Supporting Information

Hypoxia efficient and glutathione resistant cytoselective Ruthenium(II)-*p*-cymene-arylimidazophenanthroline complexes: biomolecular interaction and live cell imaging†

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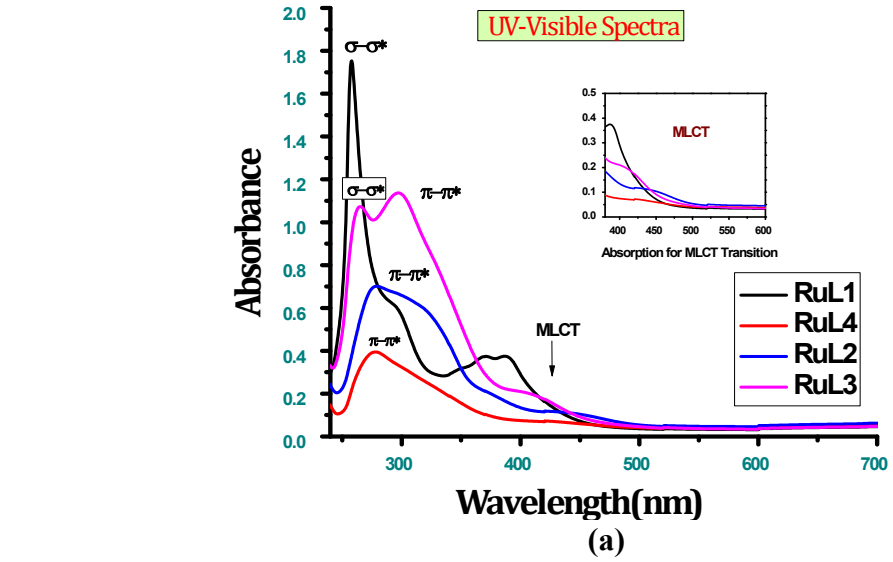
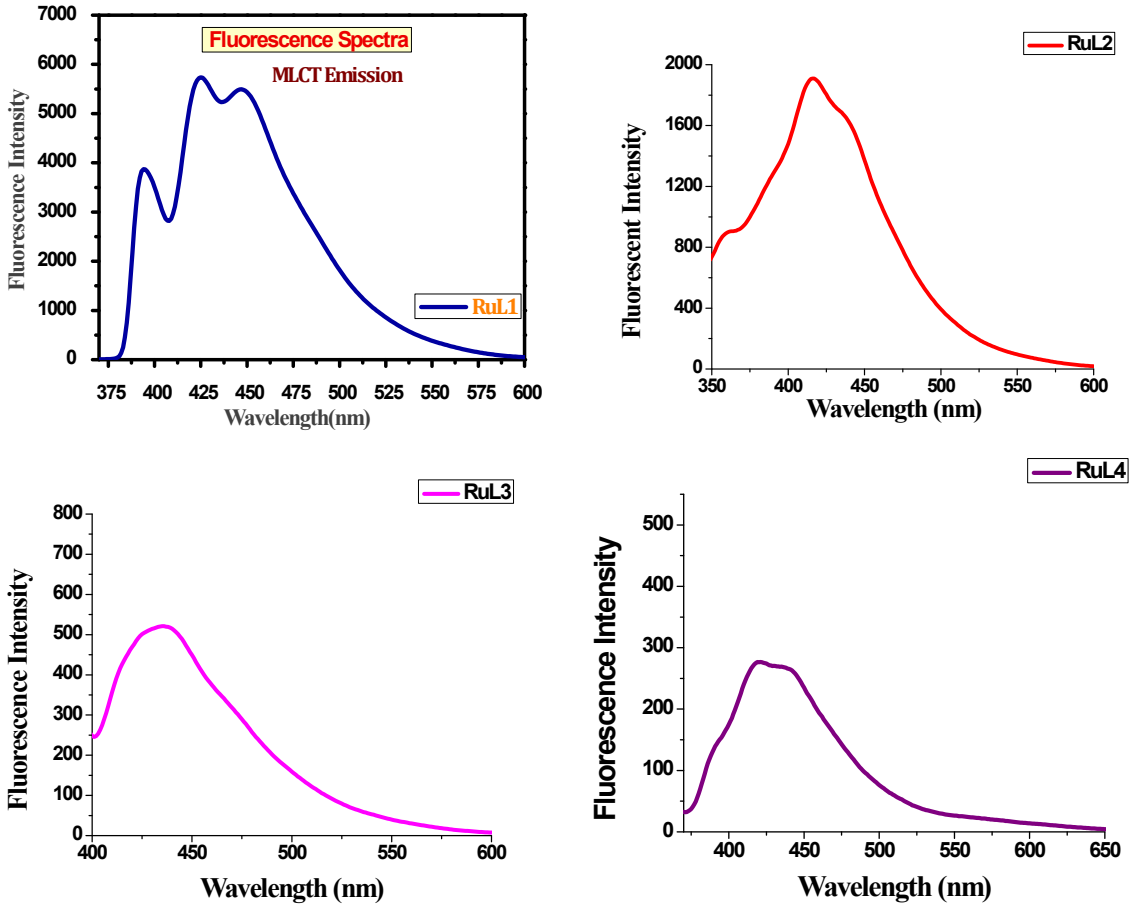


(a)



(b)

Fig. S1: (a) UV-Vis spectra (b) emission spectra of complexes RuL1–RuL4 in DMSO-water (1:1) solvent system at room temperature λex = 380 nm.

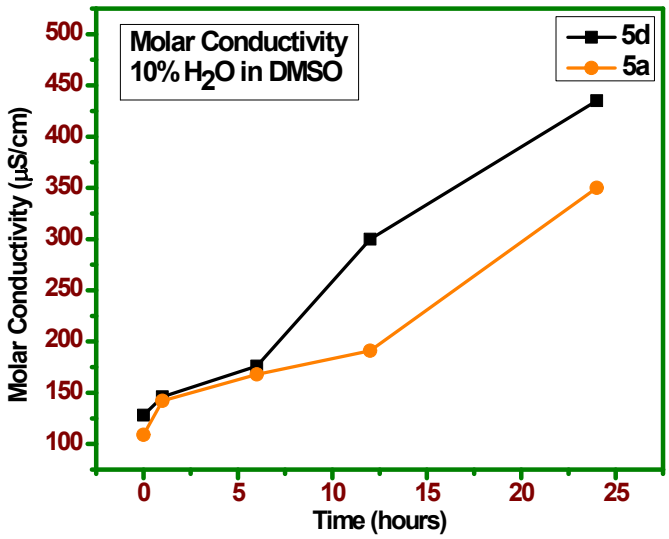


Fig. S2. Time dependent molar conductivity of compound RuL1 (black) and RuL4 (red) in 10% DMSO

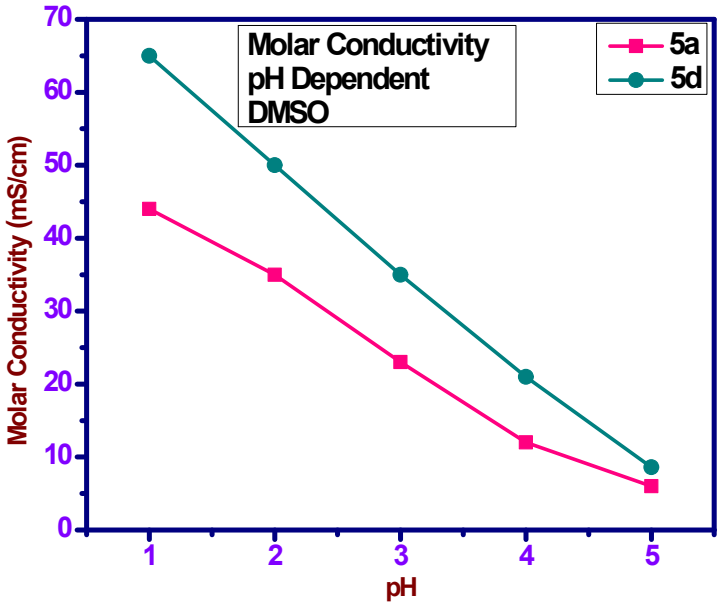


Fig. S3. PH dependent molar conductivity of compound RuL1 (Pink) and RuL4 (Green) in DMSO

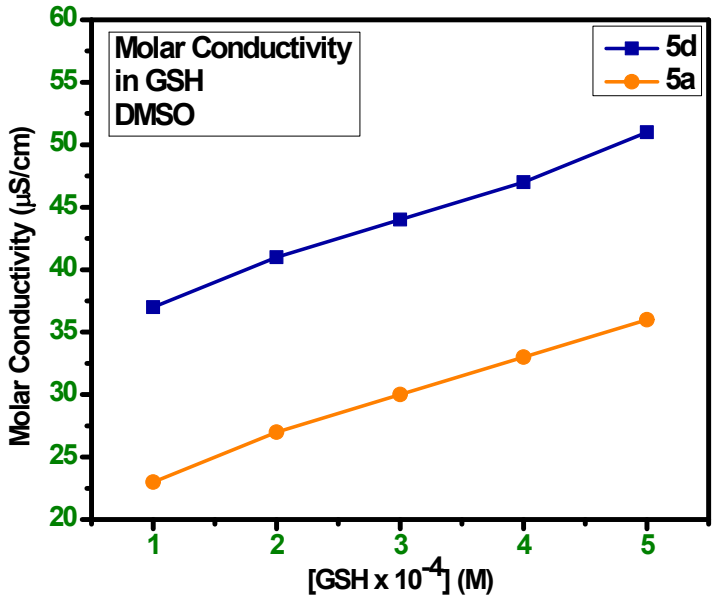


Fig. S4. GSH dependent molar conductivity of compound RuL1 (Orange)and RuL4 (blue) in DMSO

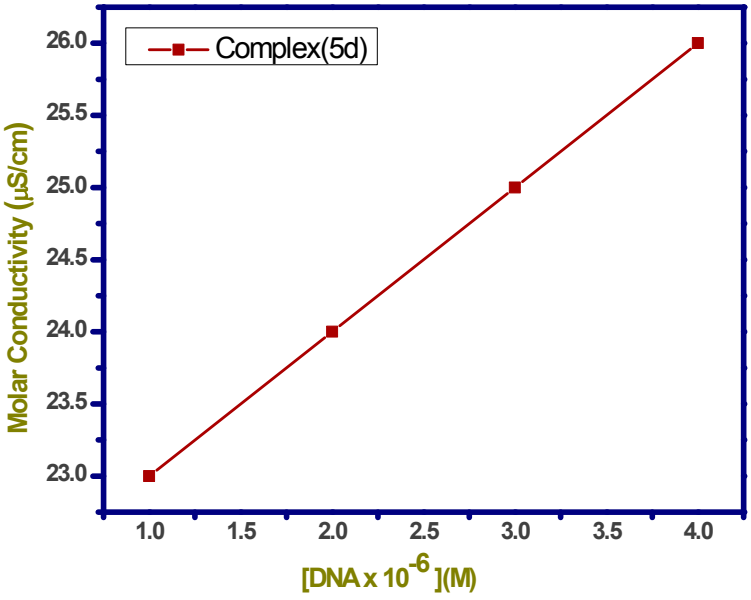
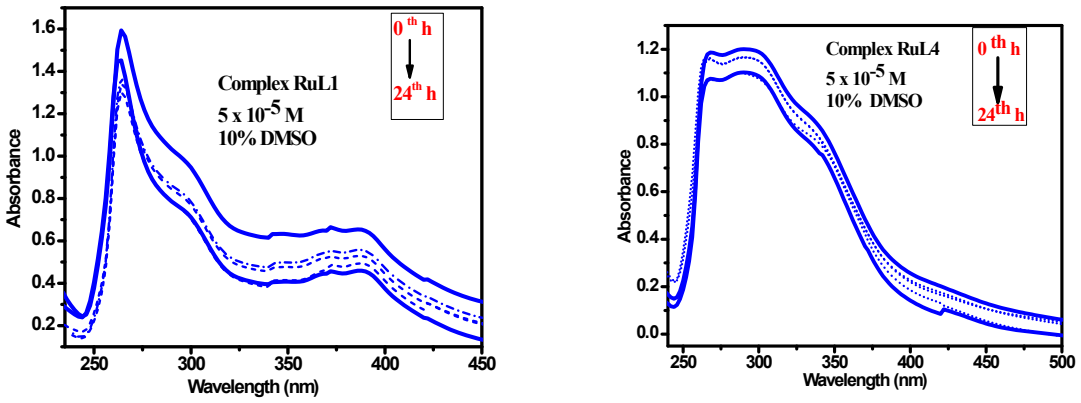
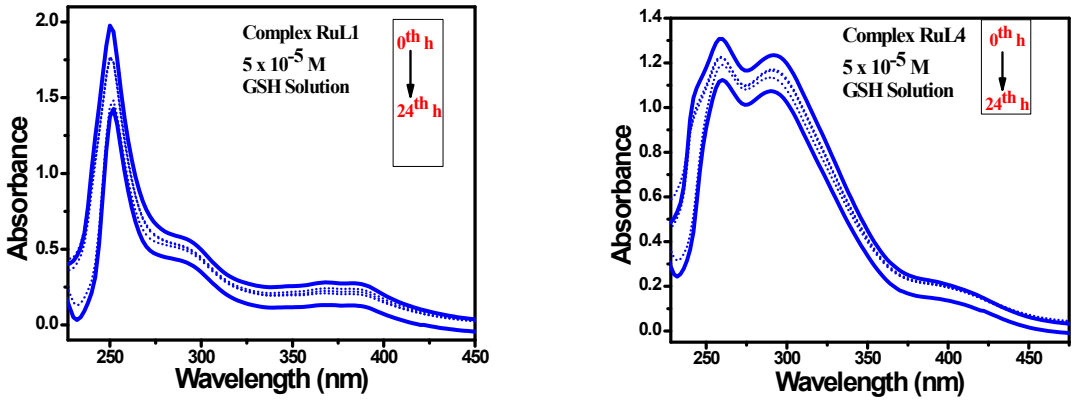


Fig. S5. Conductivity of compound RuL4 in DMSO w.r.t the increasing concentration of Ct-DNA



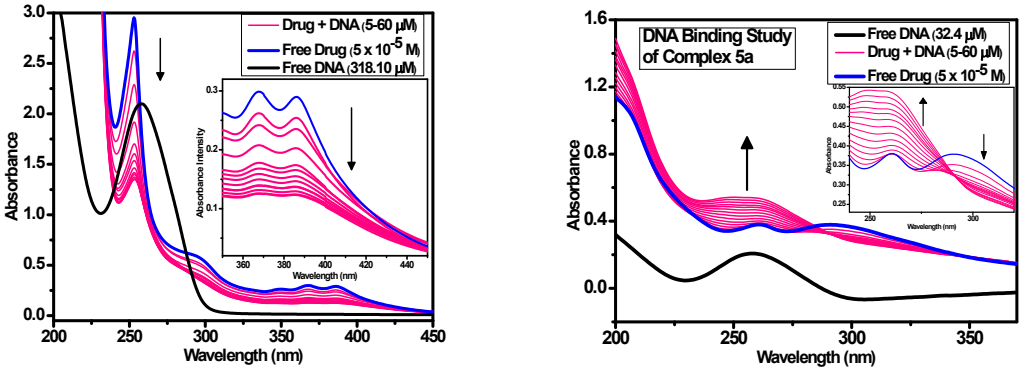
(a) (b)

Fig. S6: (a) Stability of RuL1 and (b) RuL4 in 10 % DMSO media



(a) (b)

Fig. S7: Stability of (a) RuL1 and (b) RuL4 in aqueous GSH media



(a) (b)

Fig. S8: DNA binding plots of (a) complex RuL1 and (b) complex RuL4

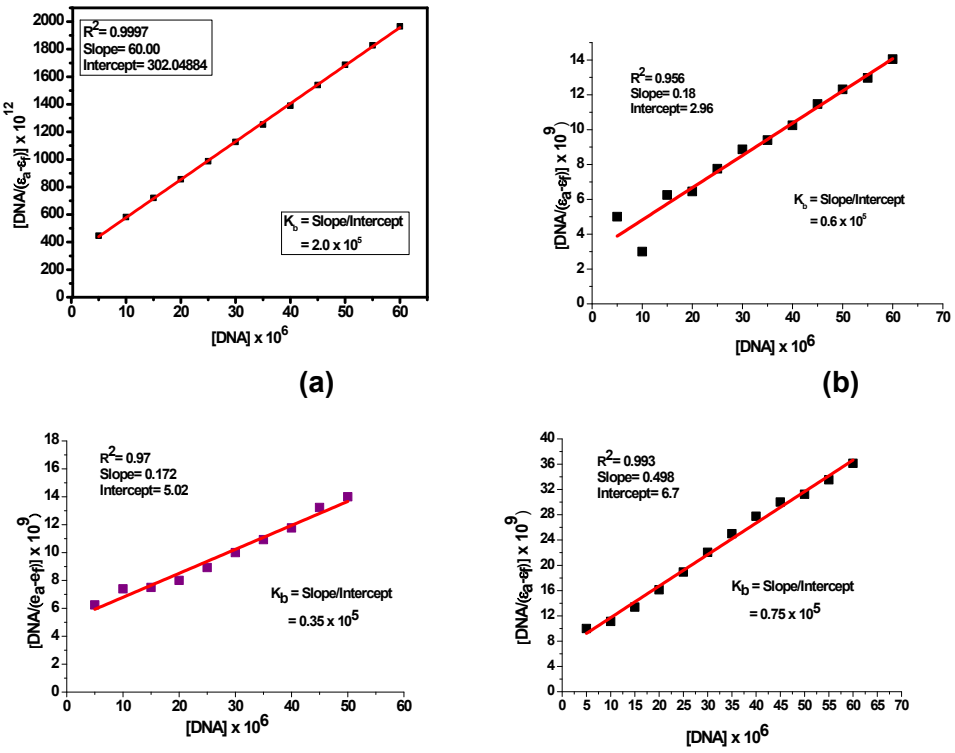


Fig. S9: [DNA]/(ε_a-ε_f) vs. [DNA] linear plots of complex RuL1 at (a) λ_{max} = 250 nm (b) λ_{max} = 300 nm (c) λ_{max} = 380 nm and complex RuL4 at (d) λ_{max} = 300 nm

