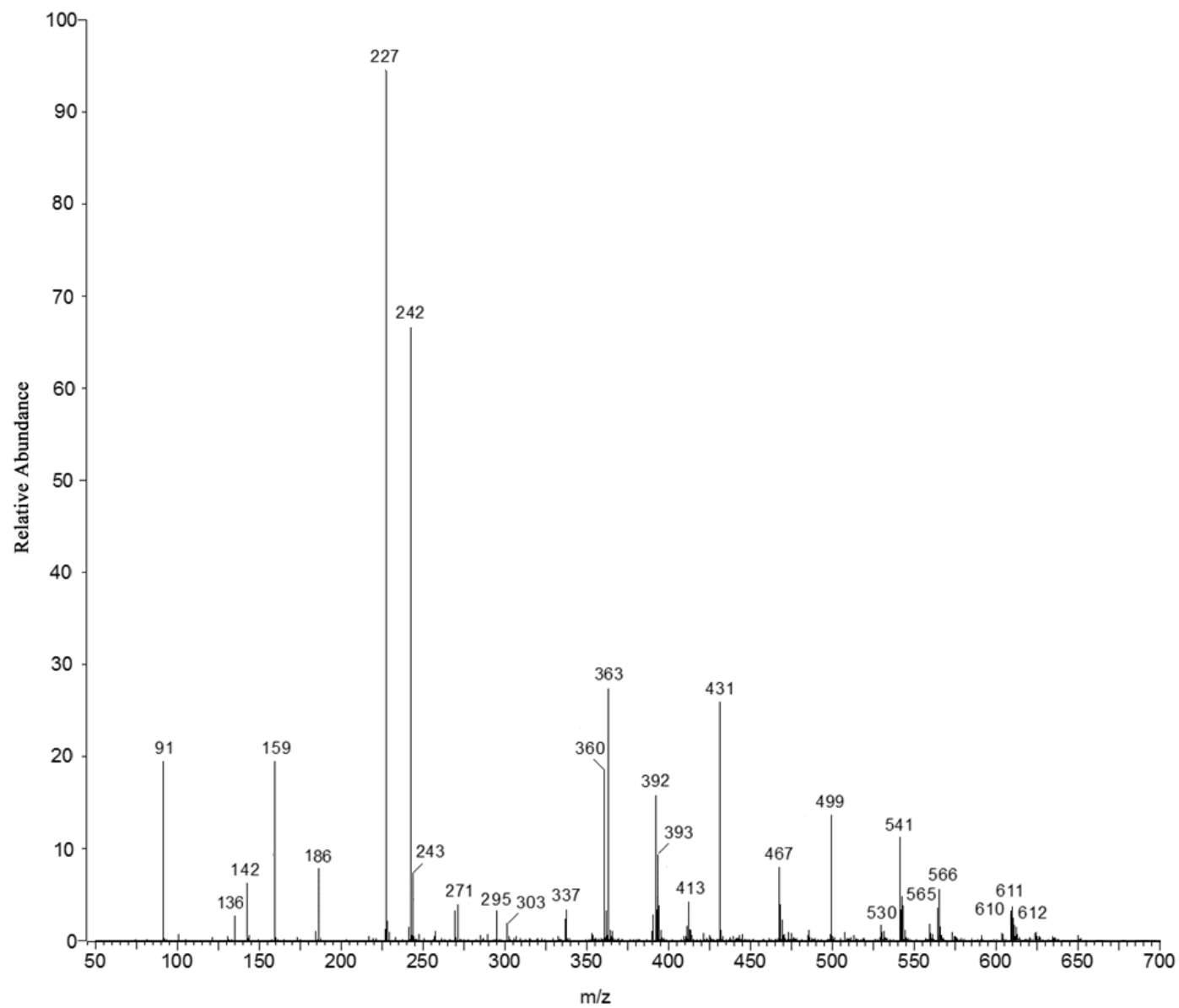


Fig. S17: MS of VOSaln-Ph complex.

