

## Supplementary Material

# New Heteroleptic 3D Metal Complexes: Synthesis, Antimicrobial and Solubilization Parameters

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**Table 1.** Physical and Analytical Data of HL<sub>1</sub> and its heteroleptic complexes (ML<sub>1</sub>Gly).

Compound	Colour	Melting Temp (°C)	Elemental analysis (%) found (calc.)				Electrical Conductance $\mu\text{S}/\text{cm}$
			C	H	N	Metal	
HL <sub>1</sub> <i>C<sub>20</sub>H<sub>18</sub>ClNO<sub>2</sub></i>	Yellow	250-254	70.65 (70.69)	5.28 (5.34)	3.90 (4.12)		3.55
CoL <sub>1</sub> Gly <i>C<sub>28</sub>H<sub>25</sub>ClCoN<sub>2</sub>O<sub>4</sub></i>	Pink	>350	60.78 (61.38)	4.49 (4.60)	5.31 (5.11)	10.57 (10.76)	18.56
NiL <sub>1</sub> Gly <i>C<sub>28</sub>H<sub>25</sub>ClNiN<sub>2</sub>O<sub>4</sub></i>	Light green	312-316	60.87 (61.41)	4.55 (4.60)	5.02 (5.12)	10.61 (10.72)	31.4
CuL <sub>1</sub> Gly <i>C<sub>28</sub>H<sub>25</sub>ClCuN<sub>2</sub>O<sub>4</sub></i>	Light Blue	>330	60.58 (60.87)	4.50 (4.56)	5.16 (5.07)	11.41 (11.50)	13.42
ZnL <sub>1</sub> Gly <i>C<sub>28</sub>H<sub>25</sub>ClZnN<sub>2</sub>O<sub>4</sub></i>	White	>350	60.63 (60.67)	4.32 (4.55)	5.00 (5.05)	11.66 (11.79)	27.9

**Table 2.** Physical and Analytical Data of HL<sub>2</sub> and its heteroleptic complexes (ML<sub>2</sub>Gly).

Compound	Colour	Melting Temp (°C)	Elemental analysis (%) found (calc.)				Electrical Conductance $\mu\text{S}/\text{cm}$
			C	H	N	Metal	
HL <sub>2</sub> <i>C<sub>13</sub>H<sub>9</sub>ClN<sub>2</sub>O<sub>6</sub>S</i>	Brown	125-128	43.55 (43.77)	2.50 (2.54)	7.67 (7.85)		-
CoL <sub>2</sub> Gly <i>C<sub>21</sub>H<sub>16</sub>ClCoN<sub>3</sub>O<sub>8</sub>S</i>	Dark brown	> 250	44.47 (44.66)	2.76 (2.86)	7.40 (7.44)	10.39 (10.43)	30.7
NiL <sub>2</sub> Gly <i>C<sub>21</sub>H<sub>16</sub>ClNiN<sub>3</sub>O<sub>8</sub>S</i>	Dark Green	333-338	44.59 (44.68)	2.85 (2.86)	7.31 (7.44)	10.22 (10.40)	4.69
CuL <sub>2</sub> Gly <i>C<sub>21</sub>H<sub>16</sub>ClCuN<sub>3</sub>O<sub>8</sub>S</i>	Brown	217-222	44.28 (44.30)	2.76 (2.83)	7.21 (7.38)	11.01 (11.16)	3.42

ZnL <sub>2</sub> Gly C <sub>21</sub> H <sub>16</sub> ClCuN <sub>3</sub> O <sub>8</sub> S	Light brown	280-282	43.89 (44.15)	2.65 (2.82)	7.31 (7.36)	11.34 (11.44)	27.9
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**Table 3.** Physical and Analytical Data of HL<sub>3</sub> and its heteroleptic complexes (ML<sub>3</sub>Gly).

Compound	Colour	Melting Temp (°C)	Elemental analysis (%) found (calc.)				Electrical Conductance $\mu$ S/cm
			C	H	N	Metal	
HL <sub>3</sub> C <sub>20</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	Bright Yellow	161-163	75.82 (75.93)	4.95 (5.10)	8.71 (8.86)		1.06
CoL <sub>3</sub> Gly C <sub>28</sub> H <sub>22</sub> CoN <sub>3</sub> O <sub>4</sub>	Velvety brown	185-190	64.04 (64.25)	4.12 (4.24)	7.89 (8.03)	11.11 (11.26)	31.7
NiL <sub>3</sub> Gly C <sub>28</sub> H <sub>22</sub> NiN <sub>3</sub> O <sub>4</sub>	Maroon	> 346	63.75 (64.28)	3.99 (4.24)	8.01 (8.03)	11.01 (11.22)	25.4
CuL <sub>3</sub> Gly C <sub>28</sub> H <sub>22</sub> CuN <sub>3</sub> O <sub>4</sub>	Dark blue	225-235	63.58 (63.69)	4.01 (4.20)	7.83 (7.96)	11.99 (12.03)	13.5
ZnL <sub>3</sub> Gly C <sub>28</sub> H <sub>22</sub> ZnN <sub>3</sub> O <sub>4</sub>	Yellow	220-222	63.40 (63.47)	3.98 (4.19)	7.59 (7.93)	12.03 (12.34)	3.57

**Table 4.** FTIR Data (cm<sup>-1</sup>) of HL<sub>1</sub> and its heteroleptic complexes (ML<sub>1</sub>Gly).

Type of Vibration (cm <sup>-1</sup> )	Water of hydration	$\nu$ (N-H) Asym. /Sym.	$\nu$ (C=O)	$\nu$ (C=N) ~shift	$\nu$ (C-O)	$\nu$ (COO <sup>-</sup> ) asym.	$\nu$ (COO <sup>-</sup> ) sym.	$\nu$ -(M-O)	$\nu$ -(M-N)
Ligand HL <sub>1</sub>	-	-	1647 (s)	1591 (s)	1215 (m)	-	-	-	-
Co(II) L <sub>1</sub> - PhGly (ternary)	3360 (w)	3246 (w) 2976 (b, w)	1645 (m)	1585 (s)	1201 (m)	1556 (s)	1357 (s)	615 (s)	597 (m) 549 (m)
Ni(II) L <sub>1</sub> - PhGly (ternary)	3363 (w)	3224 (w) 3149 (w)	1643 (w)	1581 (s)	1199 (m)	-	1409 (s)	646 (s) 617 (s)	586 (s) 509 (s)
Cu(II) L <sub>1</sub> - PhGly (ternary)	3334 (w)	3217 (w) 3047 (w)	1622 (s)	1562 (s)	-	-	1365 (s)	609 (s)	542 (m) 459 (m)
Zn(II) L <sub>1</sub> - PhGly (ternary)	3315 (w)	3255 (w) 3034 (w)	1618 (s)	1560 (s)	1197 (m)	-	1377 (s)	648 (m) 615 (s)	555 (m) 478 (s)