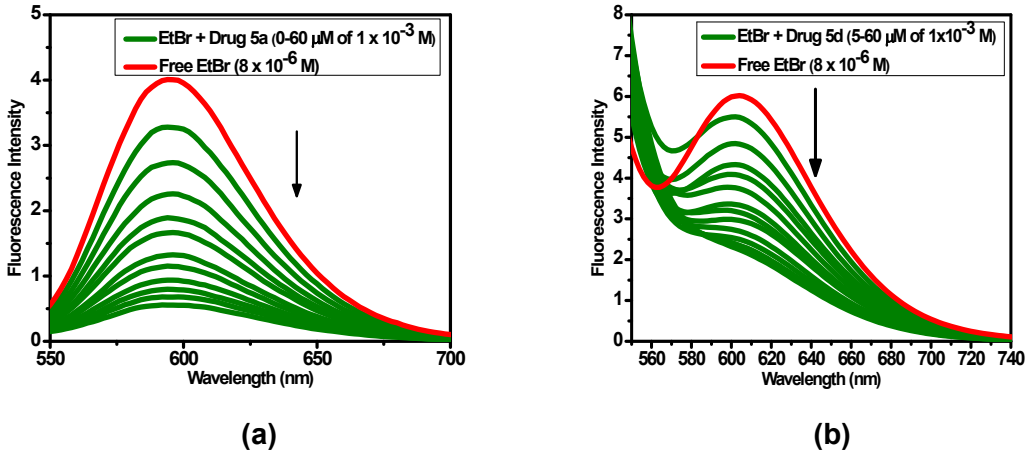


Fig. S10: EtBr quenching plots of complex (a) RuL1 and (b) RuL4

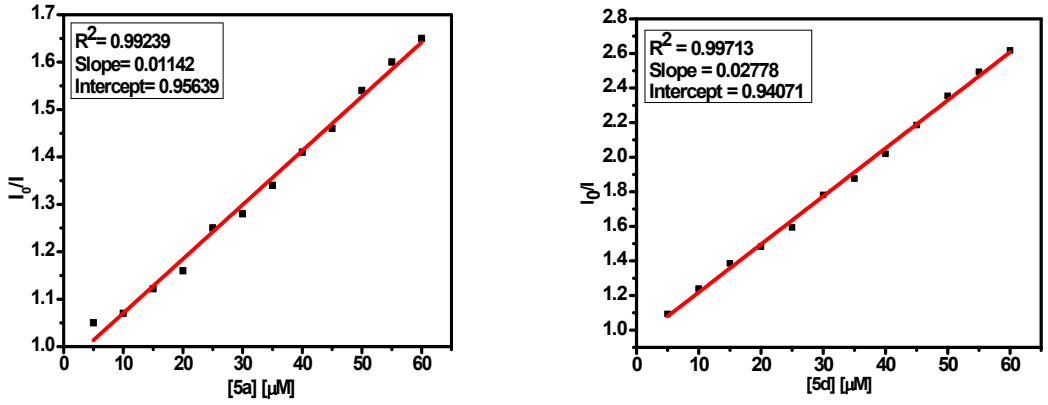


Fig. S11: Stern-Volmer plots of I_0/Ivs. complexes (a) RuL1 and (b) RuL4

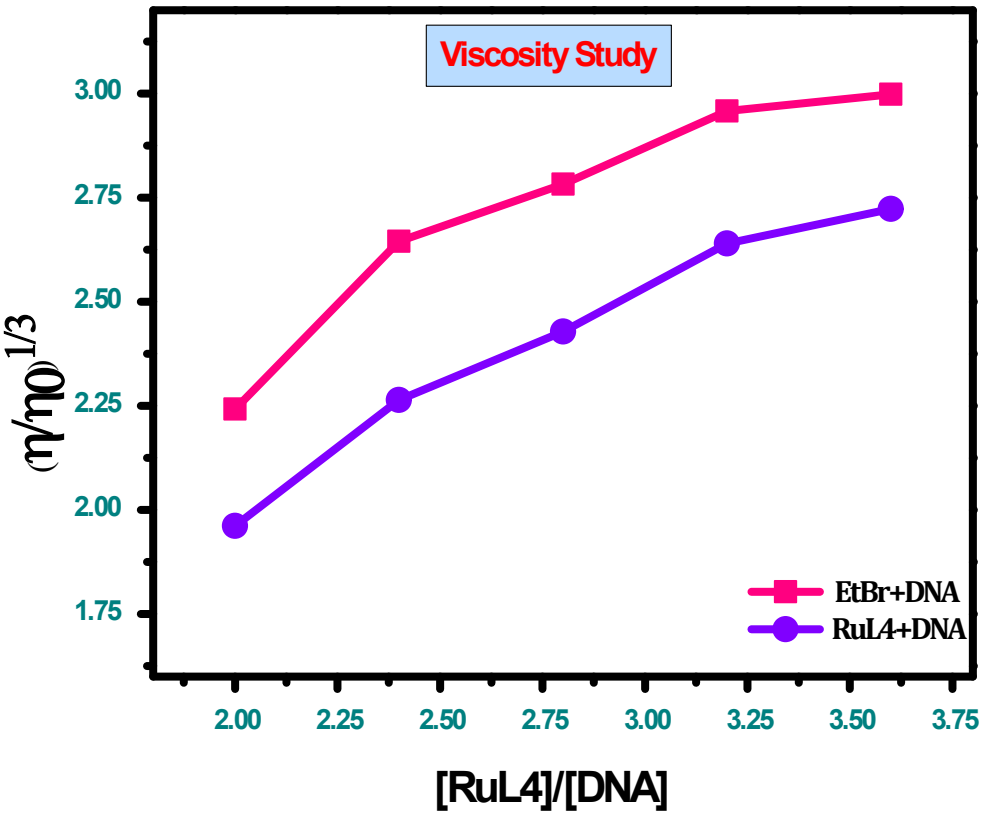
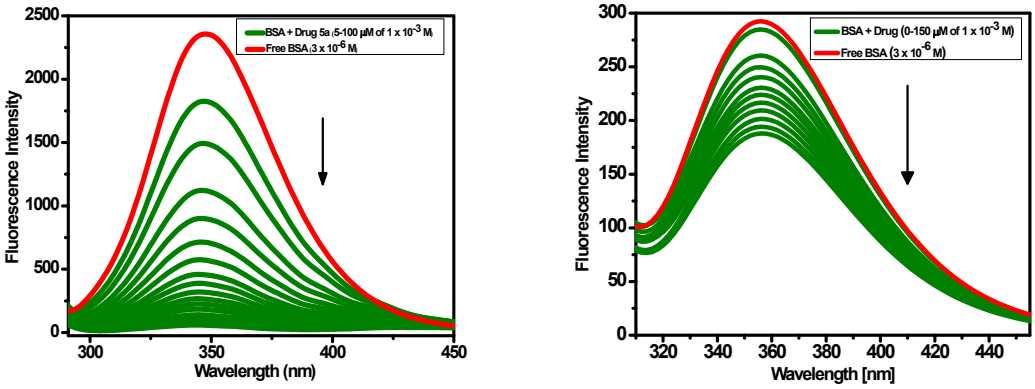
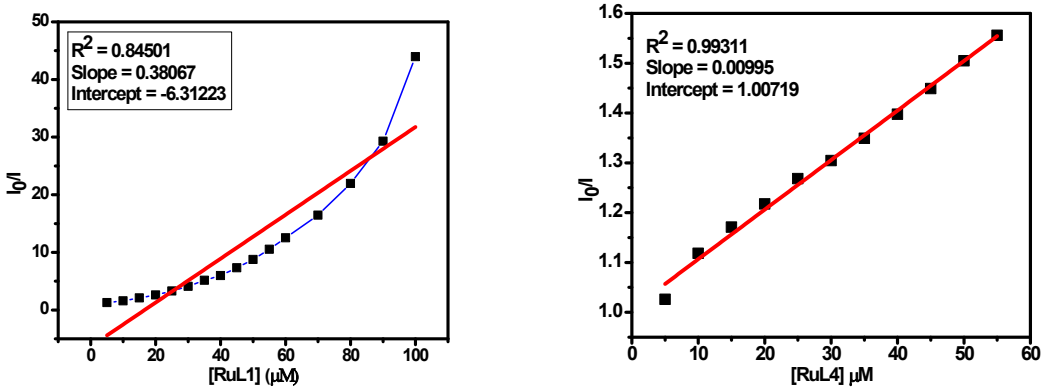


Fig. S12: Viscosity plot of complexes RuL4 and EtBr with Ct-DNA



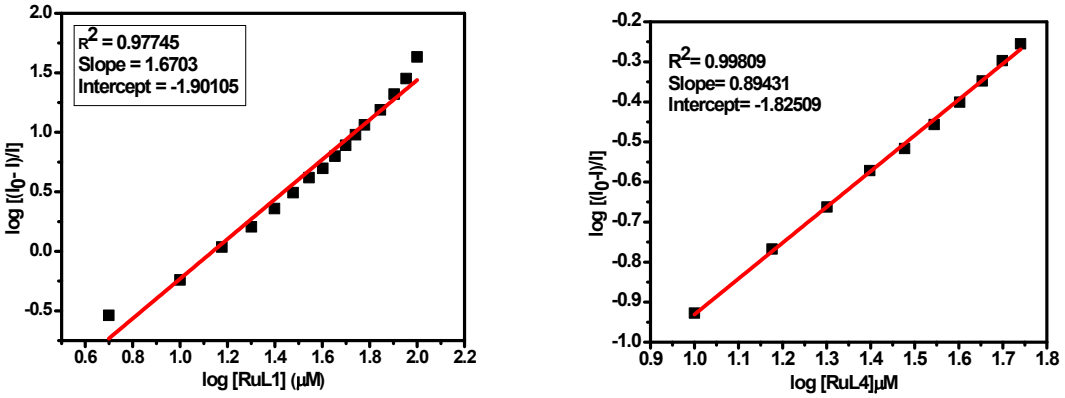
(a) (b)

Fig. S13: Interaction of complexes (a) RuL1 and (b) RuL4 with BSA



(a) (b)

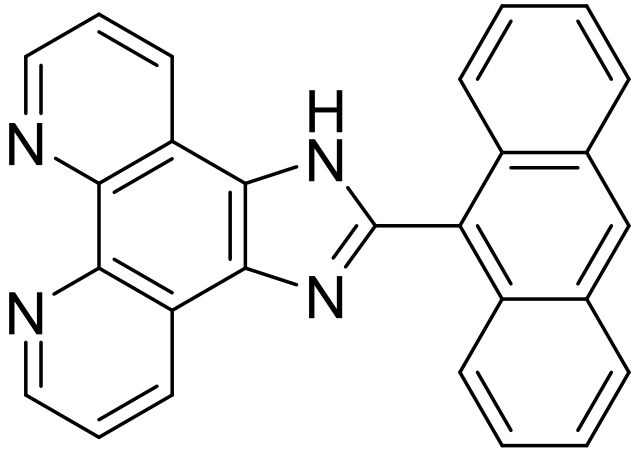
Fig. S14: Stern-Volmer plot of I_0/I vs. concentration of (a) complex RuL1 and (b) Complex RuL4



(a) (b)

Fig. S15: Scatchard plot of log($[I_0-I]/I$) vs. log[Complex] for BSA in the presence of (a) Complex RuL1 and (b) Complex RuL4

Characterization of the ligands



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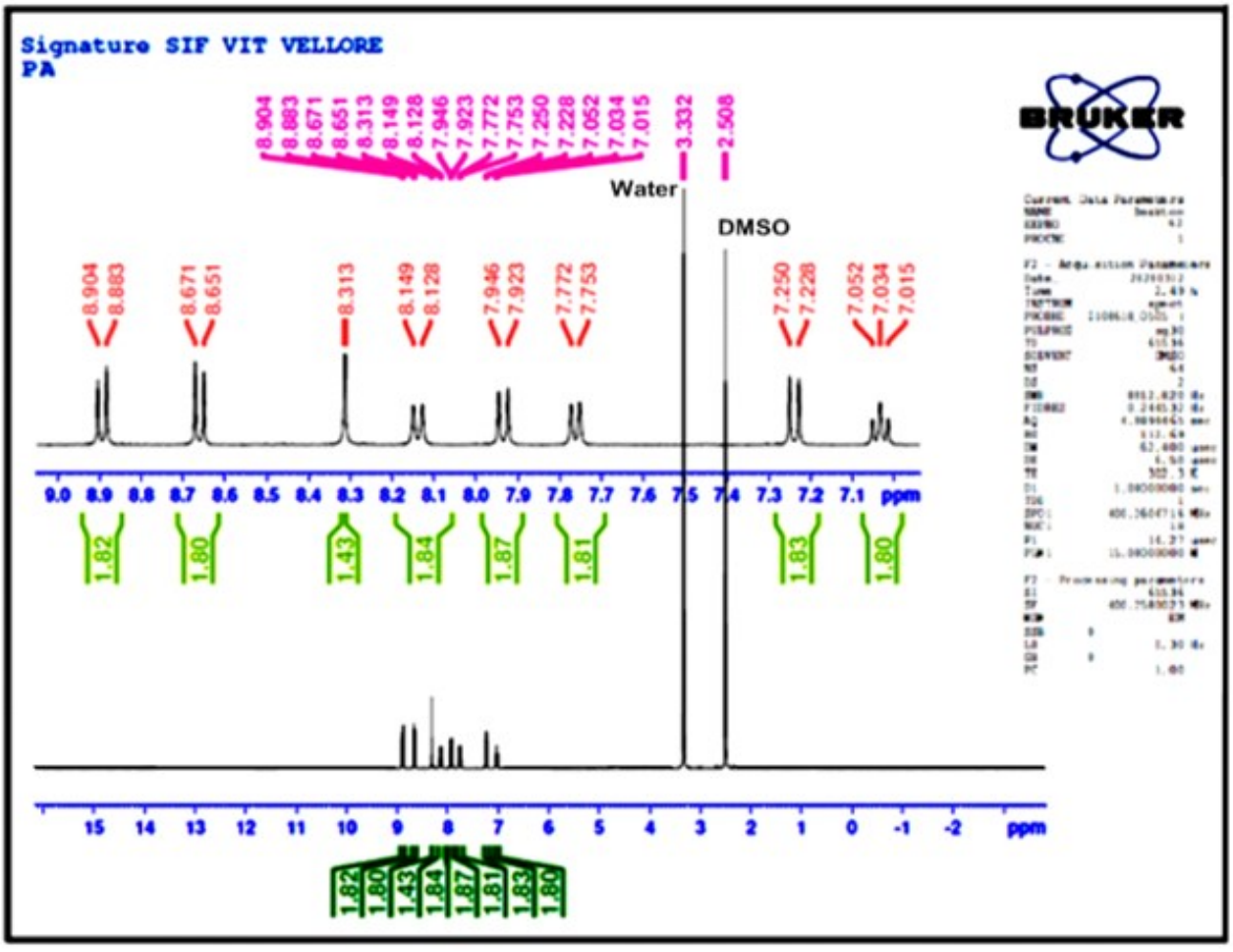

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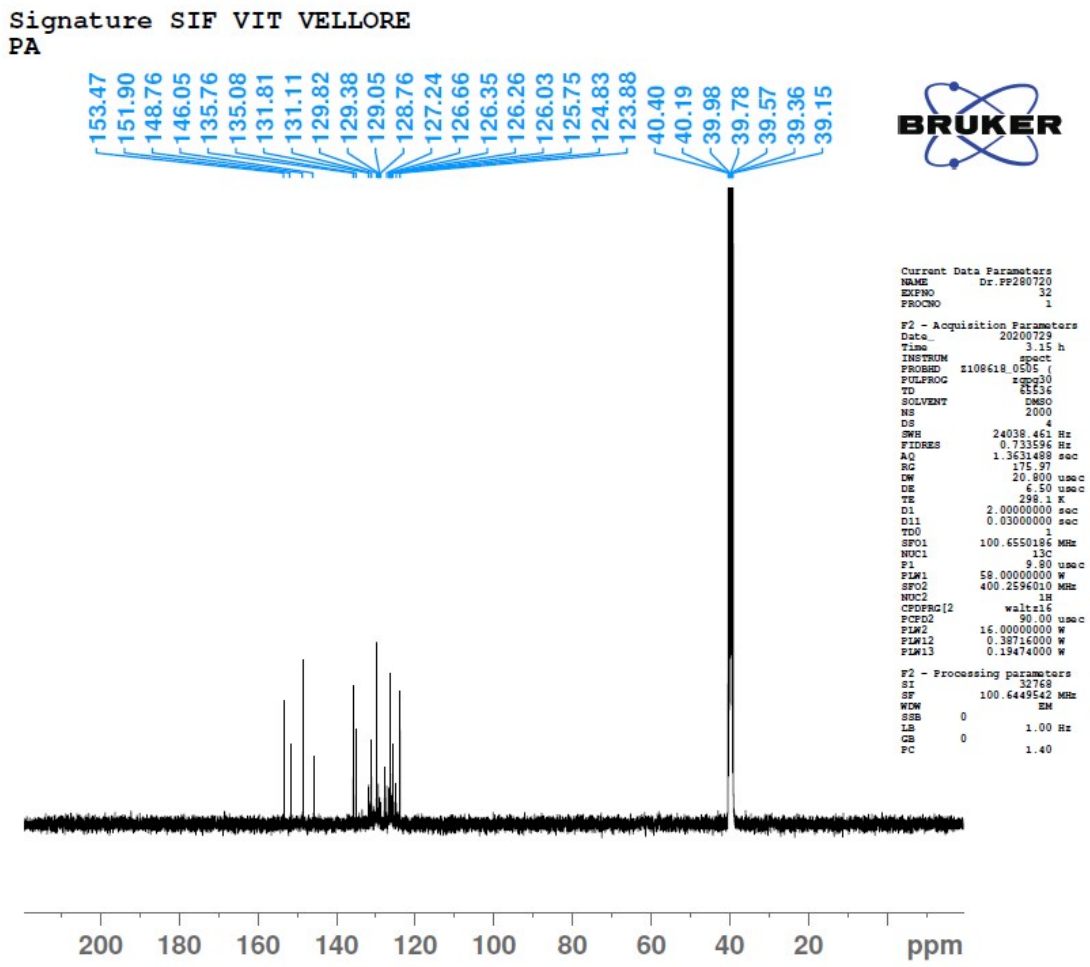
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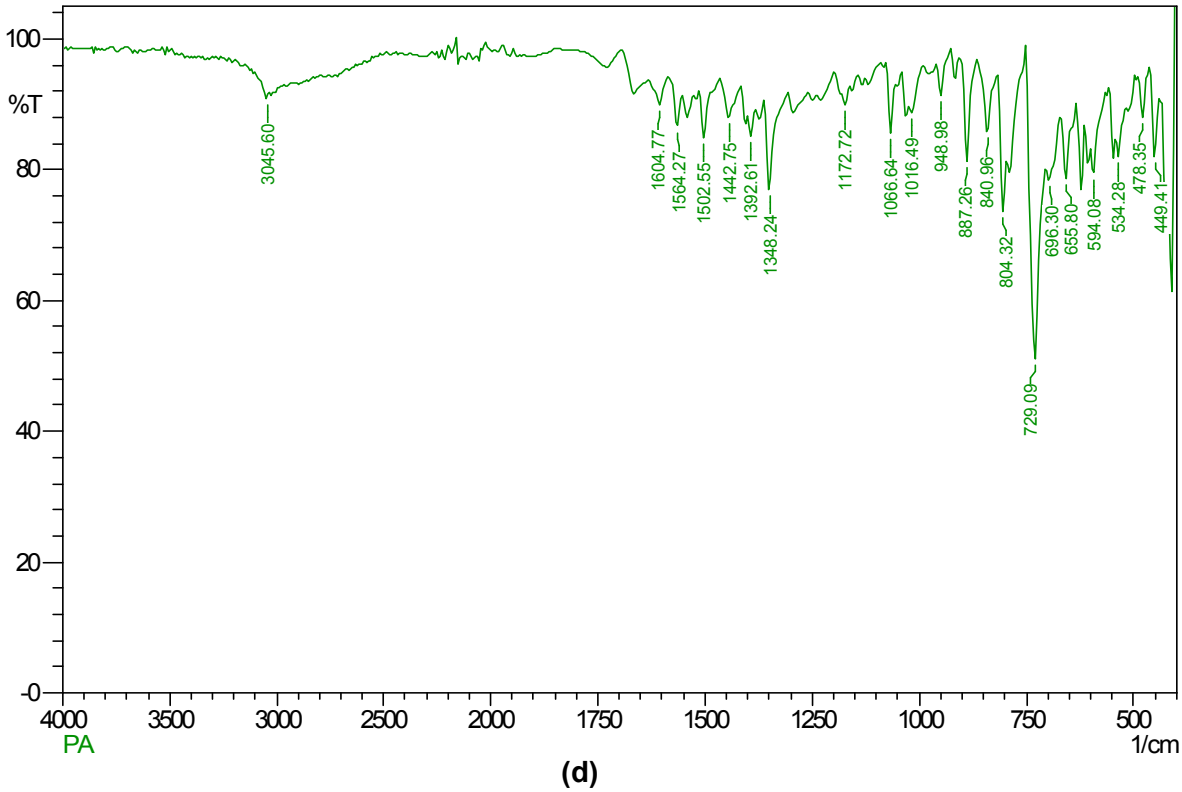
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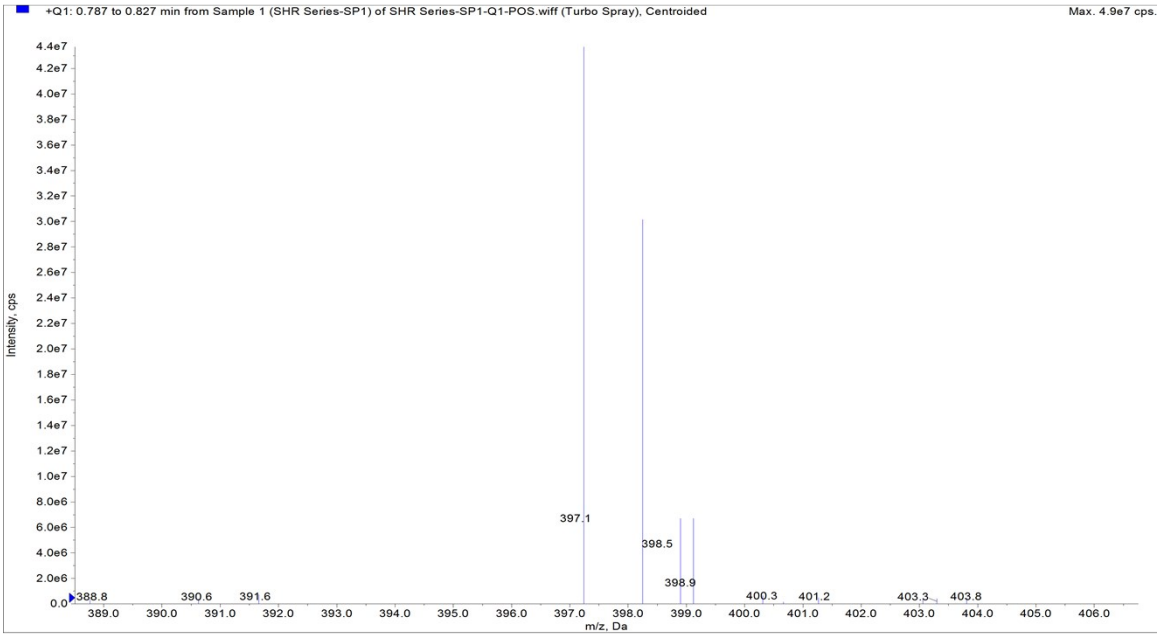
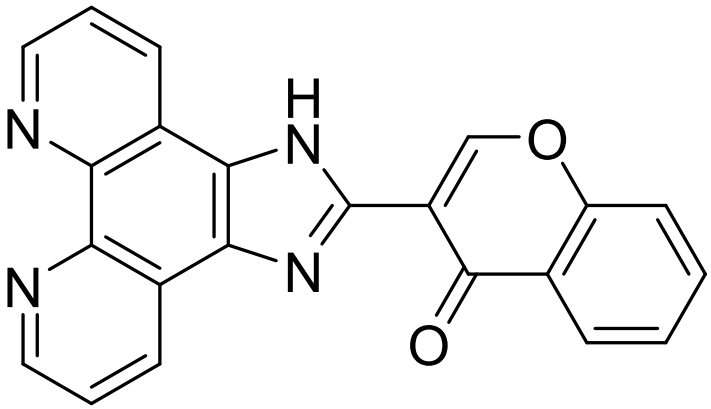


(e)

Fig. S16: Ligand L1 (a) Chemical structure (b) ^{1}H NMR (c) ^{13}C NMR (d) IR spectra, and (e) ESI-MS



