DNA targeting half sandwich Ru(II)-*p*-cymene-N^N complexes as cancer cell imaging and terminating agents: influence of regiosiomers in cytotoxicity†

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Index

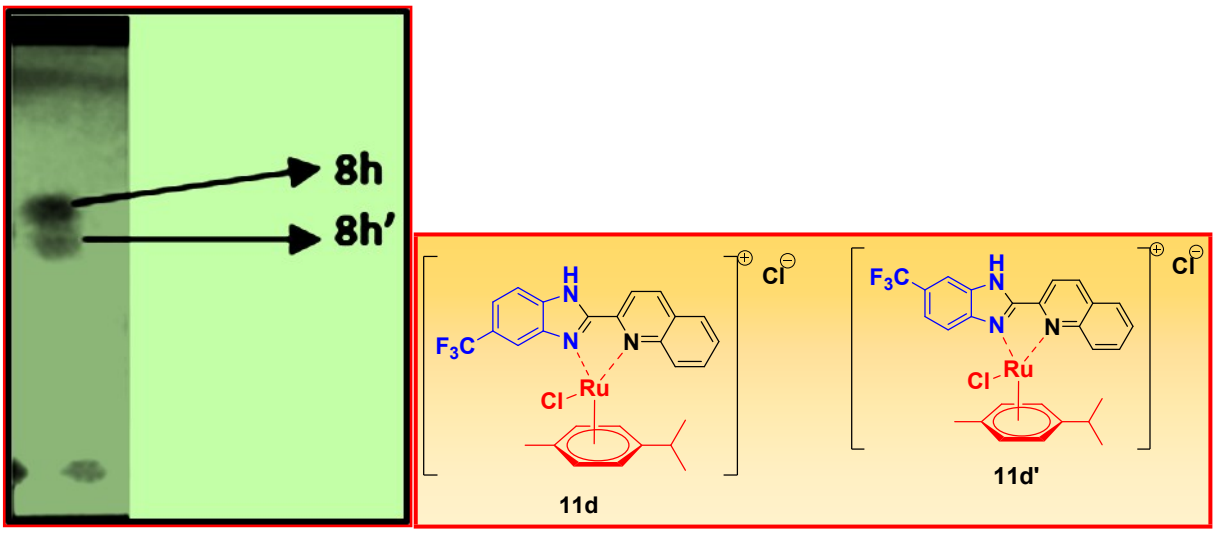
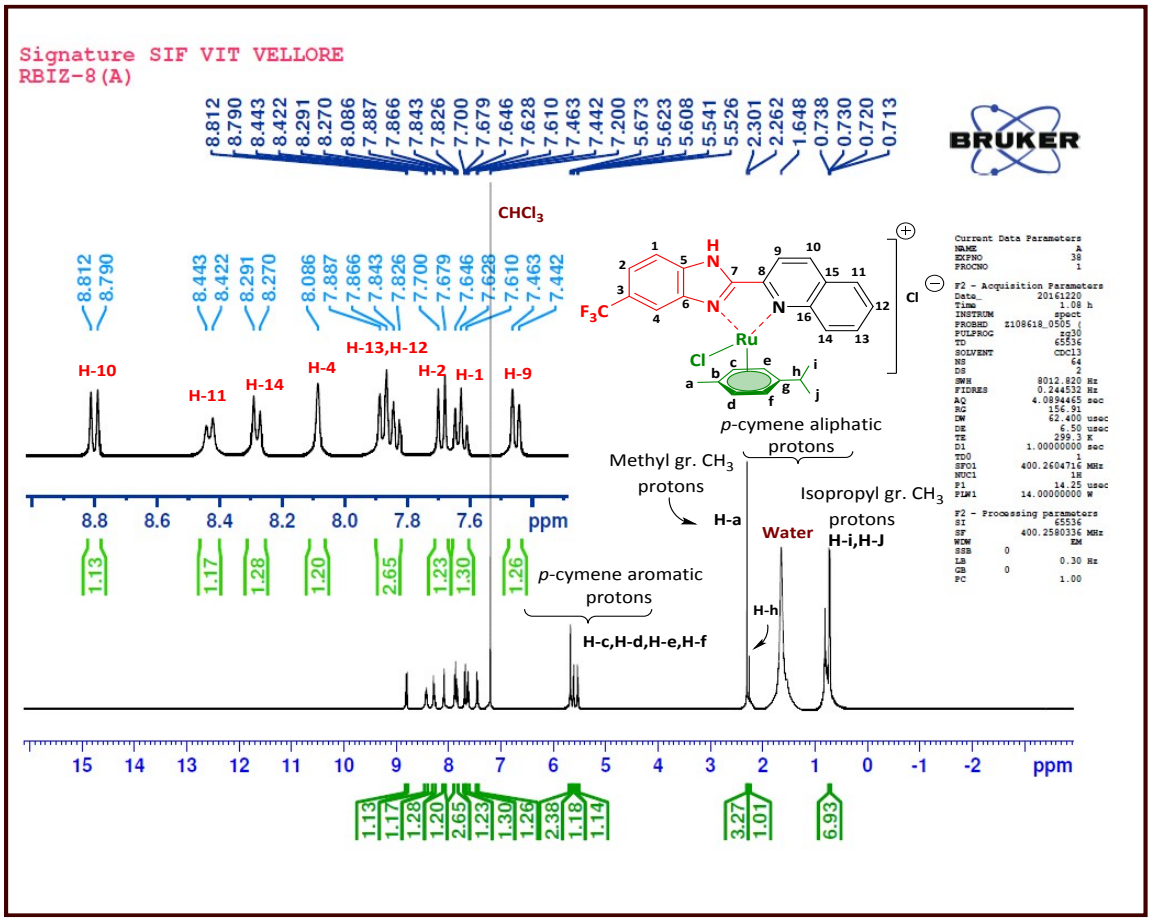
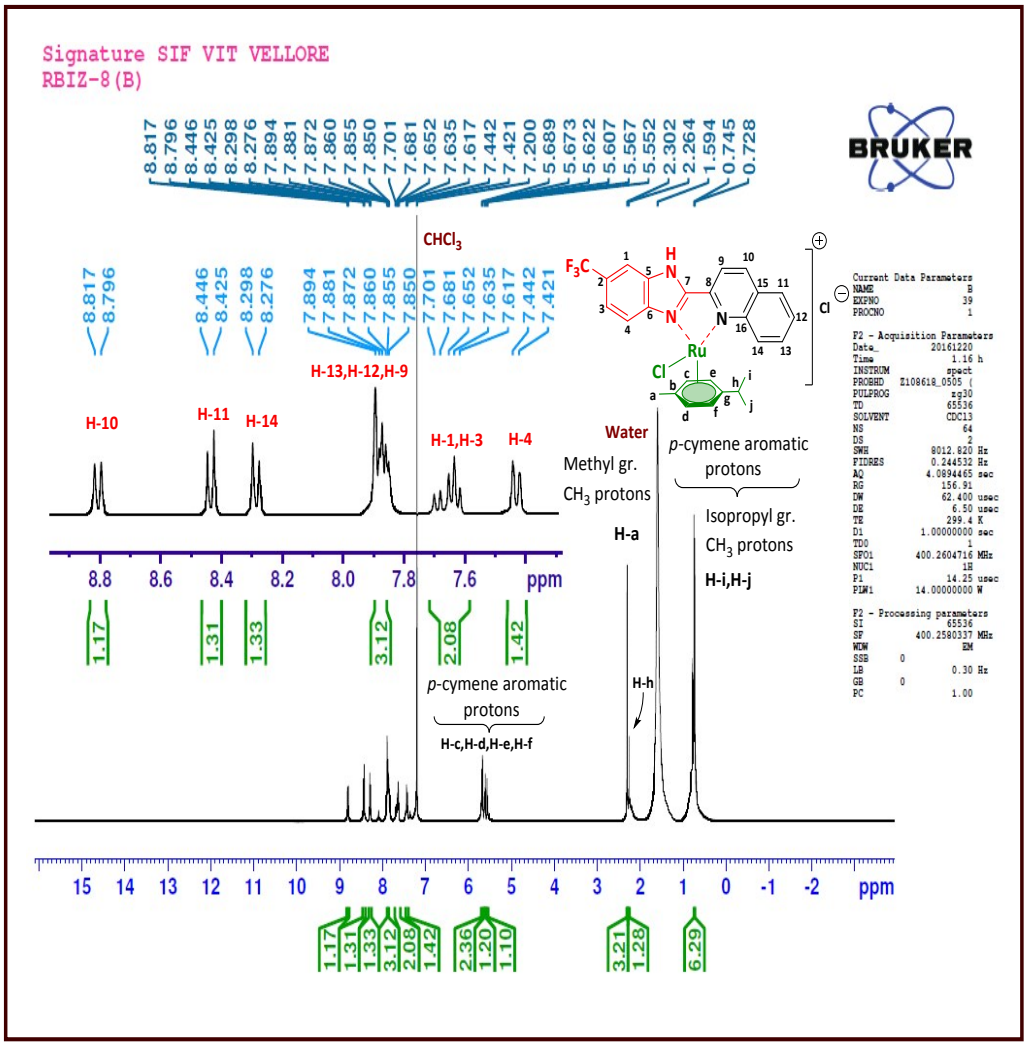


Fig. S1 TLC images of two isomers (8h = 11d and 8h′ = 11d′)



(Above)



(Below)

Fig. S2 ^{1}H NMR spectra of two separated isomers 11d (above) and 11d′ (below)

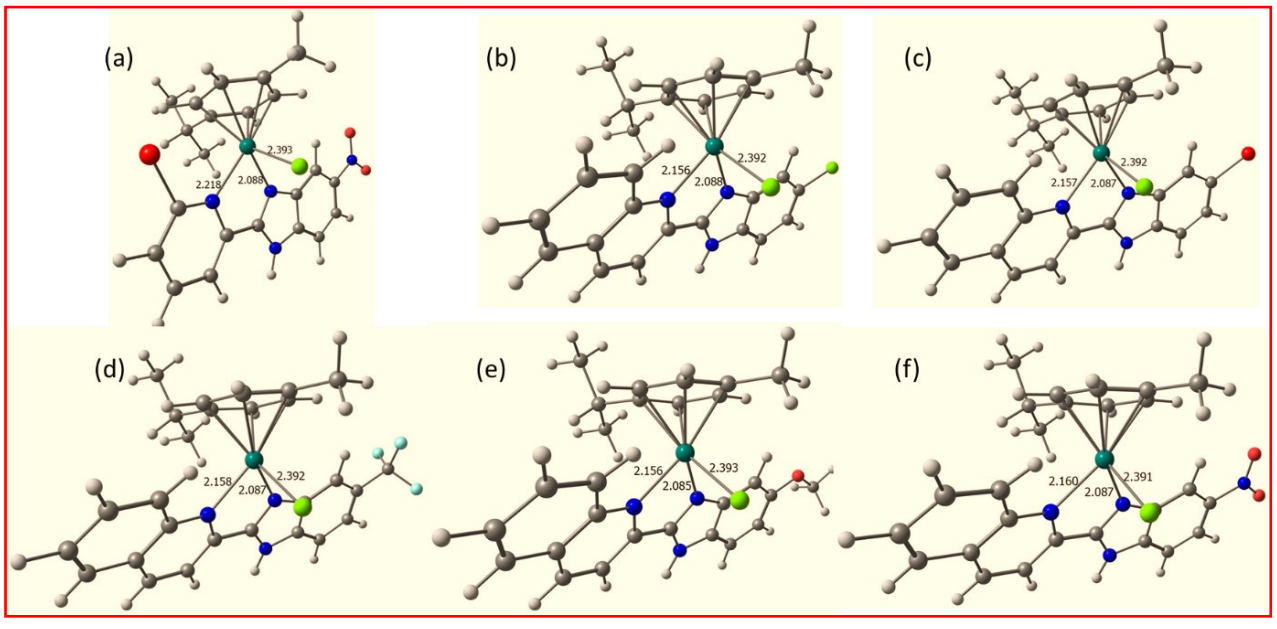


Fig. S3 DFT computed structure of the complexes (a) 5f (b) 11b (c) 11l (d) 11d (e) 11e (f) 11f.

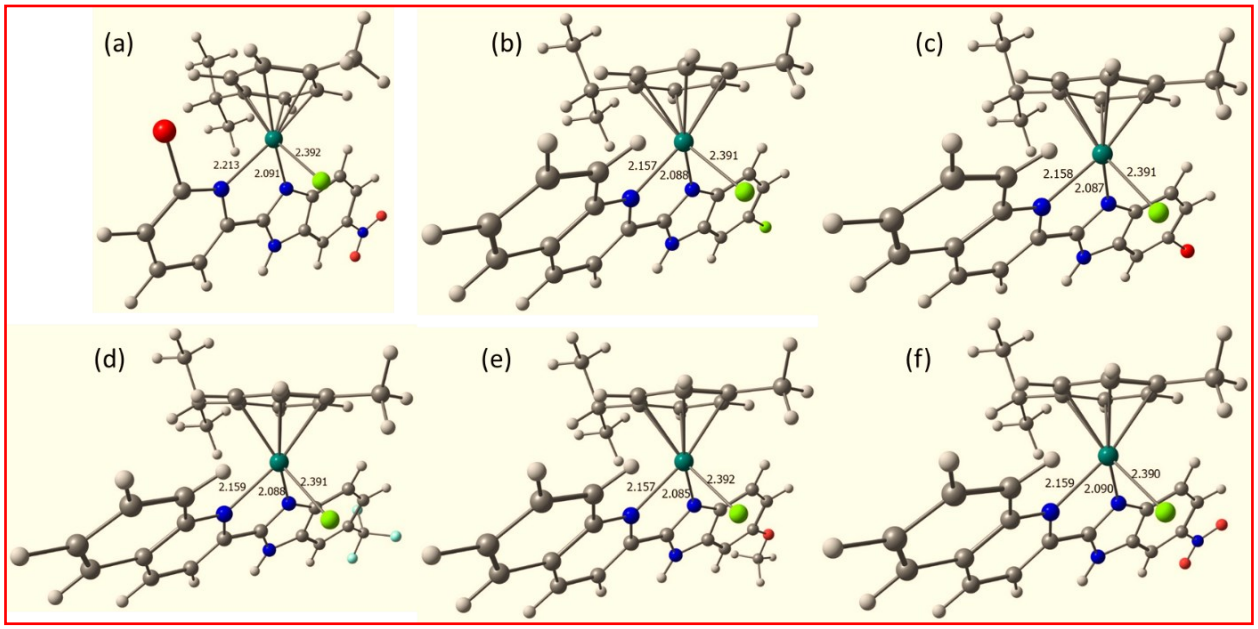


Fig. S4 DFT computed structure of the regioisomer of the complexes (a) 5f′ (b) 11b′ (c) 11l′ (d) 11d′ (e) 11e′ (f) 11f′.

Table S1 Calculated parameters of the complexes 5d, 5f, 11b, 11g, 11h, 11i, 11j and their regioisomers

Complex	Parameters of isomer 1				Parameters of isomer 2			
	E_T (a.u.)	E_{LUMO} (eV)	E_{HOMO} (eV)	ΔE	E_T (a.u.)	E_{LUMO} (eV)	E_{HOMO} (eV)	ΔE
5d	-4477.66866821	-0.16023	-0.38047	0.22024	-4477.66768295	-0.16091	-0.38127	0.22036
5f	-4345.13889634	-0.16673	-0.38417	0.21744	-4345.13700718	-0.16944	-0.38556	0.21612
11b	-2182.96620205	-0.16130	-0.37249	0.21119	-2182.96603210	-0.16110	-0.37237	0.21127
11l	-4294.27505340	-0.16094	-0.37221	0.21127	-4294.27483267	-0.16078	-0.37149	0.21071
11d	-2060.33098734	-0.16288	-0.37400	0.21112	-2060.33011619	-0.16344	-0.37499	0.21155
11e	-1837.85515419	-0.15427	-0.36065	0.20638	-1837.85717876	-0.15235	-0.35830	0.20595
11f	-1927.80137214	-0.16829	-0.37756	0.20927	-1927.79967194	-0.17050	-0.37924	0.20874

UV spectra of synthesized compounds

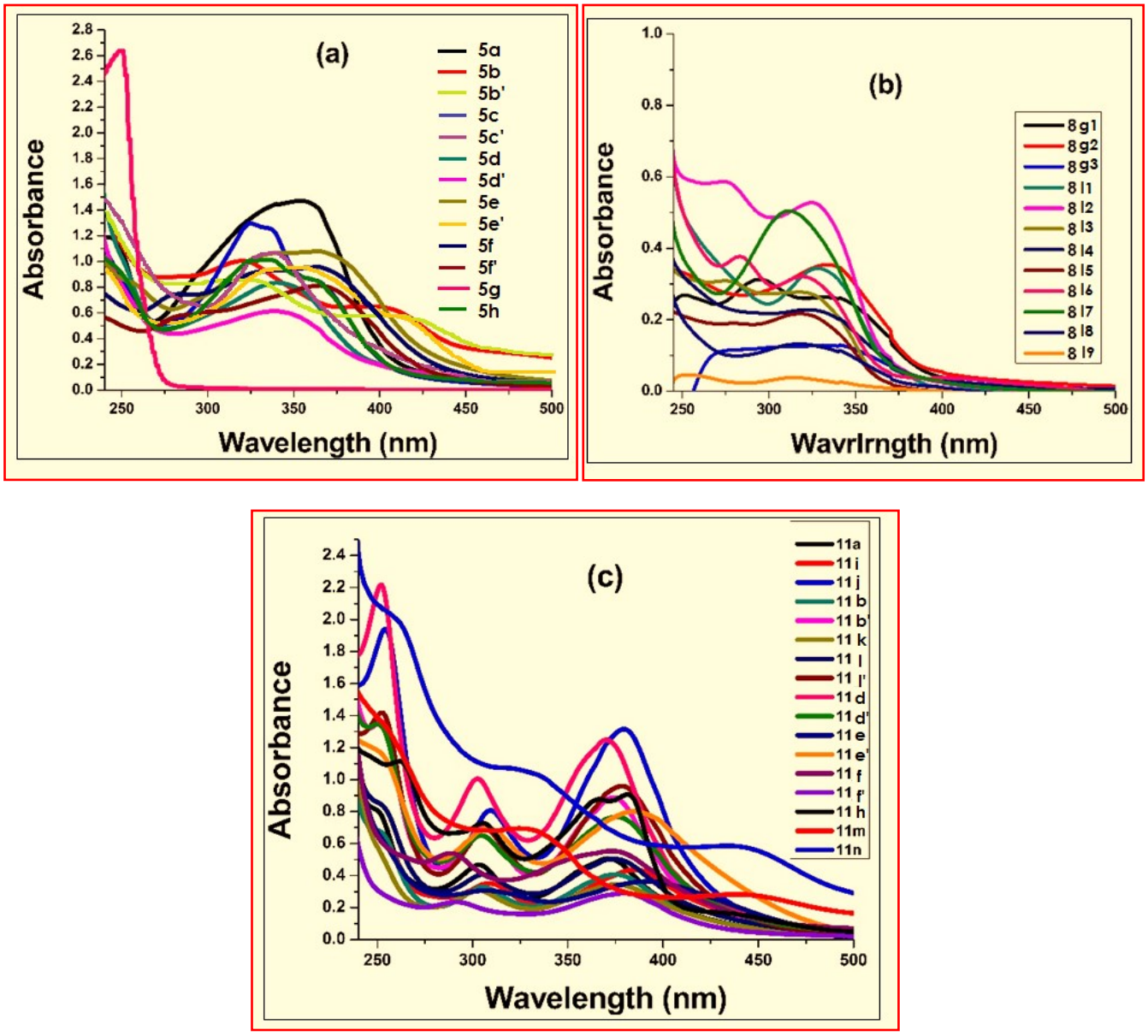


Fig. S5 UV absorption bands of (a)(η^6-*p*-cymene)Ruthenium(II)chlorido-2-(6-bromopyridinyl) BIZ, BTZ complexes; (b)(η^6-*p*-cymene)Ruthenium(II)chlorido-2-(6-arylpyridinyl) BIZ, BTZ complexes; (c)(η^6-*p*-cymene)Ruthenium(II)chlorido-2-quinolinyl BIZ, BTZ and BOZ complexes

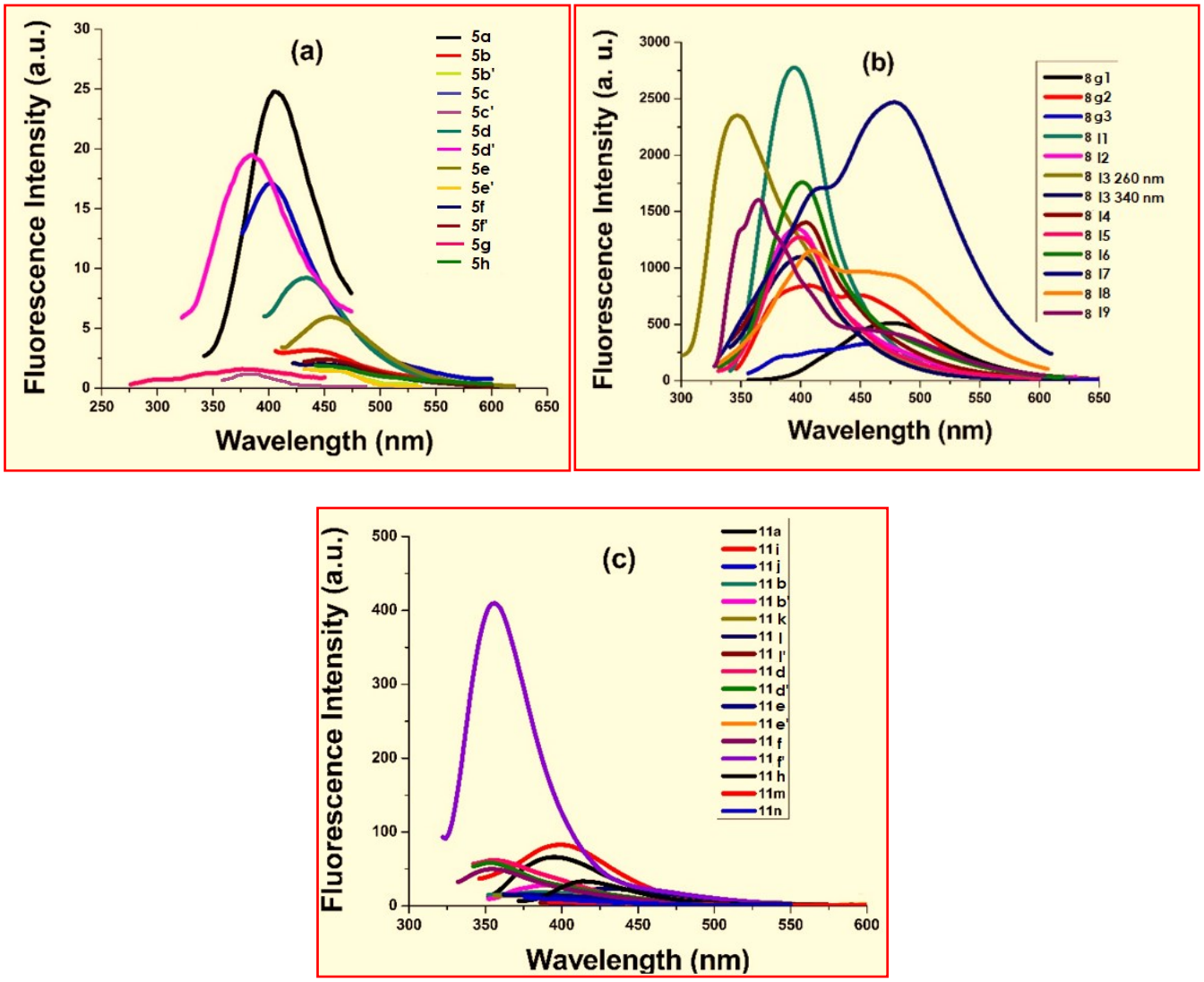


Fig. S6 Fluorescence emission bands of (a)(η^6-*p*-cymene)Ruthenium(II)chlorido-2-(6-bromopyridinyl) BIZ, BTZ complexes; (b)(η^6-*p*-cymene)Ruthenium(II)chlorido-2-(6-arylpyridinyl) BIZ, BTZ complexes (c)(η^6-*p*-cymene)Ruthenium(II)chlorido-2-quinolinyl BIZ, BTZ & BOZ complexes

Table S2 Solubility, lipophilicity and conductivity study of the synthesized ruthenium complexes

Samples	Solubility (M)[a]	Log P[b]	Λ_M[c](S cm^{2}M^{-1})	
			DMSO (pure)	DMSO (10%)
5a	0.060	0.69±0.05	28	32
5b	0.063	0.86±0.07	29	30
5b′	0.061	0.90±0.06	28	30
5c	0.068	1.4±0.07	30	35
5c′	0.065	1.29±0.05	31	34
5d	0.067	1.34±0.07	29	35
5d'	0.067	1.32±0.03	30	36
5e	0.071	0.66±0.09	31	37
5e′	0.078	0.68±0.07	32	38
5f	0.072	1.14±0.07	29	33
5f'	0.072	1.07±0.05	30	34
5g (less soluble)	0.024	0.79±0.07	32	35
5h	0.076	0.92±0.04	33	38
8g1	0.071	0.93±0.08	34	39
8g2	0.072	0.95±0.07	35	40
8g3	0.074	0.96±0.05	33	39
8l1	0.070	0.97±0.09	33	38
8l2	0.075	0.99±0.08	34	40
8l3	0.076	1.17±0.06	32	35
8l4	0.069	1.19±0.08	35	39
8l5	0.064	1.21±0.07	35	39
8l6	0.070	1.23±0.05	32	38
8l7	0.072	1.19±0.07	34	37
8l8	0.071	1.20±0.1	32	39
8l9	0.075	0.99±0.07	32	39
11a	0.069	0.92±0.08	30	37
11b	0.071	1.3±0.1	31	36
11b'	0.071	1.4±0.07	29	38
11d	0.082	1.45±0.07	28	34
11d'	0.082	1.34±0.08	29	36
11e	0.071	1.2±0.07	32	38
11e'	0.071	1.1±0.17	31	37
11f	0.069	0.97±0.1	34	36
11f'	0.069	0.92±0.08	35	40
11h	0.068	0.97±0.07	30	35
11i	0.064	1.17±0.1	32	37
11j	0.066	1.30±0.04	34	38
11k	0.067	1.35±0.08	29	35
11k′	0.062	1.34±0.09	30	40
11l	0.074	1.07±0.06	32	38
11l'	0.074	1.04±0.09	33	37
11m	0.069	0.97±0.17	34	38
11n	0.071	0.99±0.04	34	39

[a]DMSO-10% DMEM medium (1:99 v/v, comparable to cell media), [b]n-Octanol/Water Partition Coefficients, [c]Molar Conductance

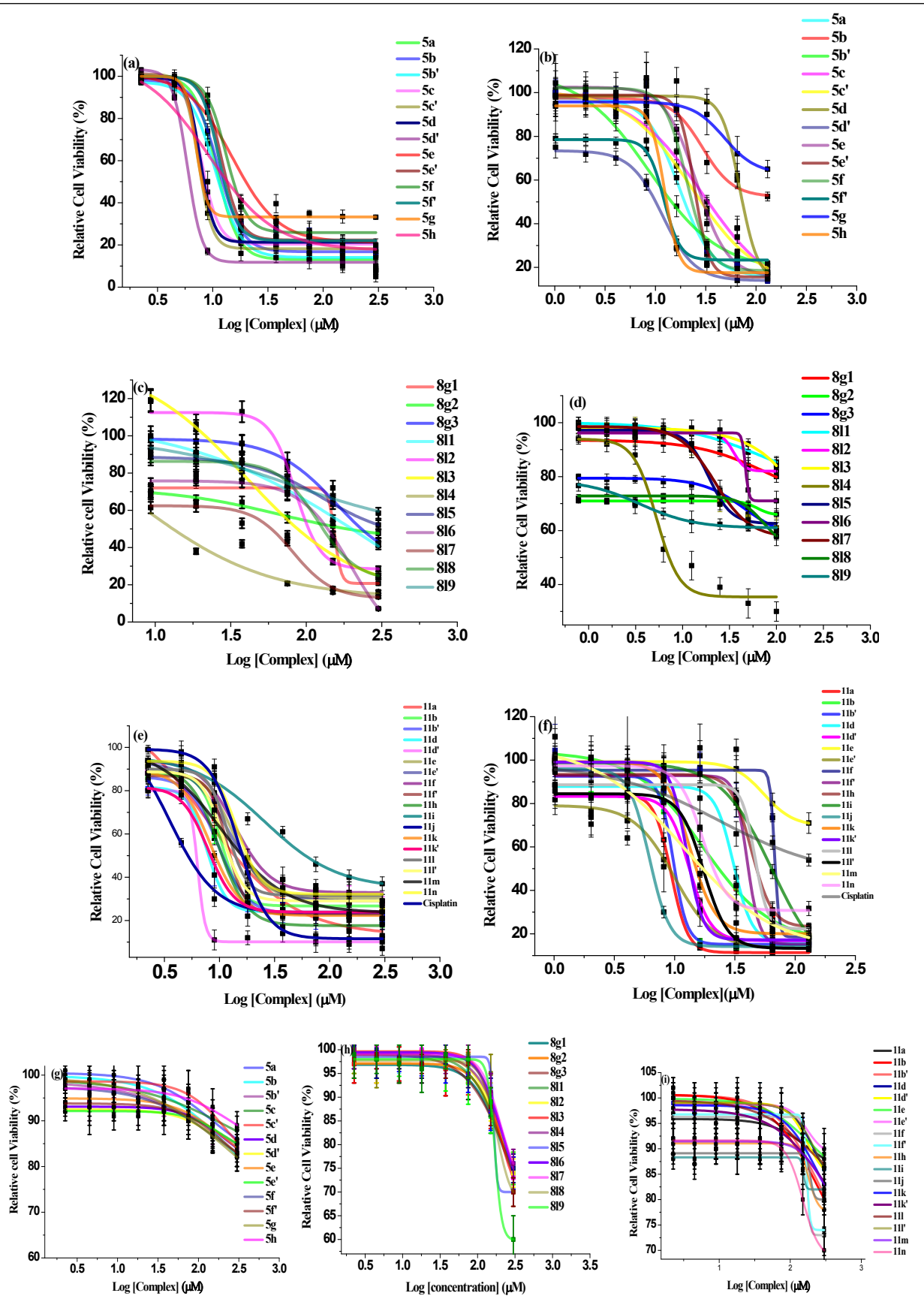
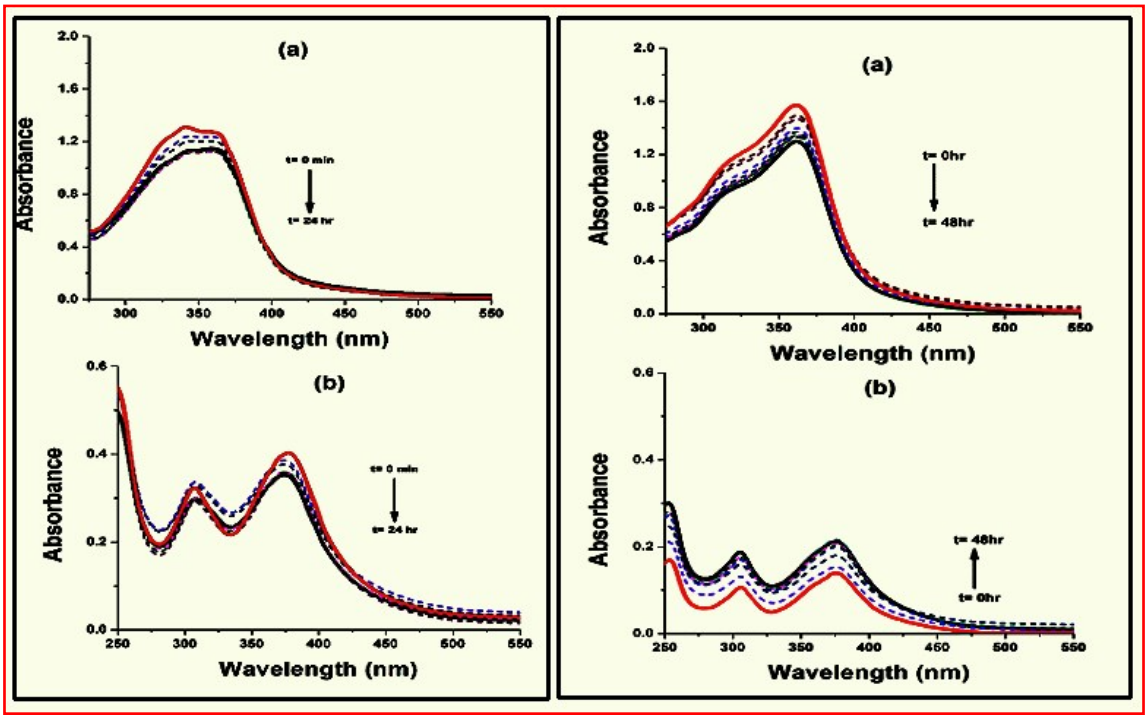
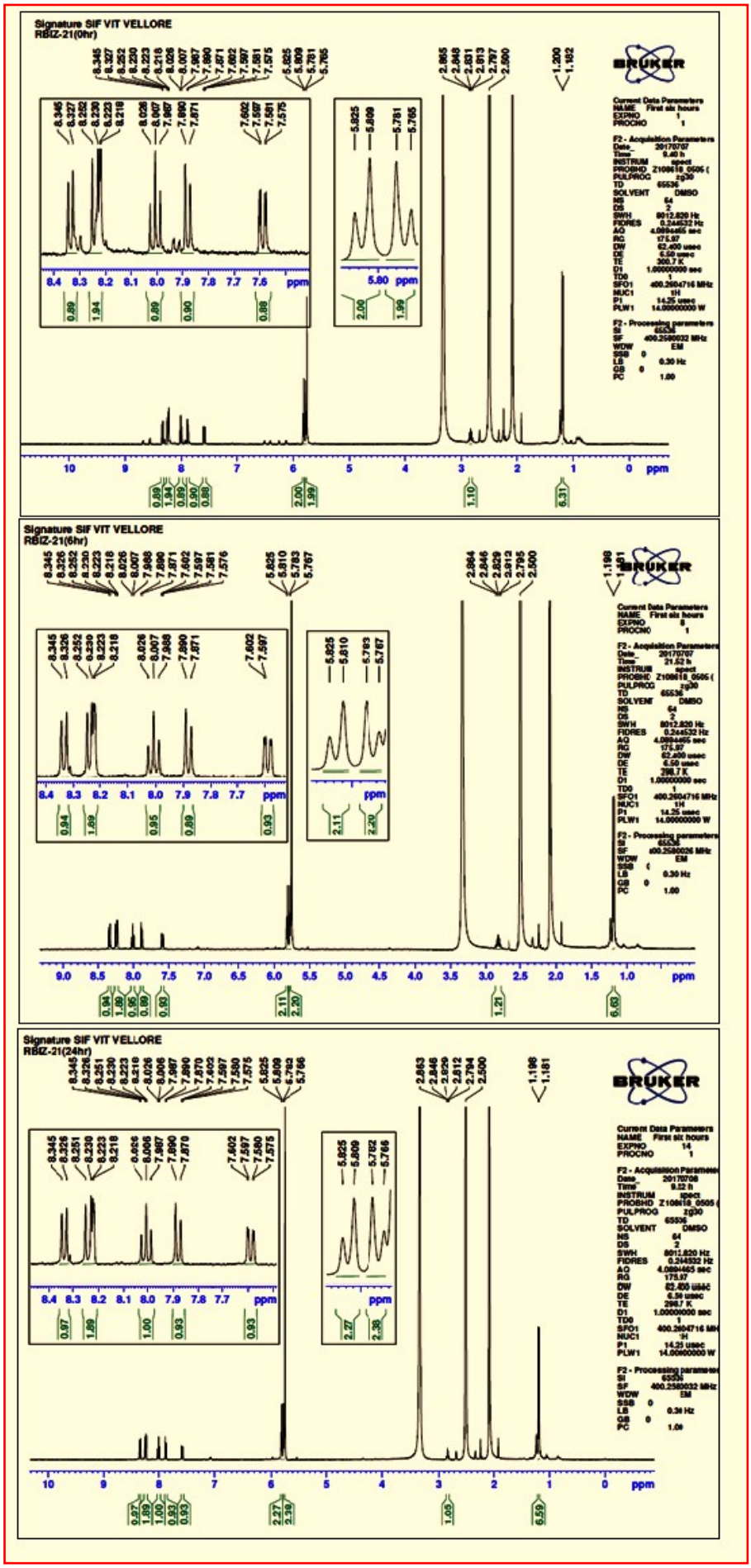


Fig. S7 Comparison of cytotoxicity for complexes 5a-h in (a) HeLa (b) CaCo-2 and (g) HEK-293 cell line; complexes 8g1-8l9 in (c) HeLa (d) CaCo-2 and (h) HEK-293 cell line; complexes 11a-n in (e) HeLa (f) CaCo-2 and (i) HEK-293 cell line



(Left) **(Right)**

Fig. S8. Left: UV-Vis absorption band of complexes (a) 5h and (b) 11j (c = 2×10^{-5} M) in 5% DMSO in phosphate buffer, pH = 7.4 with time interval. Right: UV-Vis absorption band of complexes (a) 5h and (b) 11j (c = 2×10^{-5} M) in (Water pH 7.4)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BRUKER
Signature SIF VIT VELLORE
RBIZ-21(6hr)
BRUKER
Signature SIF VIT VELLORE
RBIZ-21(24hr)
BRUKER

Fig. S9 NMR spectra of compound 5h in DMSO-d_6 recorded at 0th, 6th and 24th h after dissolving in solvent

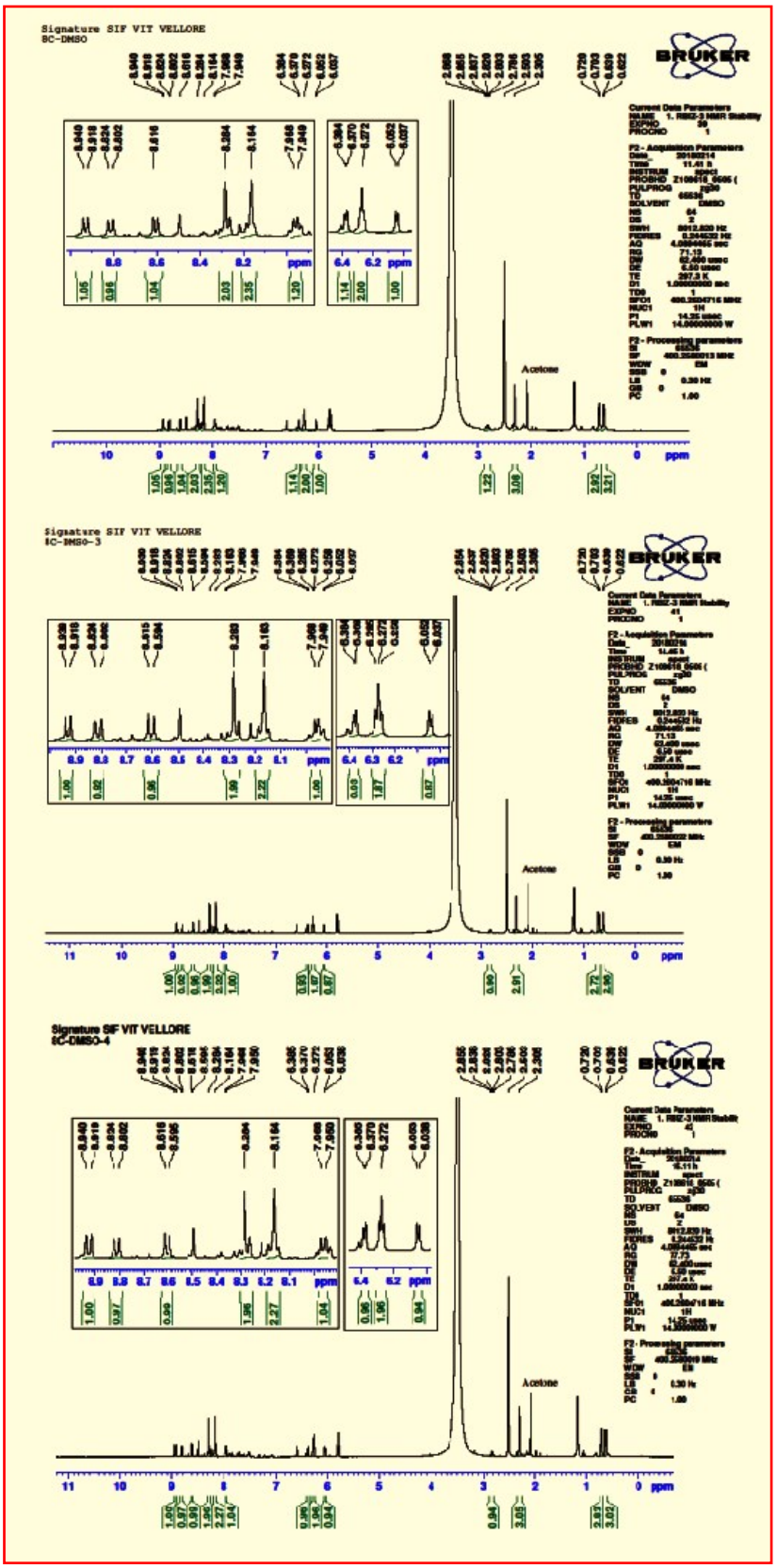


Fig. S10 NMR spectra of compound 11j in DMSO-d_6 recorded at 0th, 6th and 24th h after dissolving in solvent

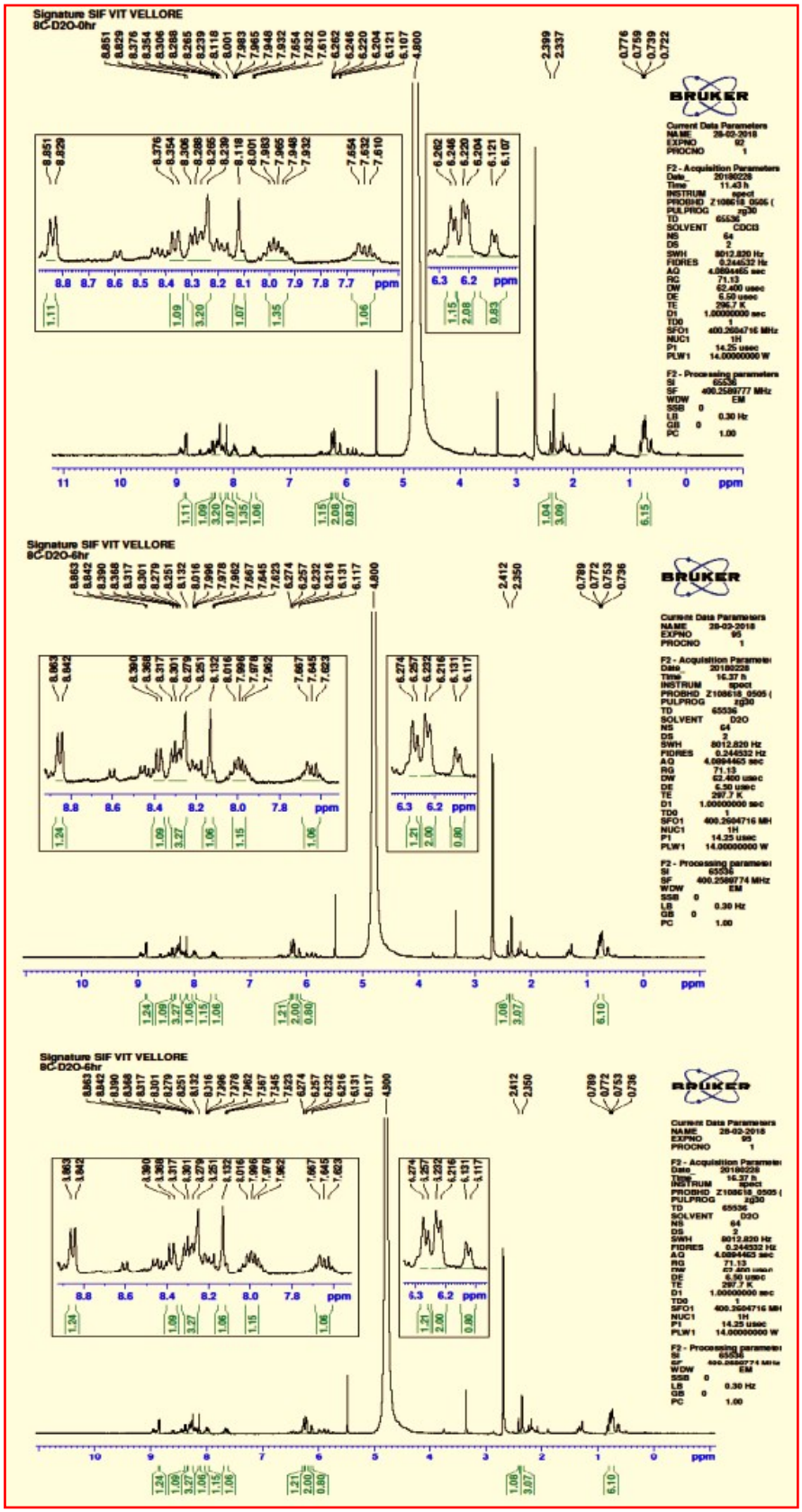


Fig. S11 NMR spectra of compound 11j in D_2O recorded at 0th, 6th and 24th hour after dissolving in solvent (PH 7.4)

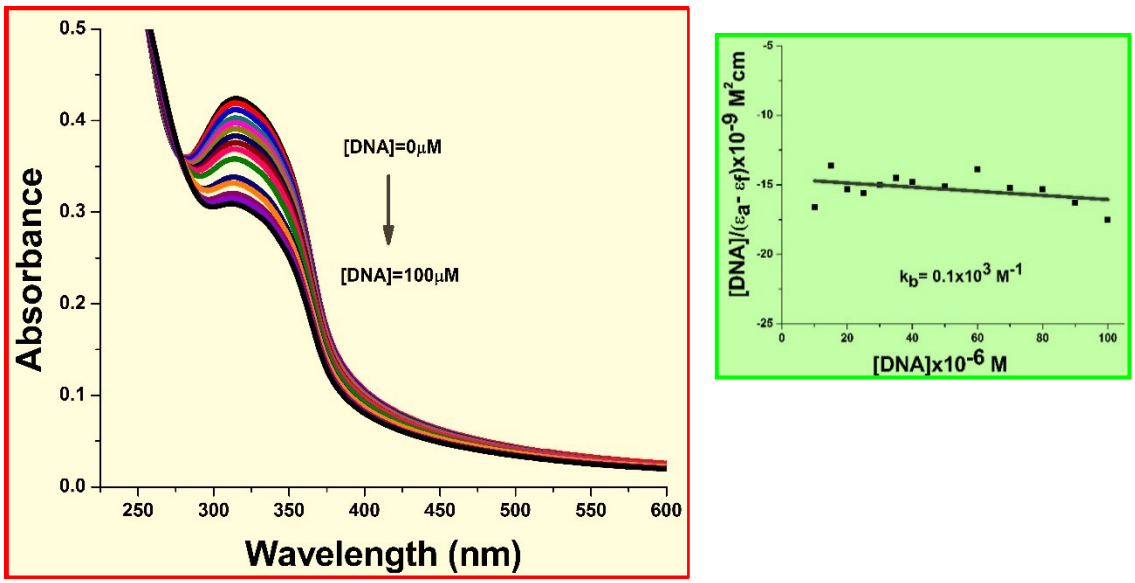


Fig. S12 UV-vis absorption spectrum of moderately potent compound 8l7 in absence and in presence of 10, 15, 20, ……. 90, 95, 100 μM of ct-DNA in TrisHCl buffer (pH 7.4, T = 25 °C). Change in absorbance with increasing DNA concentration happened in the direction of arrow. Inset: plot of [DNA]/(ε_a- ε_f) vs [DNA] for 8l7

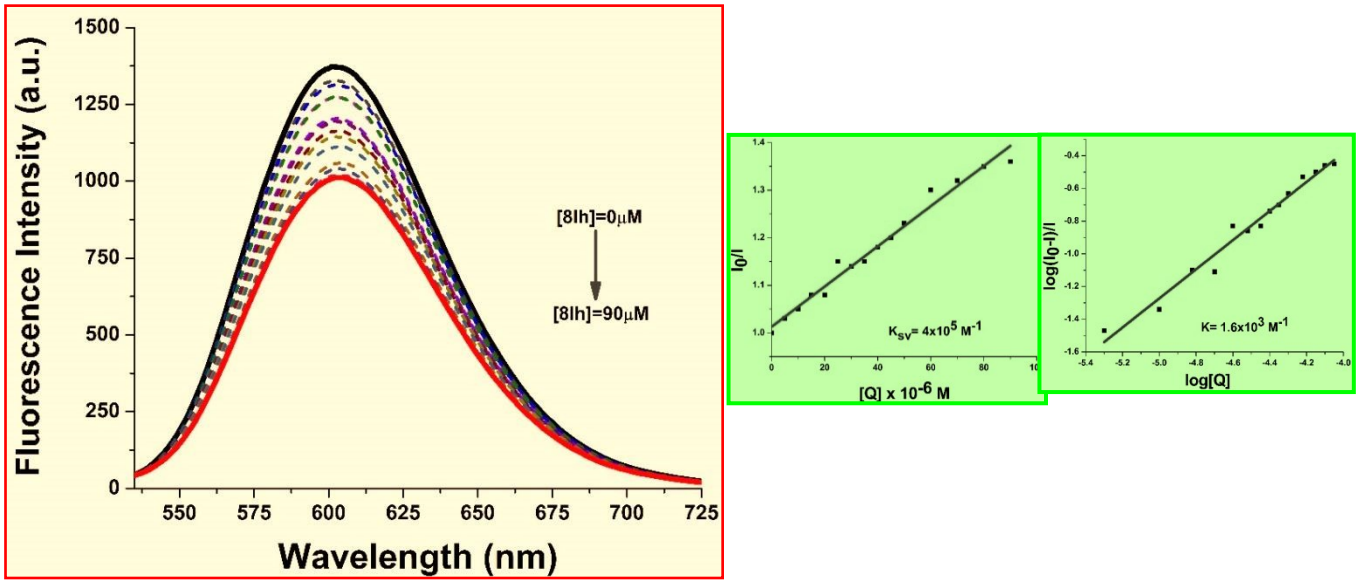


Fig. S13 Fluorescence emission spectra (λ_{ex}= 485 nm) of Ct-DNA-EtBr complex in Tris-HCl buffer (pH 7.4, T = 25 °C) in absence and presence of 5, 10, 15, 20, ….80, 85 μM of compound 8l7. Inset: plot of I_0/I *vs.* [Q]. and Plot of log [(I_0− I)/I] *vs.* log [Q] for compound 8l7

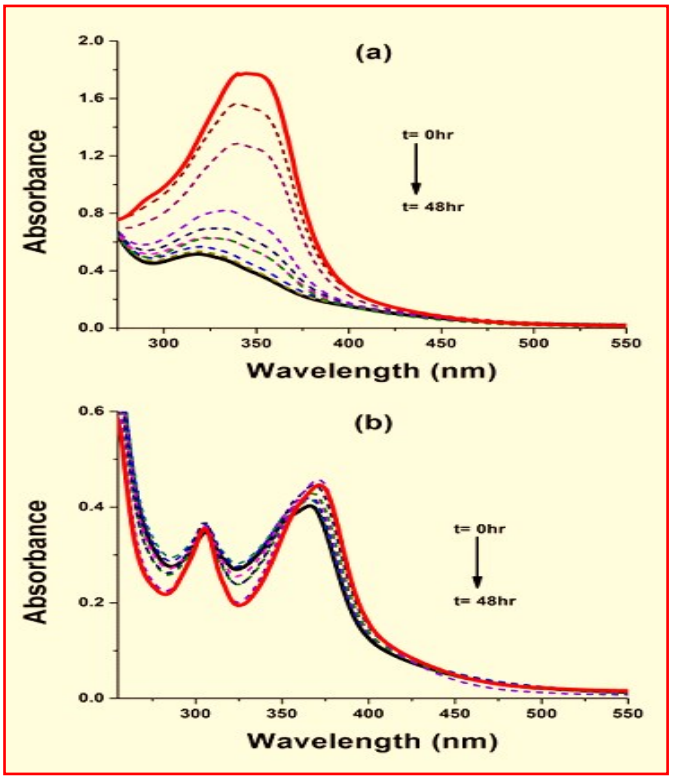
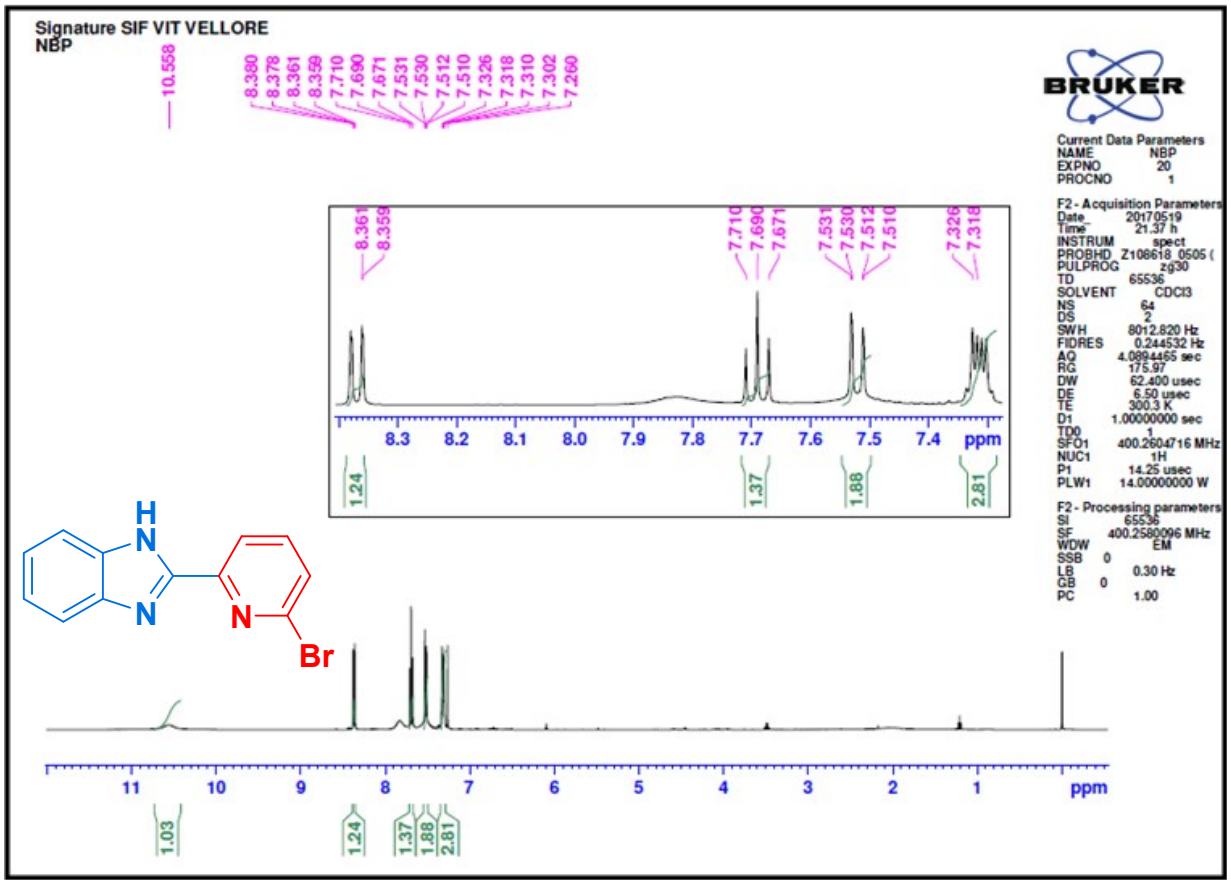


Fig. S14 UV-Vis absorption band of complexes (a) 5h and (b) 11j (c = 2×10^{-5} M) in 1 mM GSH

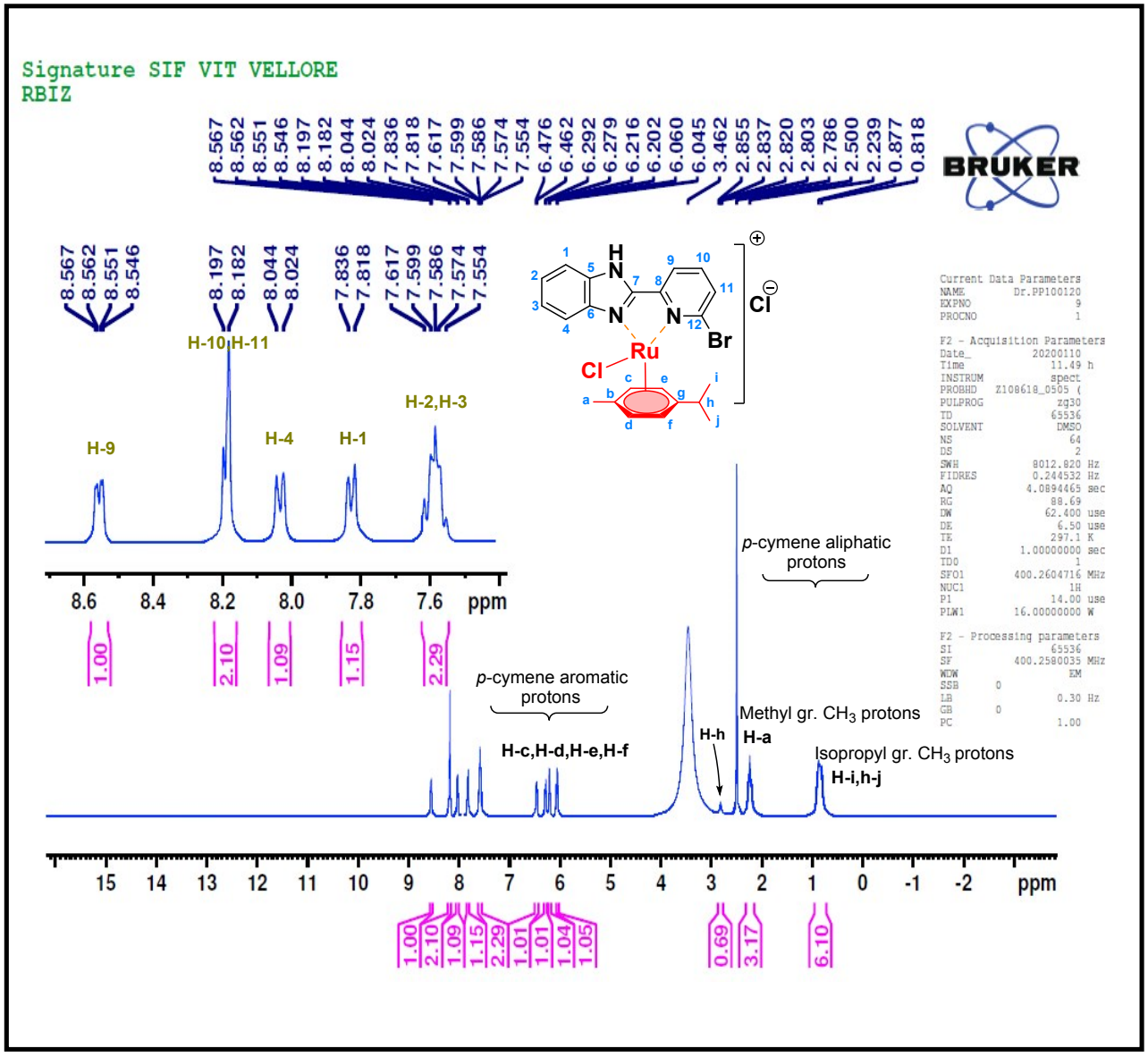
Pyridine Series

^{1}H NMR of ligand 3a

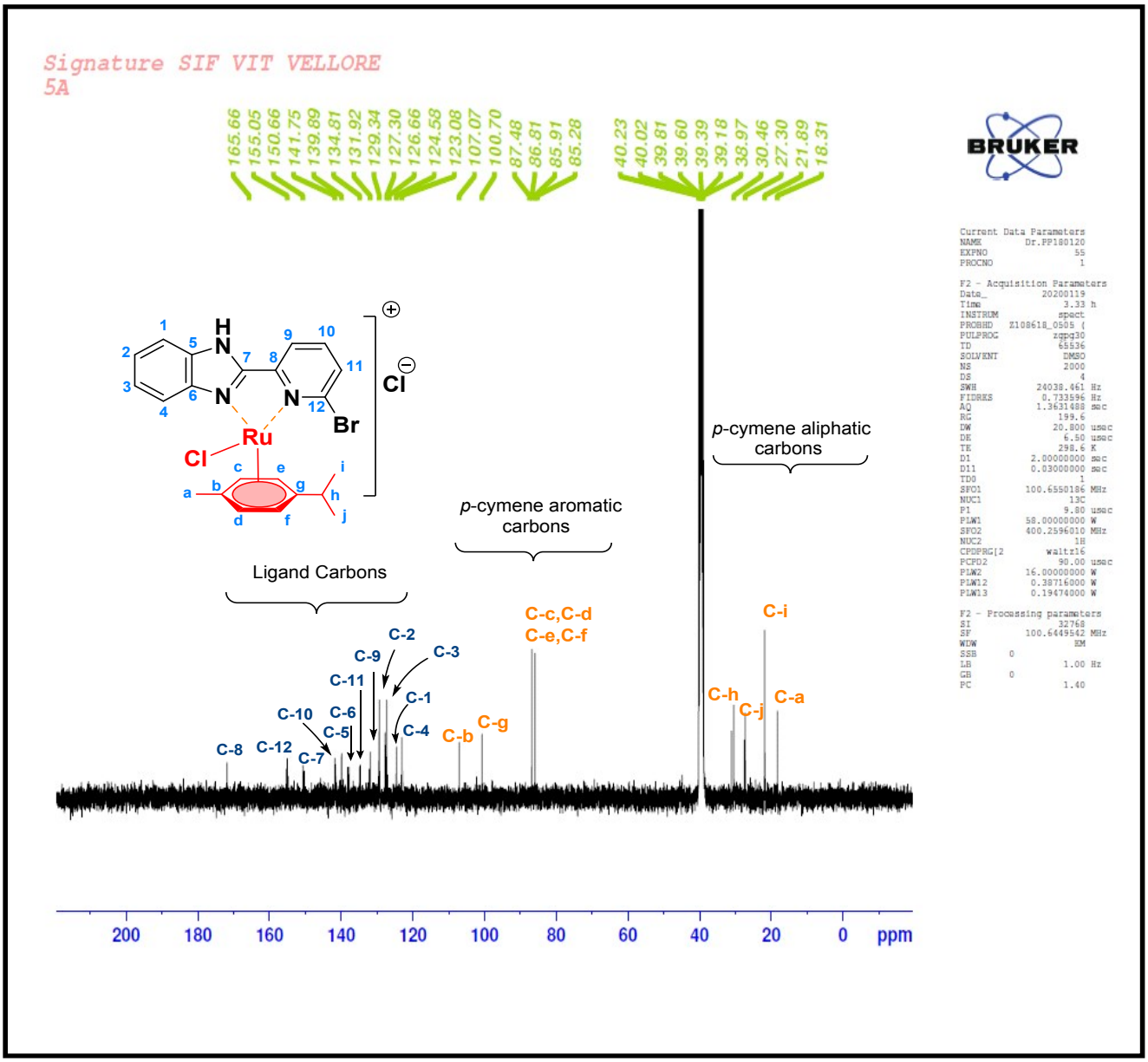


^{1}H and ^{13}C NMR of complex 5a-h

5a



5a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85.91
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18.31
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p-cymene aromatic carbons
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C-e,C-f
C-i
C-h
C-j
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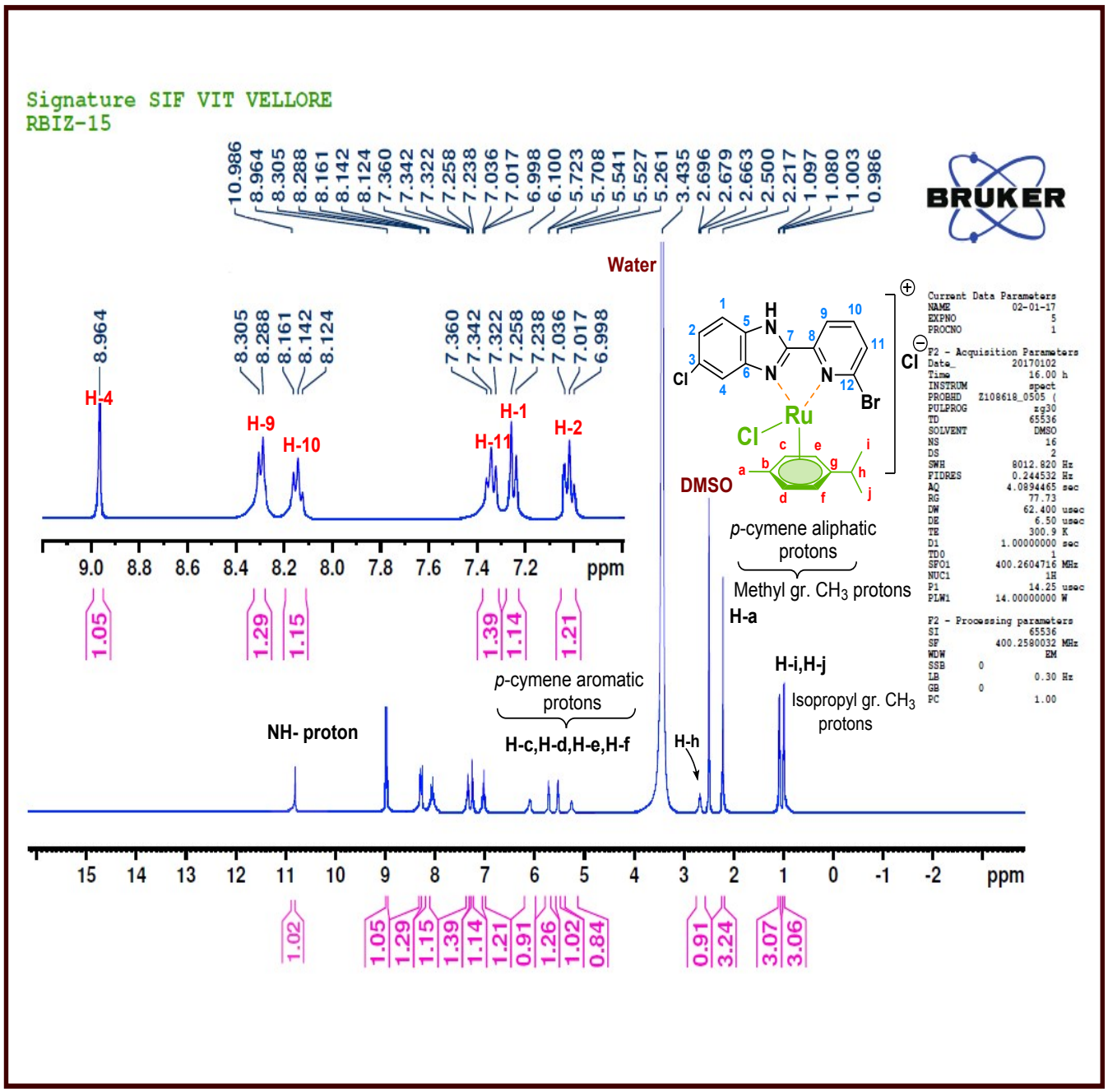
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Methyl gr. CH3 protons
H-a
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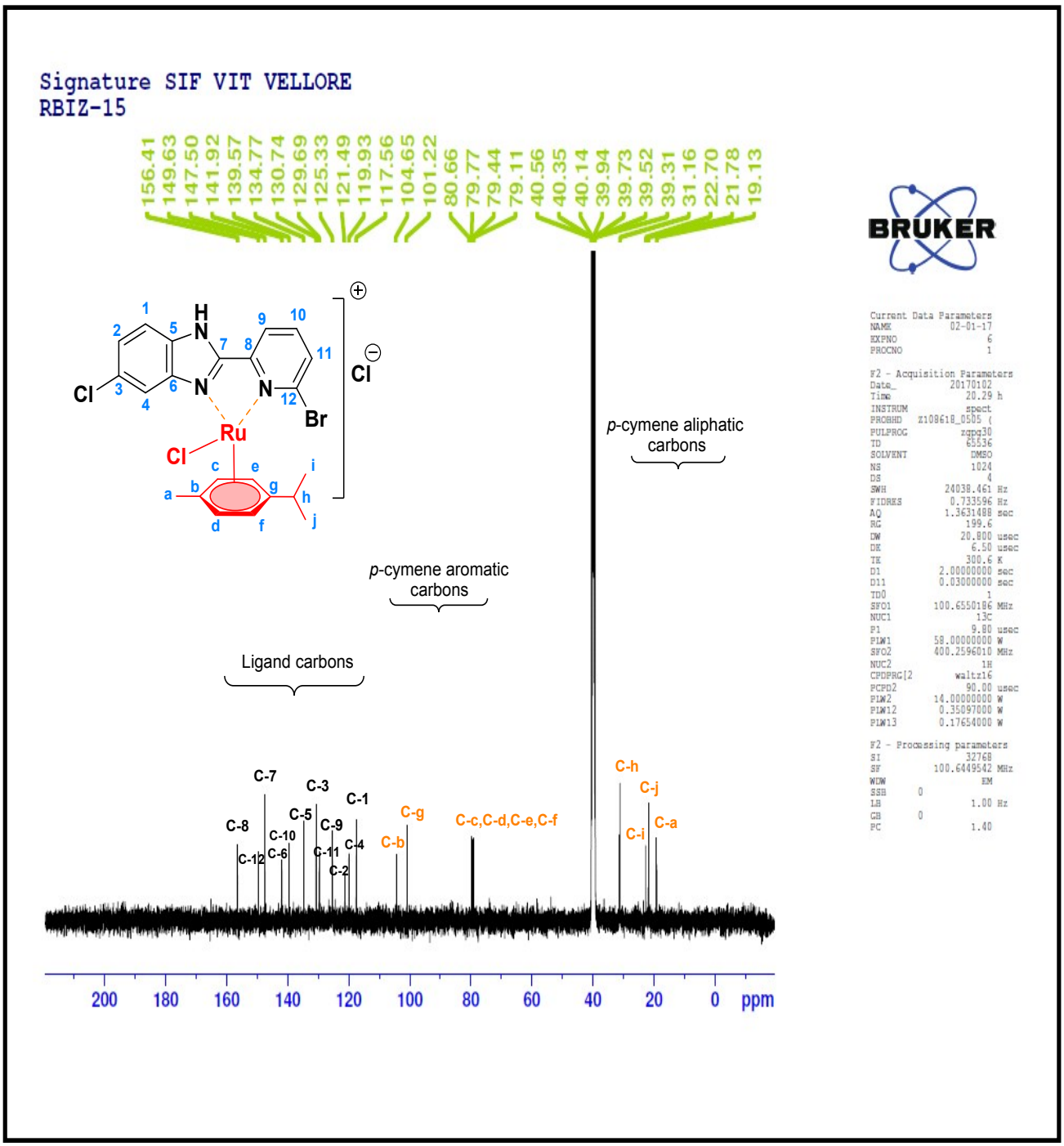
H-h
ppm