**Table 5.** FTIR Data (cm<sup>-1</sup>) of HL<sub>2</sub> and its heteroleptic complexes (ML<sub>2</sub>Gly).

Type of Vibration (cm <sup>-1</sup> )	Water of hydration	$\nu$ (=C-H) aromatic	$\nu$ (C=N) ~shift	$\nu$ -(NO <sub>2</sub> )	$\nu$ -(Sulfonic acid)	$\nu$ (C-H) sp <sup>2</sup> Aromatic (o.o.p bending)	$\nu$ -(S-O)	$\nu$ COO <sup>-</sup> asym./sym.	$\nu$ -(M-O)	$\nu$ -(M-N)
Ligand HL <sub>2</sub>	3379 (w)	3027 (w)	1627 (s)	1370 (s) 1568 (s)	1205 (m) 1276 (s)	910 (m) 806 (s)	65 8 (m)	-	-	-



Co(II) L <sub>2</sub> - PhGly (ternary)	3358 (w)	3062 (w)	1651 (s)	1556 (s) 1404 (s)	1192 (s)	931 (m) 754 (s) 698(s)	66 7 (m)	1585 (s) 1361 (s)	657 (m) 609 (s)	555 (m) 486 (s)
Ni(II)L <sub>2</sub> - PhGly (ternary)	3363 (w)	3062 (w)	1595 (s)	1475 (s) 1404 (s)	1192 (m) 1118 (s)	921 (m) 817 (s) 696 (s)	66 5 (s)	1581 1294 (s)	644 (s) 584 (s)	484 (m) 451 (s)
Cu(II)L <sub>2</sub> - PhGly (ternary)	3332 (w)	3039 (w)	1622 (s)	1493 (m) 1402 (m)	1139 (s) 1105	921 (m) 752(s) 696 (s)	67 1 (m)	1562 (s) 1357 (s)	615 (s) 597 (m)	- 441 (s)
Zn(II)L <sub>2</sub> - PhGly (ternary)	3313 (w)	3034 (w)	1616 (s)	1485 (s) 1409 (s)	1197(m) 1292 (s)	927 (m) 746 (s) 696 (s)	64 6 (m)	1562 (s) 1377 (s)	624 (s) 590 (m)	542 (m) 468 (s)

Table 6. FTIR Data (cm<sup>-1</sup>) of HL<sub>3</sub> and its heteroleptic complexes (ML<sub>3</sub>Gly).

Type of Vibration (cm <sup>-1</sup> )	Water of hydration	v(=C-H) aromatic	v(CH) sp <sup>3</sup>	v(C=N) ~shift	v- (C- O)	v(C-H) sp <sup>2</sup> aromatic (o.o.p bending)	v(COO <sup>-</sup> ) ) asym.	v(COO <sup>-</sup> ) ) sym.	v- (M- O)	v- (M- N)
Ligand HL <sub>3</sub>	O-H phenolic 3430 (w)	3055 (w)	-	1608 (s)	1274 (s)	754 (s) 854 (m)	-	-	-	-
Co(II)L <sub>3</sub> - PhGly (ternary)	3414	-	-	1630 (s)	1200 (s)	751 (s) 855 (m)	1521(s)	1357 (s)	597 (s) 511 (m)	475 (s) 412 (s)
Ni(II)L <sub>3</sub> - PhGly (ternary)	3388 (b, w)	-	2896 (w)	1601 (s)	1233 (m)	752 (s) 847 (m)	1517 (s)	1370 (s)	543 (s) 507 (m)	457 (s) 409 (s)
Cu(II)L <sub>3</sub> - PhGly (ternary)	3406 (b, w)	2906 (w)	2887 (w)	1576 (s)	1200 (m)	694 (s) 728 (s) 854 (m)	1519 (s)	1356 (s)	595 (s) 508 (s)	472 (m)
Zn(II)L <sub>3</sub> - PhGly (ternary)	-	-	2895 (w)	1613 (s)	1244 (m)	747 (s) 854 (m)	1528 (s)	1323 (s)	597 (s) 510 (s)	490 (m) 437 (m)

Comparison of Zn(II) complexes.

Type of Vibration (cm <sup>-1</sup> )	Water of hydration	v(-NH <sub>2</sub> ) sym./ asym.	v(CH) sp <sup>3</sup> and v(=C- H) Phe.	v(C=N) ~shift	v- (C- O)	v(C-H) sp <sup>2</sup> aromatic (o.o.p bending)	v(COO <sup>-</sup> ) ) asym.	v(COO <sup>-</sup> ) ) sym.	v- (M- O)	v- (M- N)
Ph-Gly	-	2975, 3167 (w)	2880 (w)	-	-	694 (s) 728 (s)	1576 (s)	1355 (s)	-	-
Zn(II)-Ph- Gly (binary)	3313 (w)	3062 3256 (w)	3034 (w)	-	-	697 (s) 746 (s)	1560 (s)	1376 (s)	586 (s)	460 (s)
Ligand HL <sub>3</sub>	O-H phenolic 3430 (w)	-	-	1608 (s)	1274 (s)	754 (s) 854 (m)	-	-	-	-

ZnL <sub>3</sub> (binary)	3453 (w)	-	3007 (w)	1612 (s)	1244 (m)	746 (s) 854 (m)	-	-	540 (s)	488 (s)
ZnL <sub>3</sub> - PhGly (ternary)	-	2965 (w) masked	2895 (w)	1613 (s)	1244 (m)	747 (s) 854 (m)	1528 (s)	1323 (s)	597 (s)	490 (m)