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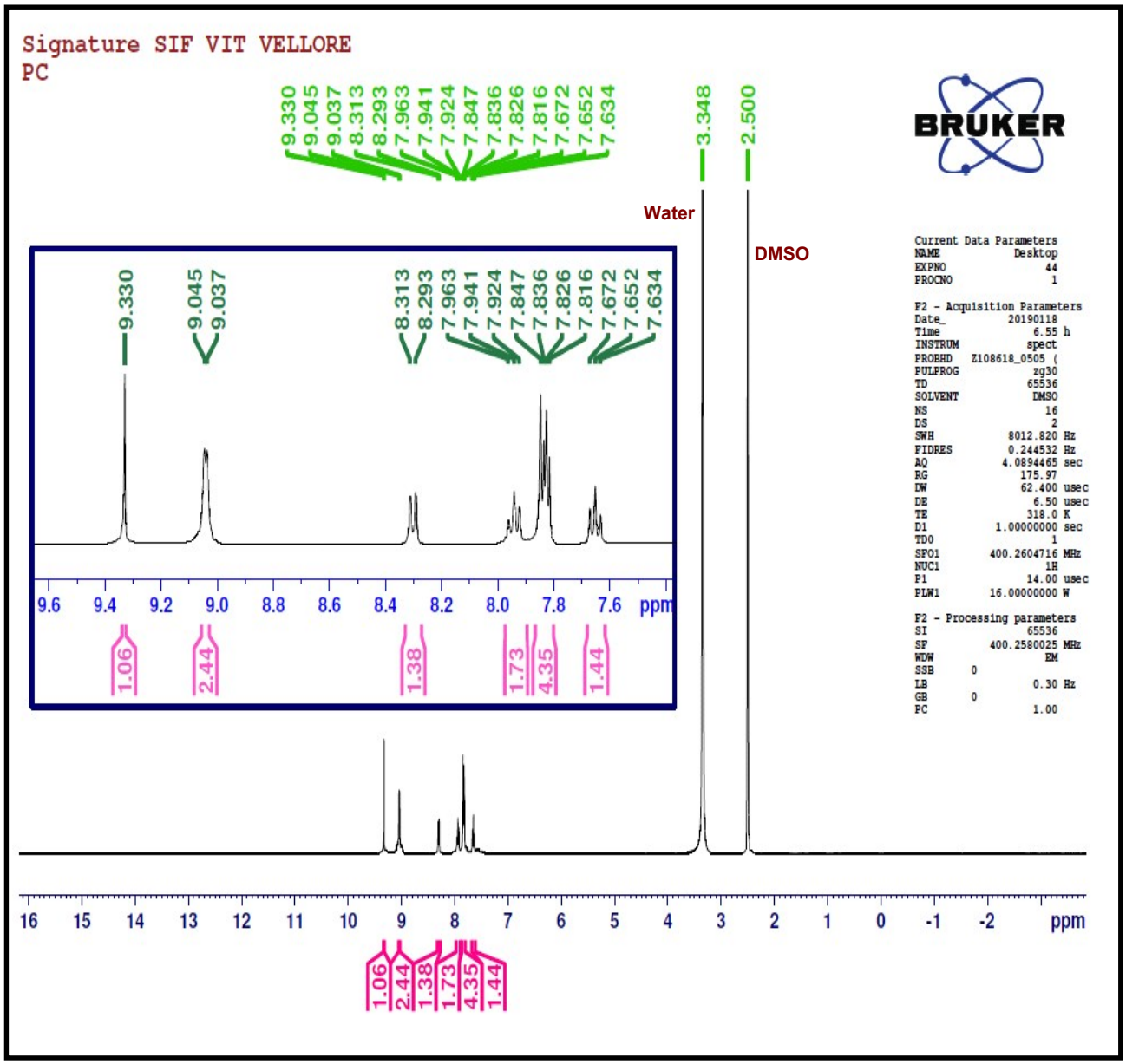
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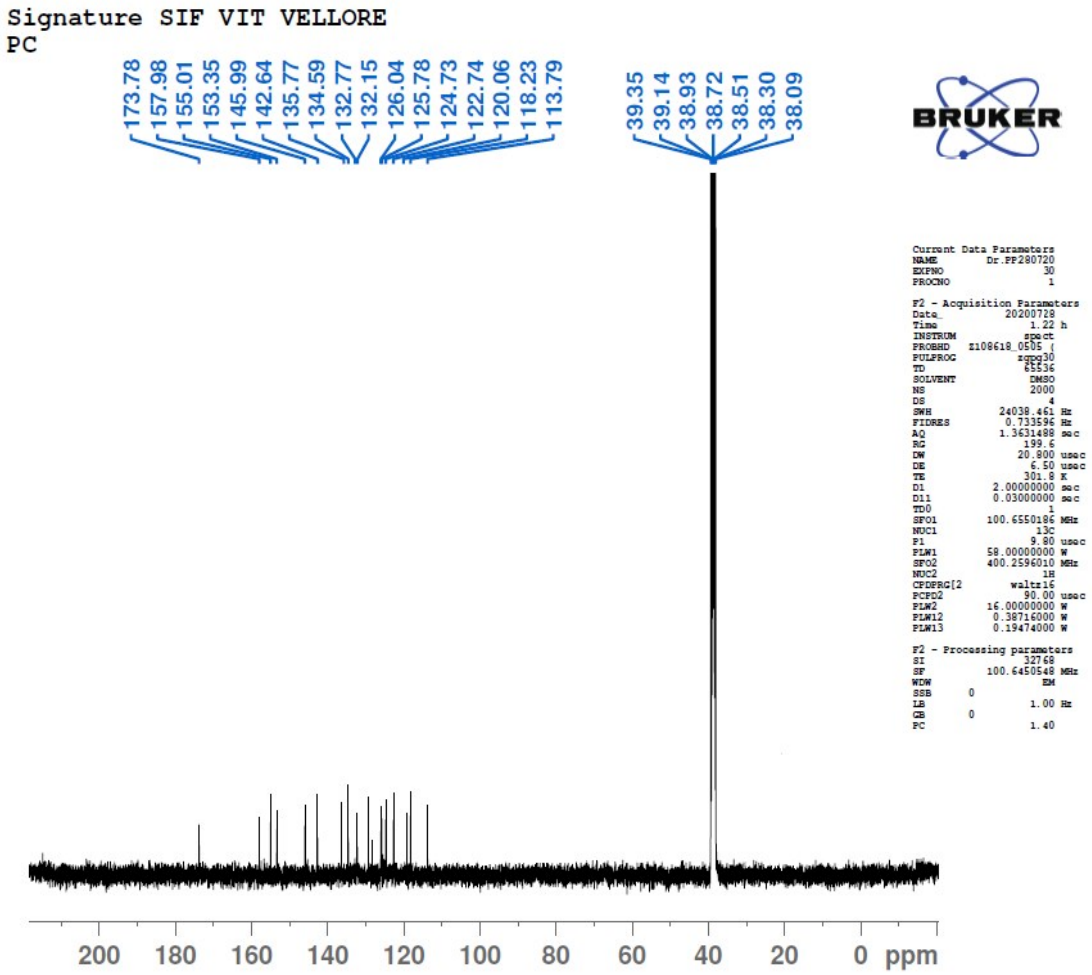
(b)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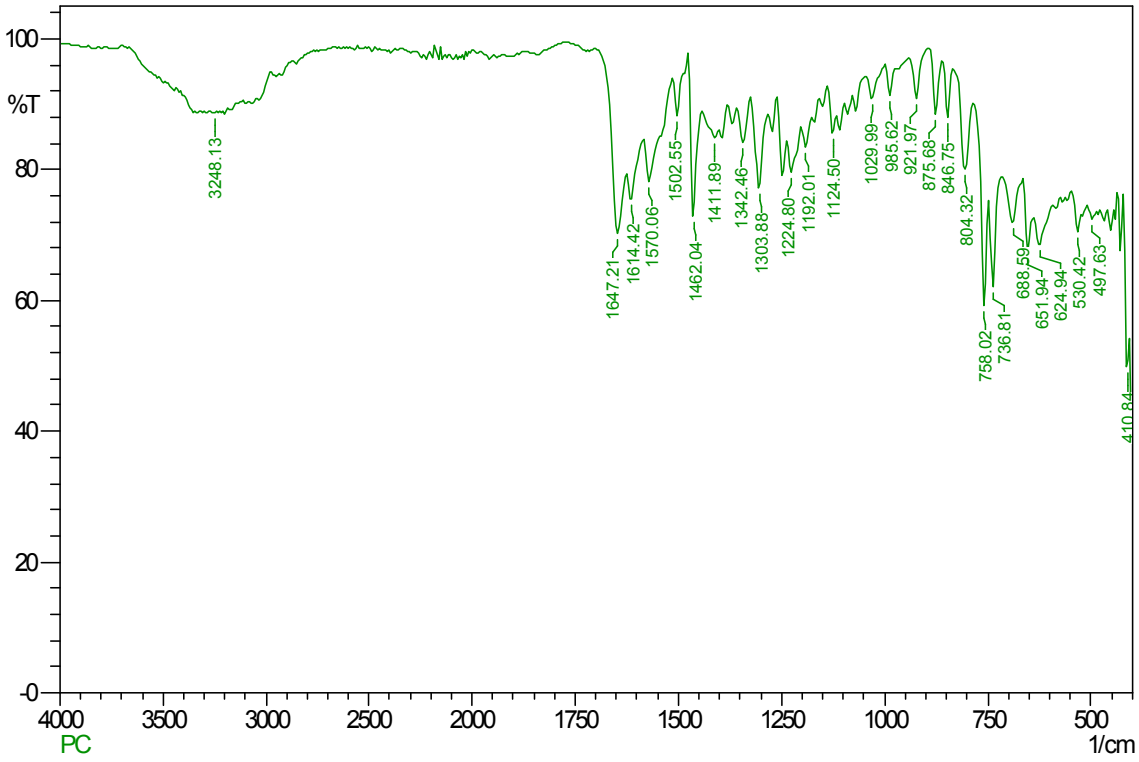
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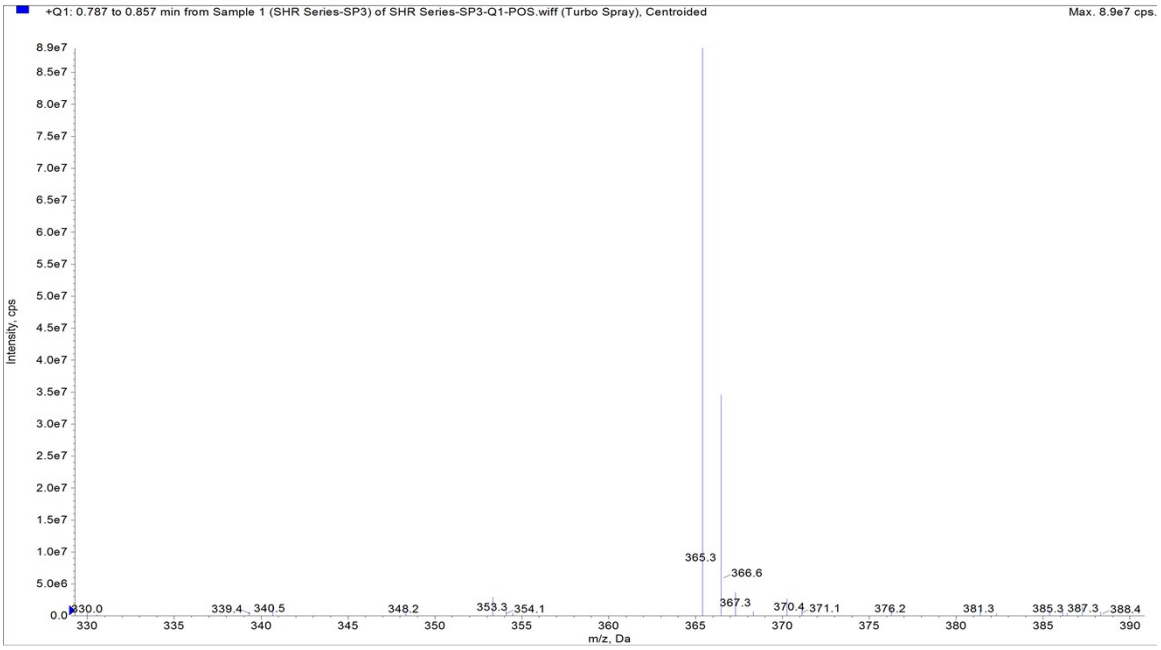
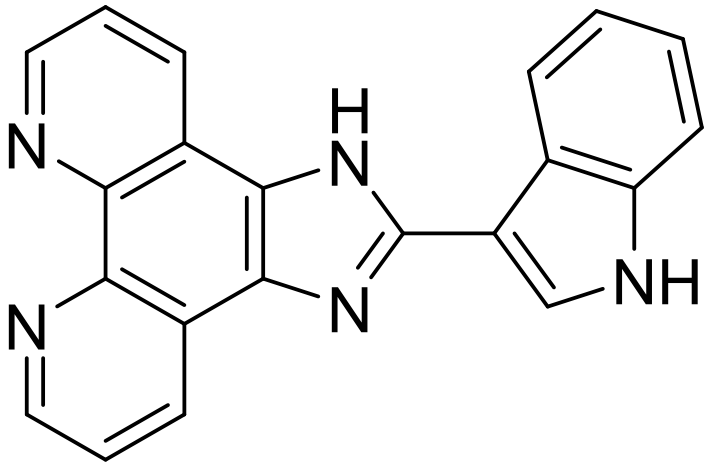


(e)

Fig. S17: Ligand L2 (a) Chemical structure (b) ^{1}H NMR (c) ^{13}C NMR (d) IR spectra, and (e) ESI-MS



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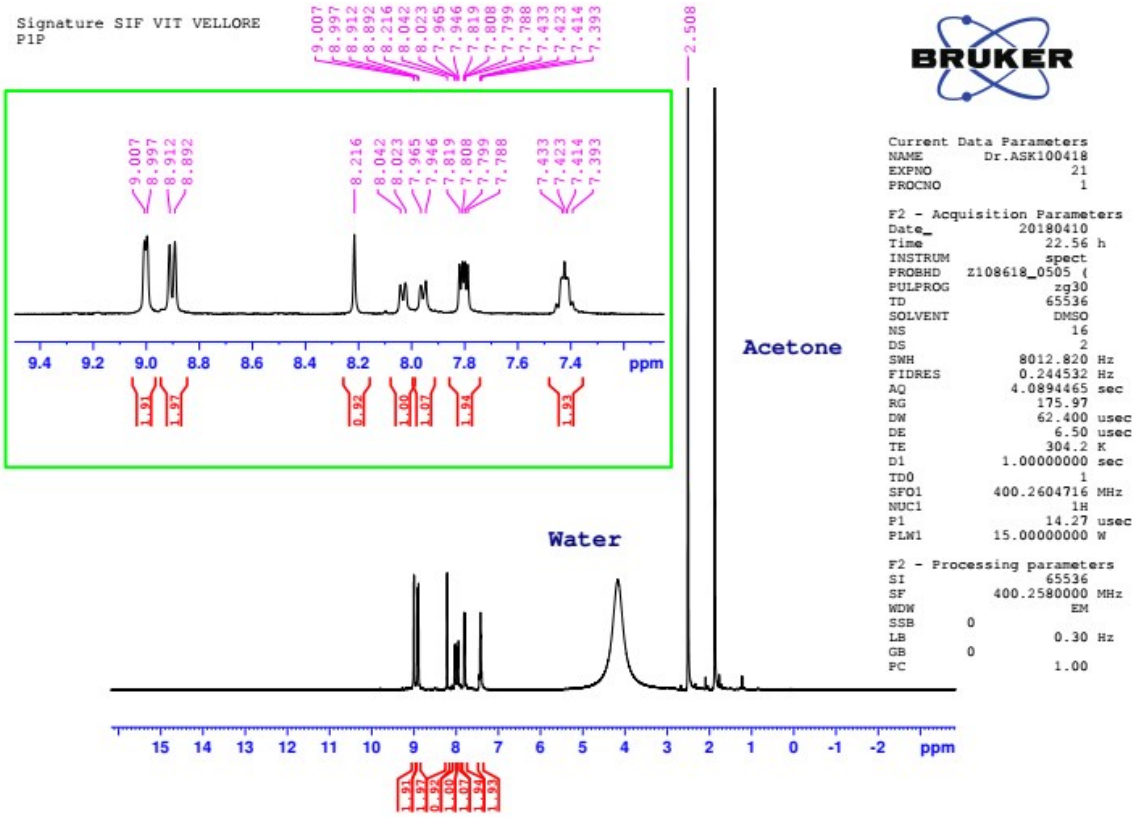
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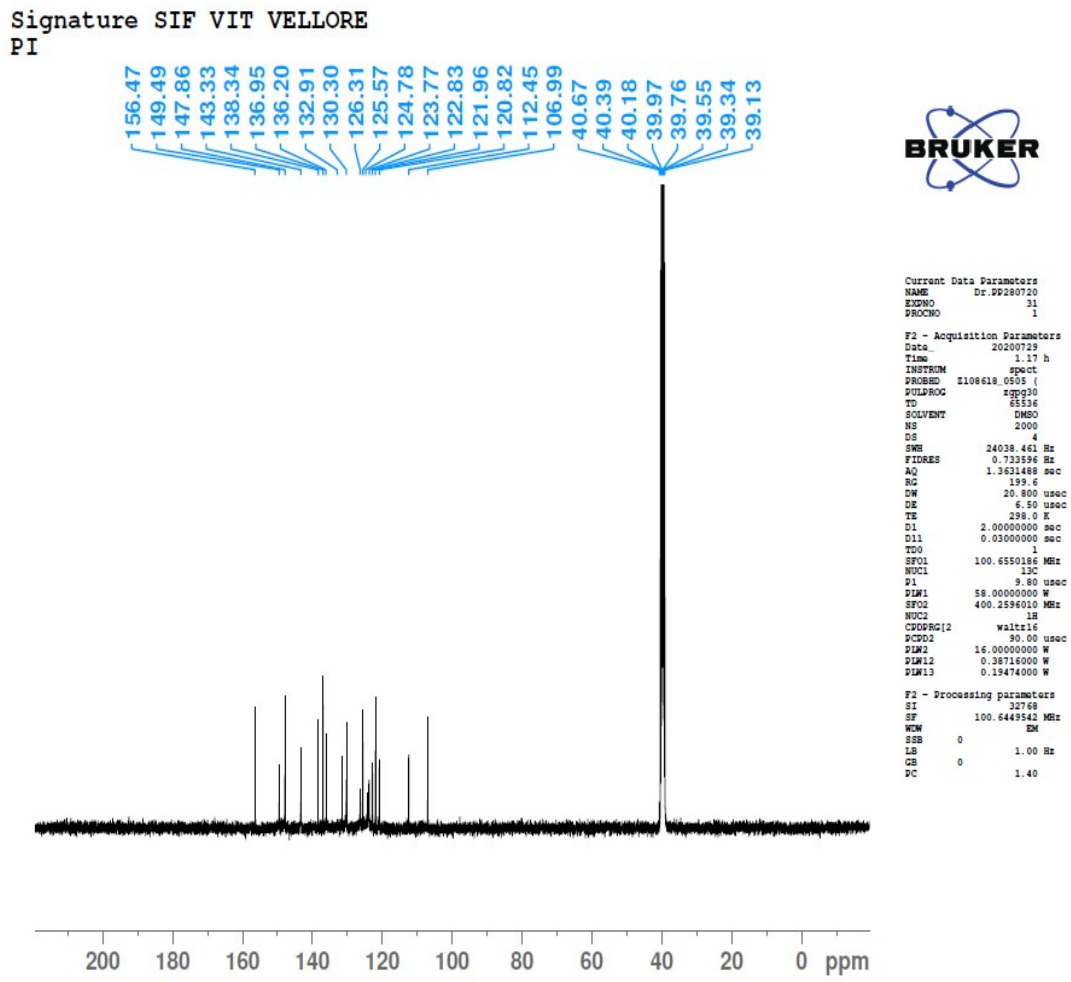
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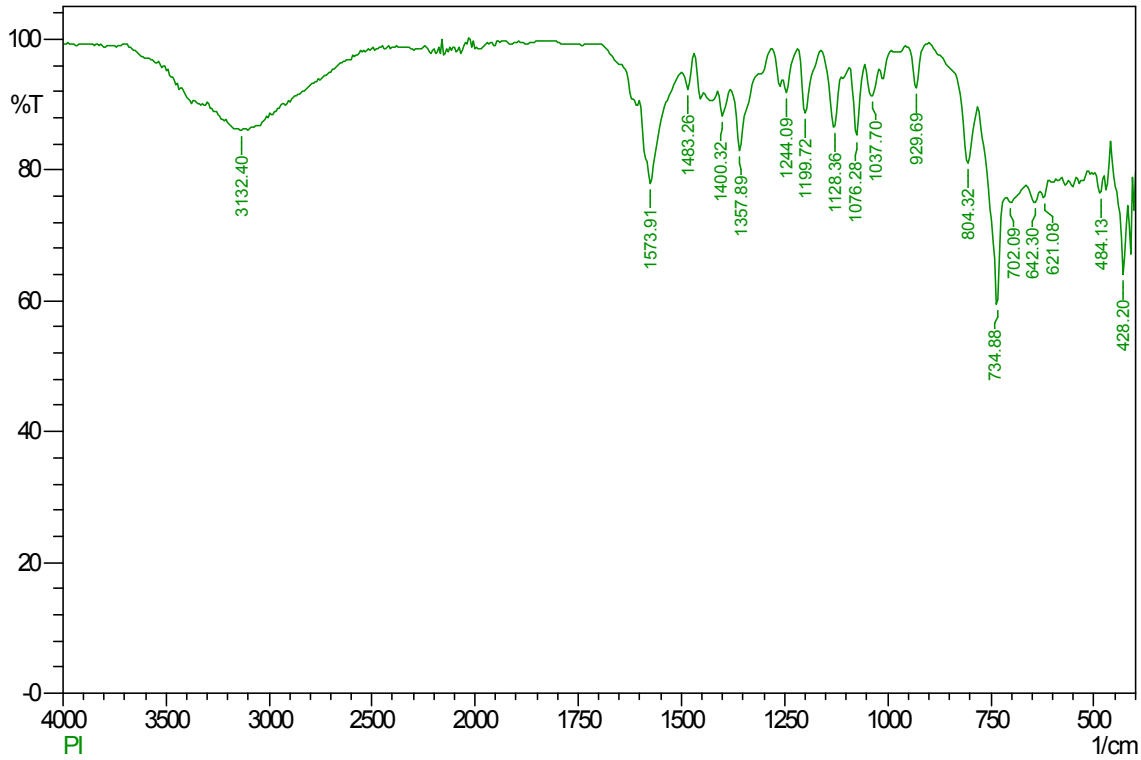
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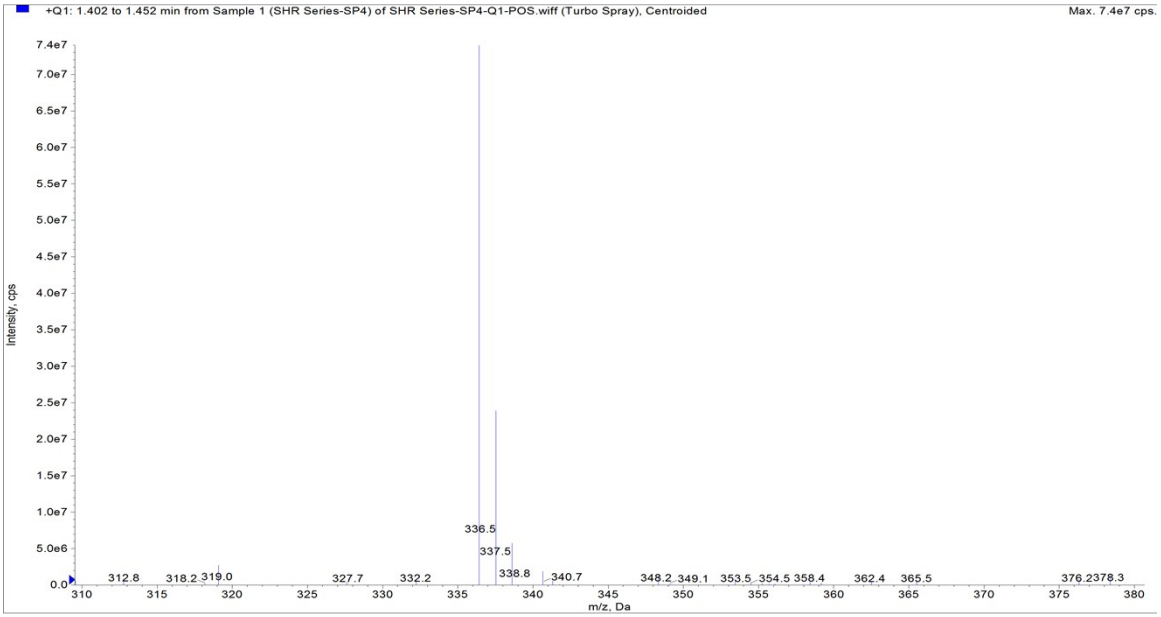
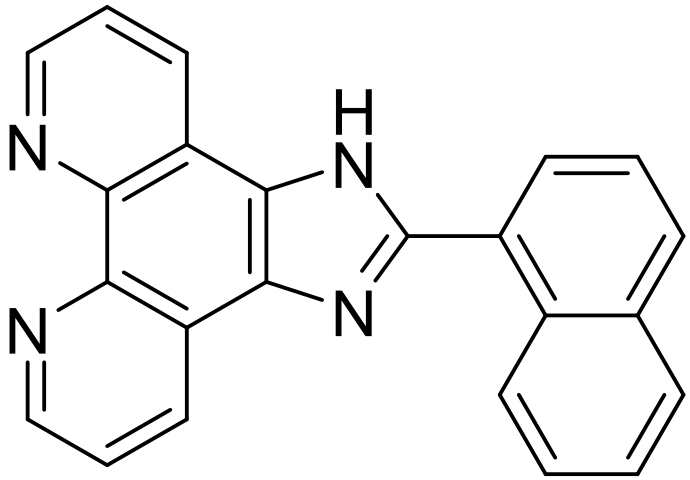