5b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Ligand carbons
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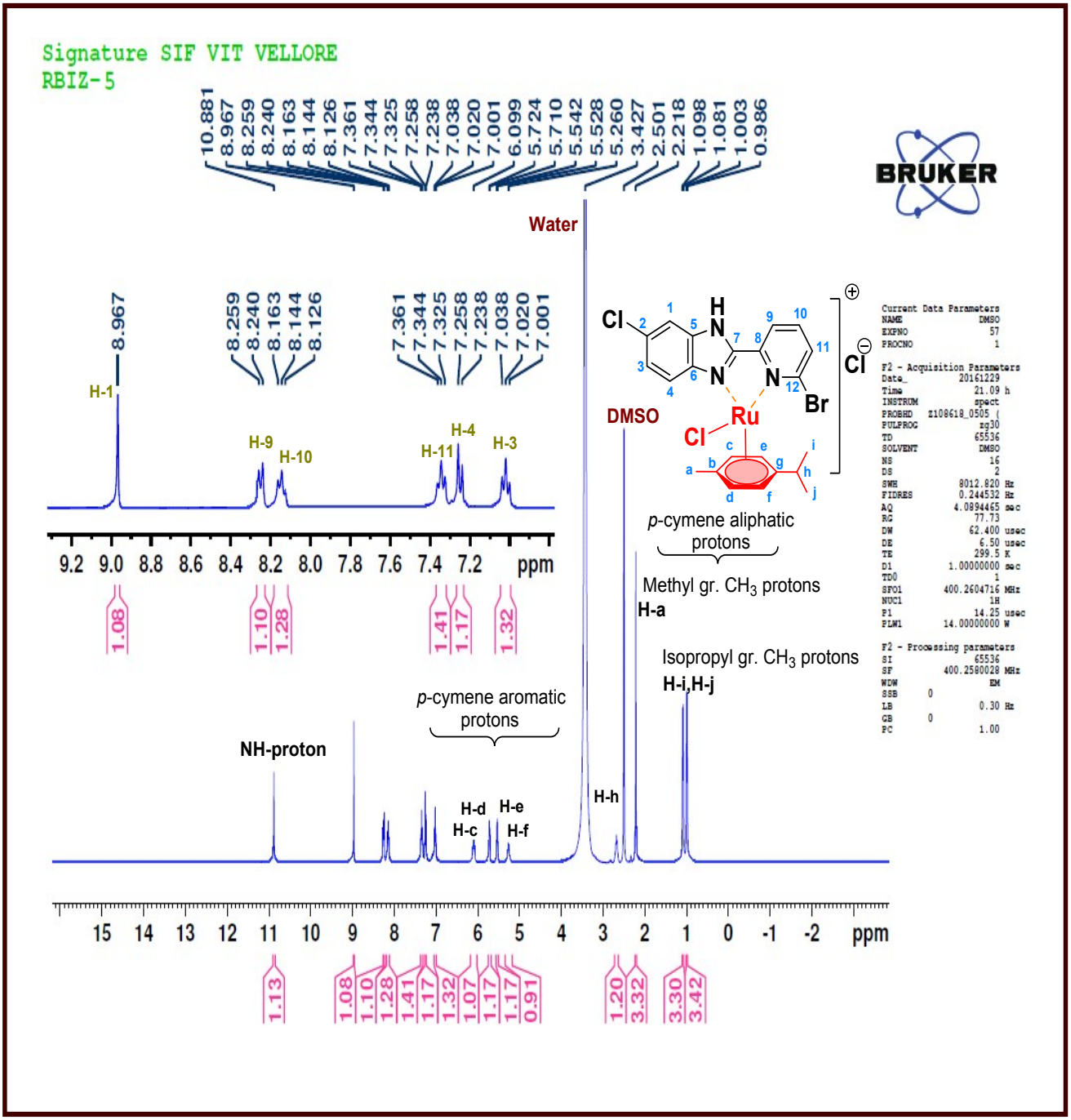
5b′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H-c
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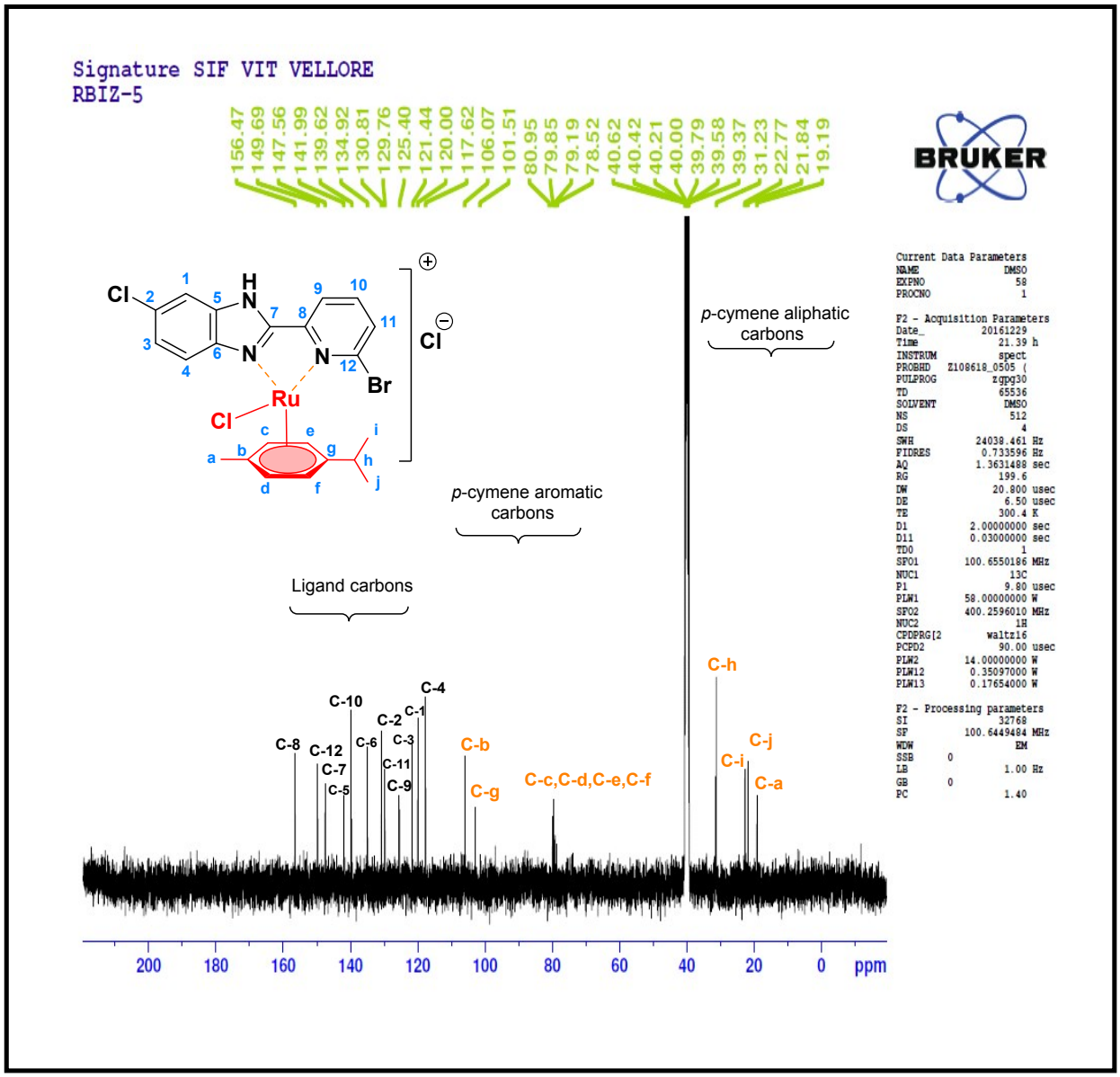
5b′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p-cymene aromatic carbons
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C-j
C-i
C-a
C-b
C-g
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NUC2 1H
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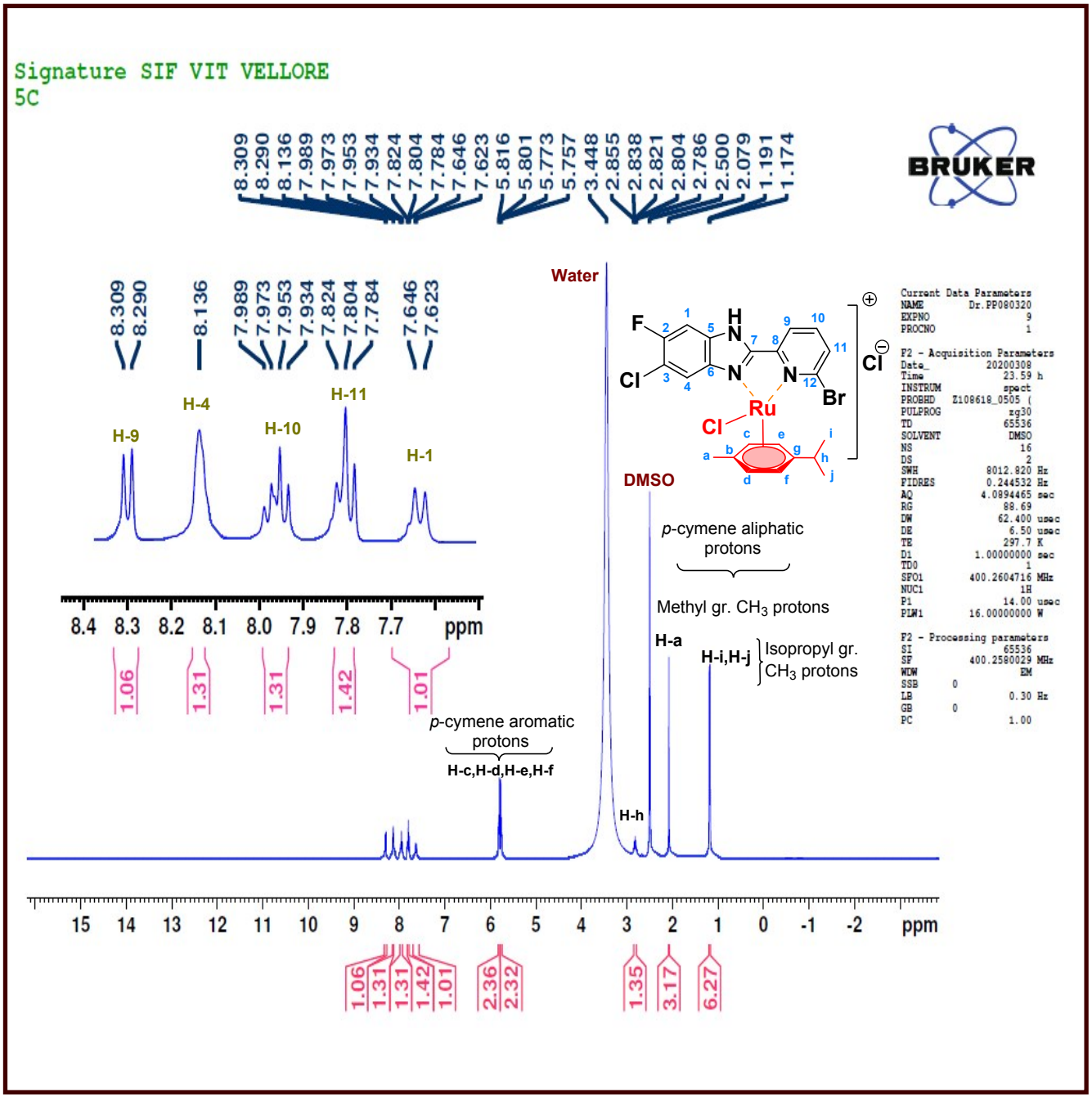
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BRUKER
H-9
H-4
H-10
H-11
H-1
Water
DMSO
H-h
H-a
H-i,H-j
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p-cymene aliphatic protons
Methyl gr. CH3 protons
p-cymene aromatic protons
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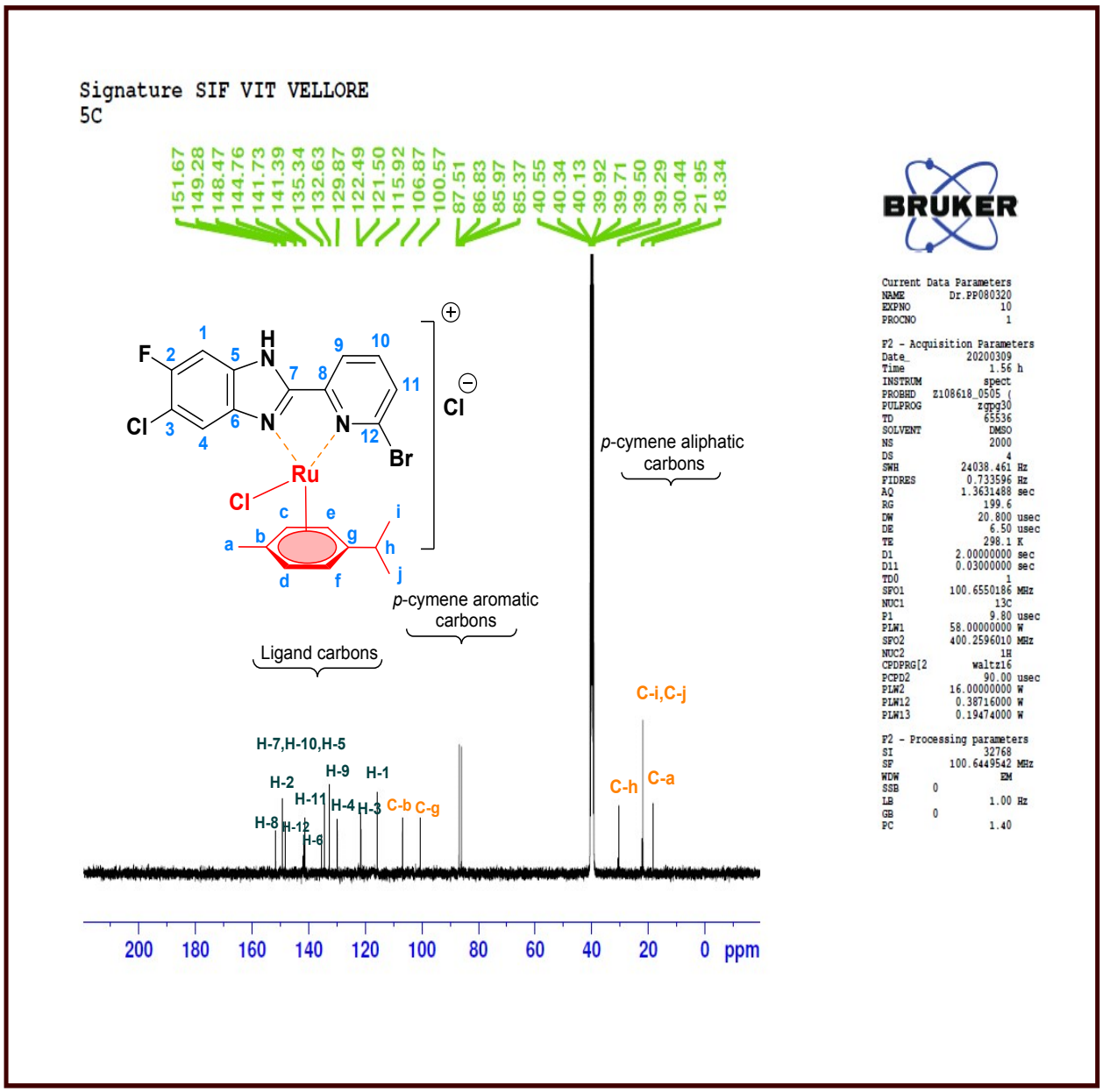
5c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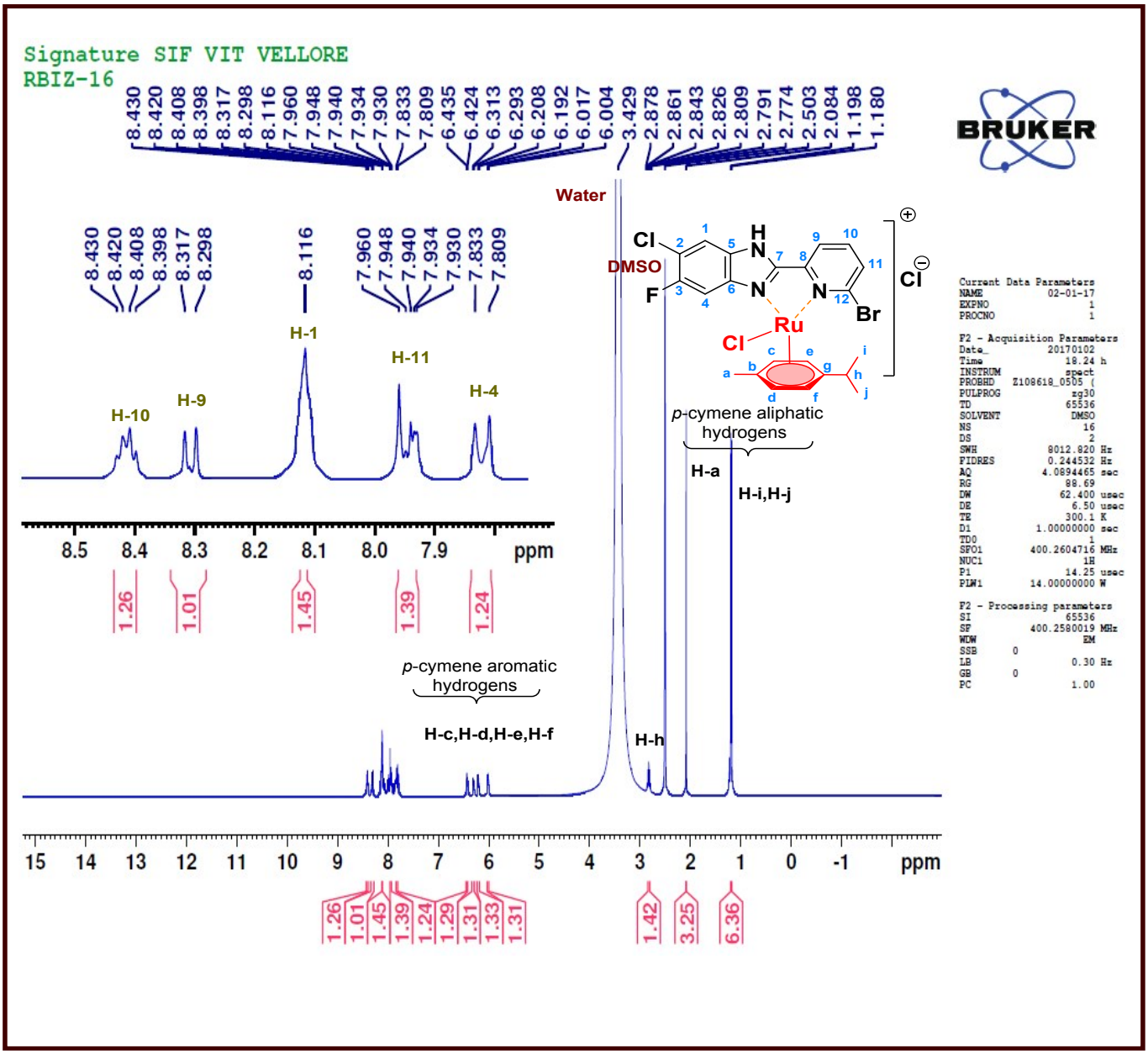
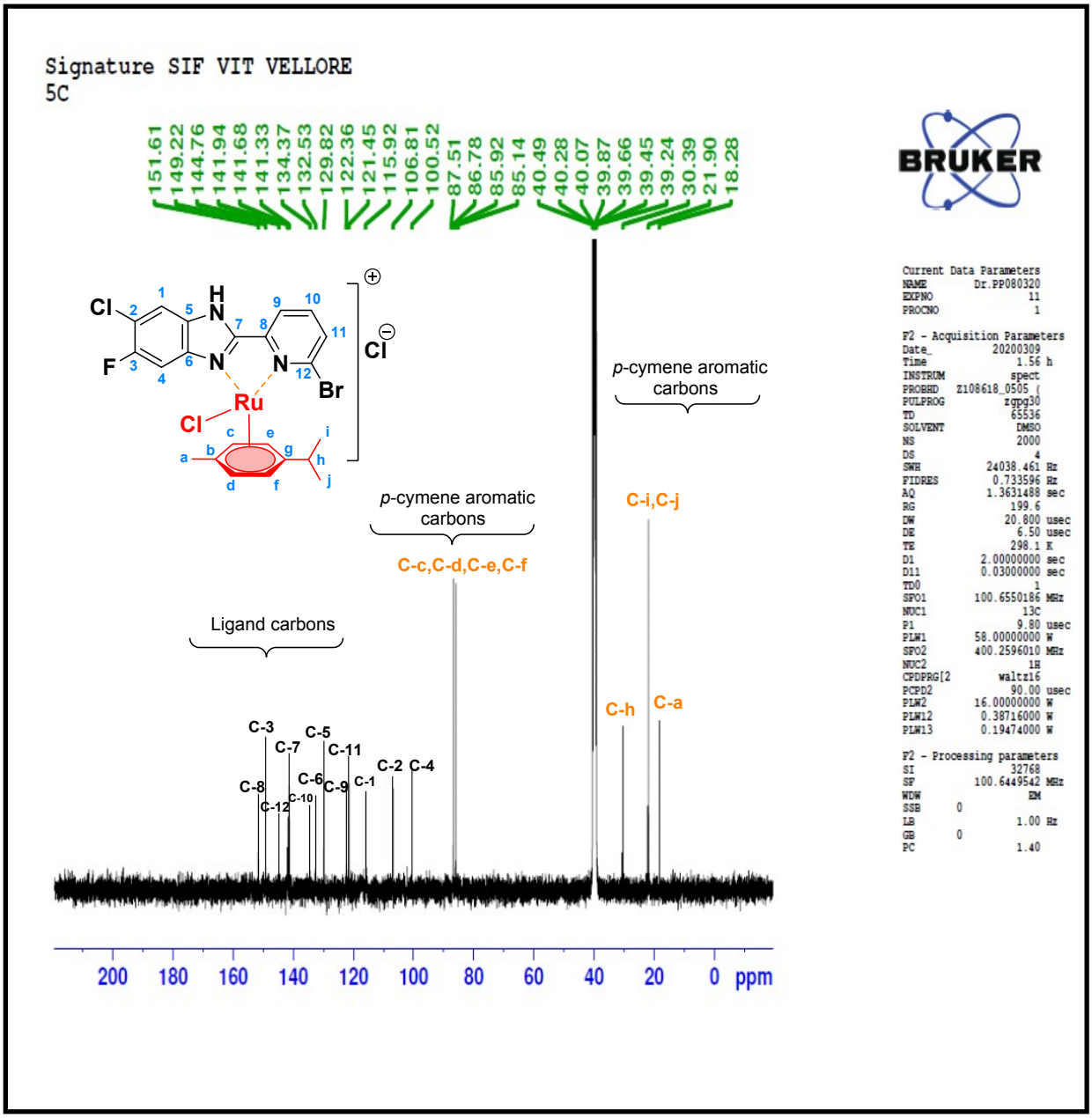
39.92
39.71
39.50
39.29
30.44
21.95
18.34
BRUKER
Current Data Parameters
NAME Dr.PP080320
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200309
Time 1.56 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 298.1 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
F
Cl
Cl
Ru
Br
N
H
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-i,C-j
C-h
C-a
H-7,H-10,H-5
H-9
H-1
H-2
H-11
H-4
H-3
C-b
C-g
H-8
H-12
H-6
200
180
160
140
120
100
80
60
40
20
0
ppm

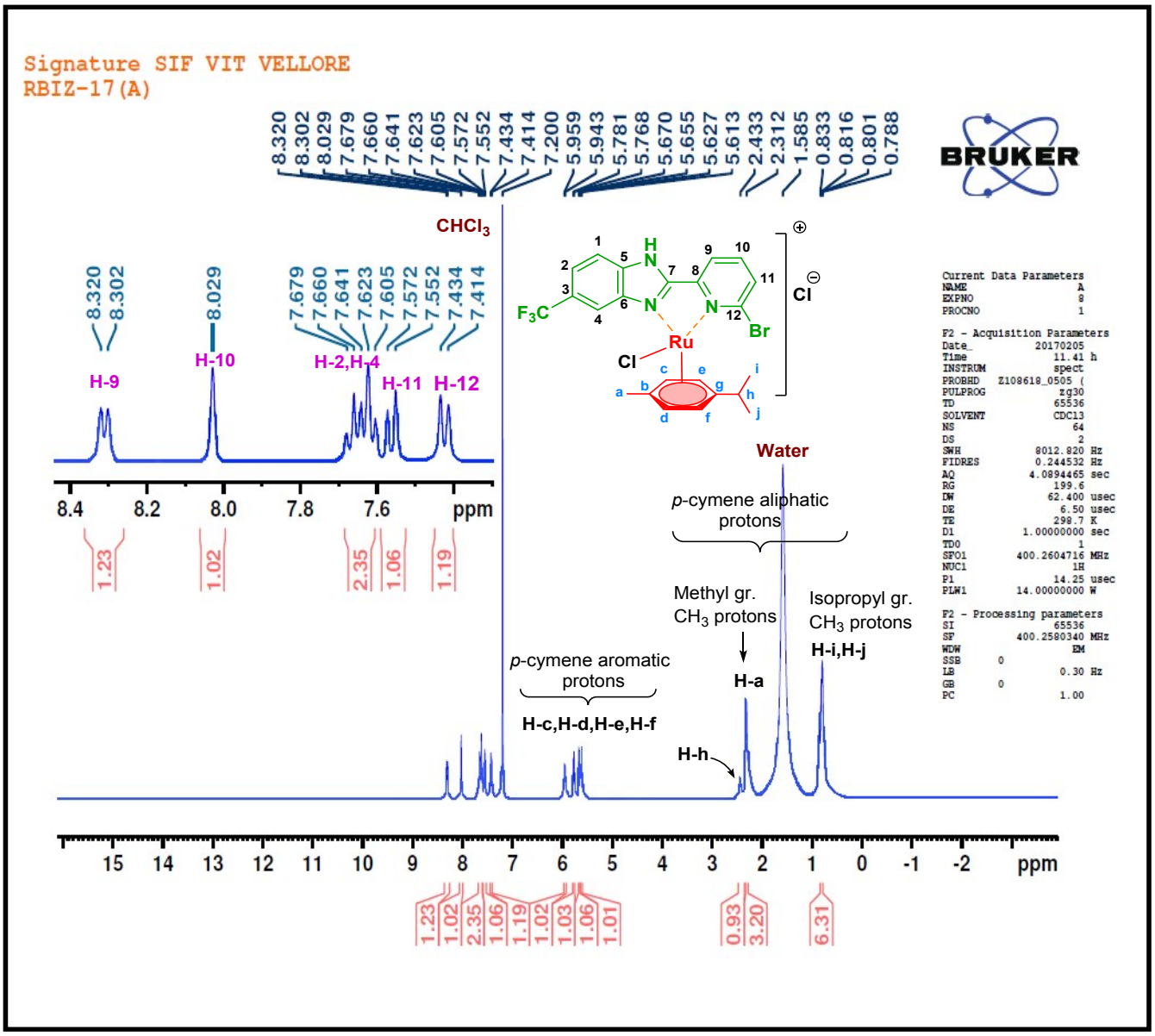
5c′


Signature SIF VIT VELLORE
RBIZ-16
BRUKER
Water
DMSO
H-1
H-10
H-9
H-11
H-4
H-a
H-i,H-j
H-h
p-cymene aromatic hydrogens
H-c,H-d,H-e,H-f
p-cymene aliphatic hydrogens
ppm

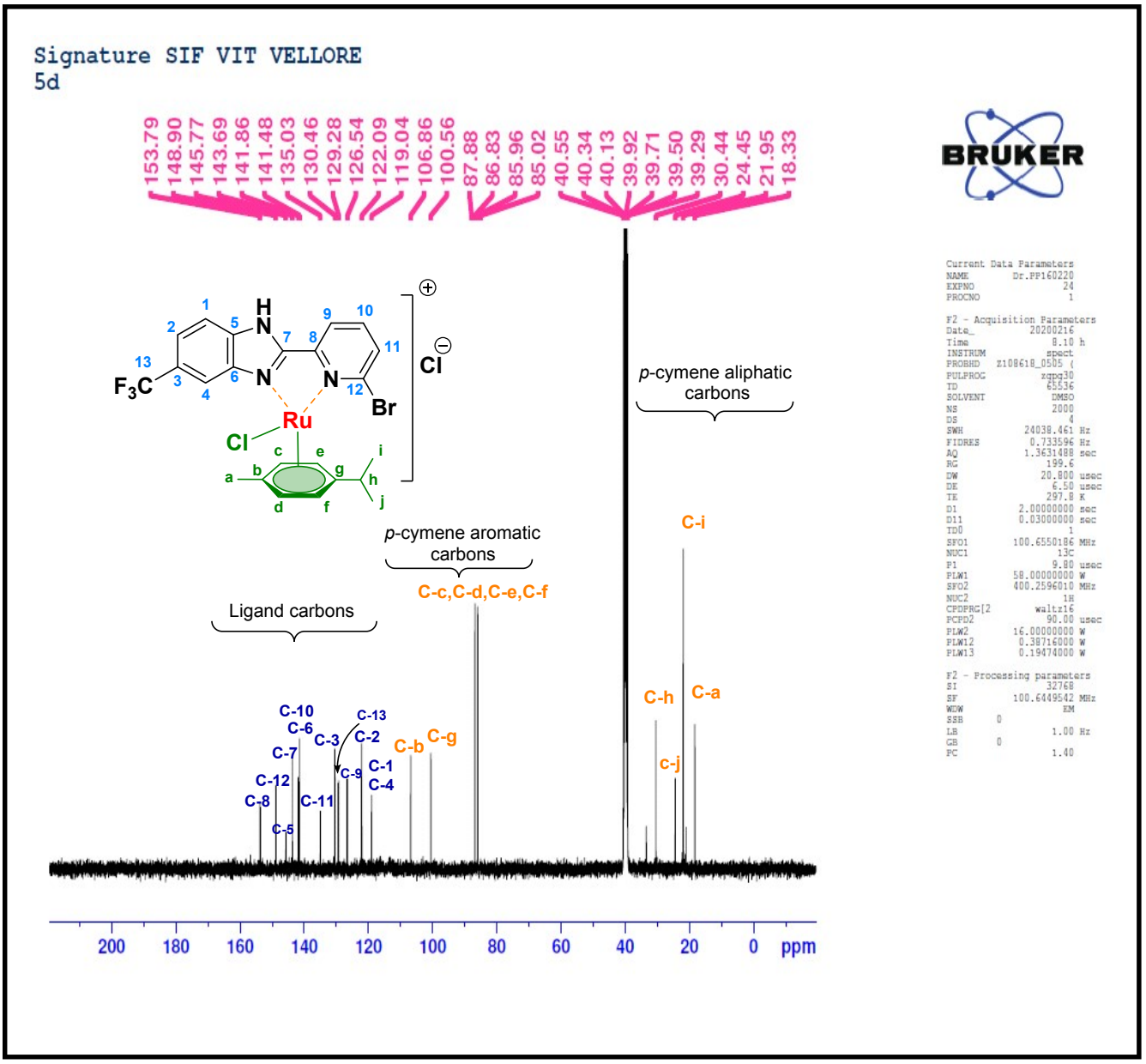
5c′


Signature SIF VIT VELLORE
5C
151.61
149.22
144.76
141.94
141.68
141.33
134.37
132.53
129.82
122.36
121.45
115.92
106.81
100.52
87.51
86.78
85.92
85.14
40.49
40.28
40.07
39.87
39.66
39.45
39.24
30.39
21.90
18.28
BRUKER
p-cymene aromatic carbons
p-cymene aromatic carbons
C-c,C-d,C-e,C-f
C-i,C-j
Ligand carbons
C-h
C-a
C-3
C-7
C-5
C-11
C-2
C-4
C-8
C-12
C-10
C-6
C-9
C-1
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Dr.PP080320
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200309
Time 1.56 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 298.1 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

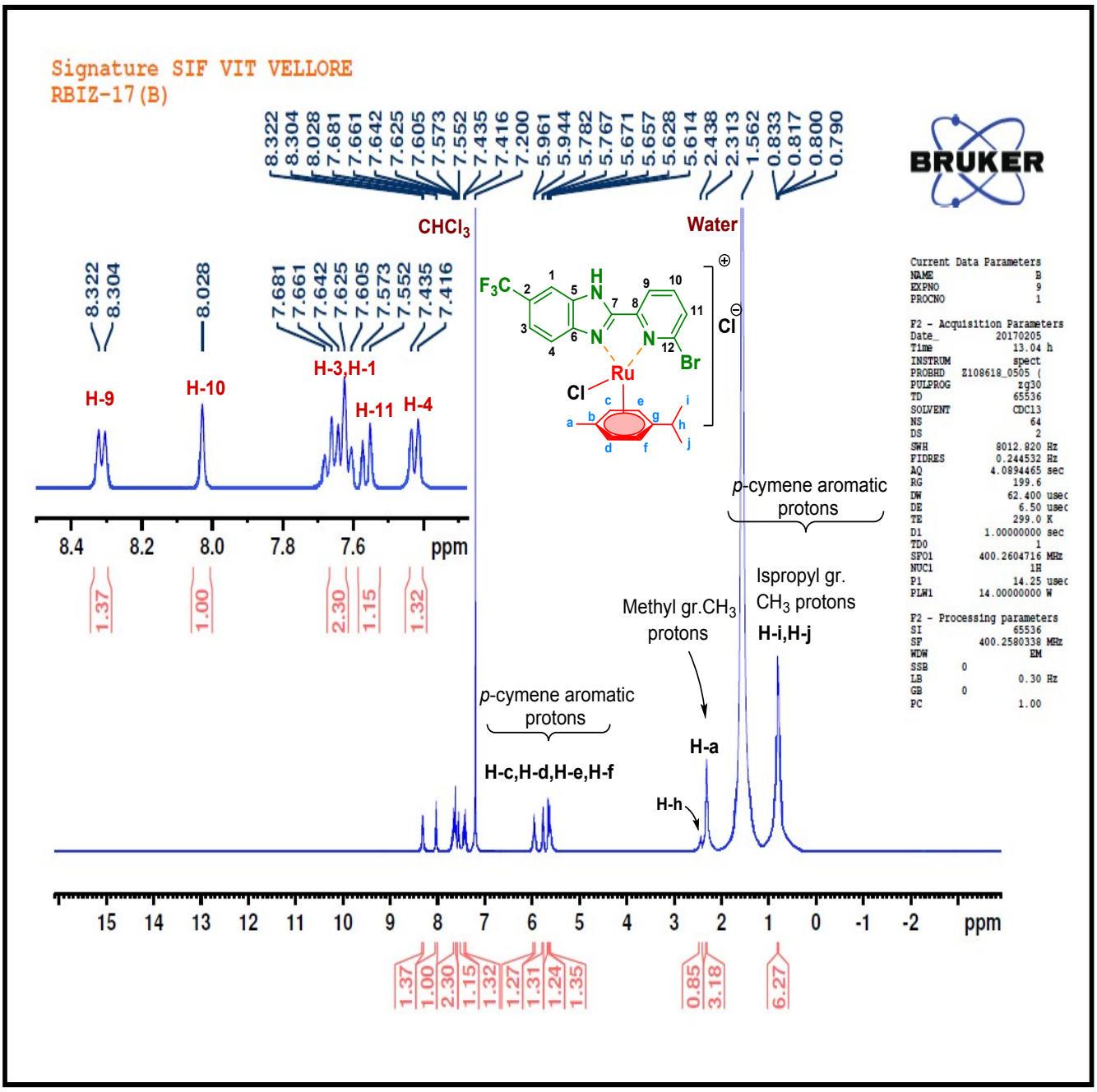
5d


Signature SIF VIT VELLORE
RBIZ-17(A)
BRUKER
8.320 8.302 8.029 7.679 7.660 7.641 7.623 7.605 7.572 7.552 7.434 7.414 7.200 5.959 5.943 5.781 5.768 5.670 5.655 5.627 5.613 2.433 2.312 1.585 0.833 0.816 0.801 0.788
CHCl3
H-9
H-10
H-2,H-4
H-11
H-12
8.4 8.2 8.0 7.8 7.6 ppm
1.23 1.02 2.35 1.06 1.19
Water
p-cymene aliphatic protons
Methyl gr. CH3 protons
Isopropyl gr. CH3 protons
H-i,H-j
H-a
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.23 1.02 2.35 1.06 1.19 1.02 1.03 1.06 1.01 0.93 3.20 6.31
Current Data Parameters
NAME A
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170205
Time 11.41 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
F2 - Processing parameters
SI 65536
SF 400.2580340 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

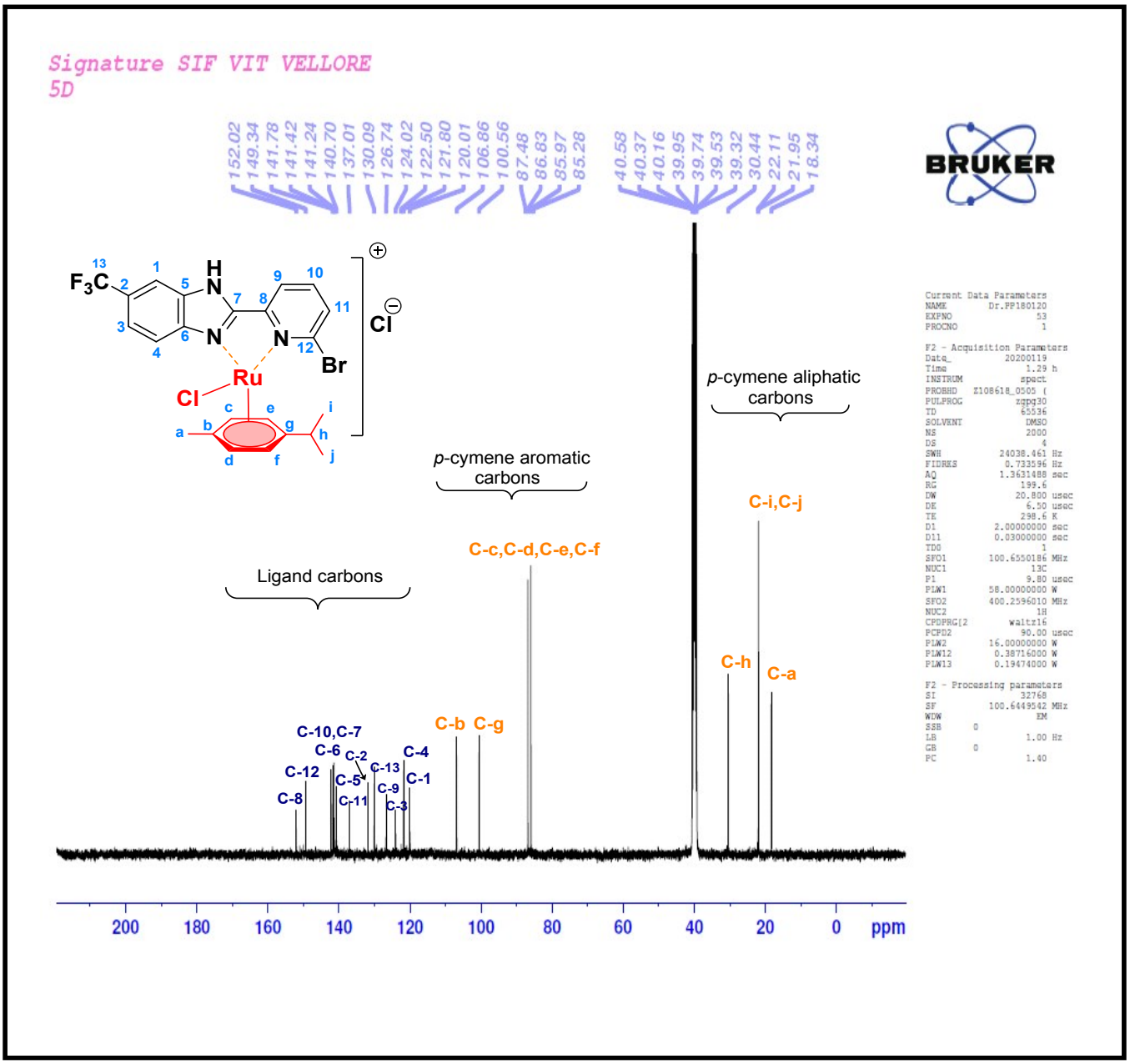
5d


Signature SIF VIT VELLORE
5d
153.79
148.90
145.77
143.69
141.86
141.48
135.03
130.46
129.28
126.54
122.09
119.04
106.86
100.56
87.88
86.83
85.96
85.02
40.55
40.34
40.13
39.92
39.71
39.50
39.29
30.44
24.45
21.95
18.33
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
C-c,C-d,C-e,C-f
Ligand carbons
C-i
C-h
C-a
c-j
C-10
C-6
C-13
C-3
C-2
C-7
C-b
C-g
C-9
C-1
C-12
C-4
C-8
C-11
C-5
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Dr.PP160220
EXPNO 24
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200216
Time 8.10 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 297.8 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

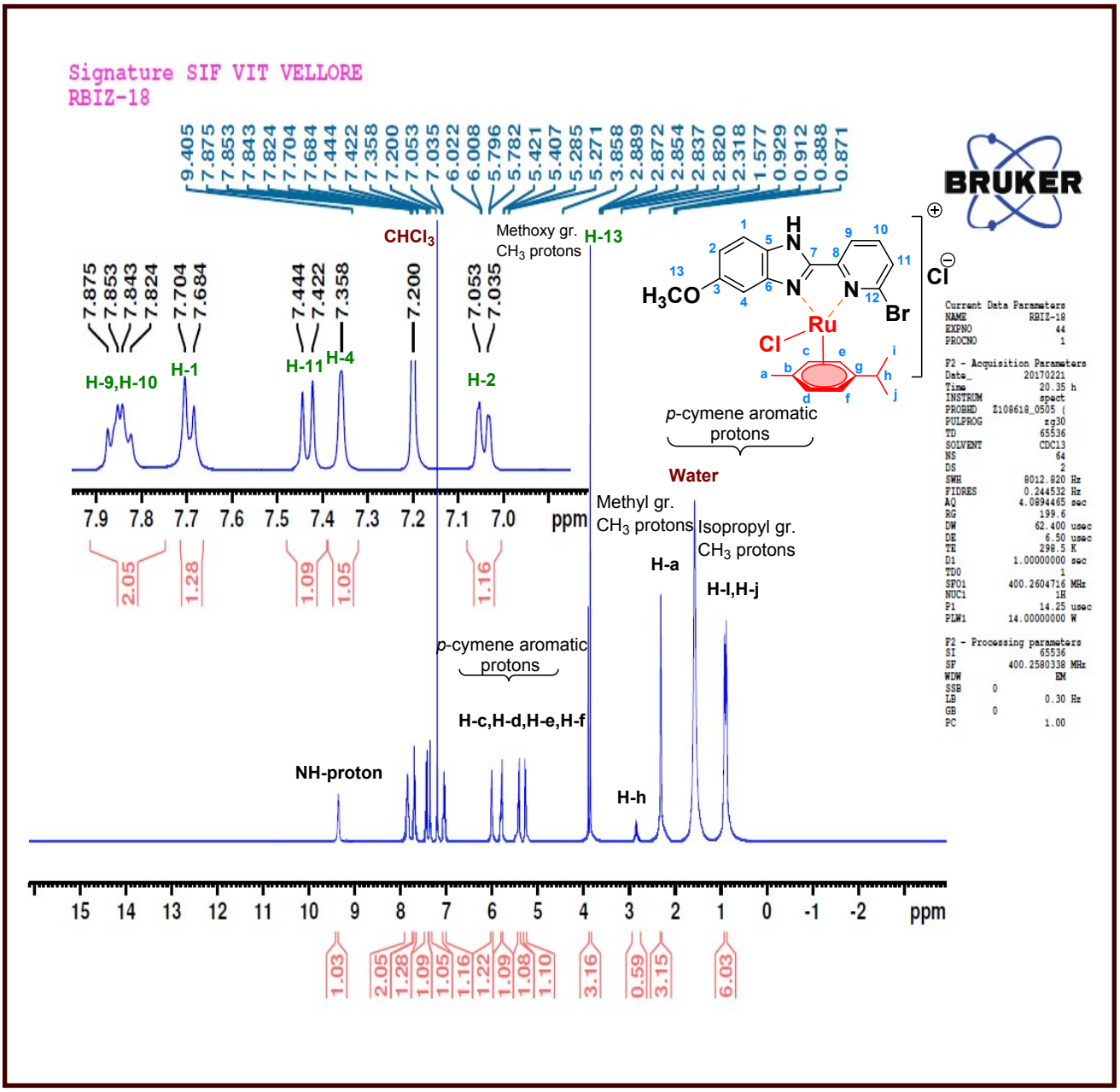
5d′


Signature SIF VIT VELLORE
RBIZ-17(B)
BRUKER
CHCl3
Water
H-9
H-10
H-3,H-1
H-11
H-4
p-cymene aromatic protons
Ispropyl gr. CH3 protons
H-i,H-j
Methyl gr.CH3 protons
H-a
H-h
p-cymene aromatic protons
H-c,H-d,H-e,H-f
ppm

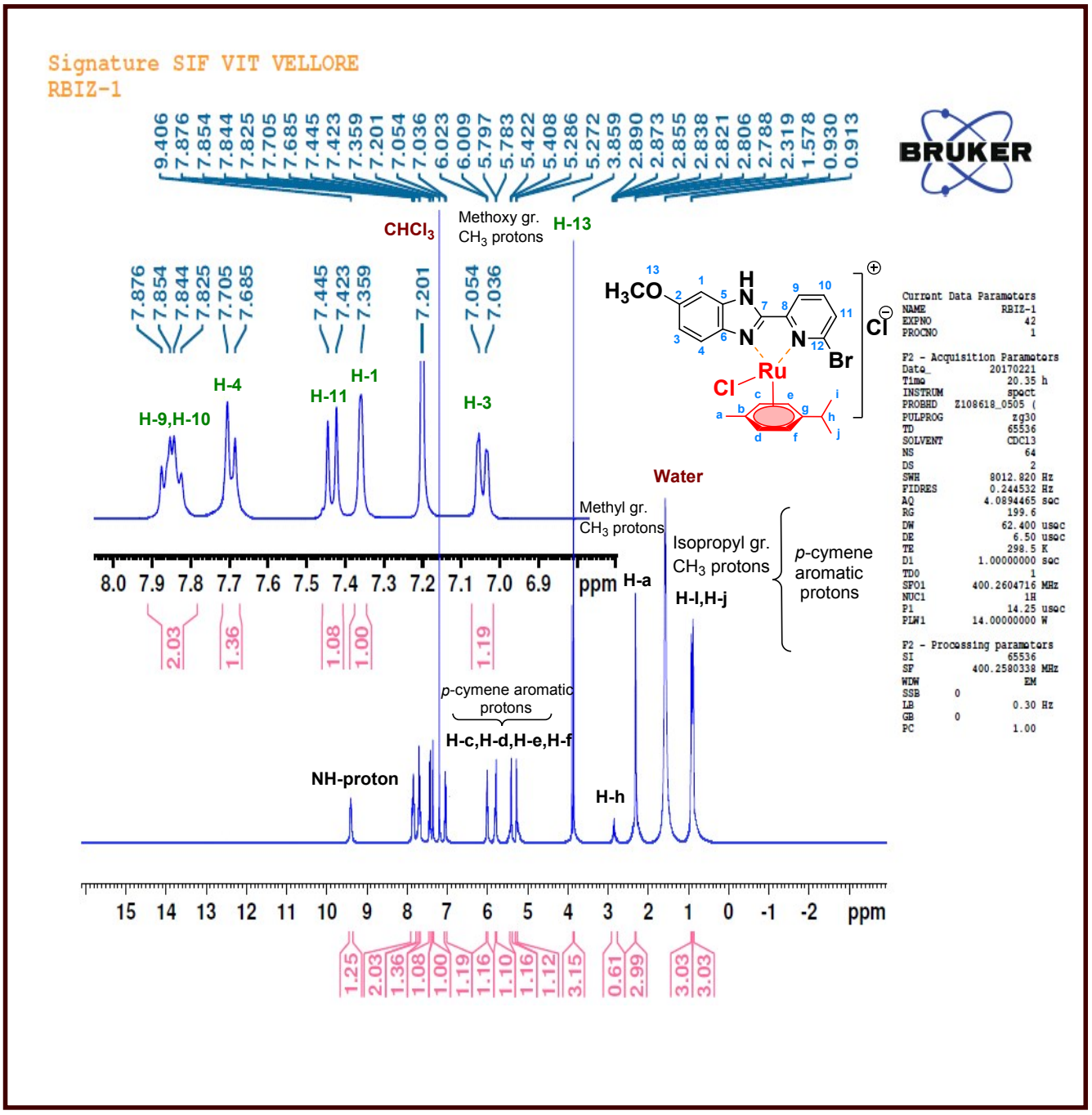
5d′


Signature SIF VIT VELLORE
5D
152.02 149.34 141.78 141.42 141.24 140.70 137.01 130.09 126.74 124.02 122.50 121.80 120.01 106.86 100.56 87.48 86.83 85.97 85.28 40.58 40.37 40.16 39.95 39.74 39.53 39.32 30.44 22.11 21.95 18.34
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-c,C-d,C-e,C-f
C-i,C-j
C-h
C-a
C-b C-g
C-10,C-7
C-6
C-2
C-4
C-12
C-13
C-5
C-1
C-9
C-8
C-11
C-3
200 180 160 140 120 100 80 60 40 20 0 ppm

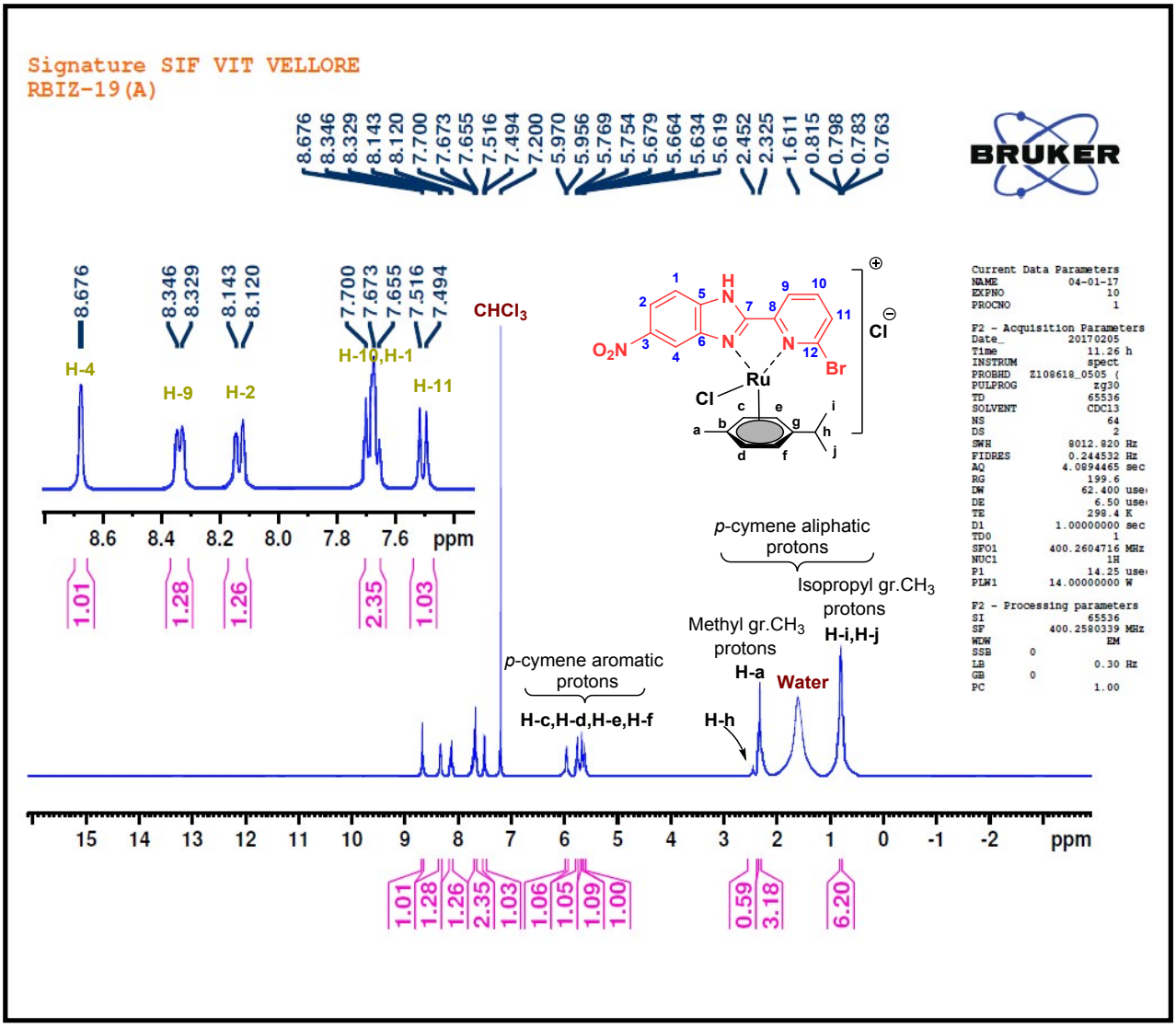
5e


Signature SIF VIT VELLORE
RBIZ-18
BRUKER
CHCl3
Methoxy gr. CH3 protons
H-13
H-9,H-10
H-1
H-11
H-4
H-2
p-cymene aromatic protons
Water
Methyl gr. CH3 protons
Isopropyl gr. CH3 protons
H-a
H-l,H-j
p-cymene aromatic protons
H-c,H-d,H-e,H-f
NH-proton
H-h
ppm

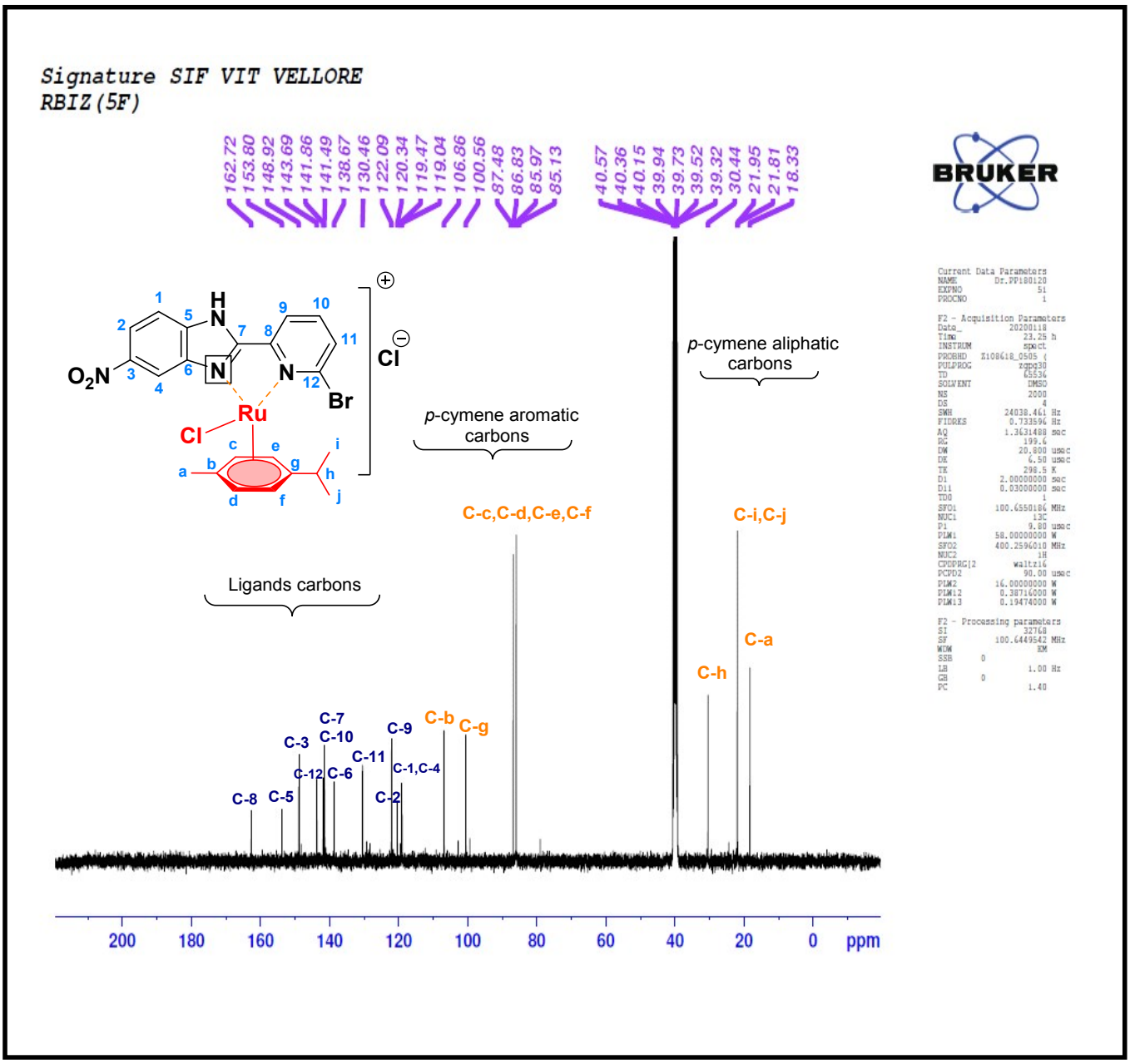
5e′


Signature SIF VIT VELLORE
RBIZ-1
BRUKER
CHCl3
Methoxy gr. CH3 protons
H-13
H-4
H-9,H-10
H-11
H-1
H-3
Water
Methyl gr. CH3 protons
Isopropyl gr. CH3 protons
H-l,H-j
p-cymene aromatic protons
H-a
p-cymene aromatic protons
H-c,H-d,H-e,H-f
NH-proton
H-h
ppm

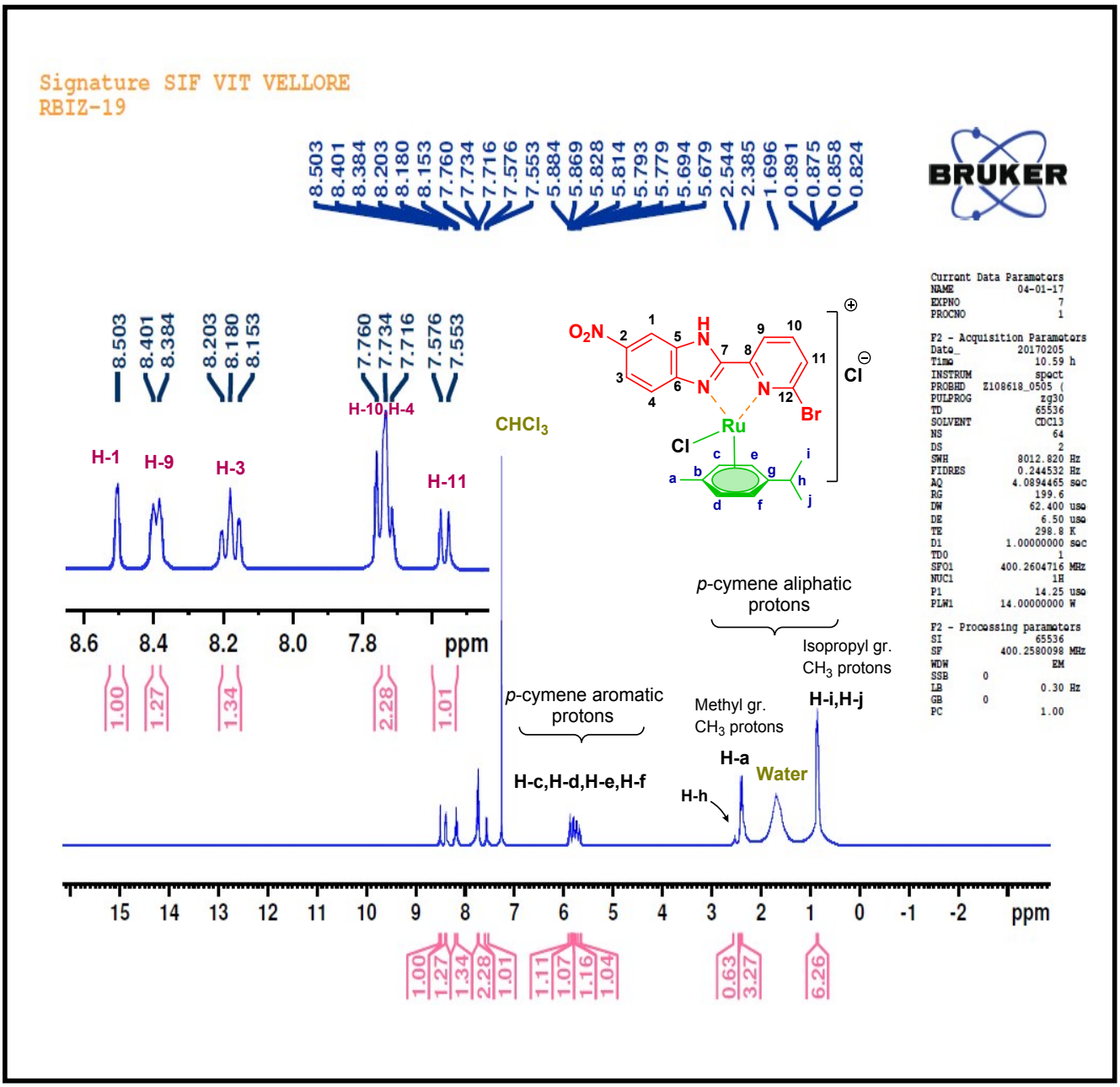
5f


Signature SIF VIT VELLORE
RBIZ-19(A)
8.676 8.346 8.329 8.143 8.120 7.700 7.673 7.655 7.516 7.494 7.200 5.970 5.956 5.769 5.754 5.679 5.664 5.634 5.619 2.452 2.325 1.611 0.815 0.798 0.783 0.763
BRUKER
H-4
H-9
H-2
H-10,H-1
H-11
CHCl3
p-cymene aromatic protons
H-c,H-d,H-e,H-f
p-cymene aliphatic protons
Isopropyl gr.CH3 protons
H-i,H-j
Methyl gr.CH3 protons
H-a
Water
H-h
Current Data Parameters
NAME 04-01-17
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170205
Time 11.26 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 use
DE 6.50 use
TE 298.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.25 use
PLW1 14.00000000 W
F2 - Processing parameters
SI 65536
SF 400.2580339 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

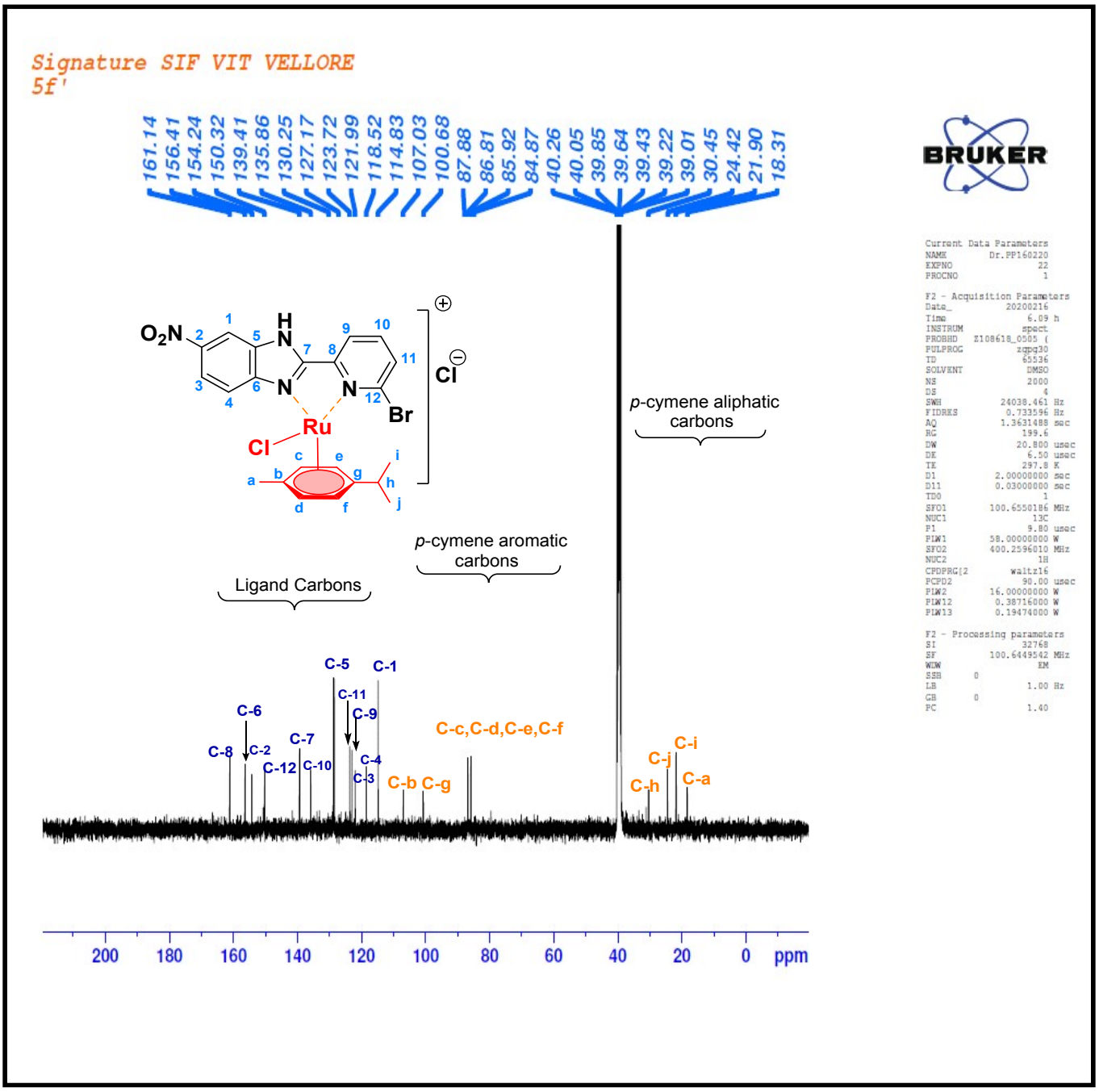
5f


Signature SIF VIT VELLORE
RBIZ(5F)
162.72
153.80
148.92
143.69
141.86
141.49
138.67
130.46
122.09
120.34
119.47
119.04
106.86
100.56
87.48
86.83
85.97
85.13
40.57
40.36
40.15
39.94
39.73
39.52
39.32
30.44
21.95
21.81
18.33
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
C-c,C-d,C-e,C-f
C-i,C-j
Ligands carbons
C-a
C-h
C-b
C-g
C-7
C-10
C-3
C-9
C-11
C-12
C-6
C-1,C-4
C-8
C-5
C-2
200
180
160
140
120
100
80
60
40
20
0
ppm

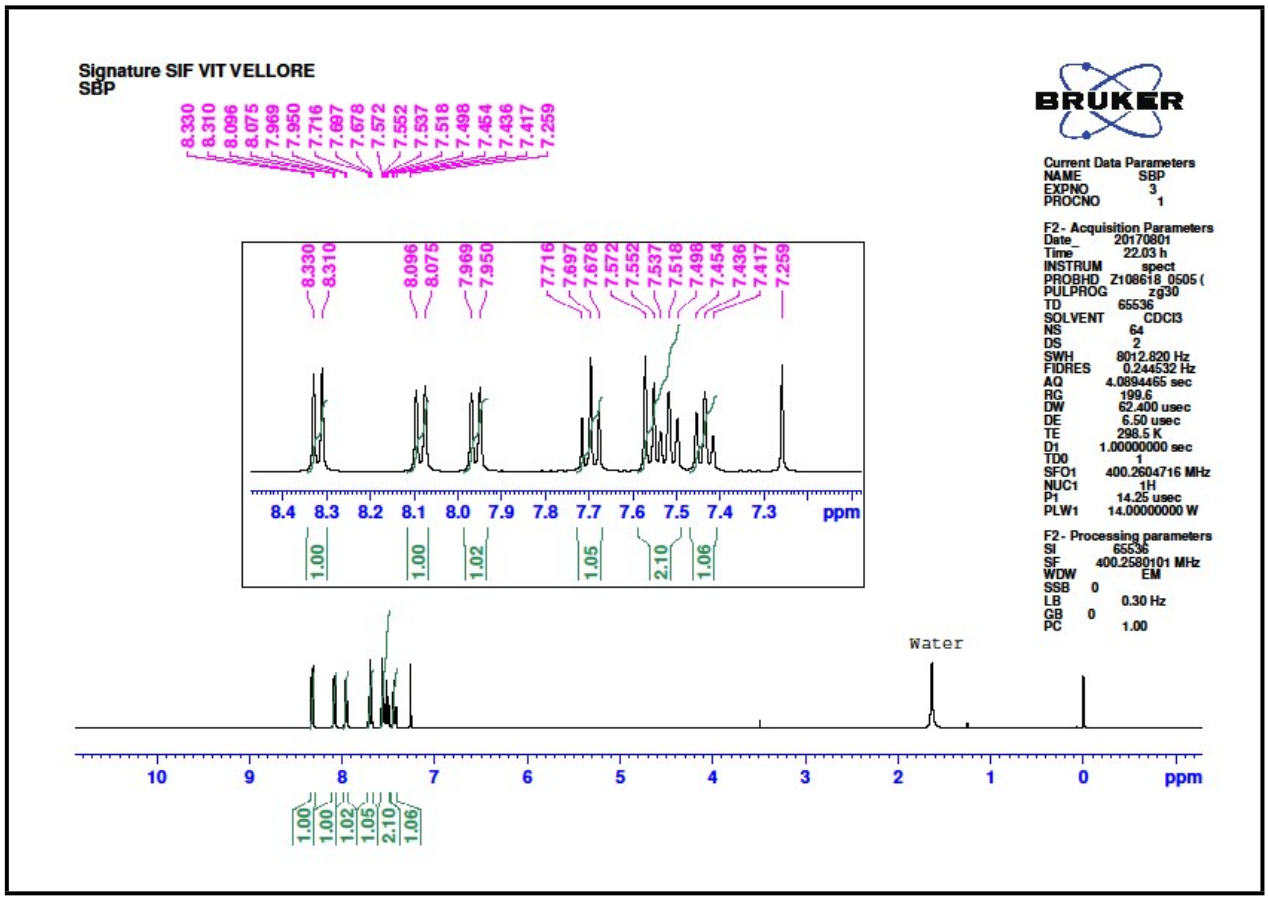
5f'


Signature SIF VIT VELLORE
RBIZ-19
BRUKER
8.503 8.401 8.384 8.203 8.180 8.153 7.760 7.734 7.716 7.576 7.553 5.884 5.869 5.828 5.814 5.793 5.779 5.694 5.679 2.544 2.385 1.696 0.891 0.875 0.858 0.824
H-1
H-9
H-3
H-10,H-4
H-11
CHCl3
p-cymene aromatic protons
H-c,H-d,H-e,H-f
p-cymene aliphatic protons
Isopropyl gr. CH3 protons
Methyl gr. CH3 protons
H-i,H-j
H-a
Water
H-h
Cl
Ru
Br
ppm
Current Data Parameters
NAME 04-01-17
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170205
Time 10.59 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
F2 - Processing parameters
SI 65536
SF 400.2580098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

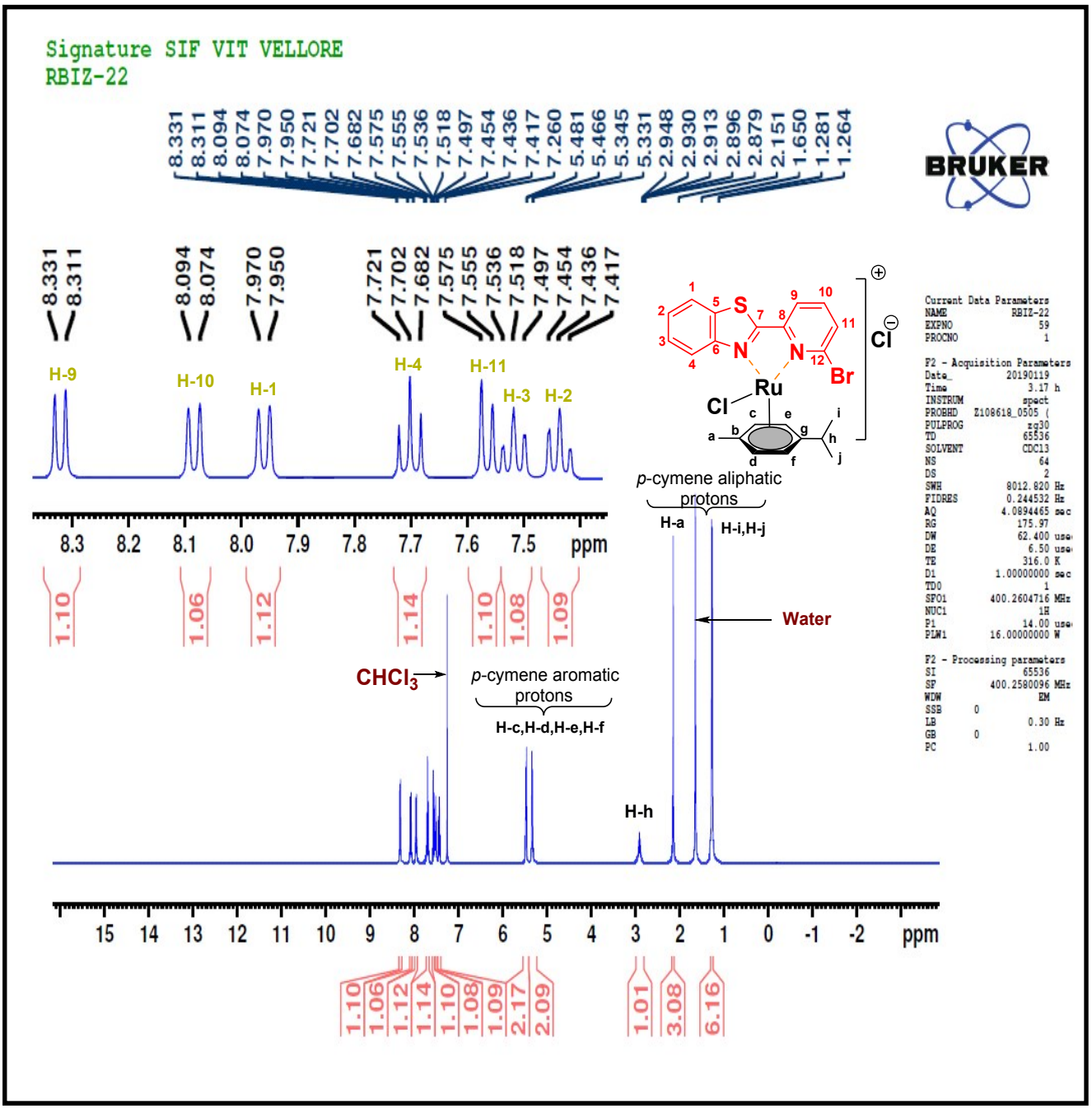
5f'


Signature SIF VIT VELLORE
5f'
161.14 156.41 154.24 150.32 139.41 135.86 130.25 127.17 123.72 121.99 118.52 114.83 107.03 100.68 87.88 86.81 85.92 84.87 40.26 40.05 39.85 39.64 39.43 39.22 39.01 30.45 24.42 21.90 18.31
BRUKER
Current Data Parameters
NAME Dr.PP160220
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200216
Time 6.09 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 297.8 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
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand Carbons
C-5 C-1 C-11 C-9 C-6 C-8 C-2 C-7 C-12 C-10 C-4 C-3 C-b C-g C-c,C-d,C-e,C-f C-i C-j C-h C-a
200 180 160 140 120 100 80 60 40 20 0 ppm

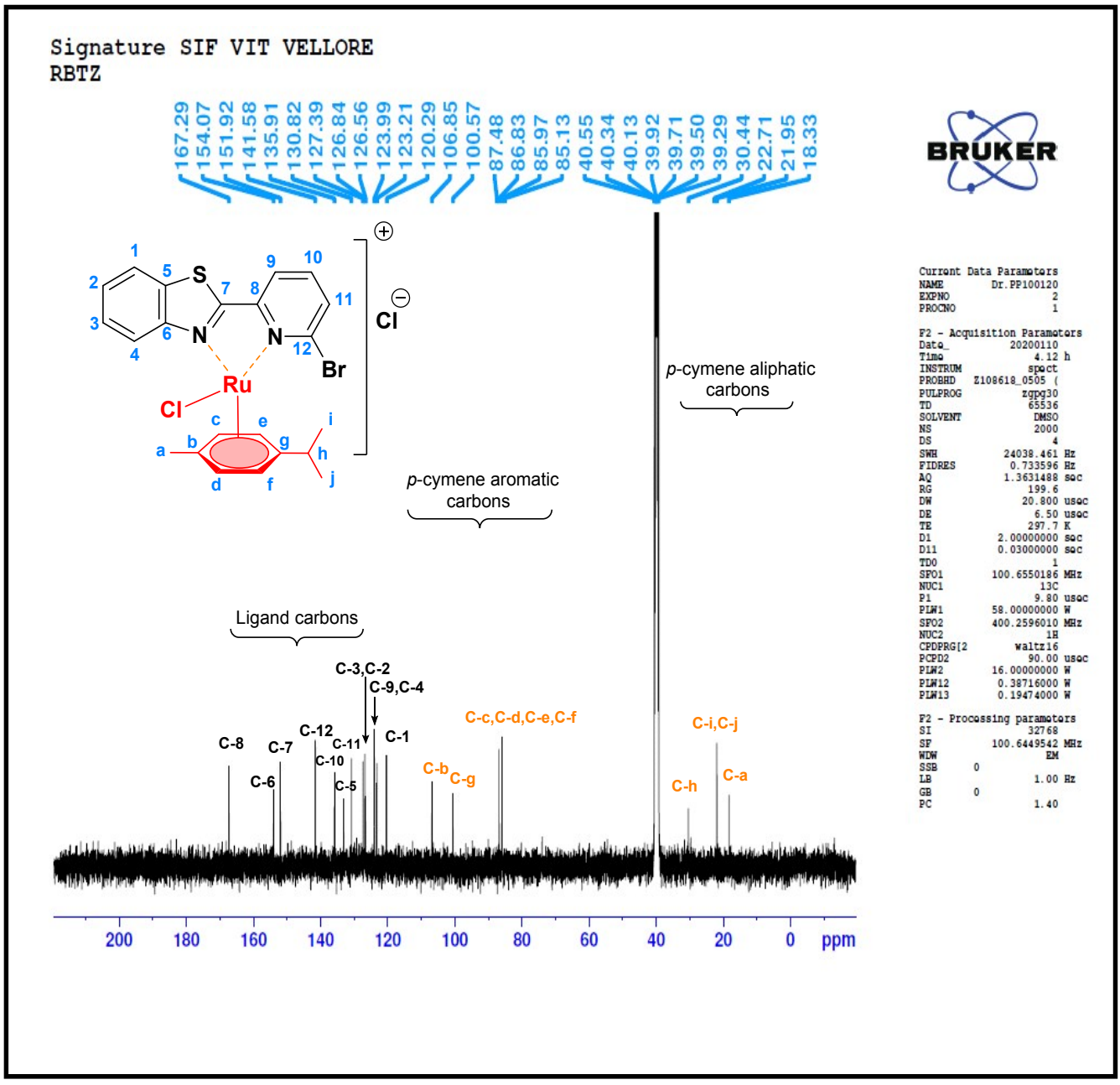
^{1}H NMR of ligand 3g



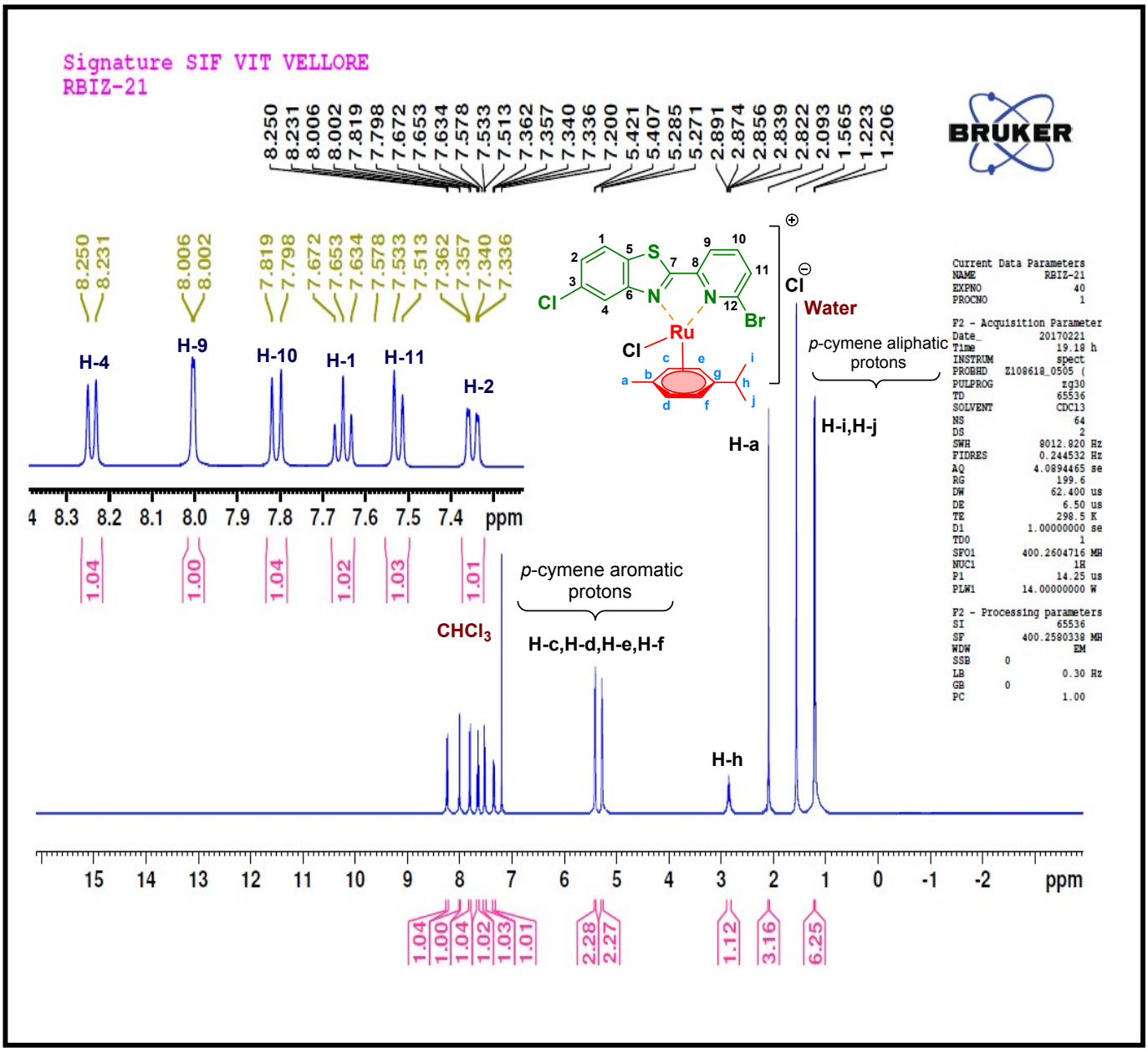
5g


Signature SIF VIT VELLORE
RBIZ-22
BRUKER
H-9
H-10
H-1
H-4
H-11
H-3
H-2
p-cymene aliphatic protons
H-a
H-i,H-j
Water
CHCl3
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
ppm

5g


Signature SIF VIT VELLORE
RBTZ
167.29
154.07
151.92
141.58
135.91
130.82
127.39
126.84
126.56
123.99
123.21
120.29
106.85
100.57
87.48
86.83
85.97
85.13
40.55
40.34
40.13
39.92
39.71
39.50
39.29
30.44
22.71
21.95
18.33
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-3,C-2
C-9,C-4
C-8
C-7
C-12
C-11
C-1
C-10
C-6
C-5
C-b
C-g
C-c,C-d,C-e,C-f
C-i,C-j
C-h
C-a
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Dr.PP100120
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200110
Time 4.12 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 297.7 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

5h


Signature SIF VIT VELLORE
RBIZ-21
BRUKER
H-4
H-9
H-10
H-1
H-11
H-2
H-a
H-h
H-i,H-j
Water
p-cymene aliphatic protons
p-cymene aromatic protons
H-c,H-d,H-e,H-f
CHCl3
Current Data Parameters
NAME RBIZ-21
EXPNO 40
PROCNO 1
F2 - Acquisition Parameter
Date_ 20170221
Time 19.18 h
INSTRUM spect
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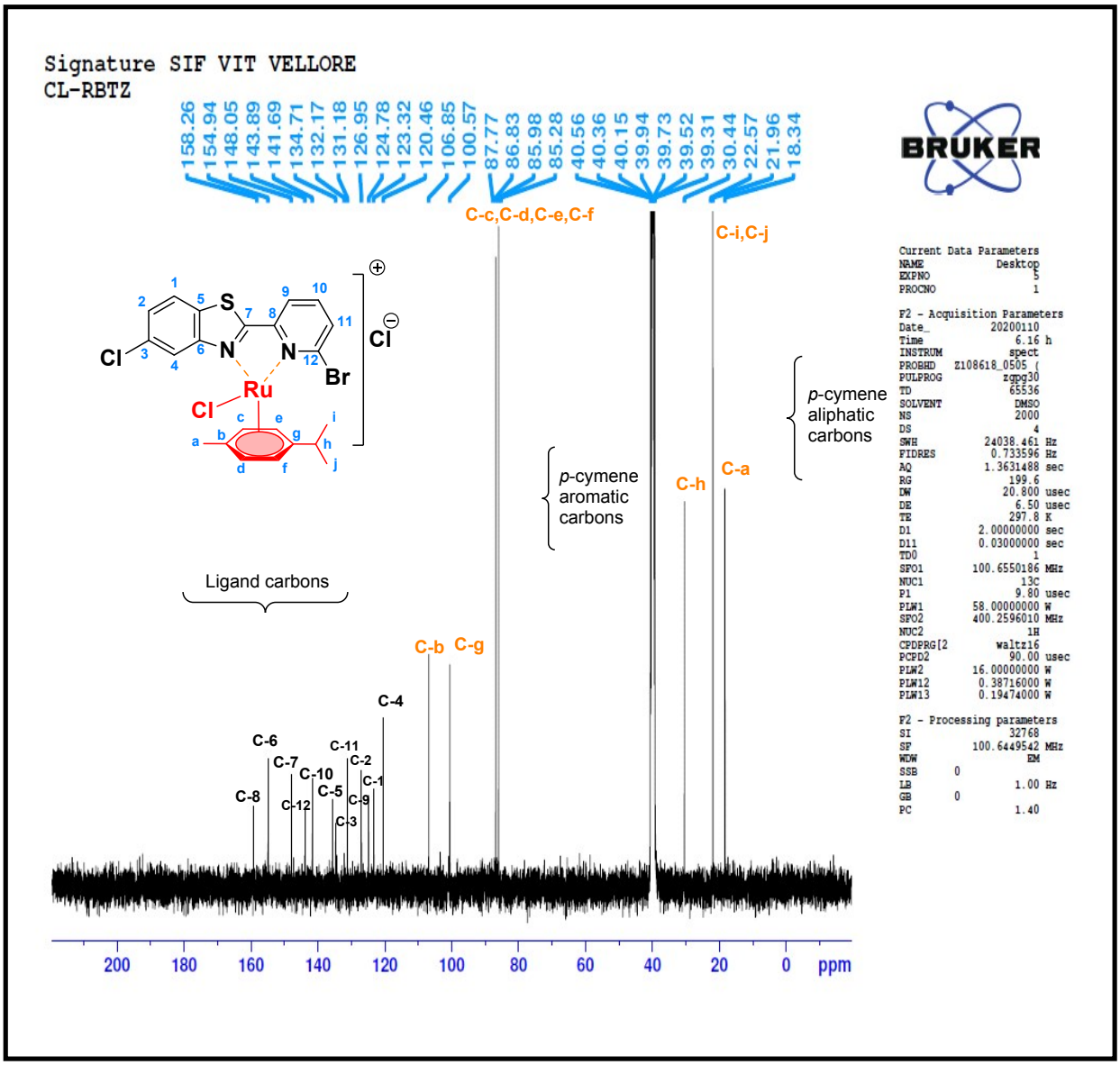
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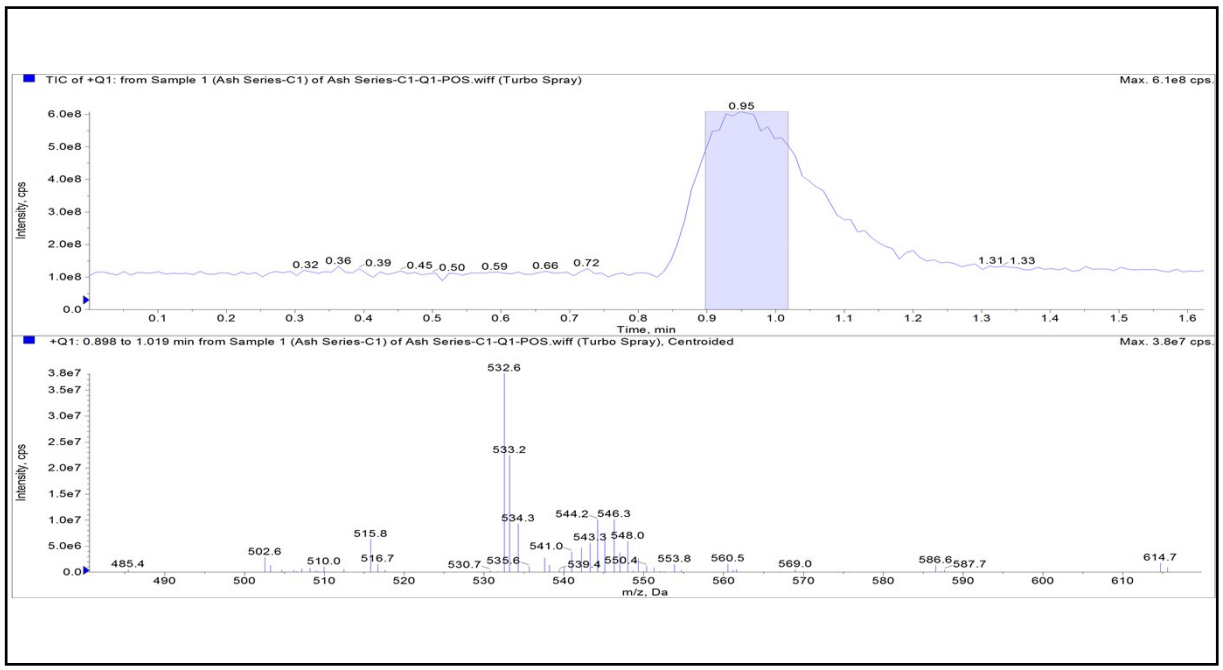
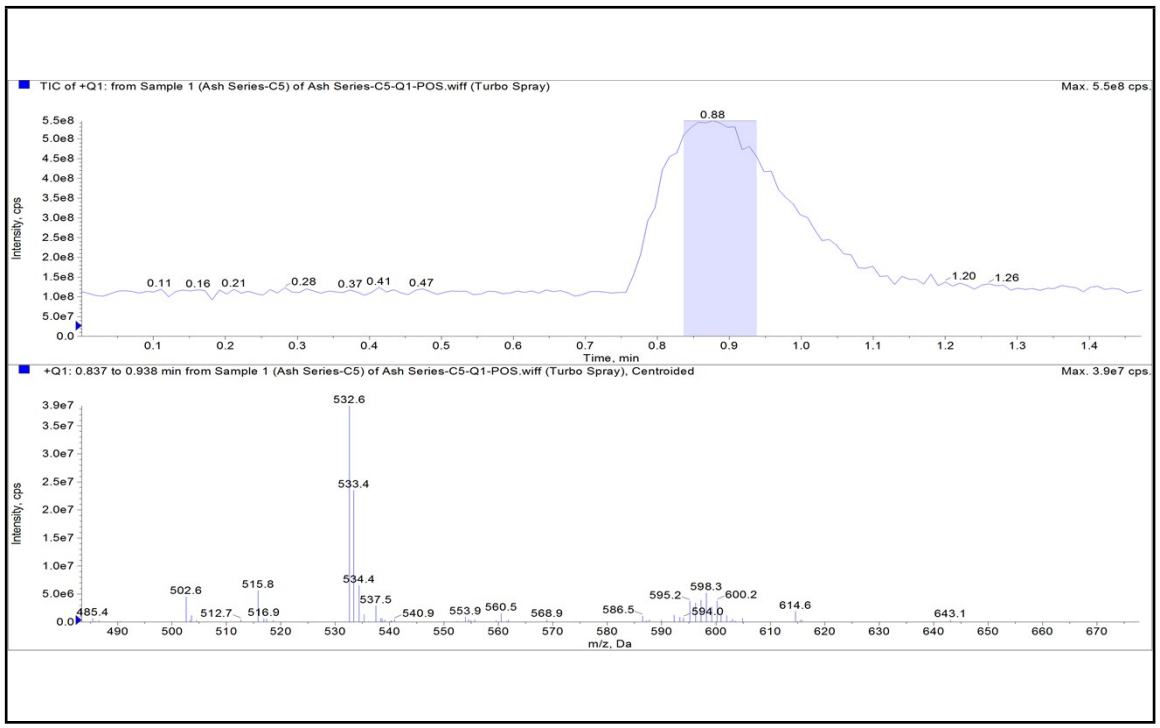
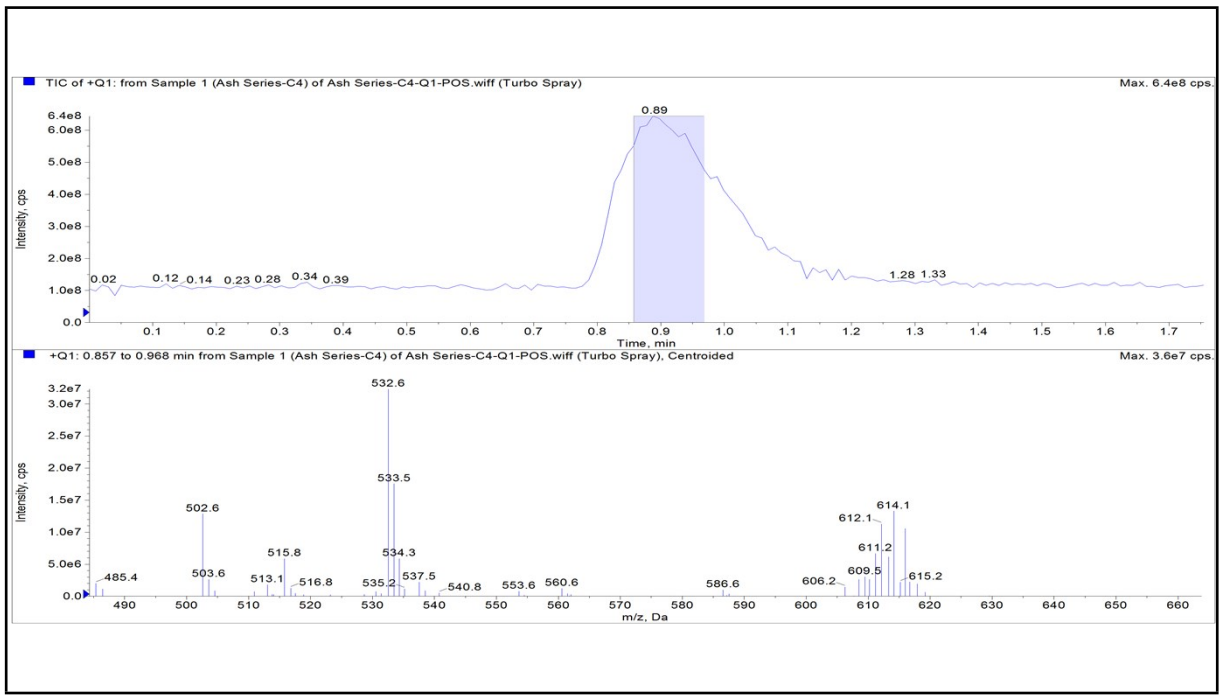