### Selected NMR and FTIR spectra's of synthesized ligands and mixed complexes

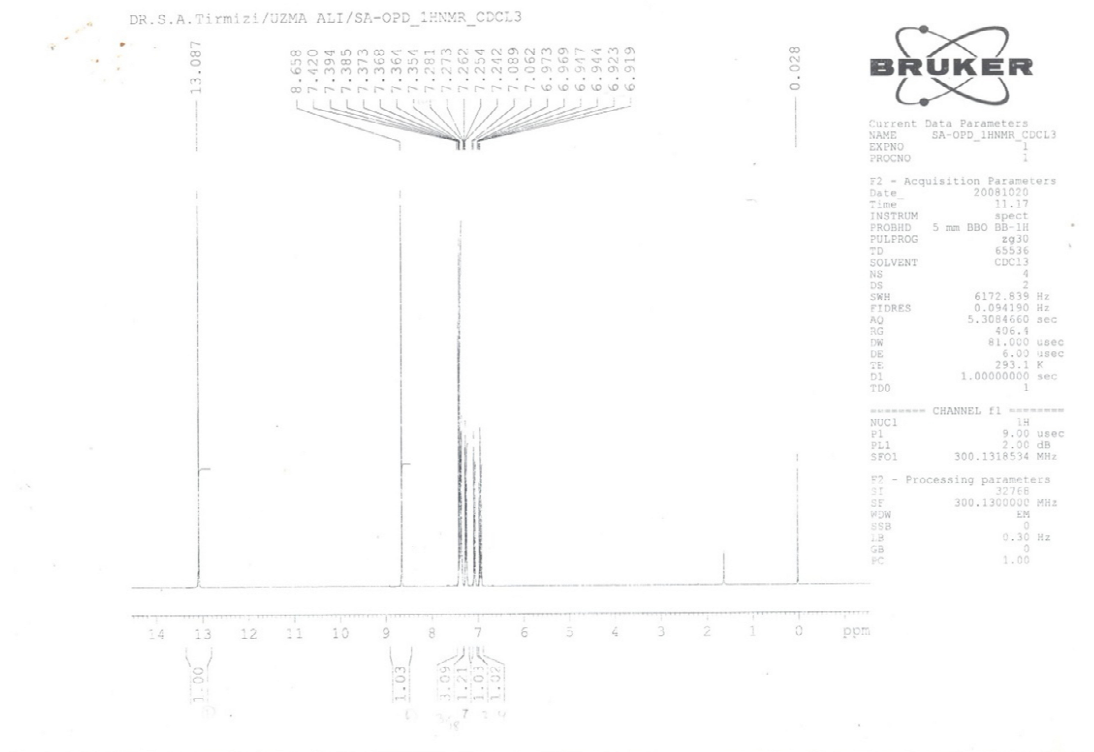
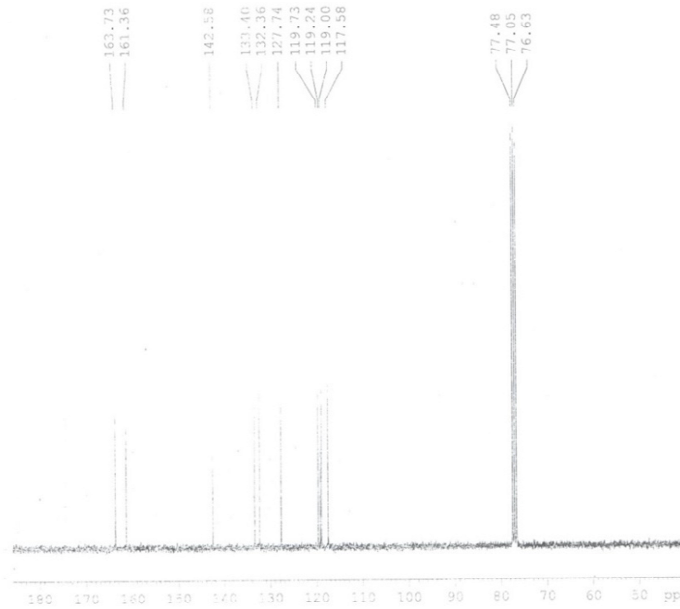


Figure 1. <sup>1</sup>H NMR spectrum of HL<sub>3</sub>.

DR.S.A.Tirmizi/UZMA ALI/SA-OPD\_13CNMR\_CDCL3



Current Data Parameters  
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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCL3  
NS 316  
DS 2  
SFR 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 1824.6  
DM 27.800 usec  
DE 4.00 usec  
TE 293.3 K  
D1 2.00000000 sec  
d11 0.20000000 sec  
DELTA 1.89999998 sec  
TDO 1

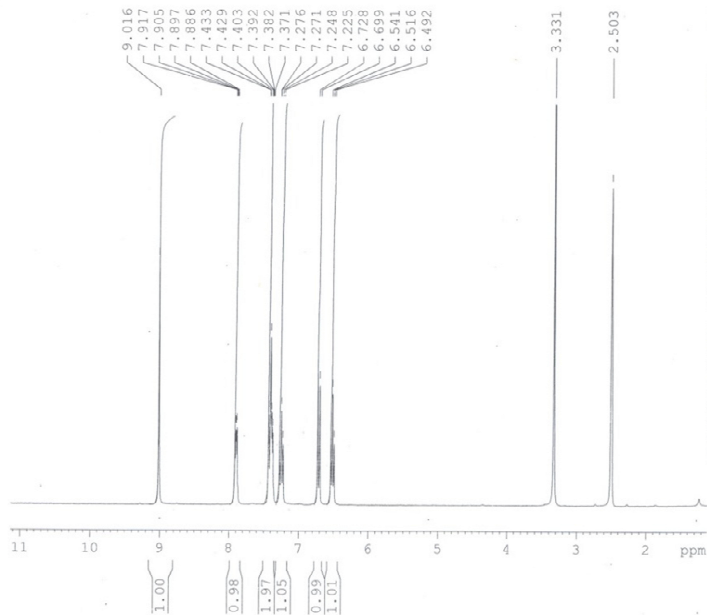
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PL1 -5.00 dB  
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PCPD2 80.00 usec  
PD 2.00 dB  
PL12 20.98 dB  
PL13 20.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
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SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Figure 2. <sup>13</sup>C NMR spectrum of HL3.

DR.S.A.Tirmizi/UZMA ALI/ZN(SA-OPD)\_1HNMR\_DMSO



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PROCNO   1

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SOLVENT  DMSO
NS        16
DS        2
SWH       6172.839 Hz
FIDRES    0.094159 Hz
AQ        5.3084660 sec
RG        645.1
DE        81.000 usec
TE        298.2 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
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PL1       2.00 dB
SFO1      300.1318534 MHz

F2 - Processing parameters
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SF        300.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
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Figure 3. <sup>1</sup>H NMR spectrum of ZnL<sub>3</sub>Gly.