(e)

Fig. S18: Ligand L3 (a) Chemical structure (b) ^{1}H NMR (c) ^{13}C NMR (d) IR spectra, and (e) ESI-MS



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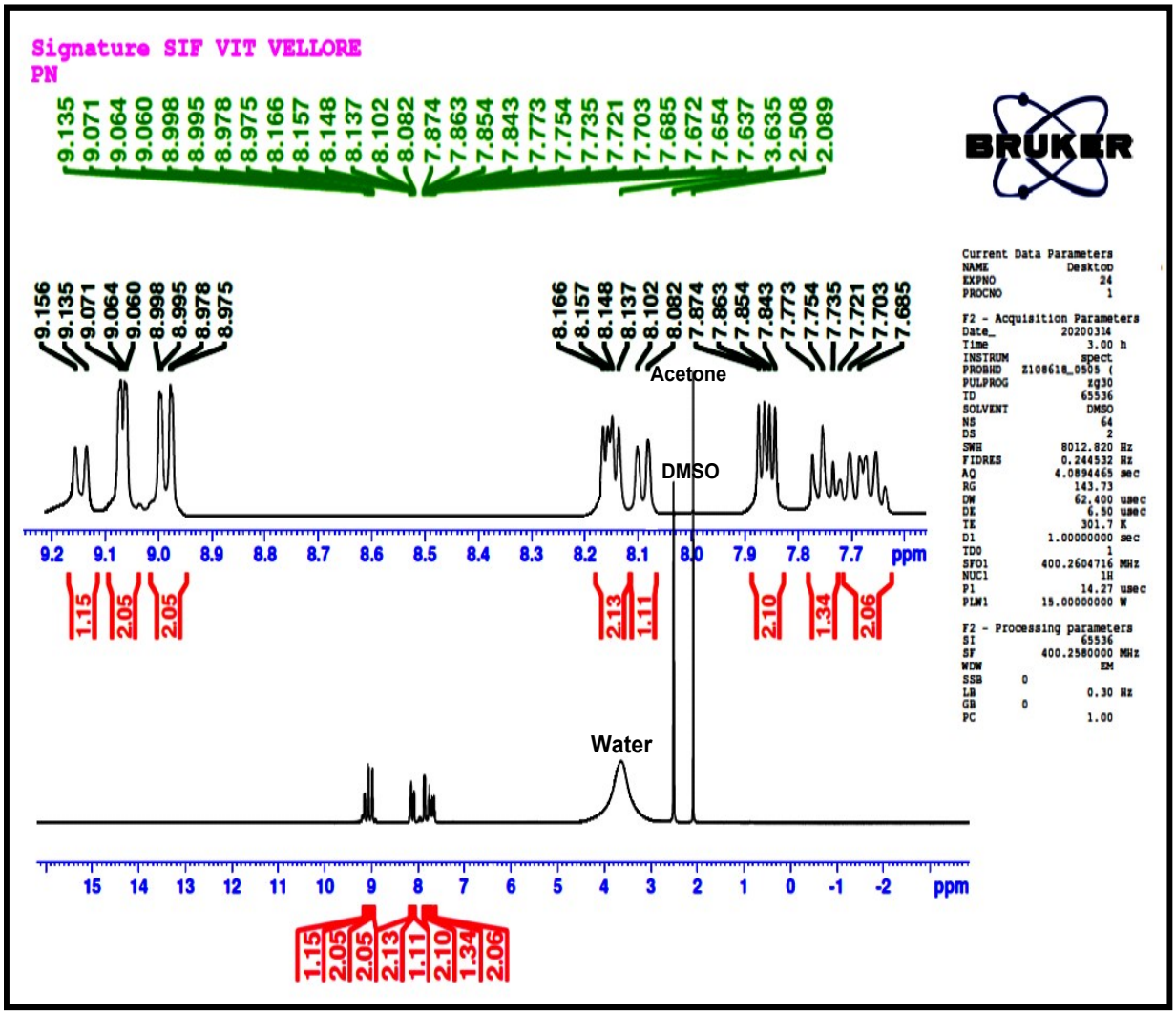
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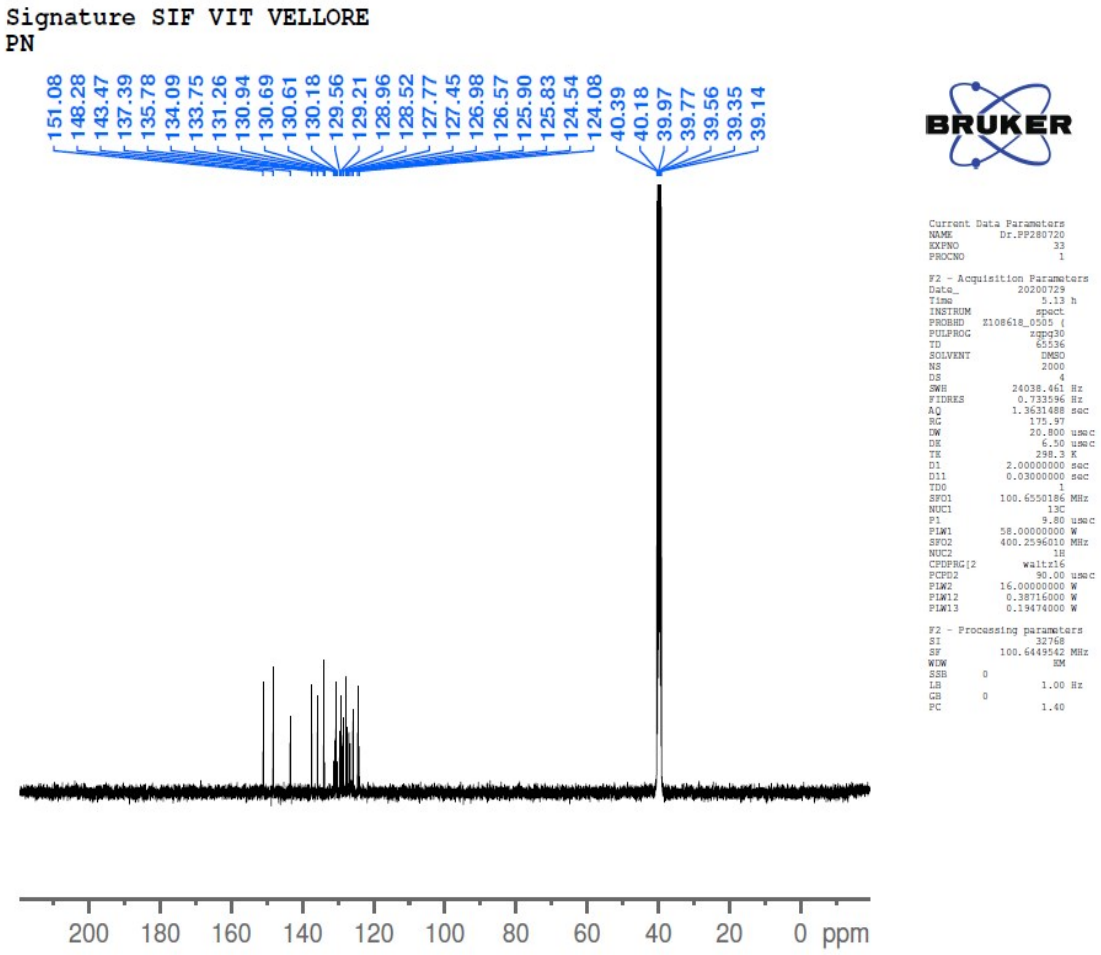
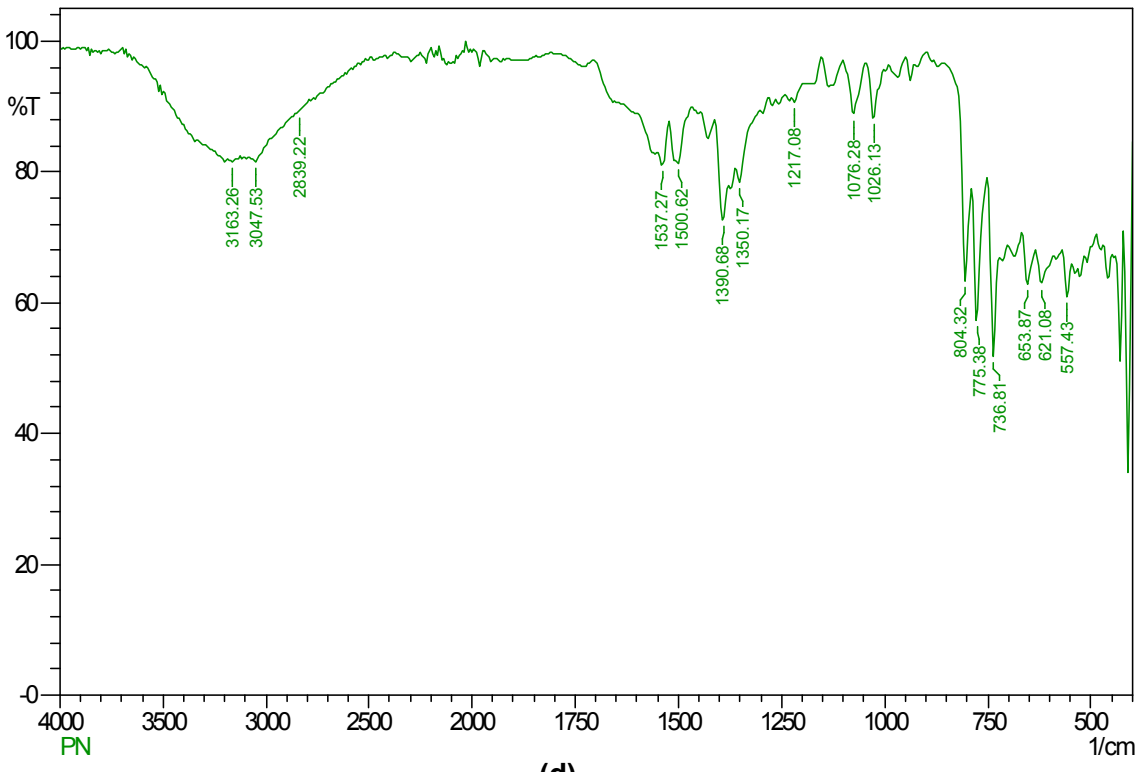
9.135 9.071 9.064 9.060 8.998 8.995 8.978 8.975 8.166 8.157 8.148 8.137 8.102 8.082 7.874 7.863 7.854 7.843 7.773 7.754 7.735 7.721 7.703 7.685 7.672 7.654 7.637 3.635 2.508 2.089
BRUKER
9.156 9.135 9.071 9.064 9.060 8.998 8.995 8.978 8.975
8.166 8.157 8.148 8.137 8.102 8.082 7.874 7.863 7.854 7.843 7.773 7.754 7.735 7.721 7.703 7.685
Acetone
DMSO
Water
9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 ppm
1.15 2.05 2.05 2.13 1.11 2.10 1.34 2.06
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.15 2.05 2.05 2.13 1.11 2.10 1.34 2.06
Current Data Parameters
NAME Desktop
EXPNO 24
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200314
Time 3.00 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 301.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.00000000 W
F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

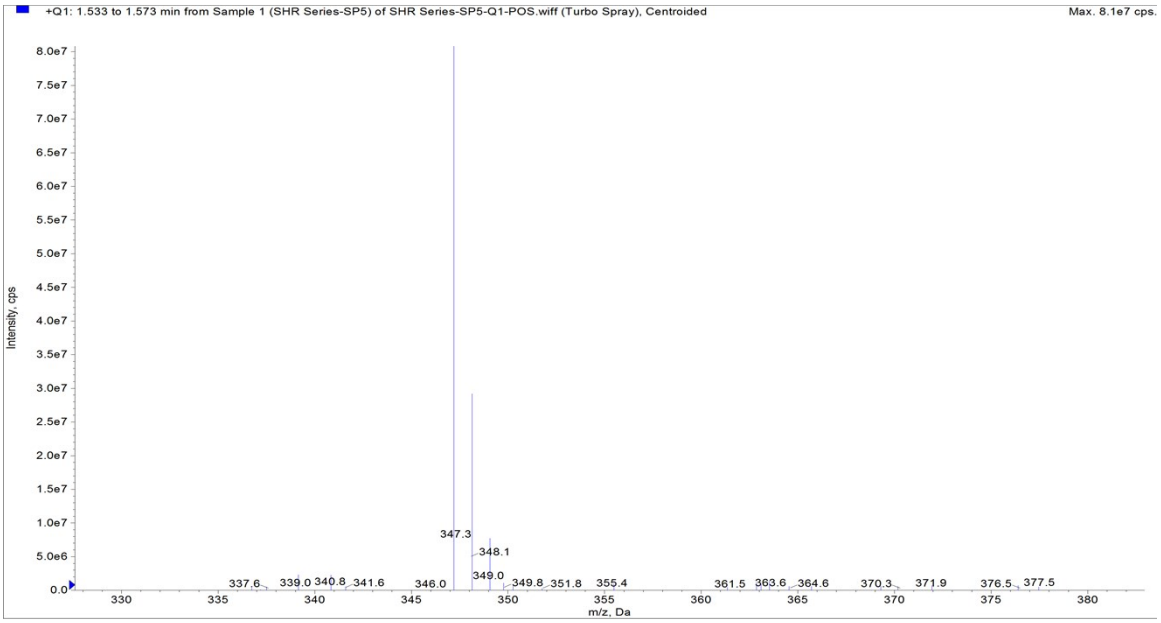
(b)


Signature SIF VIT VELLORE
PN
151.08
148.28
143.47
137.39
135.78
134.09
133.75
131.26
130.94
130.69
130.61
130.18
129.56
129.21
128.96
128.52
127.77
127.45
126.98
126.57
125.90
125.83
124.54
124.08
40.39
40.18
39.97
39.77
39.56
39.35
39.14
BRUKER
Current Data Parameters
NAME Dr.PP280720
EXPNO 33
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200729
Time 5.13 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.38716000 W
PLW13 0.19474000 W
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0 ppm

(C)

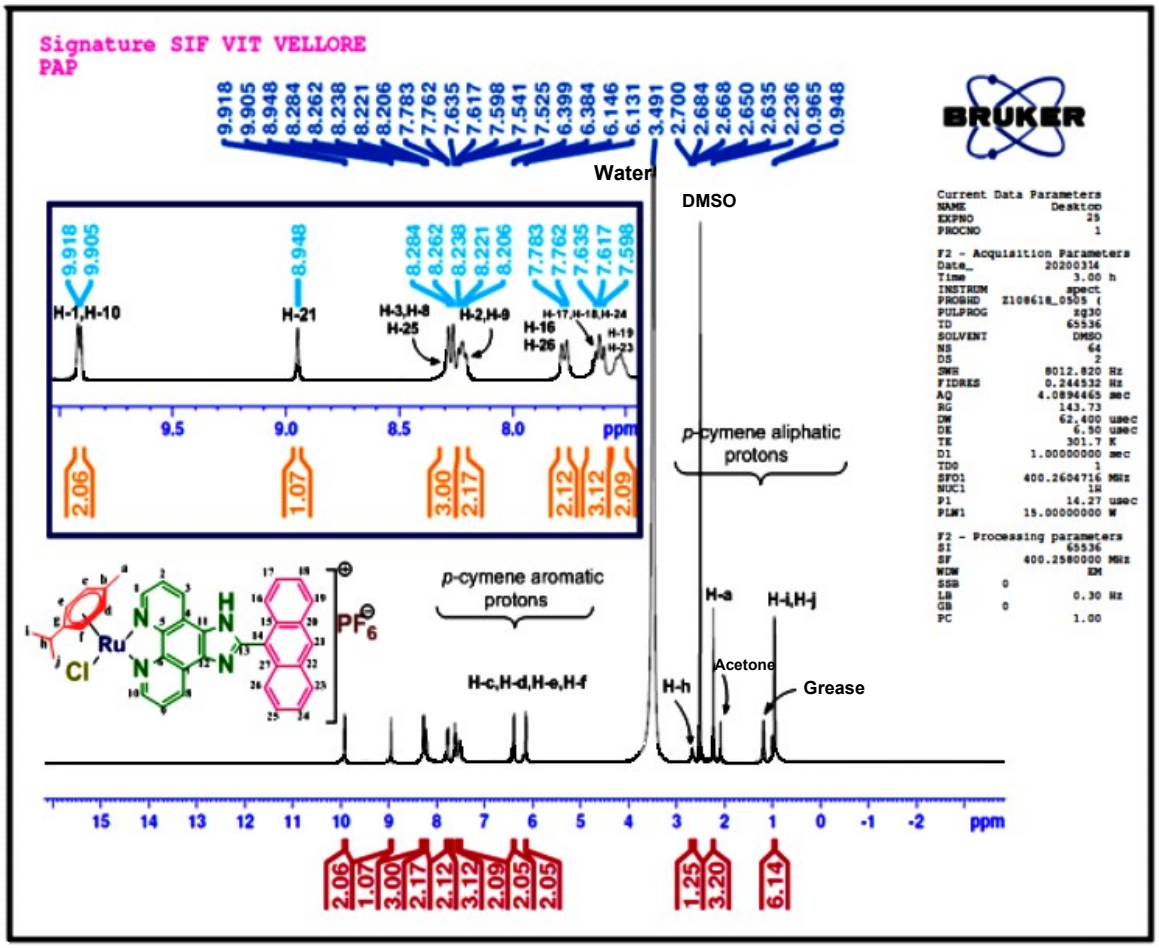

100
%T
80
60
40
20
-0
3163.26
3047.53
2839.22
1537.27
1500.62
1390.68
1350.17
1217.08
1076.28
1026.13
804.32
775.38
736.81
653.87
621.08
557.43
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
PN

(d)

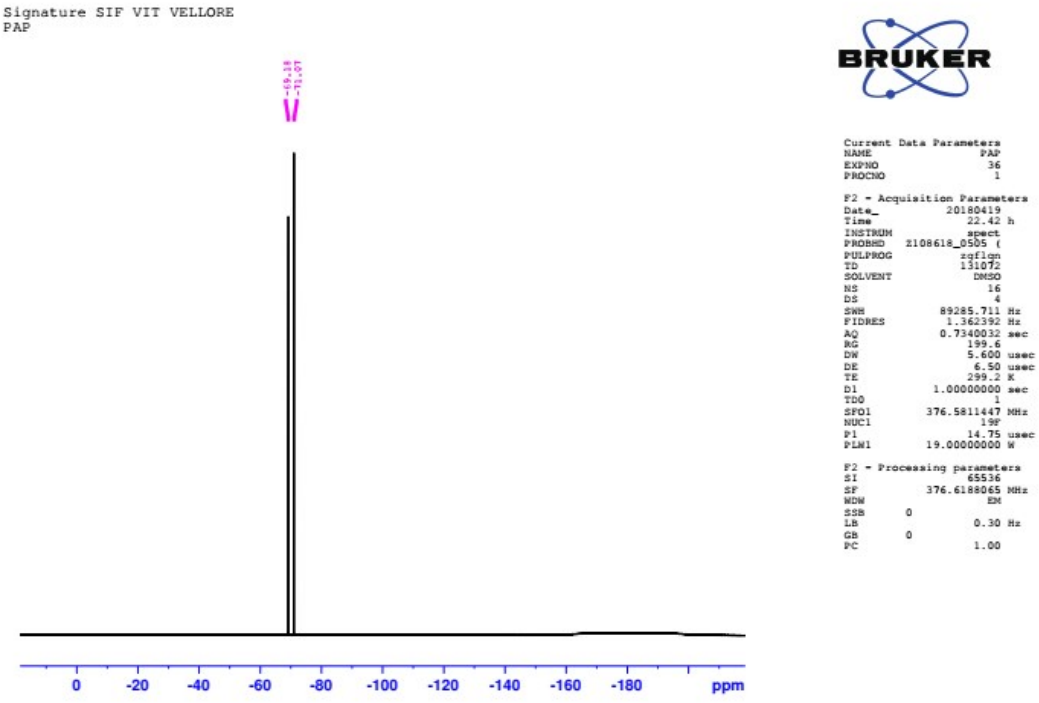


(e)

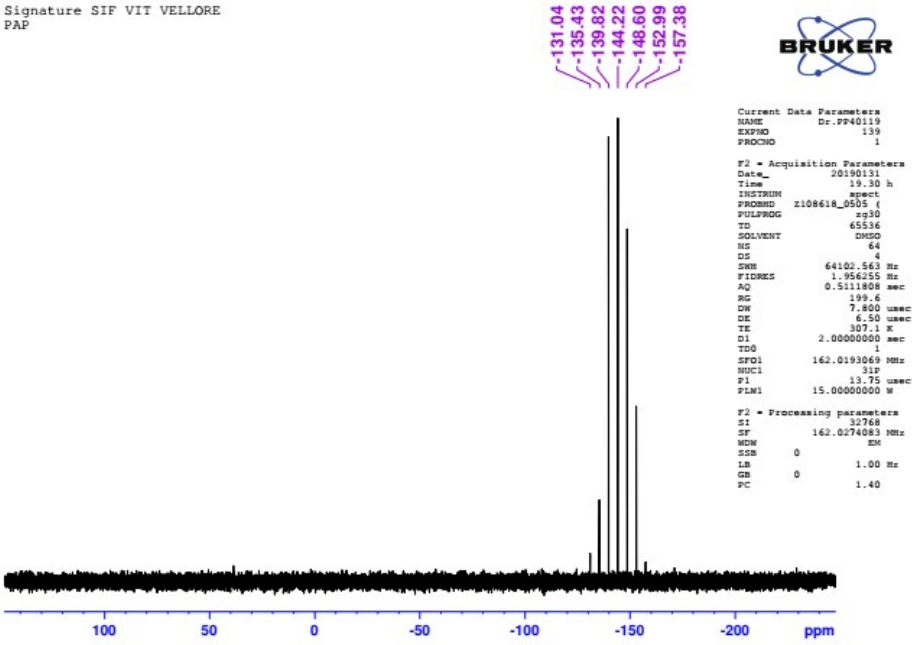
Fig. S19: Ligand L4 (a) Chemical structure (b) ^{1}H NMR (c) ^{13}C NMR (d) IR spectra, and (e) ESI-MS