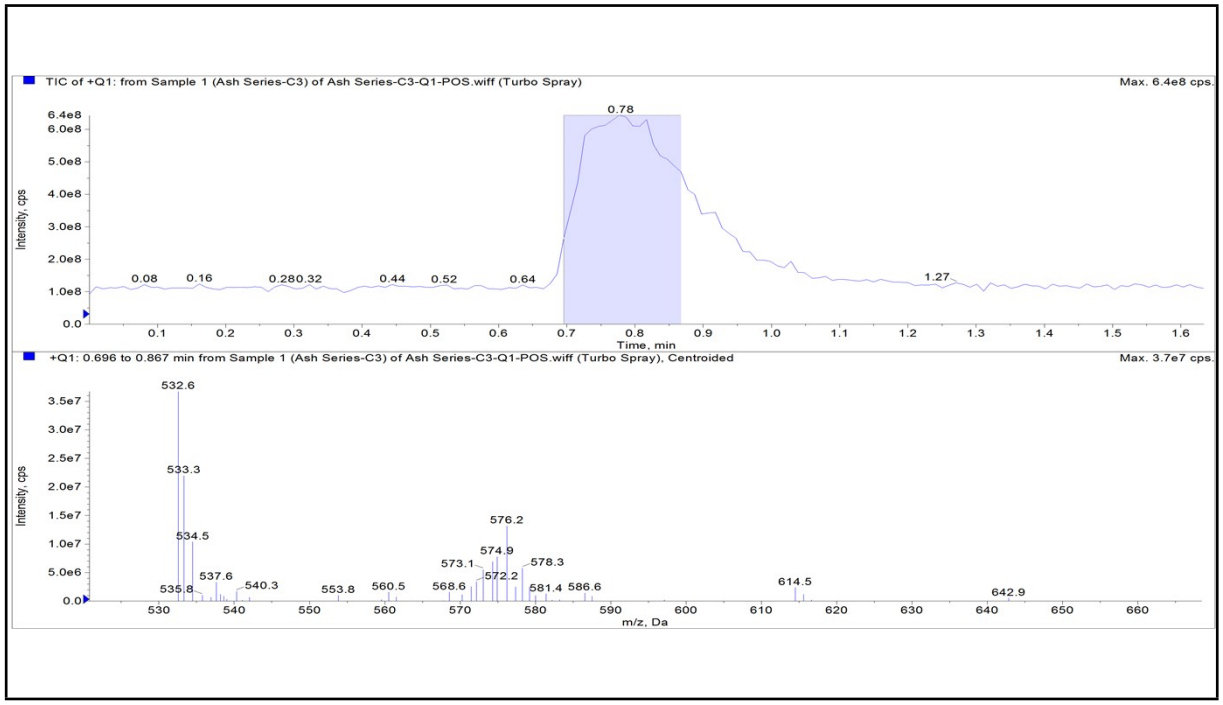
ESI-MS spectra of complex 5a



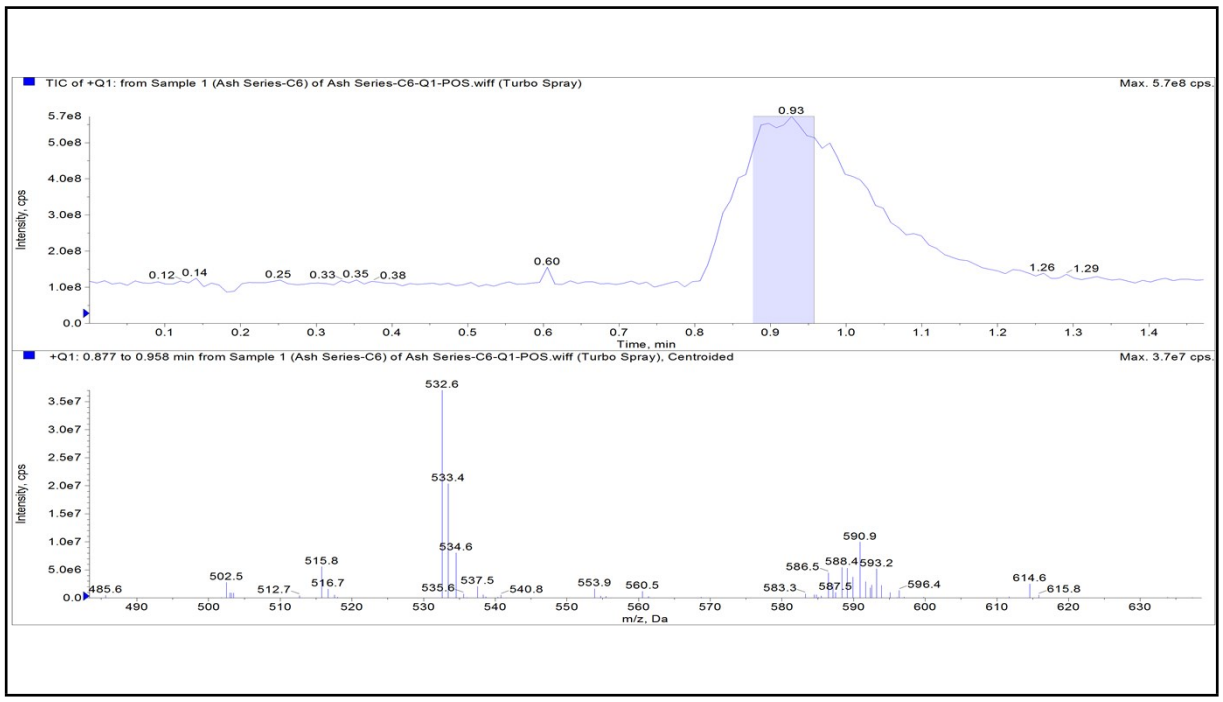
ESI-MS spectra of complex 5c



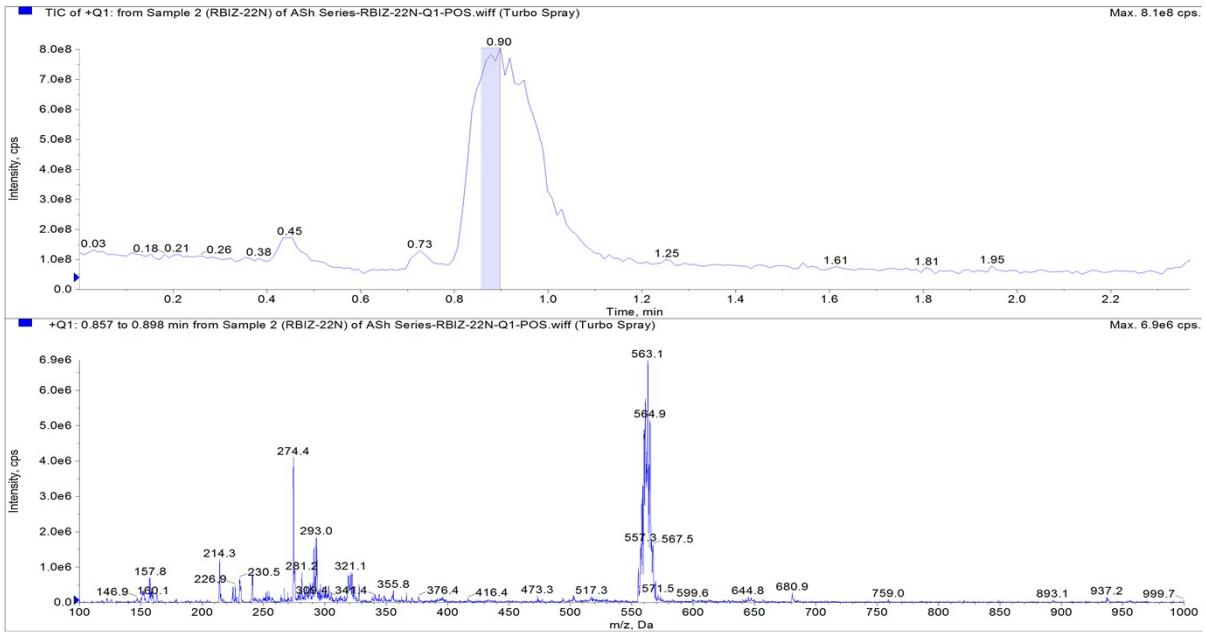
ESI-MS spectra of complex 5d



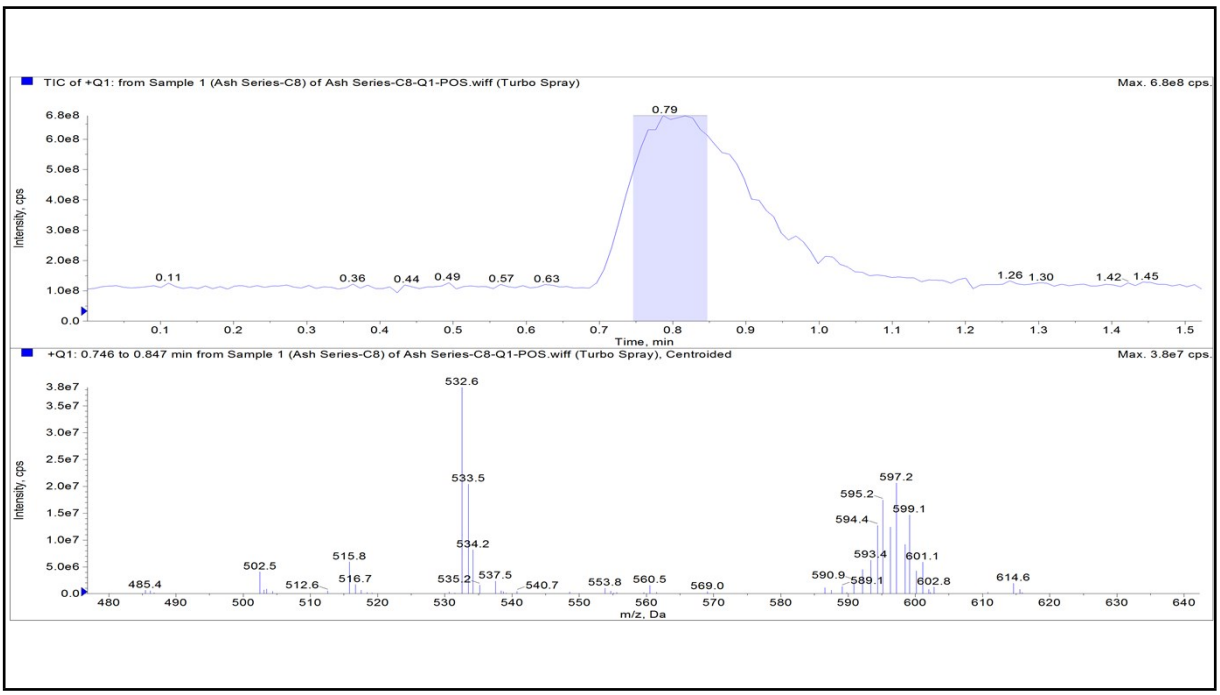
ESI-MS spectra of complex 5e



ESI-MS spectra of complex 5f

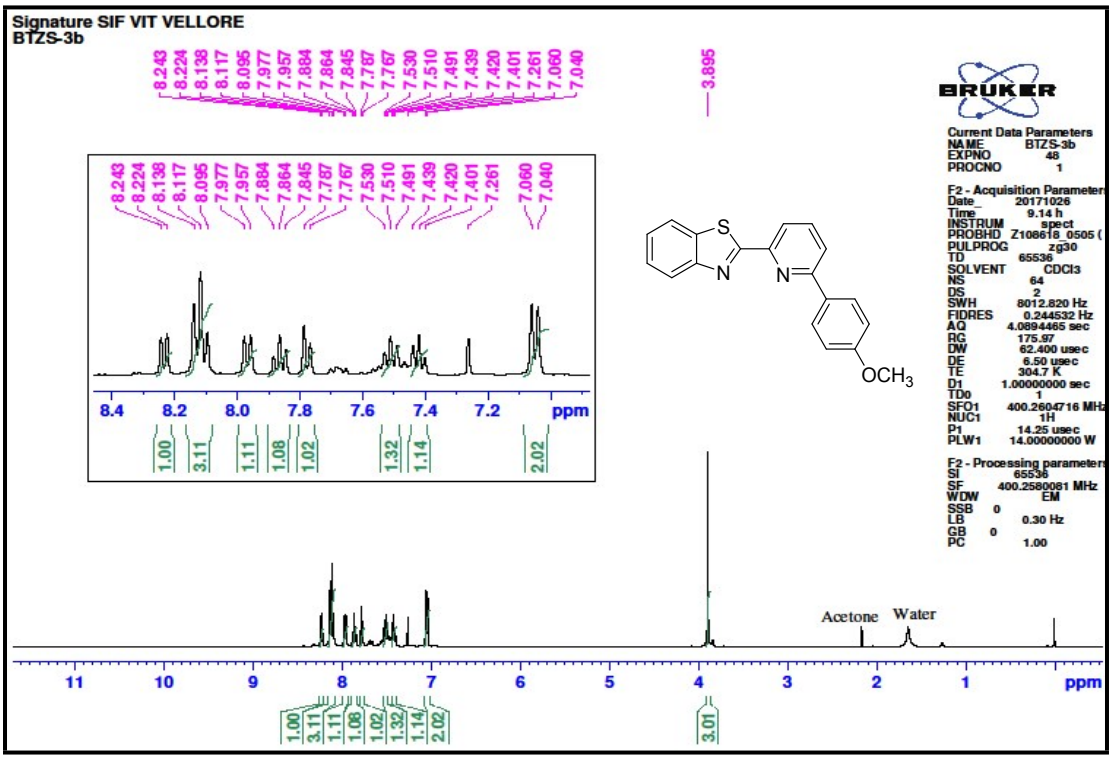


ESI-MS spectra of complex 5g

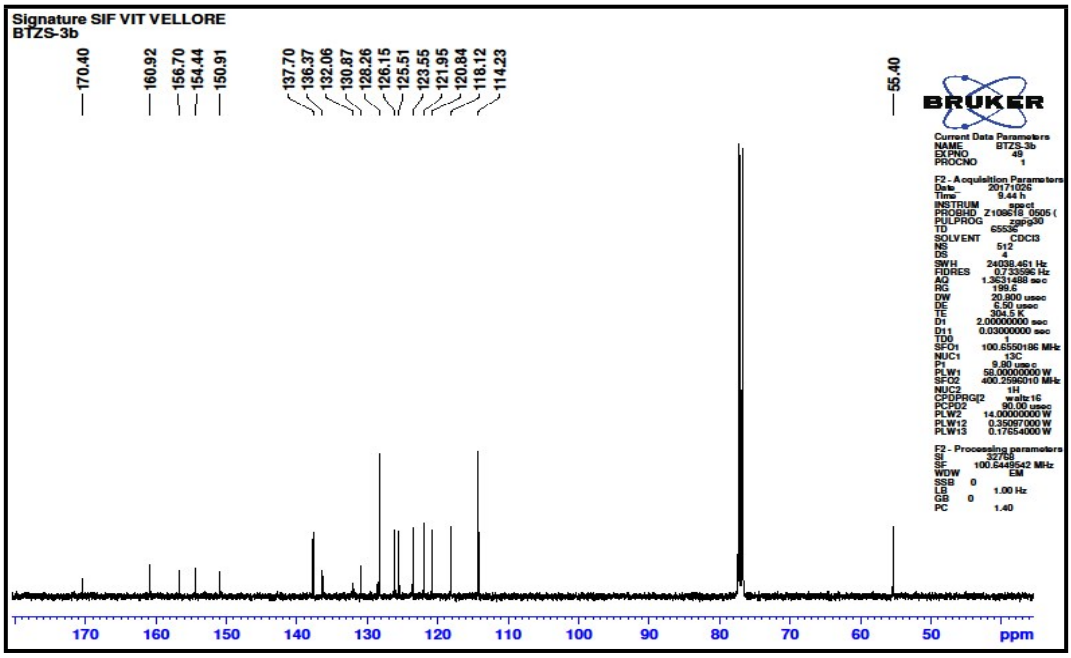


ESI-MS spectra of complex 5h

Suzuki Series

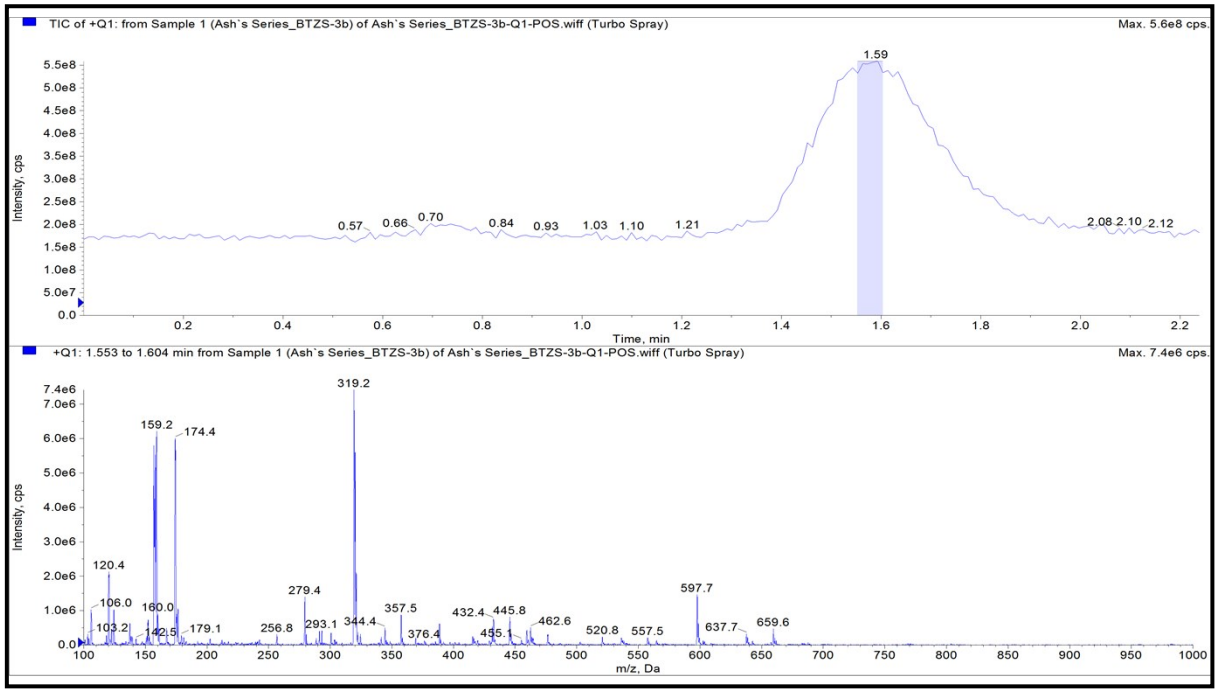


^{1}H NMR of ligand 7g1

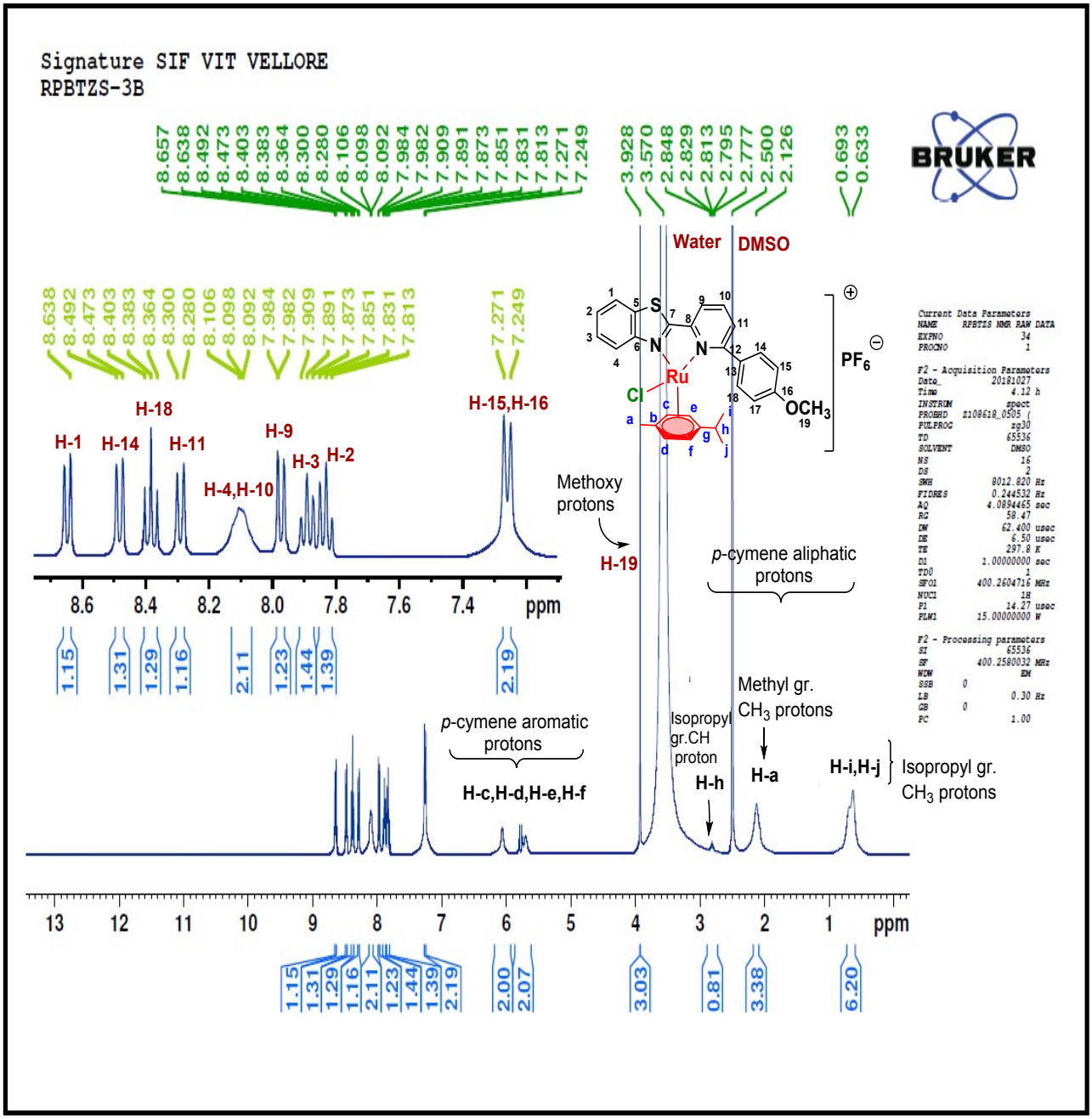


^{13}C NMR of ligand 7g1

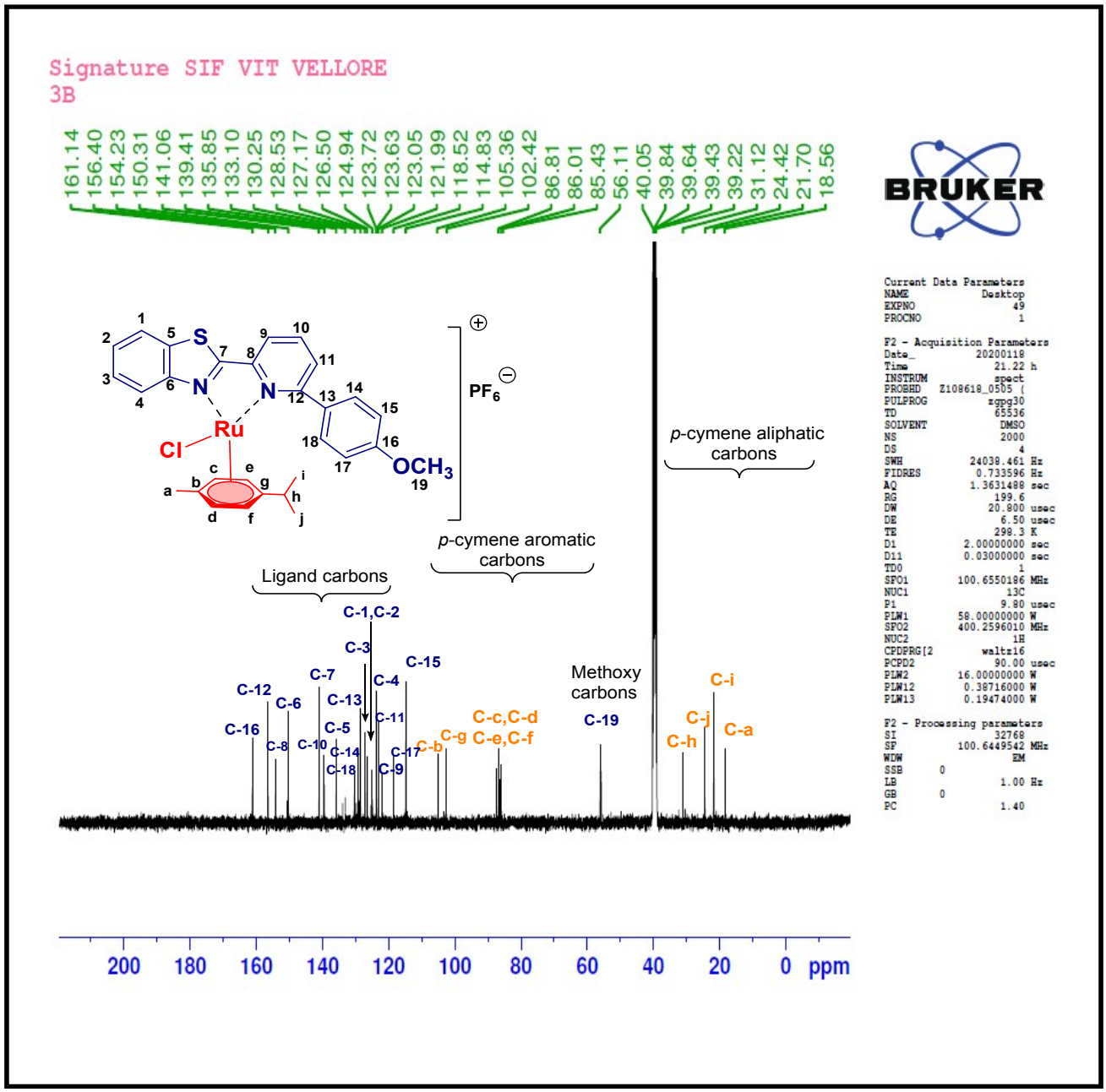
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 319.08[M+H]$^+$



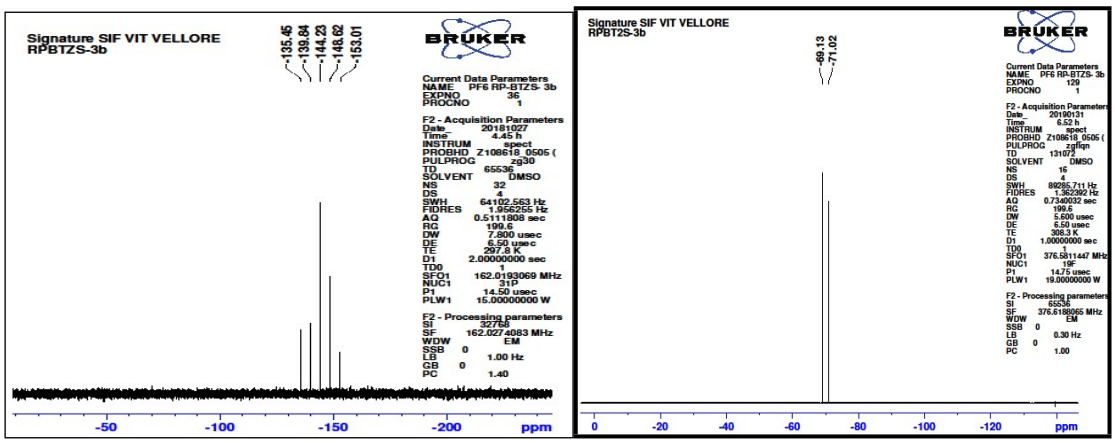
ESI-MS spectra of complex 7g1



^{1}H NMR of ligand 8g1

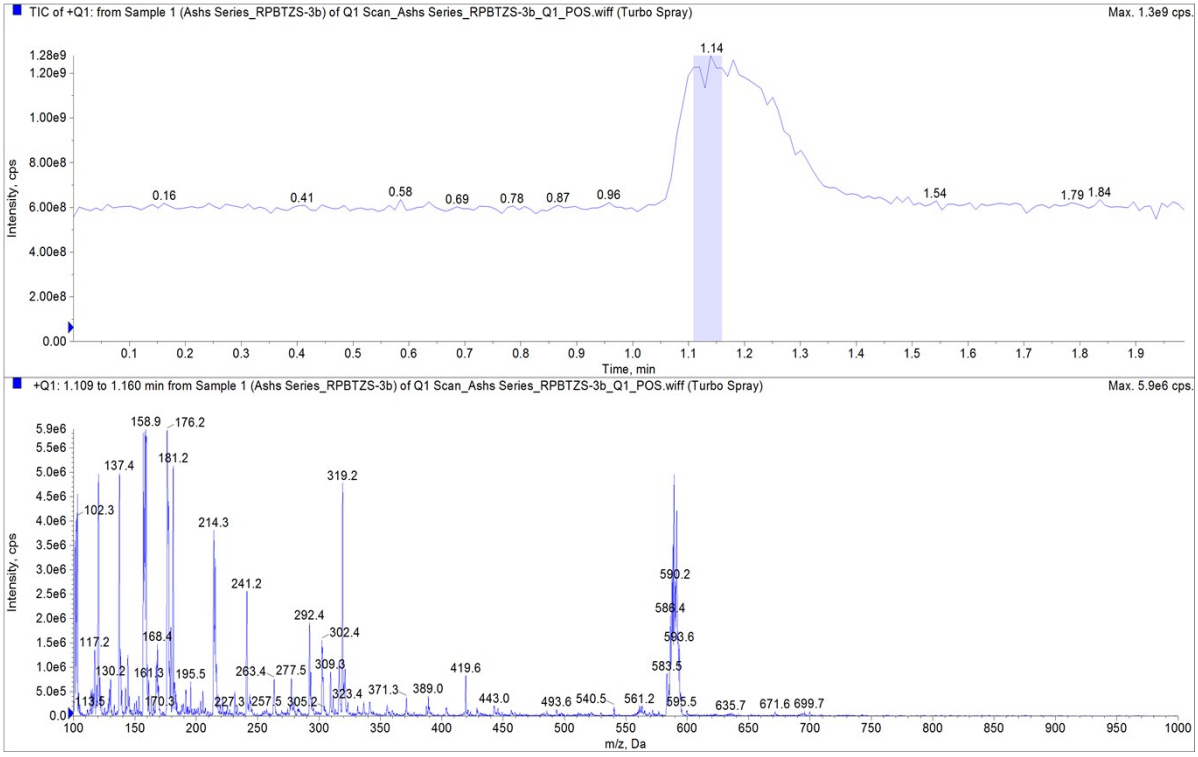


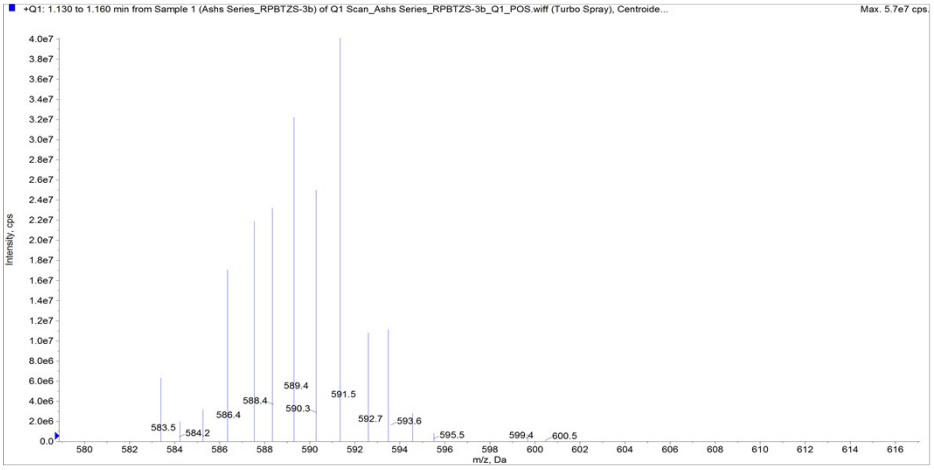
^{13}C NMR of ligand 8g1



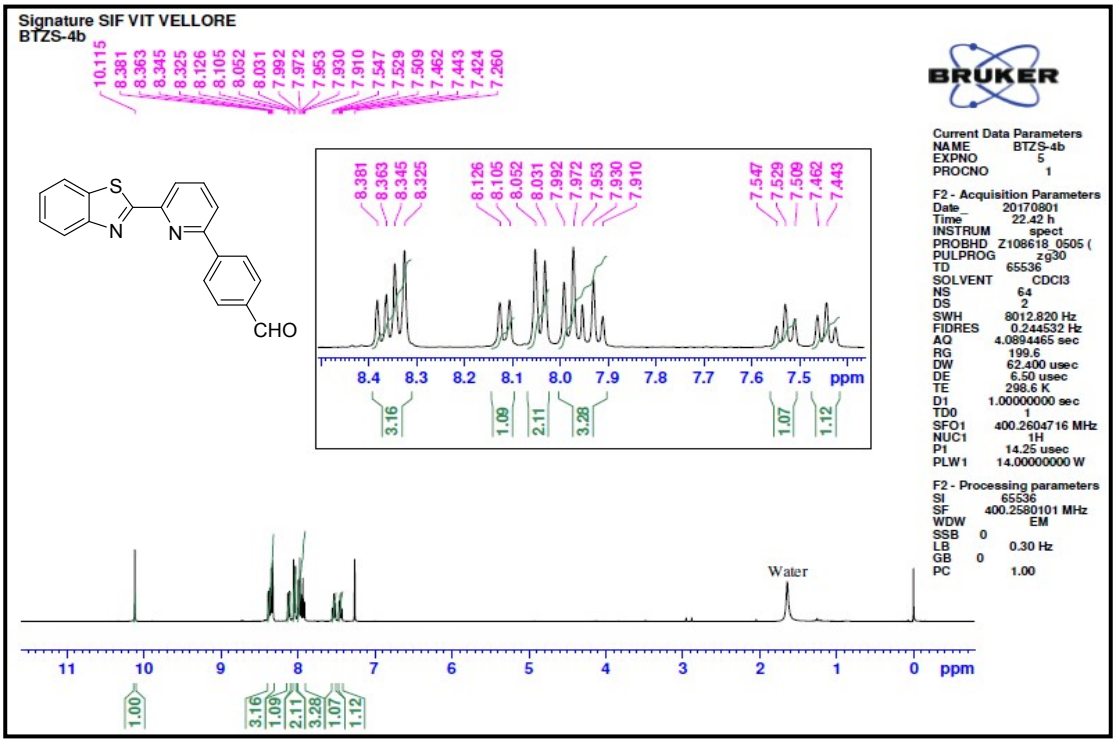
^{31}P and ^{19}F NMR of complex 8g1

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 589.06 [M$^+$]

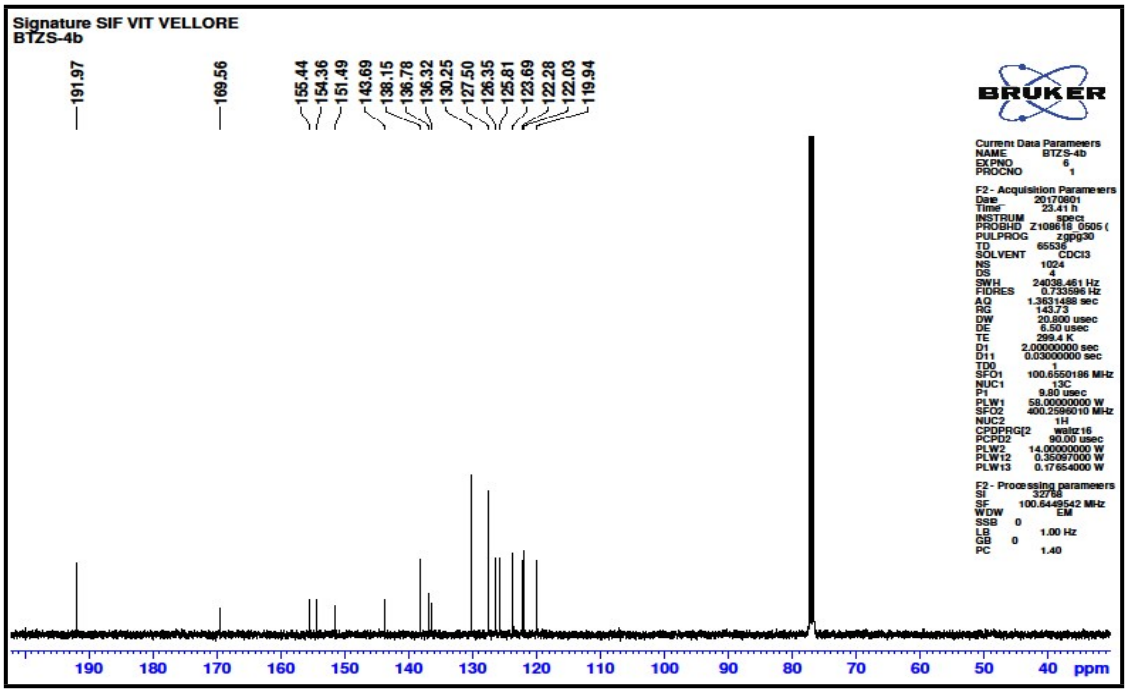




ESI-MS spectra of complex 8g1



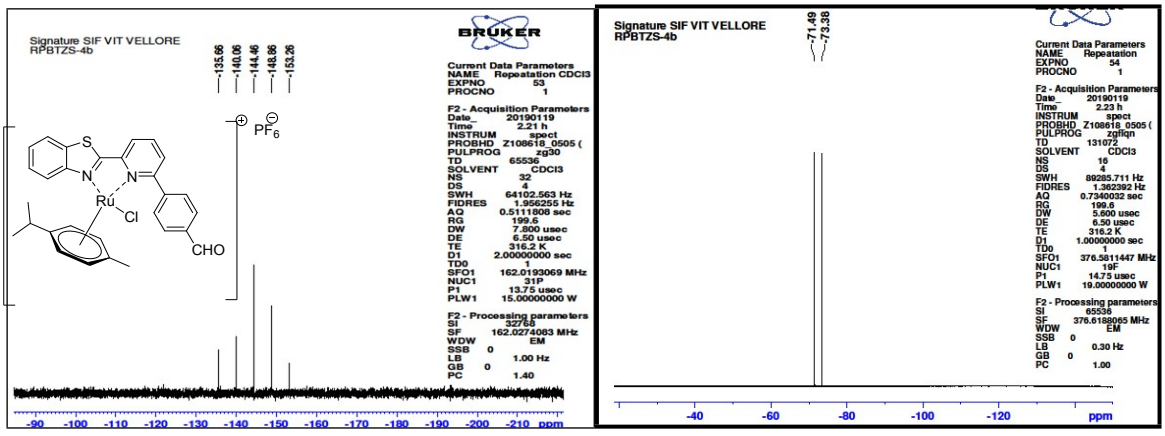
^{1}H NMR of ligand 7g2



^{1}H NMR of ligand 7g2

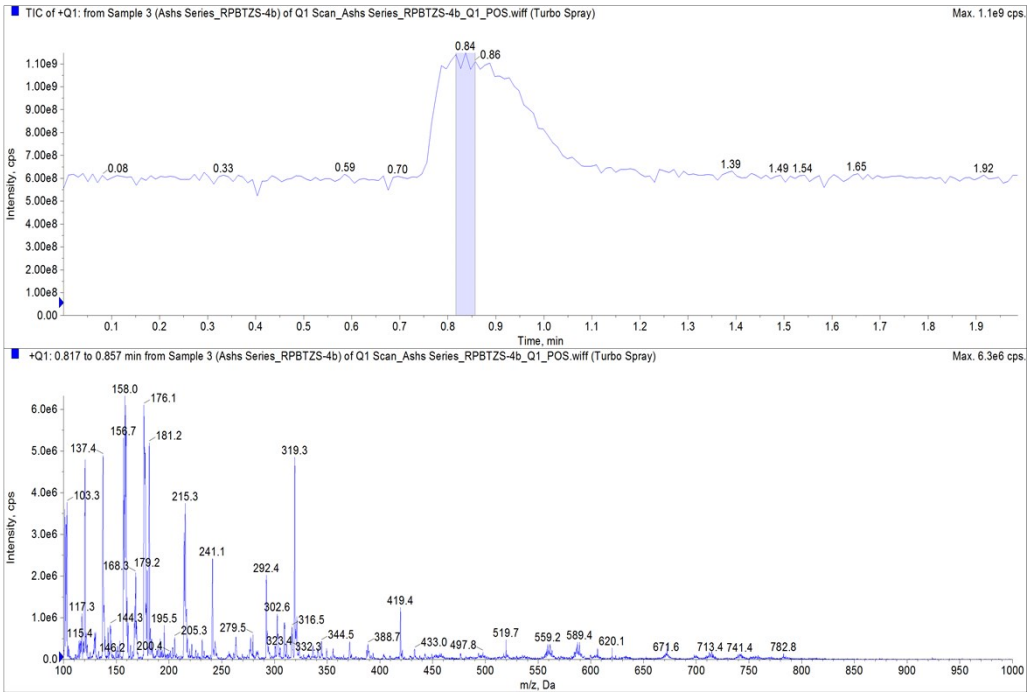
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 317.09[M+H]$^{+}$

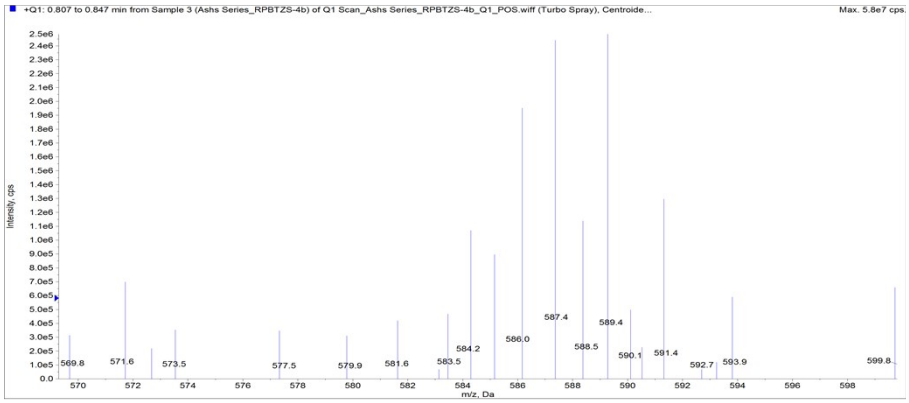
ESI-MS spectra of complex 7g2



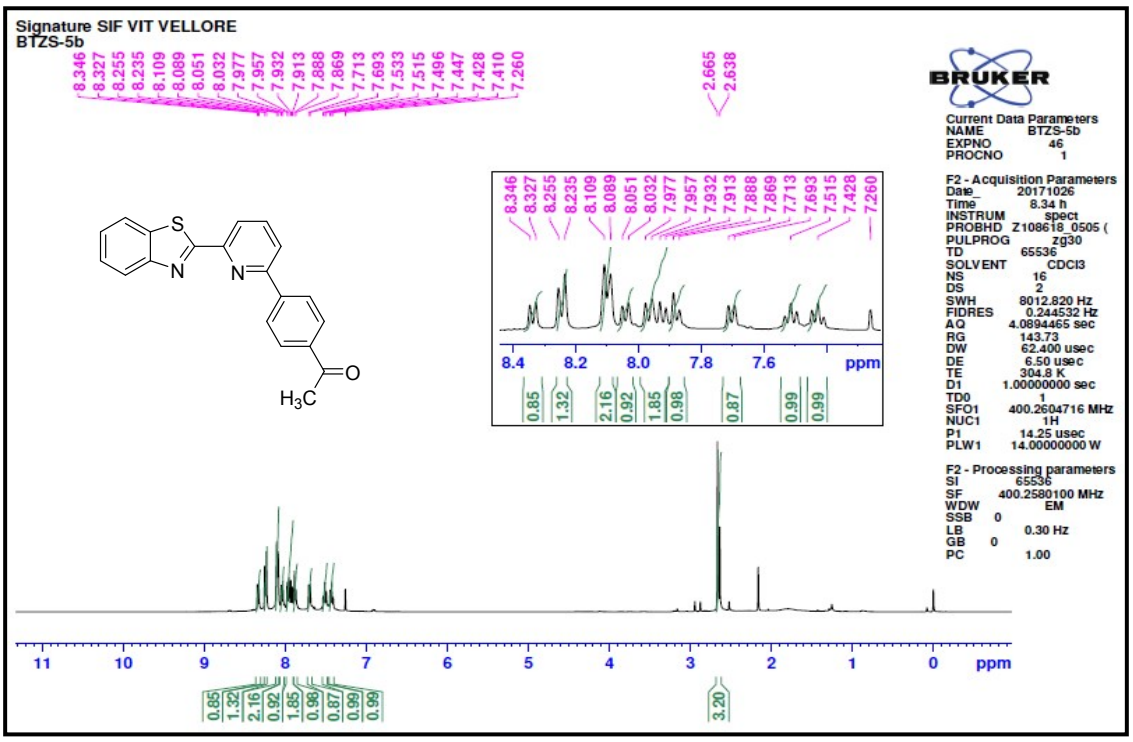
^{31}P and ^{19}F NMR of complex 8g2

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 587.05 [M+]

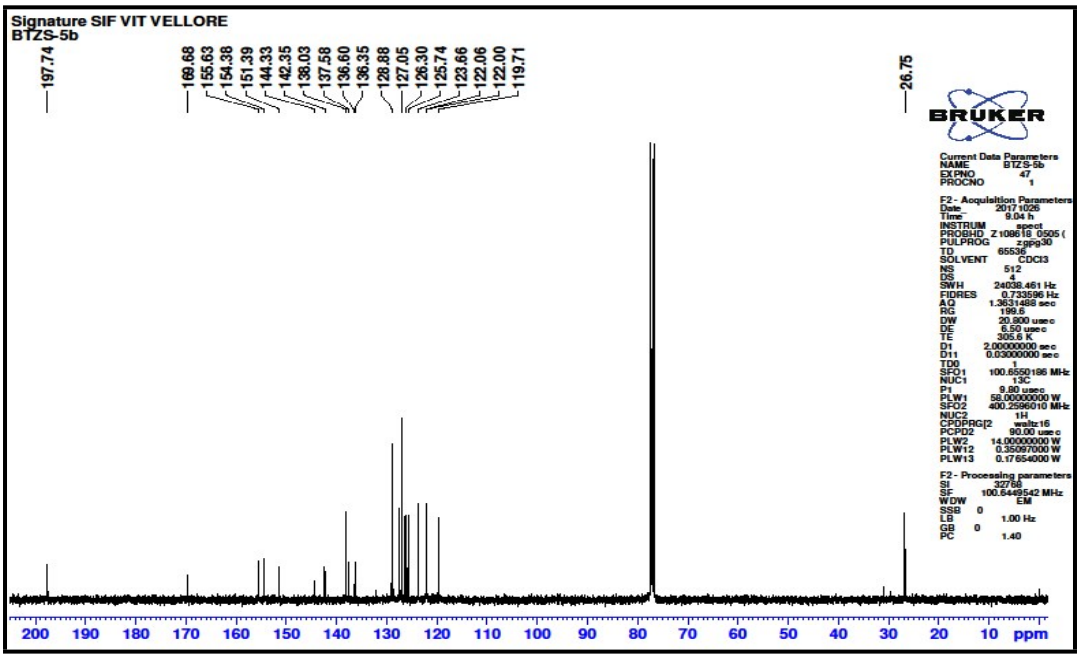




ESI-MS spectra of complex 8g2

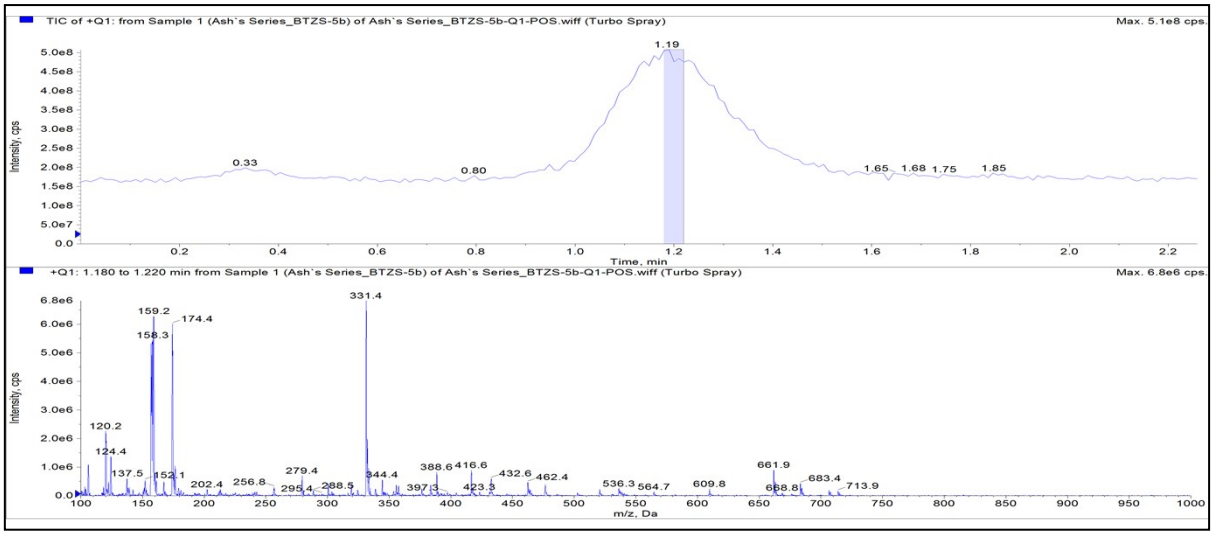


^{1}H NMR of ligand 7g3

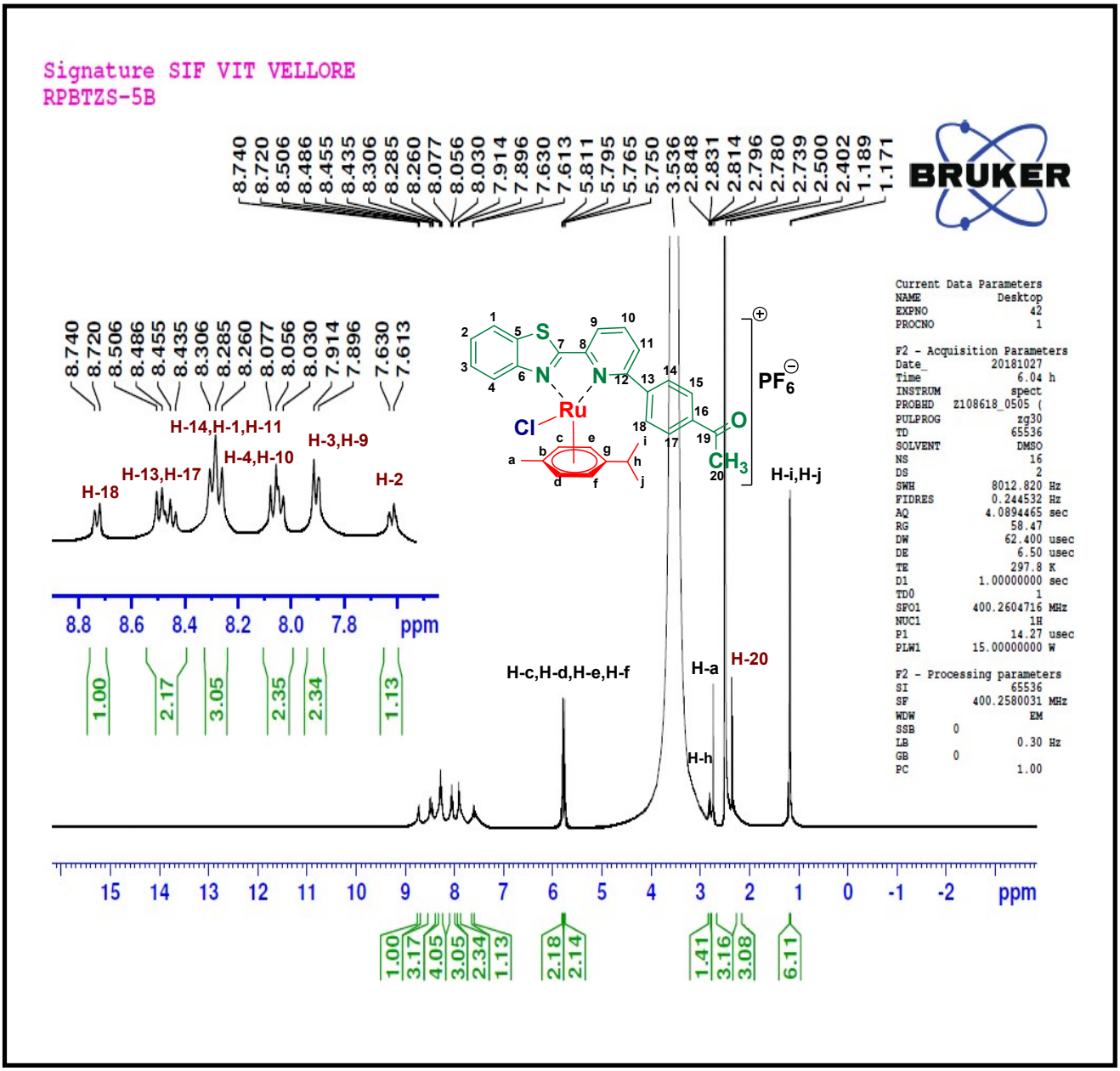


^{13}C NMR of ligand 7g3

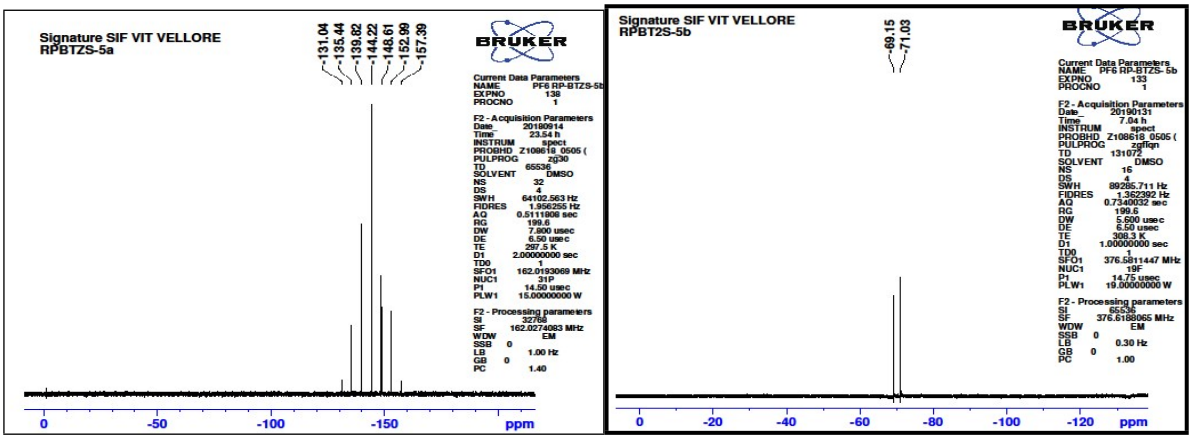
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 331.08 $[M+H]^{+}$



ESI-MS spectra of complex 7g3

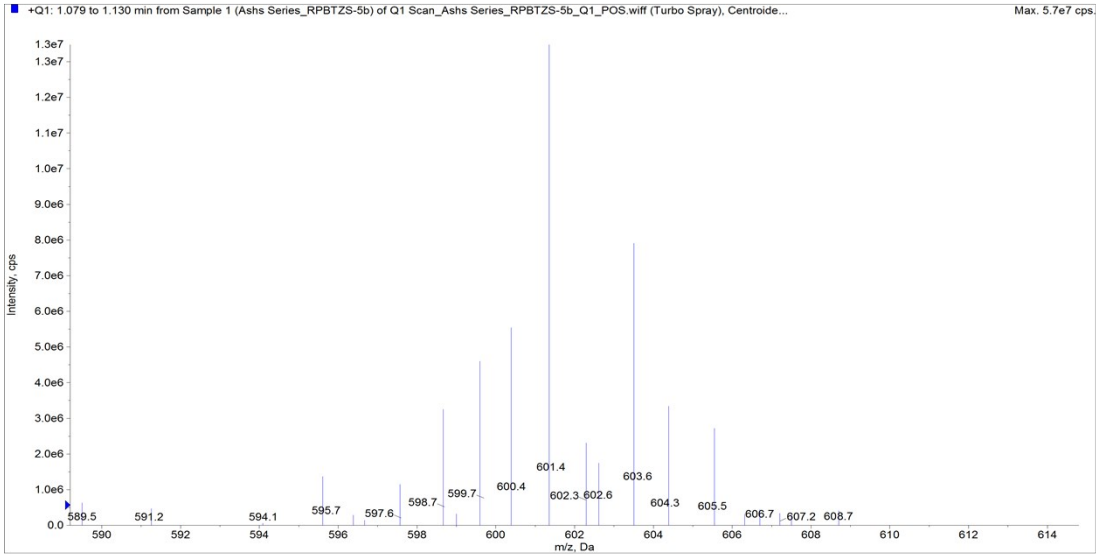


^{1}H NMR of ligand 8g3

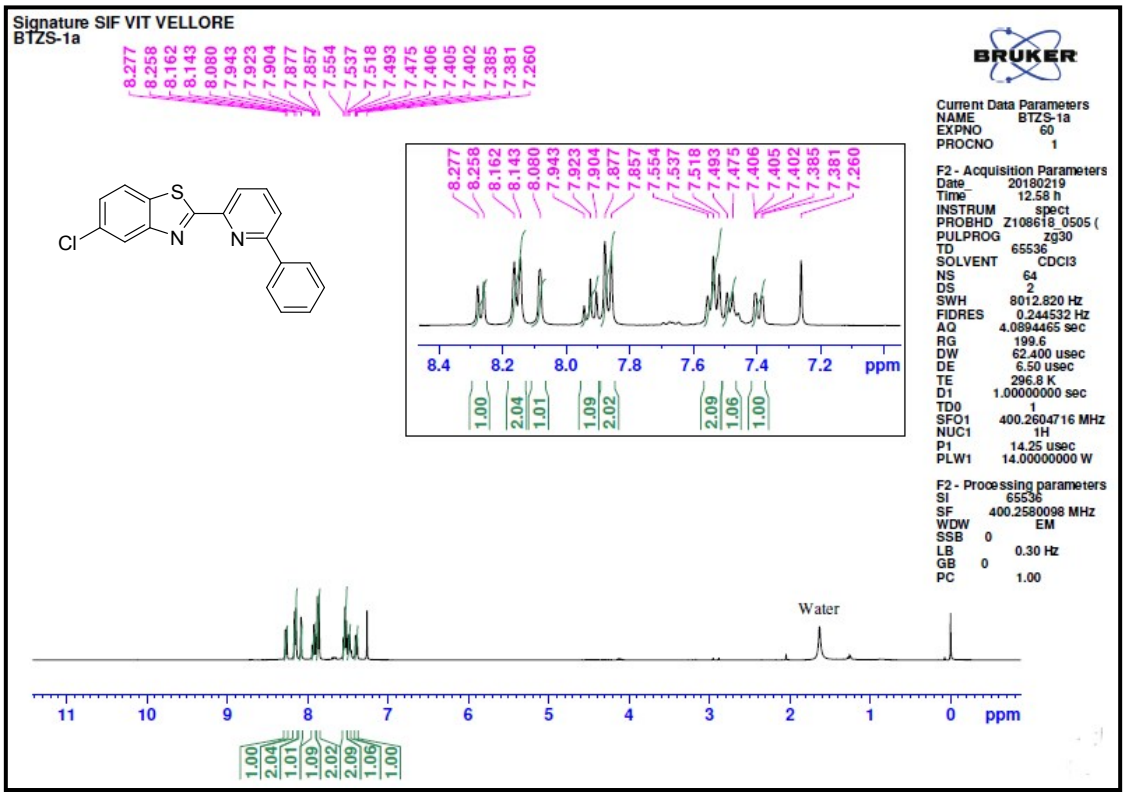


^{31}P and ^{19}F NMR of complex 8g3

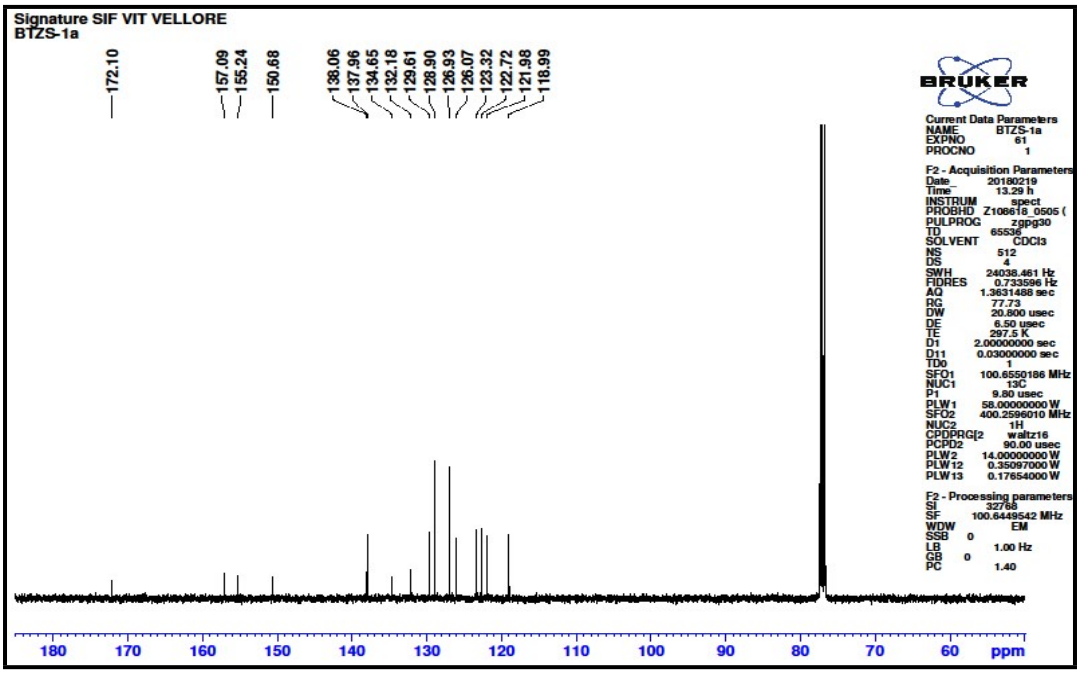
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 601.06[M^+]



ESI-MS spectra of complex 8g3

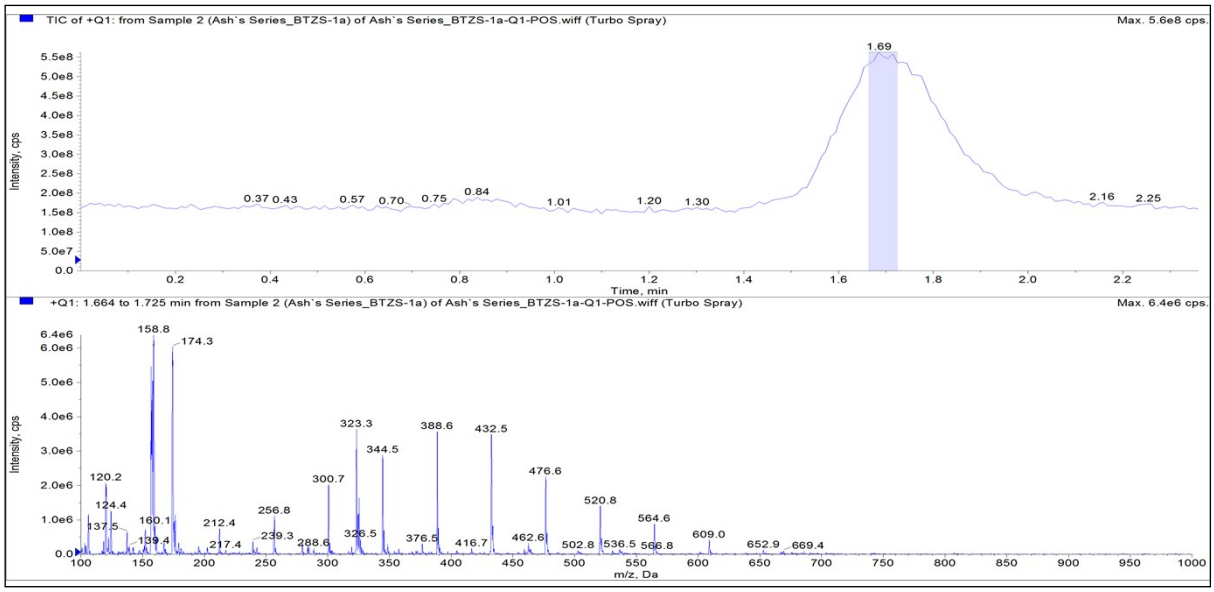


^{1}H NMR of ligand 7l1

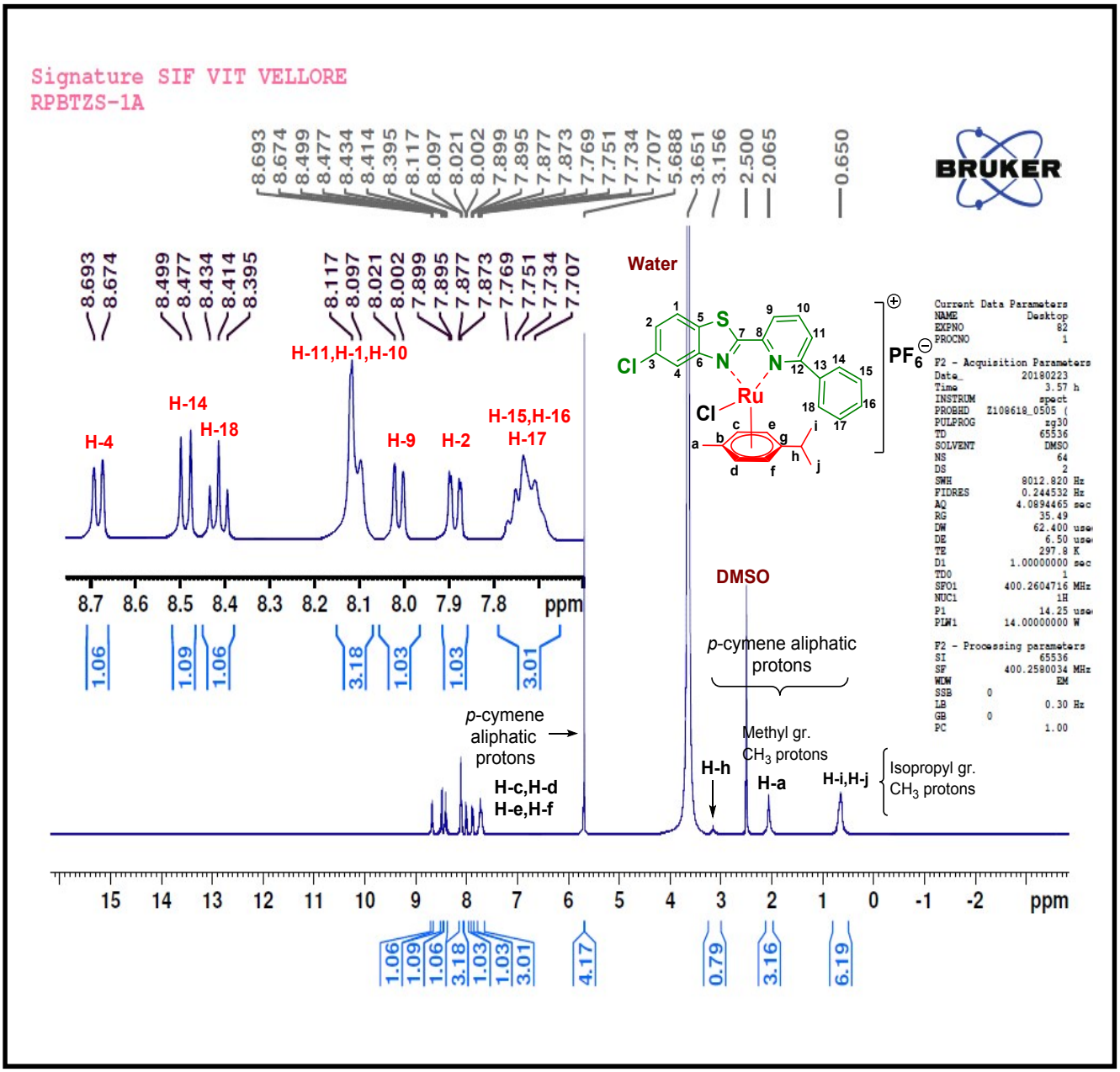


^{13}C NMR of ligand 7l1

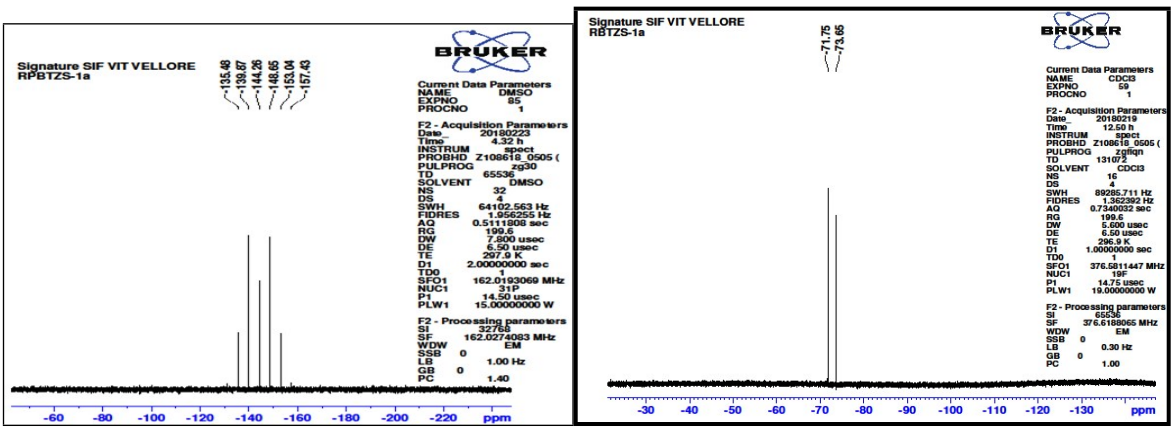
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 323.03$[M+H]^{+}$



ESI-MS spectra of complex 7l1

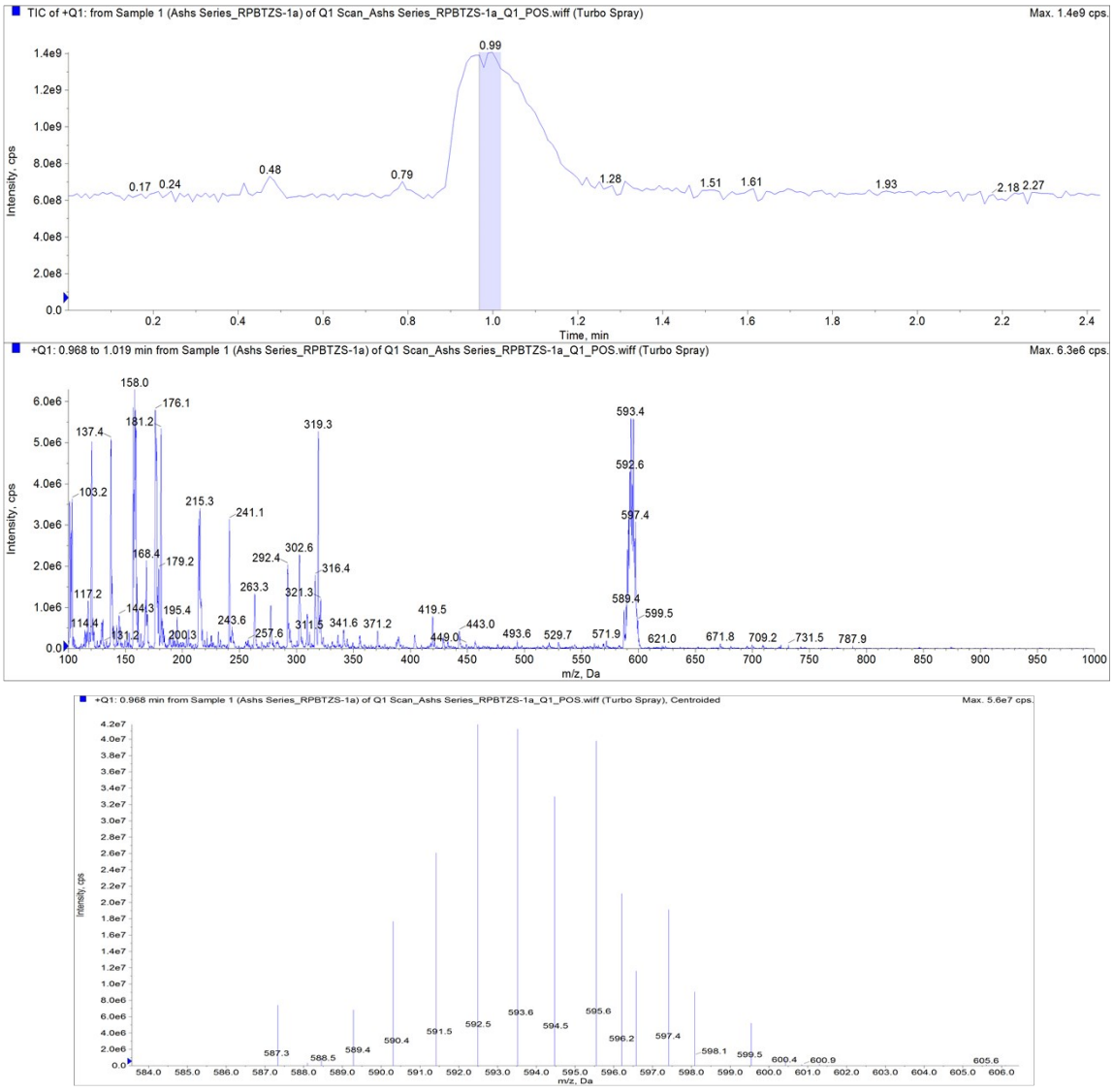


^{1}H NMR of ligand 8l1

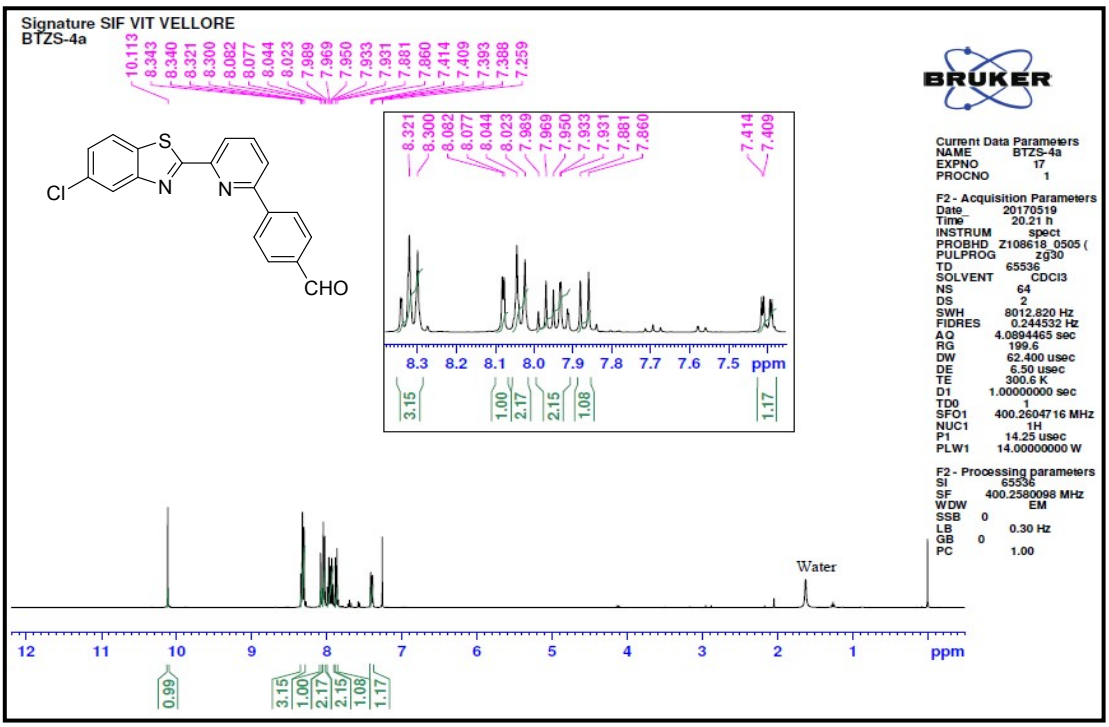


^{31}P and ^{19}F NMR of complex 8l1

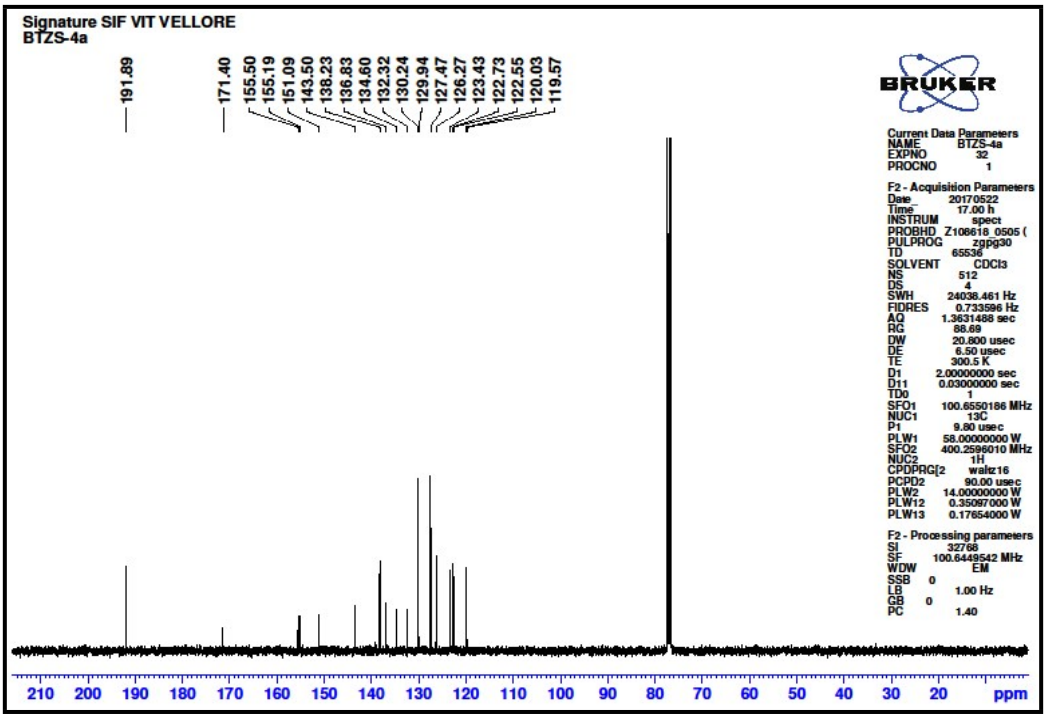
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 593.02[M^+]