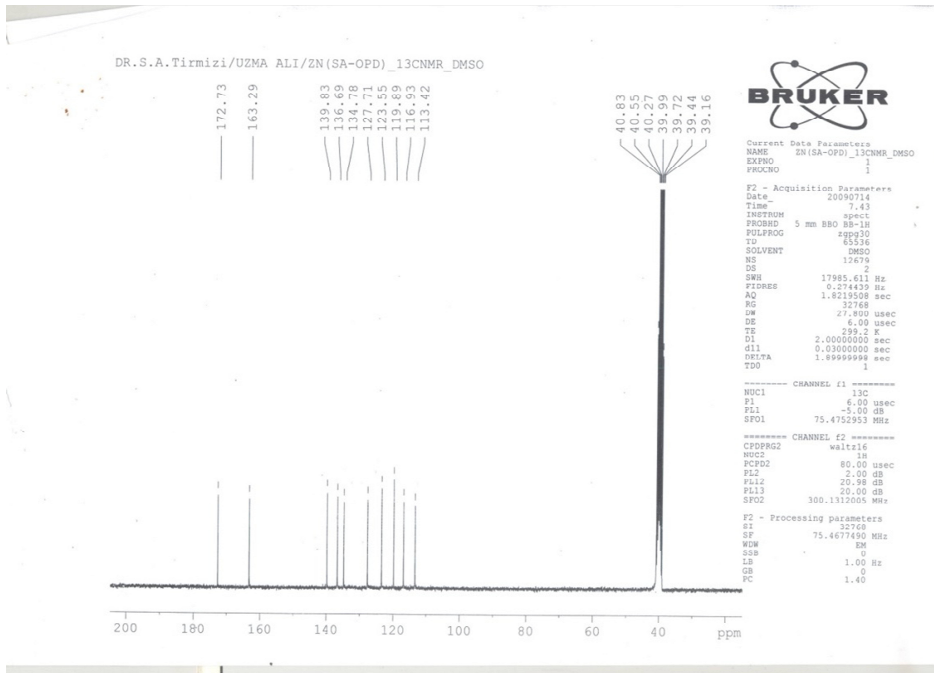


Figure 4.  $^{13}\text{C}$  NMR spectrum of ZnLaGly.

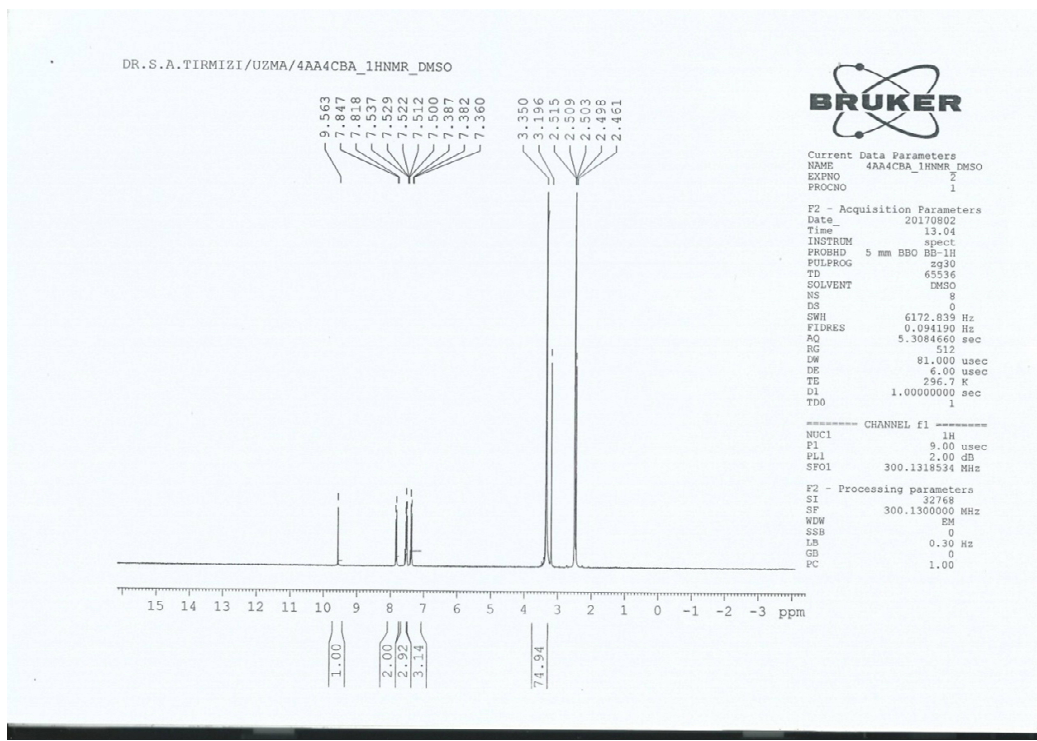
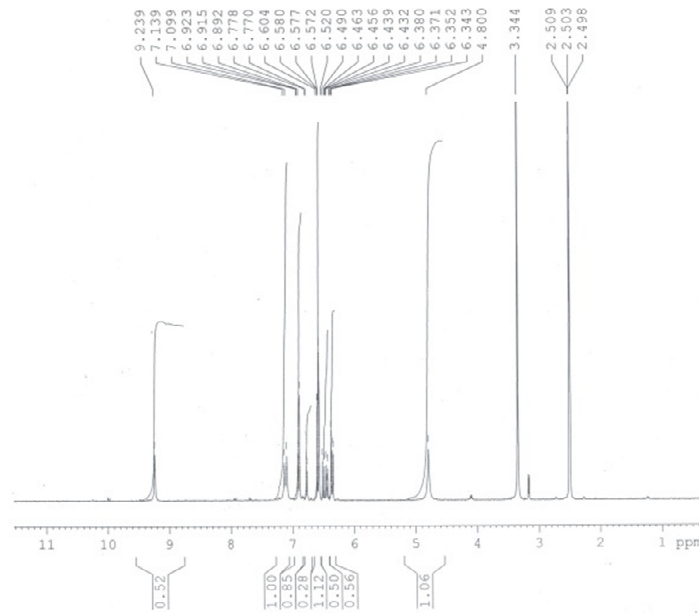


Figure 5. <sup>1</sup>H NMR spectrum of HL1.