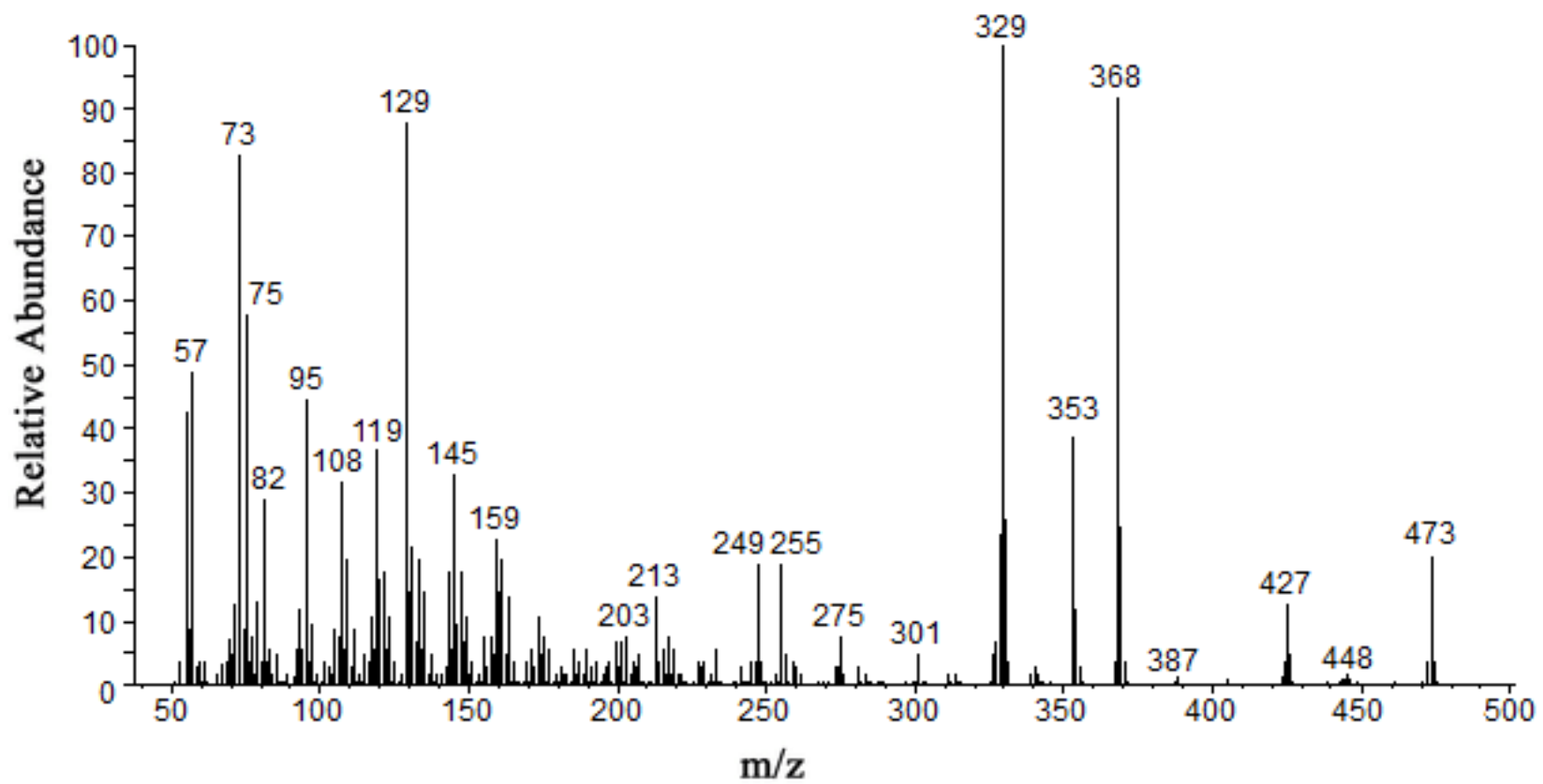


Fig. S18: MS of MnSaln complex.