Signature SIF VIT VELLORE
PAP
BRUKER
Water
DMSO
H-1,H-10
H-21
H-3,H-8
H-25
H-2,H-9
H-16
H-26
H-17,H-18,H-24
H-19
H-23
p-cymene aliphatic protons
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-a
H-i,H-j
H-h
Acetone
Grease
Ru
Cl
PF6
ppm

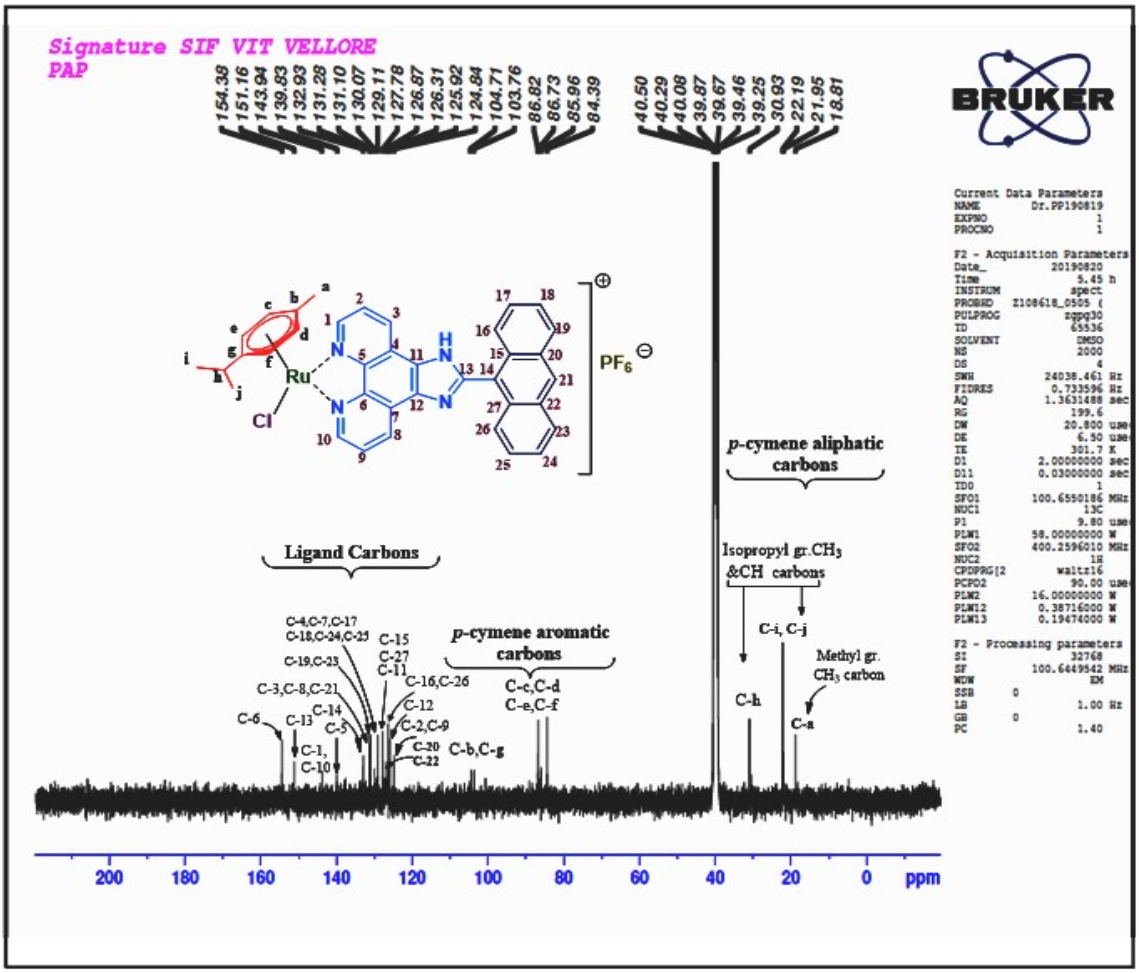
(a)


Signature SIF VIT VELLORE
PAP
BRUKER
ppm

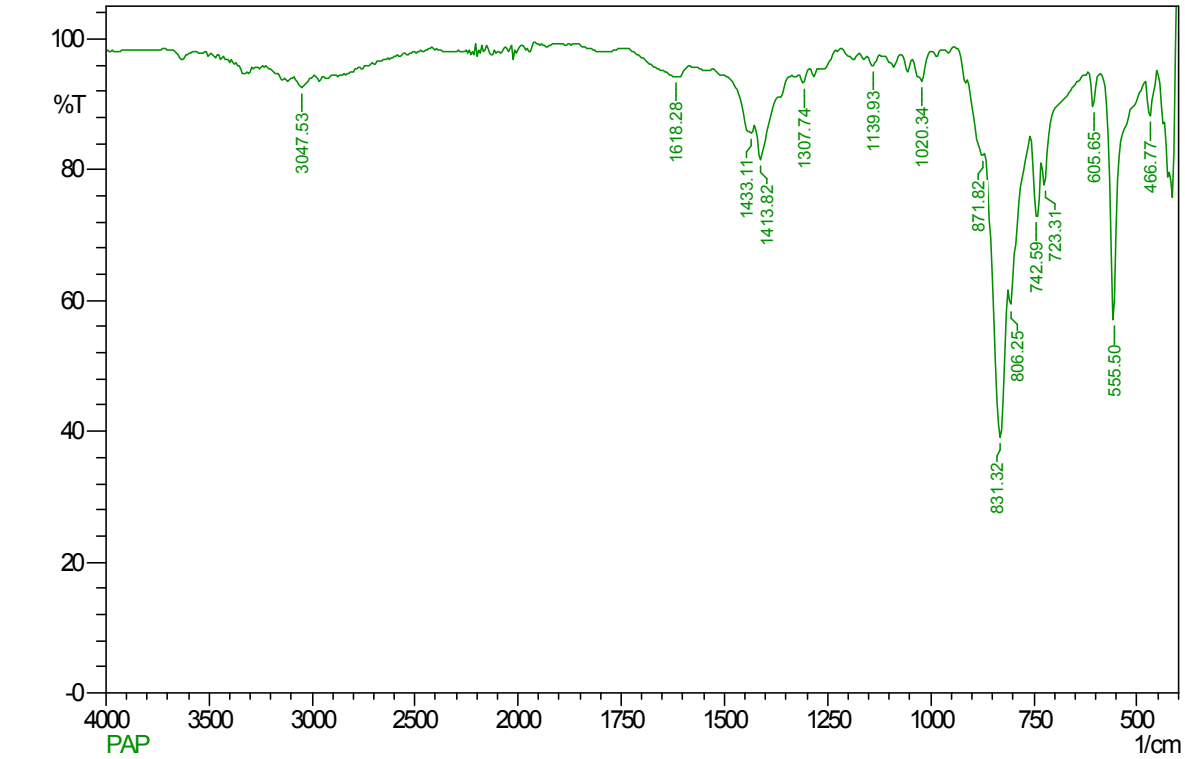
(b)


Signature SIF VIT VELLORE
PAP
-131.04
-135.43
-139.82
-144.22
-148.60
-152.99
-157.38
BRUKER
100
50
0
-50
-100
-150
-200
ppm

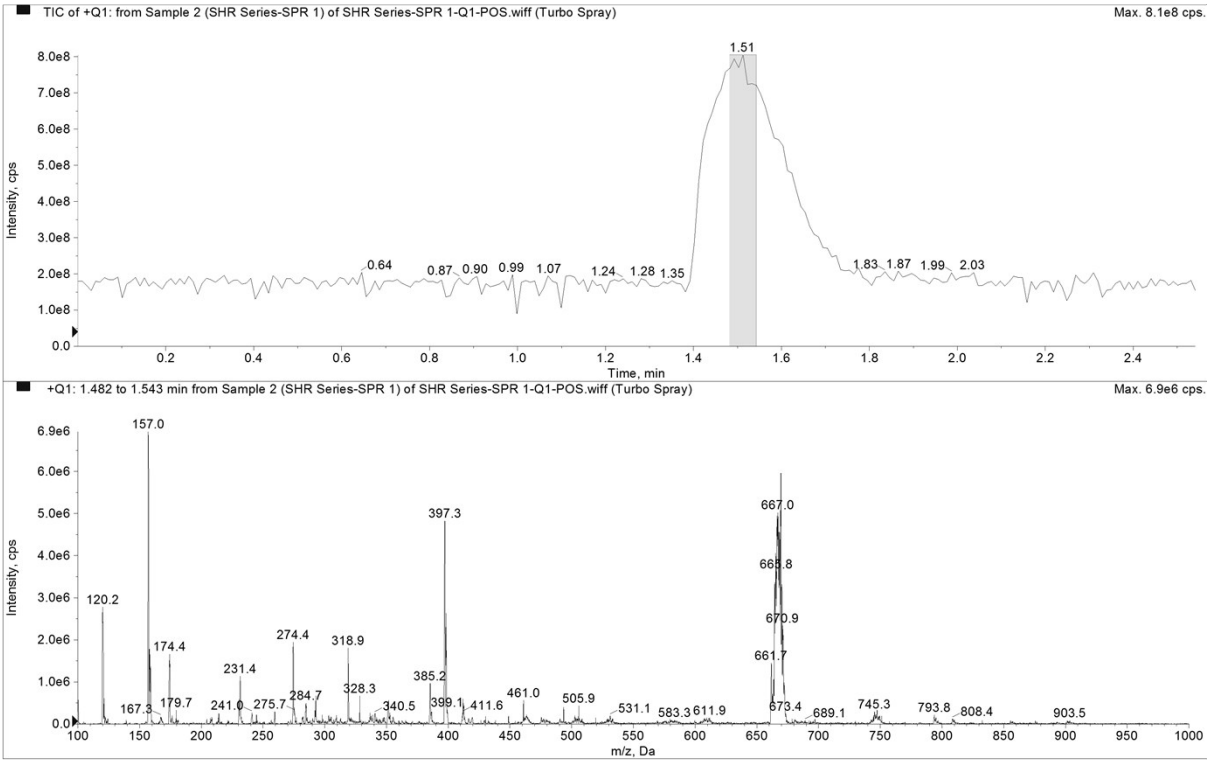
(c)

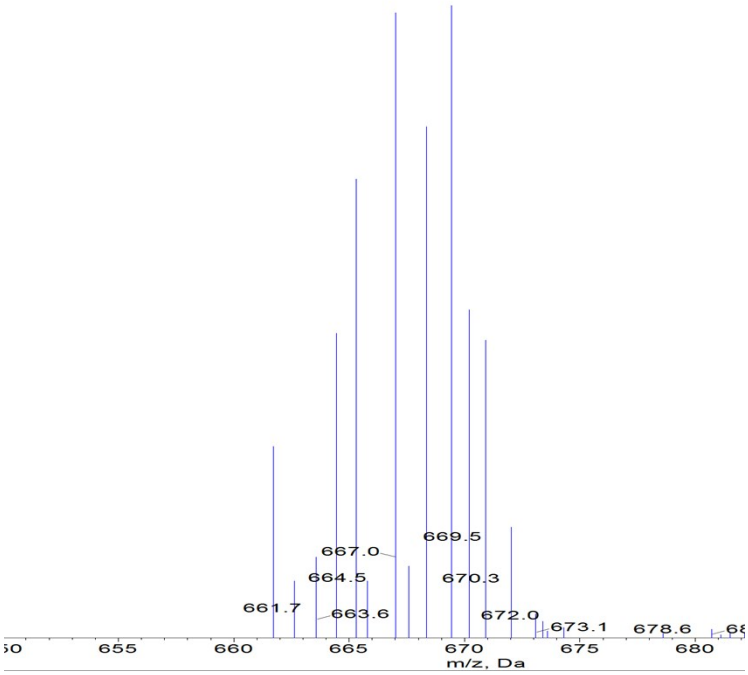

Signature SIF VIT VELLORE
PAP
BRUKER
PF6
Ligand Carbons
p-cymene aromatic carbons
p-cymene aliphatic carbons
Isopropyl gr.CH3 &CH carbons
Methyl gr. CH3 carbon
200
180
160
140
120
100
80
60
40
20
0
ppm

(d)


100
%T
80
60
40
20
-0
3047.53
1618.28
1433.11
1413.82
1307.74
1139.93
1020.34
871.82
831.32
806.25
742.59
723.31
605.65
555.50
466.77
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
PAP

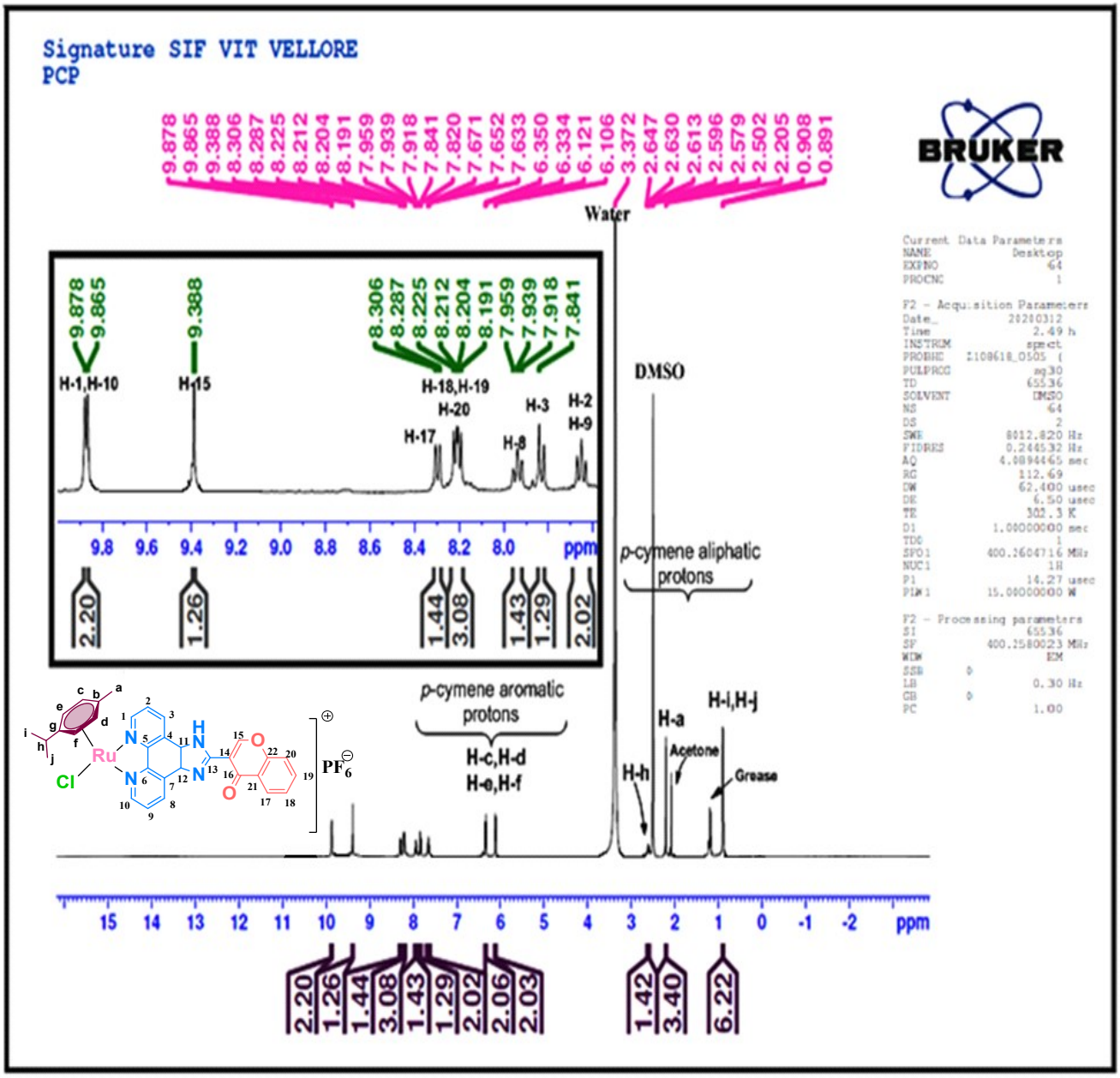
(e)


TIC of +Q1: from Sample 2 (SHR Series-SPR 1) of SHR Series-SPR 1-Q1-POS.wiff (Turbo Spray)
Max. 8.1e8 cps.
Intensity, cps
Time, min
1.51
0.64
0.87
0.90
0.99
1.07
1.24
1.28
1.35
1.83
1.87
1.99
2.03
+Q1: 1.482 to 1.543 min from Sample 2 (SHR Series-SPR 1) of SHR Series-SPR 1-Q1-POS.wiff (Turbo Spray)
Max. 6.9e6 cps.
m/z, Da
157.0
397.3
667.0
668.8
670.9
661.7
120.2
174.4
231.4
274.4
318.9
385.2
328.3
461.0
505.9
531.1
583.3
611.9
673.4
689.1
745.3
793.8
808.4
903.5

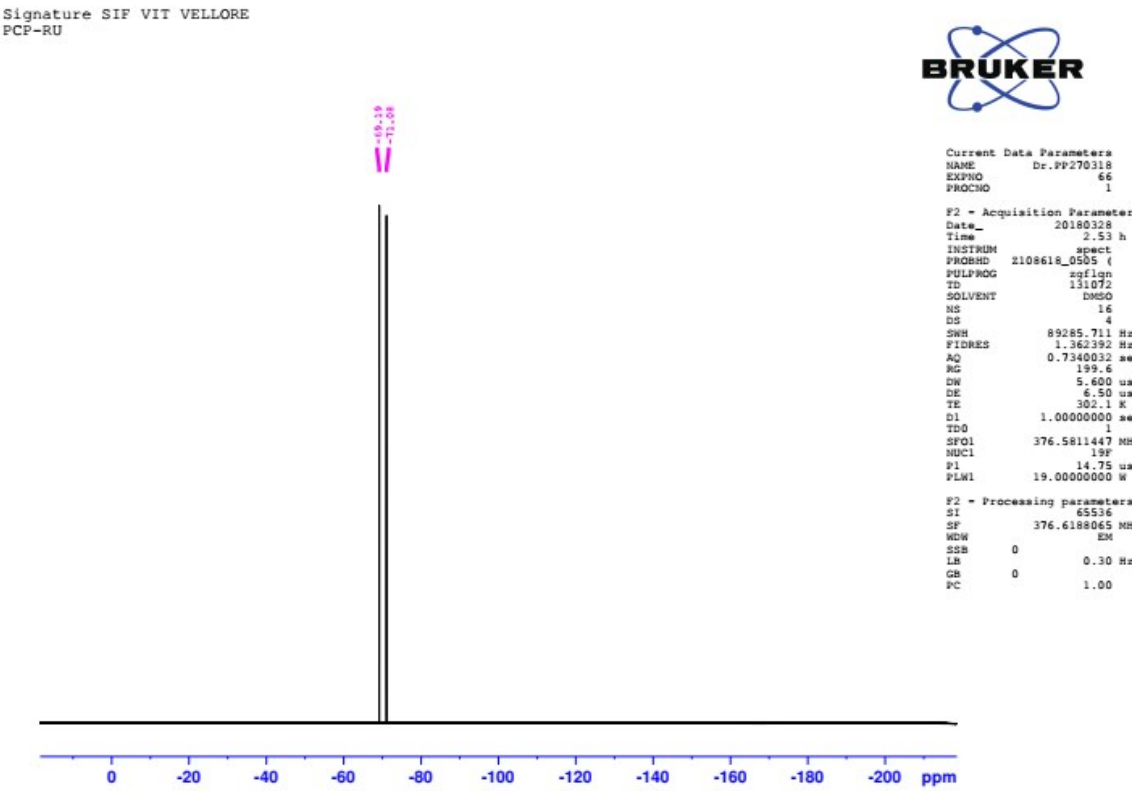


(f)

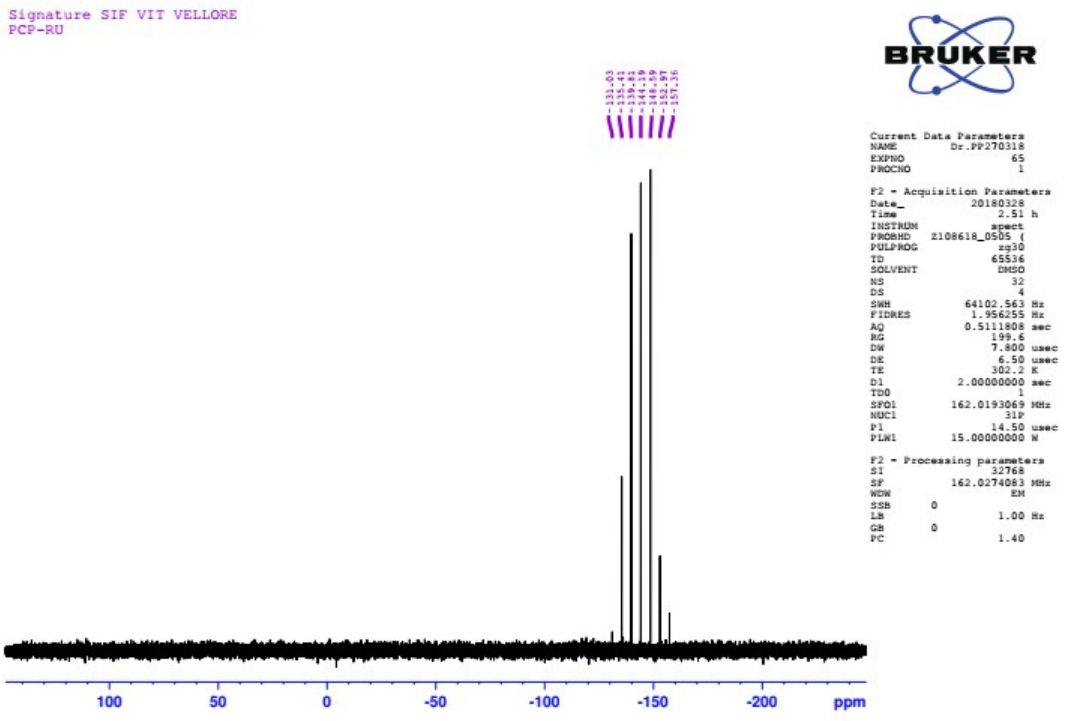
Fig. S20: Complex RuL1 (a) ^{1}H NMR (b) ^{19}F NMR (c) ^{31}P NMR (d) ^{13}C NMR (e) IR spectra, and (f) ESI-MS (Chromatogram, full spectra & Zoom scan)