DR. S. A. TIRMIZI/UZMA/PD-NAPSA4CBA\_1HNMR\_DMSO



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PROCNO 1

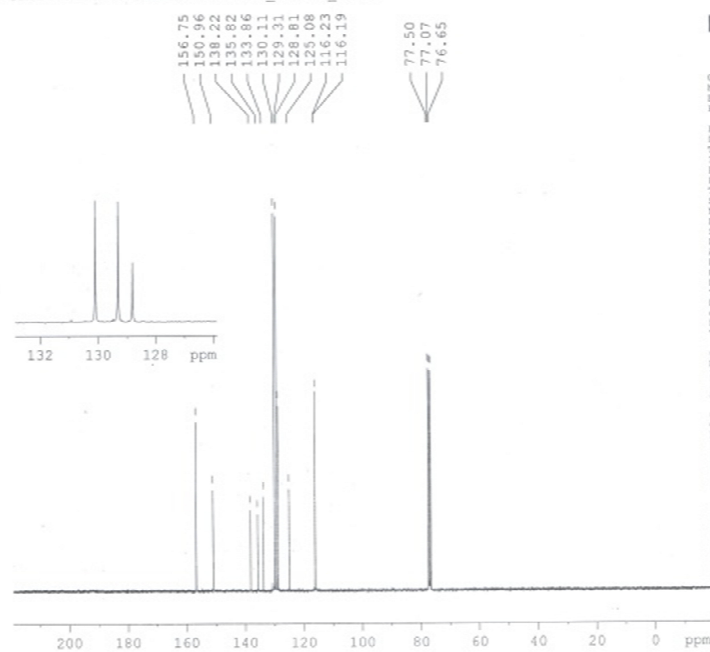
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SWH 4172.895 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 645.1
DM 01.000 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TDO 1

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PL1 2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
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RGW 8M
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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Figure 6. <sup>1</sup>H NMR spectrum of HL<sub>2</sub>.

DR.S.A.TIRMIZI/UZMA/NAPSA4CBA\_13CNMR\_CDCL3



Current Data Parameters  
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EXPNO 1  
PROCNO 1

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SWH 17985.611 Hz  
FIDRES 0.500049 Hz  
AQ 0.889604 sec  
RG 1625.5  
DW 27.850 usec  
DE 4.00 usec  
TE 295.6 K  
C1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999999 sec  
TV 1

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PL1 -5.00 dB  
SFO1 75.4752853 MHz  
----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 20.98 dB  
PL13 70.00 dB  
SFO2 300.1312005 MHz

F2 - Processing Parameters  
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WDW EM  
SSB 0  
IB 1.00 Hz  
GB 0  
PC 1.40

Figure 7. <sup>13</sup>C NMR spectrum of HL2.



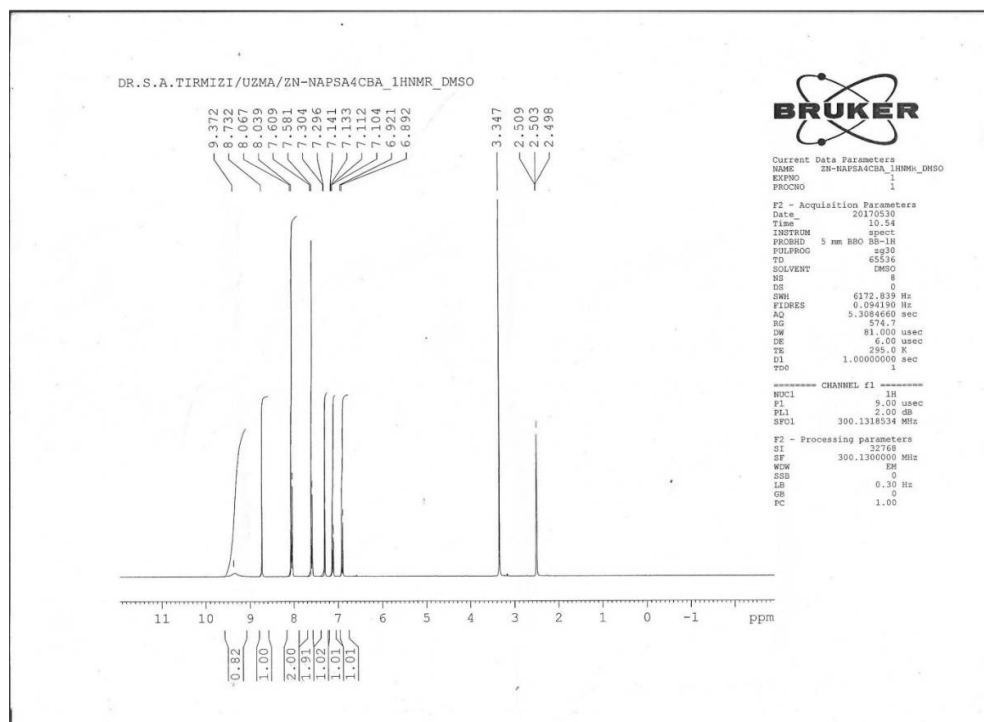


Figure 8.  $^1\text{H}$  NMR spectrum of  $\text{ZnL}_2\text{Gly}$ .

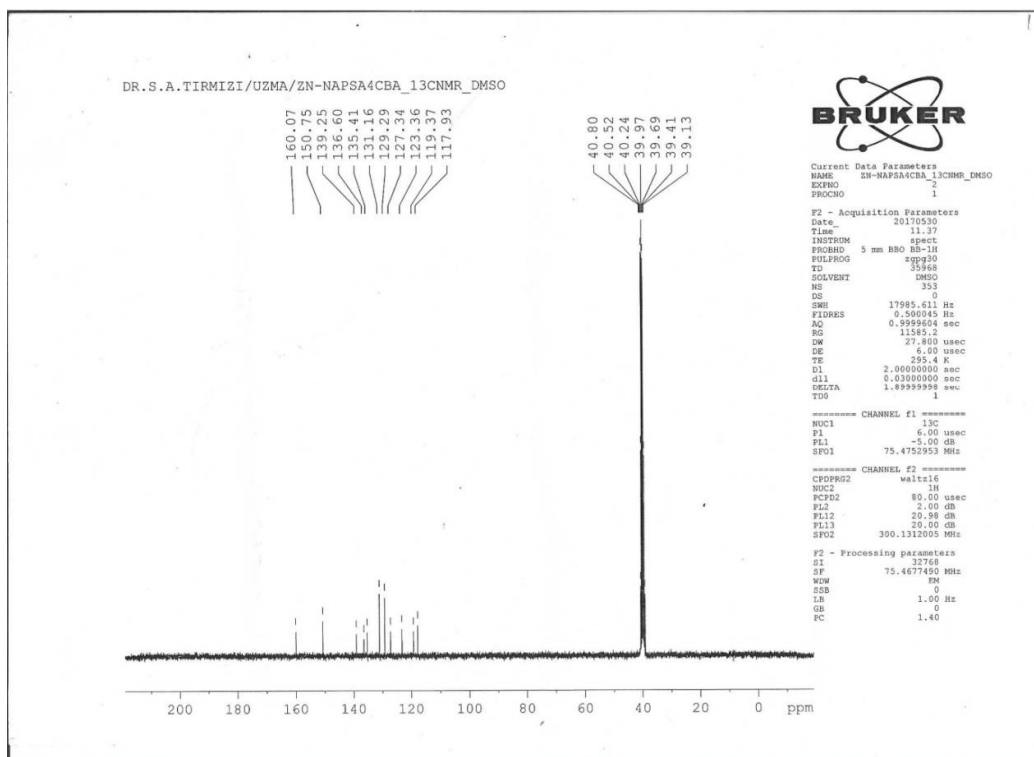


Figure 9.  $^{13}\text{C}$  NMR spectrum of ZnLzGly.