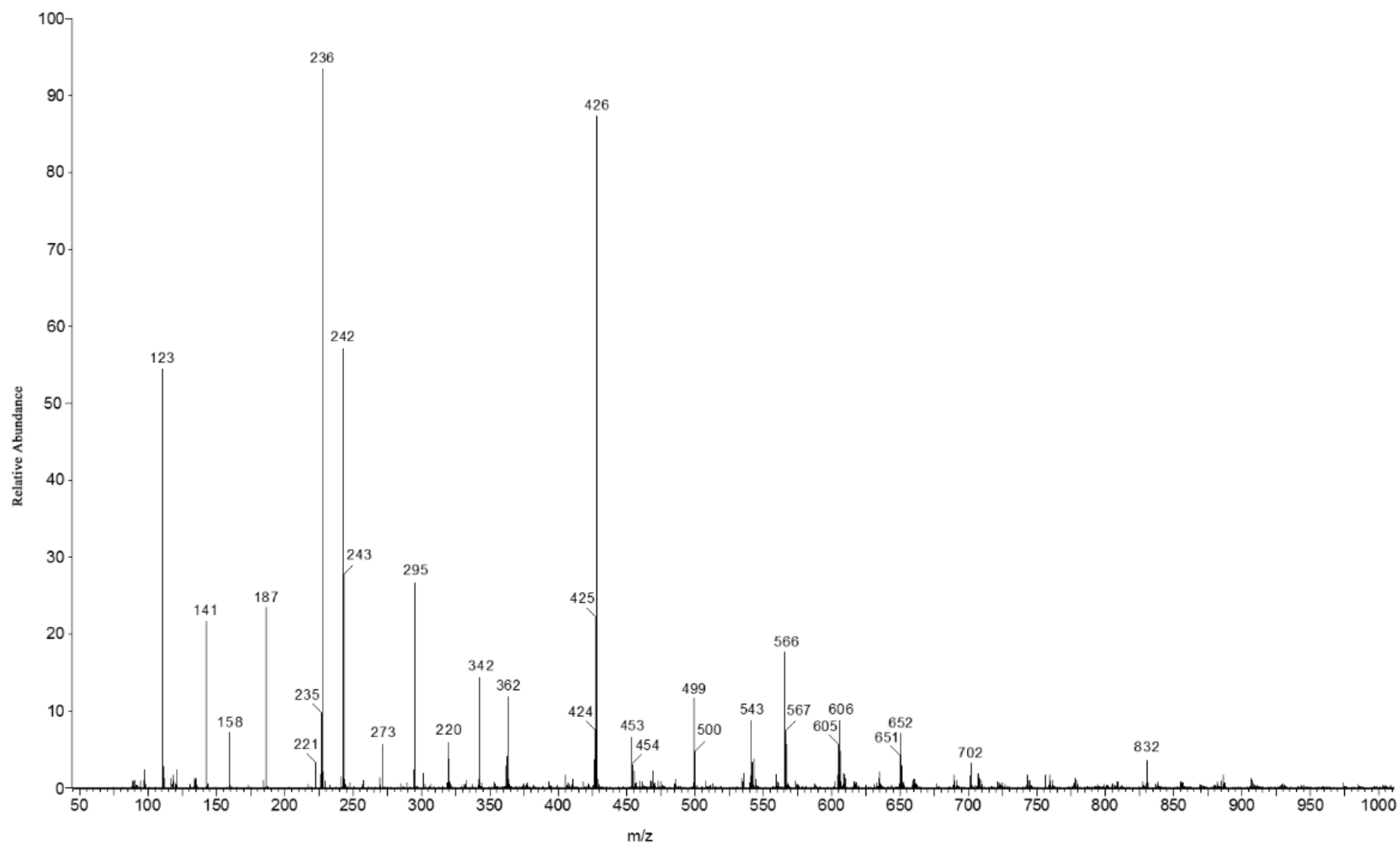


Fig. S19: MS of UO_2Saln complex.