Signature SIF VIT VELLORE
PCP
BRUKER
9.878 9.865 9.388 8.306 8.287 8.225 8.212 8.204 8.191 7.959 7.939 7.918 7.841 7.820 7.671 7.652 7.633 6.350 6.334 6.121 6.106 3.372 2.647 2.630 2.613 2.596 2.579 2.502 2.205 0.908 0.891
Water
DMSO
H-1,H-10
H-15
H-18,H-19
H-20
H-17
H-8
H-3
H-2
H-9
p-cymene aliphatic protons
p-cymene aromatic protons
H-c,H-d
H-e,H-f
H-h
H-a
H-i,H-j
Acetone
Grease
Cl
Ru
PF6
2.20 1.26 1.44 3.08 1.43 1.29 2.02 2.06 2.03 1.42 3.40 6.22
ppm

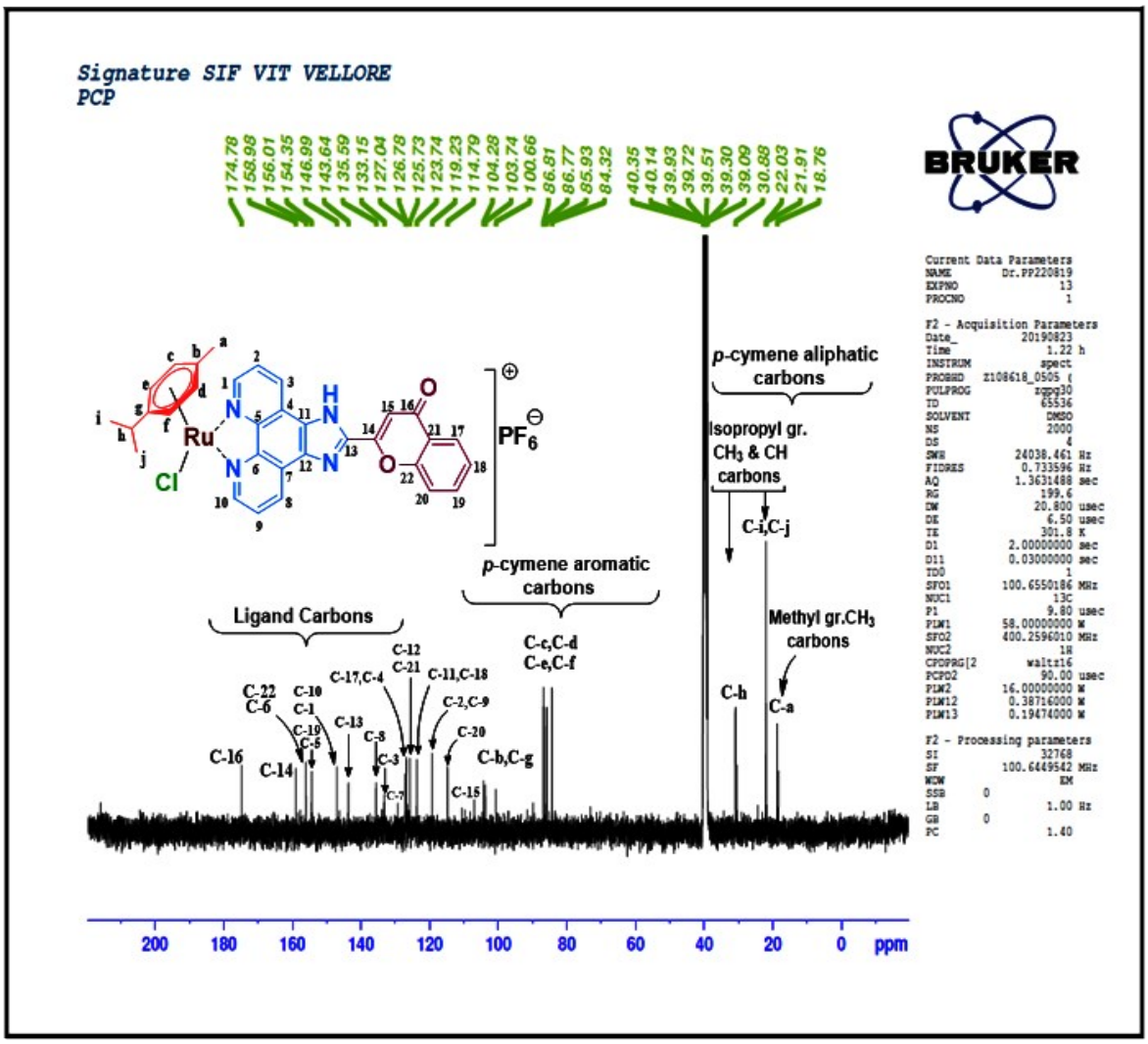
(a)


Signature SIF VIT VELLORE
PCP-RU
BRUKER
-69.19
-71.08
Current Data Parameters
NAME Dr.PP270318
EXPNO 66
PROCNO 1
F2 - Acquisition Parameter
Date_ 20180328
Time 2.53 h
INSTRUM spect
PROBHD 2108618_0505 (
PULPROG zgflqn
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 se
RG 199.6
DW 5.600 us
DE 6.50 us
TE 302.1 K
D1 1.00000000 se
TD0 1
SFO1 376.5811447 MH
NUC1 19F
P1 14.75 us
PLW1 19.00000000 W
F2 - Processing parameters
SI 65536
SF 376.6188065 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

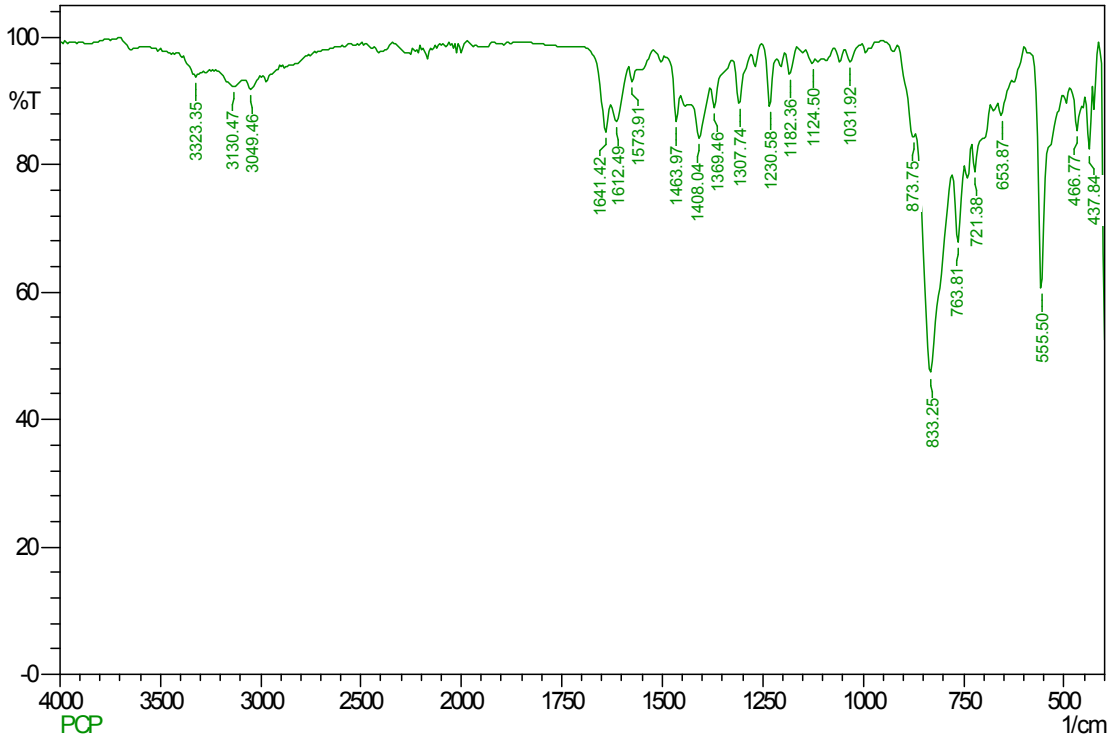
(b)


Signature SIF VIT VELLORE
PCP-RU
BRUKER
-133.03
-135.41
-139.01
-144.16
-148.59
-152.97
-157.36
Current Data Parameters
NAME Dr.PP270318
EXPNO 65
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180328
Time 2.51 h
INSTRUM spect
PROBHD 2108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 4
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 199.6
DW 7.800 usec
DE 6.50 usec
TE 302.2 K
D1 2.00000000 sec
TD0 1
SFO1 162.0193069 MHz
NUC1 31P
P1 14.50 usec
PLW1 15.00000000 W
F2 - Processing parameters
SI 32768
SF 162.0274083 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
100 50 0 -50 -100 -150 -200 ppm

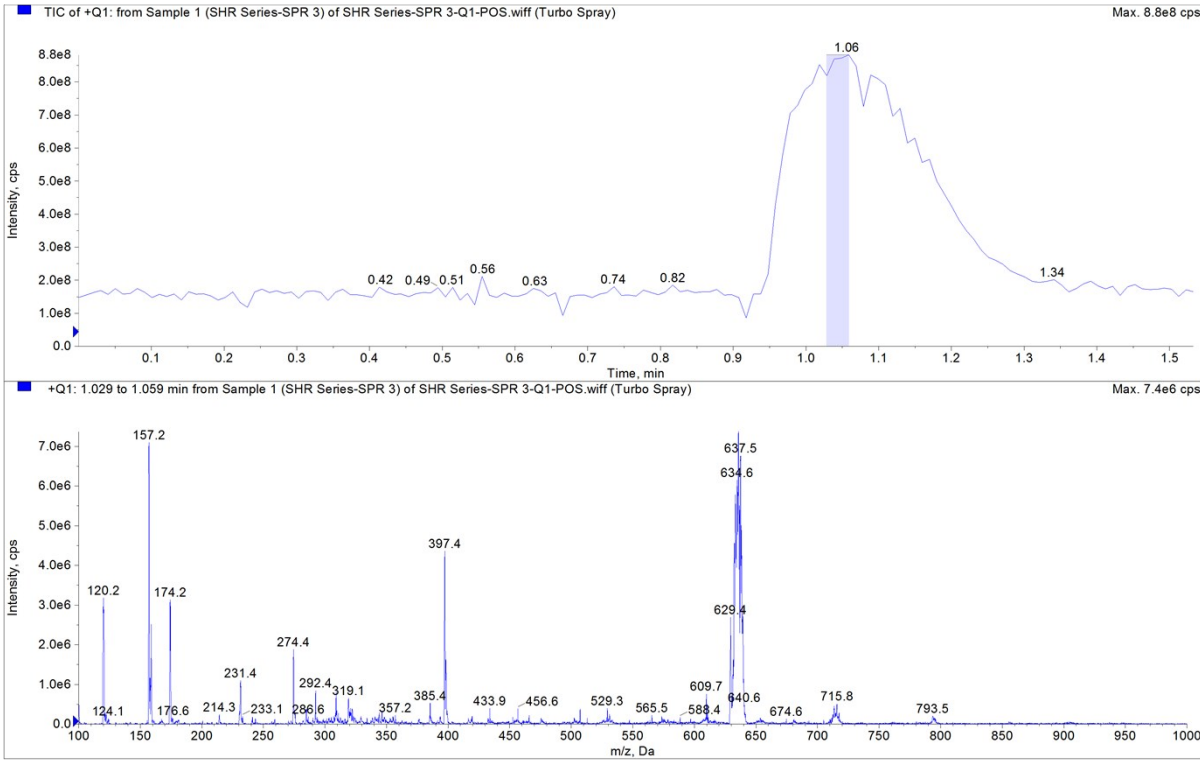
(c)

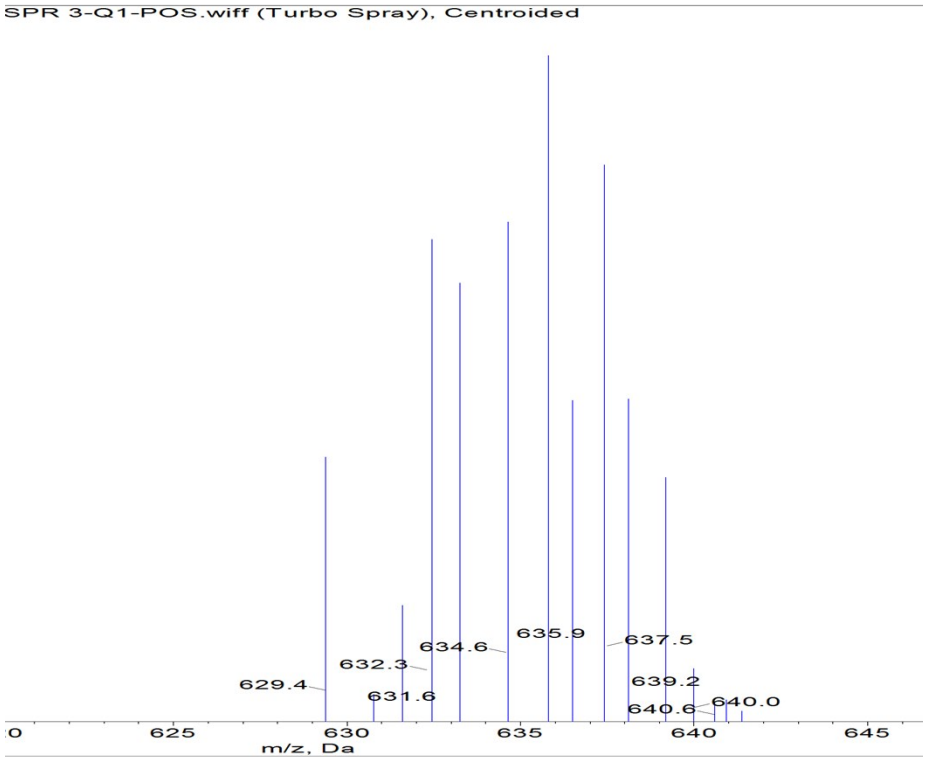

Signature SIF VIT VELLORE
PCP
174.78 158.98 156.01 154.35 146.99 143.64 135.59 133.15 127.04 126.78 125.73 123.74 119.23 114.79 104.28 103.74 100.66 86.81 86.77 85.93 84.32 40.35 40.14 39.93 39.72 39.51 39.30 39.09 30.88 22.03 21.91 18.76
BRUKER
p-cymene aliphatic carbons
Isopropyl gr. CH3 & CH carbons
C-i,C-j
Methyl gr.CH3 carbons
C-h
C-a
p-cymene aromatic carbons
C-c,C-d
C-e,C-f
Ligand Carbons
C-12
C-21
C-17,C-4
C-11,C-18
C-22
C-6
C-10
C-1
C-2,C-9
C-19
C-5
C-13
C-8
C-20
C-16
C-14
C-3
C-b,C-g
C-7
C-15
Ru
Cl
PF6
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME Dr.PP220819
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190823
Time 1.22 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 301.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.38716000 W
PLW13 0.19474000 W
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(d)


100
%T
80
60
40
20
-0
3323.35
3130.47
3049.46
1641.42
1612.49
1573.91
1463.97
1408.04
1369.46
1307.74
1230.58
1182.36
1124.50
1031.92
873.75
833.25
763.81
721.38
653.87
555.50
466.77
437.84
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
PCP

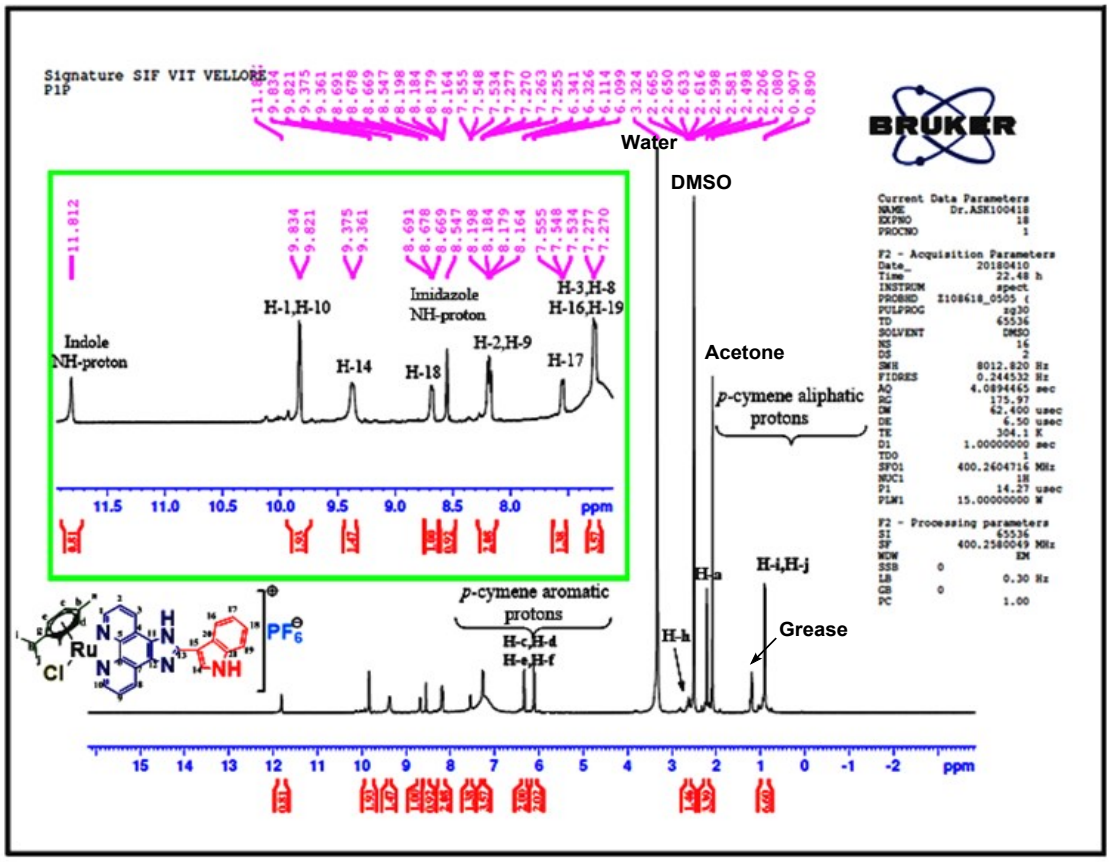
(e)


TIC of +Q1: from Sample 1 (SHR Series-SPR 3) of SHR Series-SPR 3-Q1-POS.wiff (Turbo Spray)
Max. 8.8e8 cps
Intensity, cps
Time, min
1.06
0.42
0.49
0.51
0.56
0.63
0.74
0.82
1.34
+Q1: 1.029 to 1.059 min from Sample 1 (SHR Series-SPR 3) of SHR Series-SPR 3-Q1-POS.wiff (Turbo Spray)
Max. 7.4e6 cps
m/z, Da
157.2
637.5
634.6
397.4
120.2
174.2
629.4
274.4
231.4
292.4
319.1
609.7
640.6
715.8
385.4
433.9
456.6
529.3
565.5
588.4
674.6
793.5
124.1
176.6
214.3
233.1
286.6
357.2

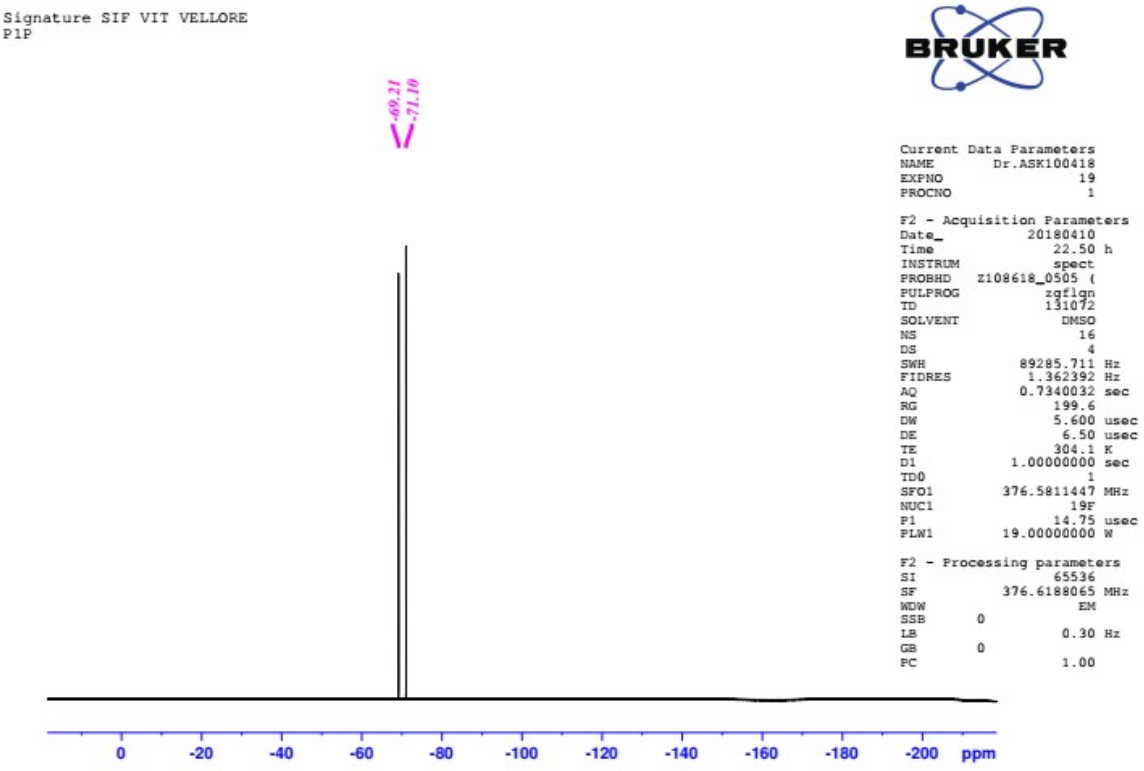


(f)