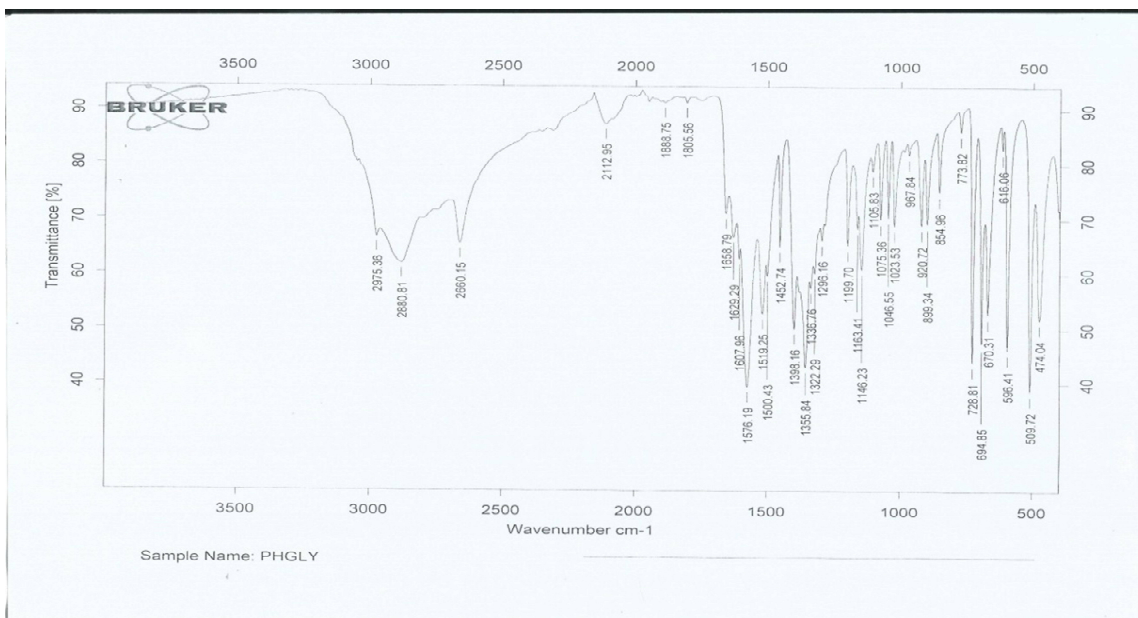


Figure 10. FTIR spectrum of  $\alpha$ -phenyl glycine.

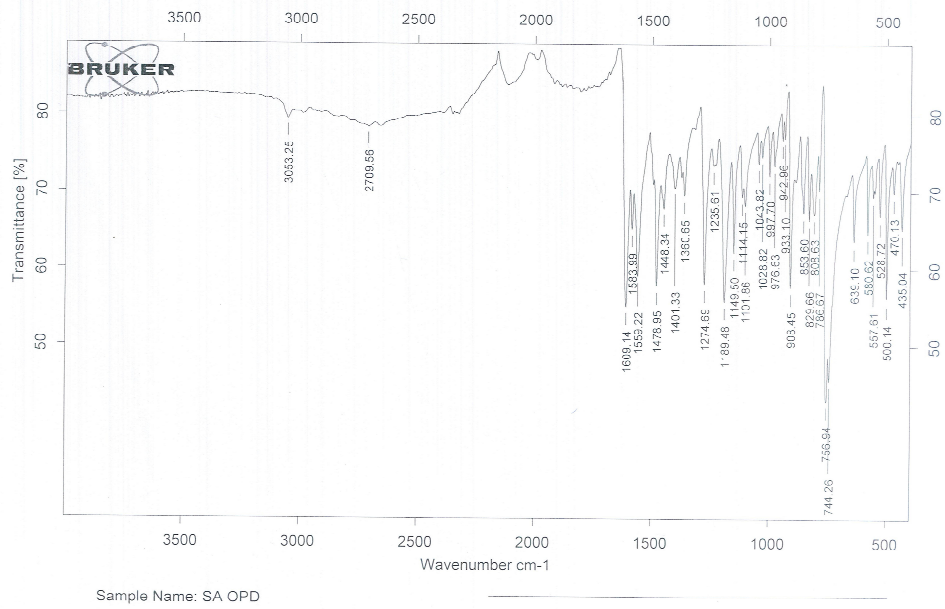
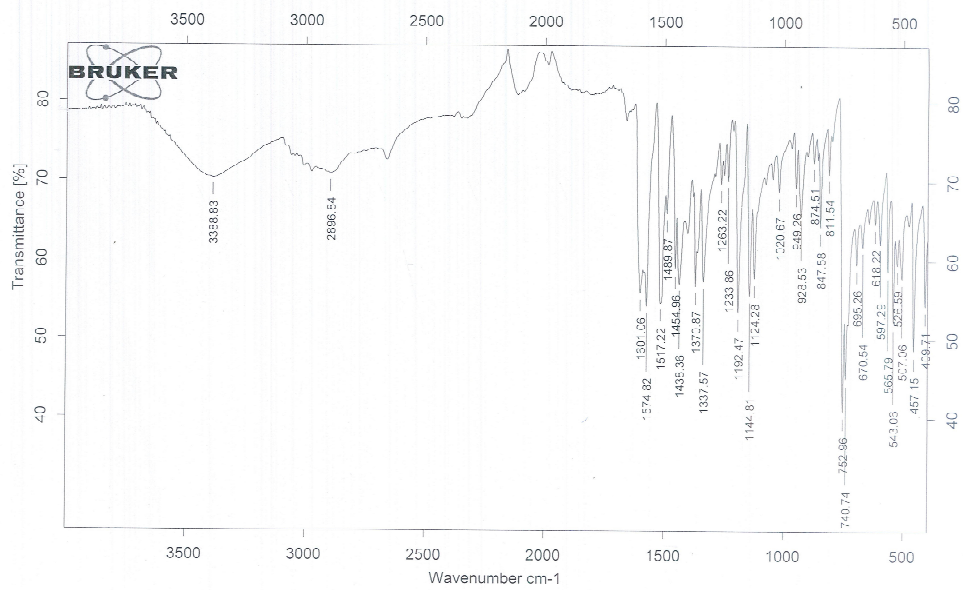


Figure 11. FTIR spectrum of HL3.