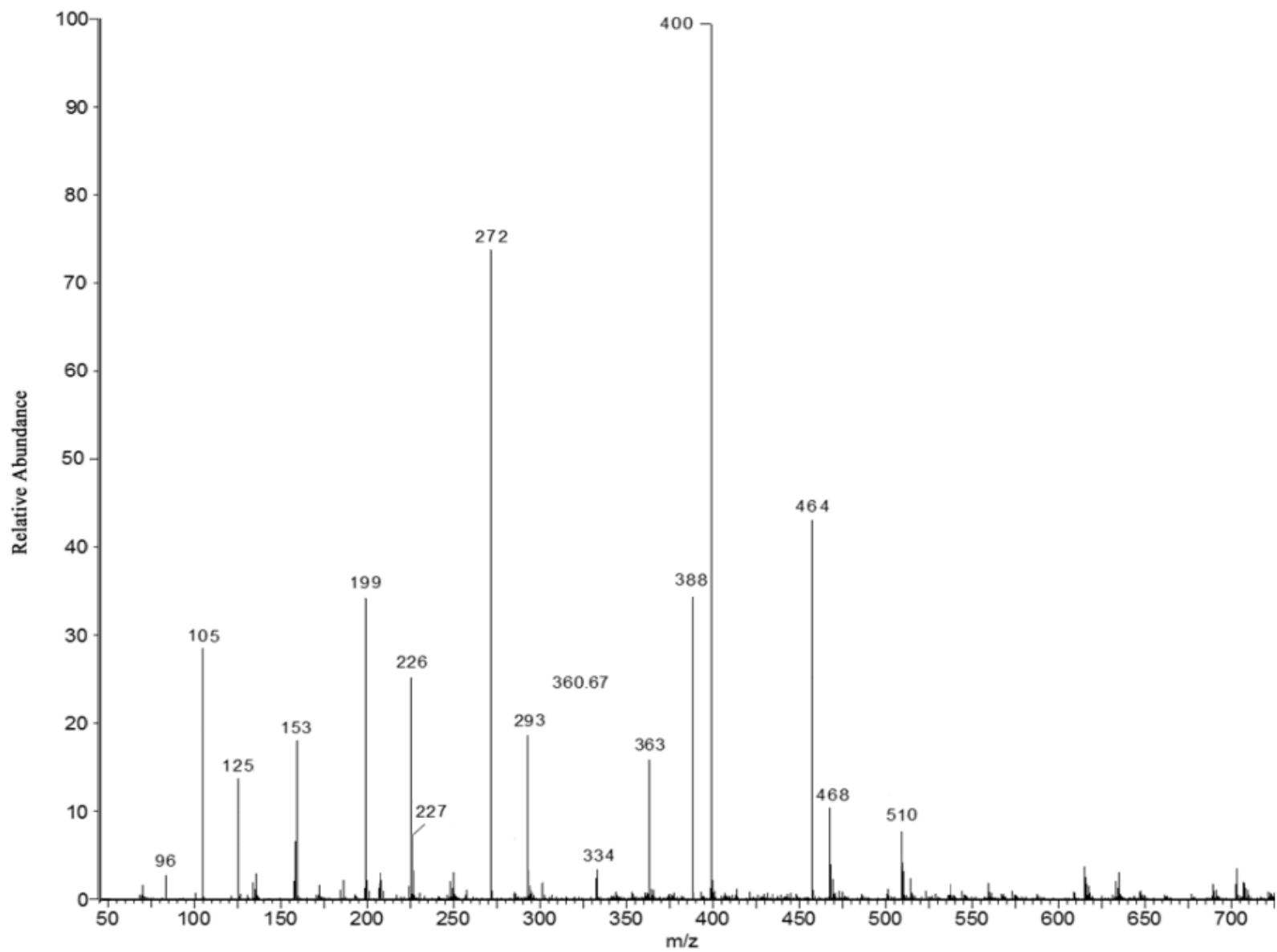


Fig. S20: MS of MoO₂Saln complex.