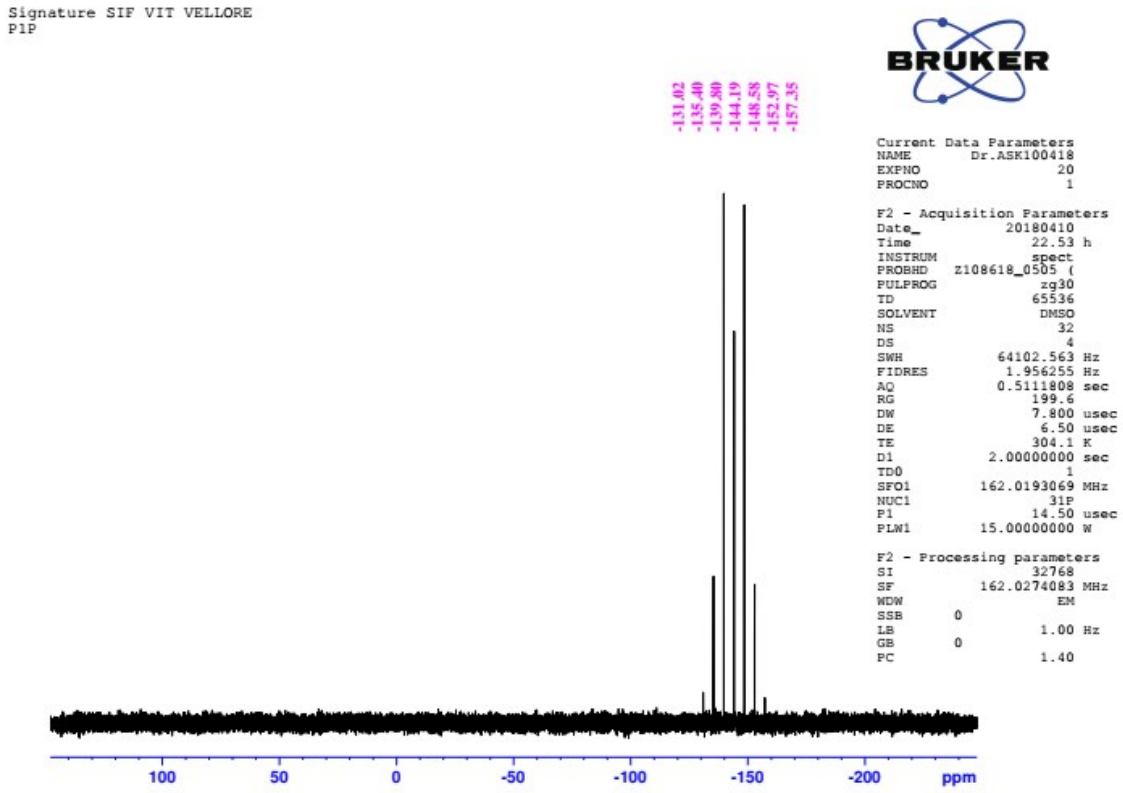
Fig. S21: Complex RuL2(a) ^{1}H NMR (b) ^{19}F NMR (c) ^{31}P NMR (d) ^{13}C NMR (e) IR spectra, and (f) ESI-MS (Chromatogram, full spectra & Zoom scan)


Signature SIF VIT VELLORE
P1P
Water
DMSO
Acetone
p-cymene aliphatic protons
p-cymene aromatic protons
Indole NH-proton
Imidazole NH-proton
H-1,H-10
H-14
H-18
H-2,H-9
H-17
H-3,H-8
H-16,H-19
H-a
H-h
H-i,H-j
H-c,H-d
H-e,H-f
Grease
PF6
Cl
Ru
NH
ppm

(a)


Signature SIF VIT VELLORE
P1P
-69.21
-71.10
ppm

(b)


Signature SIF VIT VELLORE
P1P
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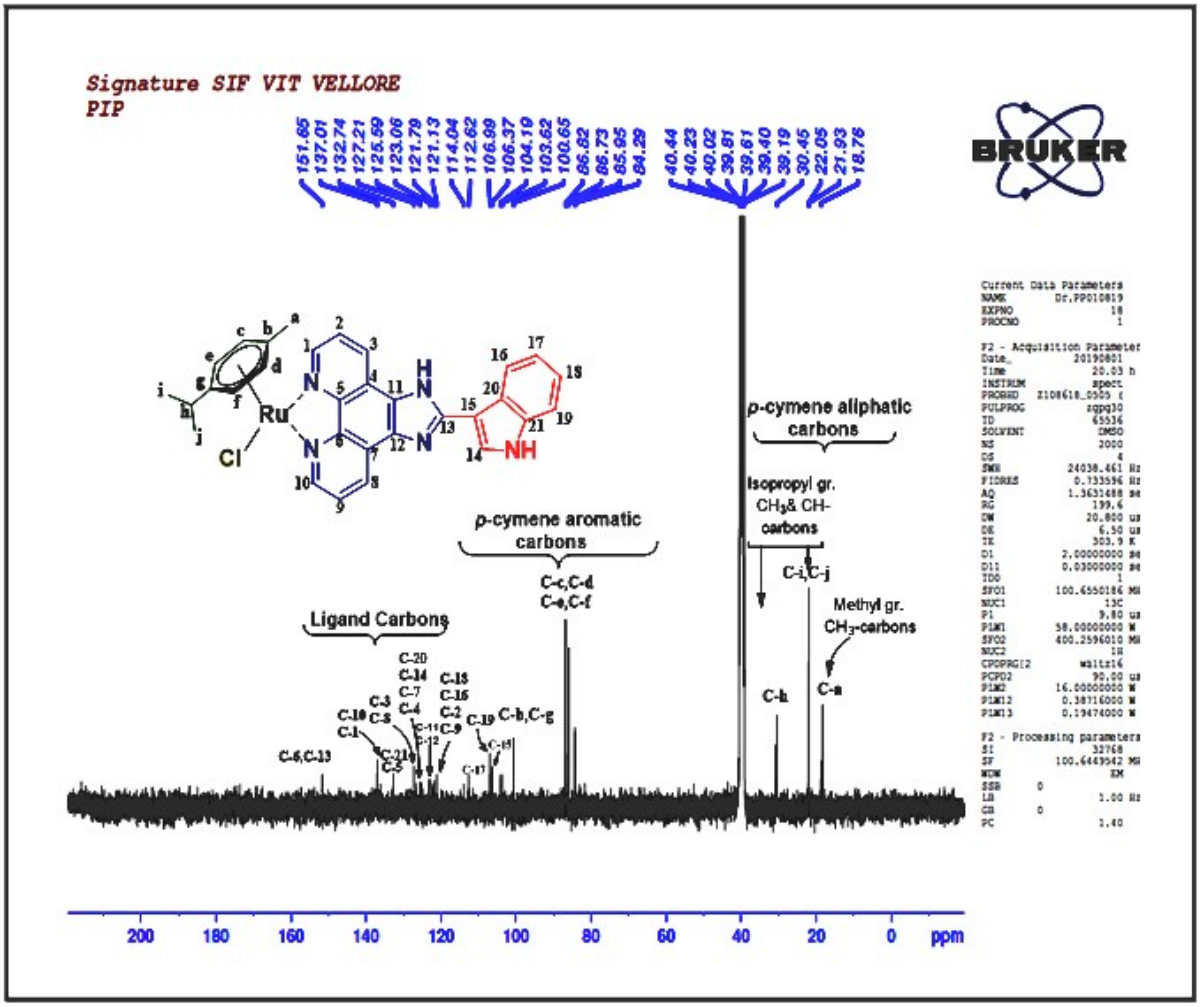
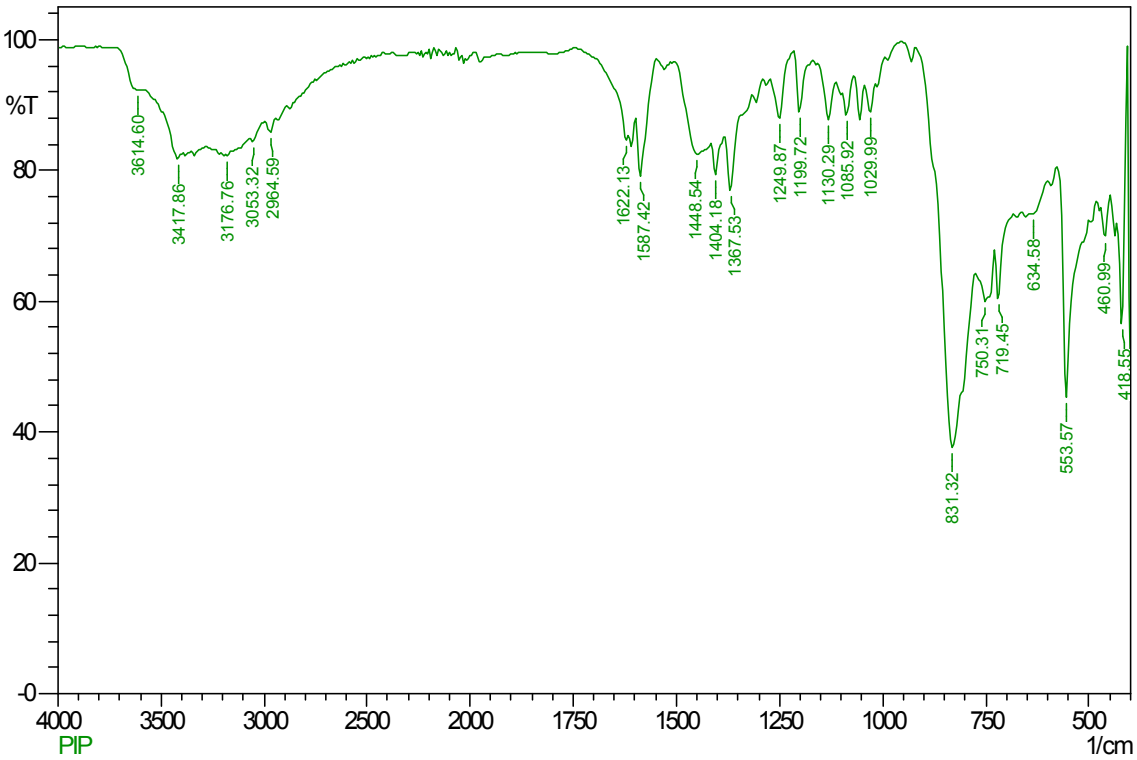
-135.40
-139.80
-144.19
-148.58
-152.97
-157.35
Current Data Parameters
NAME Dr.ASK100418
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180410
Time 22.53 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 4
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 199.6
DW 7.800 usec
DE 6.50 usec
TE 304.1 K
D1 2.00000000 sec
TD0 1
SFO1 162.0193069 MHz
NUC1 31P
P1 14.50 usec
PLW1 15.00000000 W
F2 - Processing parameters
SI 32768
SF 162.0274083 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
100
50
0
-50
-100
-150
-200
ppm

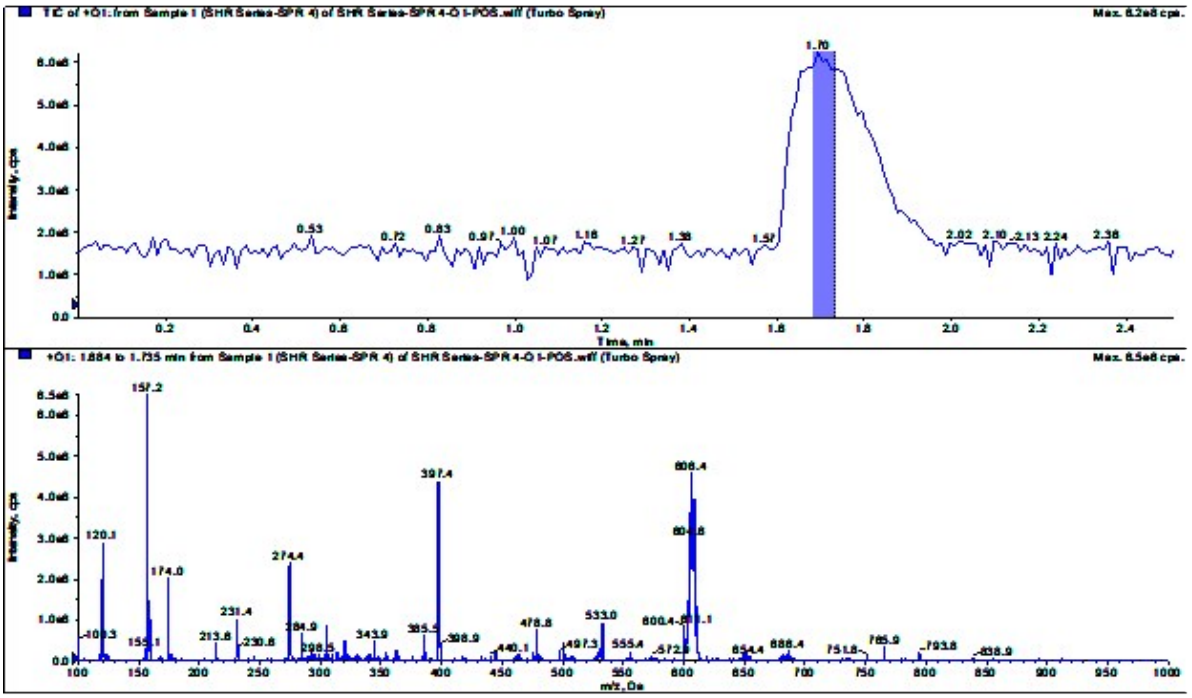
(c)

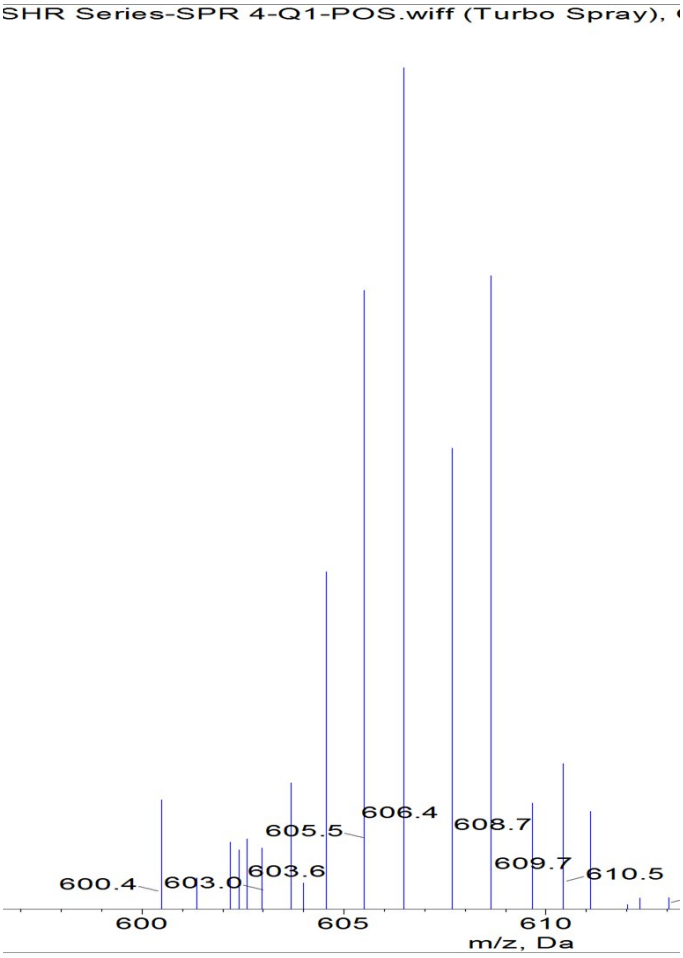

Signature SIF VIT VELLORE
PIP
151.65
137.01
132.74
127.21
125.59
123.06
121.79
121.13
114.04
112.62
106.59
106.37
104.19
103.62
100.65
86.82
86.73
85.95
84.29
40.44
40.23
40.02
39.81
39.61
39.40
39.19
30.45
22.05
21.93
18.76
p-cymene aromatic carbons
C-c,C-d
C-e,C-f
Ligand Carbons
p-cymene aliphatic carbons
Isopropyl gr. CH3& CH-carbons
C-i,C-j
Methyl gr. CH3-carbons
C-h
C-a
C-h,C-g
C-6,C-13
Current Data Parameters
NAME Dr.PP010819
EXPNO 18
PROCNO 1
F2 - Acquisition Parameter
Date_ 20190801
Time 20.03 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 se
RG 199.6
DW 20.800 us
DE 6.50 us
TE 303.9 K
D1 2.00000000 se
D11 0.03000000 se
TD0 1
SFO1 100.6550186 MH
NUC1 13C
P1 9.80 us
PLW1 58.00000000 W
SFO2 400.2596010 MH
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 us
PLW2 16.00000000 W
PLW12 0.38716000 W
PLW13 0.19474000 W
F2 - Processing parameters
SI 32768
SF 100.6449542 MH
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

(d)


100
%T
80
60
40
20
-0
3614.60
3417.86
3176.76
3053.32
2964.59
1622.13
1587.42
1448.54
1404.18
1367.53
1249.87
1199.72
1130.29
1085.92
1029.99
831.32
750.31
719.45
634.58
553.57
460.99
418.55
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
PIP

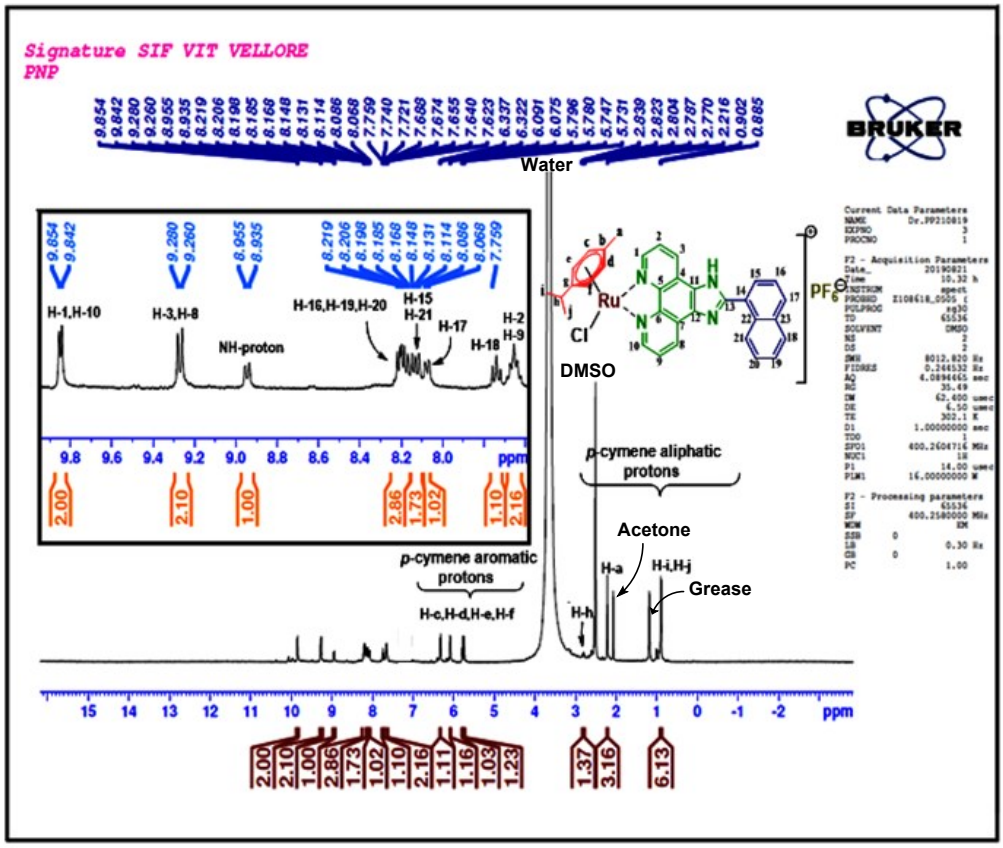
(e)


TIC of +Q1: from Sample 1 (SHR Series-SPR 4) of SHR Series-SPR 4-O I-POS.wiff (Turbo Spray)
Max. 8.2e8 cps.
Intensity, cps
Time, min
+Q1: 1.884 to 1.735 min from Sample 1 (SHR Series-SPR 4) of SHR Series-SPR 4-O I-POS.wiff (Turbo Spray)
Max. 8.5e8 cps.
m/z, Da

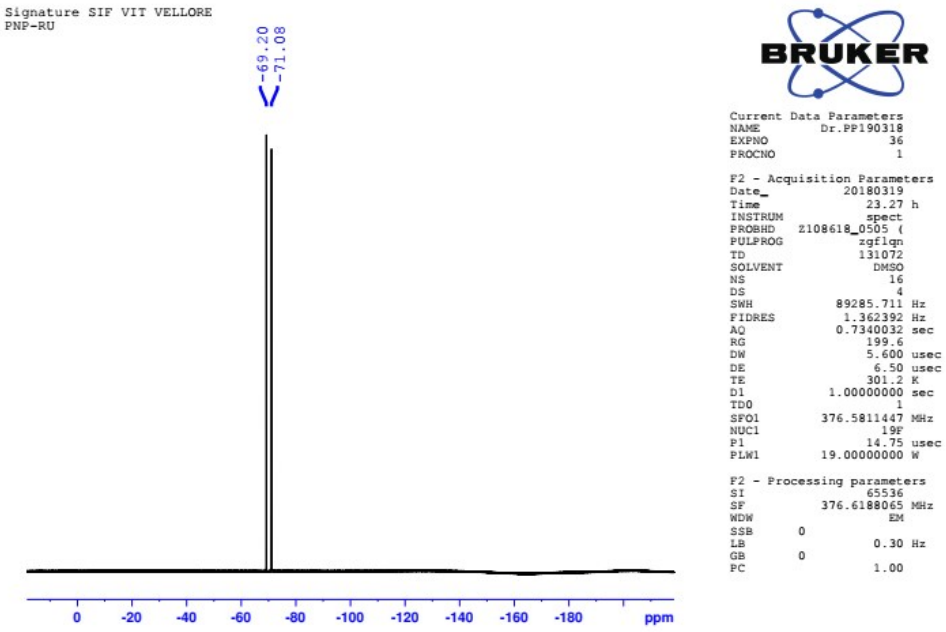


(f)