ESI-MS spectra of complex 8l1

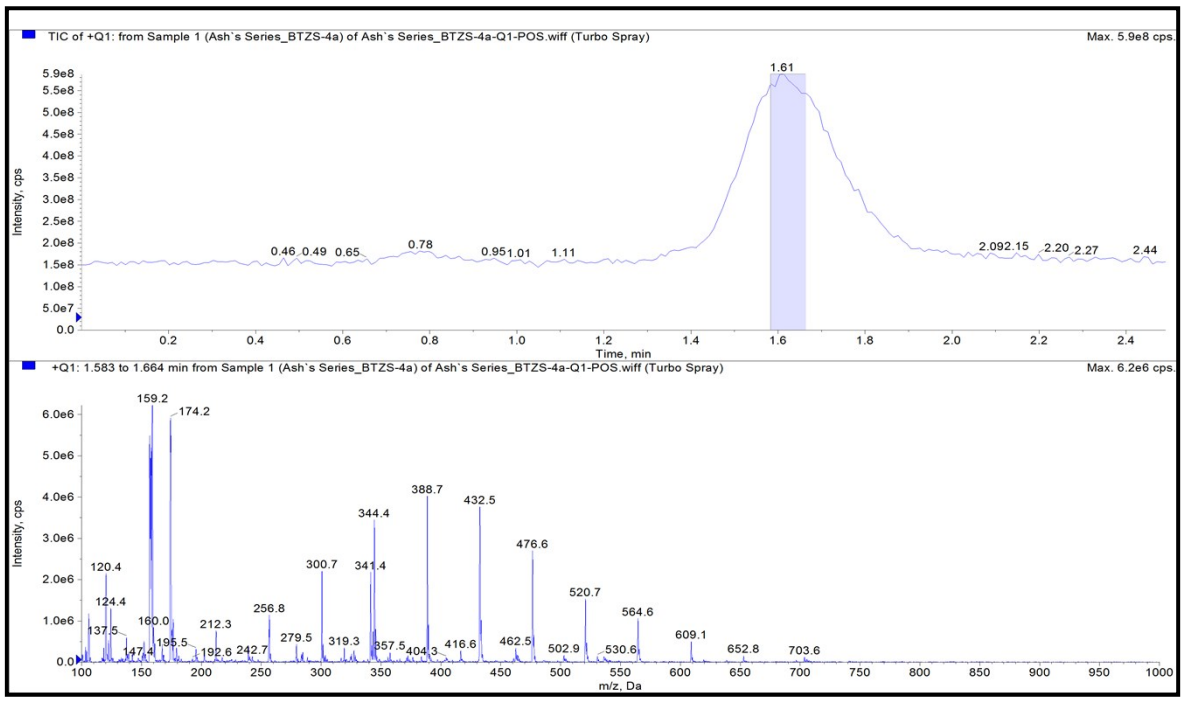


^{1}H NMR of ligand 7l2

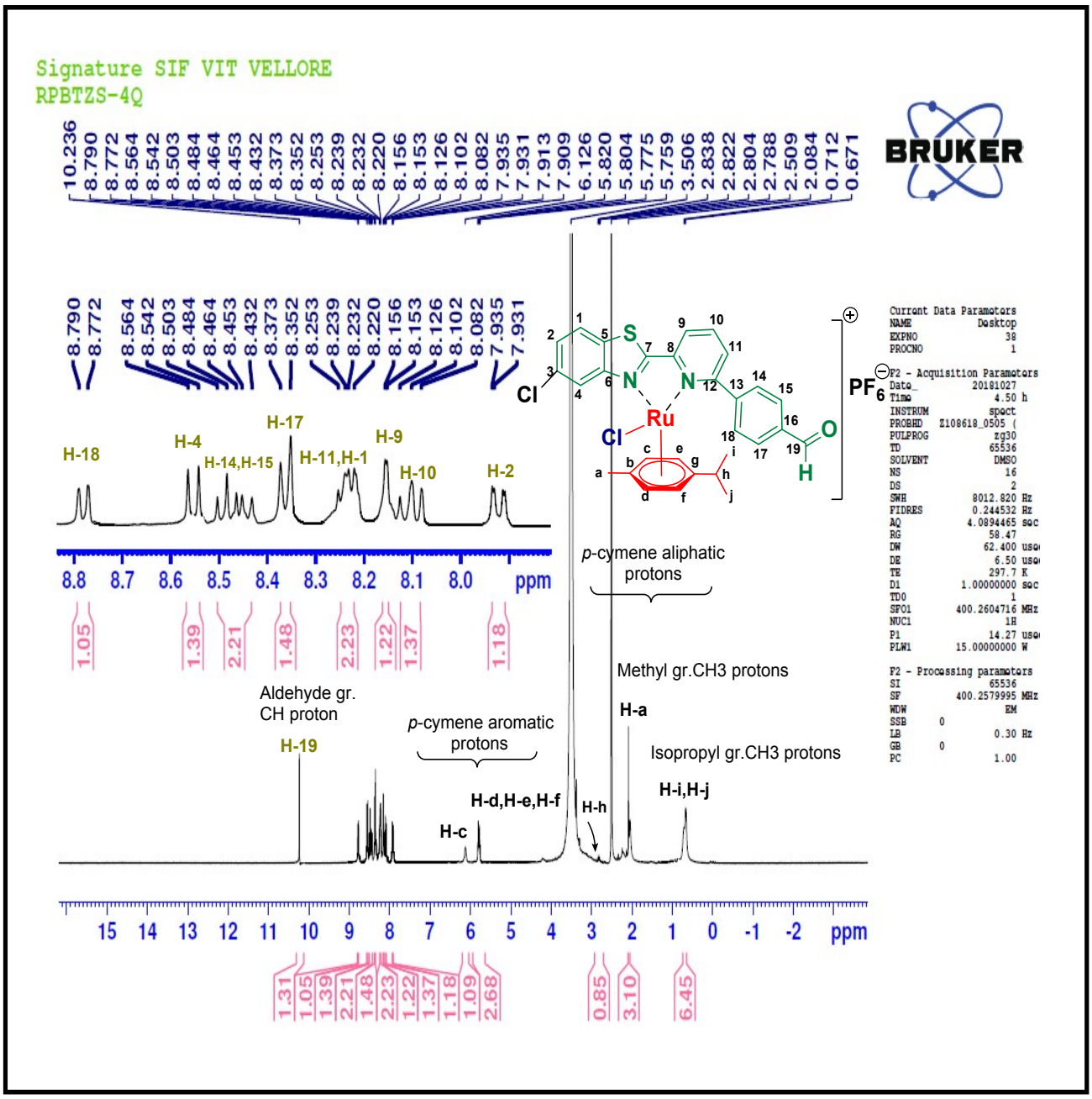


^{13}C NMR of ligand 7l2

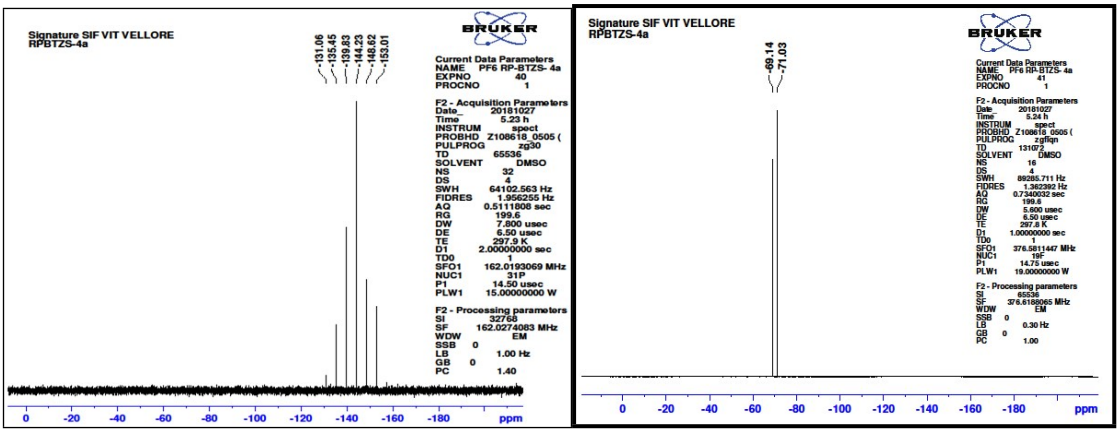
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 351.03$[M+H]^{+}$



ESI-MS spectra of complex 7l2

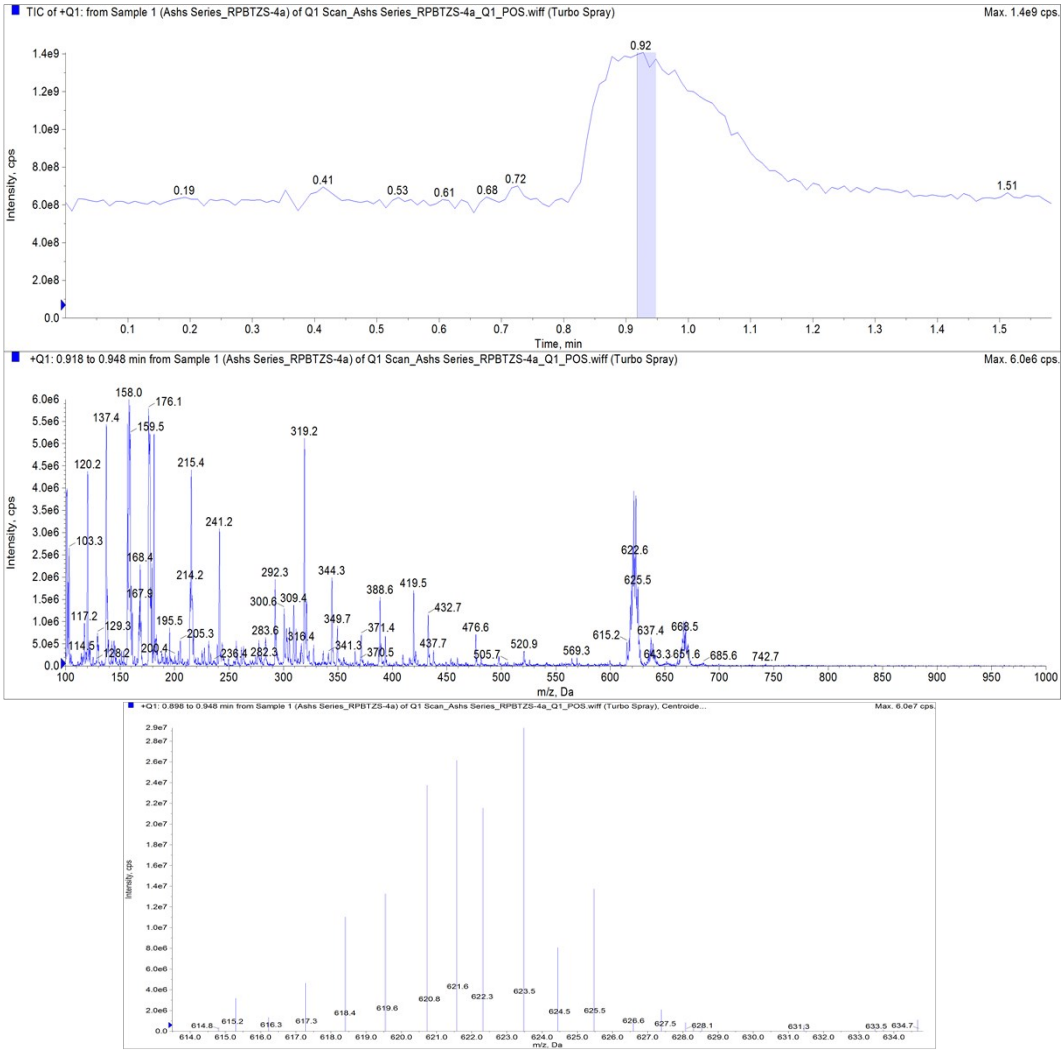


^{1}H NMR of ligand 8l2

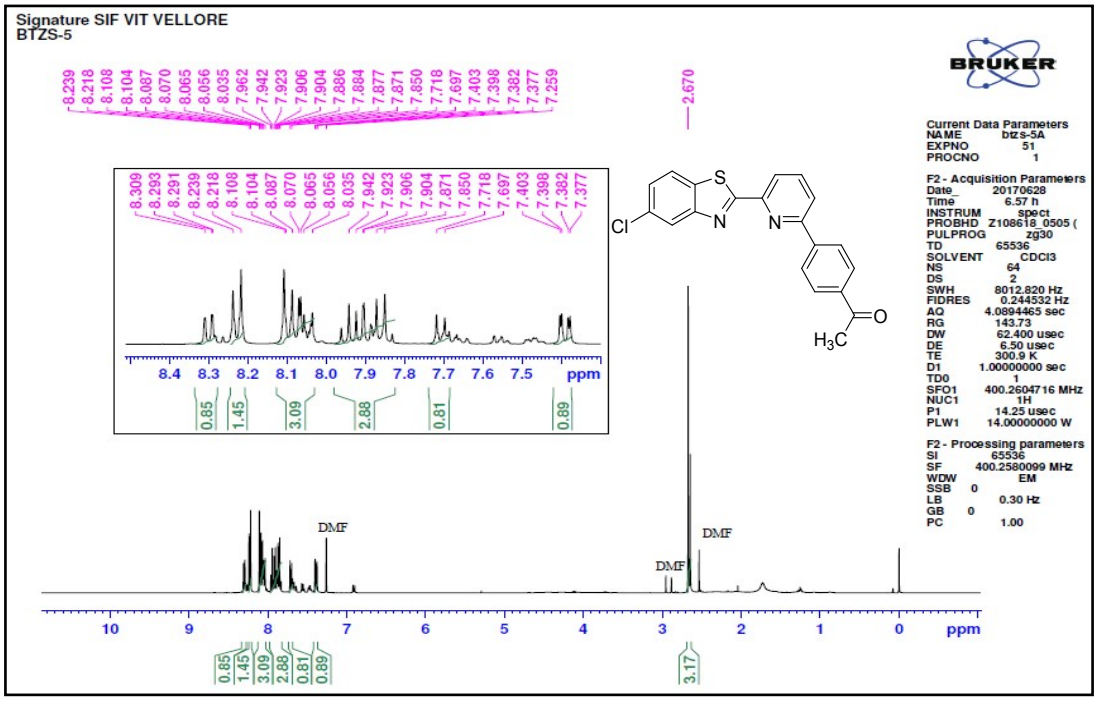


^{31}P and ^{19}F NMR of complex 8l2

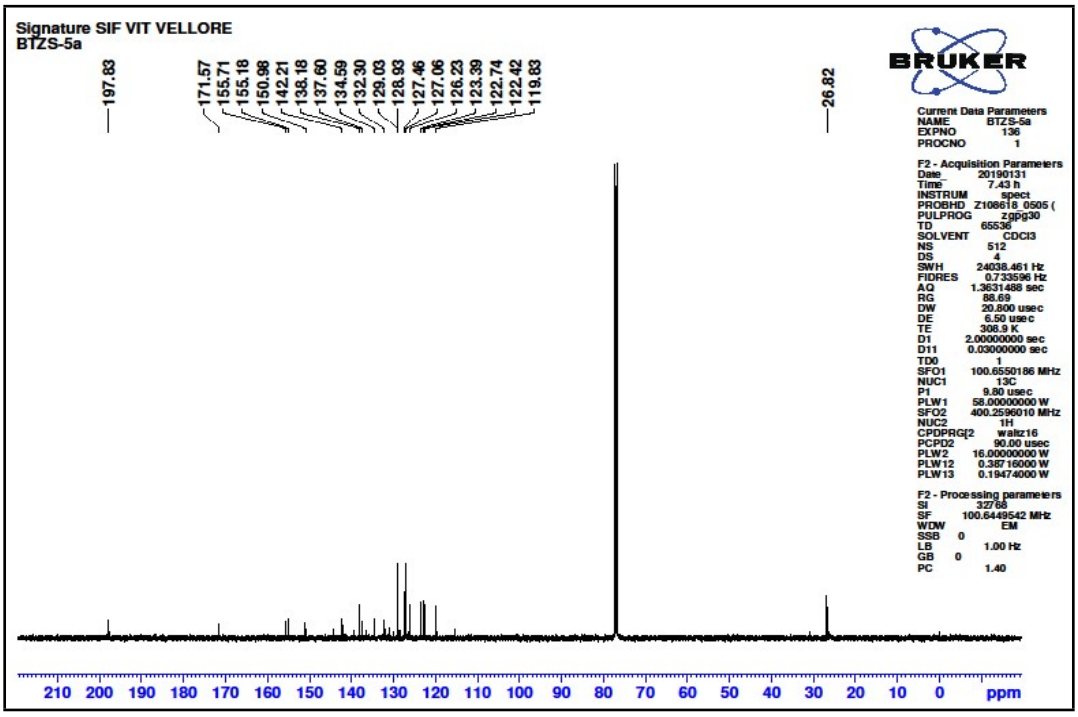
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 621.01 [M$^+$]



ESI-MS spectra of complex 8l2

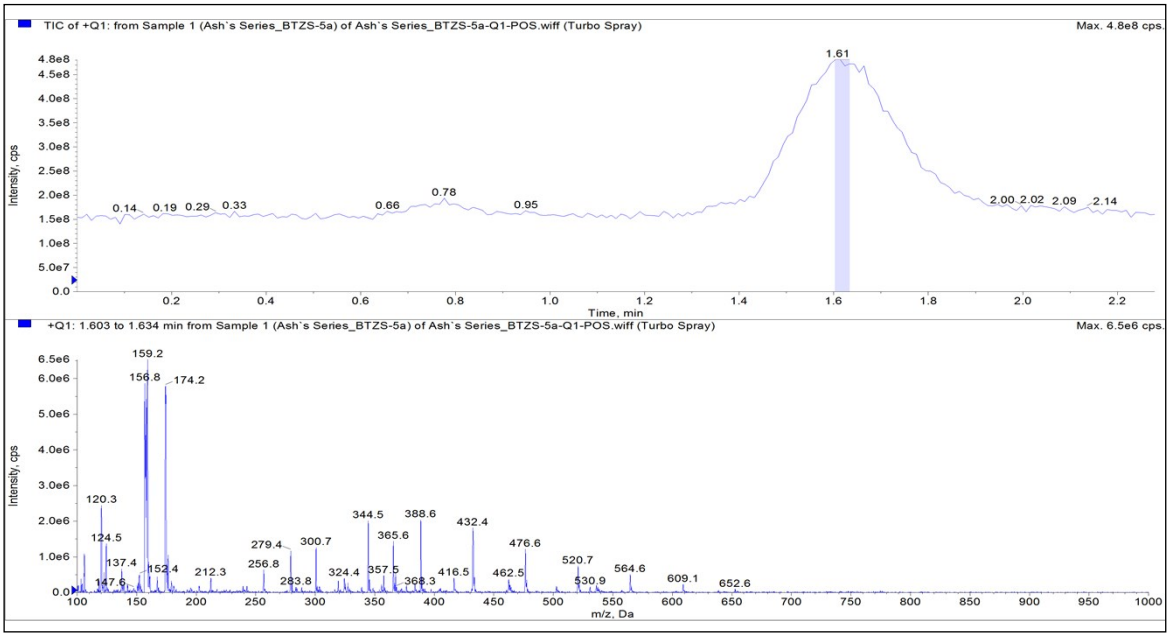


^{1}H NMR of ligand 7l3

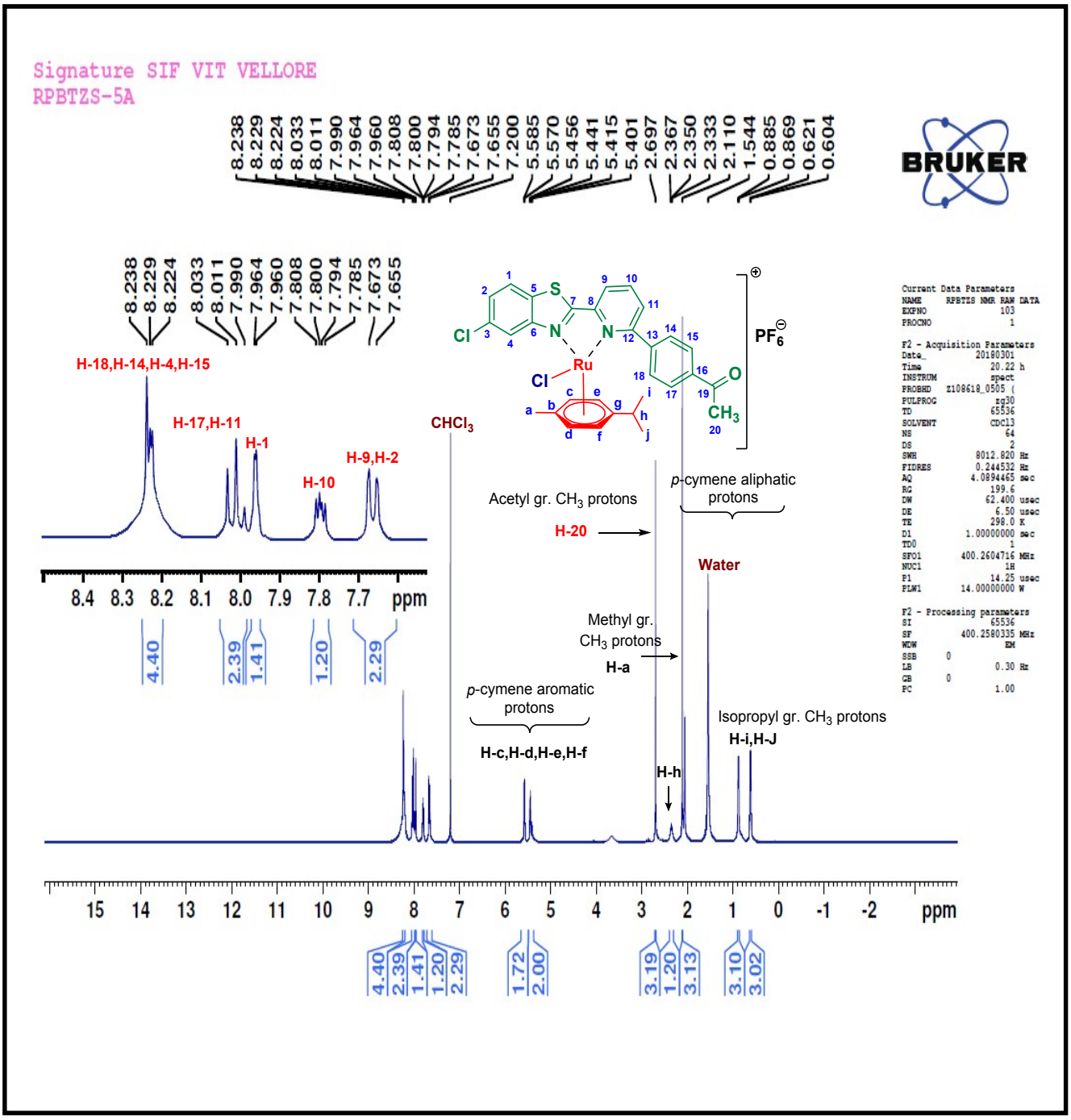


^{13}C NMR of ligand 7l3

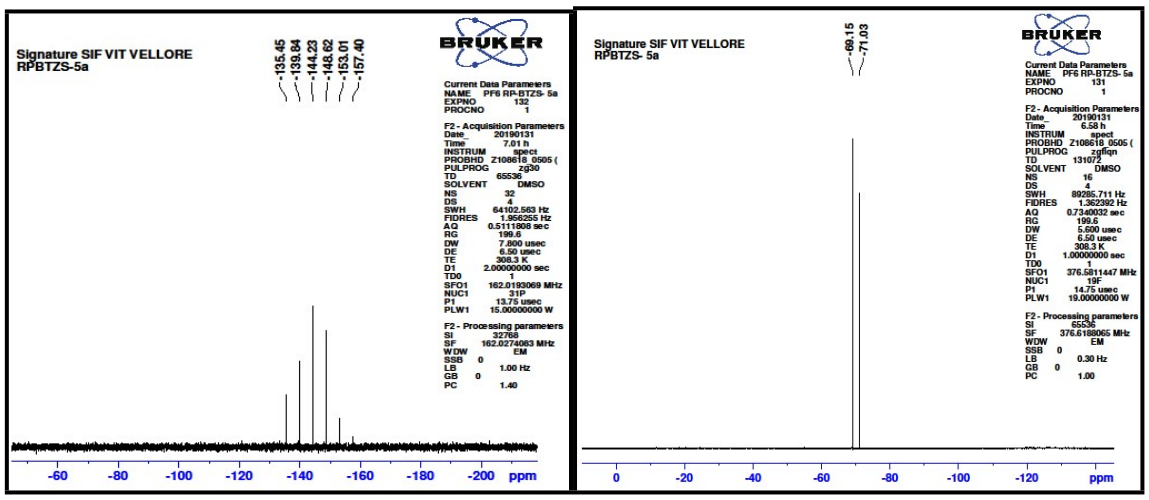
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 365.04[M+H]+



ESI-MS spectra of complex 7l3

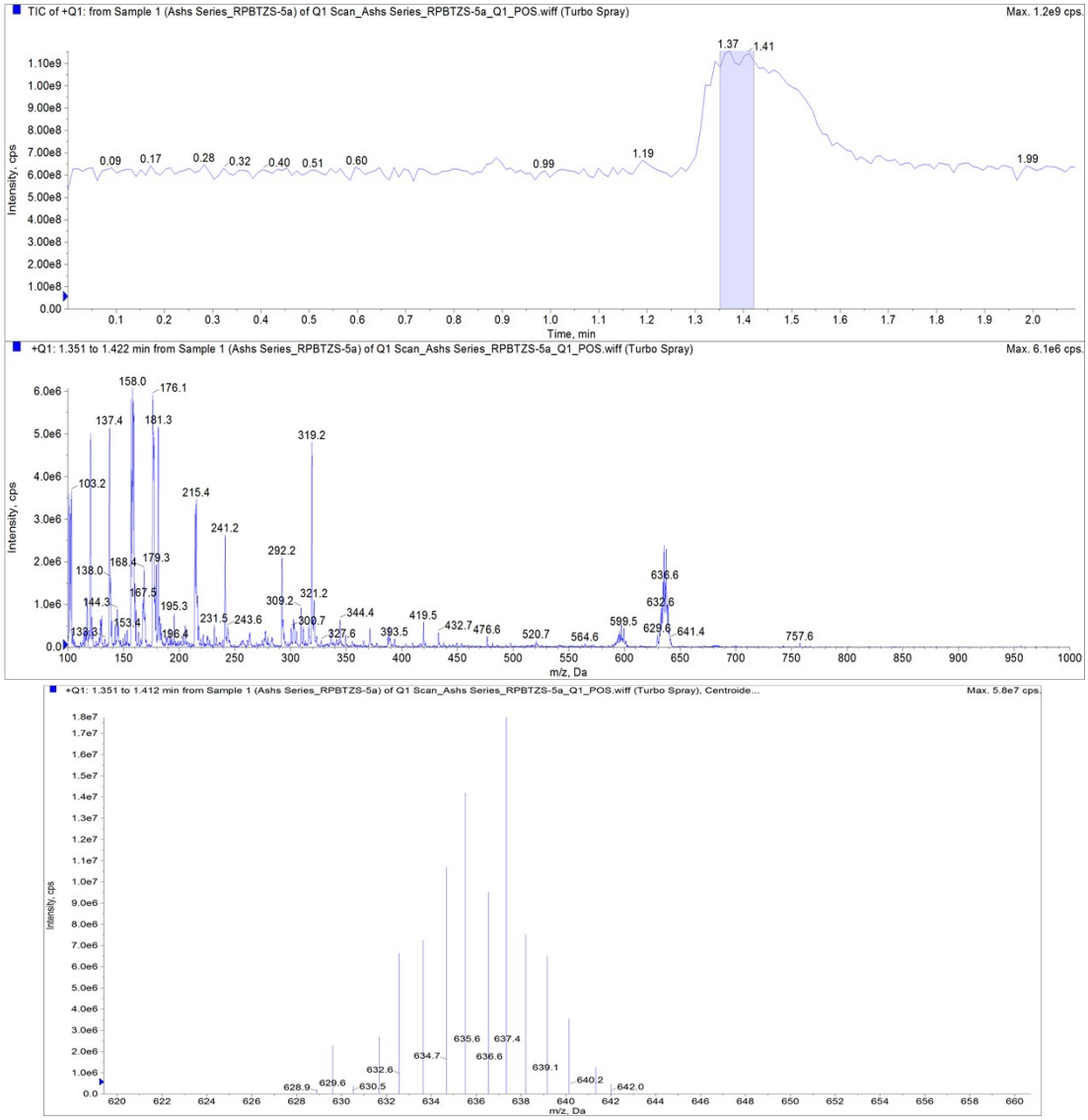


^{1}H NMR of ligand 8l3

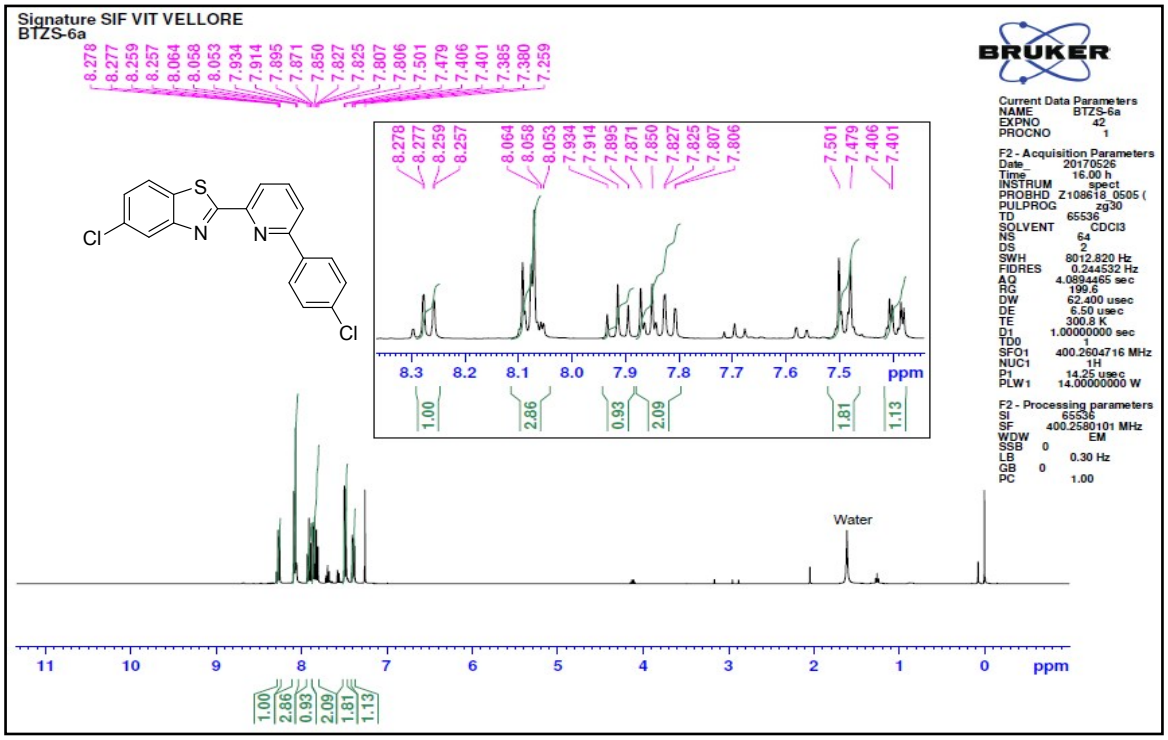


^{31}P and ^{19}F NMR of complex 8l3

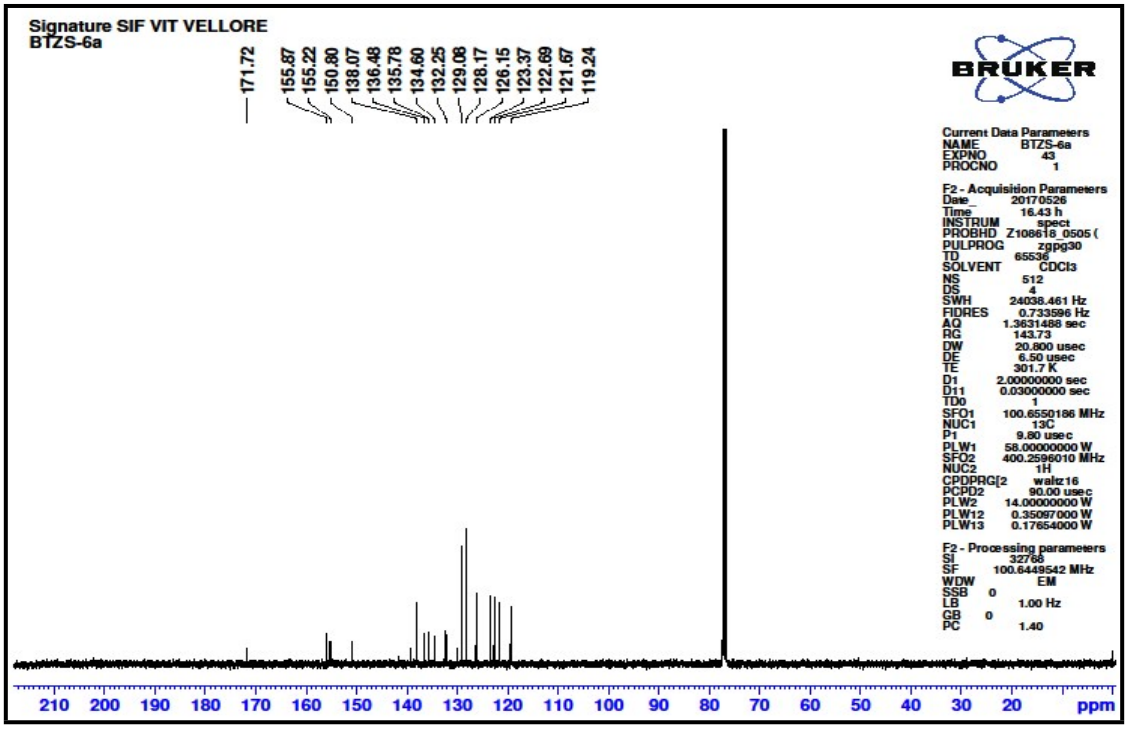
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 635.03[M$^+$]



LC-MS spectra of complex 8I3

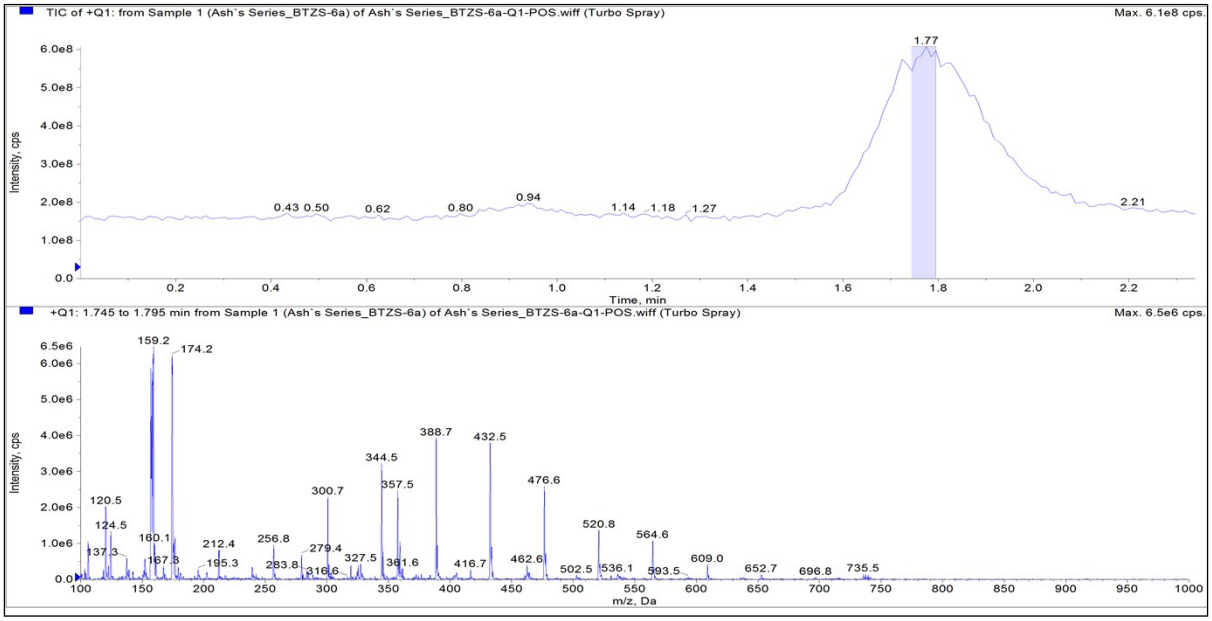


^{1}H NMR of ligand 7l4

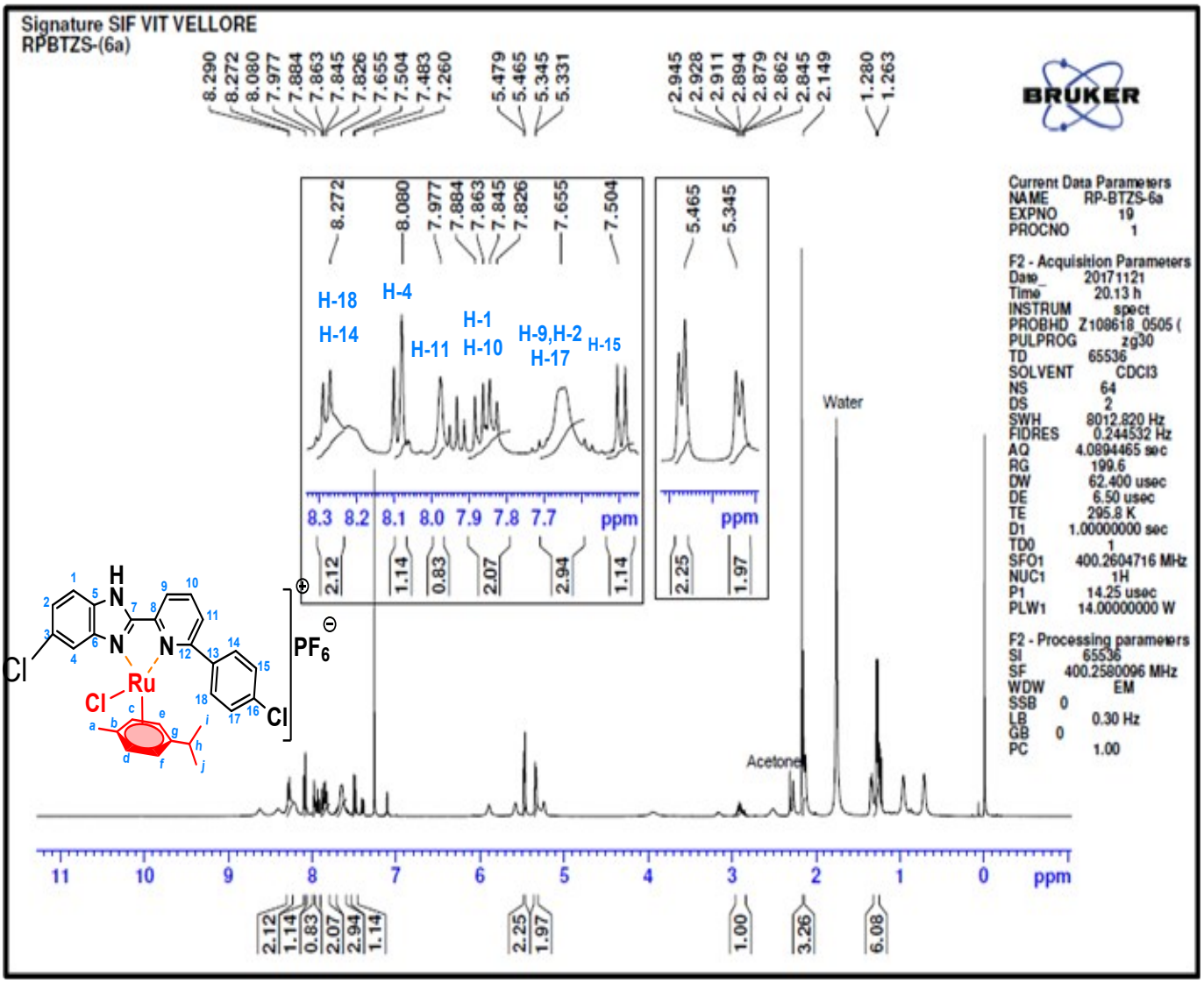


^{13}C NMR of ligand 7l4

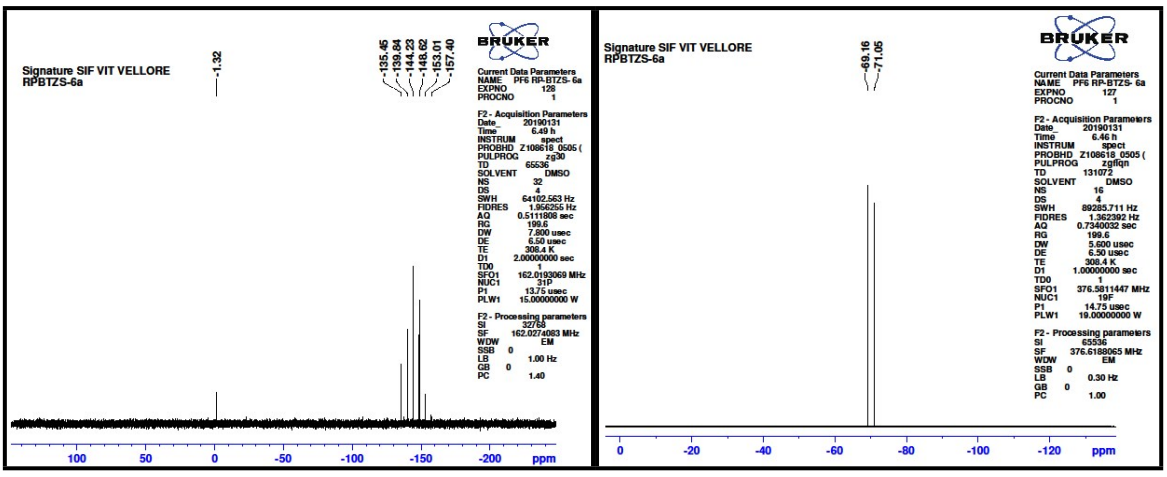
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 356.99[M+H]$^+$



ESI-MS spectra of ligand 7l4

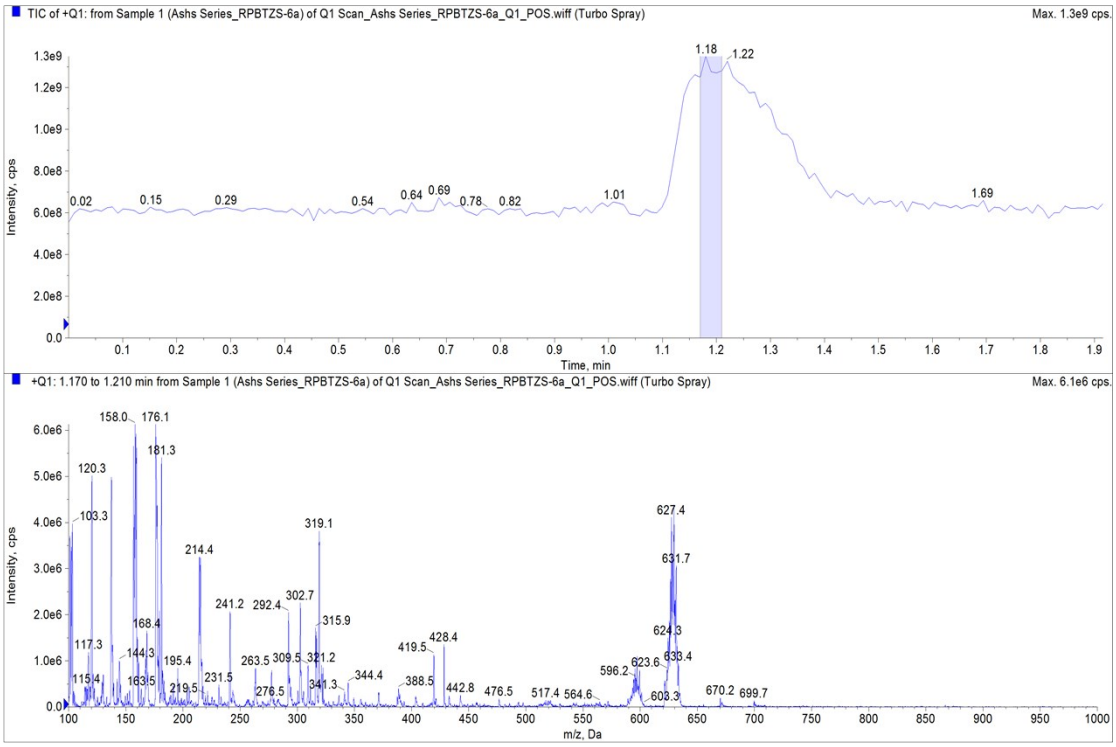


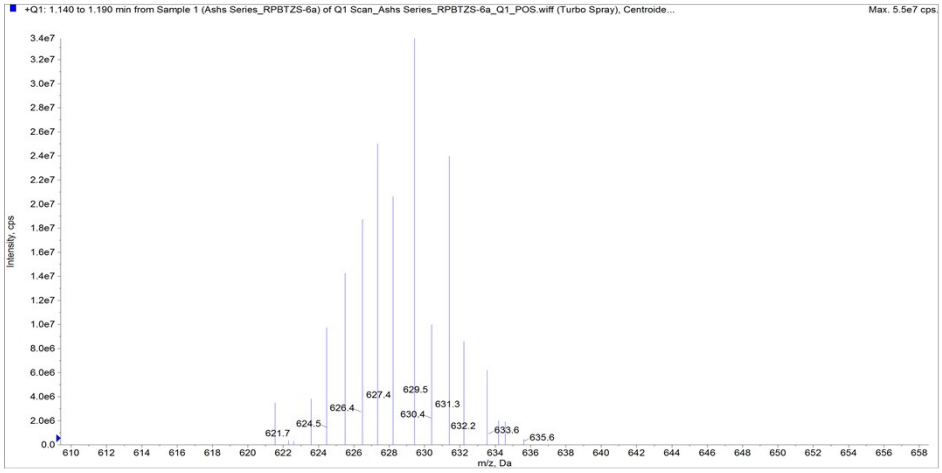
^{1}H NMR of complex 8l4



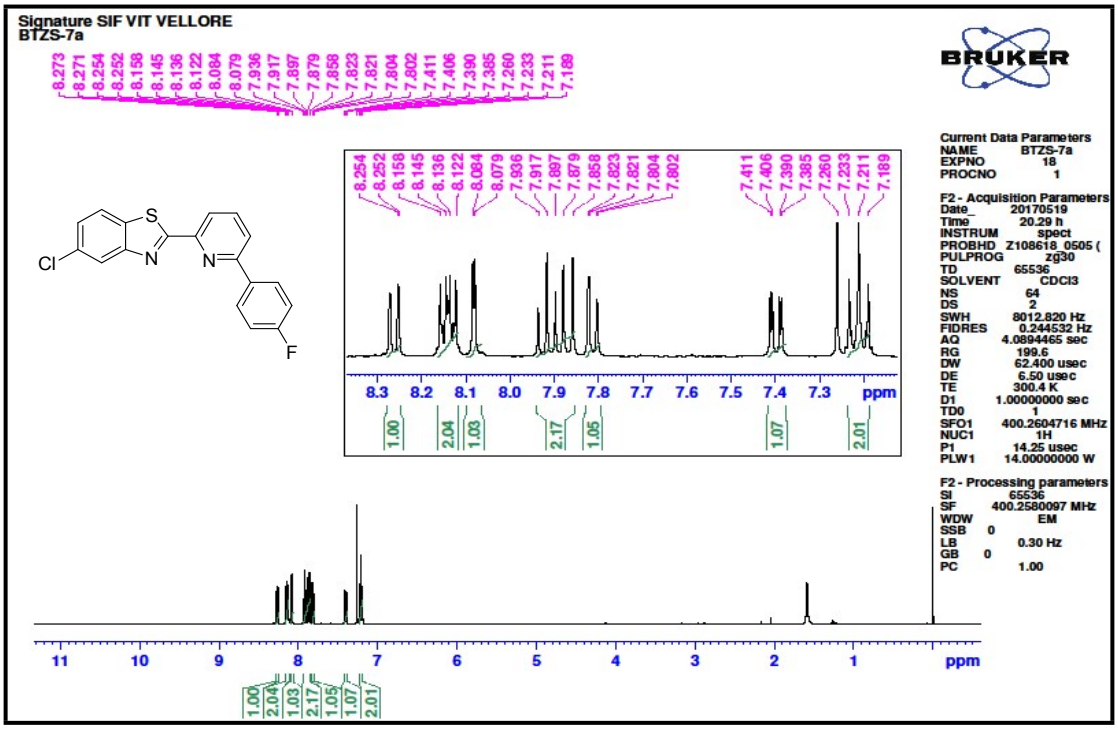
^{31}P and ^{19}F NMR of complex 8l4

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 626.98 [M$^+$]

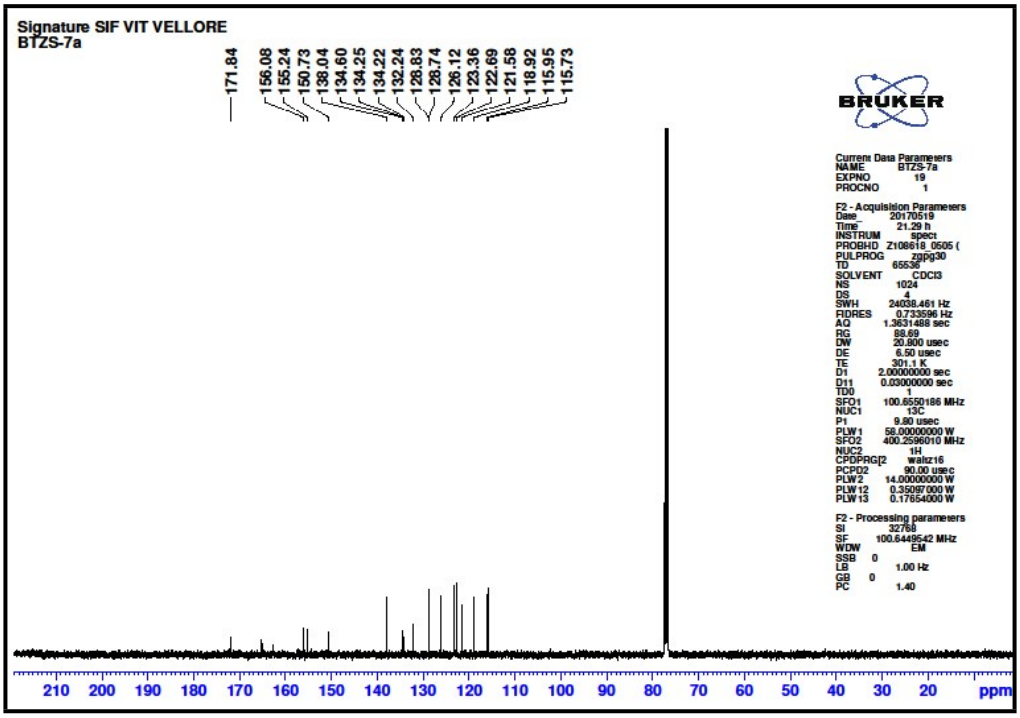




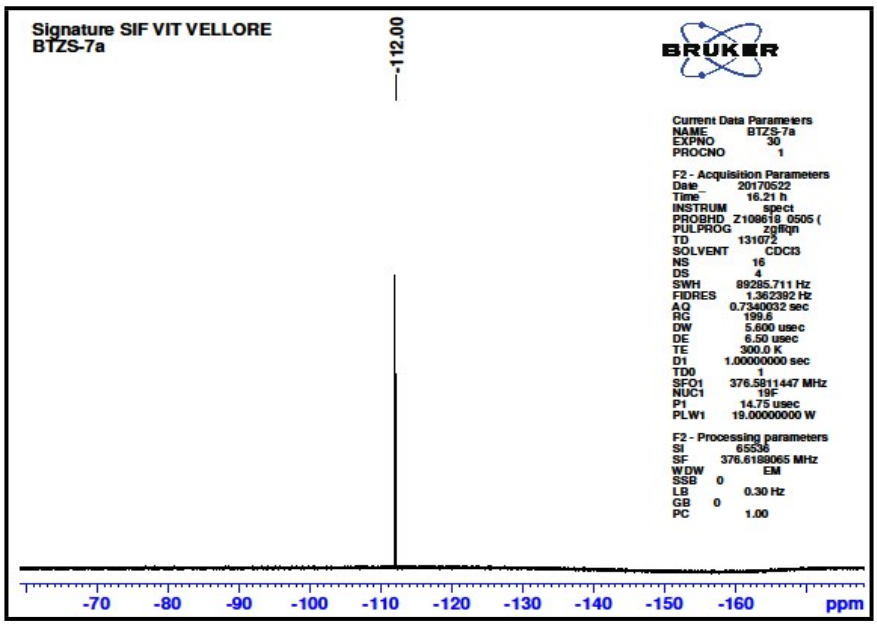
ESI-MS spectra of complex 8l4



^{1}H NMR of ligand 7l5

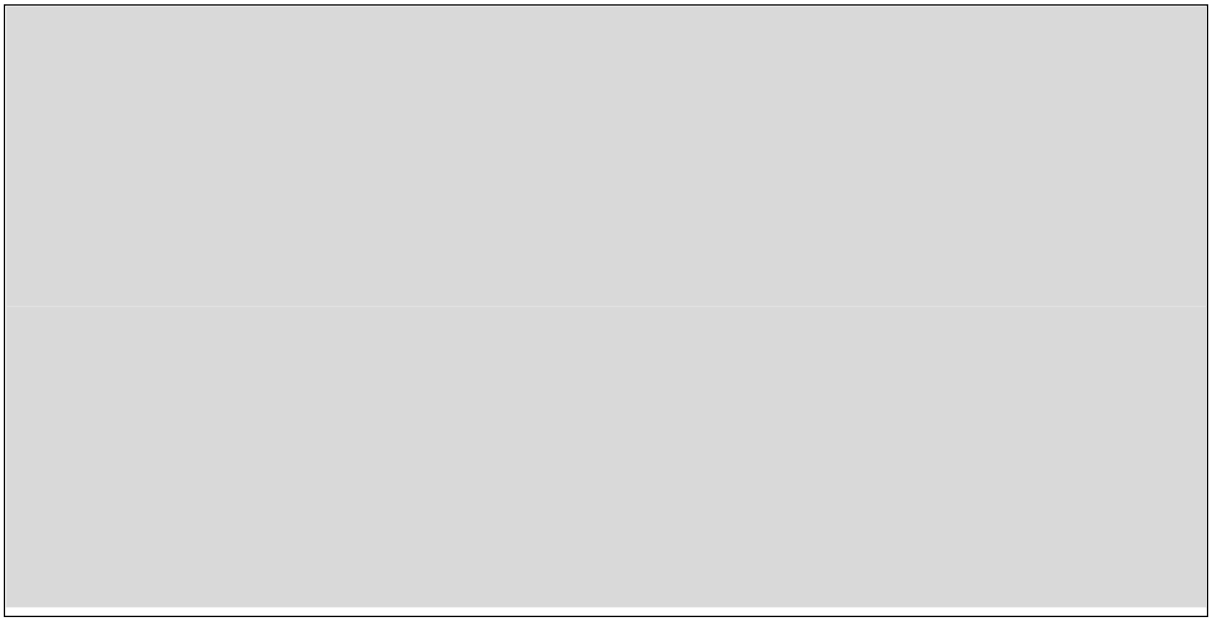


^{13}C NMR of ligand 7l5

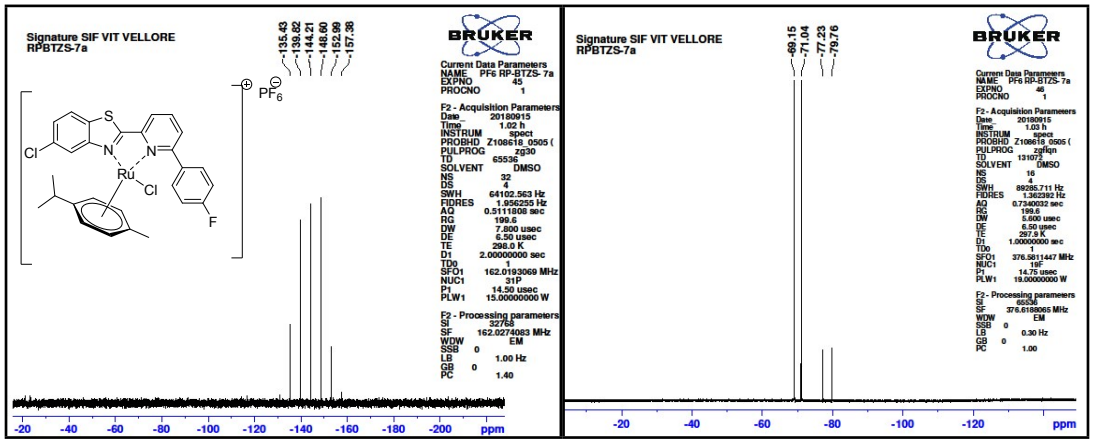


^{19}F NMR of ligand 7l5

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 341.02$[M+H]^+$

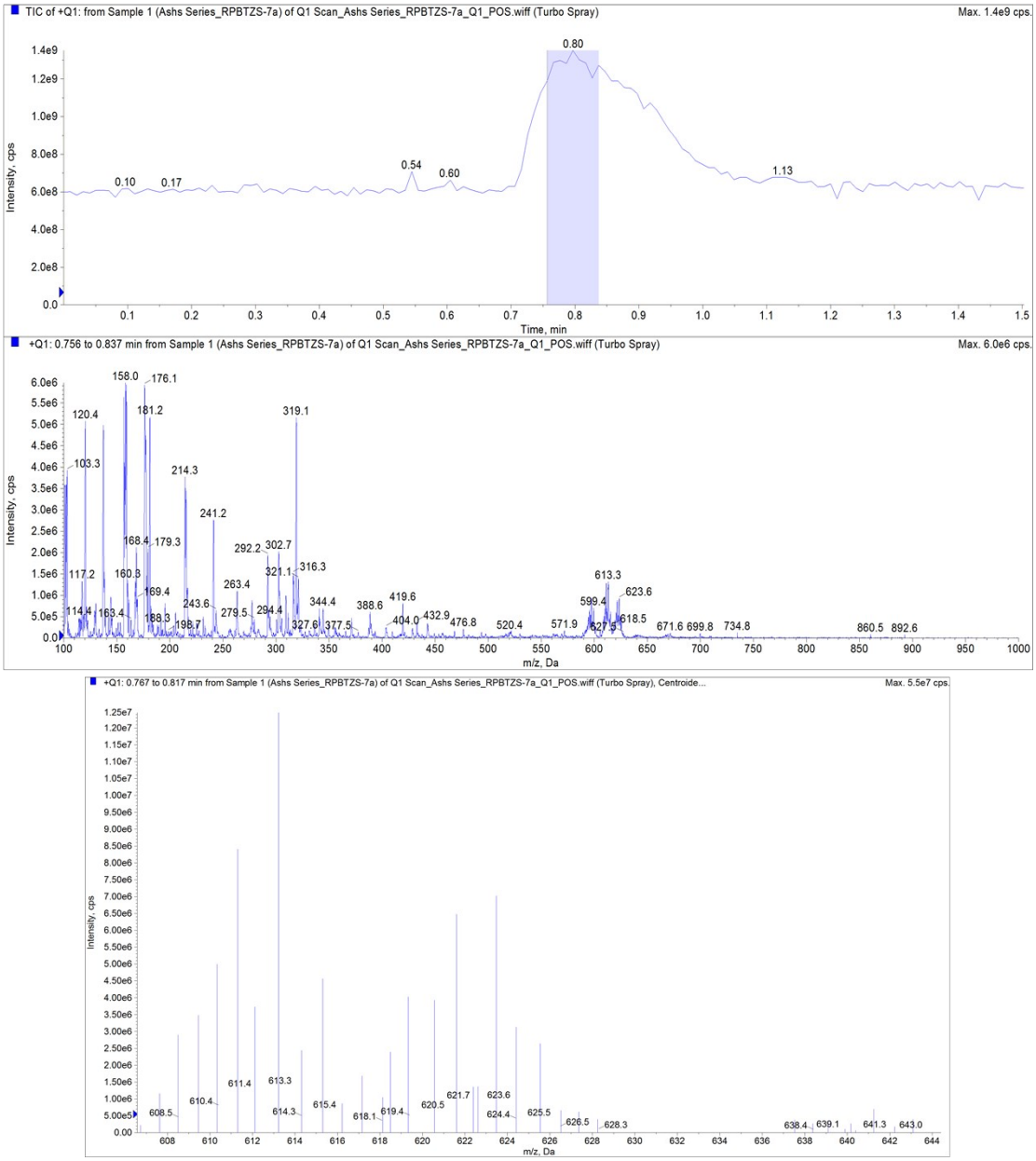


ESI-MS spectra of ligand 7l5

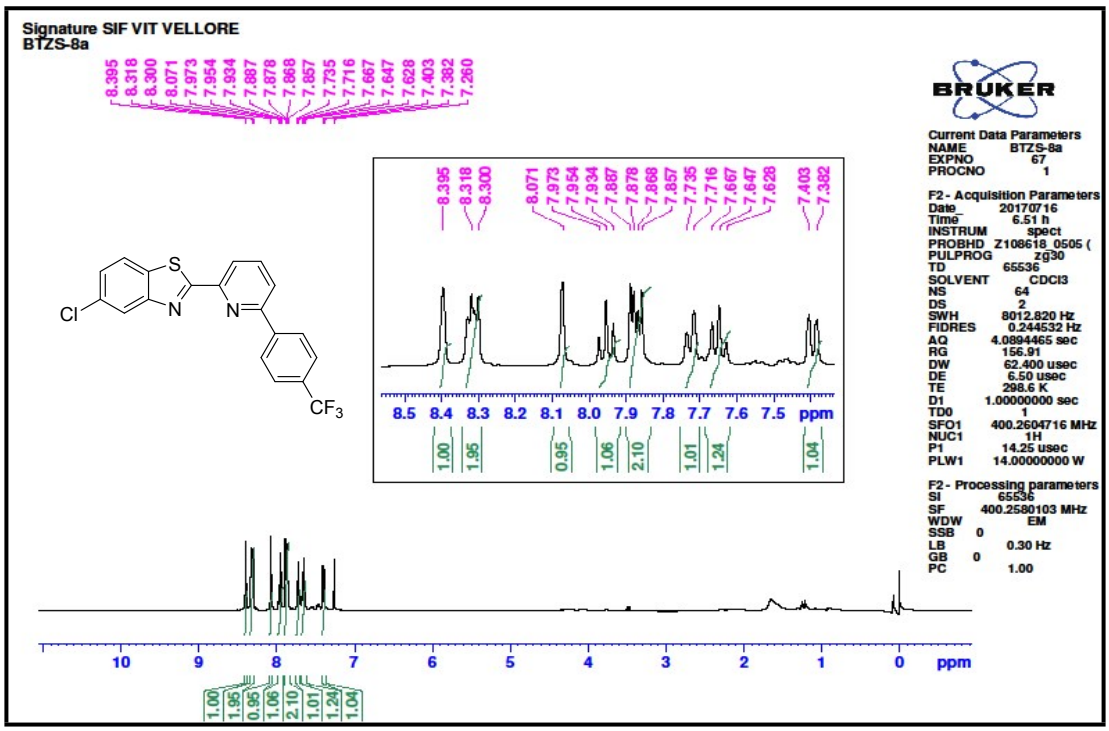


^{31}P and ^{19}F NMR of complex 8l5

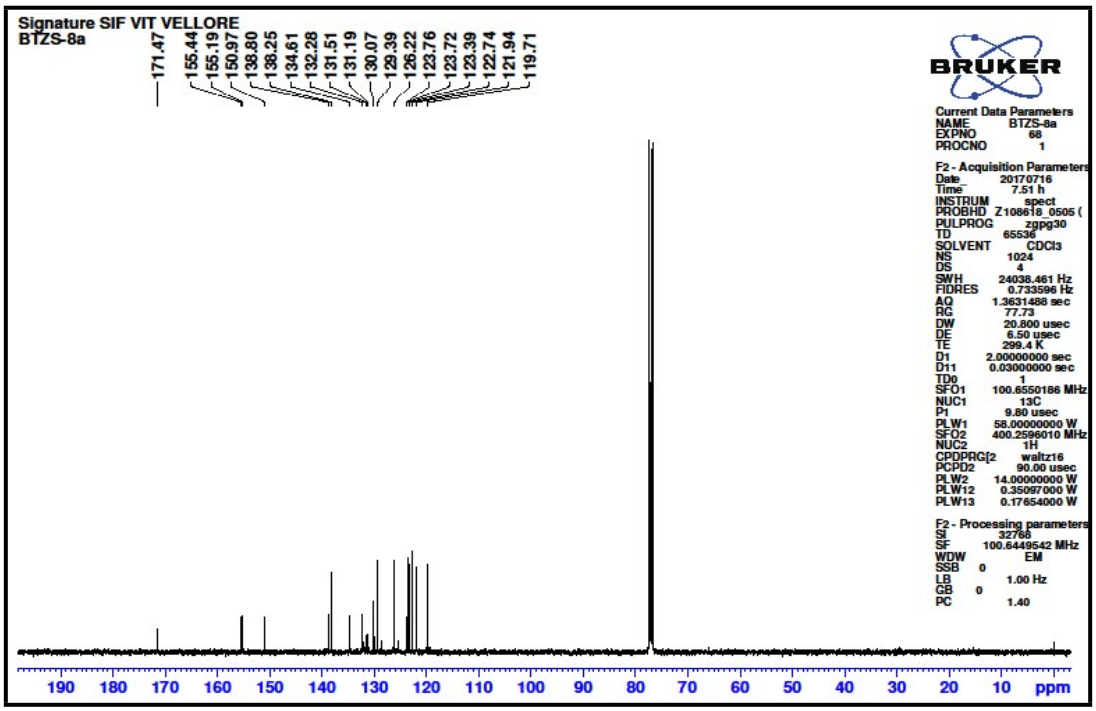
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 611.01 [M+]



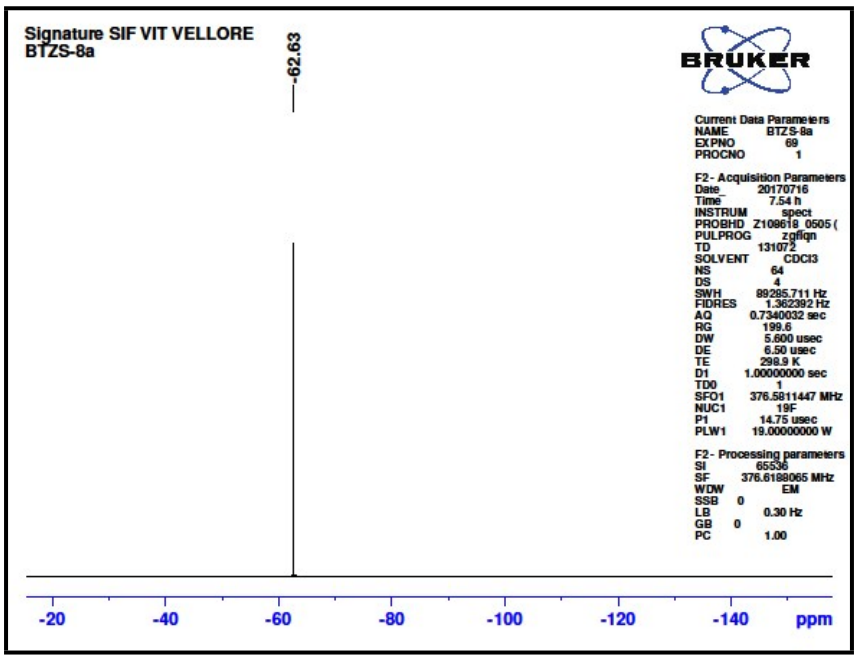
ESI-MS spectra of complex 8I5



^{1}H NMR of ligand 7l6

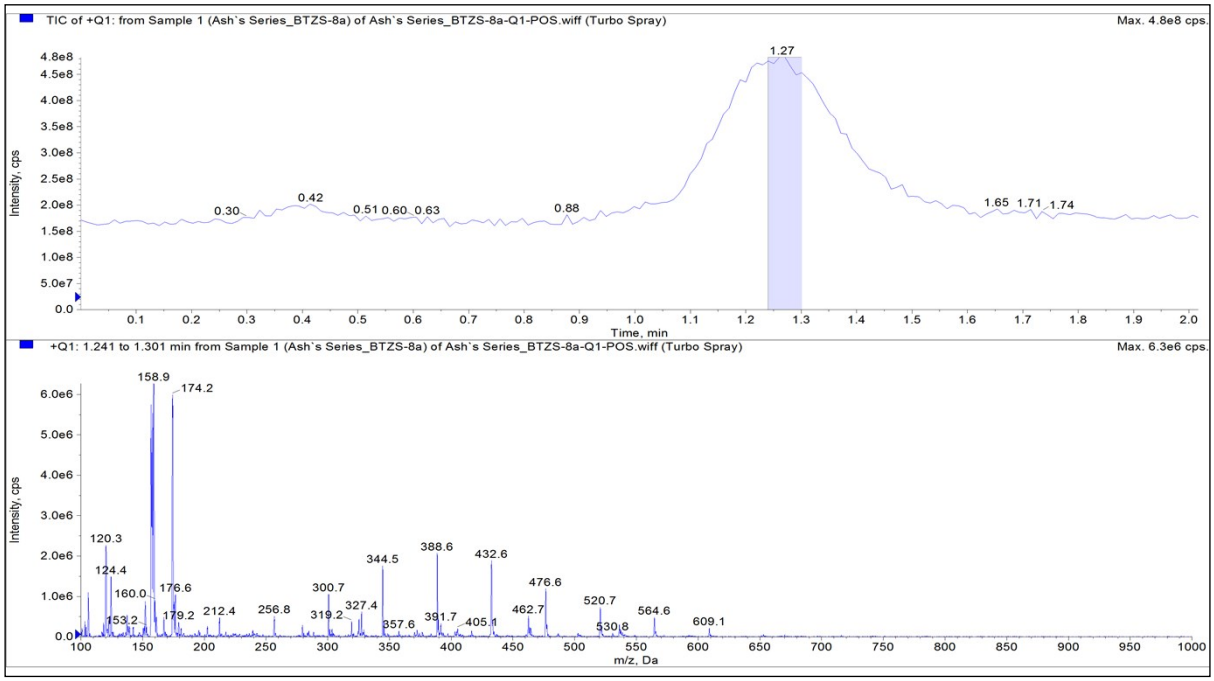


^{13}C NMR of ligand 7l6

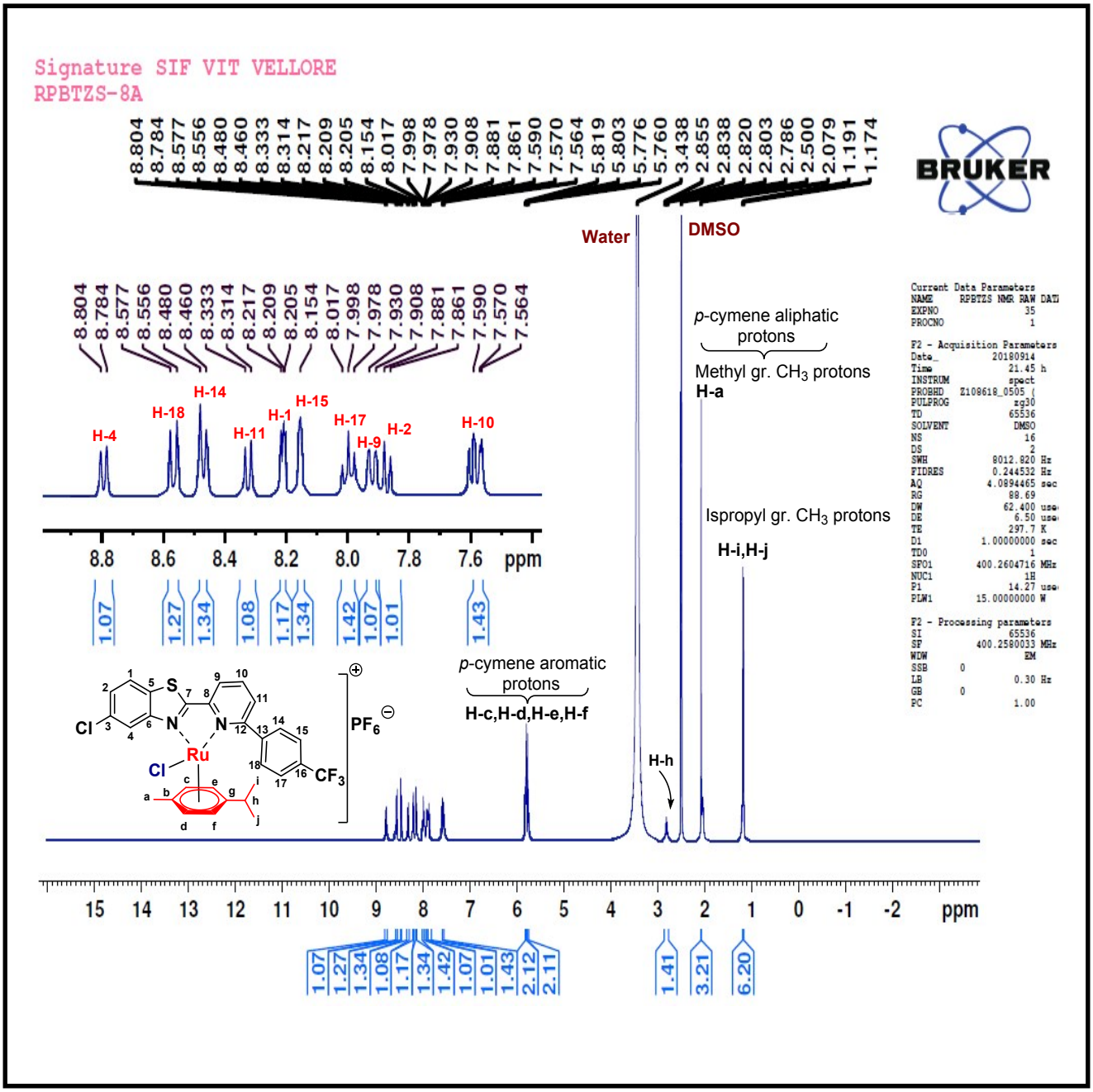


^{19}F NMR of ligand 7l6

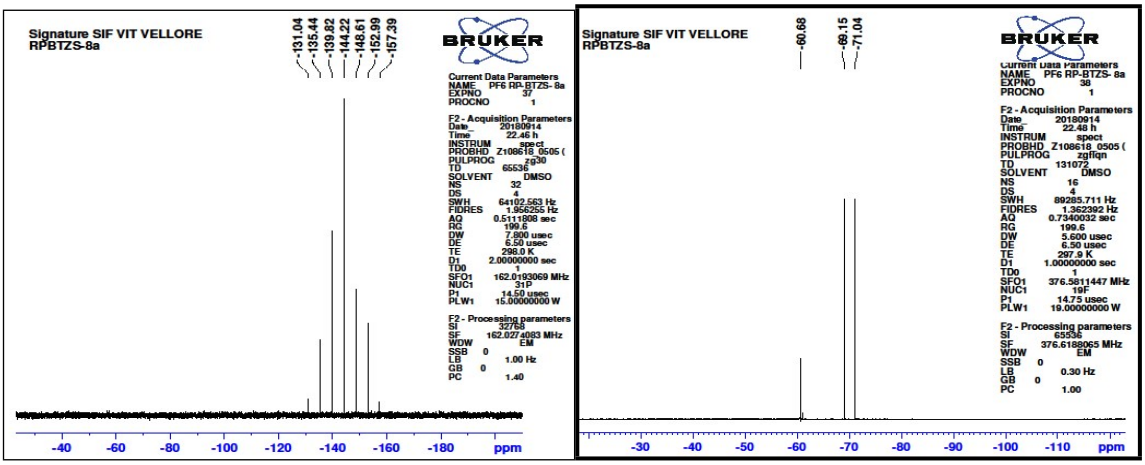
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 391.02[M+H]$^{+}$