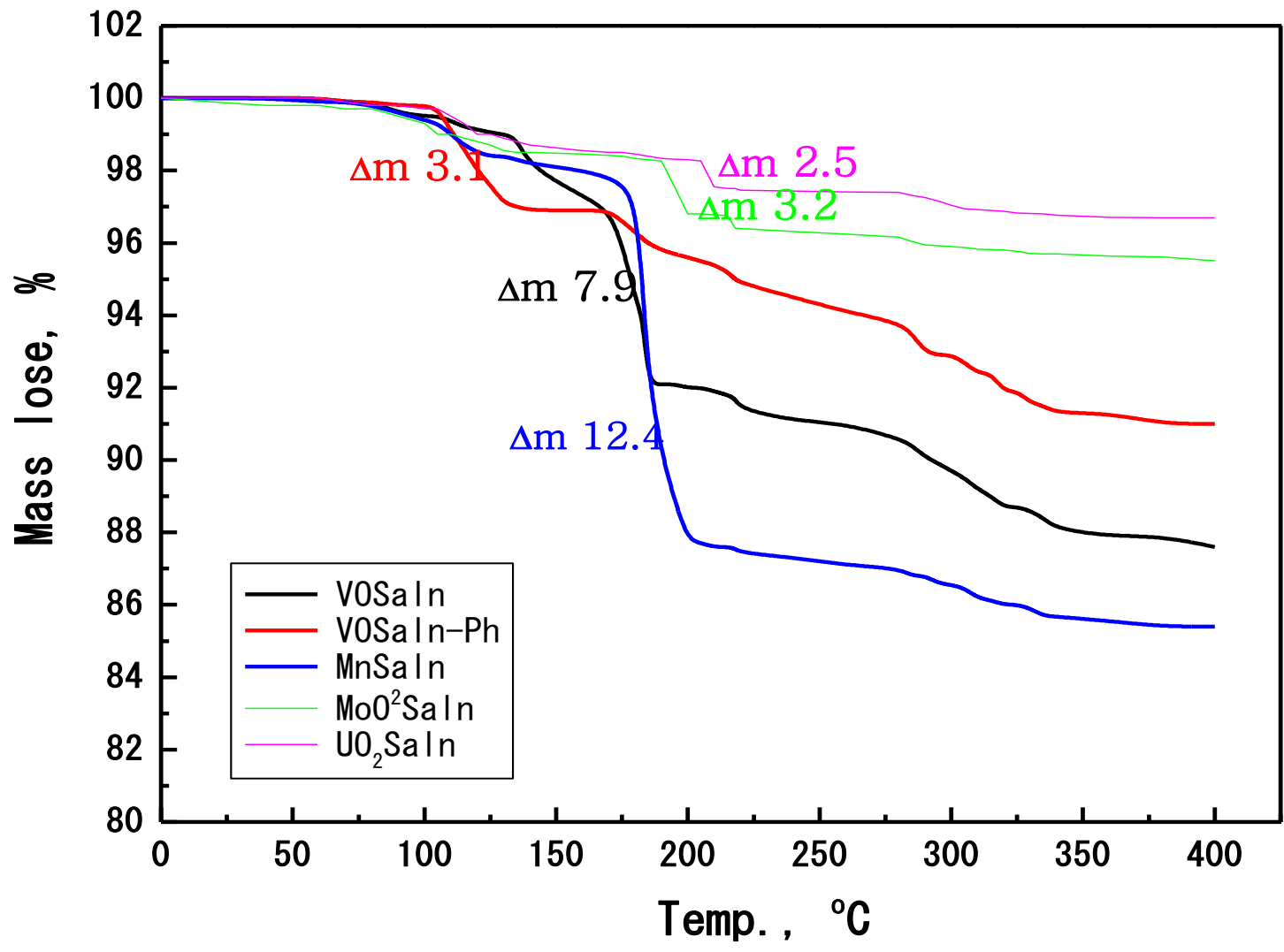


Fig. S21: TGA of MSaln complexes.

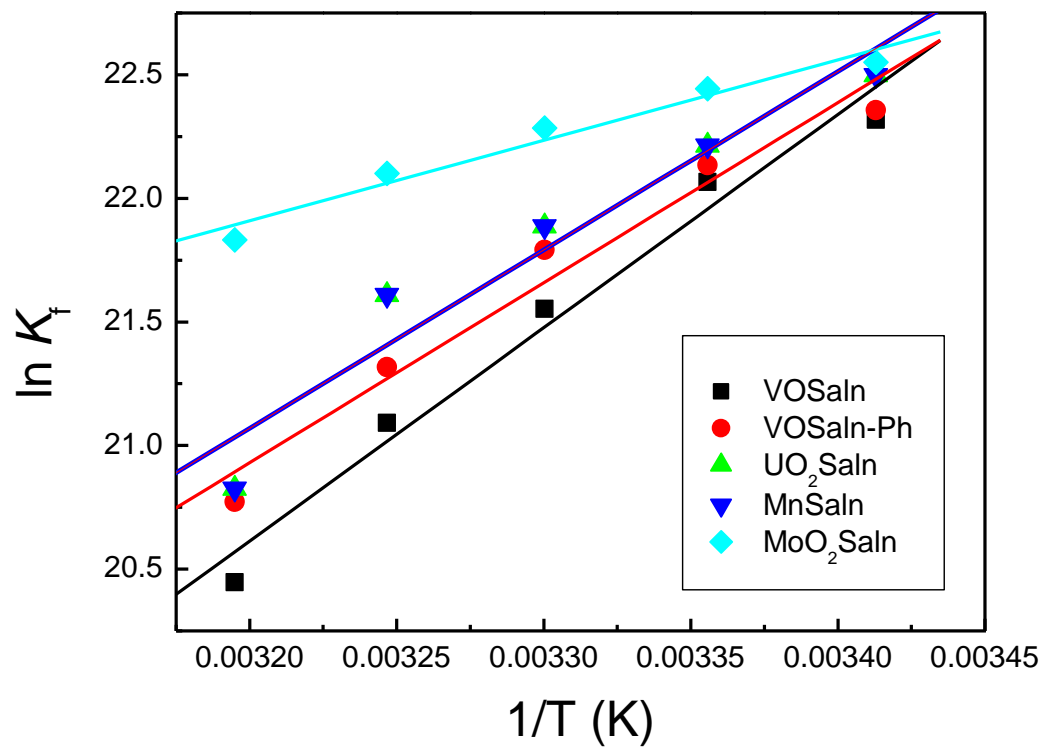


Fig. S22. Determination of thermodynamic parameters of MSalIn complexes formation from $\ln K_f$ values.