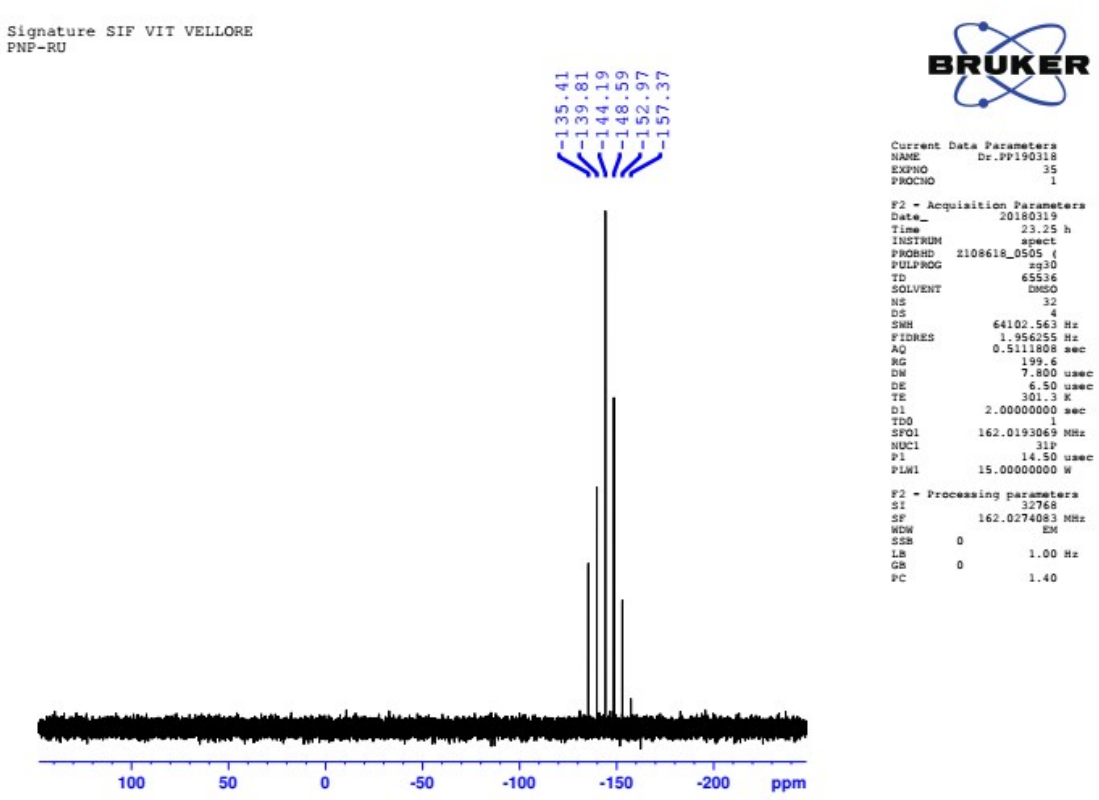
Fig. S22: Complex RuL3(a) ^{1}H NMR (b) ^{19}F NMR (c) ^{31}P NMR (d) ^{13}C NMR (e) IR spectra, and (f) ESI-MS (Chromatogram, full spectra & Zoom scan)


Signature SIF VIT VELLORE
PNP
BRUKER
Water
H-1,H-10
H-3,H-8
NH-proton
H-16,H-19,H-20
H-15
H-21
H-17
H-18
H-2
H-9
DMSO
p-cymene aliphatic protons
Acetone
H-a
H-i,H-j
Grease
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
Ru
Cl
PF6
ppm

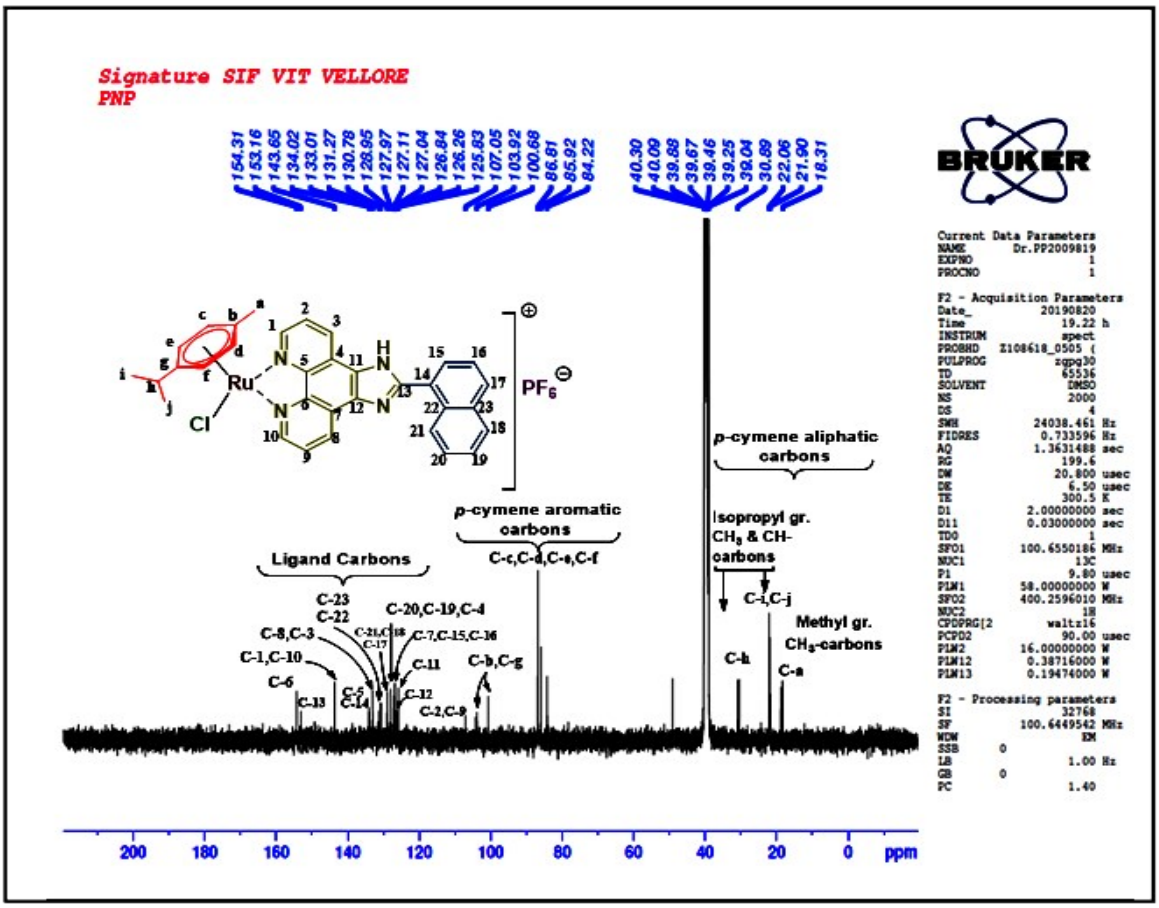
(a)


Signature SIF VIT VELLORE
PNP-RU
-69.20
-71.08
BRUKER
Current Data Parameters
NAME Dr.PP190318
EXPNO 36
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180319
Time 23.27 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgflqn
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 199.6
DW 5.600 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TD0 1
SFO1 376.5811447 MHz
NUC1 19F
P1 14.75 usec
PLW1 19.00000000 W
F2 - Processing parameters
SI 65536
SF 376.6188065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm

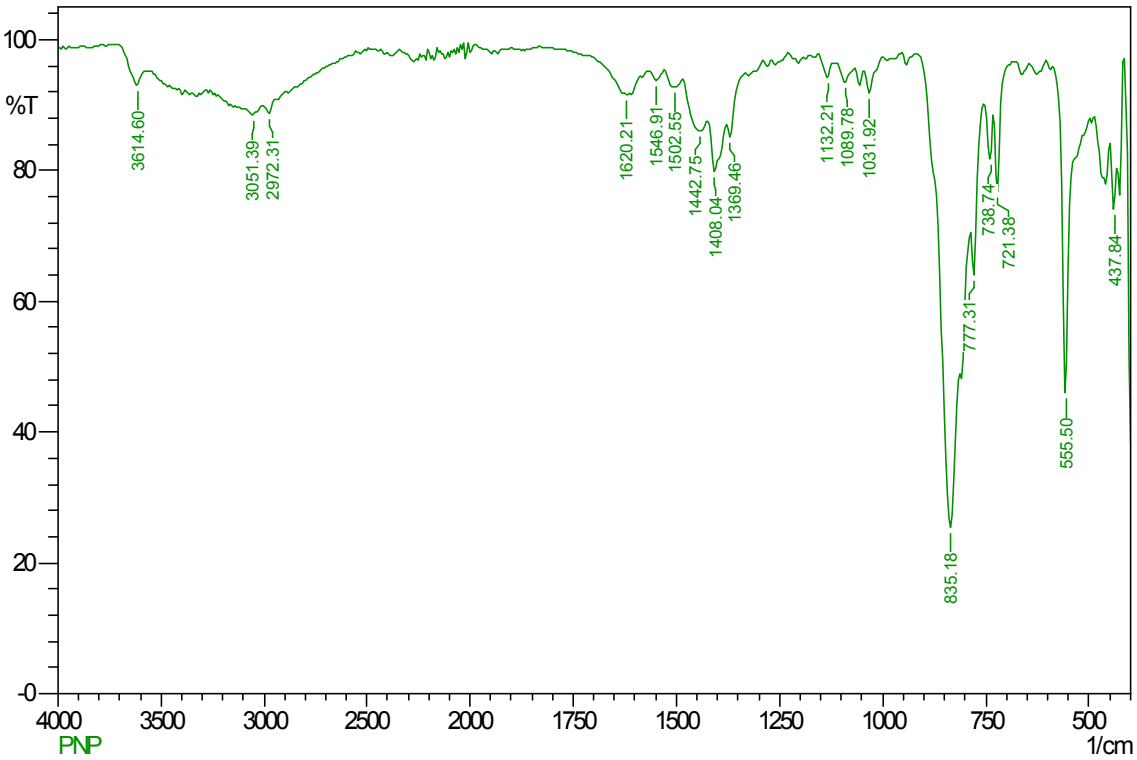
(b)


Signature SIF VIT VELLORE
PNP-RU
-135.41
-139.81
-144.19
-148.59
-152.97
-157.37
BRUKER
Current Data Parameters
NAME Dr.PP190318
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180319
Time 23.25 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 4
SWH 64102.563 Hz
FIDRES 1.956255 Hz
AQ 0.5111808 sec
RG 199.6
DW 7.800 usec
DE 6.50 usec
TE 301.3 K
D1 2.00000000 sec
TD0 1
SFO1 162.0193069 MHz
NUC1 31P
P1 14.50 usec
PLW1 15.00000000 W
F2 - Processing parameters
SI 32768
SF 162.0274083 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
100
50
0
-50
-100
-150
-200
ppm

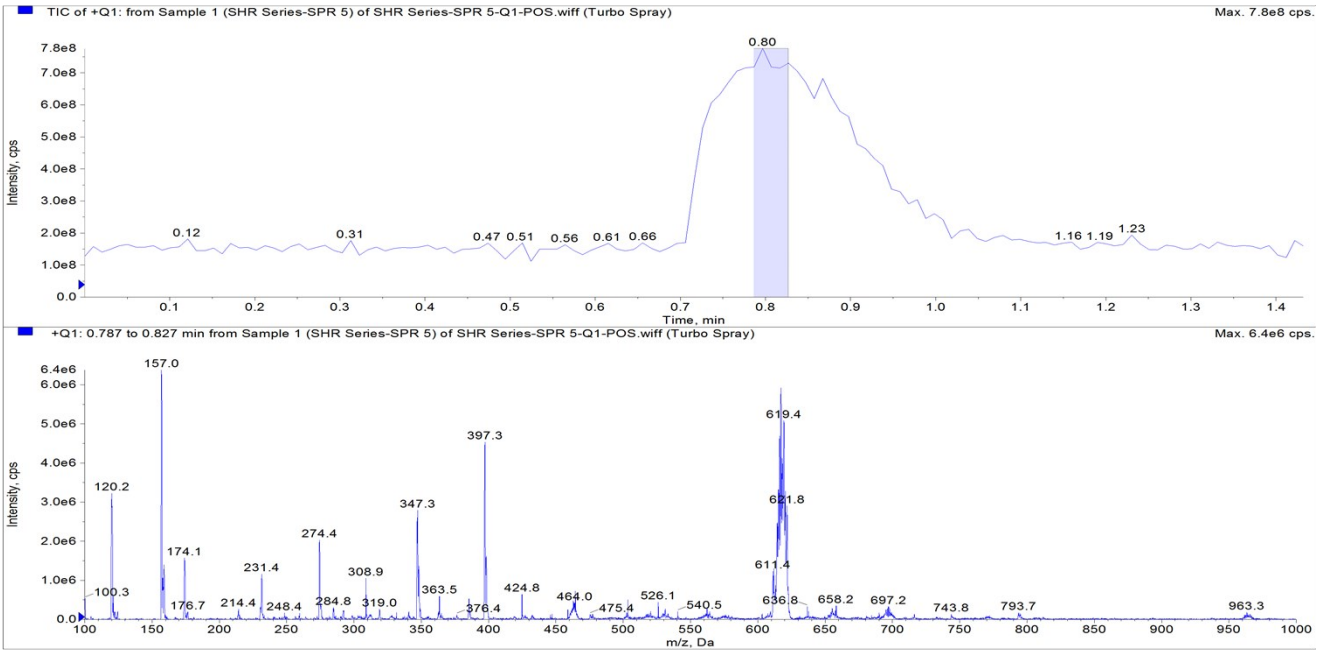
(c)

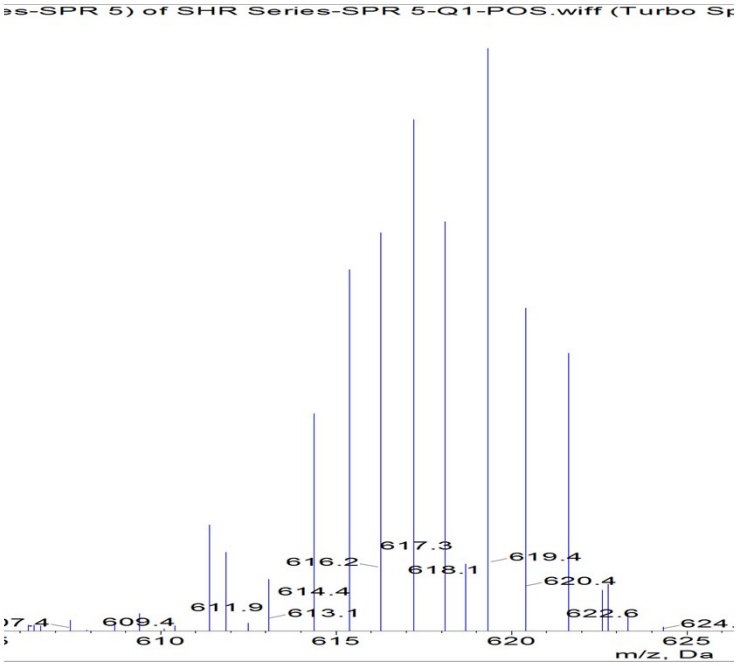

Signature SIF VIT VELLORE
PNP
154.31
153.16
143.65
134.02
133.01
131.27
130.78
128.65
127.97
127.11
127.04
126.84
126.26
125.83
107.05
103.92
100.68
86.81
85.92
84.22
40.30
40.09
39.88
39.67
39.46
39.25
39.04
30.89
22.06
21.90
18.31
PF6
Cl
Ru
p-cymene aromatic carbons
C-c,C-d,C-e,C-f
p-cymene aliphatic carbons
Isopropyl gr. CH3 & CH-carbons
C-i,C-j
Methyl gr. CH3-carbons
C-h
C-a
Ligand Carbons
C-23
C-22
C-20,C-19,C-4
C-8,C-3
C-21,C-18
C-17
C-7,C-15,C-16
C-1,C-10
C-11
C-b,C-g
C-6
C-13
C-5
C-14
C-12
C-2,C-9
BRUKER
Current Data Parameters
NAME Dr.PP2009819
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190820
Time 19.22 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.38716000 W
PLW13 0.19474000 W
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

(d)


100
%T
80
60
40
20
-0
3614.60
3051.39
2972.31
1620.21
1546.91
1502.55
1442.75
1408.04
1369.46
1132.21
1089.78
1031.92
835.18
777.31
738.74
721.38
555.50
437.84
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
PNP

(e)


TIC of +Q1: from Sample 1 (SHR Series-SPR 5) of SHR Series-SPR 5-Q1-POS.wiff (Turbo Spray)
Max. 7.8e8 cps.
Intensity, cps
Time, min
0.80
0.12
0.31
0.47
0.51
0.56
0.61
0.66
1.16
1.19
1.23
+Q1: 0.787 to 0.827 min from Sample 1 (SHR Series-SPR 5) of SHR Series-SPR 5-Q1-POS.wiff (Turbo Spray)
Max. 6.4e6 cps.
m/z, Da
157.0
120.2
174.1
100.3
231.4
274.4
308.9
347.3
363.5
397.3
424.8
464.0
526.1
540.5
619.4
621.8
611.4
636.8
658.2
697.2
743.8
793.7
963.3



(f)

Fig. S23: Complex RuL4 (a) ^{1}H NMR (b) ^{19}F NMR (c) ^{31}P NMR (d) ^{13}C NMR (e) IR spectra, and (f) ESI-MS (Chromatogram, full spectra & Zoom scan)

CHN analysis

Date of report	9/23/2019 5:26:55PM
User ID	Administrator

DATE & TIME	9/22/2019 9:25:37 PM	P_ID	VITSIFCHNS
SAMPLE ID	PAP	USER ID	Administrator
WEIGHT (mg)	1.730	MODE	CHN

		SIGNALS	
		ZR	7648
CARBON	54.44%	NR	8421
HYDROGEN	3.41%	CR	23589
NITROGEN	6.51%	HR	27080

BLANKS	-68	854	127
K FACTORS	16.177	44.698	5.740

FILL	COMB	BOOST1	BOOST2
0	0	0	0

FILL TIME 46 Seconds

DATE & TIME	9/22/2019 9:35:42 PM	P_ID	VITSIFCHNS
SAMPLE ID	PCP	USER ID	Administrator
WEIGHT (mg)	1.718	MODE	CHN

		SIGNALS	
		ZR	7646
CARBON	49.56%	NR	8511
HYDROGEN	3.14%	CR	22217
NITROGEN	7.48%	HR	25482

BLANKS	-68	854	127
K FACTORS	16.177	44.698	5.740

FILL	COMB	BOOST1	BOOST2
0	0	0	0

FILL TIME 46 Seconds

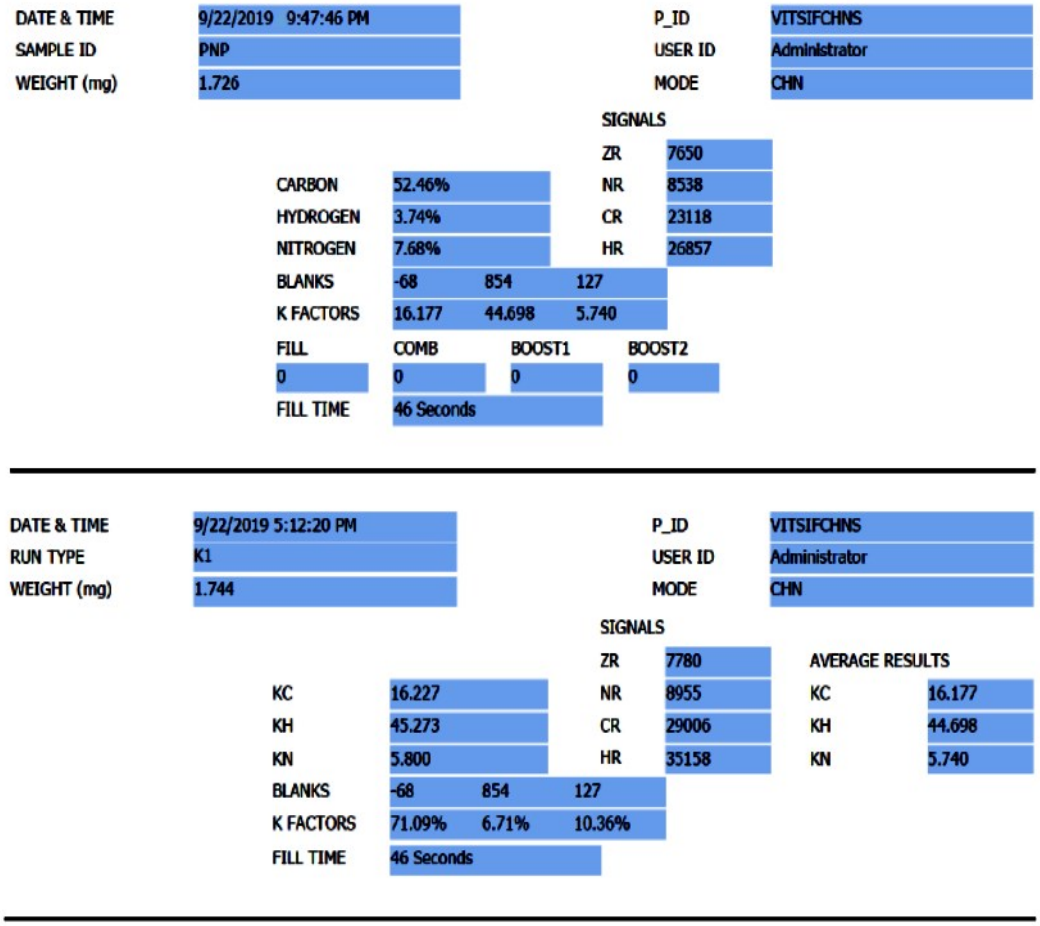
DATE & TIME	9/22/2019 9:40:55 PM	P_ID	VITSIFCHNS
SAMPLE ID	PIP	USER ID	Administrator
WEIGHT (mg)	1.722	MODE	CHN

		SIGNALS	
		ZR	7649
CARBON	49.76%	NR	8723
HYDROGEN	3.14%	CR	22517
NITROGEN	9.58%	HR	25788

BLANKS	-68	854	127
K FACTORS	16.177	44.698	5.740

FILL	COMB	BOOST1	BOOST2
0	0	0	0

FILL TIME 46 Seconds



DATE & TIME	9/22/2019 9:47:46 PM	P_ID	VITSIFCHNS
SAMPLE ID	PNP	USER ID	Administrator
WEIGHT (mg)	1.726	MODE	CHN

SIGNALS	
ZR	7650
NR	8538
CR	23118
HR	26857

CARBON	52.46%		
HYDROGEN	3.74%		
NITROGEN	7.68%		
BLANKS	-68	854	127
K FACTORS	16.177	44.698	5.740

FILL	COMB	BOOST1	BOOST2
0	0	0	0

FILL TIME 46 Seconds

DATE & TIME	9/22/2019 5:12:20 PM	P_ID	VITSIFCHNS
RUN TYPE	K1	USER ID	Administrator
WEIGHT (mg)	1.744	MODE	CHN

SIGNALS		AVERAGE RESULTS	
ZR	7780		
NR	8955	KC	16.177
CR	29006	KH	44.698
HR	35158	KN	5.740

KC	16.227		
KH	45.273		
KN	5.800		
BLANKS	-68	854	127
K FACTORS	71.09%	6.71%	10.36%

FILL TIME 46 Seconds

Fig. S24 CHN analysis: (a) PAP = RuL1 (b) PCP = RuL2 (c) PIP = RuL3 (d) PNP = RuL4