ESI-MS spectra of ligand 7l6

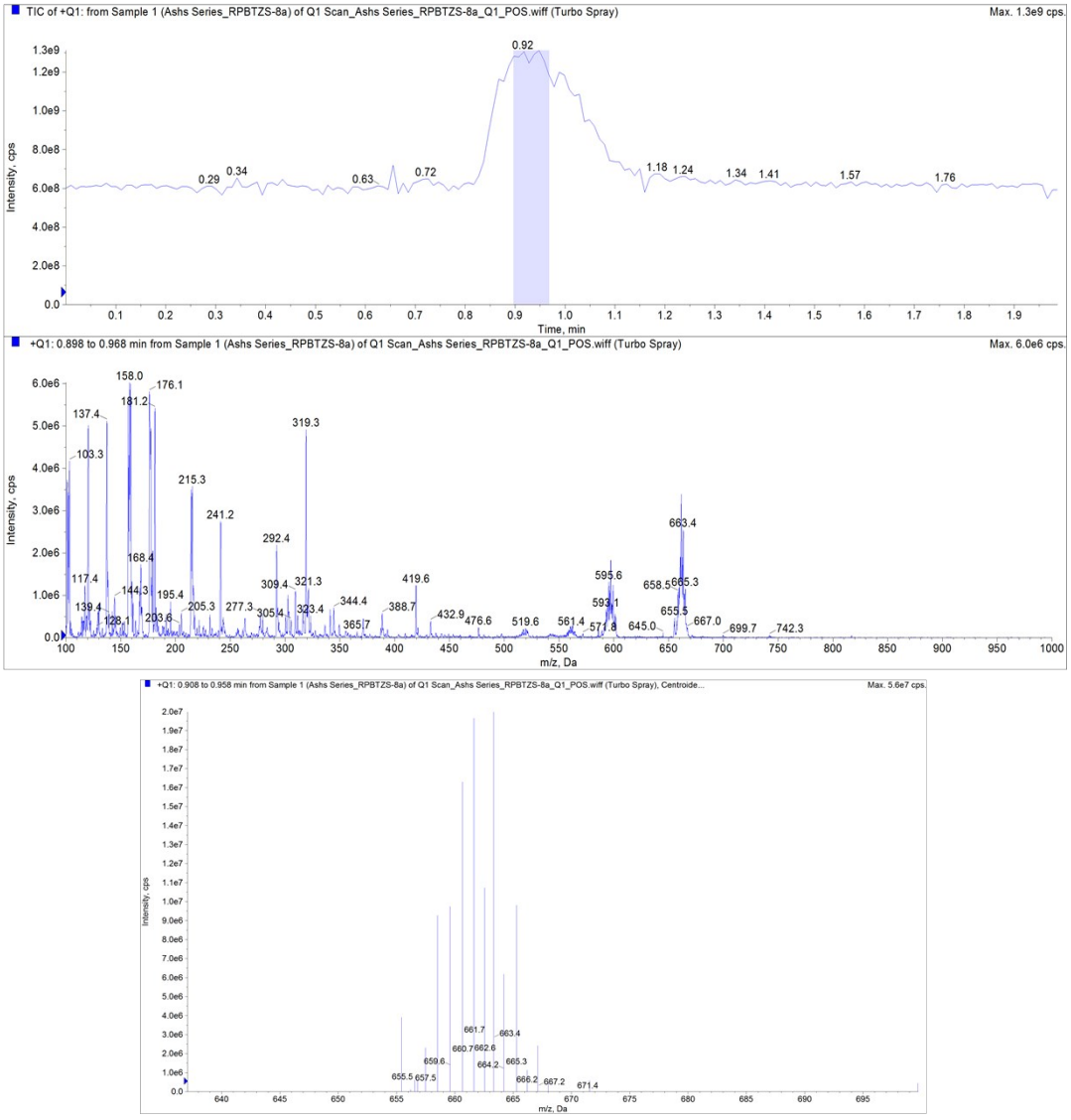


^{1}H NMR of ligand 8I6

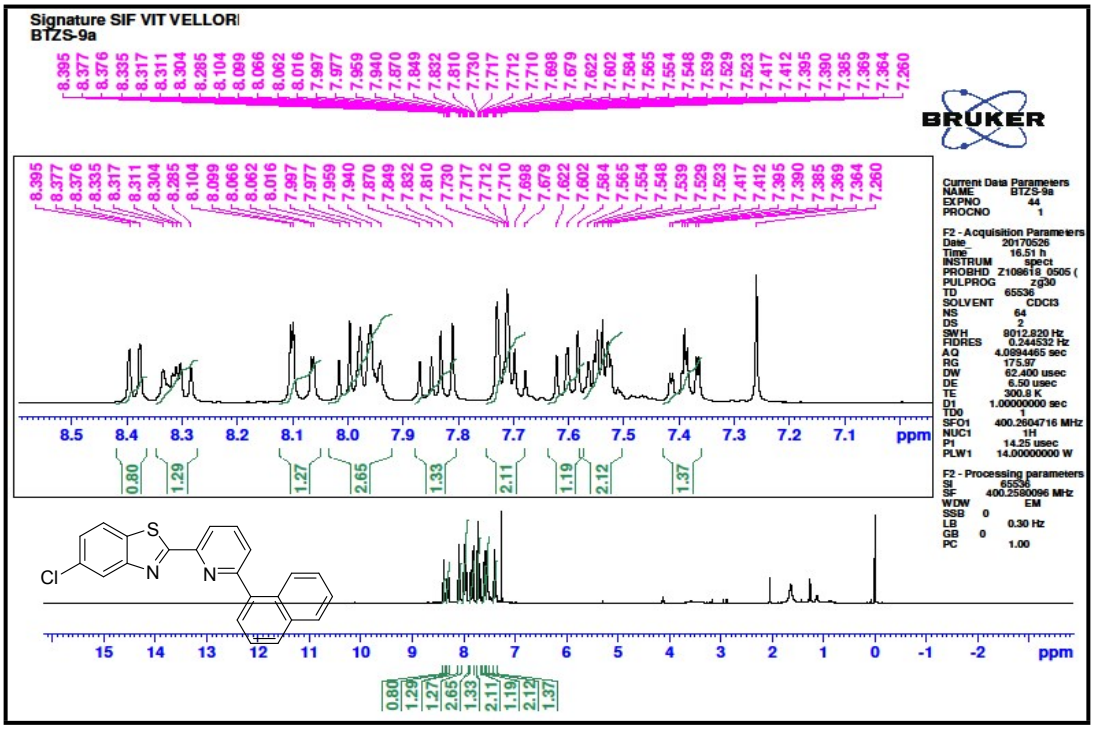


^{31}P and ^{19}F NMR of complex 8l6

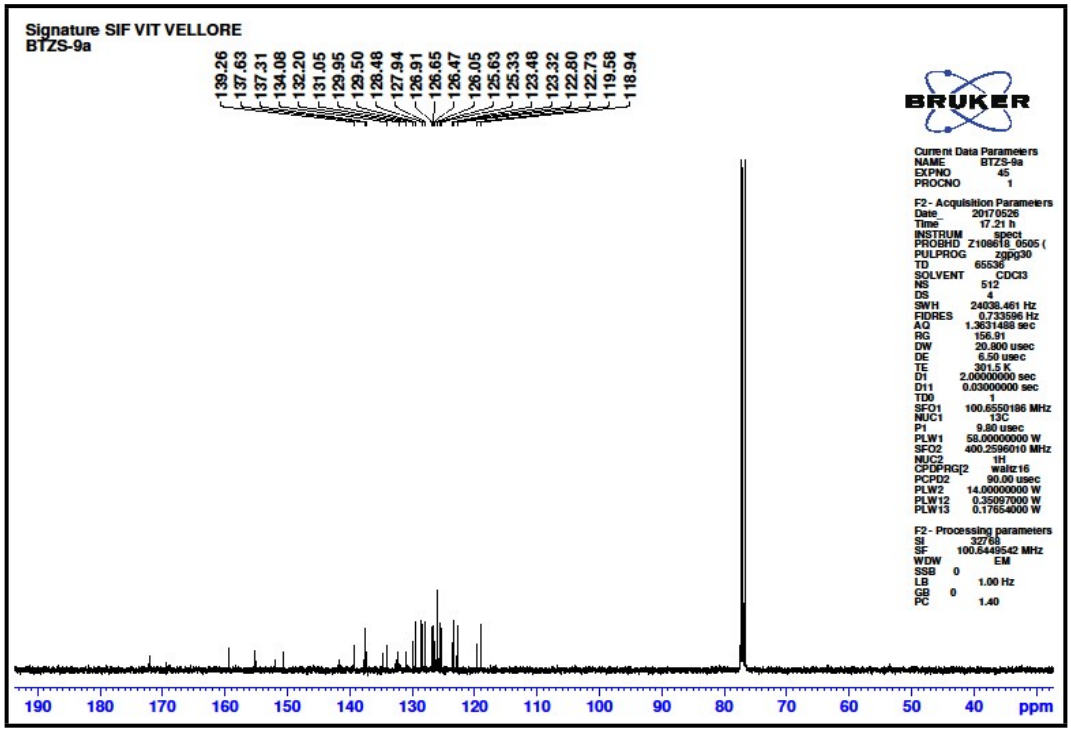
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 661.01 [M+]



ESI-MS spectra of complex 8l6

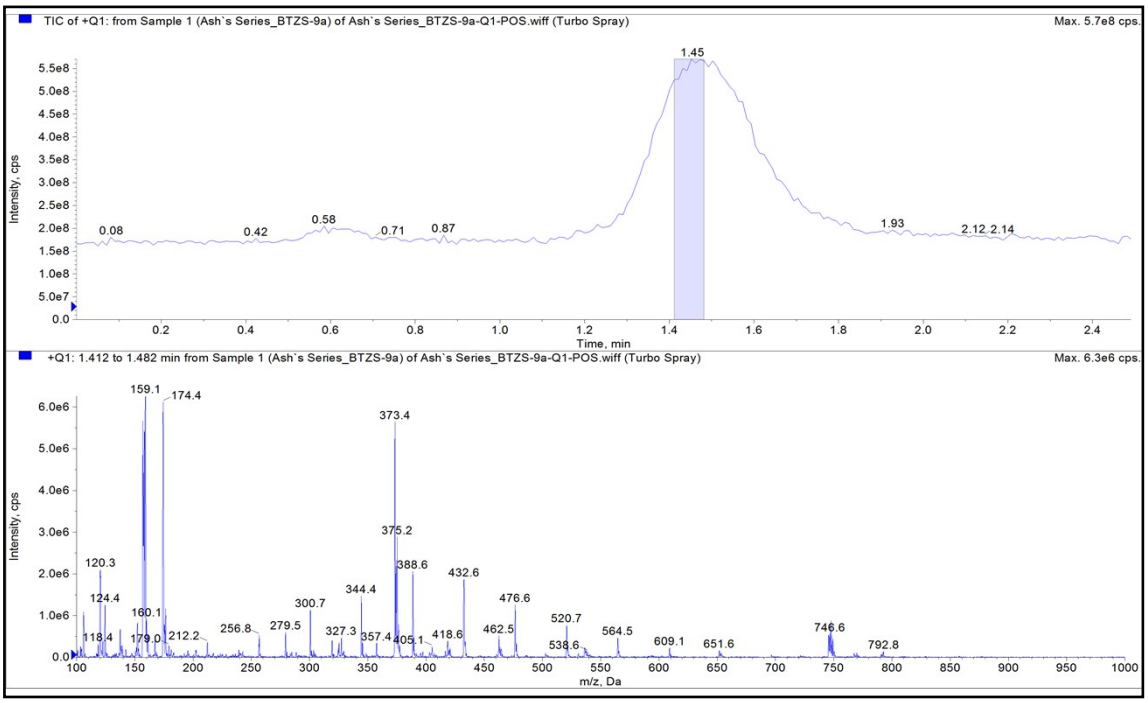


^{1}H NMR of ligand 7l7

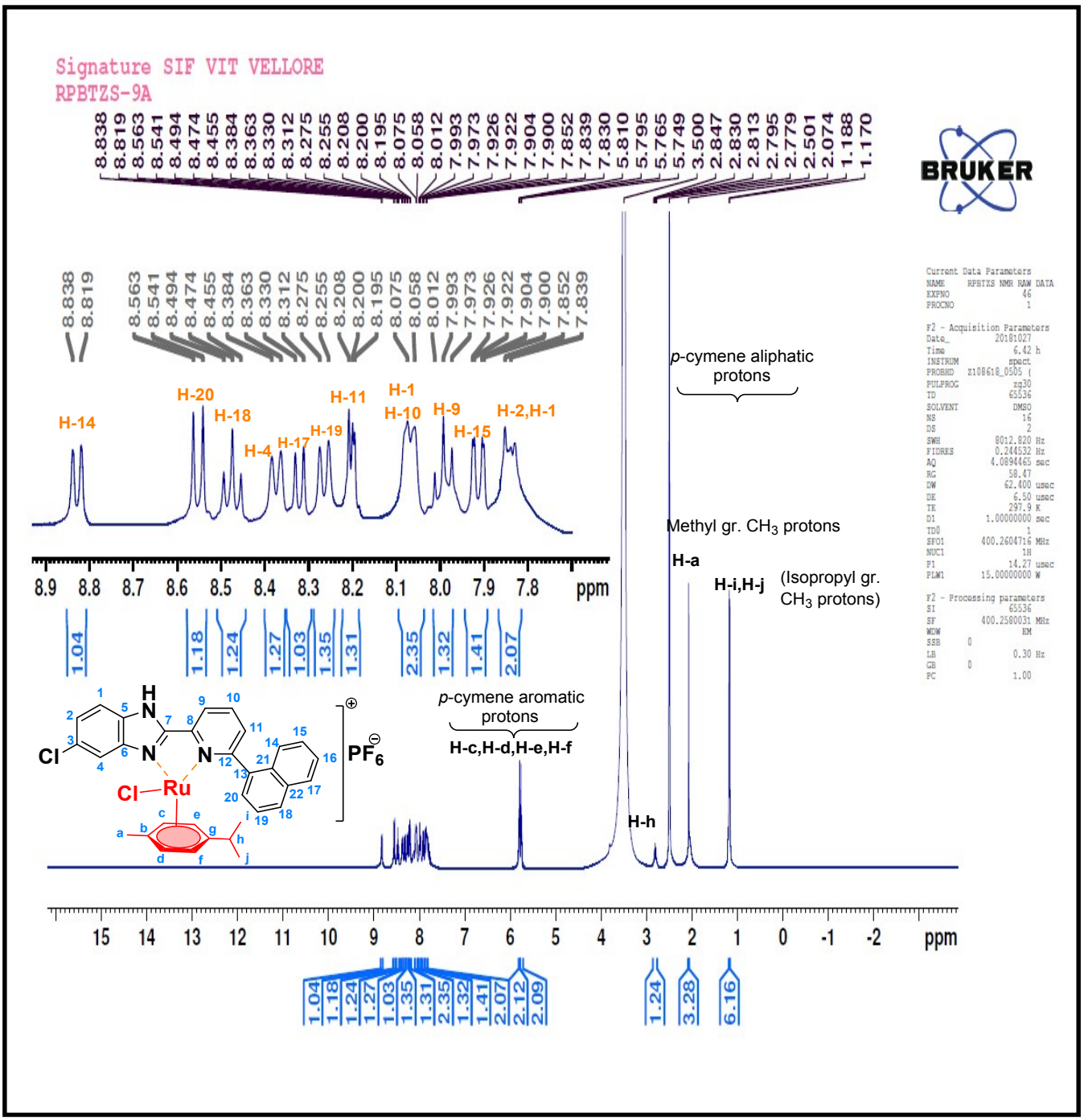


^{13}C NMR of ligand 7l7

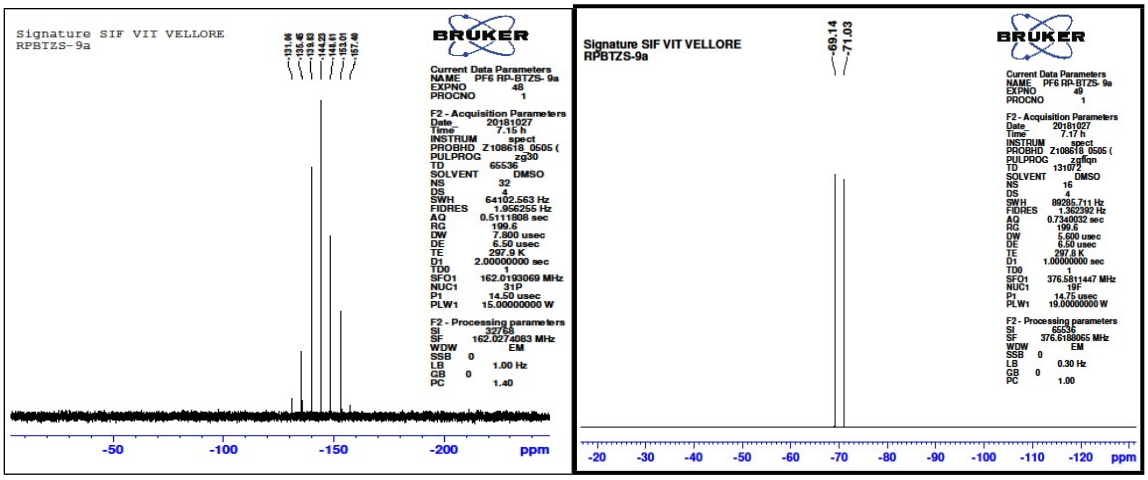
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 373.05 $[M+H]^+$



ESI-MS spectra of ligand 7l7

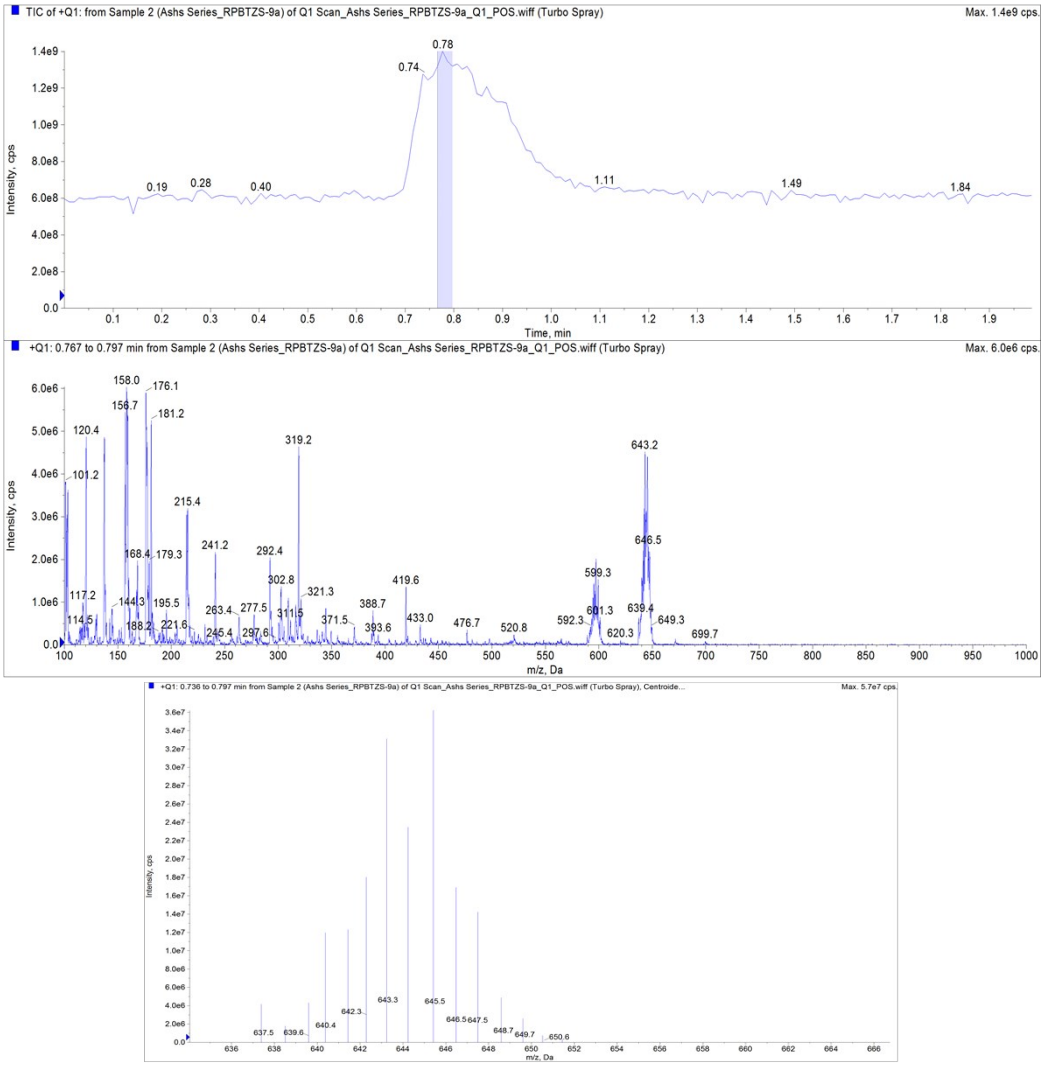


^{1}H NMR of ligand 8l7

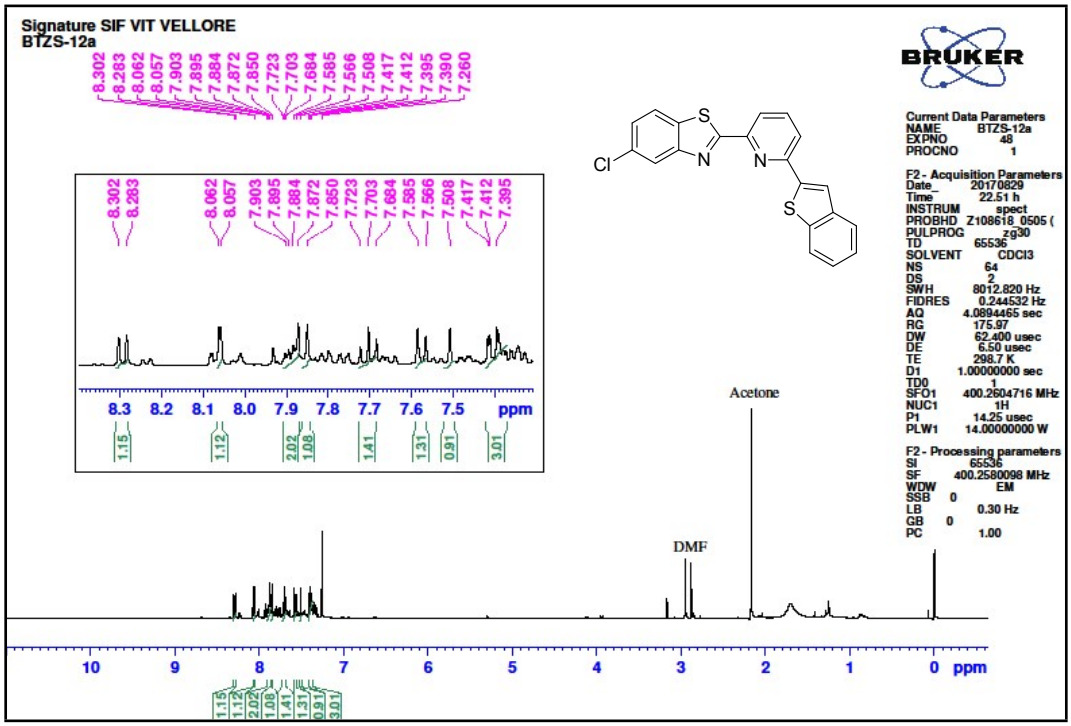


^{31}P and ^{19}F NMR of complex 8l7

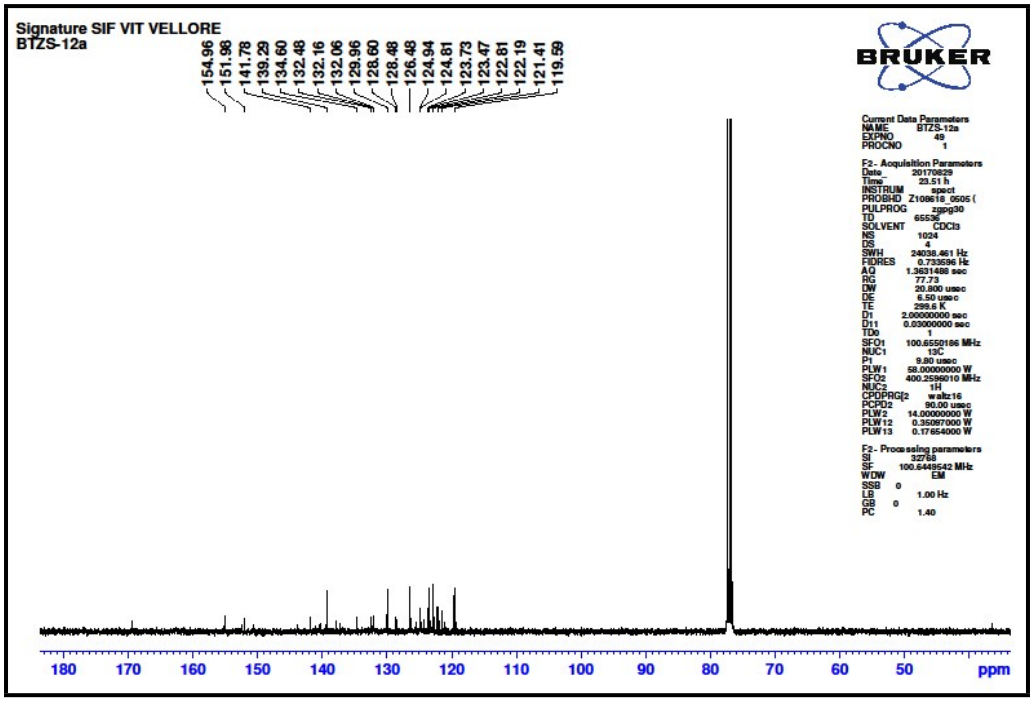
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 643.03[M$^+$]



ESI-MS spectra of complex 8I7

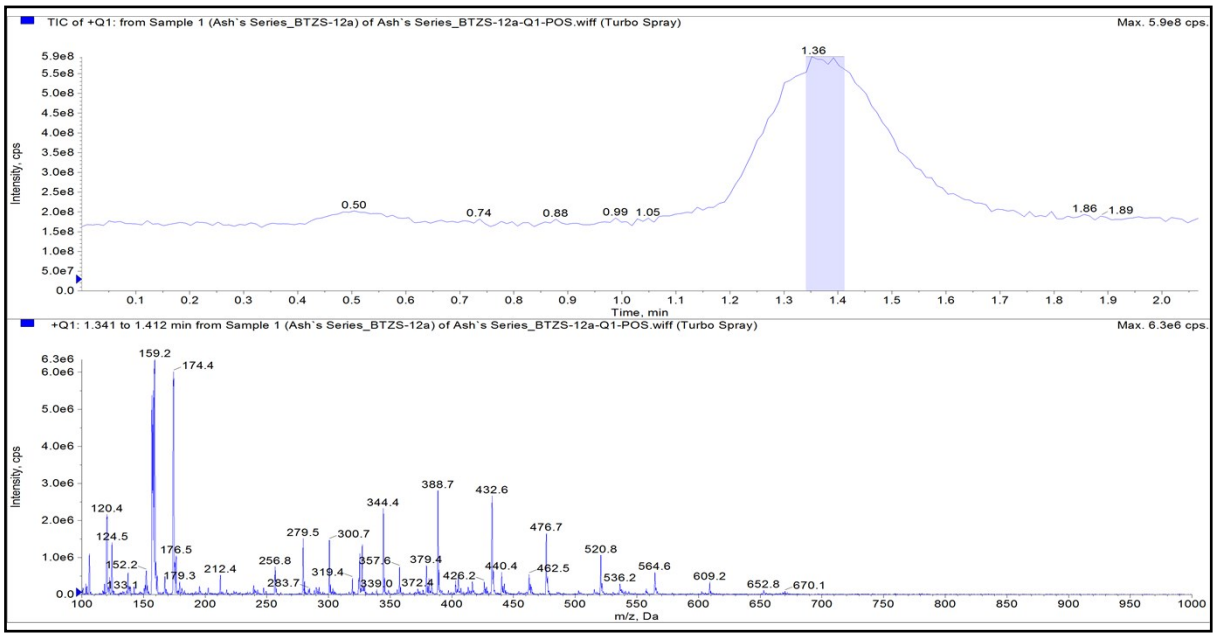


^{1}H NMR of ligand 7l8

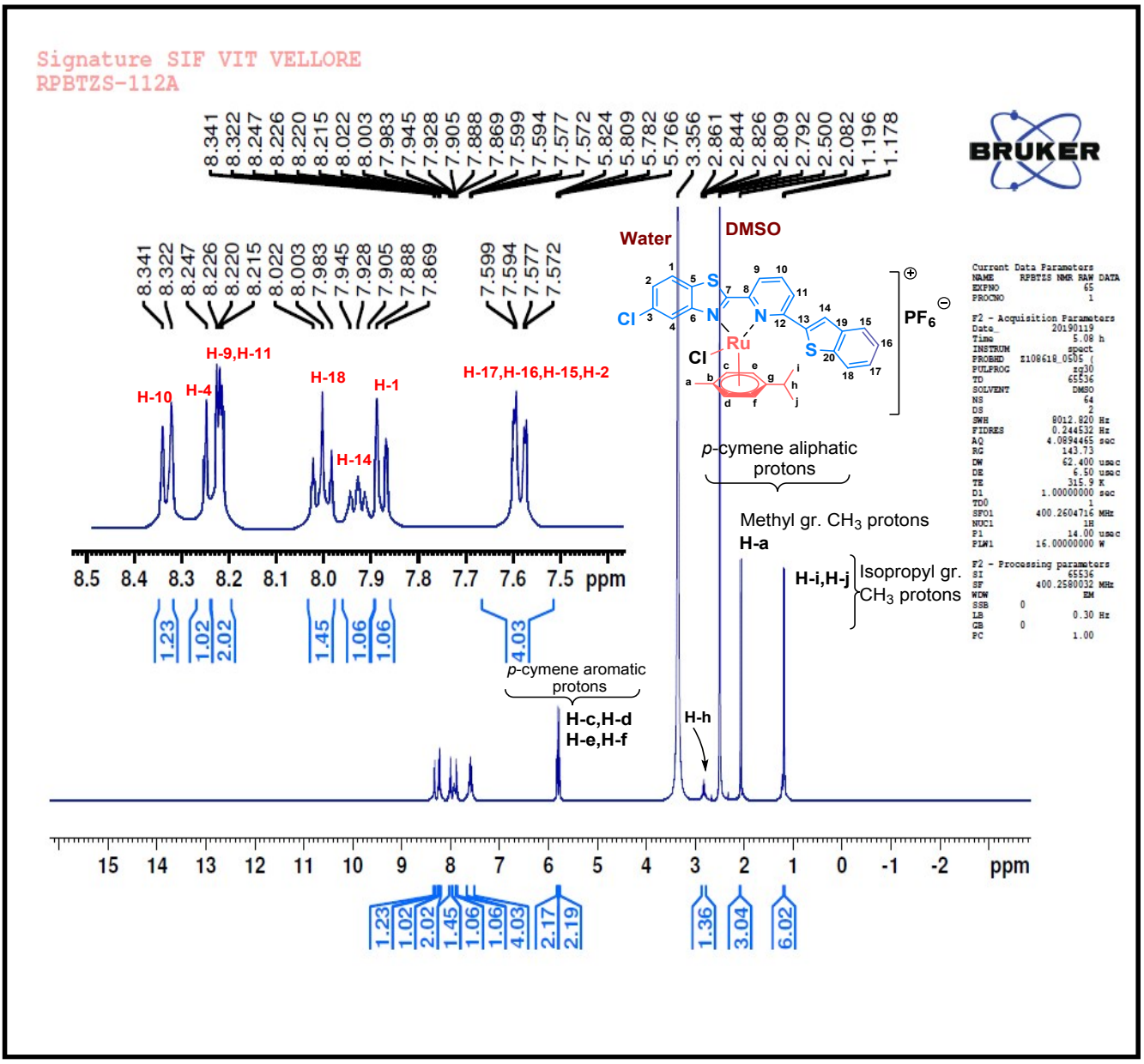


^{13}C NMR of ligand 7l8

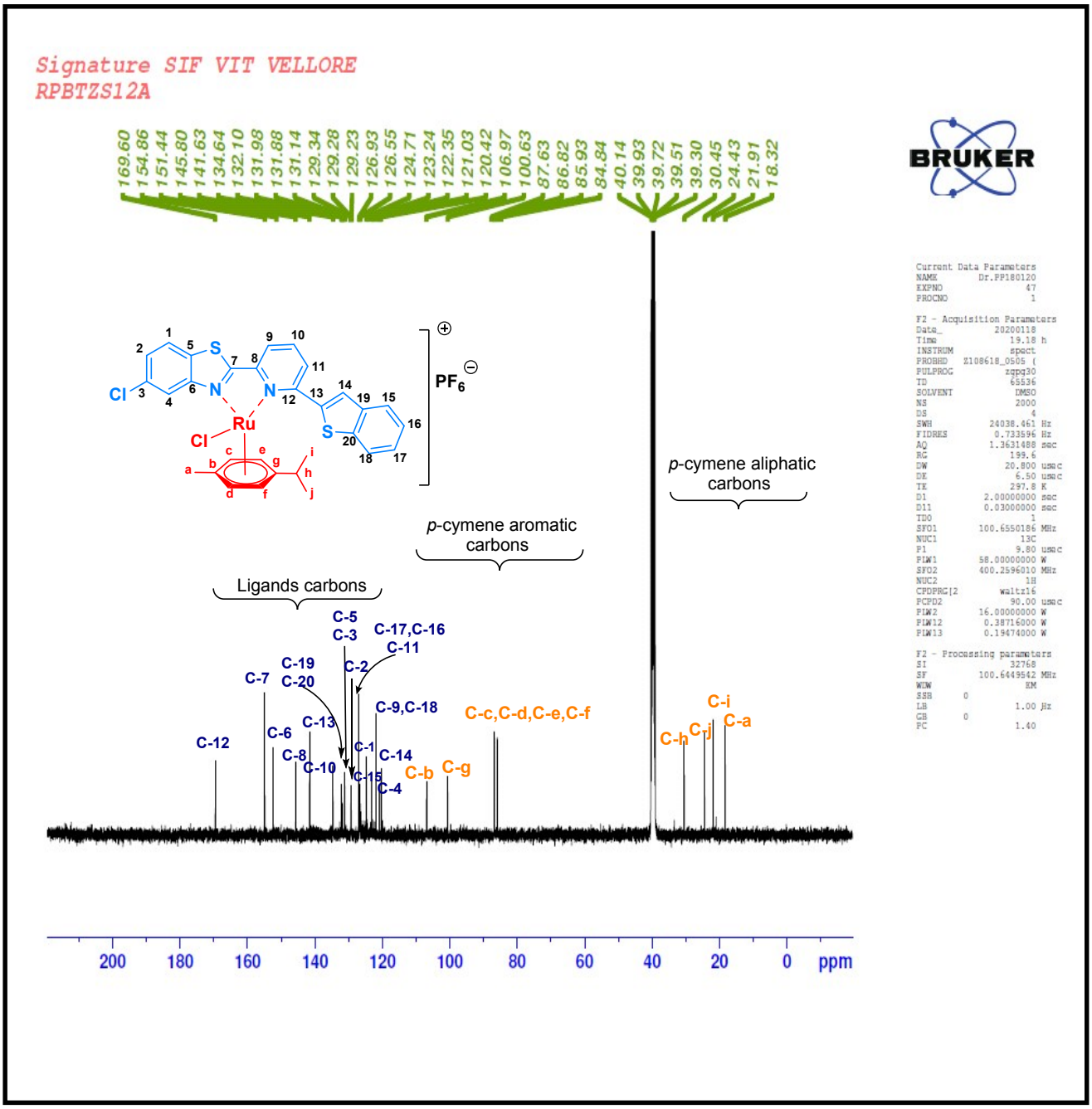
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 379.01 $[M+H]^+$



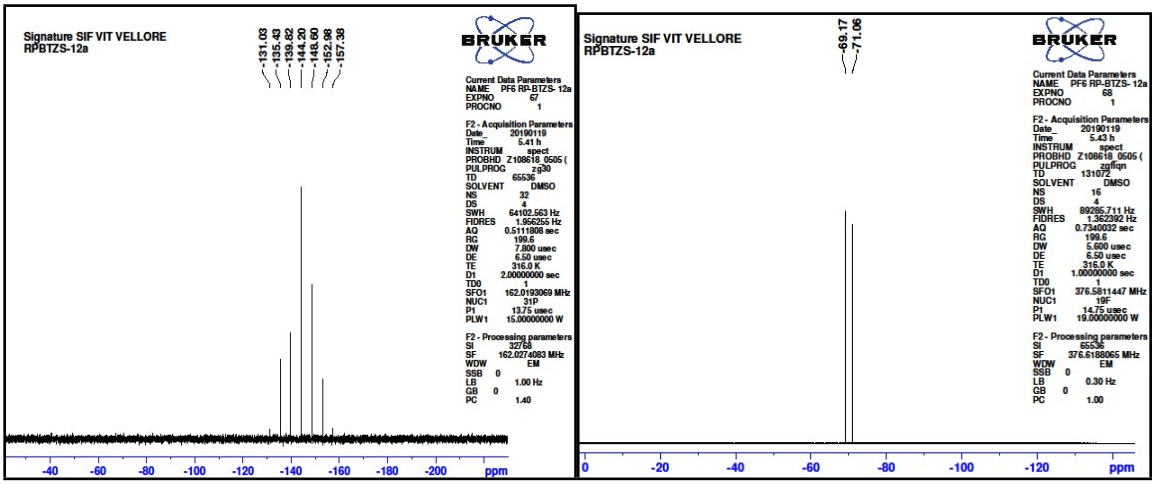
ESI-MS spectra of ligand 7l8



^{1}H NMR of ligand 8I8

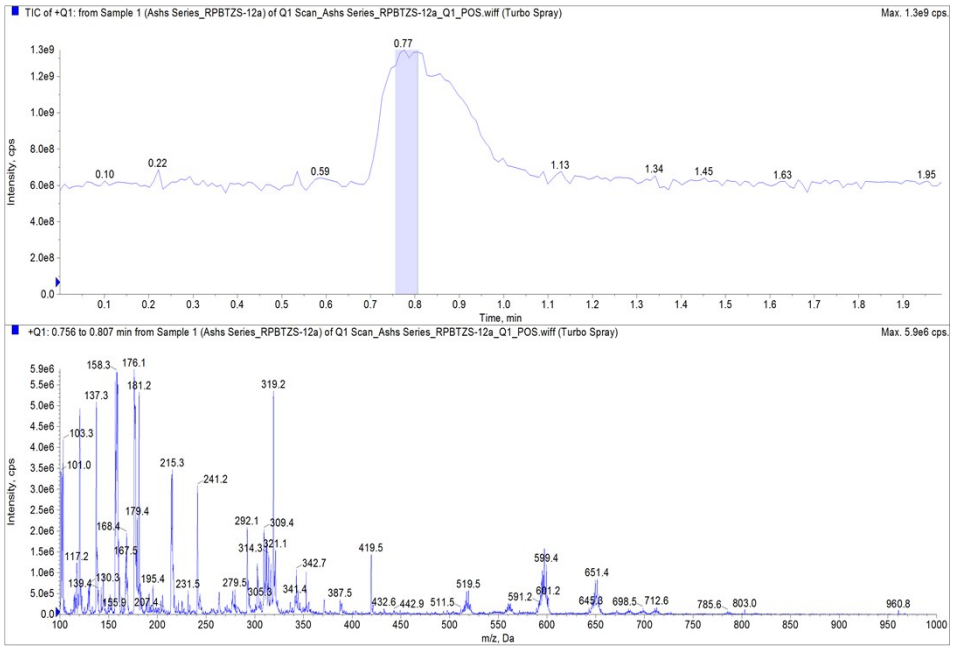


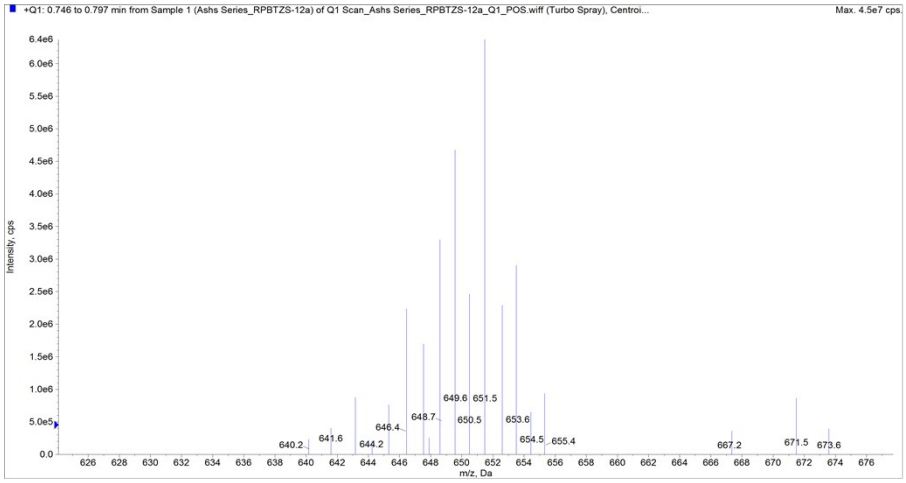
^{13}C NMR of ligand 8l8



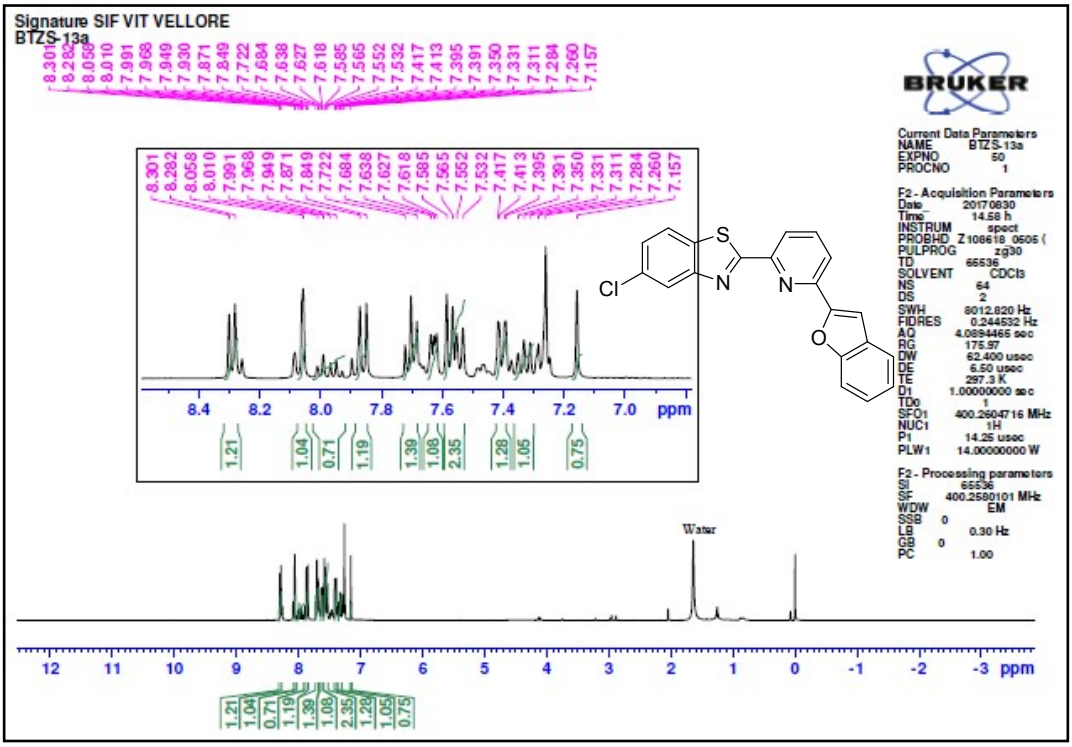
^{31}P and ^{19}F NMR of complex 8l8

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 648.99[M$^+$]

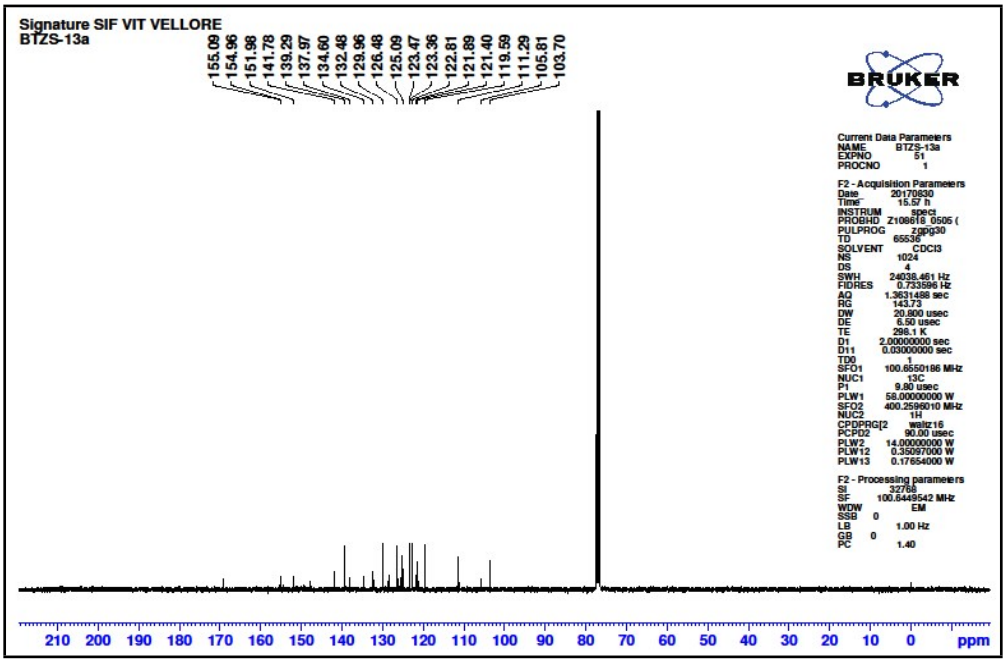




ESI-MS spectra of complex 8l8

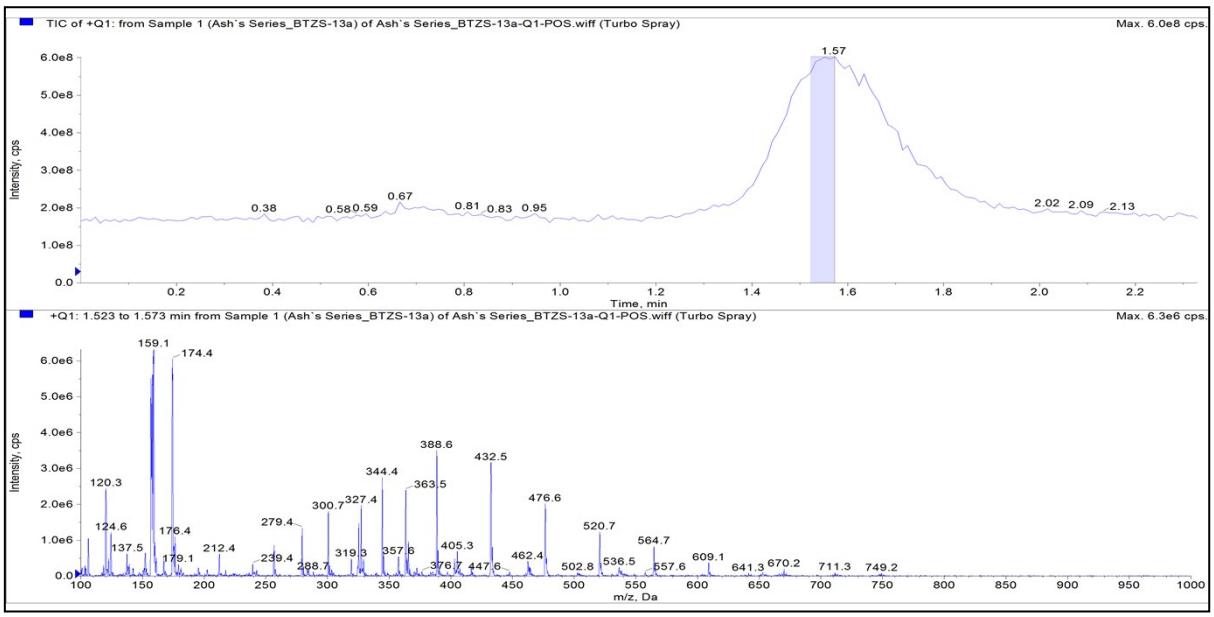


^{1}H NMR of ligand 7l9

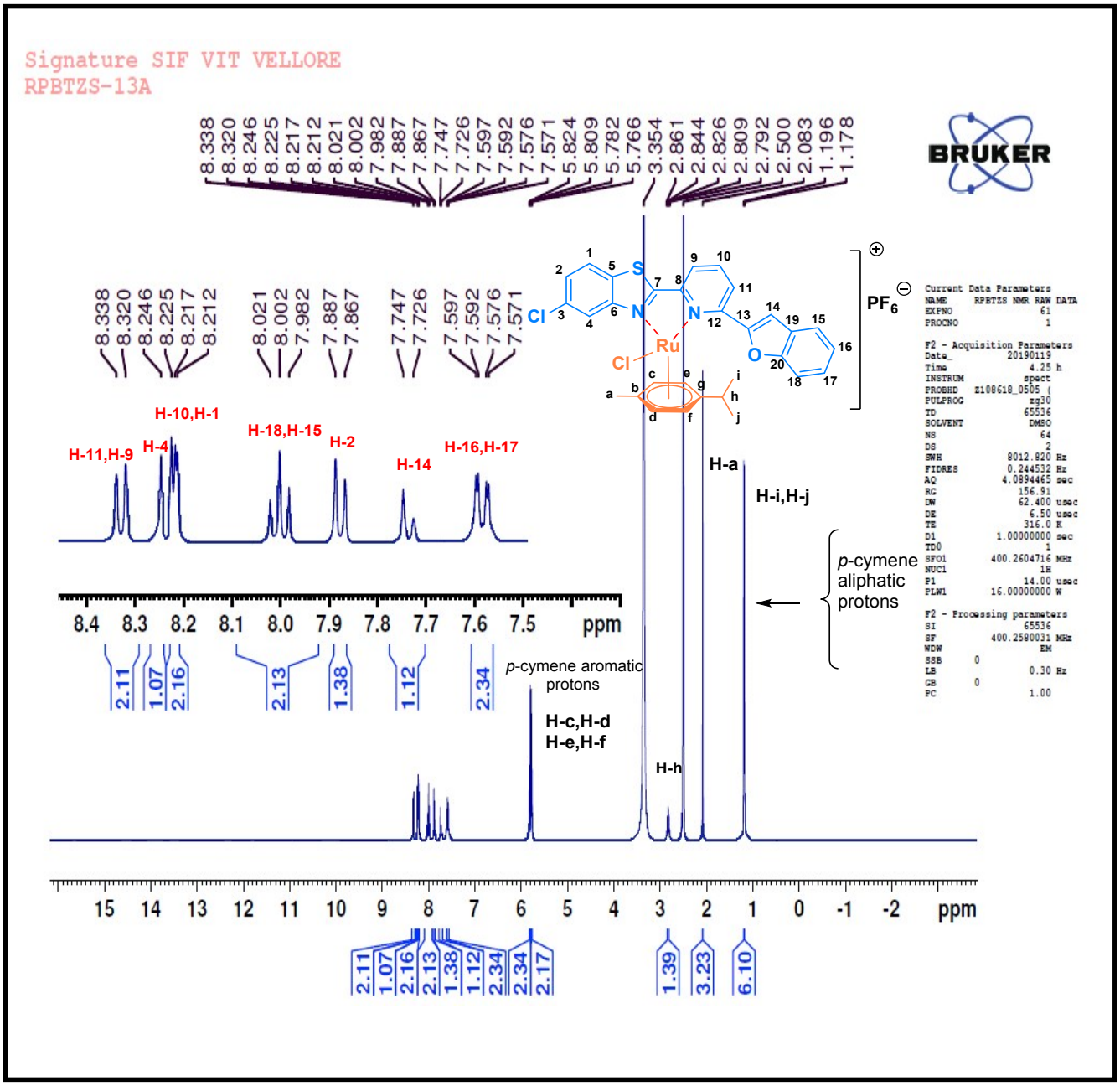


^{13}C NMR of ligand 7l9

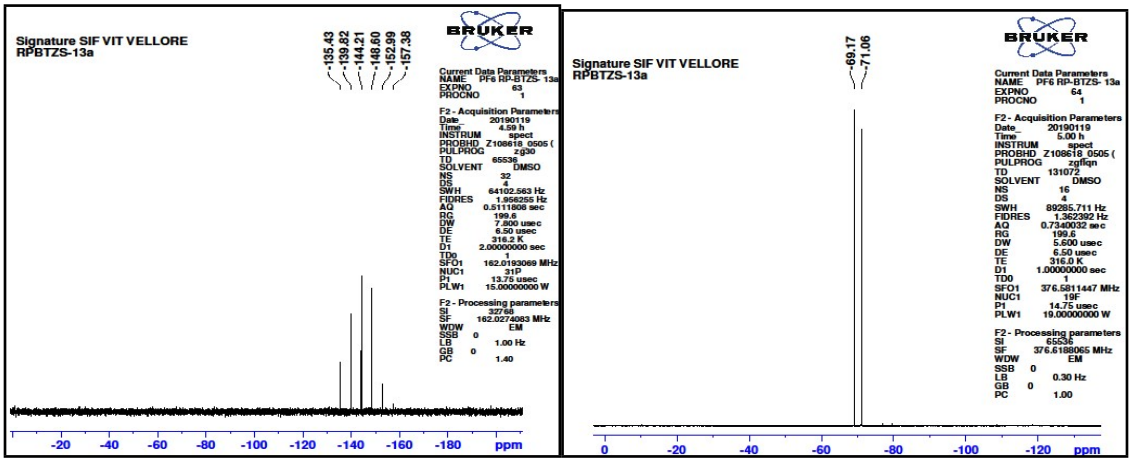
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 364.03 $[M+H]^+$



ESI-MS spectra of ligand 7l9

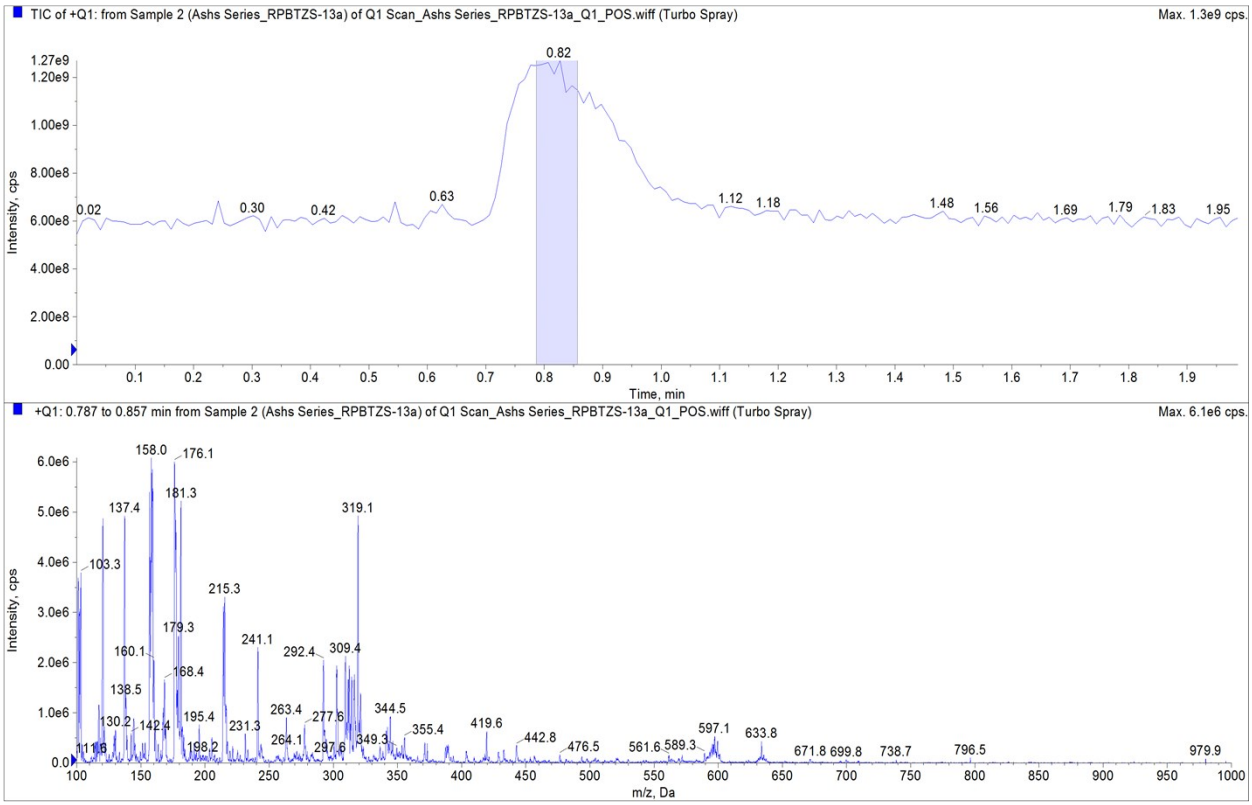


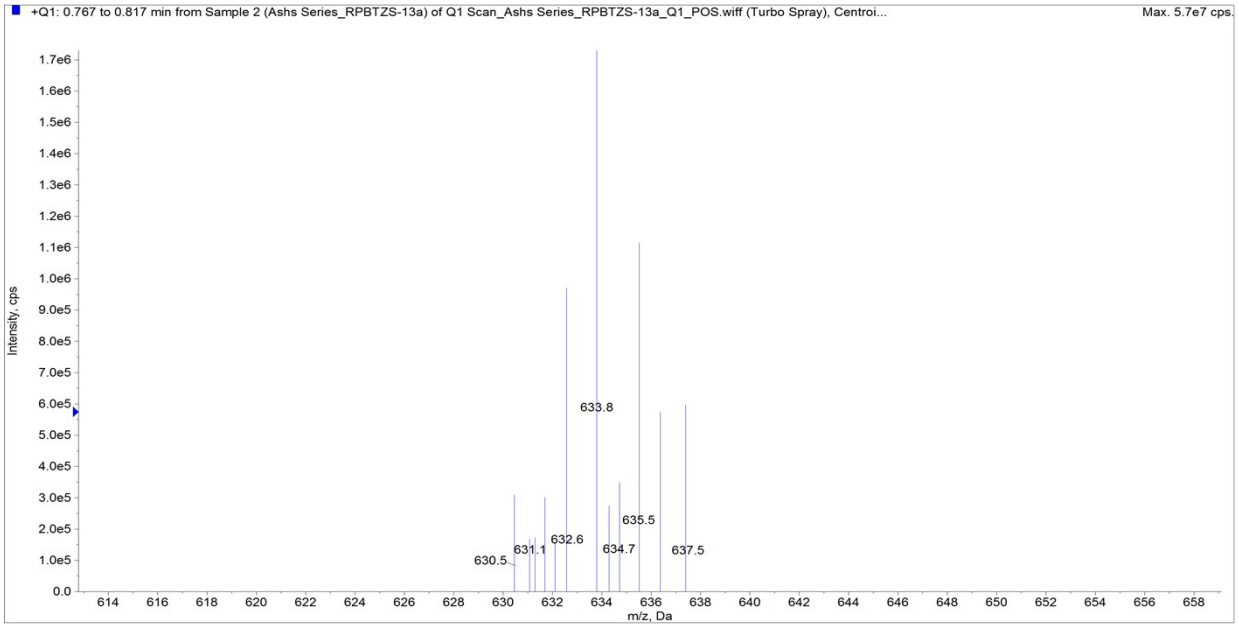
^{1}H NMR of ligand 8l9



^{31}P and ^{19}F NMR of complex 8l9

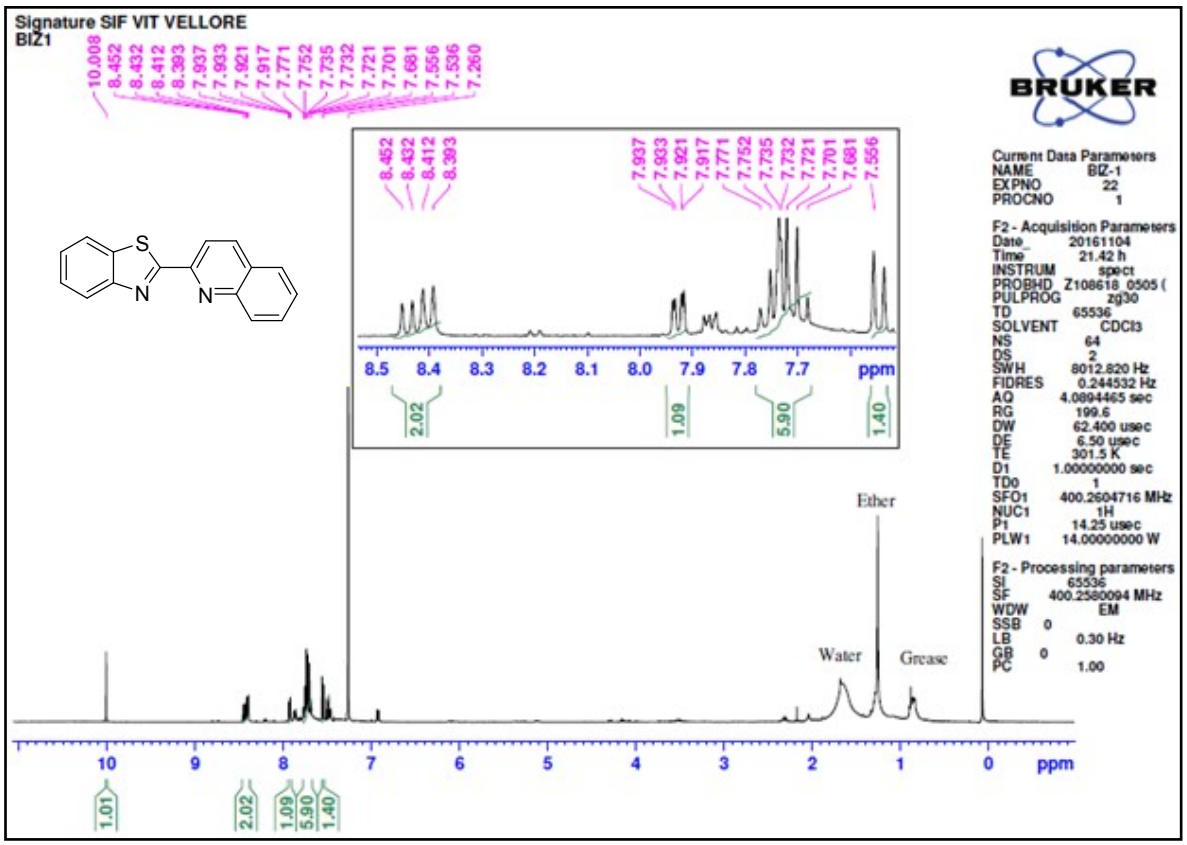
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 633.01 [M+]



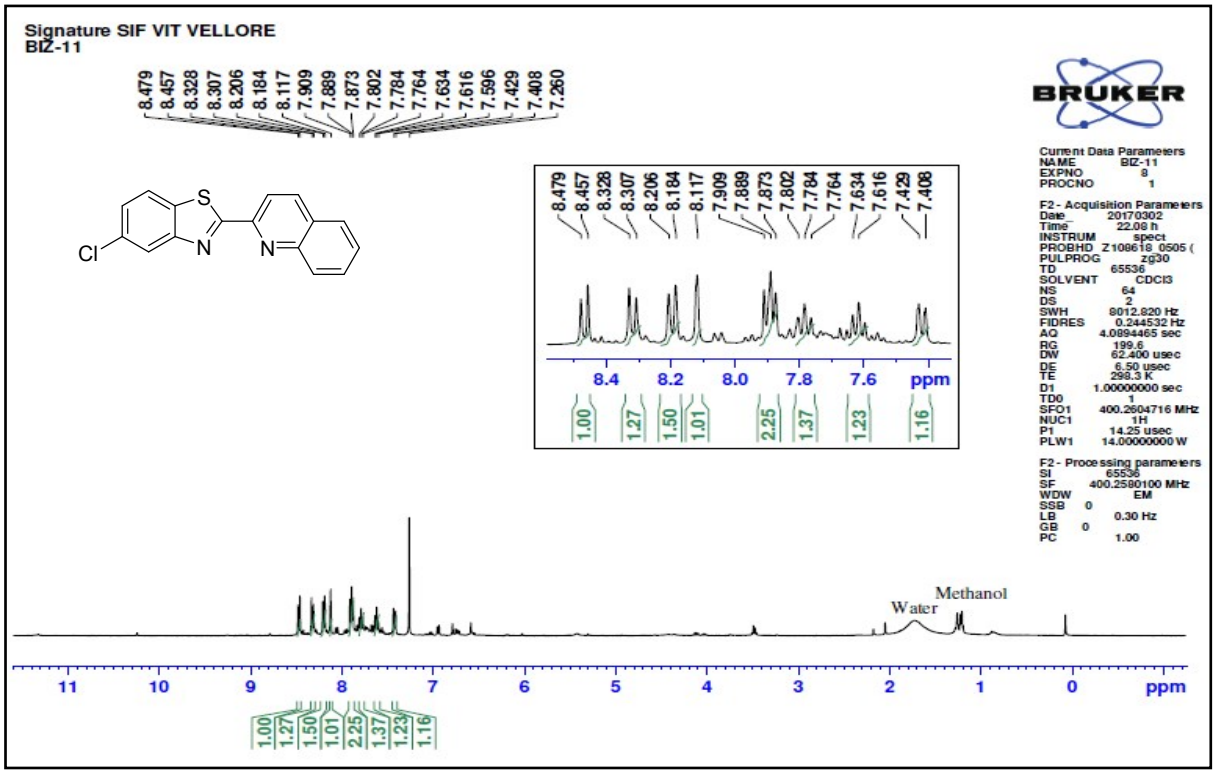


ESI-MS spectra of complex 8l9

Quinoline Series



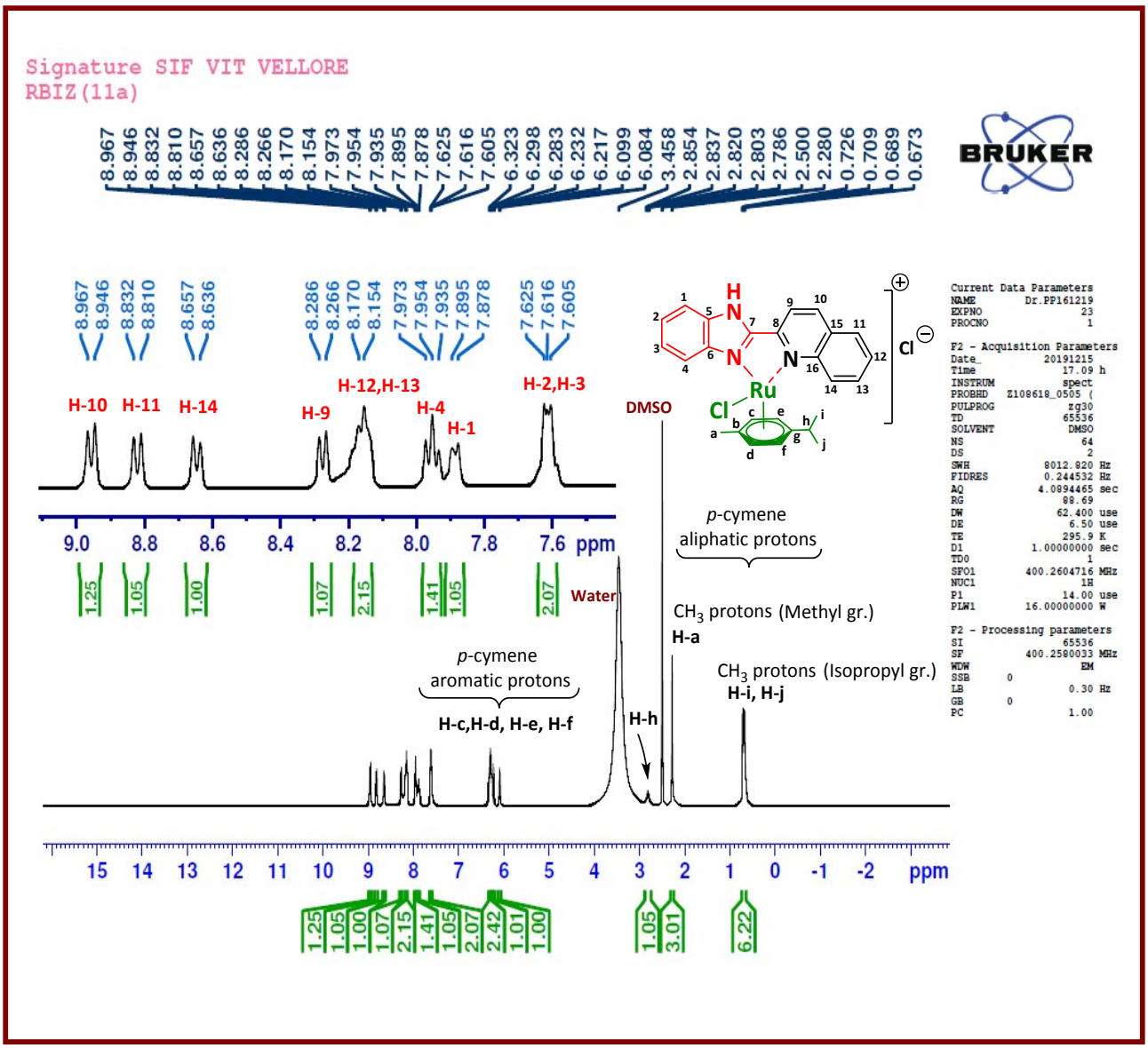
^{1}H NMR of ligand 10a



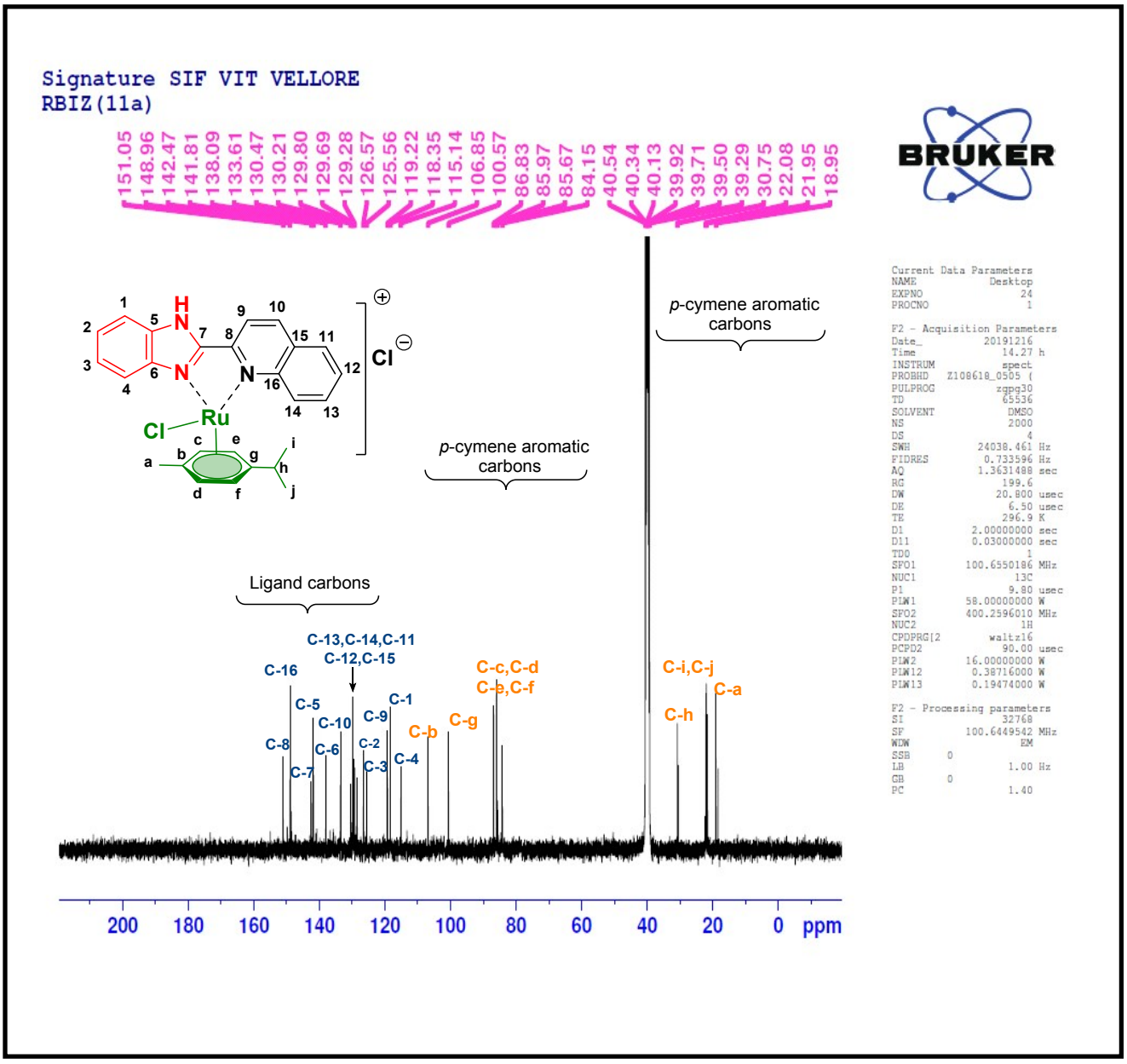
^{1}H NMR of ligand 10h

^{1}H and ^{13}C NMR of complex 11a-11n

11a



11a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p-cymene aromatic carbons
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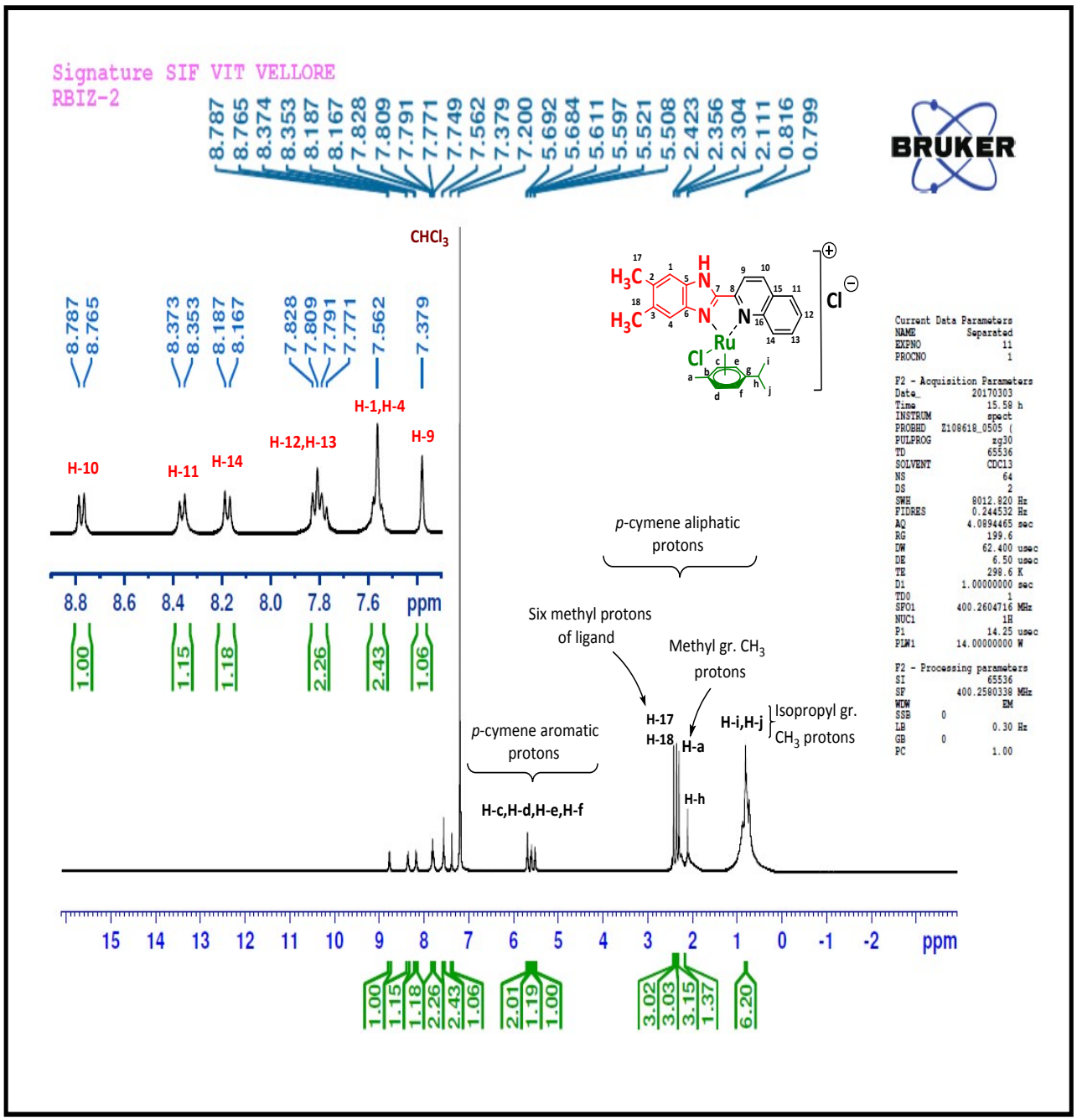
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Six methyl protons of ligand
Methyl gr. CH3 protons
H-17
H-18
H-a
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Isopropyl gr. CH3 protons
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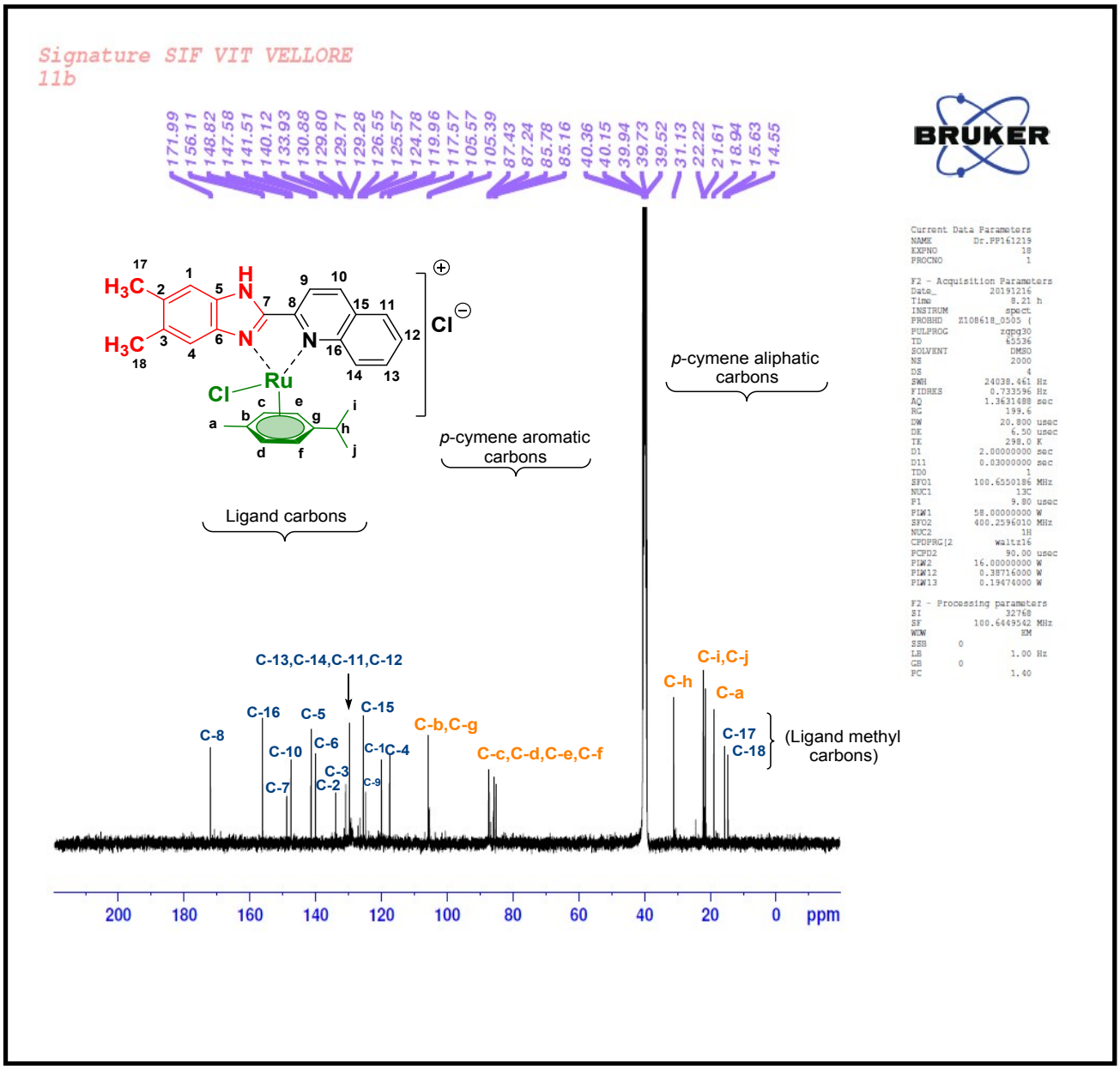
Cl
ppm