Sample Name: NISAOPSPHGLY

Figure 12. FTIR spectrum of NiL<sub>3</sub>Gly.

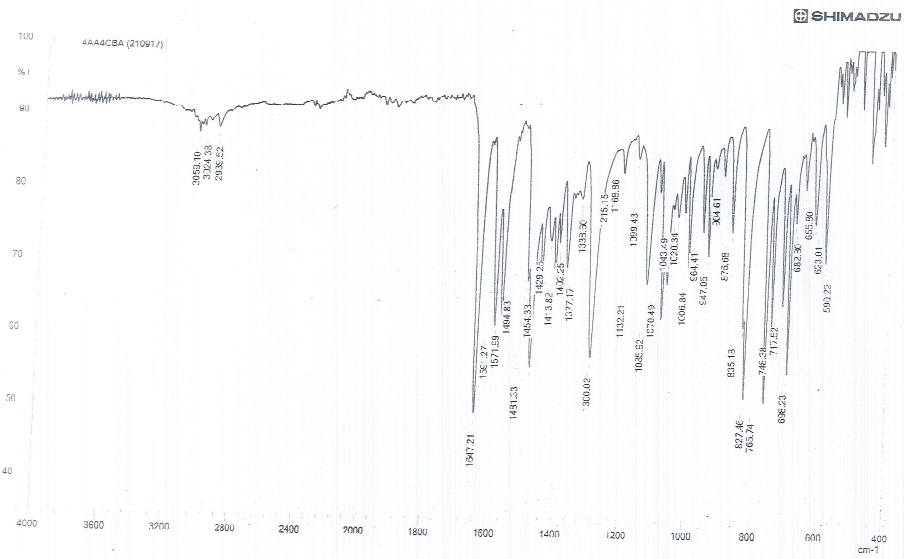


Figure 13. FTIR spectrum of HL1.

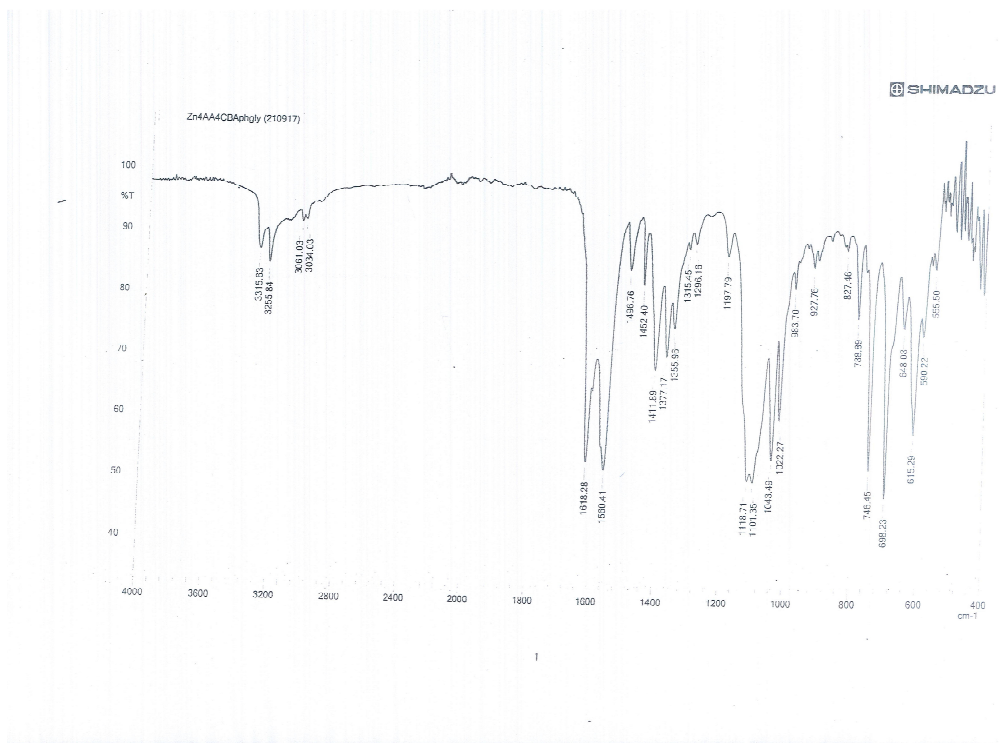
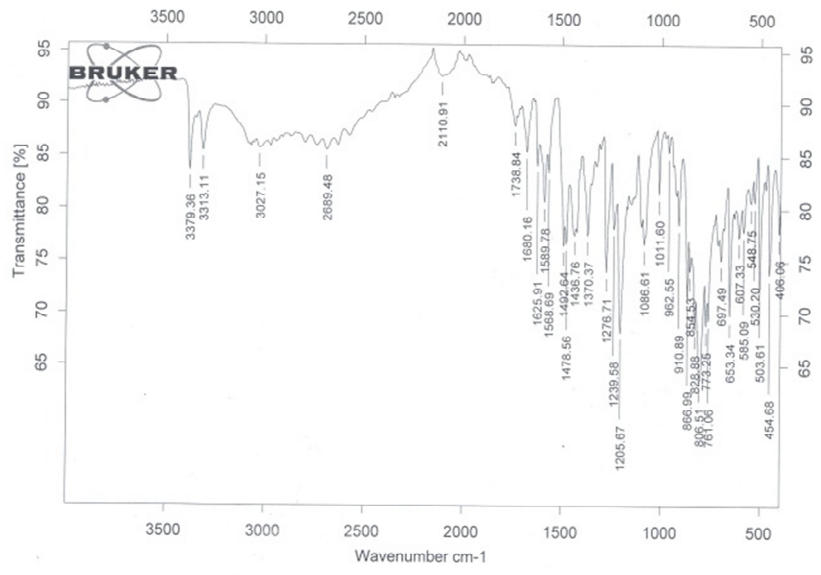


Figure 14. FTIR spectrum of ZnLiGly.