11i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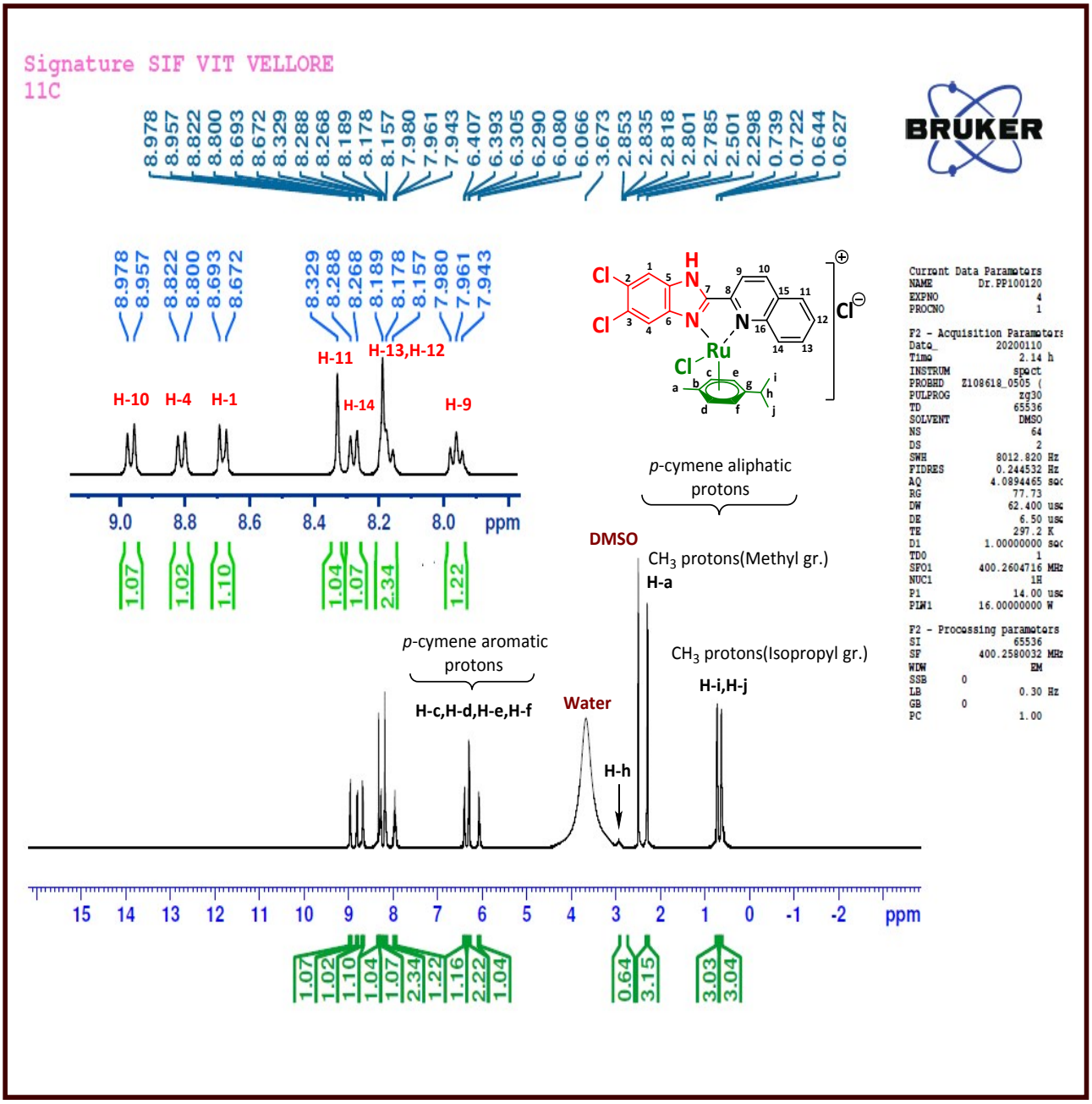
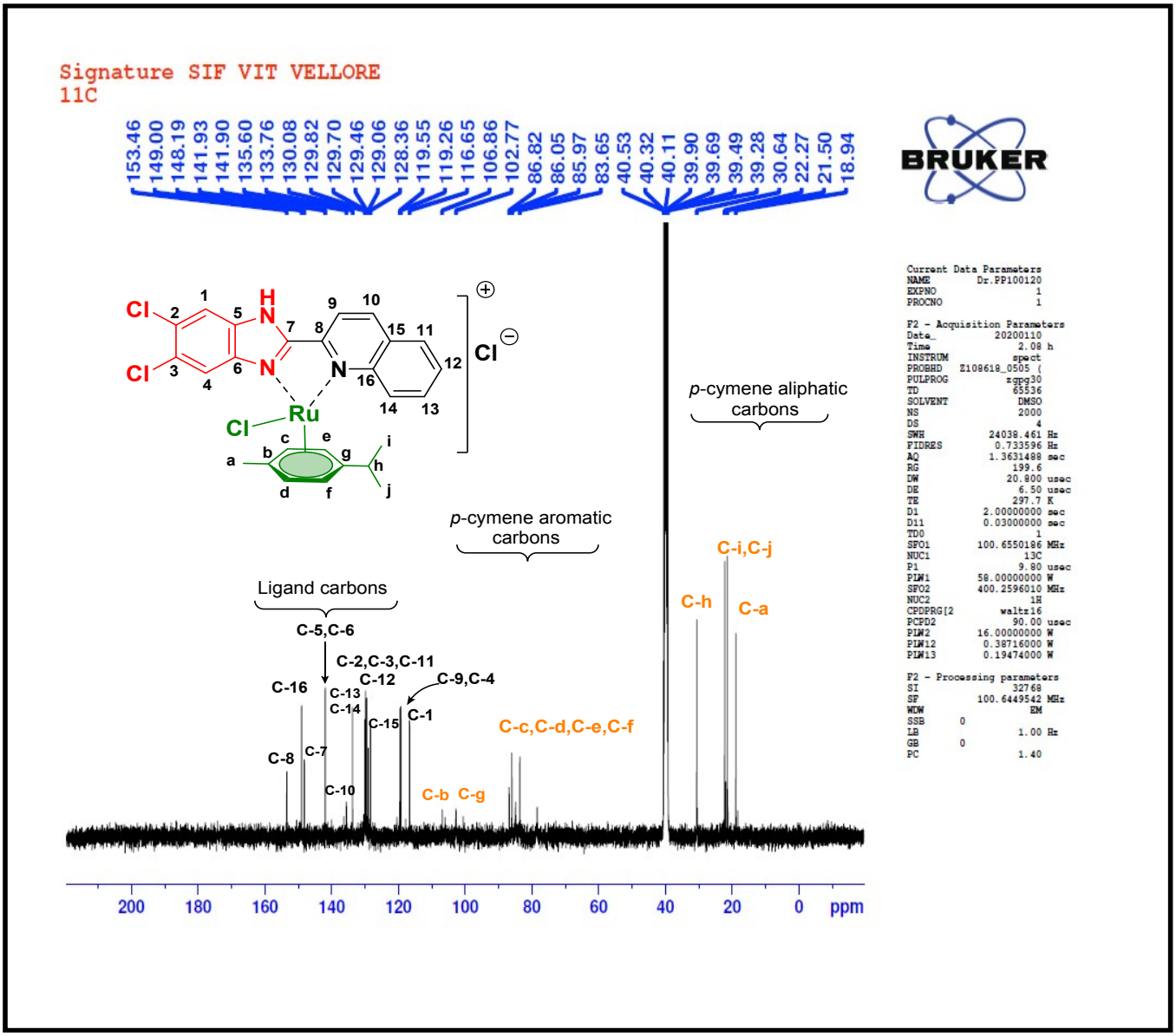
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-13,C-14,C-11,C-12
C-16
C-5
C-15
C-8
C-10
C-6
C-1
C-4
C-3
C-7
C-2
C-9
C-b,C-g
C-c,C-d,C-e,C-f
C-h
C-i,C-j
C-a
C-17
C-18
(Ligand methyl carbons)
200
180
160
140
120
100
80
60
40
20
0
ppm

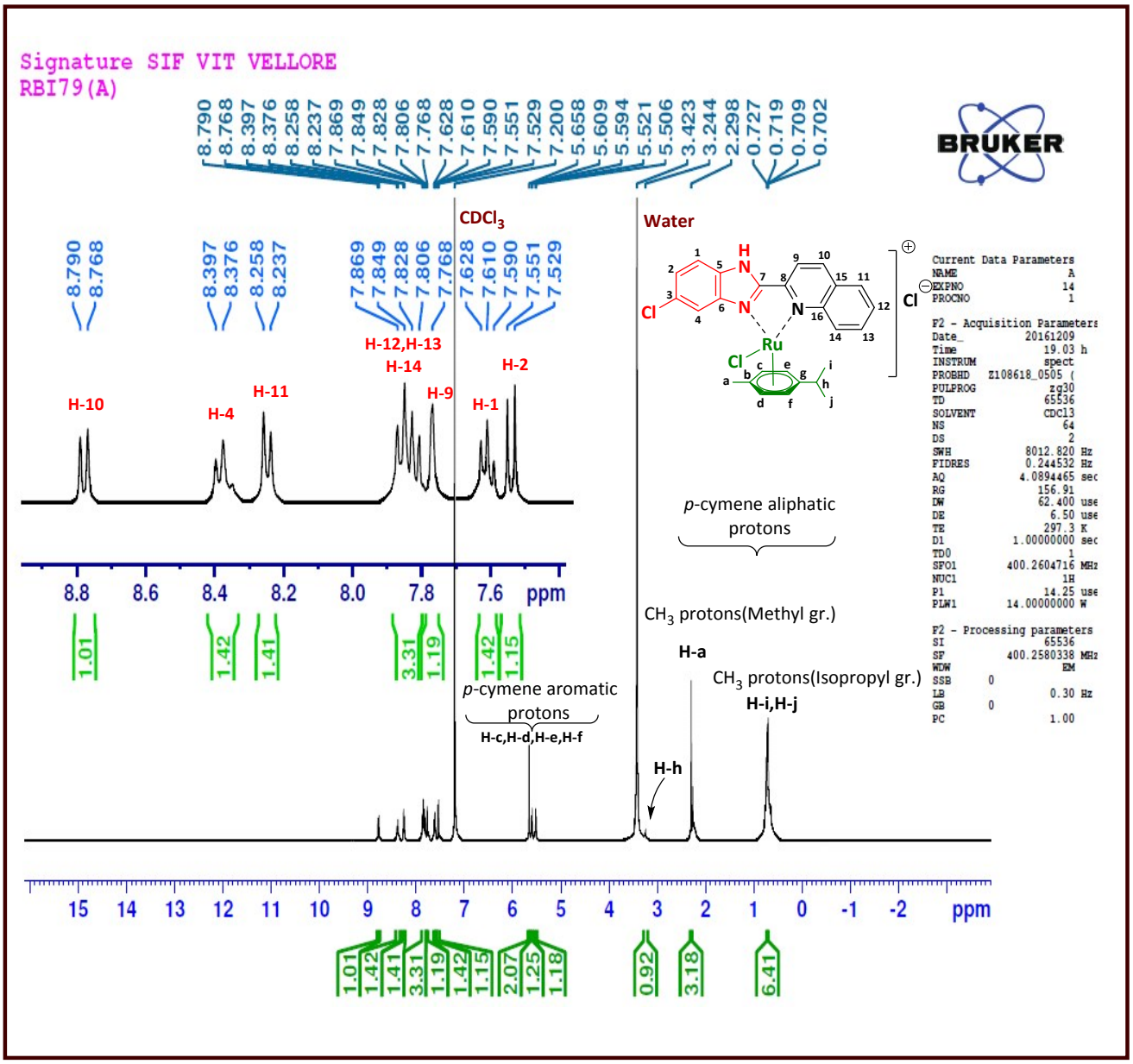
11j


Signature SIF VIT VELLORE
11C
BRUKER
8.978 8.957 8.822 8.800 8.693 8.672 8.329 8.288 8.268 8.189 8.178 8.157 7.980 7.961 7.943 6.407 6.393 6.305 6.290 6.080 6.066 3.673 2.853 2.835 2.818 2.801 2.785 2.501 2.298 0.739 0.722 0.644 0.627
H-10 H-4 H-1 H-11 H-14 H-13,H-12 H-9
9.0 8.8 8.6 8.4 8.2 8.0 ppm
1.07 1.02 1.10 1.04 1.07 2.34 1.22
p-cymene aliphatic protons
DMSO
CH3 protons(Methyl gr.)
H-a
p-cymene aromatic protons
H-c,H-d,H-e,H-f
Water
H-h
CH3 protons(Isopropyl gr.)
H-i,H-j
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.07 1.02 1.10 1.04 1.07 2.34 1.22 1.16 2.22 1.04
0.64 3.15
3.03 3.04
Current Data Parameters
NAME Dr.PP100120
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200110
Time 2.14 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 77.73
DW 62.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.00 usec
PLW1 16.00000000 W
F2 - Processing parameters
SI 65536
SF 400.2580032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

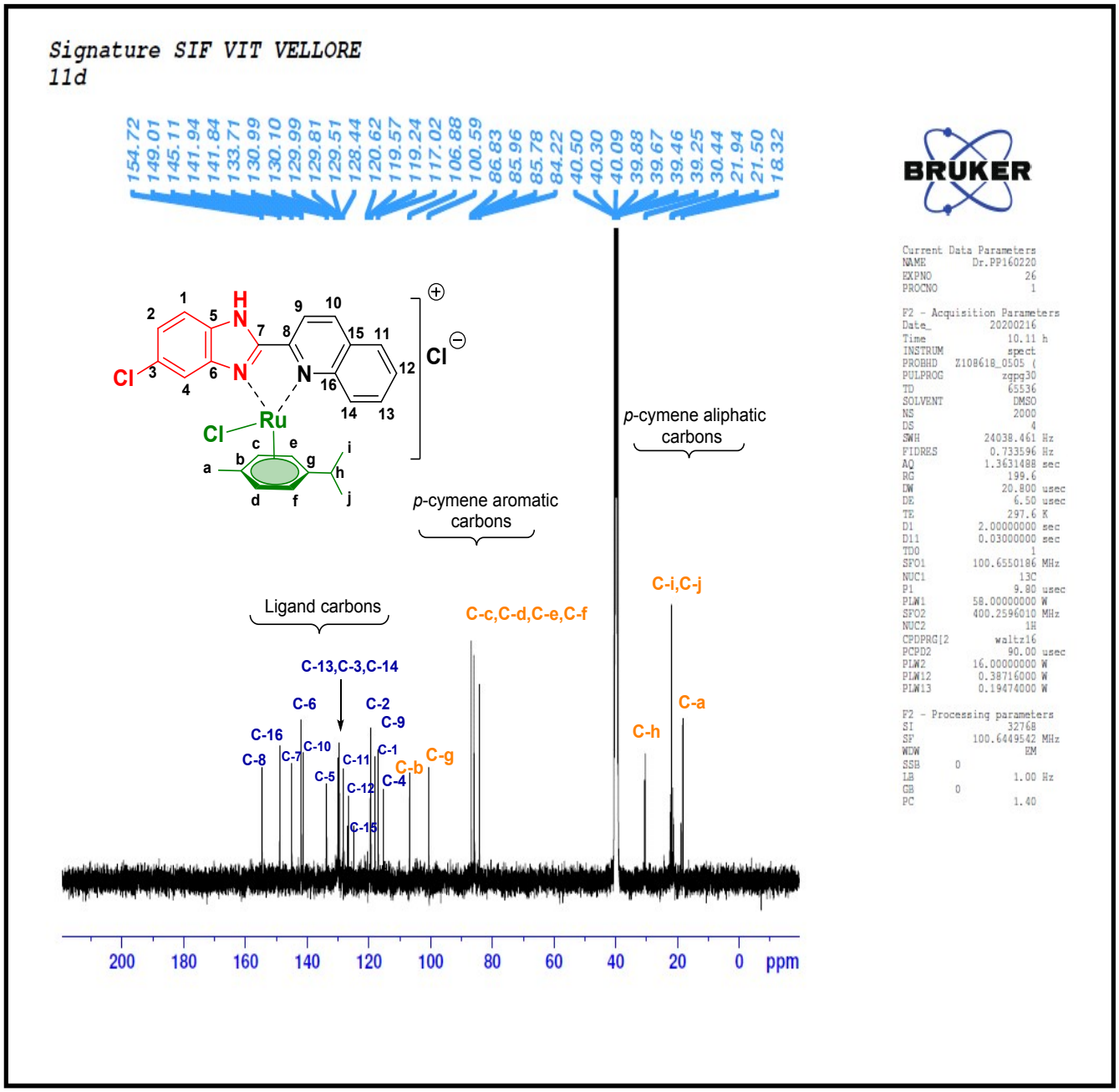
11j


Signature SIF VIT VELLORE
11C
153.46 149.00 148.19 141.93 141.90 135.60 133.76 130.08 129.82 129.70 129.46 129.06 128.36 119.55 119.26 116.65 106.86 102.77 86.82 86.05 85.97 83.65 40.53 40.32 40.11 39.90 39.69 39.49 39.28 30.64 22.27 21.50 18.94
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-5,C-6
C-2,C-3,C-11
C-16
C-13
C-14
C-12
C-9,C-4
C-15
C-1
C-8
C-7
C-10
C-b C-g
C-c,C-d,C-e,C-f
C-h
C-i,C-j
C-a
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME Dr.PP100120
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200110
Time 2.08 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 297.7 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

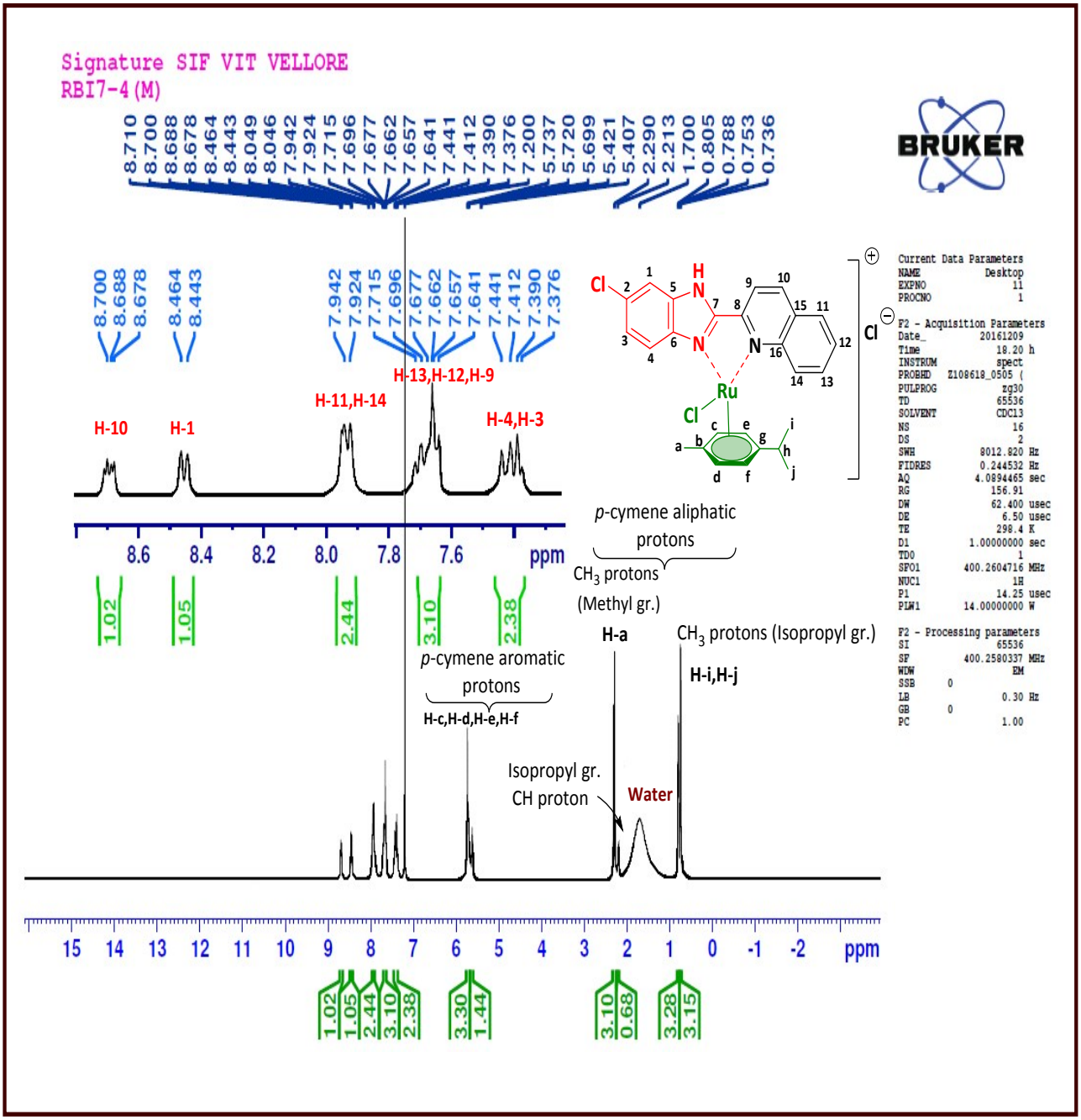
11b


Signature SIF VIT VELLORE
RBI79(A)
BRUKER
CDCl3
Water
H-10
H-4
H-11
H-12,H-13
H-14
H-9
H-1
H-2
p-cymene aliphatic protons
CH3 protons(Methyl gr.)
H-a
CH3 protons(Isopropyl gr.)
H-i,H-j
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
ppm

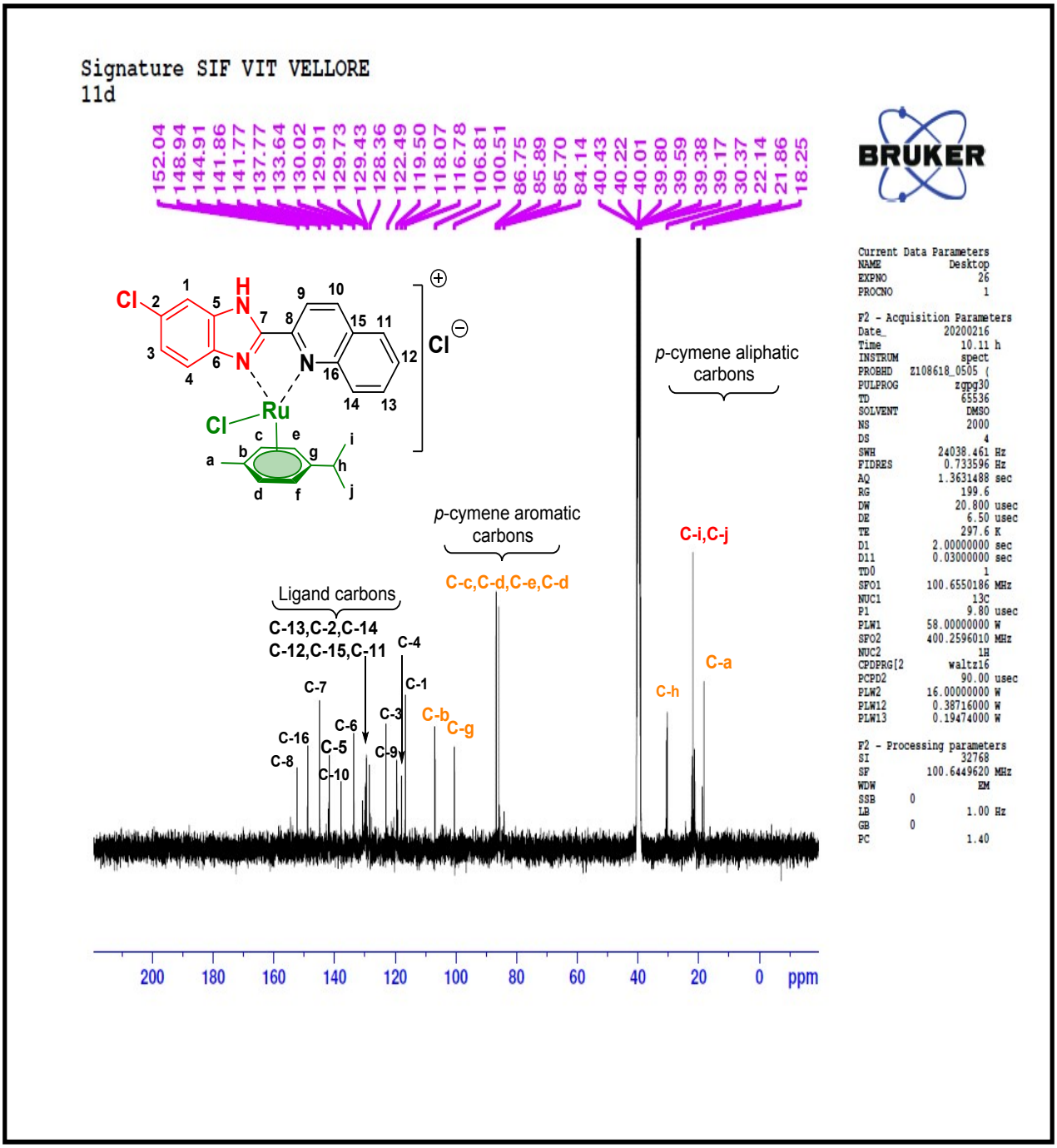
11b


Signature SIF VIT VELLORE
11d
154.72 149.01 145.11 141.94 141.84 133.71 130.99 130.10 129.99 129.81 129.51 128.44 120.62 119.57 119.24 117.02 106.88 100.59 86.83 85.96 85.78 84.22 40.50 40.30 40.09 39.88 39.67 39.46 39.25 30.44 21.94 21.50 18.32
BRUKER
Current Data Parameters
NAME Dr.PP160220
EXPNO 26
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200216
Time 10.11 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 297.6 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
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-c,C-d,C-e,C-f
C-i,C-j
C-13,C-3,C-14
C-6
C-2
C-9
C-16
C-10
C-1
C-8
C-7
C-11
C-g
C-b
C-5
C-4
C-12
C-15
C-h
C-a
200 180 160 140 120 100 80 60 40 20 0 ppm

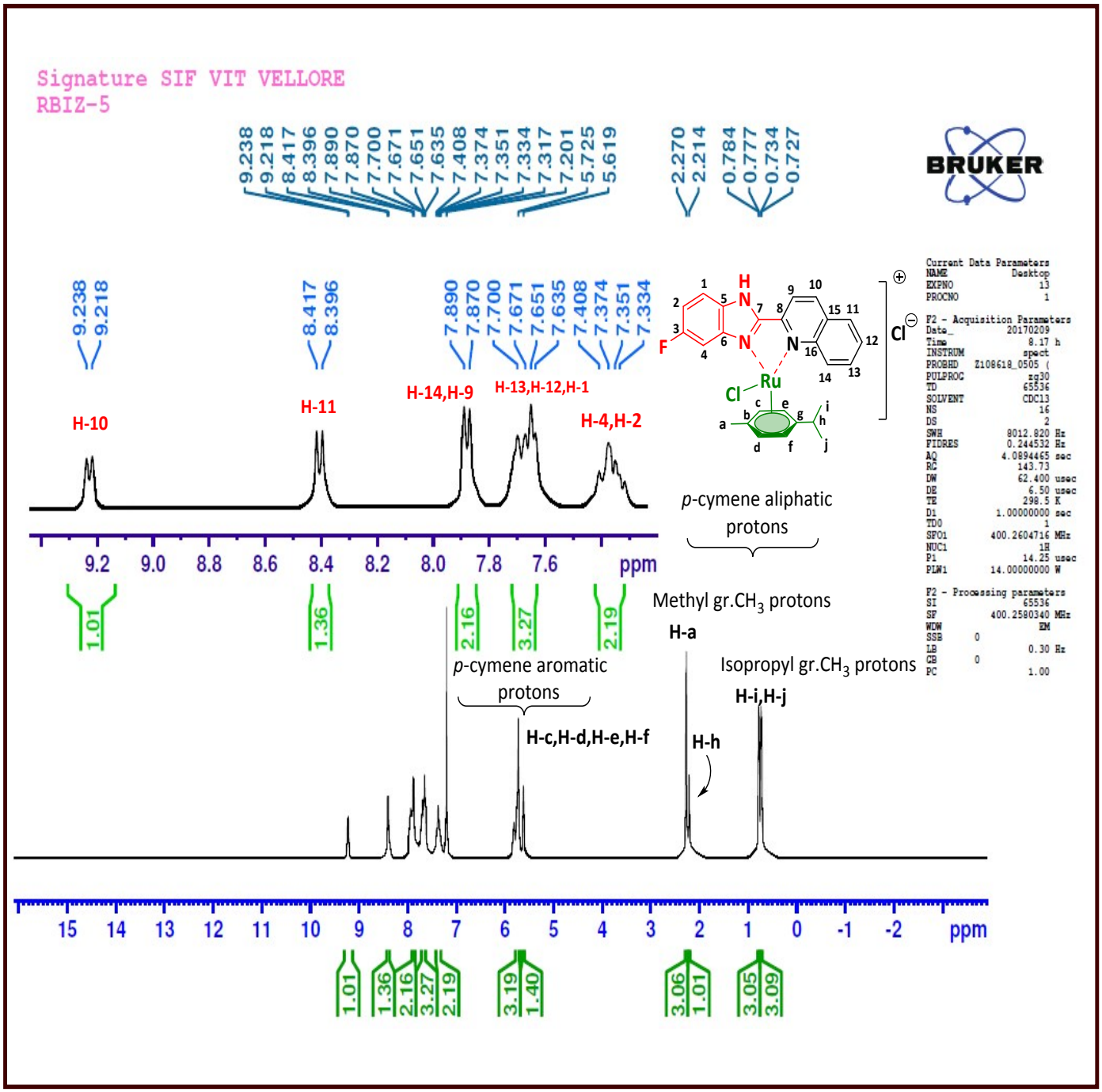
11b′


Signature SIF VIT VELLORE
RBI7-4 (M)
BRUKER
H-10
H-1
H-11,H-14
H-13,H-12,H-9
H-4,H-3
p-cymene aliphatic protons
CH3 protons (Methyl gr.)
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-a
CH3 protons (Isopropyl gr.)
H-i,H-j
Isopropyl gr. CH proton
Water
ppm

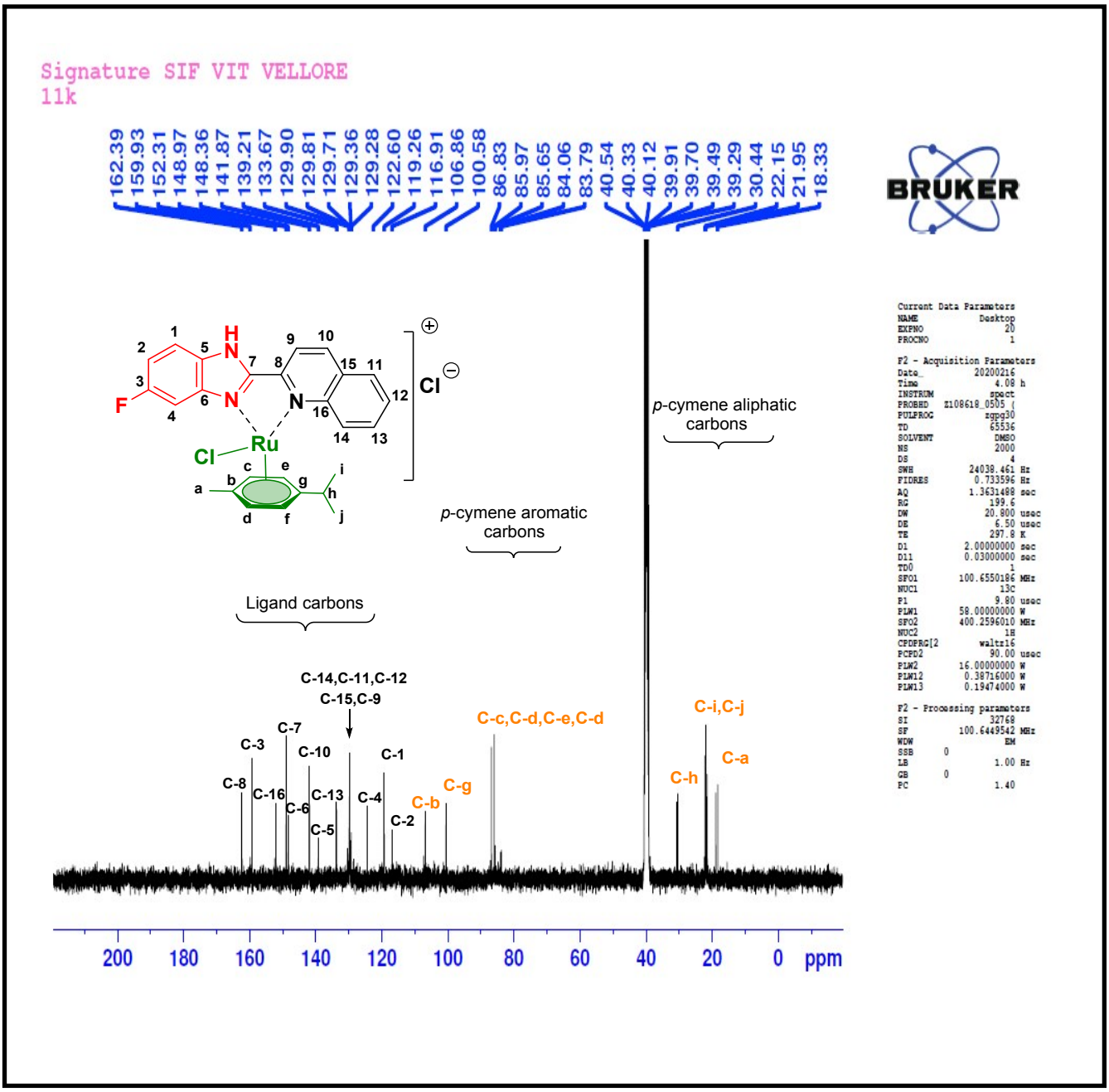
11b′


Signature SIF VIT VELLORE
11d
152.04
148.94
144.91
141.86
141.77
137.77
133.64
130.02
129.91
129.73
129.43
128.36
122.49
119.50
118.07
116.78
106.81
100.51
86.75
85.89
85.70
84.14
40.43
40.22
40.01
39.80
39.59
39.38
39.17
30.37
22.14
21.86
18.25
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
C-c,C-d,C-e,C-d
Ligand carbons
C-13,C-2,C-14
C-12,C-15,C-11
C-4
C-7
C-1
C-6
C-3
C-b
C-g
C-16
C-5
C-9
C-8
C-10
C-i,C-j
C-a
C-h
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Desktop
EXPNO 26
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200216
Time 10.11 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 297.6 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 100.6449620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

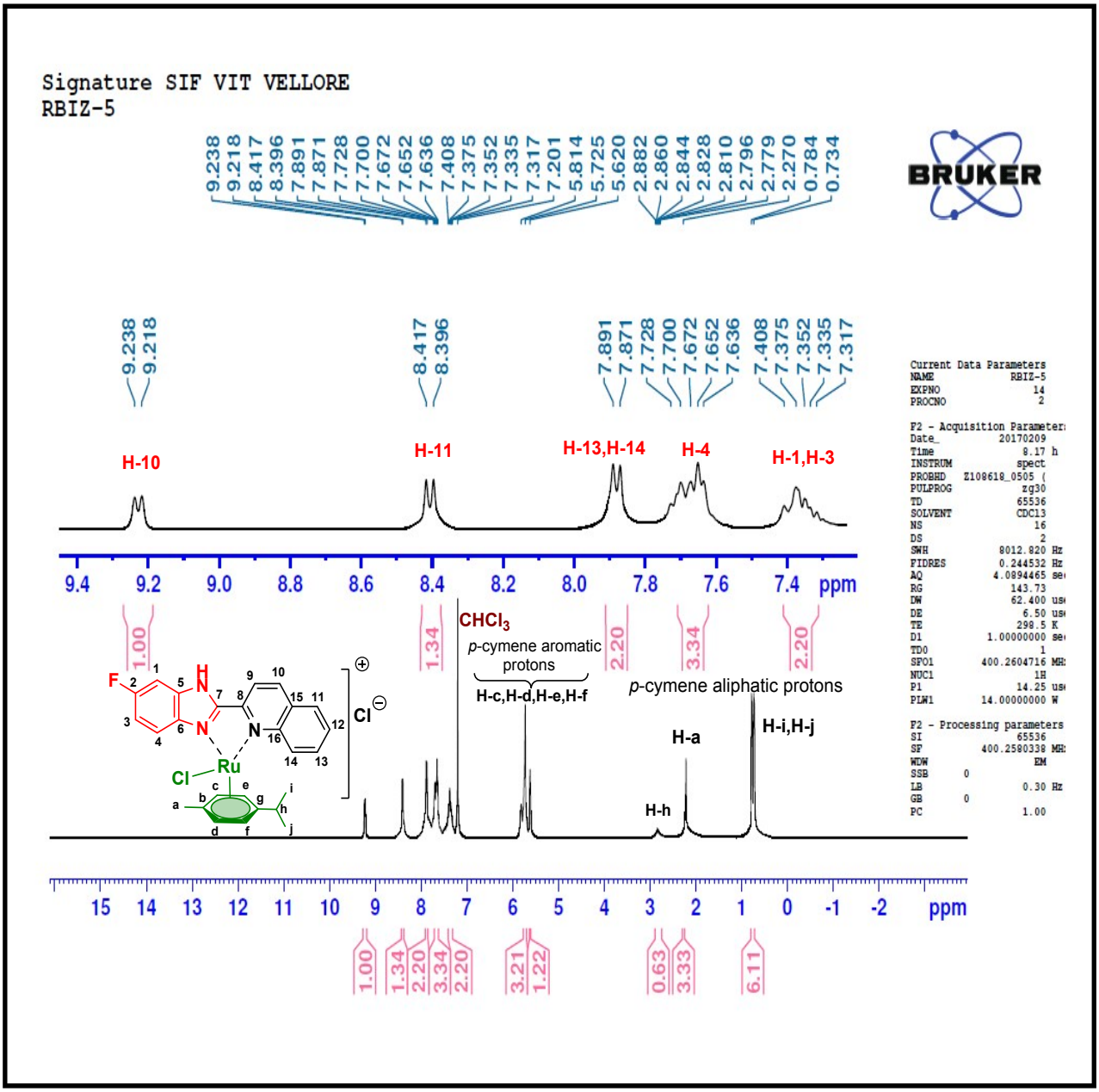
11k


Signature SIF VIT VELLORE
RBIZ-5
BRUKER
H-10
H-11
H-14,H-9
H-13,H-12,H-1
H-4,H-2
p-cymene aliphatic protons
Methyl gr.CH3 protons
H-a
Isopropyl gr.CH3 protons
H-i,H-j
H-h
p-cymene aromatic protons
H-c,H-d,H-e,H-f
ppm

11k

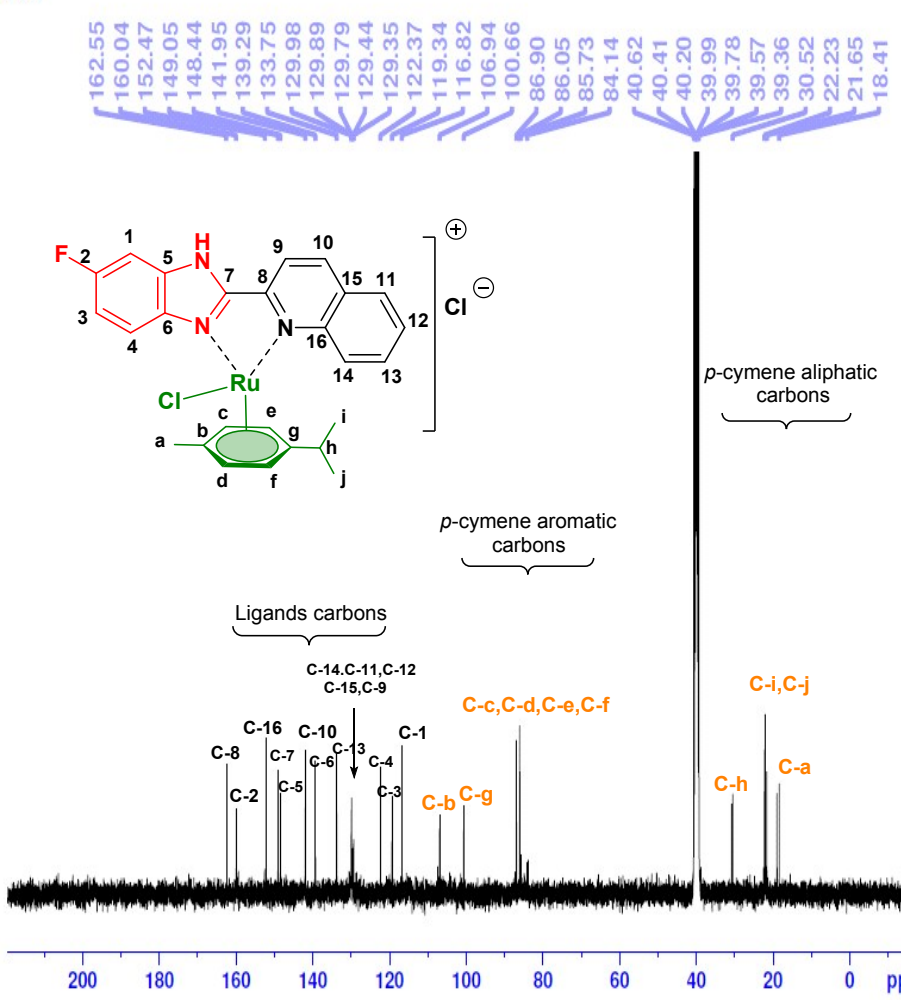

Signature SIF VIT VELLORE
11k
162.39 159.93 152.31 148.97 148.36 141.87 139.21 133.67 129.90 129.81 129.71 129.36 129.28 122.60 119.26 116.91 106.86 100.58 86.83 85.97 85.65 84.06 83.79 40.54 40.33 40.12 39.91 39.70 39.49 39.29 30.44 22.15 21.95 18.33
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-14,C-11,C-12
C-15,C-9
C-7
C-3
C-10
C-1
C-8
C-16
C-6
C-13
C-4
C-5
C-2
C-b
C-g
C-c,C-d,C-e,C-d
C-h
C-i,C-j
C-a
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME Desktop
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200216
Time 4.08 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 297.8 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

11k′


Signature SIF VIT VELLORE
RBIZ-5
BRUKER
H-10
H-11
H-13,H-14
H-4
H-1,H-3
CHCl3
p-cymene aromatic protons
H-c,H-d,H-e,H-f
p-cymene aliphatic protons
H-a
H-h
H-i,H-j
Cl
Ru
F
ppm

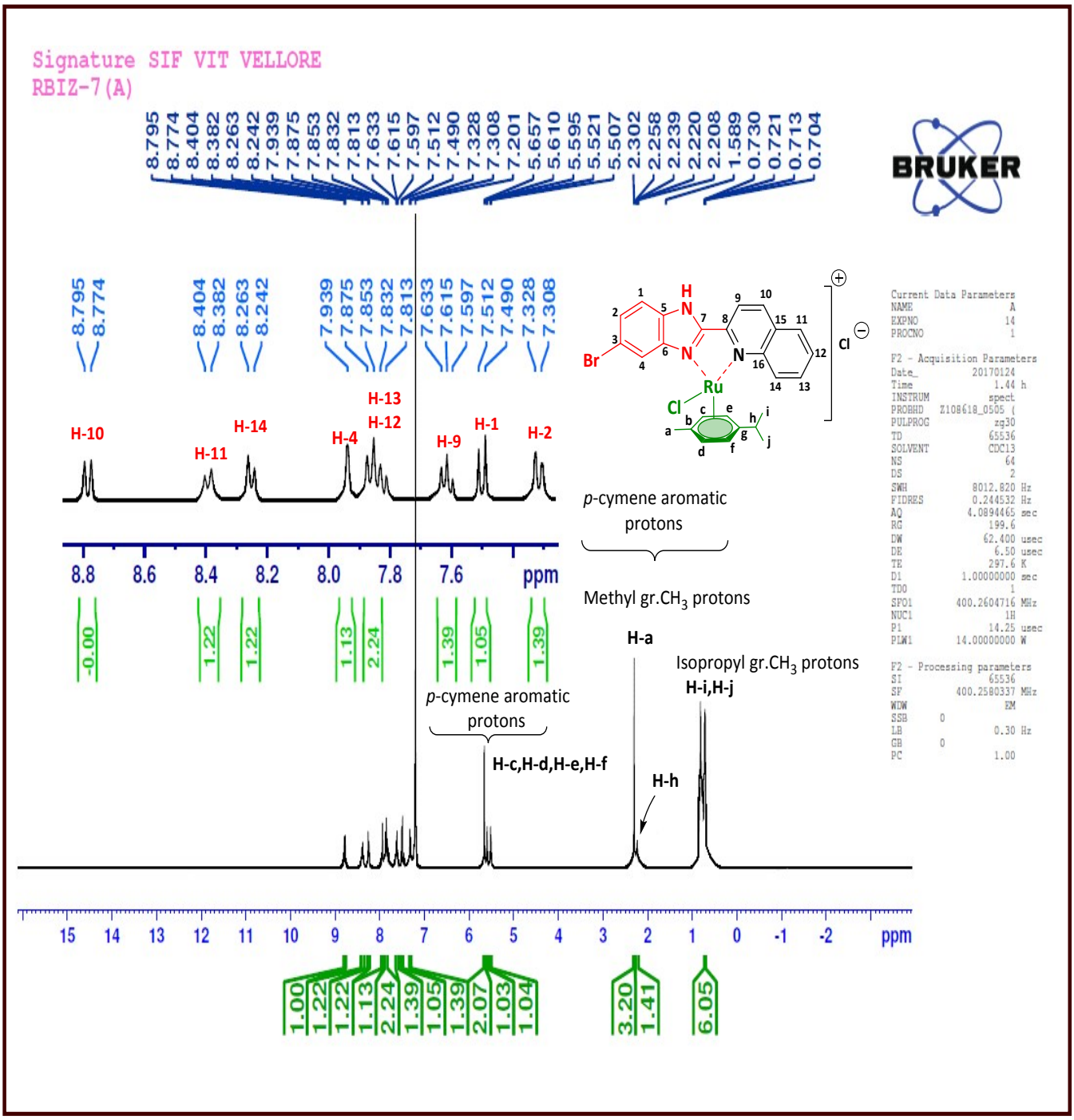
11k′

Signature SIF VIT VELLORE
11k

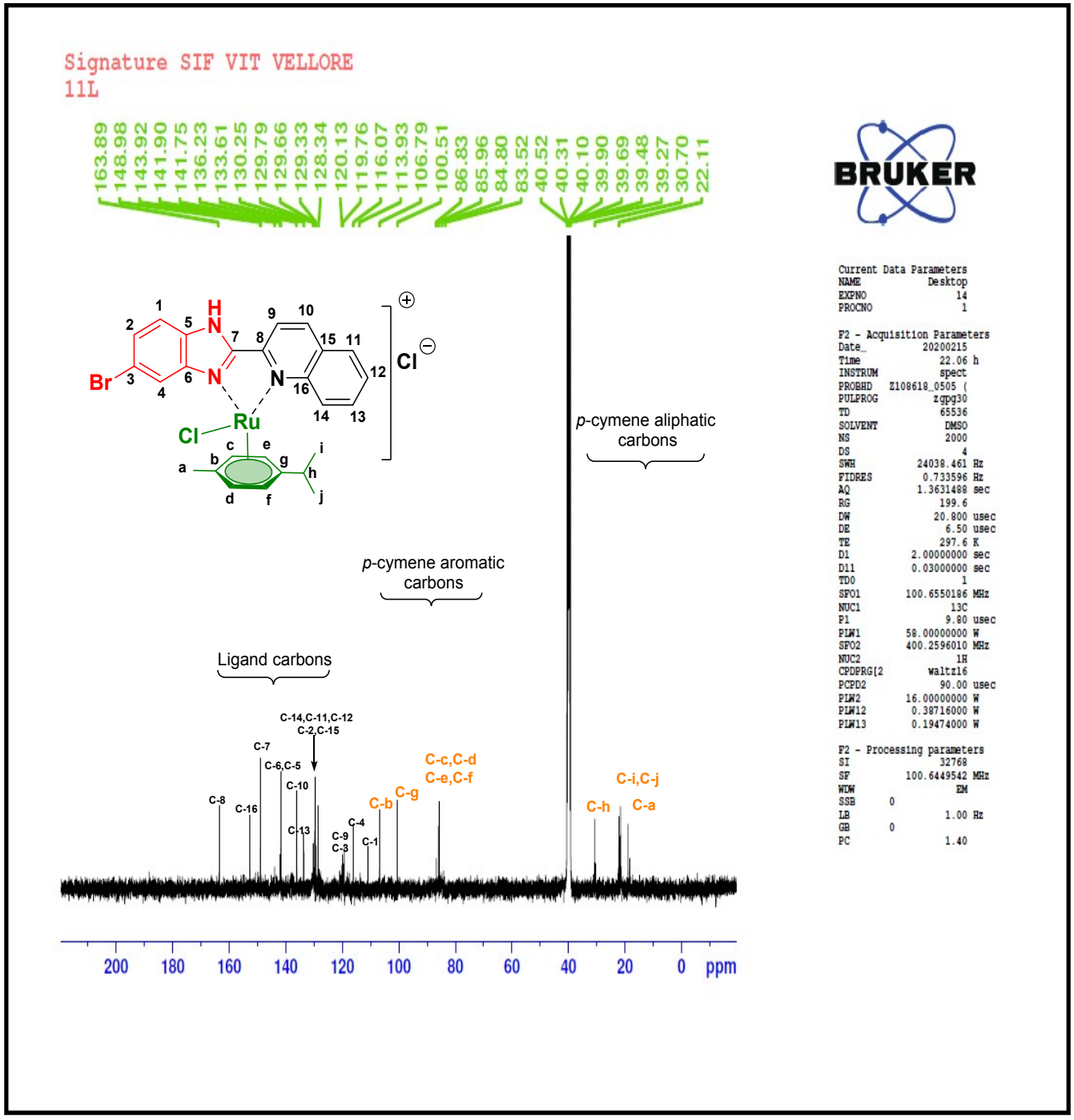



```
Current Data Parameters
NAME          Dr.PP160220
EXPNO                  21
PROCNO                  2

F2 - Acquisition Parameters
Date_            20200216
Time                4.08 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 use
DE                 6.50 use
TE                297.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         100.6550186 MHz
NUC1                13C
P1                 9.80 use
PLW1         58.00000000 W
SFO2         400.2596010 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 use
PLW2         16.00000000 W
PLW12         0.38716000 W
PLW13         0.19474000 W

F2 - Processing parameters
SI                  32768
SF           100.6449464 MHz
WDW                    EM
SSB          0
LB                 1.00 Hz
GB           0
PC                 1.40
```

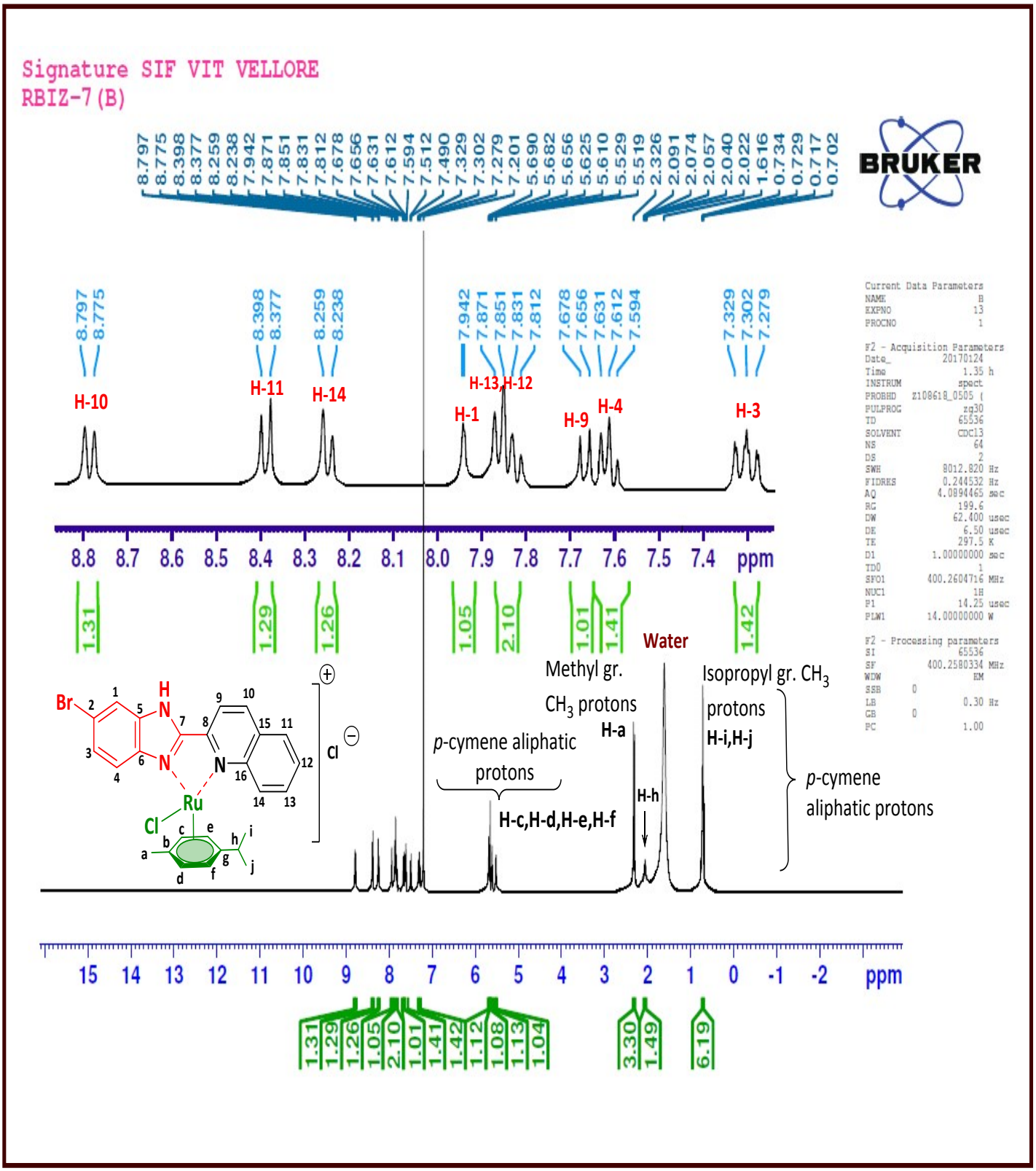
111


Signature SIF VIT VELLORE
RBIZ-7(A)
BRUKER
H-10
H-11
H-14
H-4
H-13
H-12
H-9
H-1
H-2
p-cymene aromatic protons
Methyl gr.CH3 protons
H-a
Isopropyl gr.CH3 protons
H-i,H-j
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
ppm

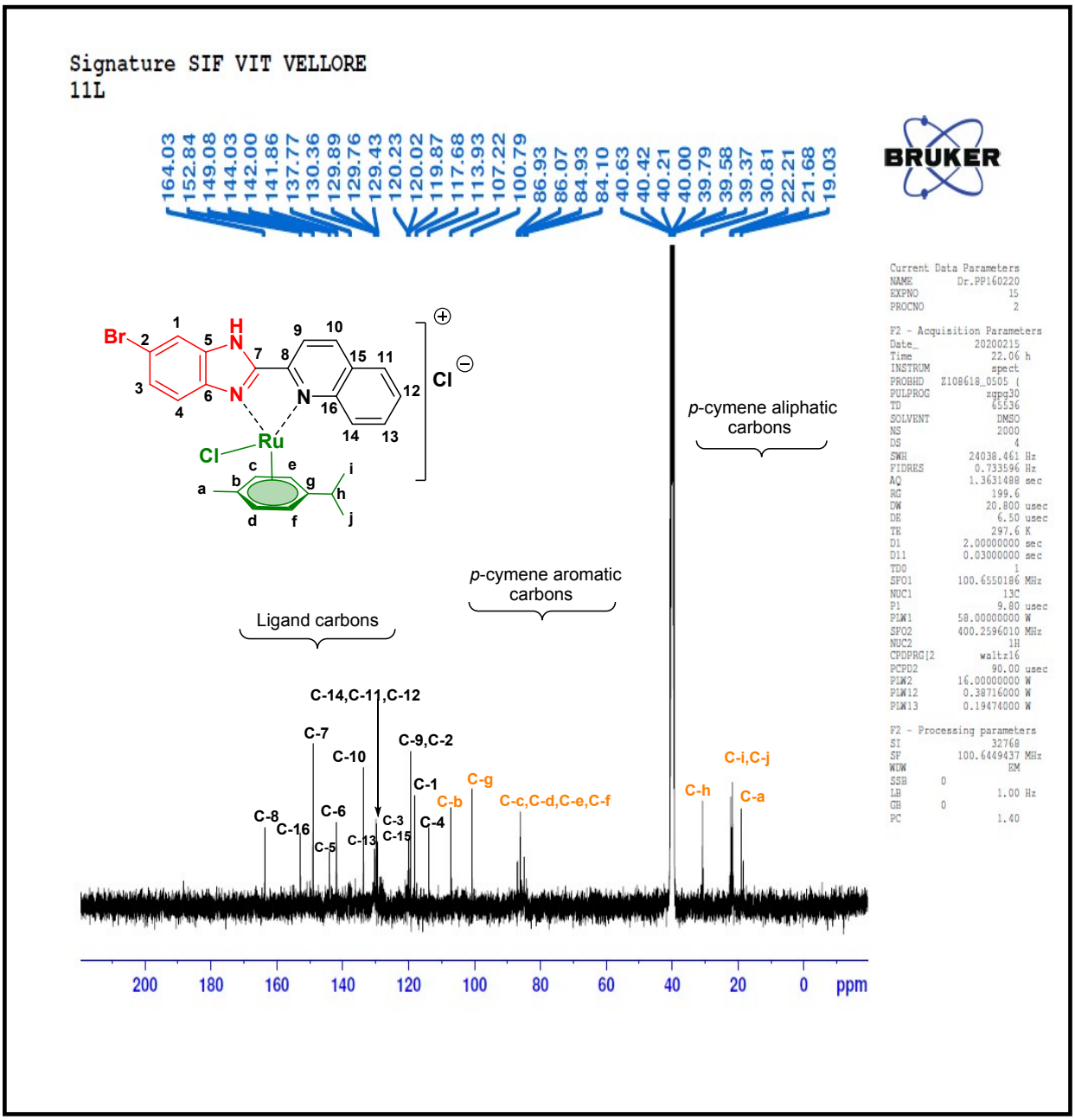
111


Signature SIF VIT VELLORE
11L
163.89 148.98 143.92 141.90 141.75 136.23 133.61 130.25 129.79 129.66 129.33 128.34 120.13 119.76 116.07 113.93 106.79 100.51 86.83 85.96 84.80 83.52 40.52 40.31 40.10 39.90 39.69 39.48 39.27 30.70 22.11
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-14,C-11,C-12
C-2,C-15
C-7
C-6,C-5
C-10
C-8
C-16
C-13
C-9
C-3
C-4
C-1
C-b
C-g
C-c,C-d
C-e,C-f
C-h
C-i,C-j
C-a
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME Desktop
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200215
Time 22.06 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 297.6 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

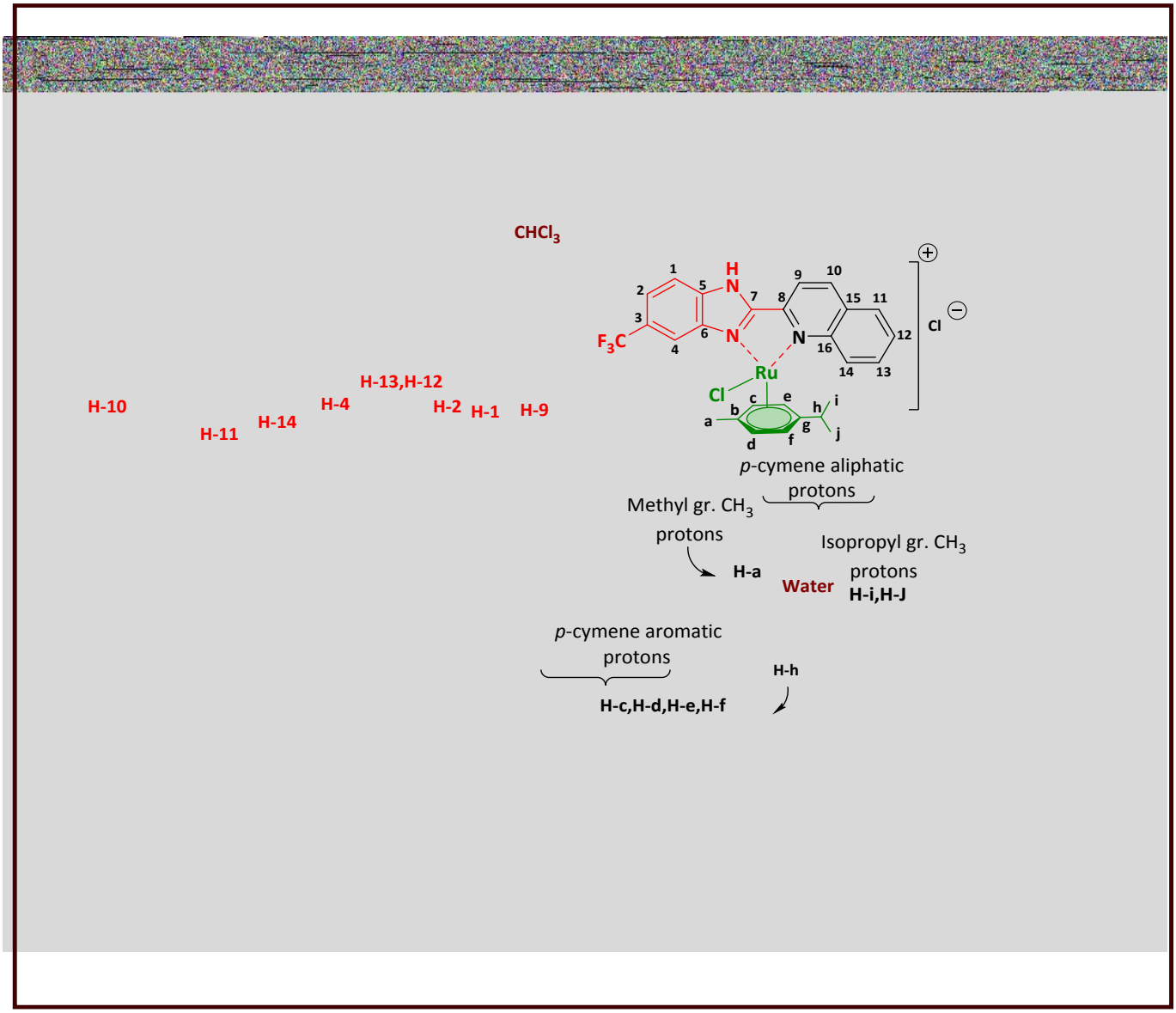
11l′


Signature SIF VIT VELLORE
RBIZ-7 (B)
BRUKER
H-10
H-11
H-14
H-13,H-12
H-1
H-9
H-4
H-3
Water
Methyl gr.
CH3 protons
H-a
Isopropyl gr. CH3
protons
H-i,H-j
p-cymene aliphatic
protons
H-c,H-d,H-e,H-f
H-h
p-cymene
aliphatic protons
Br
Cl
Ru
ppm

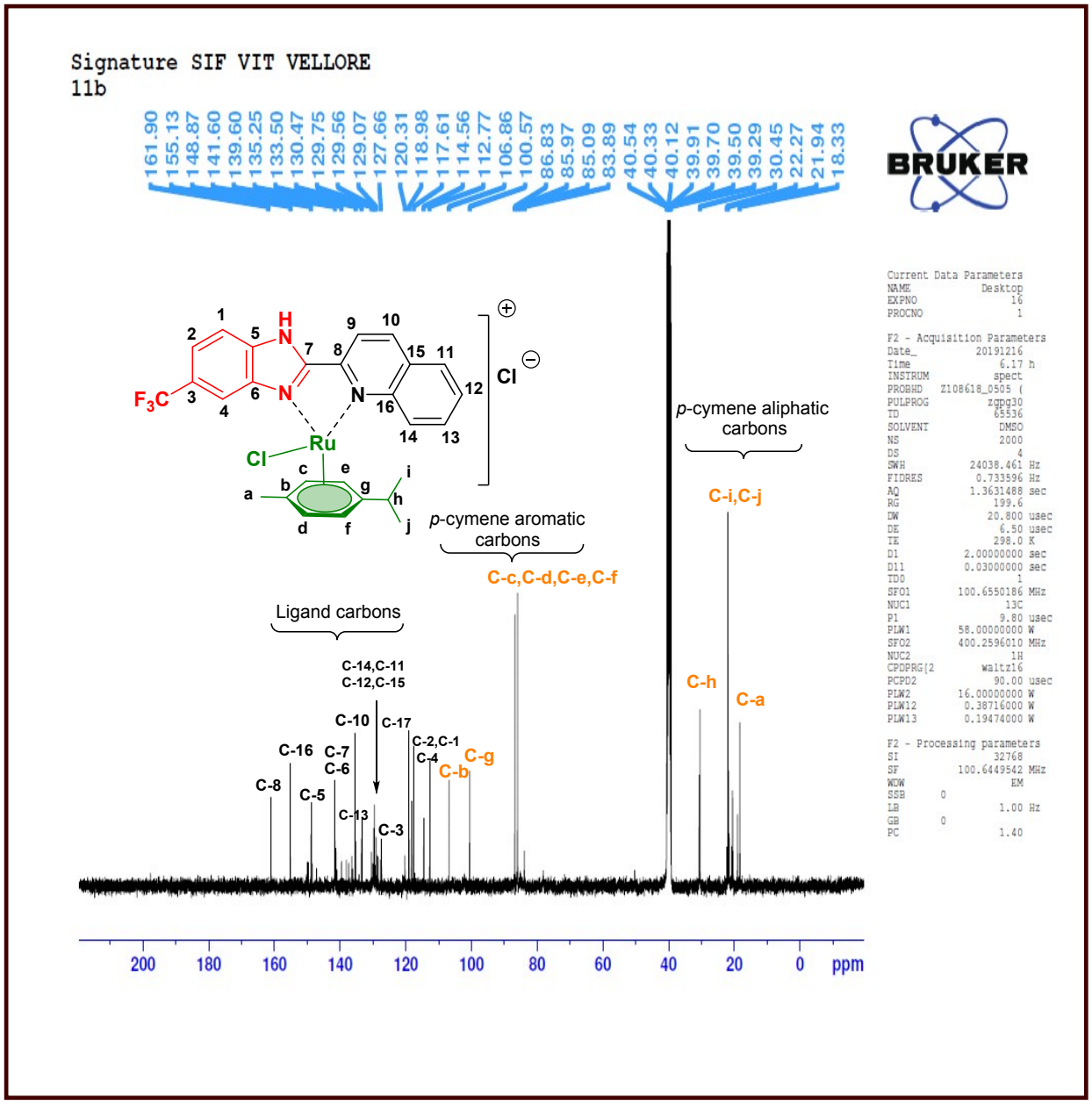
11l′


Signature SIF VIT VELLORE
11L
164.03
152.84
149.08
144.03
142.00
141.86
137.77
130.36
129.89
129.76
129.43
120.23
120.02
119.87
117.68
113.93
107.22
100.79
86.93
86.07
84.93
84.10
40.63
40.42
40.21
40.00
39.79
39.58
39.37
30.81
22.21
21.68
19.03
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-14,C-11,C-12
C-7
C-10
C-9,C-2
C-1
C-g
C-b
C-c,C-d,C-e,C-f
C-i,C-j
C-h
C-a
C-8
C-16
C-6
C-5
C-13
C-3
C-15
C-4
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Dr.PP160220
EXPNO 15
PROCNO 2
F2 - Acquisition Parameters
Date_ 20200215
Time 22.06 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 297.6 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 100.6449437 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

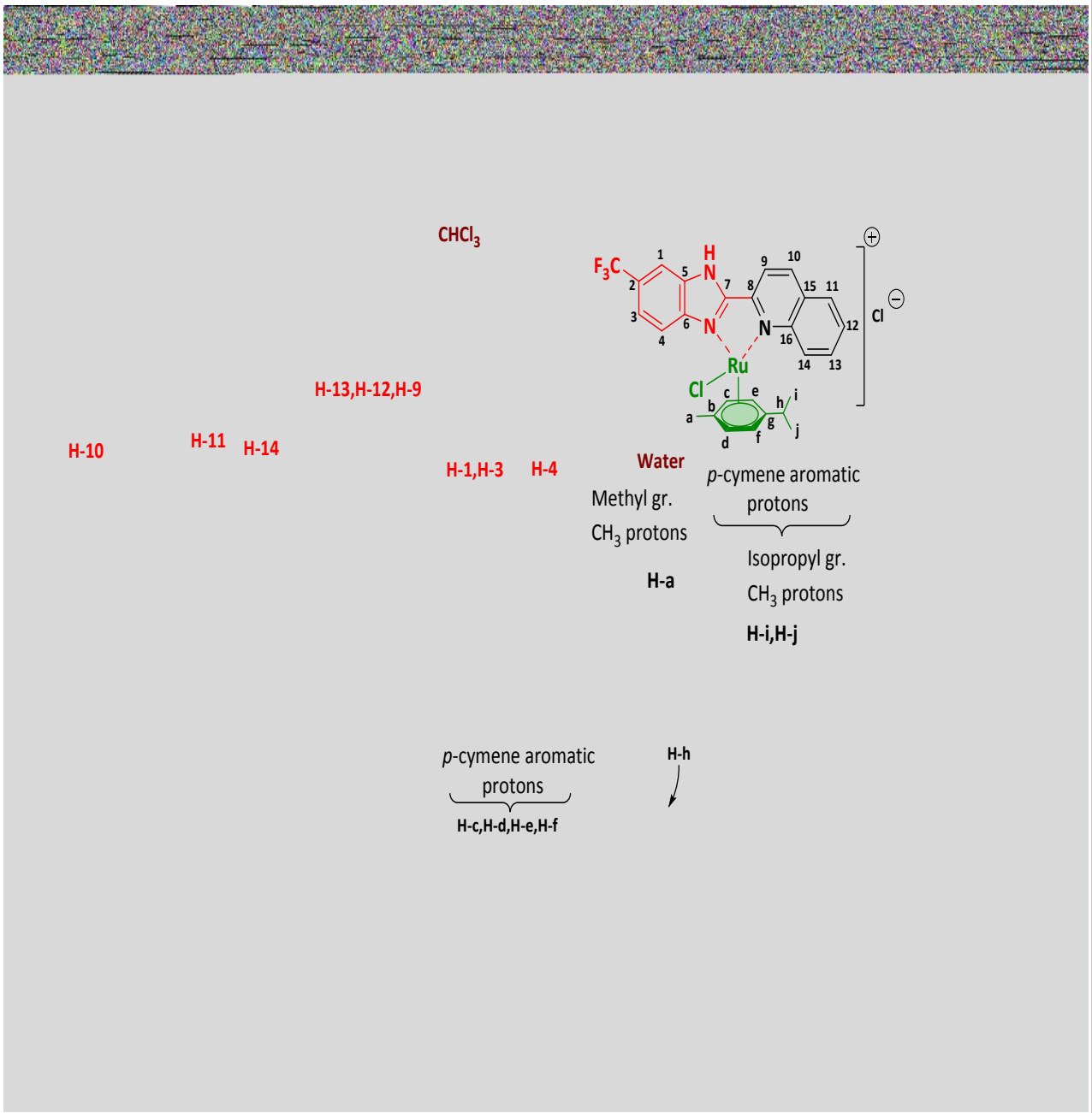
11d


CHCl3
H-10
H-11
H-14
H-4
H-13,H-12
H-2
H-1
H-9
p-cymene aliphatic protons
Methyl gr. CH3 protons
H-a
Isopropyl gr. CH3 protons
H-i,H-J
Water
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
Cl
Ru

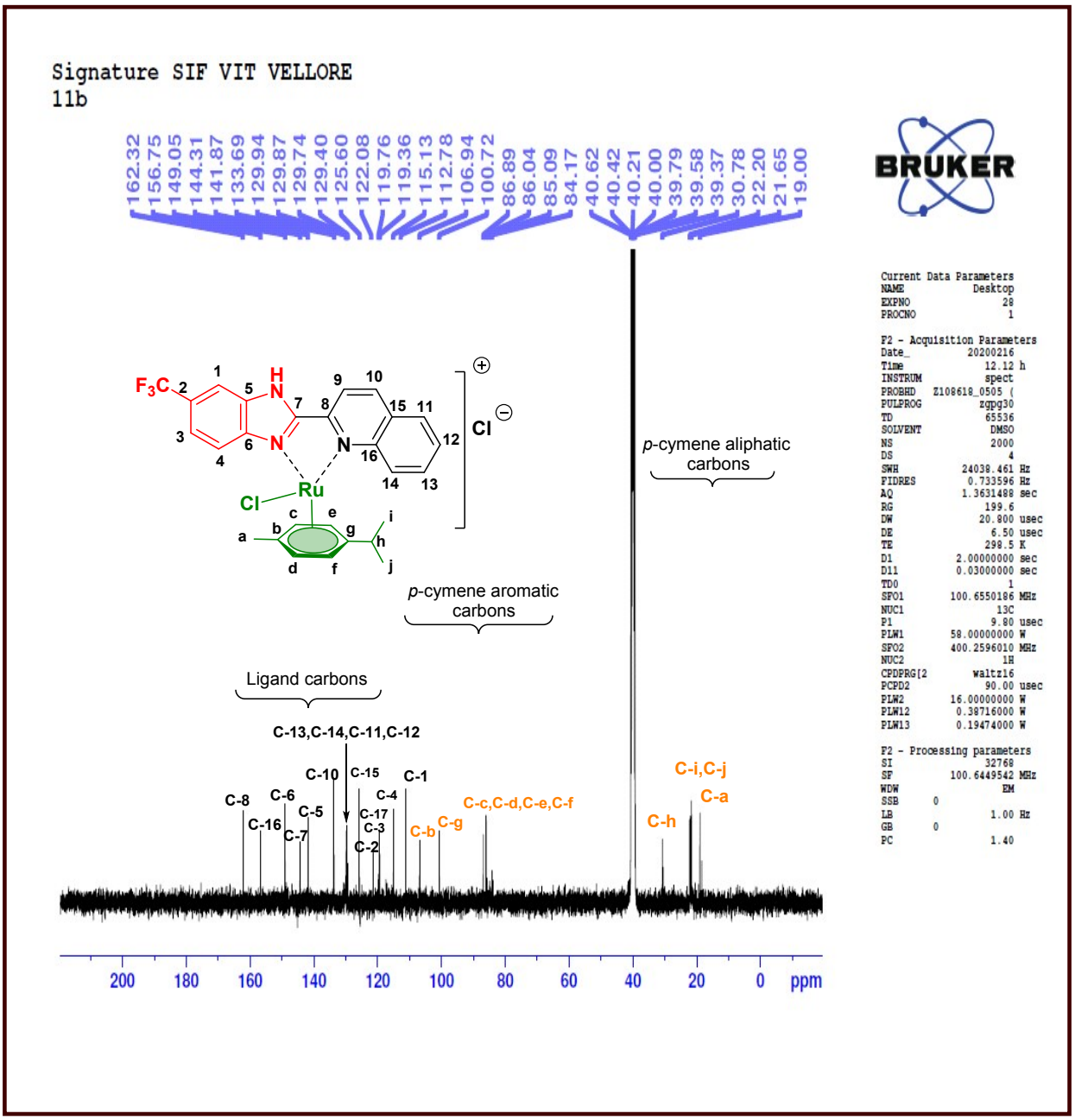
11d


Signature SIF VIT VELLORE
11b
161.90 155.13 148.87 141.60 139.60 135.25 133.50 130.47 129.75 129.56 129.07 127.66 120.31 118.98 117.61 114.56 112.77 106.86 100.57 86.83 85.97 85.09 83.89 40.54 40.33 40.12 39.91 39.70 39.50 39.29 30.45 22.27 21.94 18.33
BRUKER
Current Data Parameters
NAME Desktop
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191216
Time 6.17 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 298.0 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
p-cymene aliphatic carbons
C-i,C-j
C-h
C-a
p-cymene aromatic carbons
C-c,C-d,C-e,C-f
Ligand carbons
C-14,C-11
C-12,C-15
C-10
C-17
C-16
C-7
C-6
C-2,C-1
C-4
C-g
C-b
C-8
C-5
C-13
C-3
200 180 160 140 120 100 80 60 40 20 0 ppm

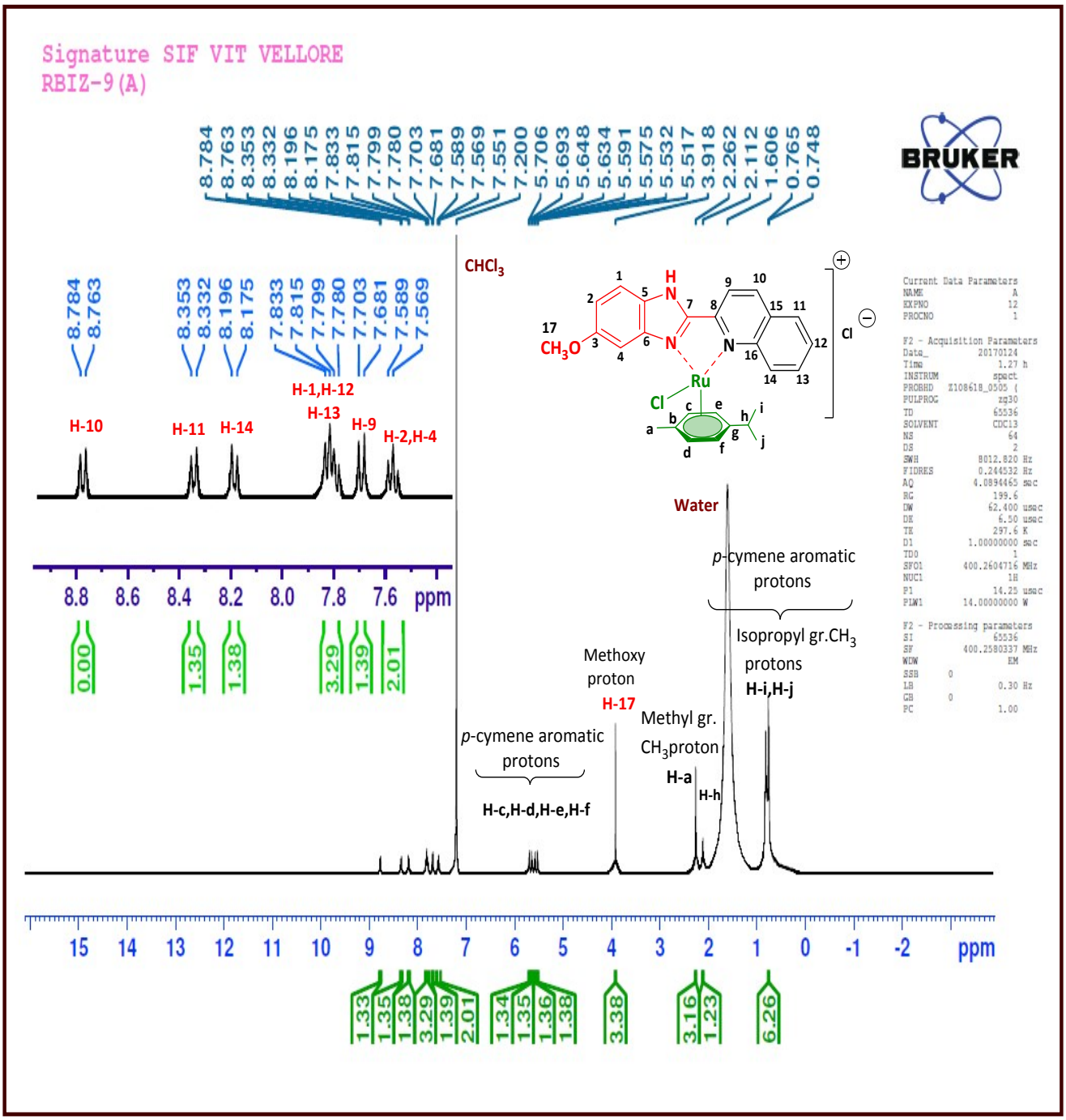
11d′


CHCl3
H-13,H-12,H-9
H-10
H-11
H-14
H-1,H-3
H-4
Water
Methyl gr.
CH3 protons
H-a
p-cymene aromatic protons
Isopropyl gr.
CH3 protons
H-i,H-j
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
F3C
H
N
N
N
Ru
Cl
Cl

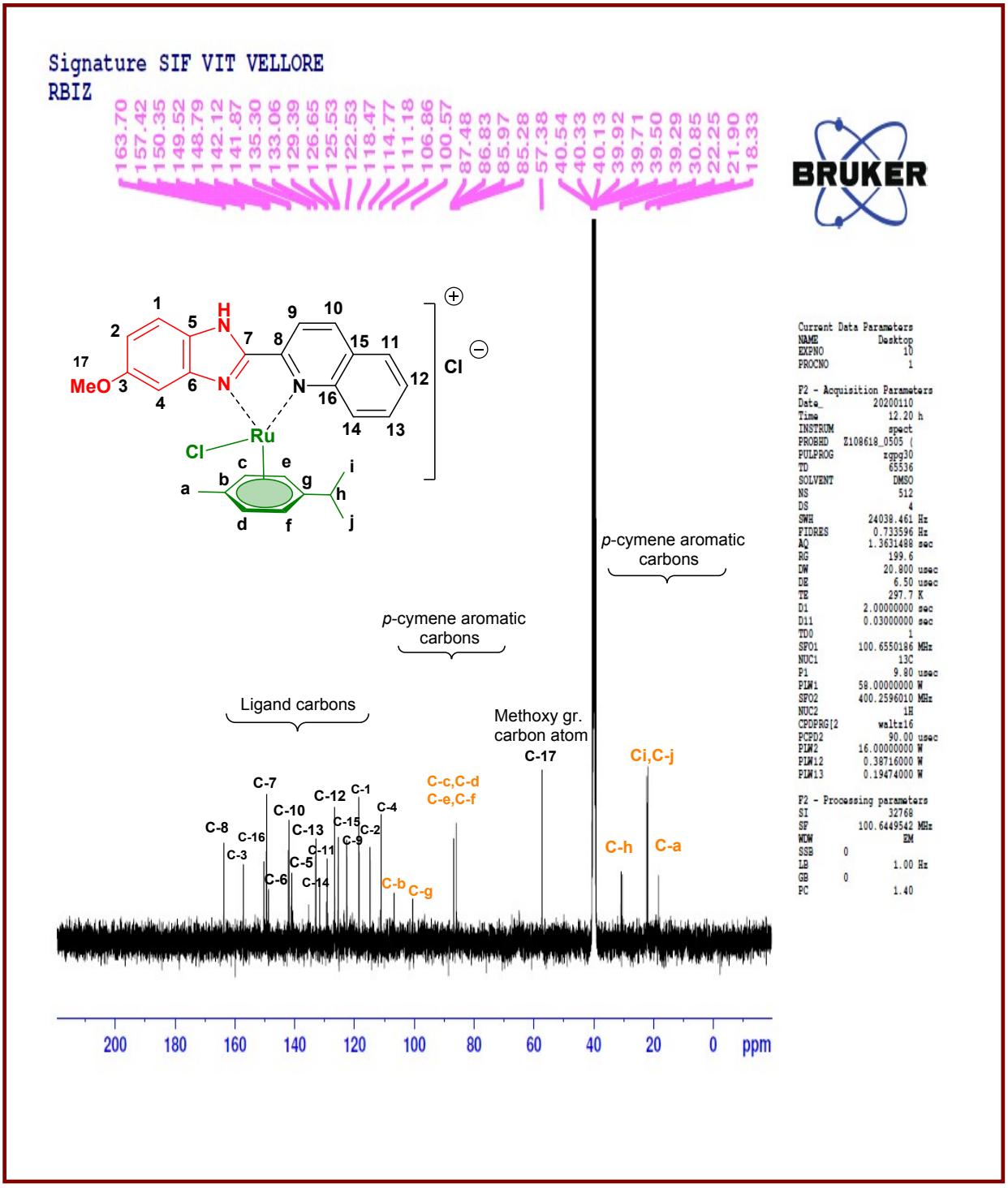
11d′


Signature SIF VIT VELLORE
11b
162.32
156.75
149.05
144.31
141.87
133.69
129.94
129.87
129.74
129.40
125.60
122.08
119.76
119.36
115.13
112.78
106.94
100.72
86.89
86.04
85.09
84.17
40.62
40.42
40.21
40.00
39.79
39.58
39.37
30.78
22.20
21.65
19.00
BRUKER
Current Data Parameters
NAME Desktop
EXPNO 28
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200216
Time 12.12 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 298.5 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
F3C
H
N
Cl
Ru
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-13,C-14,C-11,C-12
C-10
C-15
C-1
C-8
C-6
C-4
C-16
C-5
C-17
C-7
C-3
C-2
C-b
C-g
C-c,C-d,C-e,C-f
C-h
C-i,C-j
C-a
200
180
160
140
120
100
80
60
40
20
0
ppm

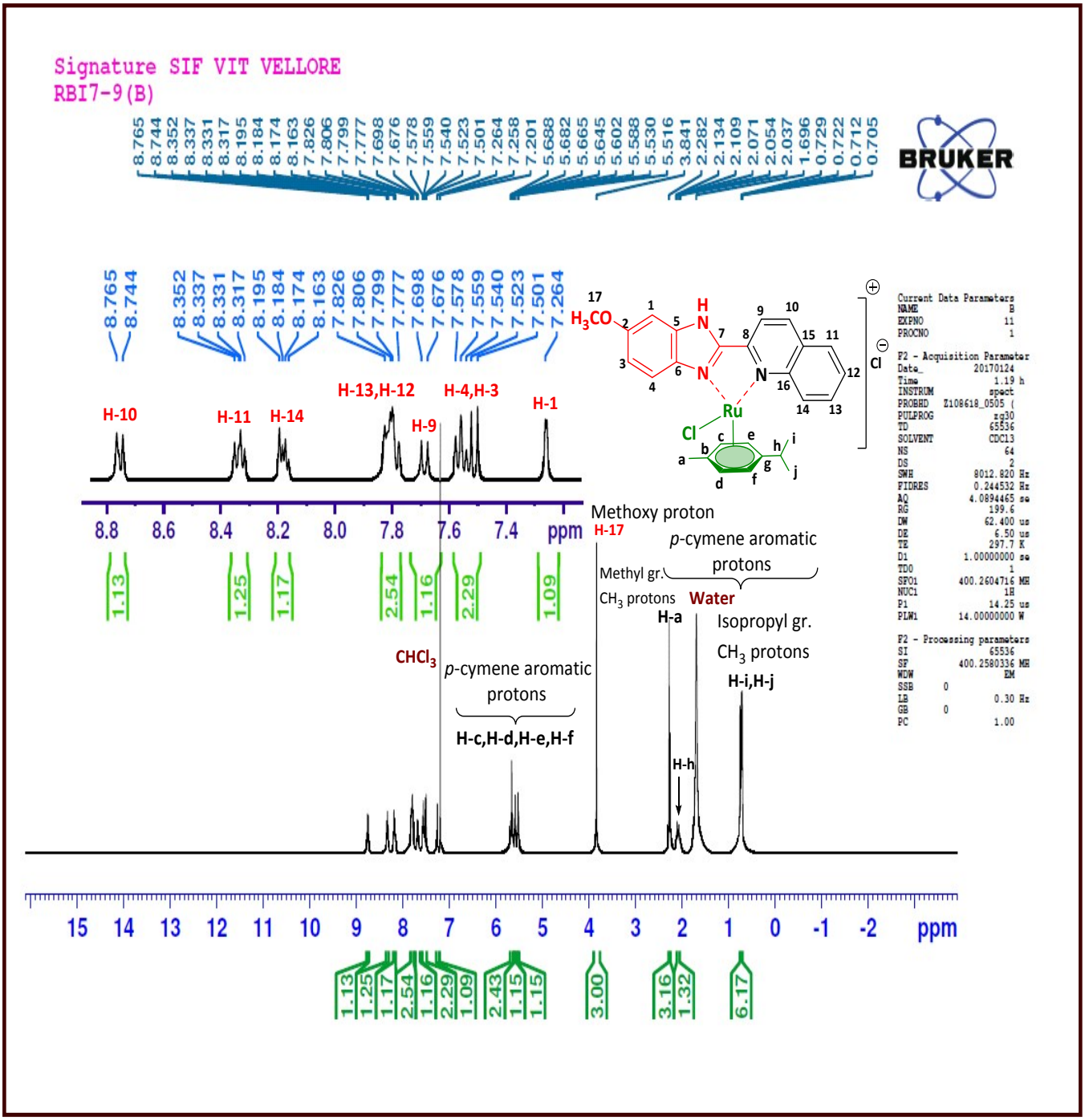
11e


Signature SIF VIT VELLORE
RBIZ-9(A)
BRUKER
8.784 8.763 8.353 8.332 8.196 8.175 7.833 7.815 7.799 7.780 7.703 7.681 7.589 7.569 7.551 7.200 5.706 5.693 5.648 5.634 5.591 5.575 5.532 5.517 3.918 2.262 2.112 1.606 0.765 0.748
CHCl3
H-10
H-11
H-14
H-13
H-9
H-2,H-4
H-1,H-12
8.8 8.6 8.4 8.2 8.0 7.8 7.6 ppm
0.00 1.35 1.38 3.29 1.39 2.01
Water
p-cymene aromatic protons
Isopropyl gr.CH3 protons
H-i,H-j
Methoxy proton
H-17
Methyl gr. CH3proton
H-a
H-h
p-cymene aromatic protons
H-c,H-d,H-e,H-f
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.33 1.35 1.38 3.29 1.39 2.01 1.34 1.35 1.36 1.38 3.38 3.16 1.23 6.26
Cl
Ru
CH3O
Current Data Parameters
NAME A
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Data_ 20170124
Time 1.27 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
F2 - Processing parameters
SI 65536
SF 400.2580337 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

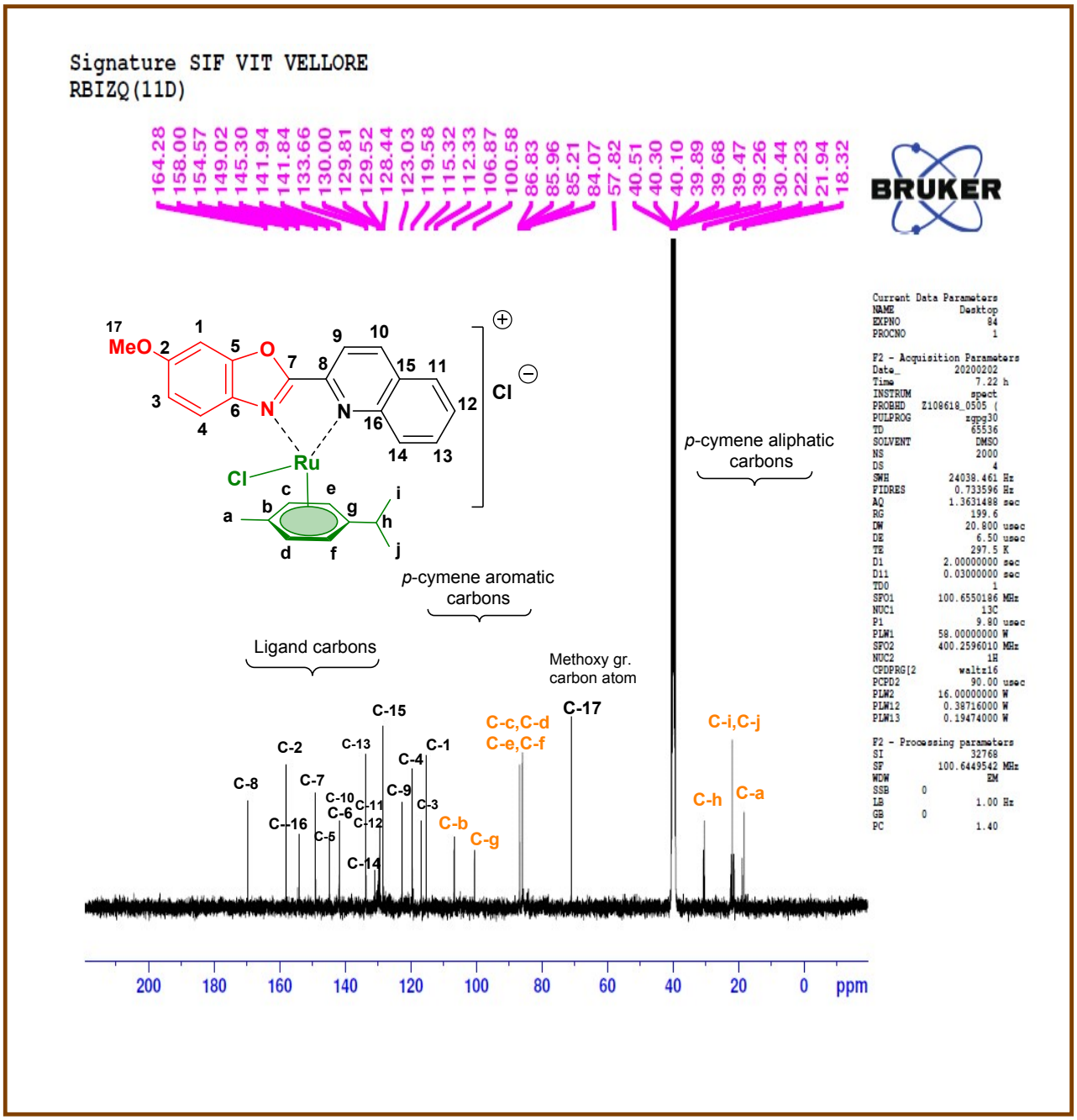
11e


Signature SIF VIT VELLORE
RBIZ
163.70 157.42 150.35 149.52 148.79 142.12 141.87 135.30 133.06 129.39 126.65 125.53 122.53 118.47 114.77 111.18 106.86 100.57 87.48 86.83 85.97 85.28 57.38 40.54 40.33 40.13 39.92 39.71 39.50 39.29 30.85 22.25 21.90 18.33
BRUKER
MeO
Cl
Ru
p-cymene aromatic carbons
p-cymene aromatic carbons
Ligand carbons
Methoxy gr. carbon atom
C-17
C-c,C-d
C-e,C-f
Ci,C-j
C-h
C-a
C-b
C-g
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME Desktop
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200110
Time 12.20 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
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 297.7 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

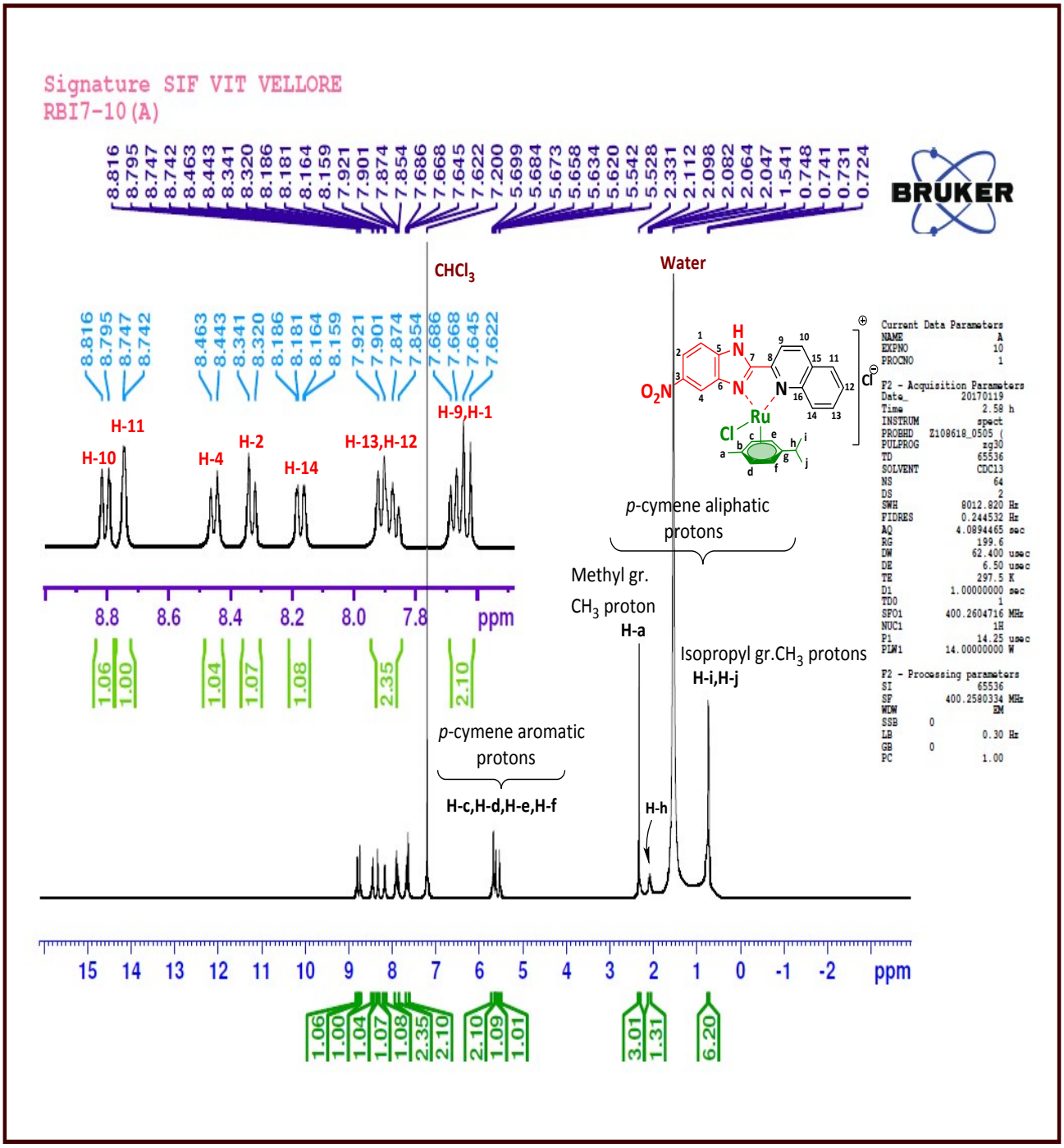
11e′


Signature SIF VIT VELLORE
RBI7-9(B)
BRUKER
H-10
H-11
H-14
H-13,H-12
H-9
H-4,H-3
H-1
Methoxy proton
H-17
p-cymene aromatic protons
Methyl gr.
CH3 protons
Water
H-a
Isopropyl gr.
CH3 protons
H-i,H-j
CHCl3
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
Cl
Ru
Current Data Parameters
F2 - Acquisition Parameter
F2 - Processing parameters
ppm

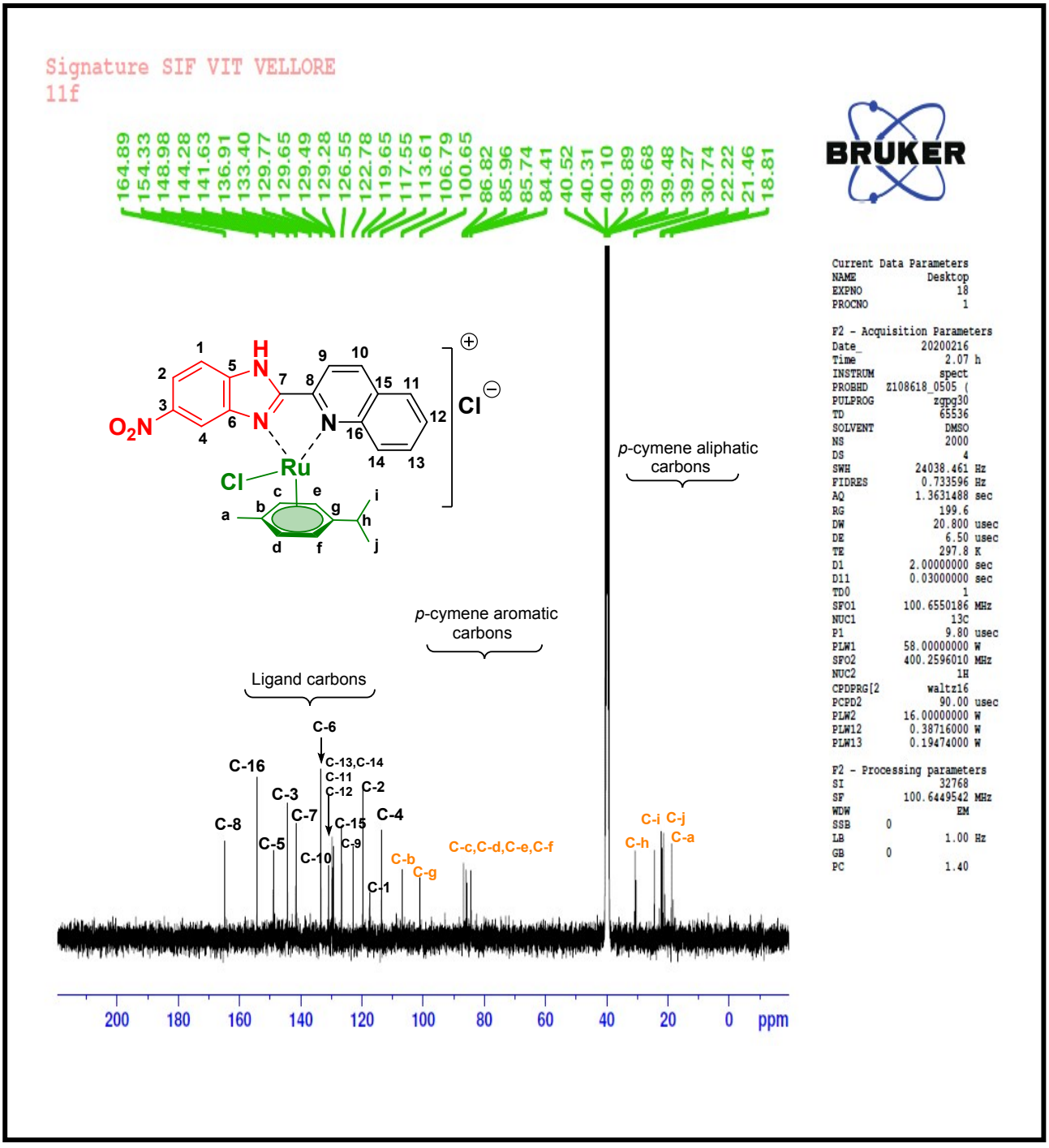
11e′


Signature SIF VIT VELLORE
RBIZQ(11D)
164.28 158.00 154.57 149.02 145.30 141.94 141.84 133.66 130.00 129.81 129.52 128.44 123.03 119.58 115.32 112.33 106.87 100.58 86.83 85.96 85.21 84.07 57.82 40.51 40.30 40.10 39.89 39.68 39.47 39.26 30.44 22.23 21.94 18.32
BRUKER
MeO
Cl
Ru
p-cymene aromatic carbons
p-cymene aliphatic carbons
Ligand carbons
Methoxy gr. carbon atom
C-15
C-2
C-13
C-1
C-4
C-c,C-d
C-e,C-f
C-17
C-i,C-j
C-8
C-7
C-10
C-11
C-9
C-3
C-6
C-12
C-16
C-5
C-b
C-g
C-14
C-h
C-a
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME Desktop
EXPNO 84
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200202
Time 7.22 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 297.5 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

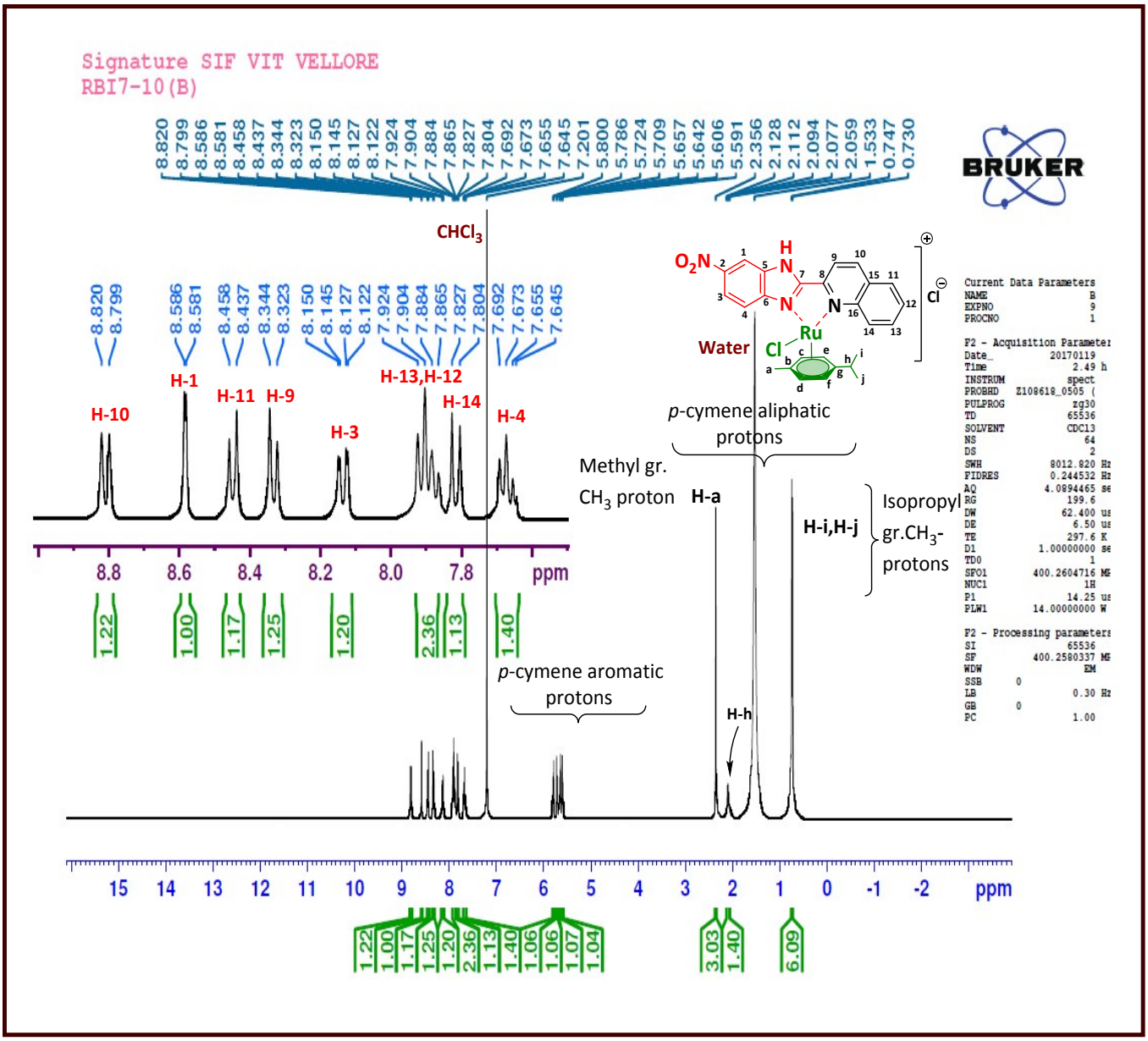
11f


Signature SIF VIT VELLORE
RBI7-10 (A)
BRUKER
CHCl3
Water
H-11
H-10
H-4
H-2
H-14
H-13,H-12
H-9,H-1
p-cymene aliphatic protons
Methyl gr.
CH3 proton
H-a
Isopropyl gr.CH3 protons
H-i,H-j
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
ppm

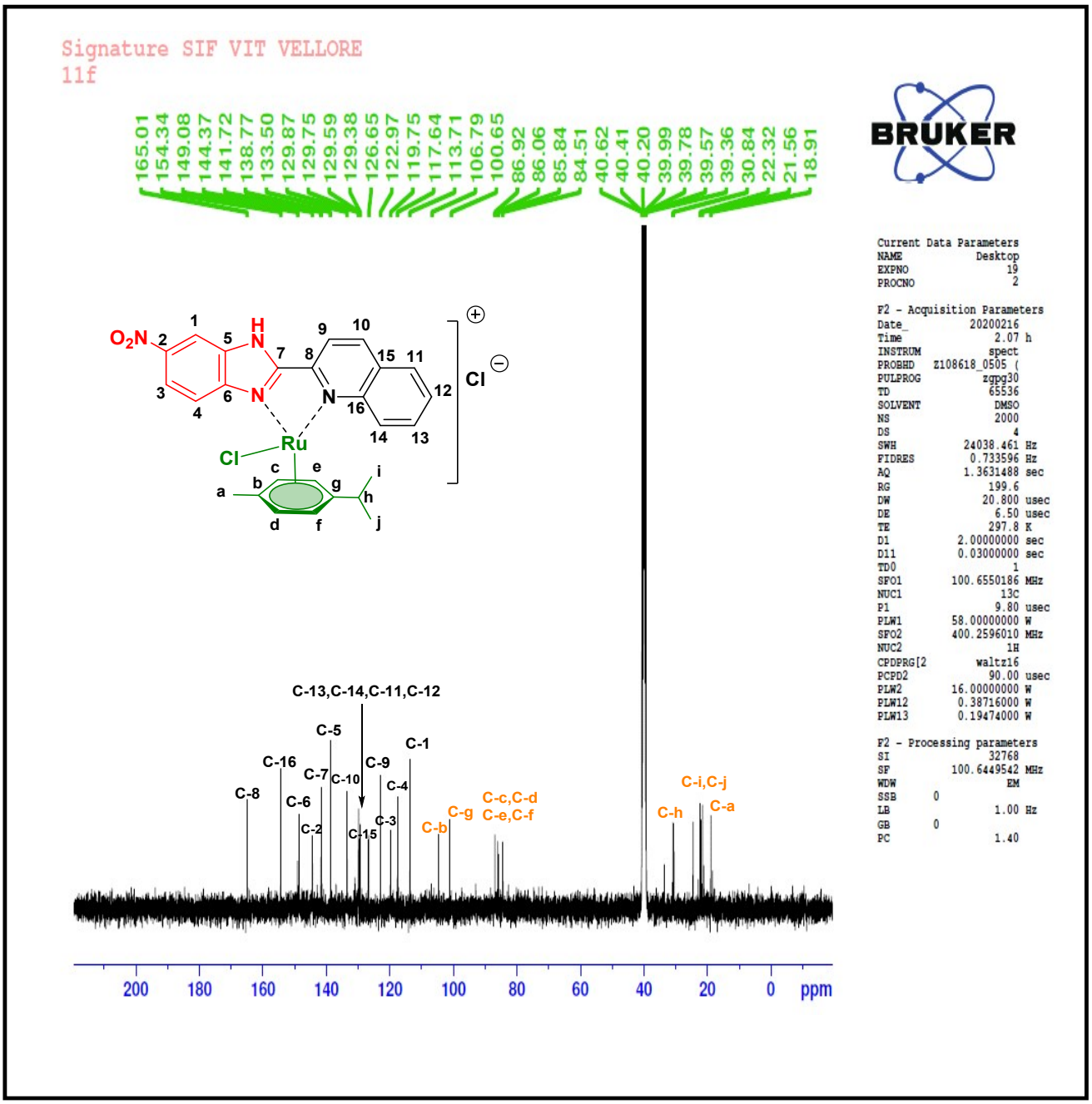
11f


Signature SIF VIT VELLORE
11f
164.89 154.33 148.98 144.28 141.63 136.91 133.40 129.77 129.65 129.49 129.28 126.55 122.78 119.65 117.55 113.61 106.79 100.65 86.82 85.96 85.74 84.41 40.52 40.31 40.10 39.89 39.68 39.48 39.27 30.74 22.22 21.46 18.81
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-6
C-16
C-13,C-14
C-11
C-12
C-2
C-3
C-7
C-15
C-4
C-8
C-5
C-9
C-10
C-b
C-g
C-1
C-c,C-d,C-e,C-f
C-i C-j
C-h
C-a
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME Desktop
EXPNO 18
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200216
Time 2.07 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 297.8 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

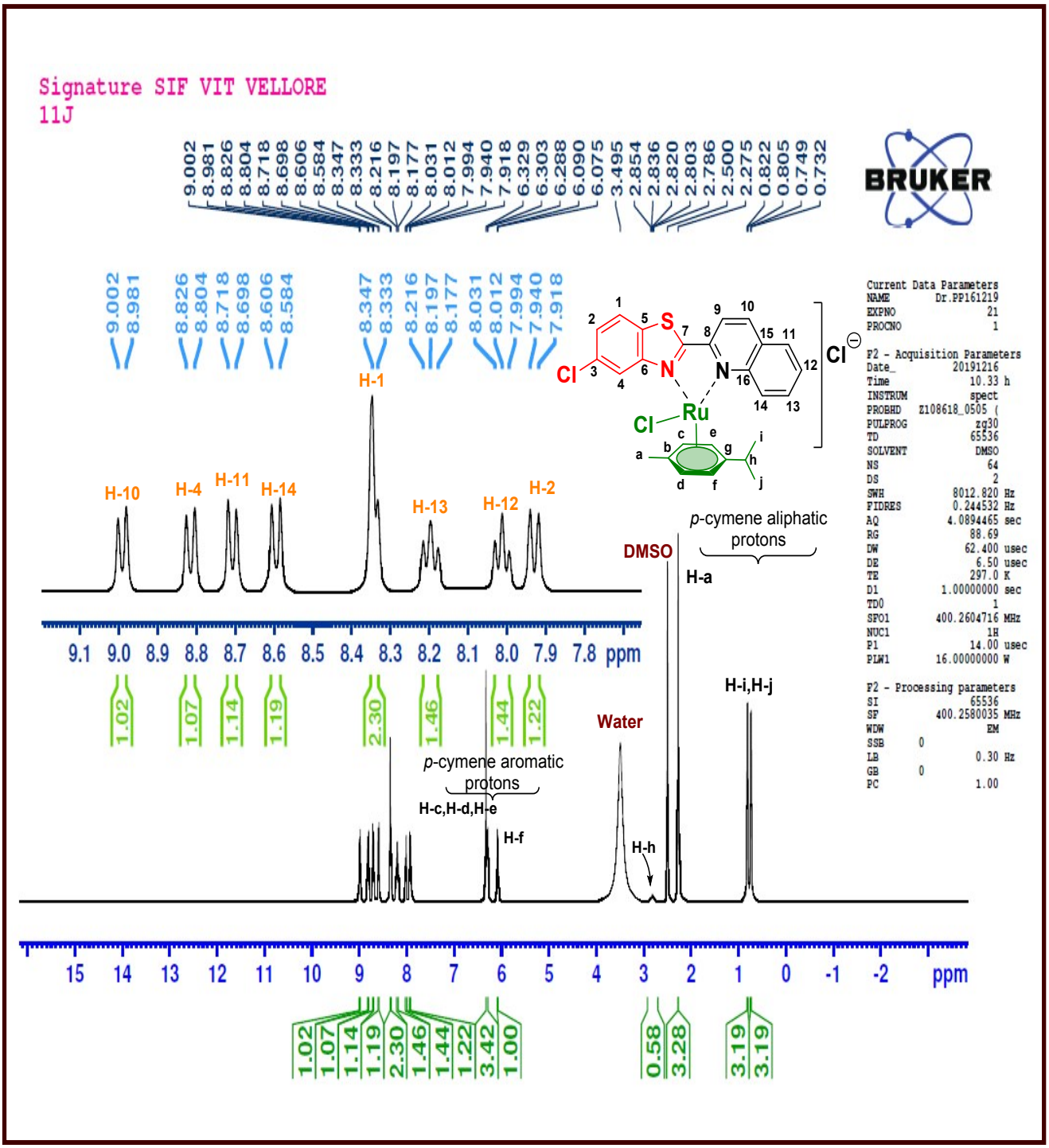
11f′


Signature SIF VIT VELLORE
RBI7-10(B)
BRUKER
CHCl3
Water
H-10
H-1
H-11
H-9
H-3
H-13,H-12
H-14
H-4
p-cymene aliphatic protons
Methyl gr. CH3 proton
H-a
H-i,H-j
Isopropyl gr.CH3-protons
p-cymene aromatic protons
H-h
ppm

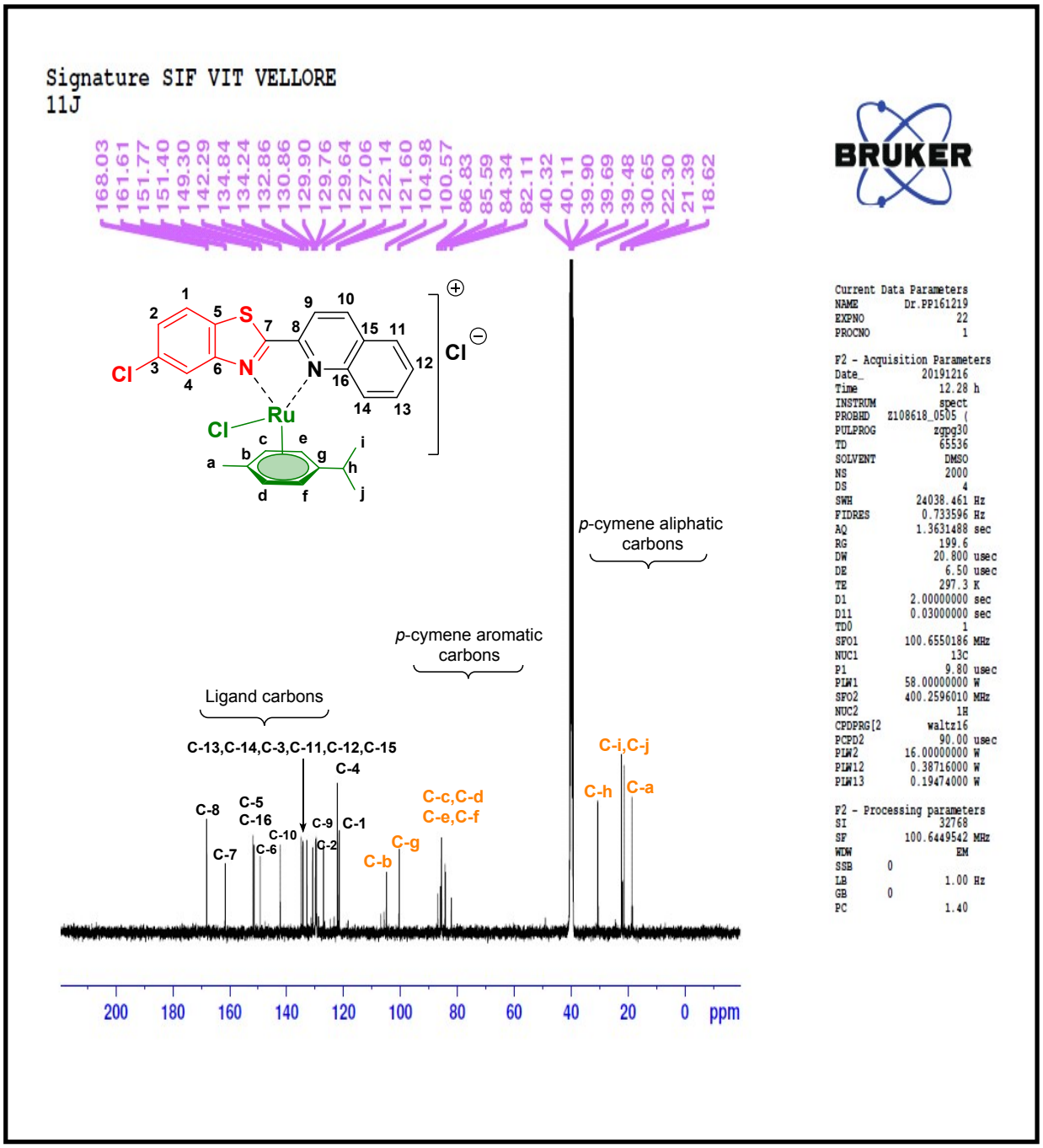
11f′


Signature SIF VIT VELLORE
11f
165.01
154.34
149.08
144.37
141.72
138.77
133.50
129.87
129.75
129.59
129.38
126.65
122.97
119.75
117.64
113.71
106.79
100.65
86.92
86.06
85.84
84.51
40.62
40.41
40.20
39.99
39.78
39.57
39.36
30.84
22.32
21.56
18.91
BRUKER
Current Data Parameters
NAME Desktop
EXPNO 19
PROCNO 2
F2 - Acquisition Parameters
Date_ 20200216
Time 2.07 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 297.8 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
O2N
H
N
Cl
Ru
C-13,C-14,C-11,C-12
C-5
C-1
C-16
C-9
C-7
C-10
C-4
C-8
C-6
C-3
C-2
C-15
C-b
C-g
C-c,C-d
C-e,C-f
C-h
C-i,C-j
C-a
200
180
160
140
120
100
80
60
40
20
0
ppm

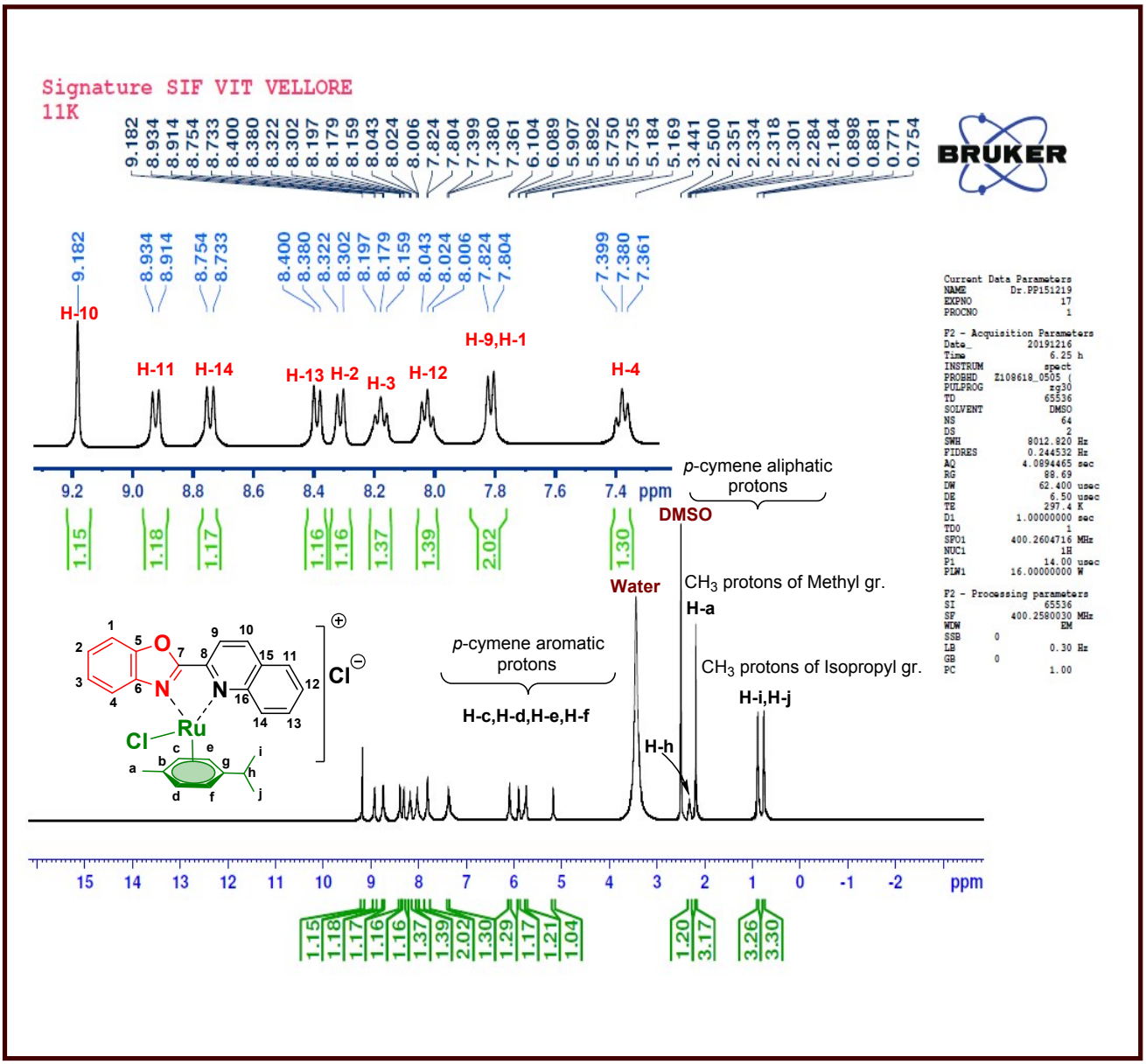
11h


Signature SIF VIT VELLORE
11J
BRUKER
H-1
H-10
H-4
H-11
H-14
H-13
H-12
H-2
DMSO
H-a
p-cymene aliphatic protons
Water
H-i,H-j
p-cymene aromatic protons
H-c,H-d,H-e
H-f
H-h
Cl
Ru
Current Data Parameters
NAME Dr.PP161219
EXPNO 21
PROCNO 1
P2 - Acquisition Parameters
Date_ 20191216
Time 10.33 h
INSTRUM spect
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 88.69
DW 62.400 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.00 usec
PLW1 16.00000000 W
P2 - Processing parameters
SI 65536
SF 400.2580035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

11h


Signature SIF VIT VELLORE
11J
168.03
161.61
151.77
151.40
149.30
142.29
134.84
134.24
132.86
130.86
129.90
129.76
129.64
127.06
122.14
121.60
104.98
100.57
86.83
85.59
84.34
82.11
40.32
40.11
39.90
39.69
39.48
30.65
22.30
21.39
18.62
BRUKER
p-cymene aliphatic carbons
p-cymene aromatic carbons
Ligand carbons
C-13,C-14,C-3,C-11,C-12,C-15
C-4
C-8
C-5
C-16
C-7
C-10
C-6
C-9
C-2
C-1
C-b
C-g
C-c,C-d
C-e,C-f
C-h
C-i,C-j
C-a
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Dr.PP161219
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191216
Time 12.28 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 297.3 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

11m


Signature SIF VIT VELLORE
11K
BRUKER
H-10
H-11
H-14
H-13
H-2
H-3
H-12
H-9,H-1
H-4
p-cymene aliphatic protons
DMSO
Water
CH3 protons of Methyl gr.
H-a
p-cymene aromatic protons
H-c,H-d,H-e,H-f
CH3 protons of Isopropyl gr.
H-i,H-j
H-h
Cl
Ru
ppm

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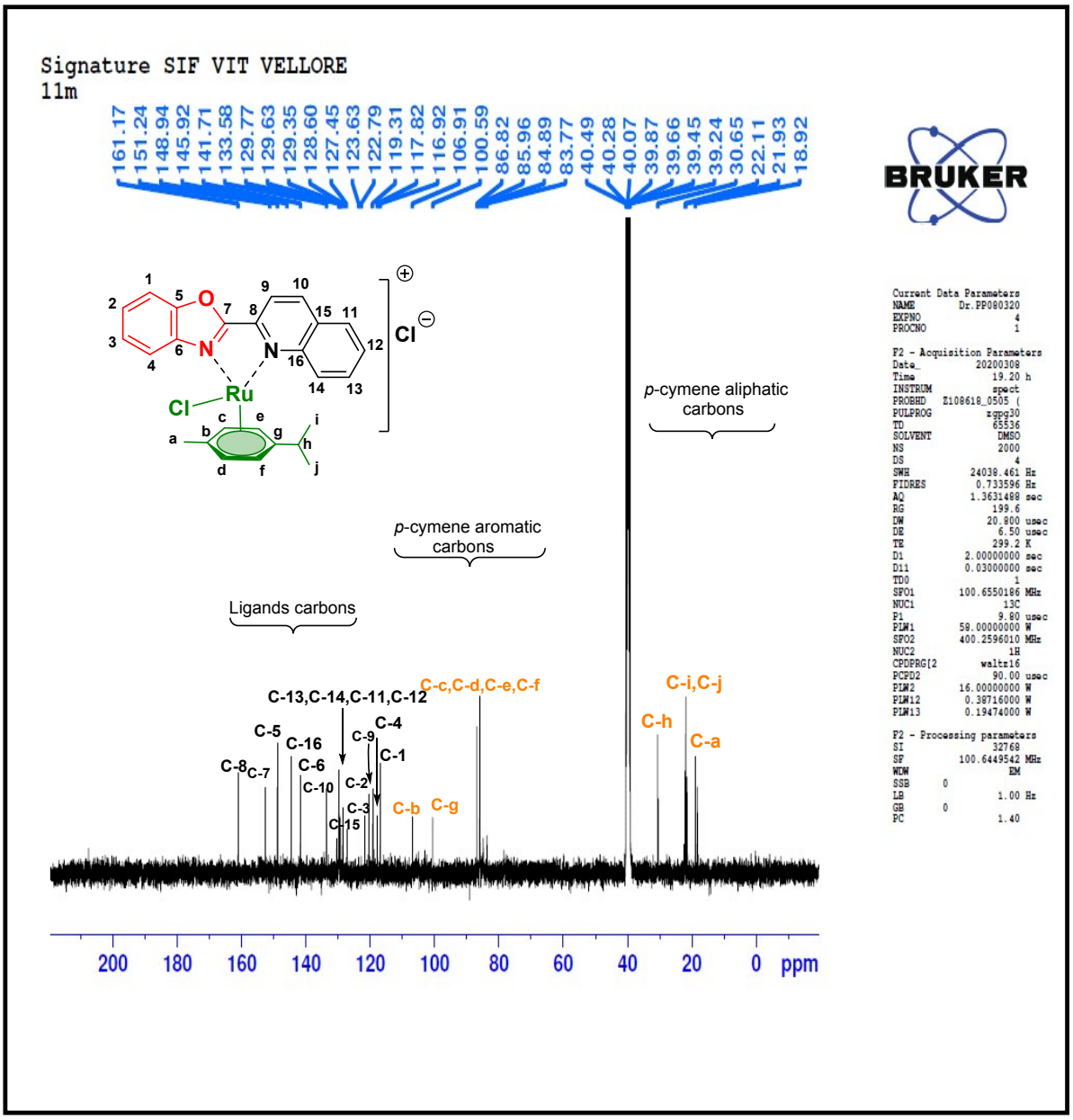
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p-cymene aromatic carbons
Ligands carbons
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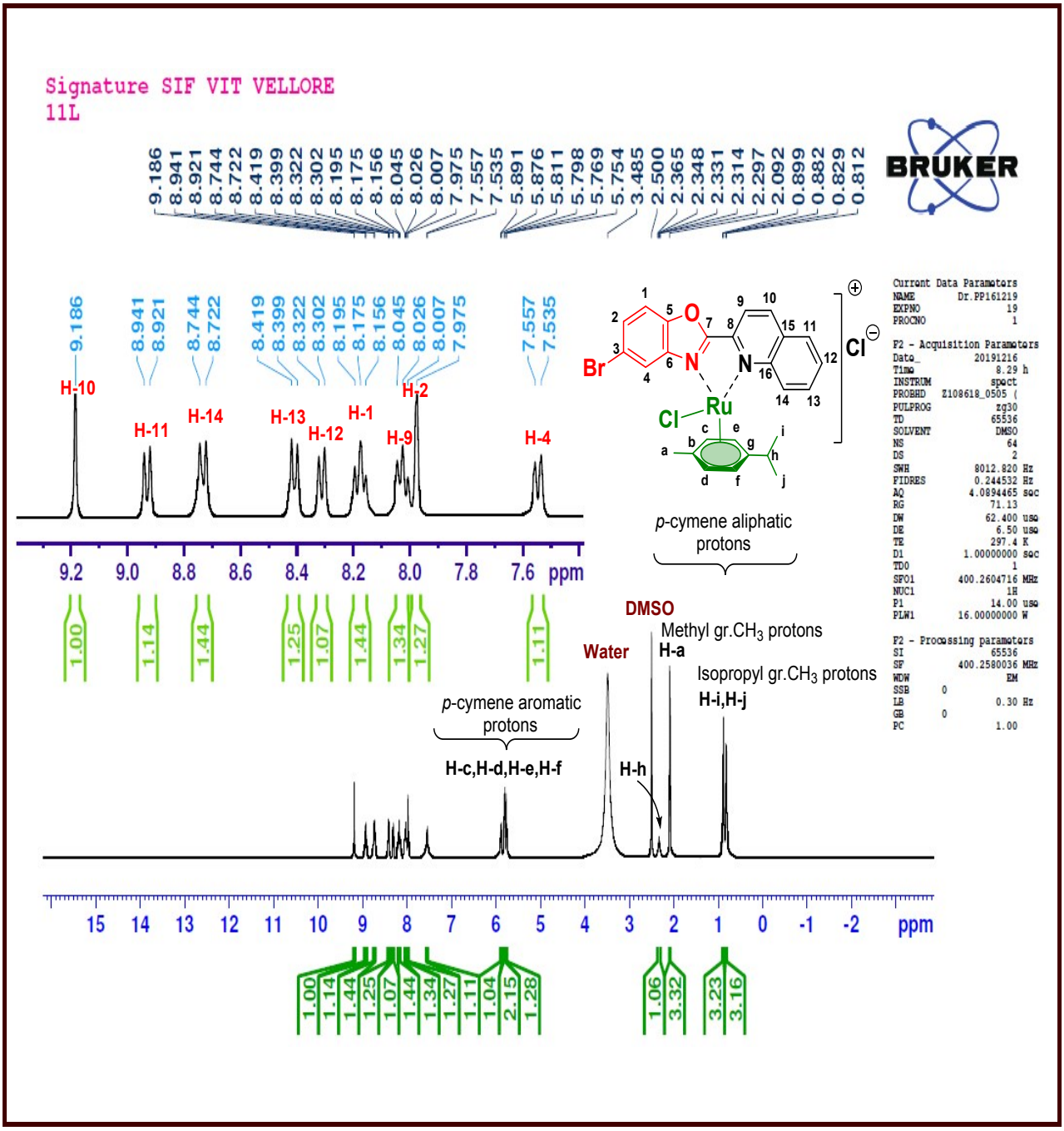
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H-10
H-11
H-14
H-13
H-12
H-1
H-9
H-2
H-4
9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 ppm
1.00 1.14 1.44 1.25 1.07 1.44 1.34 1.27 1.11
p-cymene aliphatic protons
DMSO
Methyl gr.CH3 protons
H-a
Water
Isopropyl gr.CH3 protons
H-i,H-j
p-cymene aromatic protons
H-c,H-d,H-e,H-f
H-h
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.00 1.14 1.44 1.25 1.07 1.44 1.34 1.27 1.11 1.04 2.15 1.28
1.06 3.32
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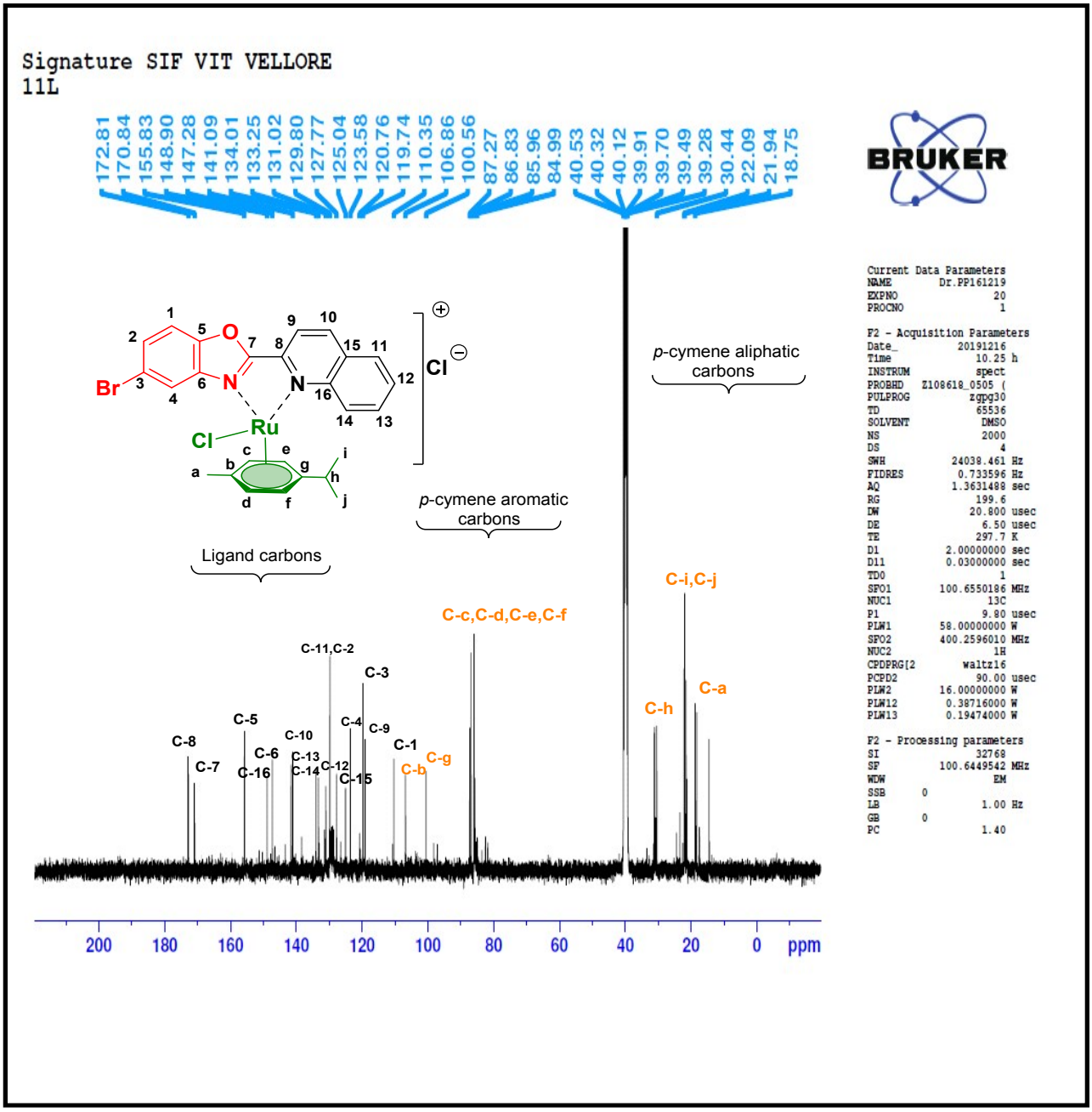
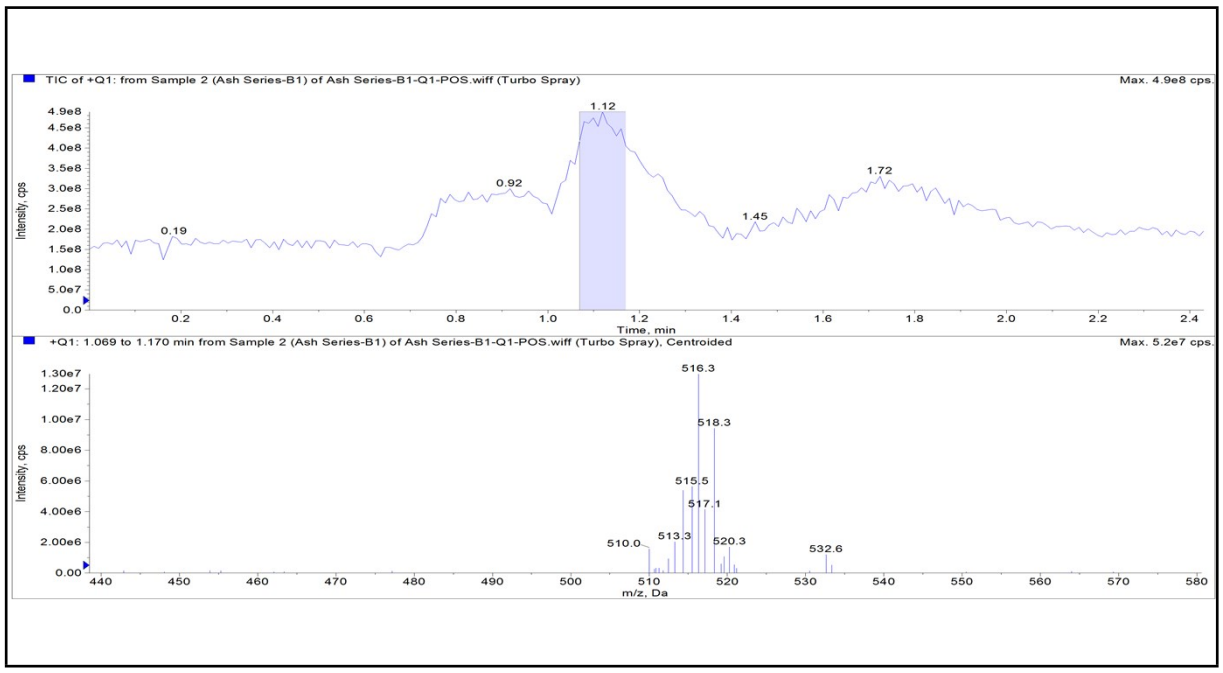
11n

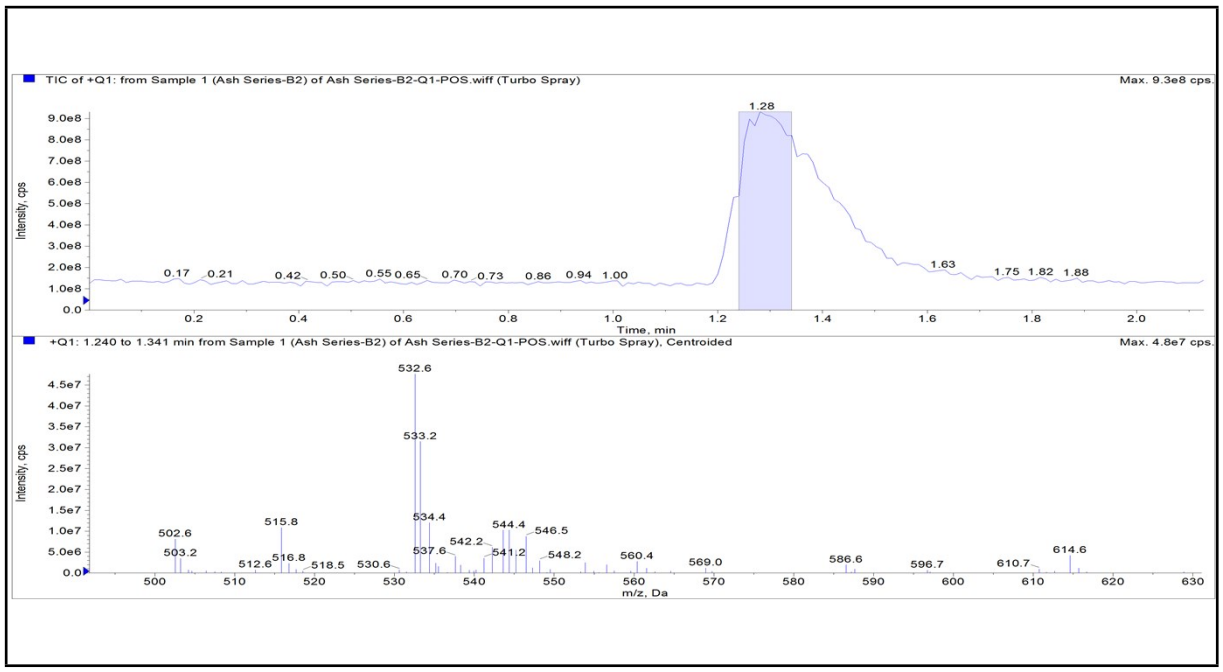


TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 516.08 [M+]



ESI-MS spectra of complex 11a

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 544.11 [M⁺]



ESI-MS spectra of complex 11i

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 584.0 [M⁺]

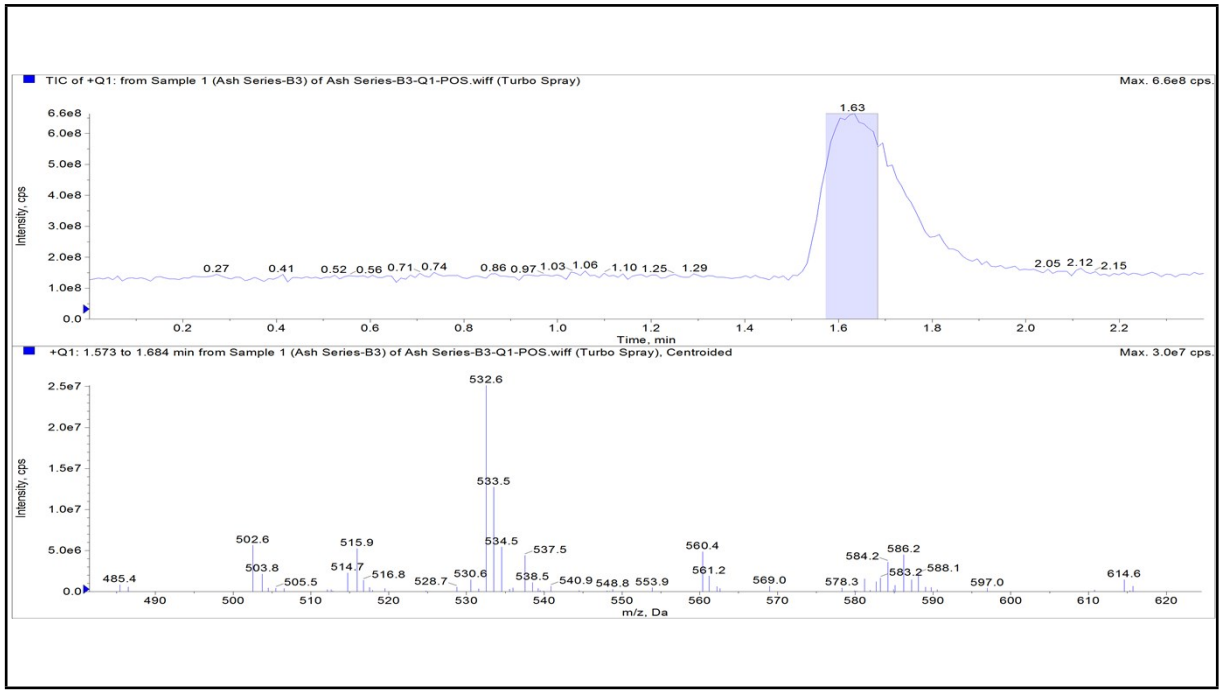
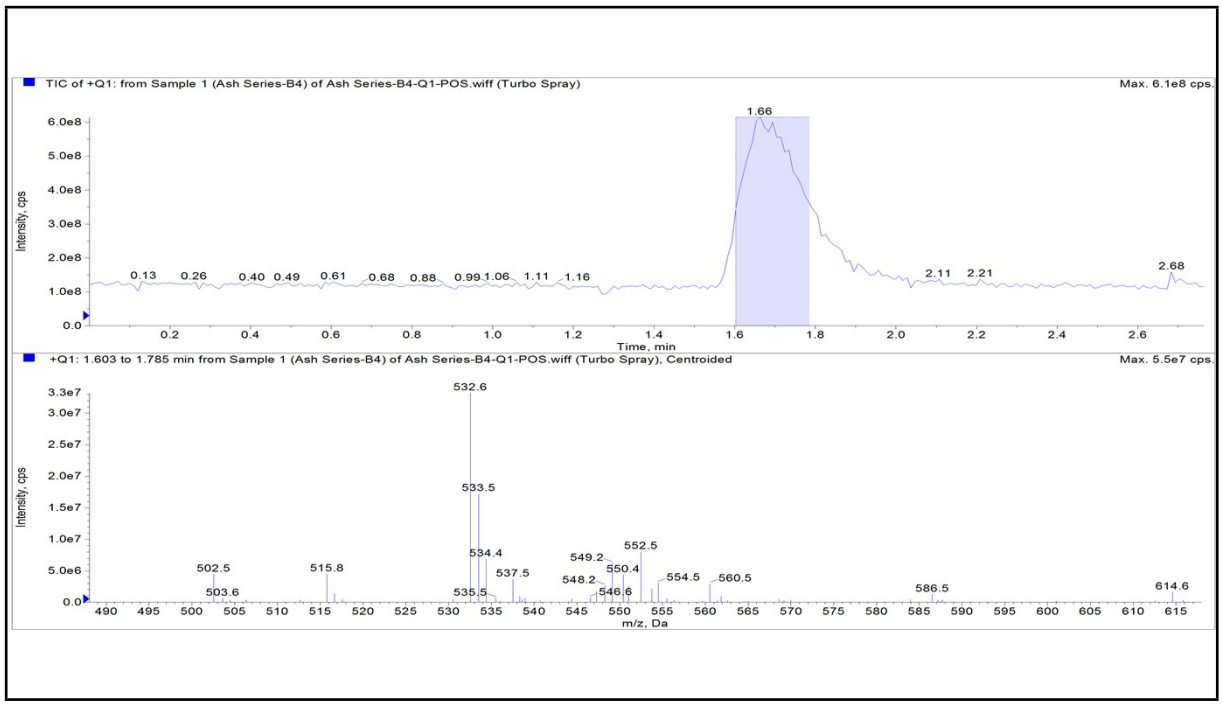


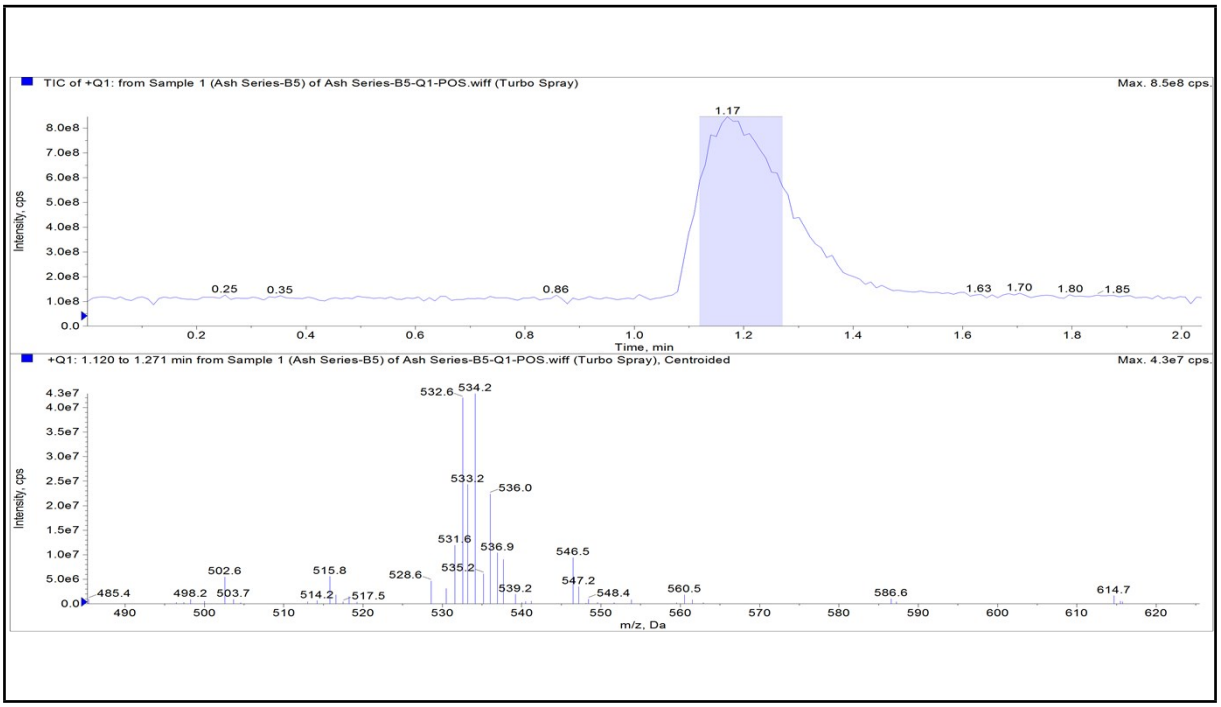
Figure S98- LC-MS spectra of complex 11j

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 550.0 [M+]



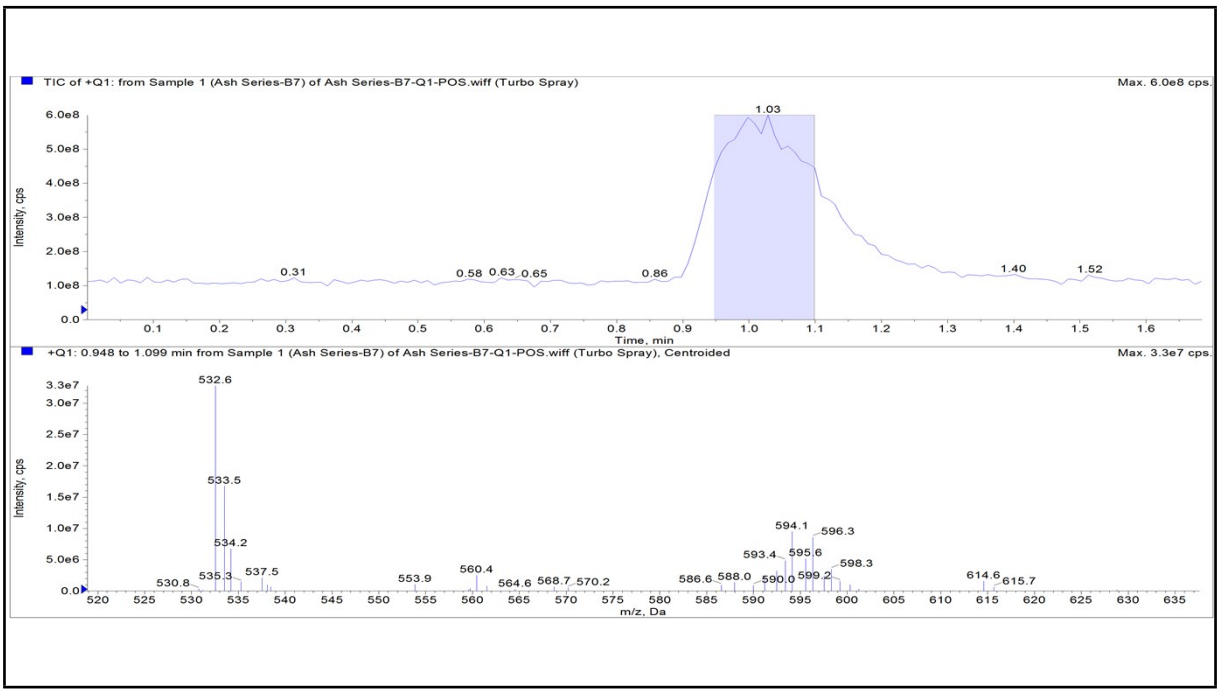
ESI-MS spectra of complex 11b

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 534.10 [M+]



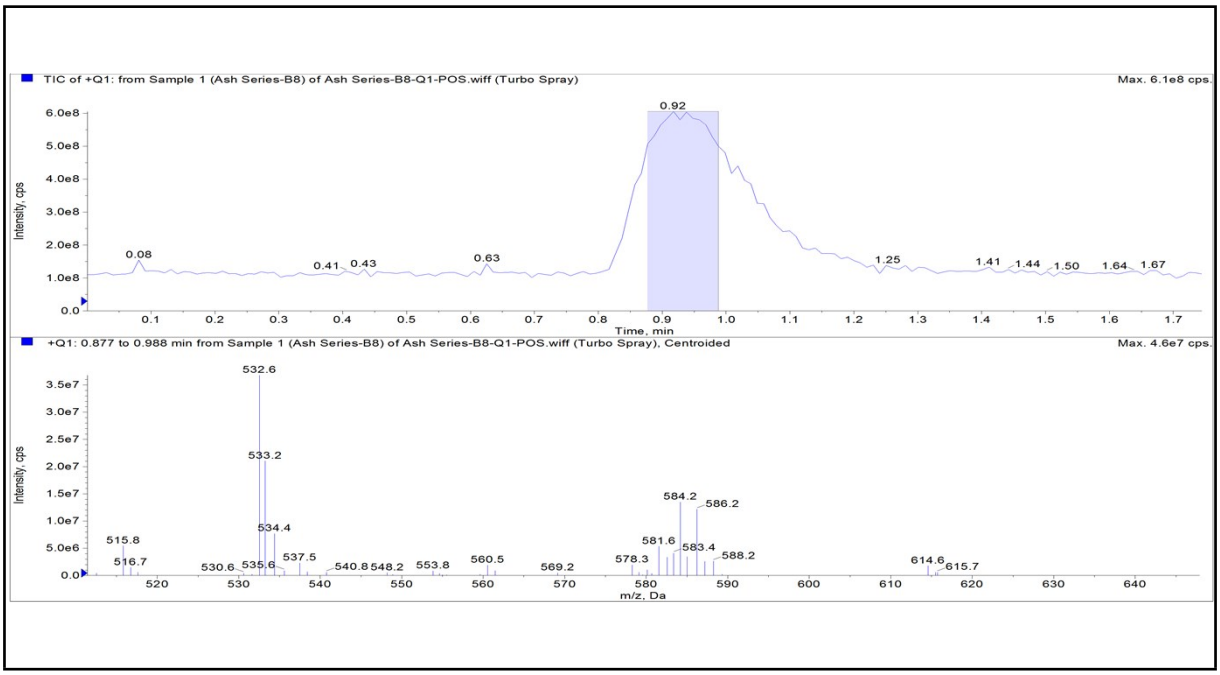
ESI-MS spectra of complex 11k

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 593.99 [M+]



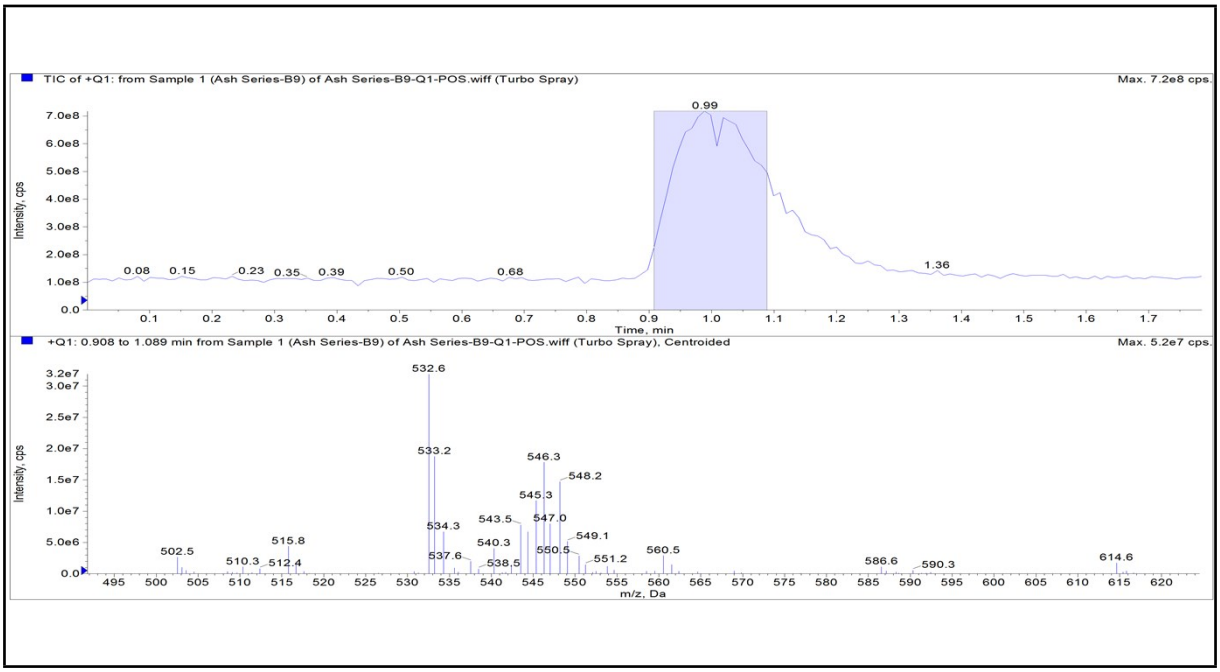
ESI-MS spectra of complex 11l

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 584.06 [M+]



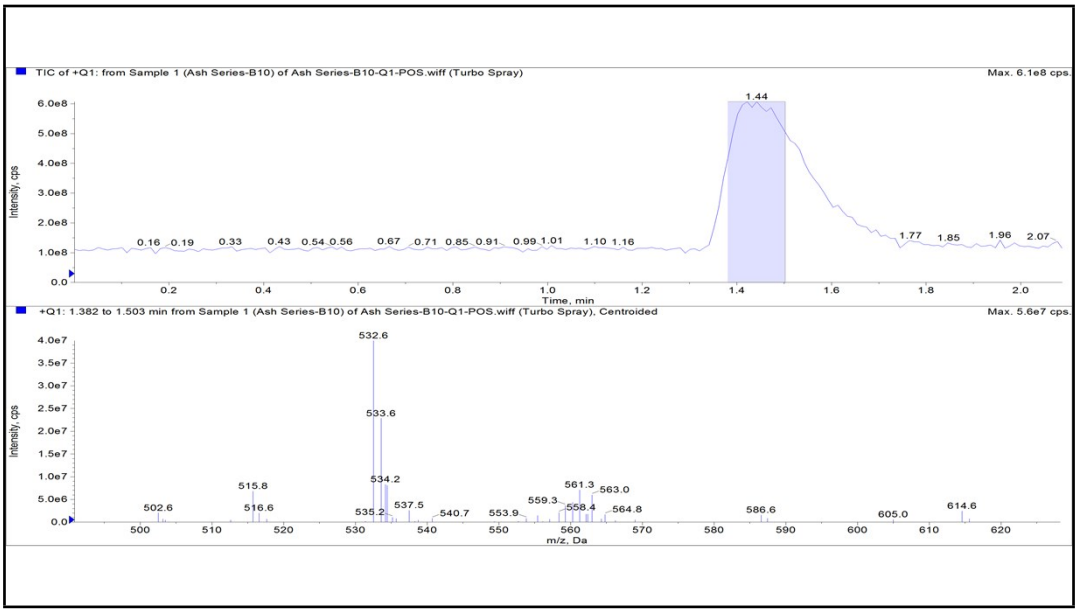
ESI-MS spectra of complex 11d

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 546.09 [M+]