Sample Name: NAPSA4CBA

Figure 15. FTIR spectrum of HL<sub>2</sub>.



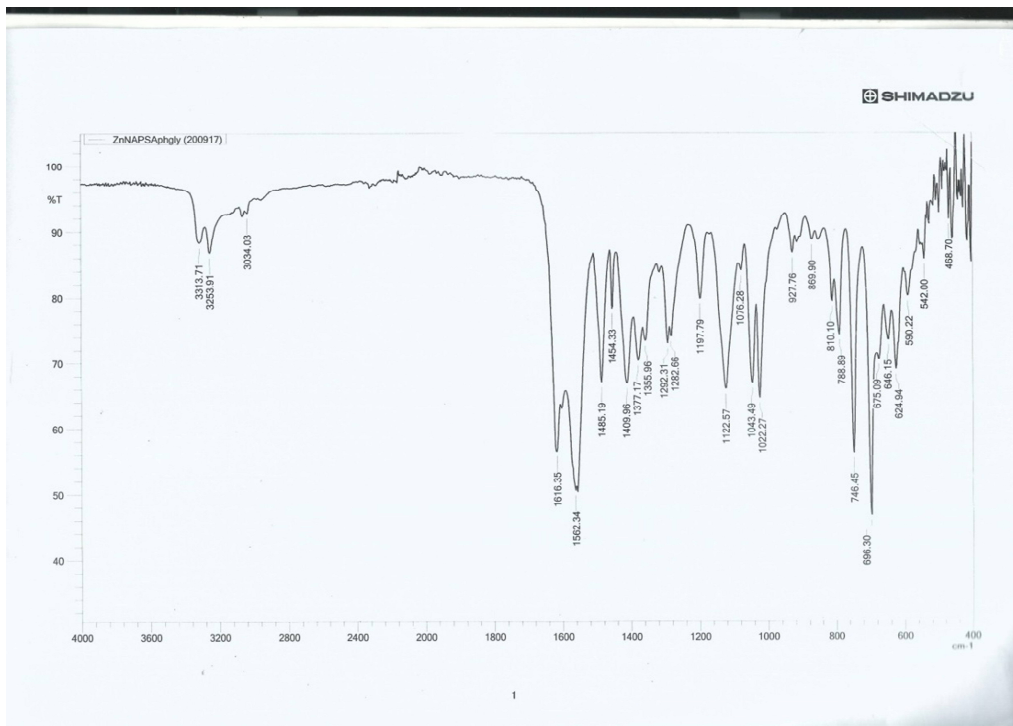
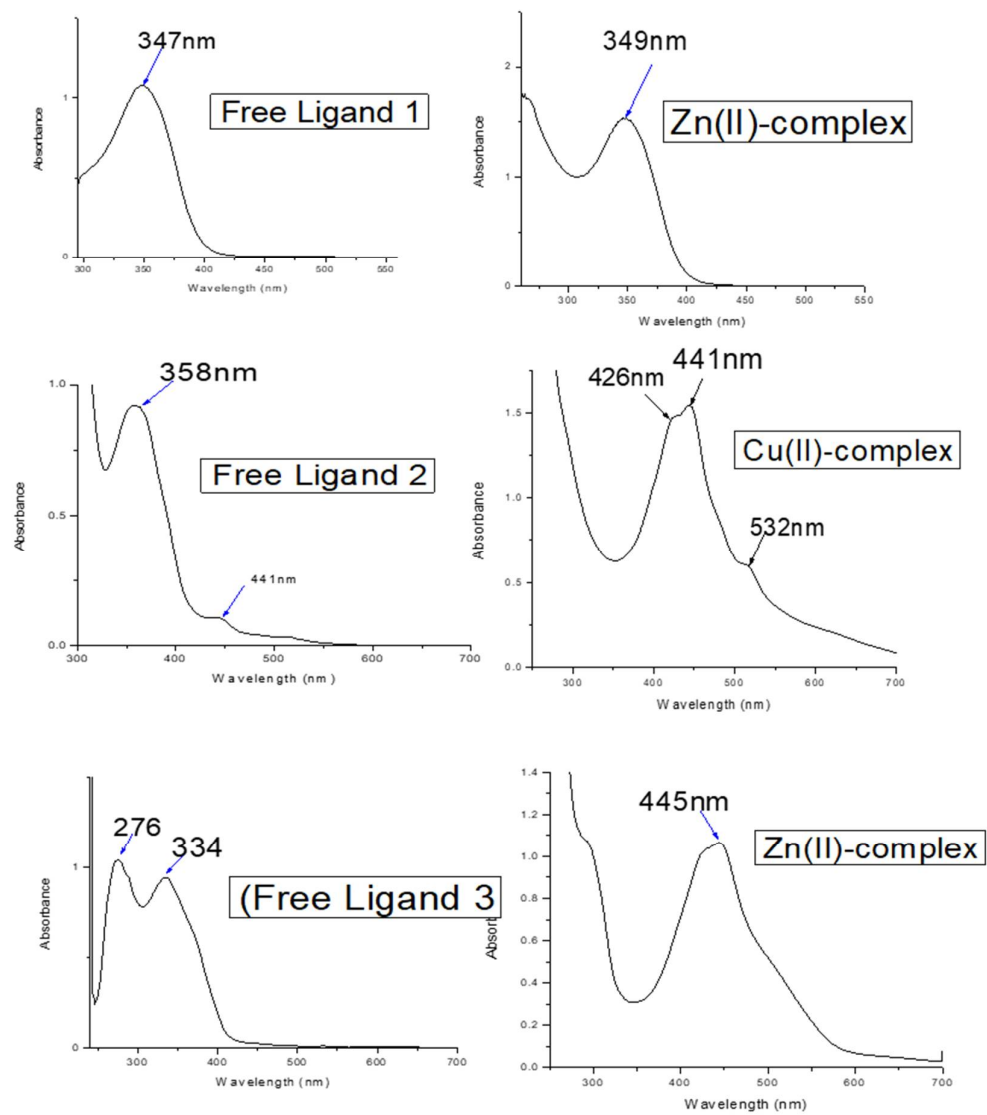


Figure 16. FTIR spectrum of ZnL<sub>2</sub>Gly.



**Figure 17.** Electronic spectra of ligands (HL<sub>1</sub>, HL<sub>2</sub>, HL<sub>3</sub>) and selected spectra of metal complexes.