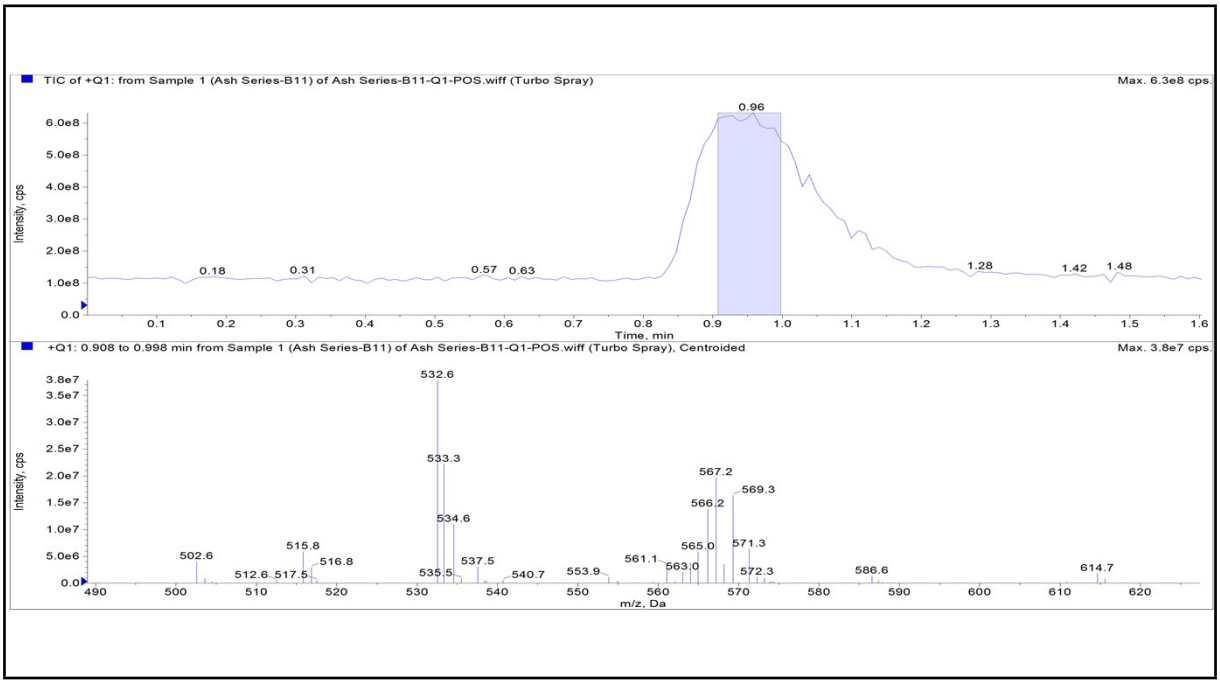
ESI-MS spectra of complex 11e

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 561.06 [M+]



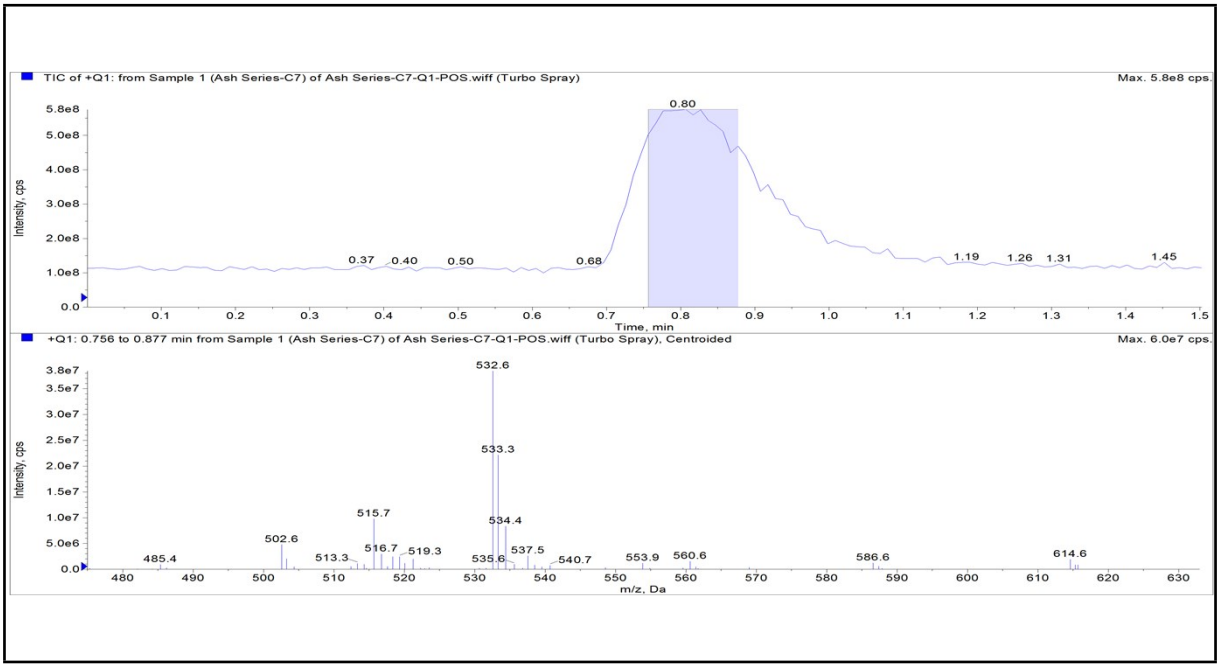
ESI-MS spectra of complex 11f

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 567.00 [M+]



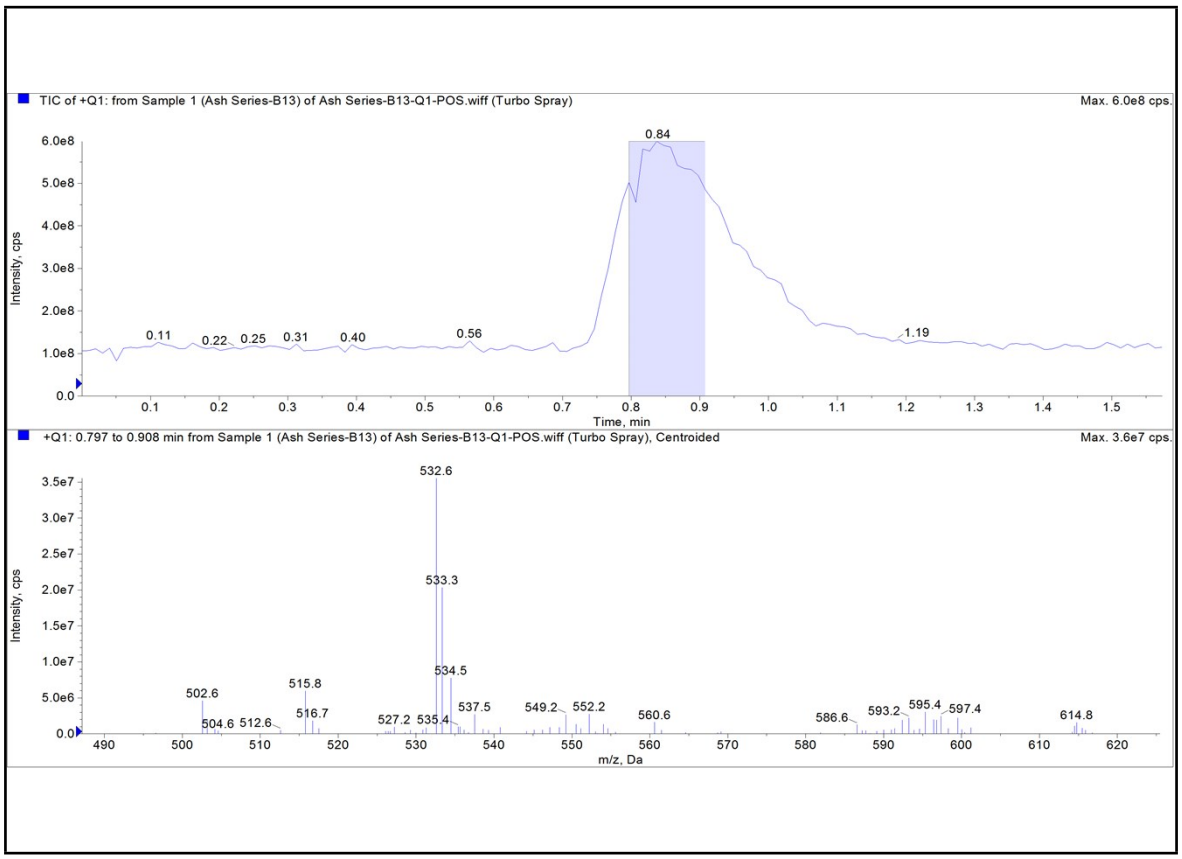
ESI-MS spectra of complex 11h

TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 517.06 [M+]



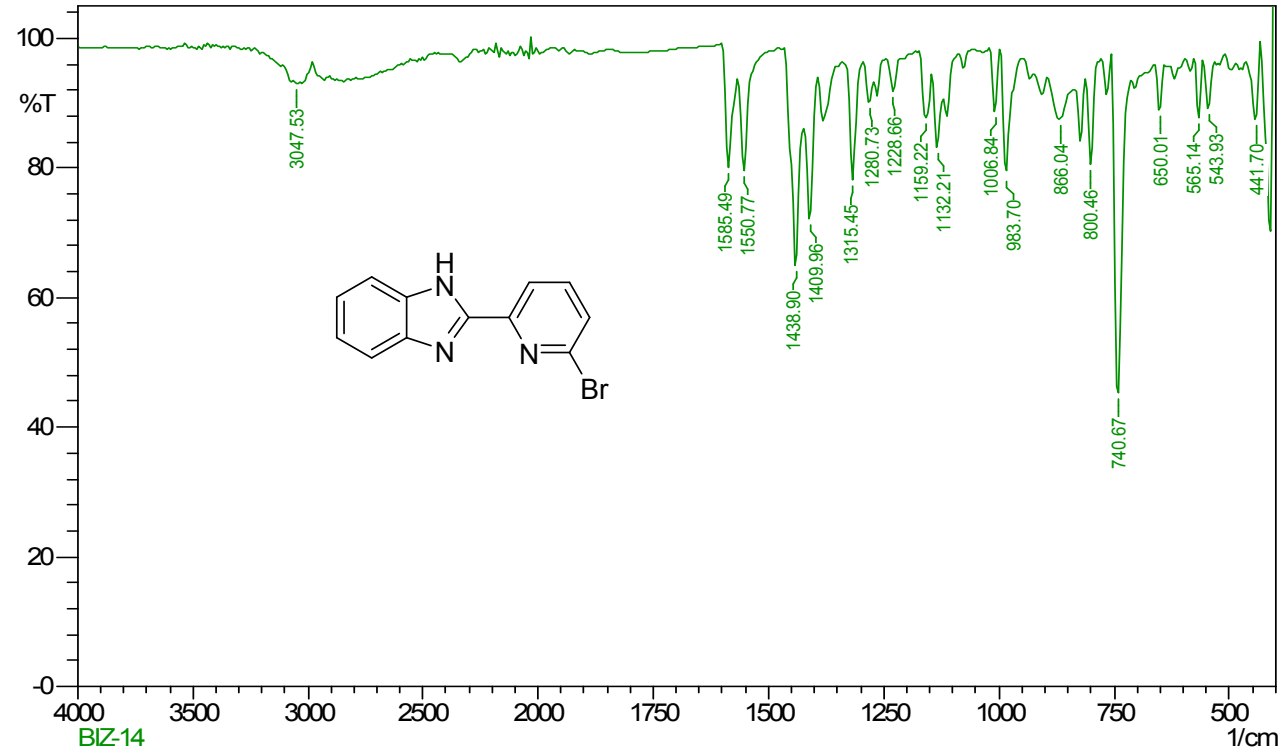
ESI-MS spectra of complex 11m

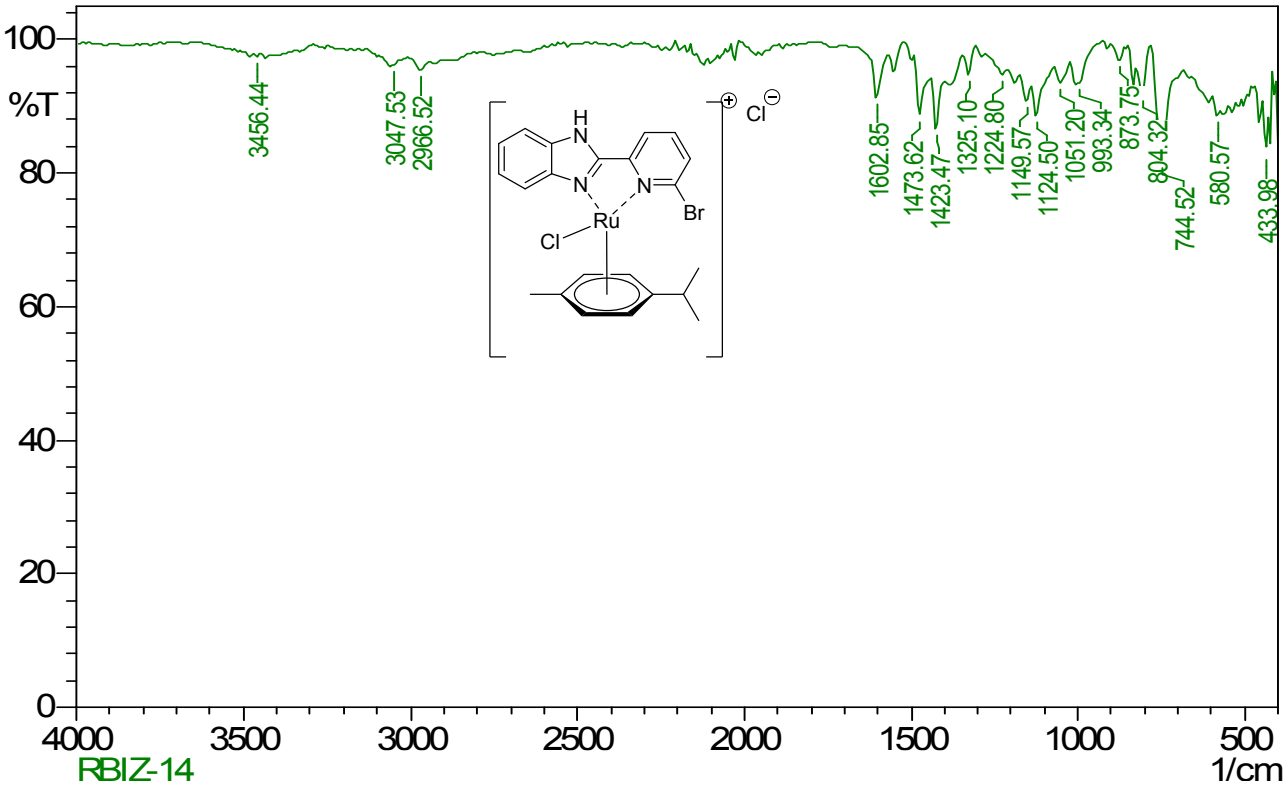
TOTAL ION CHROMATOGRAM AND MOLECULAR ION (Q1) FOR 594.97 [M$^+$]



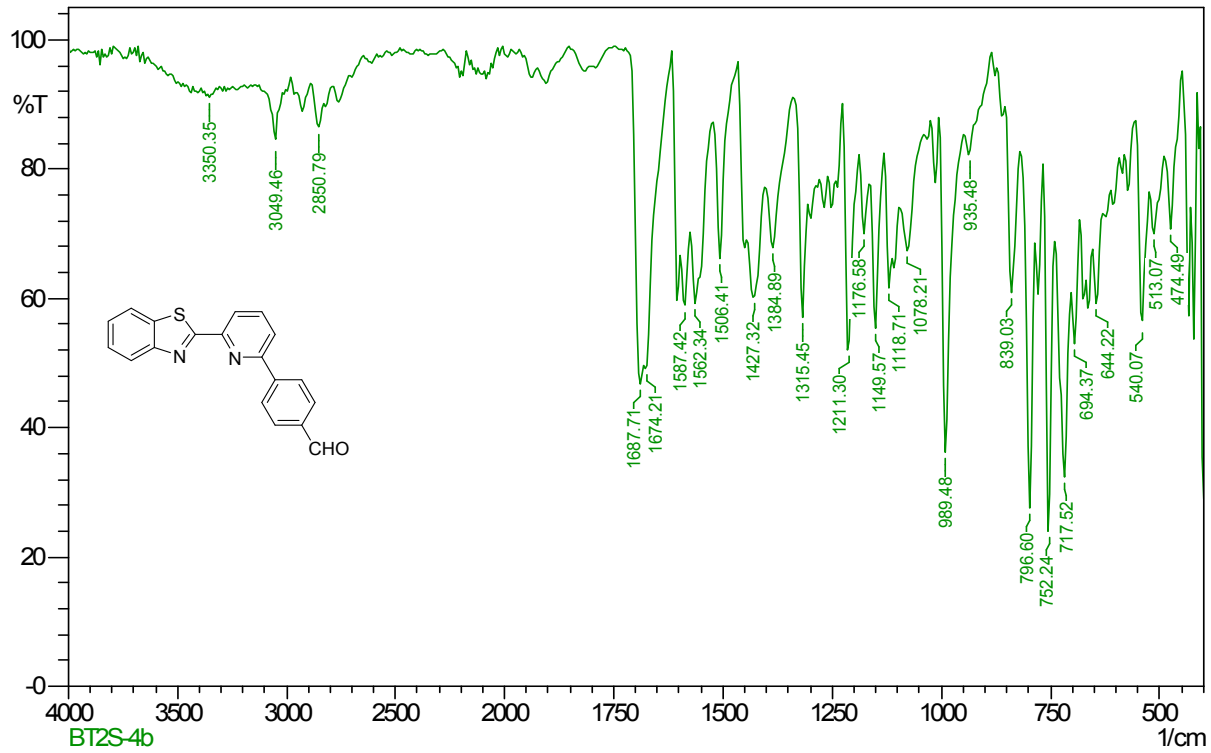
ESI-MS spectra of complex 11n

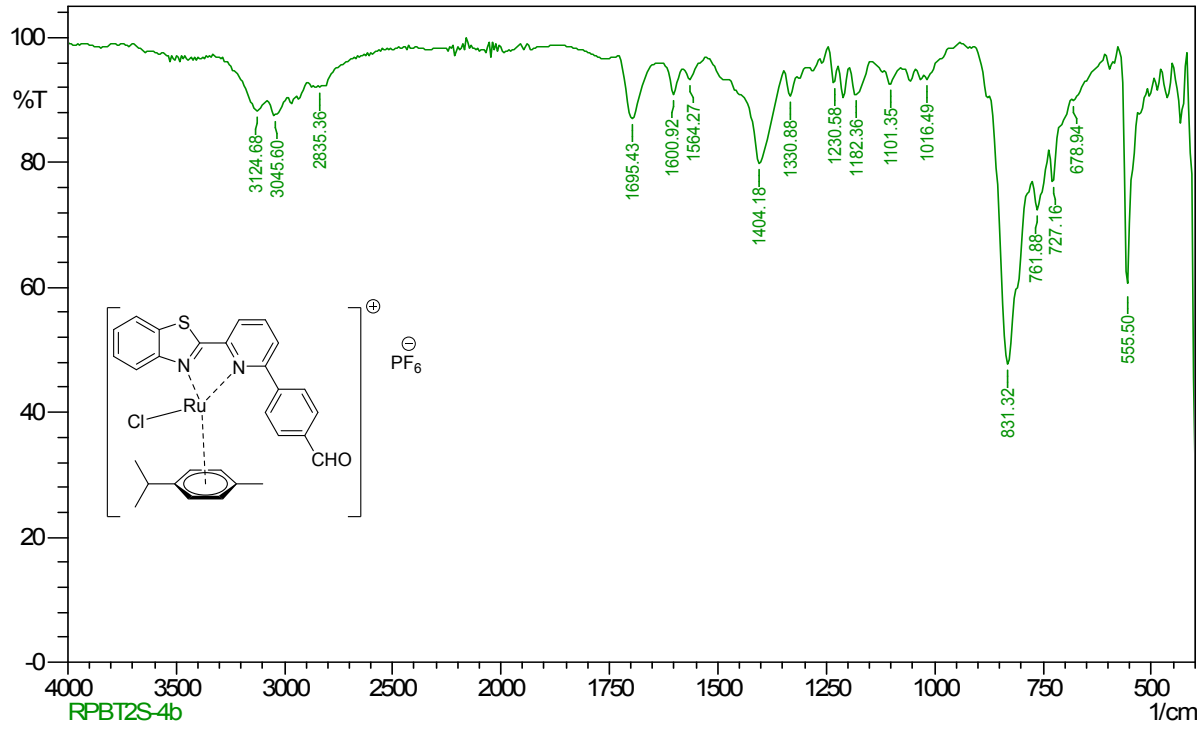
Confirmation of Complex Formation by IR Spectroscopy



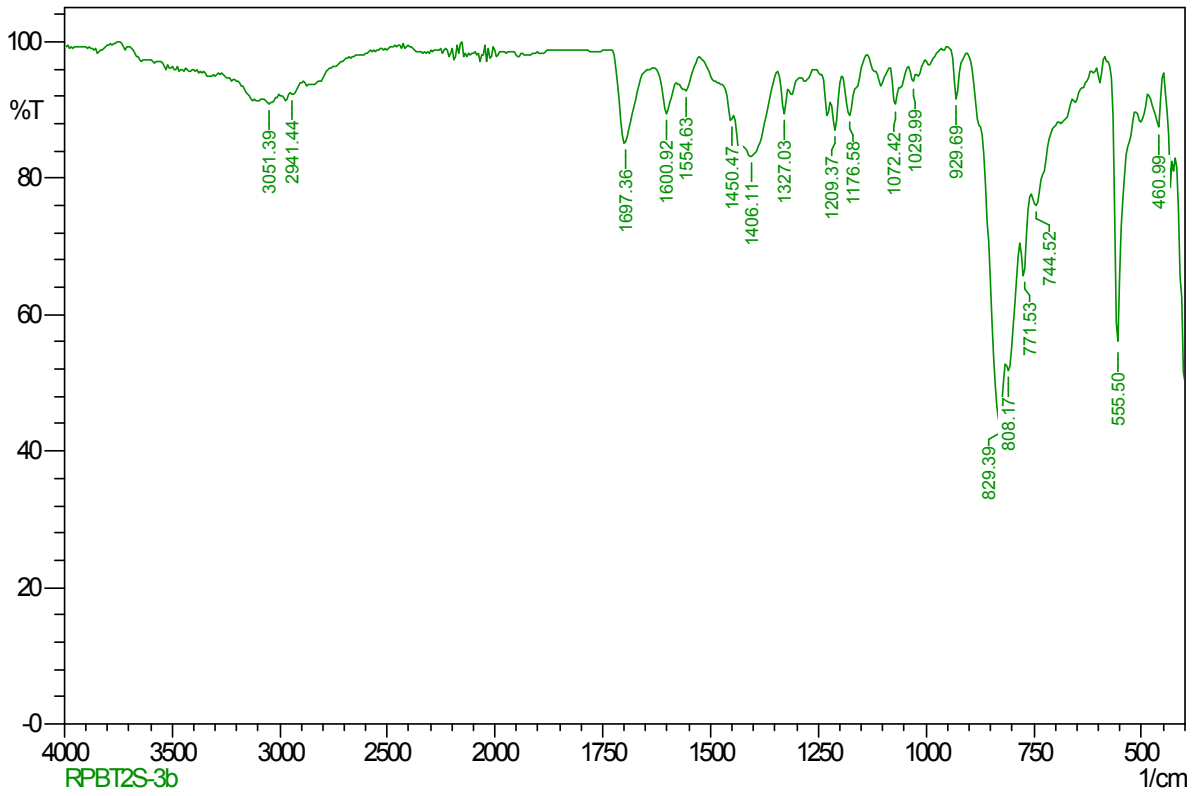


IR Spectra of ligand 3a (above) and complex 5a (below)

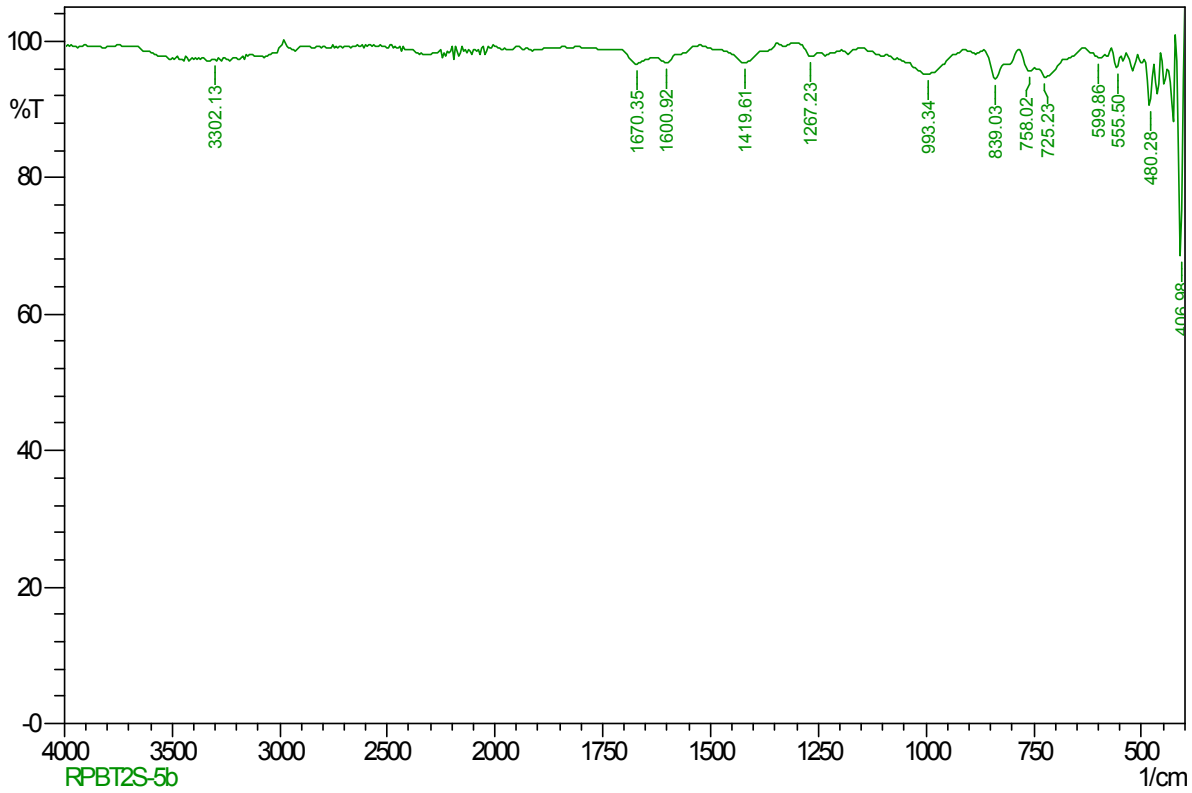




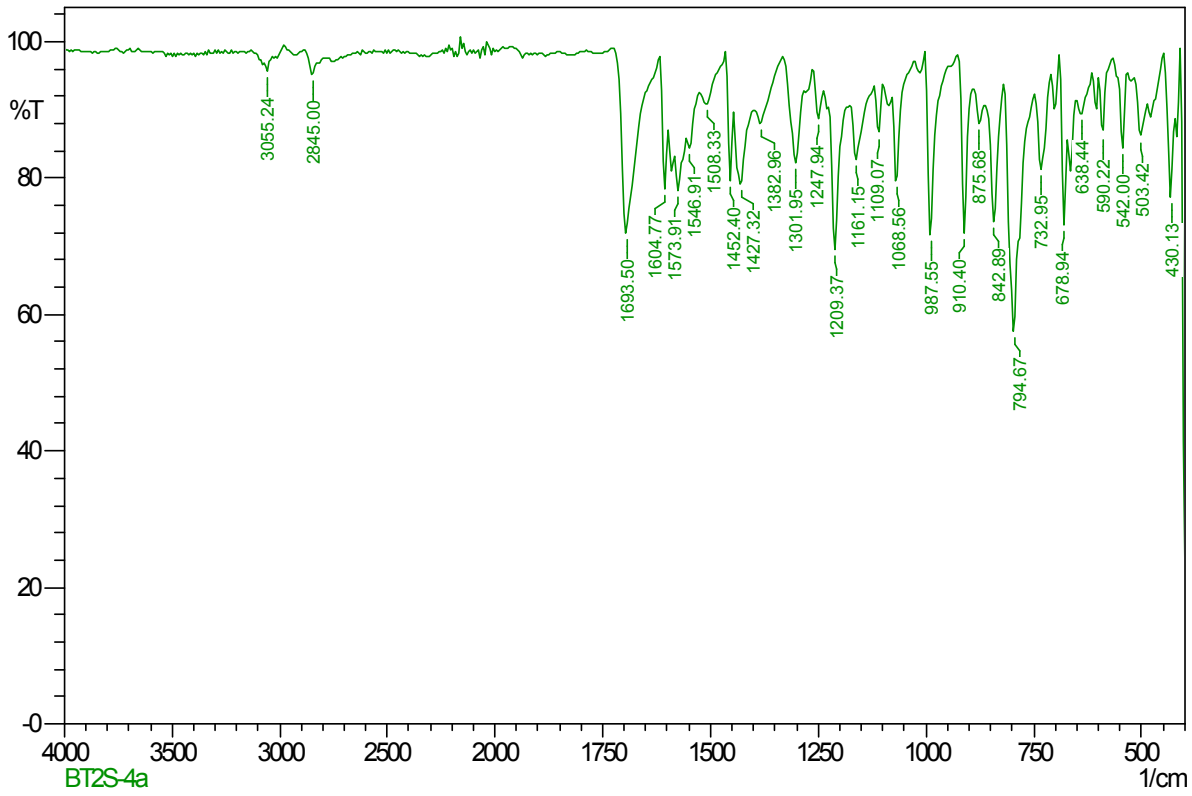
IR Spectra of ligand 7g2 (above) and complex 8g2 (below)

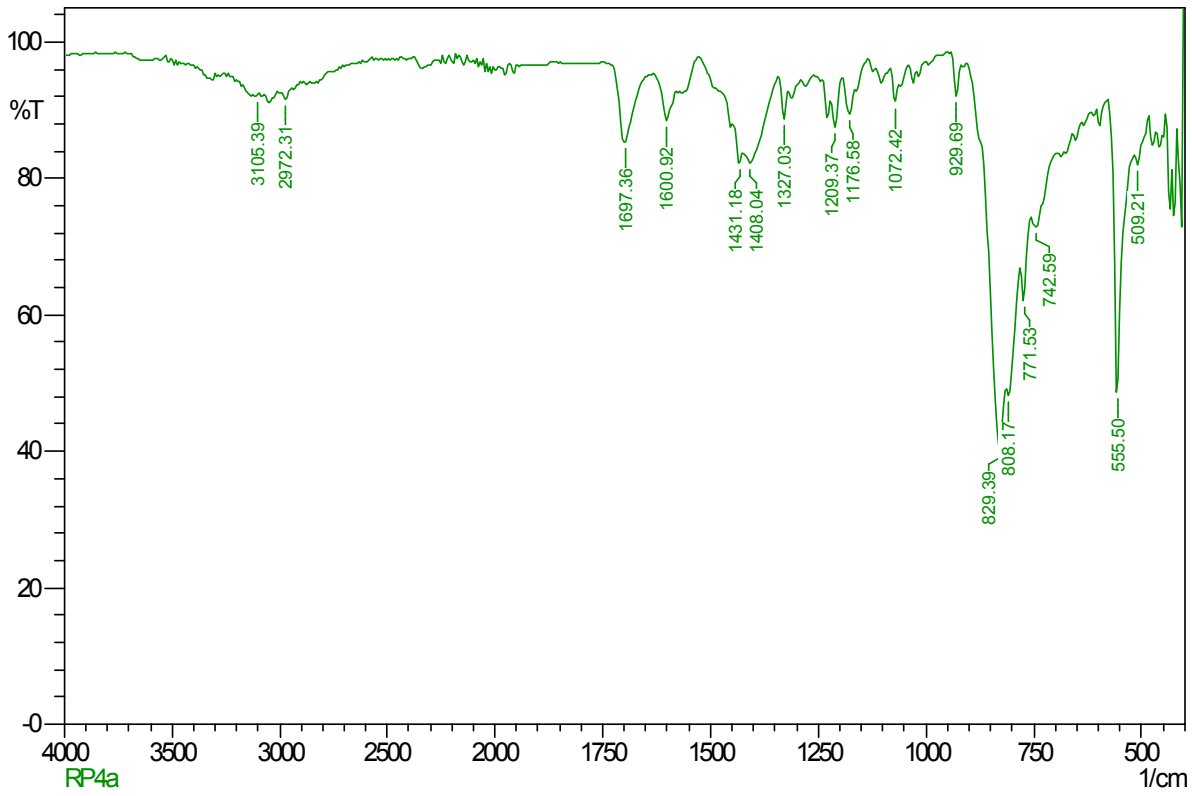


IR Spectra of complex 8g1

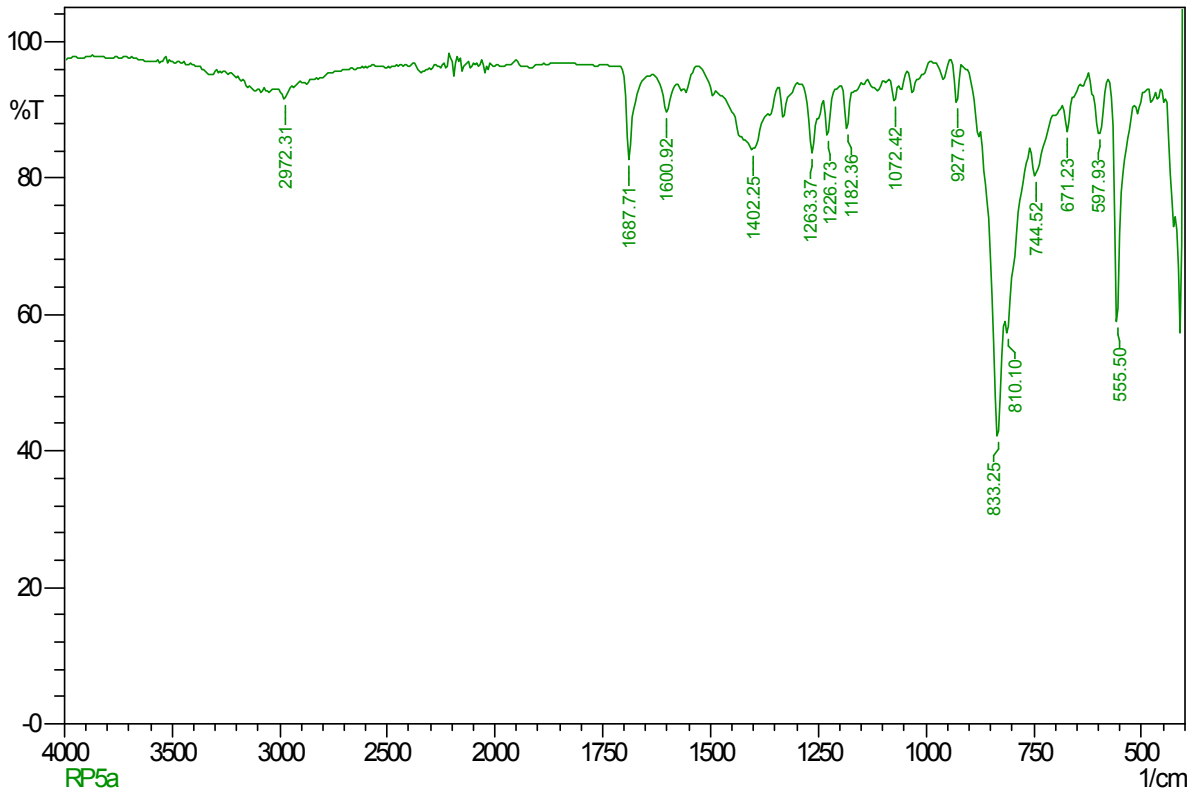


IR Spectra of complex 8g3

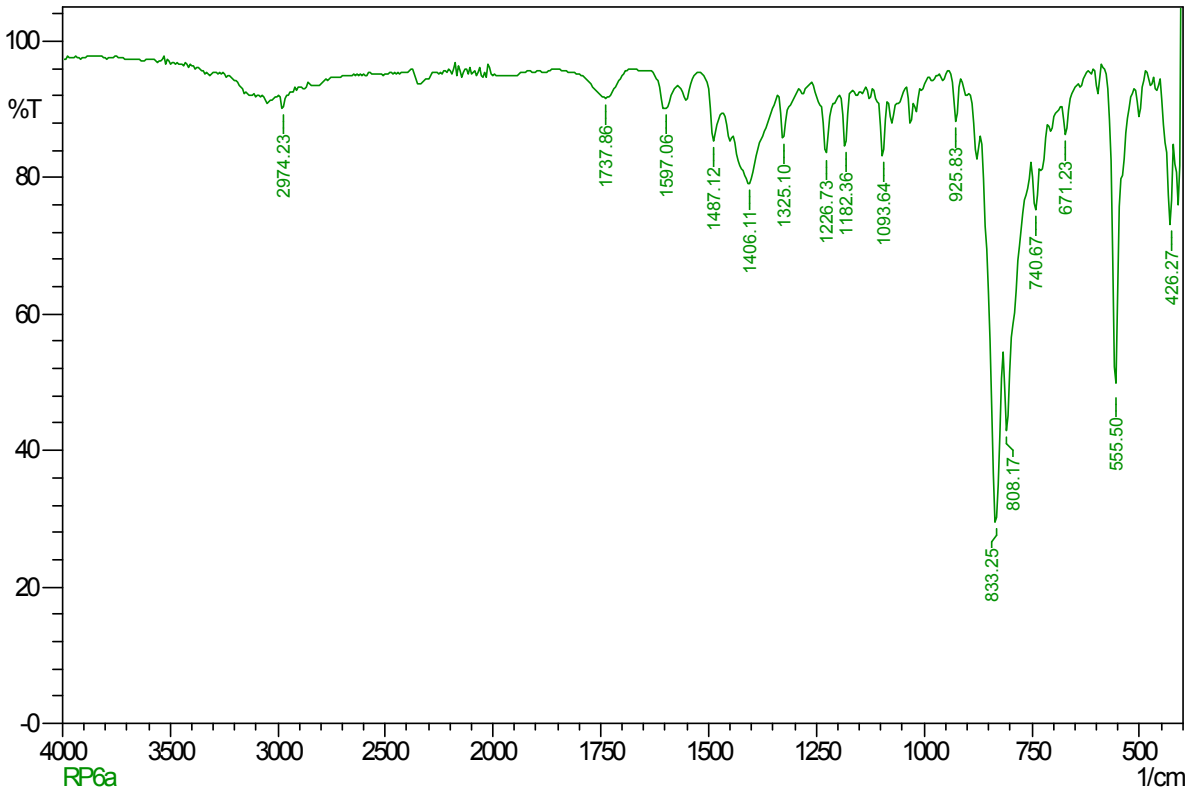




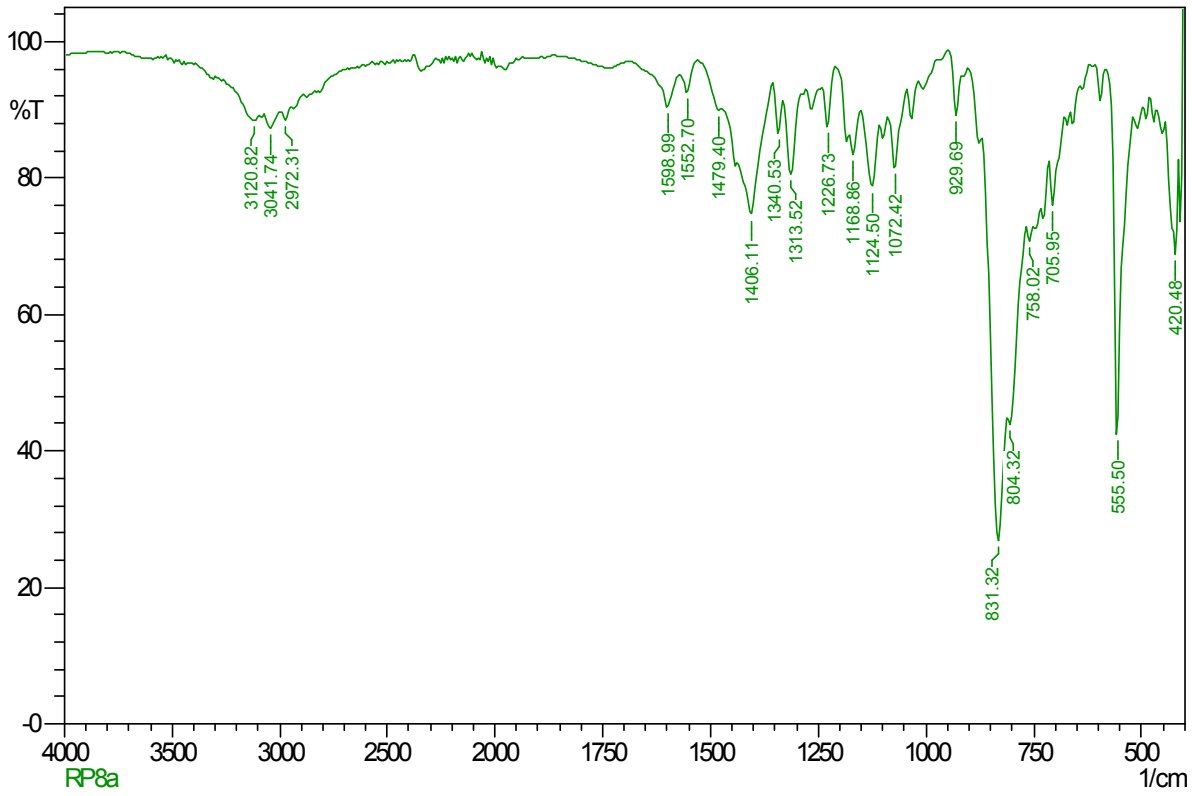
IR Spectra of ligand 7I2 (above) and complex 8I2 (below)



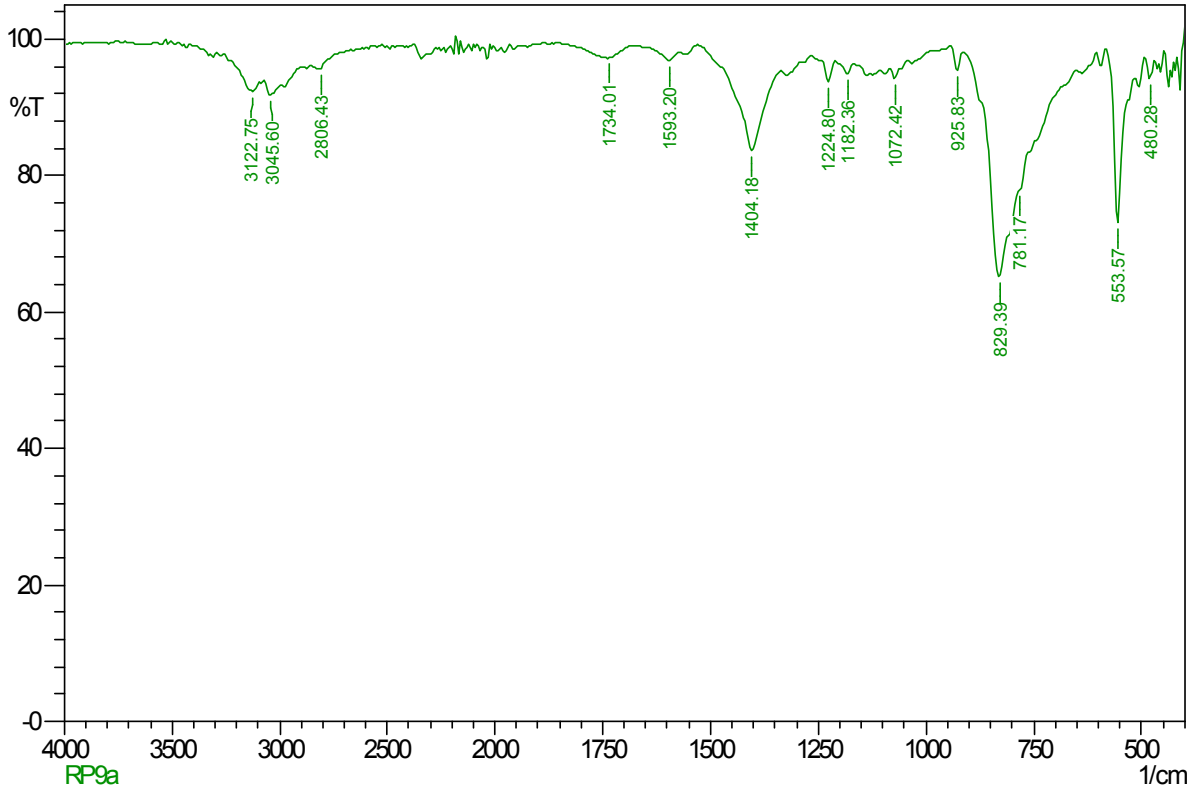
IR Spectra of complex 8I3



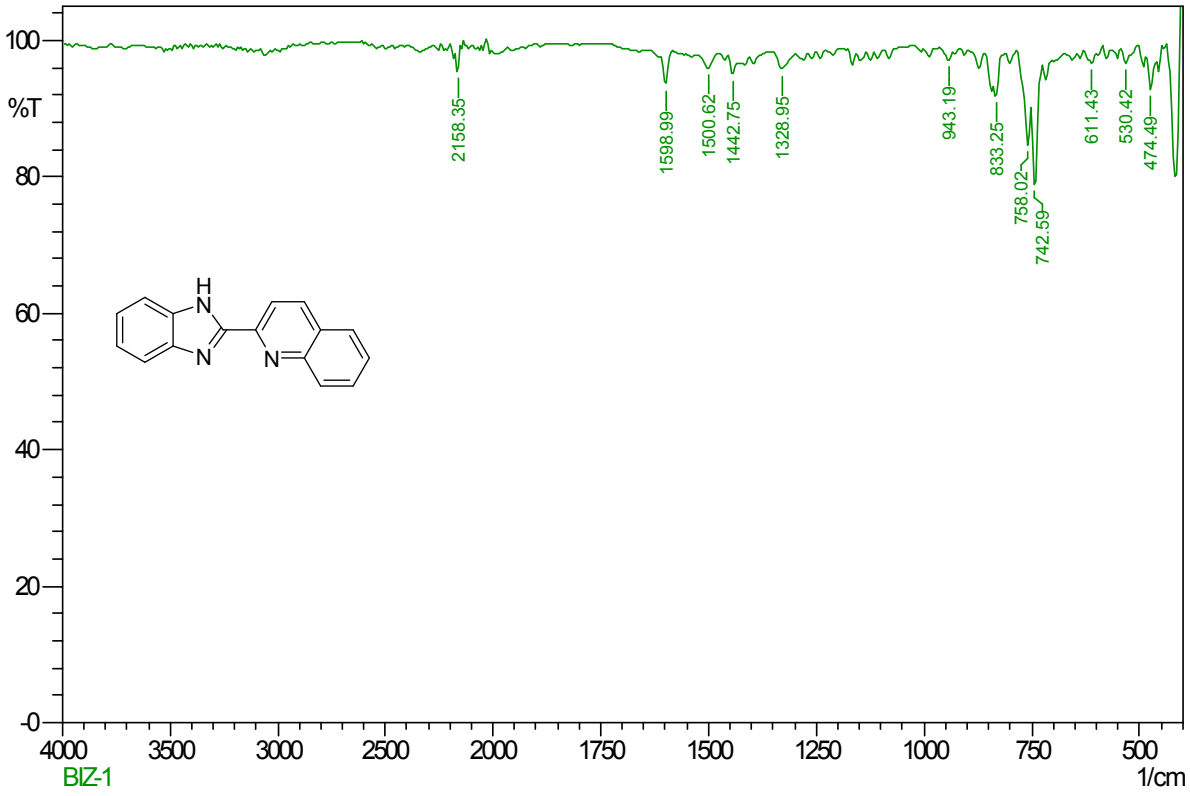
IR Spectra of complex 8I4

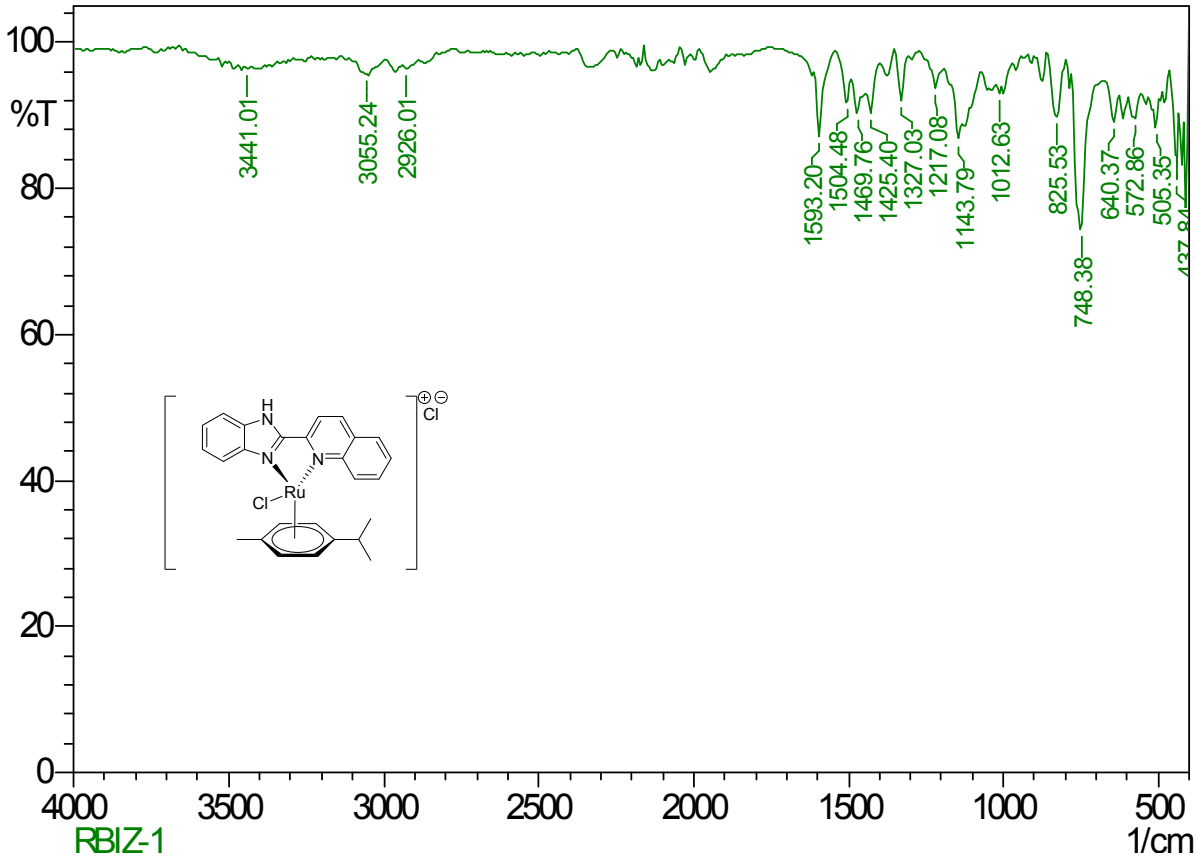


IR Spectra of complex 8I6

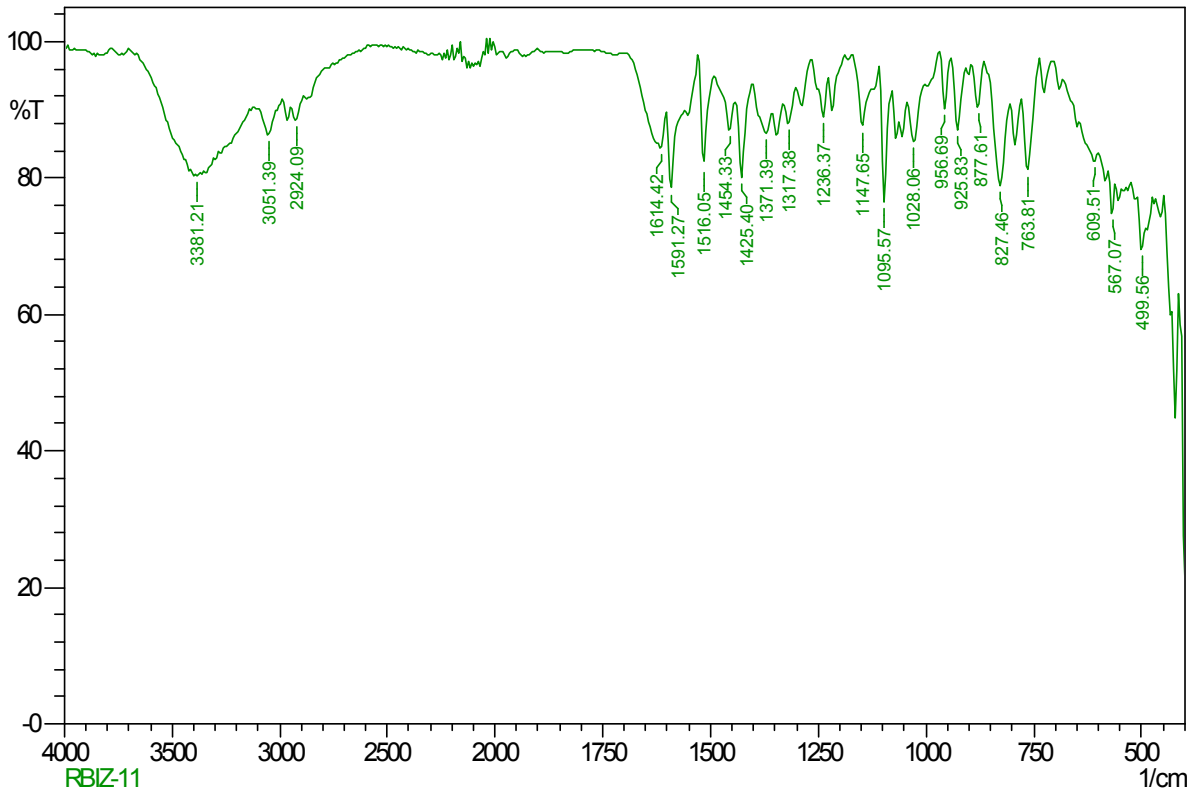


IR Spectra of complex 8I7





IR Spectra of ligand 10a (above) and complex 11a (below)



IR Spectra of complex 11l

Single crystal X-ray data

Table S3. Crystal data and structure refinement for7l1.

Identification code	shelx	
Empirical formula	C18 H11 Cl N2 S	
Formula weight	322.80	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.565(3) Å	a= 90°.
	b = 11.256(3) Å	b= 100.628(11)°.
	c = 11.423(3) Å	g = 90°.
Volume	1461.5(6) $Å^3$	
Z	4	
Density (calculated)	1.467 Mg/m^3	
Absorption coefficient	0.400 mm^{-1}	
F(000)	664	
Crystal size	0.150 x 0.120 x 0.100 mm^3	
Theta range for data collection	2.547 to 33.814°.	
Index ranges	-17<=h<=17, -17<=k<=17, -17<=l<=17	
Reflections collected	42615	
Independent reflections	5814 [R(int) = 0.0772]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7466 and 0.6349	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5814 / 0 / 199	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0441, wR2 = 0.0946	
R indices (all data)	R1 = 0.1269, wR2 = 0.1324	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.229 and -0.247 $e.Å^{-3}$	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rpbtz. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4925(2)	2398(2)	5073(2)	39(1)
C(2)	4082(2)	1743(2)	5531(2)	42(1)
C(3)	3504(2)	856(2)	4840(2)	43(1)
C(4)	3734(2)	577(2)	3713(2)	47(1)
C(5)	4573(2)	1215(2)	3266(2)	46(1)
C(6)	5162(2)	2127(2)	3941(2)	40(1)
C(7)	6229(2)	3802(2)	4974(2)	40(1)
C(8)	6978(2)	4849(2)	5304(2)	41(1)
C(9)	6918(2)	5477(2)	6337(2)	48(1)
C(10)	7644(2)	6443(2)	6599(2)	53(1)
C(11)	8403(2)	6738(2)	5850(2)	51(1)
C(12)	8433(2)	6063(2)	4835(2)	42(1)
C(13)	9282(2)	6298(2)	4032(2)	43(1)
C(14)	10031(2)	7278(2)	4184(2)	59(1)
C(15)	10853(2)	7445(2)	3459(2)	65(1)
C(16)	10951(2)	6659(2)	2575(2)	58(1)
C(17)	10208(2)	5693(2)	2406(2)	59(1)
C(18)	9388(2)	5515(2)	3128(2)	51(1)
N(1)	5543(1)	3350(1)	5641(1)	43(1)
N(2)	7708(1)	5126(1)	4561(1)	42(1)
S(1)	6212(1)	3106(1)	3602(1)	46(1)
Cl(1)	2413(1)	57(1)	5367(1)	63(1)

Table S5. Bond lengths [Å] and angles [°] for 7l1.

C(1)-N(1)	1.382(2)
C(1)-C(2)	1.399(2)
C(1)-C(6)	1.403(2)
C(2)-C(3)	1.368(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.398(3)
C(3)-Cl(1)	1.7435(19)
C(4)-C(5)	1.379(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.385(3)
C(5)-H(5)	0.9300
C(6)-S(1)	1.7359(18)
C(7)-N(1)	1.300(2)
C(7)-C(8)	1.470(3)
C(7)-S(1)	1.7487(18)
C(8)-N(2)	1.340(2)
C(8)-C(9)	1.388(3)
C(9)-C(10)	1.373(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.374(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.392(3)
C(11)-H(11)	0.9300
C(12)-N(2)	1.348(2)
C(12)-C(13)	1.486(3)
C(13)-C(18)	1.380(3)
C(13)-C(14)	1.394(3)
C(14)-C(15)	1.383(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.363(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.377(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.382(3)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
N(1)-C(1)-C(2)	124.66(16)

N(1)-C(1)-C(6)	115.40(15)
C(2)-C(1)-C(6)	119.90(17)
C(3)-C(2)-C(1)	117.98(16)
C(3)-C(2)-H(2)	121.0
C(1)-C(2)-H(2)	121.0
C(2)-C(3)-C(4)	122.62(17)
C(2)-C(3)-Cl(1)	119.02(14)
C(4)-C(3)-Cl(1)	118.35(15)
C(5)-C(4)-C(3)	119.41(18)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	119.16(17)
C(4)-C(5)-H(5)	120.4
C(6)-C(5)-H(5)	120.4
C(5)-C(6)-C(1)	120.93(16)
C(5)-C(6)-S(1)	129.72(14)
C(1)-C(6)-S(1)	109.33(13)
N(1)-C(7)-C(8)	123.88(16)
N(1)-C(7)-S(1)	116.27(14)
C(8)-C(7)-S(1)	119.83(13)
N(2)-C(8)-C(9)	123.81(18)
N(2)-C(8)-C(7)	115.74(16)
C(9)-C(8)-C(7)	120.45(17)
C(10)-C(9)-C(8)	117.63(19)
C(10)-C(9)-H(9)	121.2
C(8)-C(9)-H(9)	121.2
C(9)-C(10)-C(11)	119.4(2)
C(9)-C(10)-H(10)	120.3
C(11)-C(10)-H(10)	120.3
C(10)-C(11)-C(12)	120.23(19)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
N(2)-C(12)-C(11)	120.67(18)
N(2)-C(12)-C(13)	116.70(17)
C(11)-C(12)-C(13)	122.59(17)
C(18)-C(13)-C(14)	117.35(19)
C(18)-C(13)-C(12)	120.58(17)
C(14)-C(13)-C(12)	122.02(19)
C(15)-C(14)-C(13)	120.9(2)
C(15)-C(14)-H(14)	119.5

C(13)-C(14)-H(14)	119.5
C(16)-C(15)-C(14)	121.0(2)
C(16)-C(15)-H(15)	119.5
C(14)-C(15)-H(15)	119.5
C(15)-C(16)-C(17)	118.8(2)
C(15)-C(16)-H(16)	120.6
C(17)-C(16)-H(16)	120.6
C(16)-C(17)-C(18)	120.7(2)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(13)-C(18)-C(17)	121.3(2)
C(13)-C(18)-H(18)	119.4
C(17)-C(18)-H(18)	119.4
C(7)-N(1)-C(1)	110.29(15)
C(8)-N(2)-C(12)	118.21(16)
C(6)-S(1)-C(7)	88.68(9)

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters ($Å^2 x\ 10^3$)forrpbtz. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(1)	44(1)	33(1)	3(1)	9(1)	3(1)
C(2)	46(1)	51(1)	32(1)	3(1)	13(1)	-2(1)
C(3)	43(1)	45(1)	42(1)	6(1)	13(1)	-1(1)
C(4)	56(1)	42(1)	44(1)	-4(1)	12(1)	-2(1)
C(5)	57(1)	47(1)	40(1)	-3(1)	20(1)	2(1)
C(6)	43(1)	42(1)	36(1)	3(1)	15(1)	4(1)
C(7)	40(1)	43(1)	38(1)	3(1)	9(1)	4(1)
C(8)	37(1)	42(1)	42(1)	6(1)	6(1)	5(1)
C(9)	45(1)	53(1)	48(1)	-1(1)	10(1)	5(1)
C(10)	52(1)	54(1)	53(1)	-11(1)	7(1)	5(1)
C(11)	45(1)	45(1)	60(1)	-5(1)	5(1)	-1(1)
C(12)	37(1)	37(1)	48(1)	2(1)	2(1)	4(1)
C(13)	37(1)	40(1)	50(1)	6(1)	3(1)	4(1)
C(14)	62(1)	50(1)	65(1)	-1(1)	13(1)	-10(1)
C(15)	59(1)	58(1)	78(2)	9(1)	13(1)	-17(1)
C(16)	46(1)	63(1)	68(1)	15(1)	15(1)	-1(1)
C(17)	54(1)	59(1)	68(1)	-1(1)	21(1)	1(1)
C(18)	44(1)	47(1)	65(1)	-1(1)	14(1)	-4(1)
N(1)	45(1)	51(1)	36(1)	-1(1)	11(1)	-4(1)
N(2)	41(1)	40(1)	44(1)	3(1)	7(1)	1(1)
S(1)	53(1)	47(1)	42(1)	2(1)	22(1)	-3(1)
Cl(1)	63(1)	69(1)	60(1)	2(1)	23(1)	-21(1)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)for 7l1.

	x	y	z	U(eq)
H(2)	39201905	628251		
H(4)	3325-34	326956		
H(5)	47401036	252056		
H(9)	64045251	683458		
H(10)	76226893	727764		
H(11)	88977391	602261		
H(14)	99787826	478071		
H(15)	113478104	357878		
H(16)	115096774	209570		
H(17)	102585156	179971		
H(18)	88984853	300362		

Table S8. Torsion angles [°] for 7l1.

N(1)-C(1)-C(2)-C(3)	177.05(17)
C(6)-C(1)-C(2)-C(3)	-0.6(3)
C(1)-C(2)-C(3)-C(4)	0.8(3)
C(1)-C(2)-C(3)-Cl(1)	-177.90(14)
C(2)-C(3)-C(4)-C(5)	-0.2(3)
Cl(1)-C(3)-C(4)-C(5)	178.47(15)
C(3)-C(4)-C(5)-C(6)	-0.5(3)
C(4)-C(5)-C(6)-C(1)	0.7(3)
C(4)-C(5)-C(6)-S(1)	-177.65(15)
N(1)-C(1)-C(6)-C(5)	-177.99(17)
C(2)-C(1)-C(6)-C(5)	-0.1(3)
N(1)-C(1)-C(6)-S(1)	0.7(2)
C(2)-C(1)-C(6)-S(1)	178.52(14)
N(1)-C(7)-C(8)-N(2)	174.08(17)
S(1)-C(7)-C(8)-N(2)	-6.9(2)
N(1)-C(7)-C(8)-C(9)	-5.0(3)
S(1)-C(7)-C(8)-C(9)	173.92(14)
N(2)-C(8)-C(9)-C(10)	0.6(3)
C(7)-C(8)-C(9)-C(10)	179.70(17)
C(8)-C(9)-C(10)-C(11)	-0.9(3)
C(9)-C(10)-C(11)-C(12)	0.0(3)
C(10)-C(11)-C(12)-N(2)	1.2(3)
C(10)-C(11)-C(12)-C(13)	-176.38(18)
N(2)-C(12)-C(13)-C(18)	-6.3(3)
C(11)-C(12)-C(13)-C(18)	171.31(18)
N(2)-C(12)-C(13)-C(14)	176.36(18)
C(11)-C(12)-C(13)-C(14)	-6.0(3)
C(18)-C(13)-C(14)-C(15)	-0.6(3)
C(12)-C(13)-C(14)-C(15)	176.8(2)
C(13)-C(14)-C(15)-C(16)	0.2(4)
C(14)-C(15)-C(16)-C(17)	0.5(4)
C(15)-C(16)-C(17)-C(18)	-0.8(3)
C(14)-C(13)-C(18)-C(17)	0.2(3)
C(12)-C(13)-C(18)-C(17)	-177.21(19)
C(16)-C(17)-C(18)-C(13)	0.5(3)
C(8)-C(7)-N(1)-C(1)	178.07(16)
S(1)-C(7)-N(1)-C(1)	-0.9(2)
C(2)-C(1)-N(1)-C(7)	-177.60(17)

C(6)-C(1)-N(1)-C(7)	0.1(2)
C(9)-C(8)-N(2)-C(12)	0.5(3)
C(7)-C(8)-N(2)-C(12)	-178.57(15)
C(11)-C(12)-N(2)-C(8)	-1.4(3)
C(13)-C(12)-N(2)-C(8)	176.27(15)
C(5)-C(6)-S(1)-C(7)	177.57(19)
C(1)-C(6)-S(1)-C(7)	-0.93(14)
N(1)-C(7)-S(1)-C(6)	1.12(15)
C(8)-C(7)-S(1)-C(6)	-177.92(15)

Symmetry transformations used to generate equivalent atoms:

Table S9. Hydrogen bonds for 7l2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5)...N(1)#1	0.93	2.59	3.425(2)	150.5

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z-1/2

Characterization data for some selected ligands (3a, 3l, 10a, and 10l) and complexes (5a-5l and 11a-11n):

2-(6-bromopyridin-2-yl)-1H-benzo[d]imidazole (3a): Yield: 95%; R_f (25% ethylacetate in hexane): 0.23; IR (cm^{-1}): υ 3047, 1585, 1550, 1438, 1409, 1315, 983, 740; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.30-7.33 (m, 3H, ArCH), 7.52 (dd, J_1= 0.8 Hz, J_2= 8.0 Hz 2H, ArCH), 7.69 (t, *J* = 8.0 Hz, 1H, ArCH), 8.37 (dd, J_1= 0.8 Hz, J_2= 7.6, 1H, ArCH), 10.55 (br s, 1H, ArNH); ESI-MS (CH_3OH): m/z 273.99 $[M+H]^+$.``````

[(η^6-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-1H-benzo[d]imidazole}]Cl (5a):
123.41 mg (0.021 mmol, 92%); *Mr* ($C_{22}H_{22}N_3BrCl_2Ru$) = 583.31 g/mol; Anal. Calcd.for $C_{22}H_{22}N_3BrCl_2Ru$ (%): C 45.53, H 3.82, N 7.24. Found: C 45.23, H 3.38, N 6.86; Mp: 224-226°C decomp.; R_f (100% ethyl acetate): 0.28; IR (cm^{-1}): υ 3445, 3047, 2966, 1602, 1473, 1423, 993, 744; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 0.82-0.88 (brm, 6H, *p*-cymCH_3, H-i, H-j), 2.24 (s, 3H, *p*-cymCH_3, H-a), 2.79-2.86 (m, 1H, *p*-cym CH, H-h), 6.05 (d, *J* = 8.0 Hz, 1H, *p*-cym ArCH, H-f), 6.21 (d, *J* = 8.0 Hz, 1H, *p*-cym ArCH, H-e), 6.28 (d, *J* = 5.2 Hz, 1H, *p*-cym ArCH, H-d), 6.46 (d, *J* = 5.6 Hz, 1H, *p*-cym ArCH, H-c), 7.55-7.62 (m, 2H, ArCH, H-2, H-3), 7.83 (d, *J* = 7.2 Hz, 1H, ArCH, H-1), 8.03 (d, *J* = 8.0 Hz, 1H, ArCH, H-4), 8.17 (d, *J* = 6.0 Hz, 2H, ArCH, H-10, H-11), 8.55-8.57 (m, 1H, ArCH, H-9); ^{13}C NMR (100 MHz, DMSO-d^6): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-i, *p*-cymene), 27.3 (Me, C-j, *p*-cymene), 30.5 (CH, C-h, *p*-cymene), 85.3 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.5 (ArCH, C-c, *p*-cymene), 100.7 (ArC, C-g, *p*-cymene), 107.1 (ArC, C-b, *p*-cymene), 123.1 (ArCH, C-4), 124.6 (ArCH, C-1), 126.6 (ArCH, C-3), 127.3 (ArCH, C-2), 129.3 (ArCH, C-9), 131.9 (ArCH, C-11), 134.8 (ArC, C-6), 139.9 (ArC, C-5), 141.7 (ArCH, C-10), 150.7 (ArC, C-7), 155.0 (ArC, C-12), 165.6 (ArC, C-8); ESI-MS (CH_3OH): m/z 543.97 $[M-Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-5-chloro-1H-benzo[d]imidazole}]Cl (5b): 49.5 mg (0.081 mmol, 46 %); *Mr* ($C_{22}H_{22}N_3BrCl_2Ru$) = 614.75 g/mol; Anal. Calcd.for $C_{22}H_{21}N_3BrCl_3Ru$ (%): C 42.98, H 3.44, N 6.84. Found: C 42.71, H 3.67, N 6.69.; Mp: 225-228°C decomp.; R_f (100% ethyl acetate): 0.25; IR (cm^{-1}): υ 3441, 3045, 2963, 1600, 1453, 1413, 990, 742; ^{1}H NMR (400 MHz, DMSO-d^6): δ (ppm) 0.99 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-j), 1.09 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-i), 2.22 (s, 3H, *p*-cym CH_3, H-a), 2.66-2.69 (m, 1H, *p*-cym CH, H-h), 5.26 (brs, 1H, *p*-cym ArH, H-f), 5.53 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.71 (d,1H, *J* = 6.0 Hz, *p*-cym ArCH, H-d), 6.10 (brs, 1H, *p*-cym ArH, H-c), 7.02 (t, 1H, *J* = 7.6 Hz, ArH, H-2), 7.24 (d, *J* = 8.0 Hz, 1H, ArH, H-1), 7.34 (t, 1H, *J* = 8.0 Hz, ArH, H-11), 8.14 (t, 1H, *J* = 7.2 Hz, ArH, H-10), 8.29 (d, *J* = 6.8 Hz, ArH, H -9), 8.96 (s, 1H, ArH, H-4), 10.98 (s, 1H, ArNH); ^{13}C NMR (100 MHz, DMSO-d^6): δ 19.1 (Me, C-a, *p*-cymene), 21.8 (Me, C-j, *p*-cymene), 22.7 (Me, C-i, *p*-cymene), 31.2 (CH, C-h, *p*-cymene), 79.1 (ArCH, C-f, *p*-cymene), 79.4 (ArCH, C-e, *p*-cymene), 79.8 (ArCH, C-d, *p*-cymene), 80.6 (ArCH, C-c, *p*-cymene), 101.2 (ArC, C-g, *p*-cymene), 104.6 (ArC, C-b, *p*-cymene), 117.6 (ArCH, C-1), 119.9 (ArCH, C-4), 121.5 (ArCH, C-2), 125.3 (ArCH, C-9), 129.7 (ArCH, C-11), 130.7 (ArC, C-3), 134.8 (ArC, C-5), 139.6 (ArCH, C-10), 141.9 (ArC, C-6), 147.5 (ArC, C-7), 149.6 (ArC, C-12), 156.4 (ArC, C-8); ESI-MS (CH_3OH): m/z 577.93 $[M-Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-6-chloro-1H-benzo[d]imidazole}]Cl (5b'): 47.4 mg (0.077 mmol, 44 %); *Mr* ($C_{22}H_{22}N_3BrCl_2Ru$) = 614.75 g/mol; Anal. Calcd.for $C_{22}H_{21}N_3BrCl_3Ru$ (%): C 42.98, H 3.44, N 6.84. Found: C 42.69, H 3.71, N 6.63.; Mp: 225-228°C decomp.; R_f (100% ethyl acetate): 0.22; IR (cm^{-1}): υ 3441, 3045, 2963, 1600, 1453, 1413, 990, 742; ^{1}H NMR (400 MHz, DMSO-d^6): δ (ppm) 0.99 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-j), 1.08 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-i), 2.22 (s, 3H, *p*-cym CH_3, H-a), 2.65-2.69 (m, 1H, *p*-cym CH, H-h), 5.26 (brs, 1H, *p*-cym ArH, H-f), 5.53 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.71 (d,1H, *J* =

5.6 Hz, *p*-cym ArH, H-d), 6.09 (brs, 1H, *p*-cym ArH, H-c), 7.02 (t, 1H, J = 7.6 Hz, ArH, H-3), 7.24 (d, 1H, *J* = 8.0 Hz, ArH, H-4), 7.34 (t, 1H, J = 7.6 Hz, ArH, H-11), 8.14 (t, 1H, *J* = 7.2 Hz, ArH, H-10), 8.25 (d, 1H, *J* = 7.6 Hz, H-9), 8.96 (s, 1H, ArH, H-1), 10.88 (s, 1H, ArNH); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 19.2 (Me, C-a, *p*-cymene), 21.8 (Me, C-j, *p*-cymene), 22.8 (Me, C-i, *p*-cymene), 31.2 (CH, C-h, *p*-cymene), 78.5 (ArCH, C-f, *p*-cymene), 79.2 (ArCH, C-e, *p*-cymene), 79.8 (ArCH, C-d, *p*-cymene), 80.9 (ArCH, C-c, *p*-cymene), 101.5 (ArC, C-g, *p*-cymene), 106.1 (ArC, C-b, *p*-cymene), 117.6 (ArCH, C-4), 120.0 (ArCH, C-1), 121.4 (ArCH, C-3), 125.4 (ArCH, C-9), 129.8 (ArCH, C-11), 130.8 (ArC, C-2), 134.9 (ArC, C-6), 139.6 (ArCH, C-10), 142.0 (ArC, C-5), 147.5 (ArC, C-7), 149.7 (ArC, C-12), 156.5 (ArC, C-8); ESI-MS (CH_3OH): m/z 577.93 $[M-Cl]^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-5-chloro-6-fluoro-1H-benzo[d]imidazole}]Cl (5c): 45.30 mg (0.072 mmol, 46%); *Mr* ($C_{22}H_{20}N_3BrCl_3FRu$) = 632.74 g/mol; Anal. Calcd.for $C_{22}H_{20}N_3BrCl_3FRu$ (%):C 41.76, H 3.19, N 6.64. Found: C 41.41, H 3.48, N 6.71; Mp: 226-228°C decomp.; R_f (100% ethyl acetate): 0.20;IR (cm^{-1}): υ 3444, 3051, 2958, 1607, 1454, 1414, 991, 743; ^{1}H NMR (400 MHz, DMSO-*d*^{6}): δ (ppm) = 1.18 (d, 6H, *J* = 6.8 Hz, *p*-cym CH_3, Hi, Hj), 2.08 (s, 3H, *p*-cymCH_3, Ha), 2.79-2.87 (m, 1H, *p*-cymCH, Hh), 5.76 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, He, Hf), 5.81 (d, 2H, *J* = 6.8 Hz, *p*-cym ArH, Hc, Hd), 7.63 (d, 1H, *J* = 9.2 Hz, ArH, H1), 7.80 (t, 1H, *J* = 8 Hz, ArH, H11), 7.93-7.99 (m, 1H, ArH, H10), 8.14 (s, 1H, ArH, H4), 8.30 (d, 2H, *J* = 7.6 Hz, ArH, H9); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-i,C-j, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 85.4 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.5 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 115.9 (ArCH, C-1), 121.5 (ArCH, C-3), 122.5 (ArC, C-4), 129.9 (ArCH, C-9), 132.6 (ArCH, C-11), 135.3 (ArC, C-6), 141.4 (ArC, C-5), 141.7 (ArCH, C-10) 144.8 (ArC, C-7), 148.5 (ArC, C-12), 149.3 (ArC, C-2), 151.7 (ArC, C-8); ESI-MS (CH_3OH): m/z 595.92 $[M-Cl]^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-5-fluoro-6-chloro-1H-benzo[d]imidazole}]Cl (5c′): 43.34 mg (0.069 mmol, 44%); *Mr* ($C_{22}H_{20}N_3BrCl_3FRu$) = 632.74 g/mol; Anal. Calcd.for $C_{22}H_{20}N_3BrCl_3FRu$ (%):C 41.76, H 3.19, N 6.64. Found: C 41.49, H 3.36, N 6.72; Mp: 227-229°C decomp.; R_f (100% ethyl acetate): 0.22;^{1}H NMR (400 MHz, DMSO-*d*^{6}): δ (ppm) = 1.19 (d, 6H, *J* = 7.2 Hz, *p*-cym CH_3, Hi, Hj), 2.08 (s, 3H, *p*-cymCH_3, Ha), 2.83 (sept, 1H, *J* = 6.8 Hz, *p*-cymCH, Hh), 6.01 (d, 1H, *J* = 5.2 Hz, *p*-cym ArH, Hf), 6.20 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, He), 6.30 (d, 2H, *J* = 8.0 Hz, *p*-cym ArH, Hd), 6.43 (d, 2H, *J* = 4.4 Hz, *p*-cym ArH, He),7.82 (d, 1H, *J* = 9.2 Hz, ArH, H4), 7.93-7.96 (m, 1H, ArH, H11), 8.12 (s, 1H, ArH, H1), 8.31 (d, 1H, *J* = 7.6 Hz, ArCH, H9), 8.40-8.43 (m, 1H, ArH, H10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.2 (Me, C-a, *p*-cymene), 21.9 (Me, C-i,C-j, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 85.1 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.5 (ArCH, C-c, *p*-cymene), 100.5 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 115.9 (ArCH, C-4), 121.4 (ArC, C-2), 122.4 (ArCH, C-1), 129.8 (ArCH, C-11), 132.5 (ArCH, C-9), 134.4 (ArC, C-5), 141.3 (ArC, C-6), 141.7 (ArCH, C-10) 141.9 (ArC, C-7), 144.8 (ArC, C-12), 149.2 (ArC, C-3), 151.6 (ArC, C-8); ESI-MS (CH_3OH): m/z 595.92 $[M-Cl]^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-5-(trifluoromethyl)-1H-benzo[d]imidazole}]Cl (5d): 43.2 mg (0.067 mmol, 47 %); *Mr* ($C_{23}H_{21}N_3BrCl_2F_3Ru$) = 648.31 g/mol; Anal. calcd for $C_{23}H_{21}BrCl_2F_3N_3Ru$ (%): C 42.61, H 3.26, N 6.48. Found: C 42.29, H 3.54, N 6.13.; Mp: 222-224°C; R_f (100% ethyl acetate): 0.26; Mp: 222-224°C decomp.; R_f (100% ethyl acetate): 0.22; IR (cm^{-1}): υ 3443, 3047, 2958, 1600, 1456, 1415, 1321, 991, 743; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.79 (d, 3H, *J* = 5.2 Hz, *p*-cymCH_3, H-j), 0.82 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-i), 2.31 (s, *p*-cymCH_3, H-a), 2.43 (brs, 1H, *p*-*p*-cym CH, H-h), 5.62 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.66 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.77 (d, 1H, *J* = 5.2

Hz, *p*-cym ArH, H-d), 5.95 (d, 1H, *J* = 6.4 Hz, *p*-cym ArH, H-c), 7.42 (d, 1H, *J* = 8.0 Hz, ArH, H-12), 7.56 (d, 1H, *J* = 8.0 Hz, ArH, H-11), 7.61-7.68 (m, 2H, ArH, H-2, H-4), 8.03 (s, 1H, ArH, H-10), 8.31 (d, 1H, *J* = 8.2 Hz, H-9); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-i, *p*-cymene), 24.4 (Me, C-j, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 85.0 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.8 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 119.0 (ArCH, C-1, C-4), 122.1 (ArCH, C-2), 126.5 (ArCH, C-9), 129.3 (ArC, C-13), 130.5 (ArC, C-3), 135.0 (ArCH, C-11), 141.5 (ArC, C-6), 141.9 (ArCH, C-10), 143.7 (ArC, C-7), 145.7 (ArC, C-5), 148.9 (ArC, C-12), 153.8 (ArC, C-8); ESI-MS (CH_3OH): m/z 611.97 [M-Cl]$^+$;

[(*η*^{6}-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-6-(trifluoromethyl)-1H-benzo[d]imidazole}]Cl (5d´): 40.5 mg (0.062 mmol, 44 %); *Mr* ($C_{23}H_{21}N_3BrCl_2F_3Ru$) = 648.31 g/mol; Anal. calcd for $C_{23}H_{21}BrCl_2F_3N_3Ru$ (%): C 42.61, H 3.26, N 6.48. Found: C 42.38, H 3.47, N 6.20; Mp: 223-226°C decomp.; R_f (100% ethyl acetate): 0.18; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.80 (d, 3H, *J* = 4.0 Hz, *p*-cymCH_3, H-j), 0.82 (d, 3H, *J* = 6.4 Hz, *p*-cymCH_3, H-i), 2.31 (s, *p*-cymCH_3, H-a), 2.44 (brs, 1H, *p*-*p*-cym CH, H-h), 5.62 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.66 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.77 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-d), 5.95 (d, 1H, *J* = 6.8 Hz, *p*-cym ArH, H-c), 7.43 (d, 1H, *J* = 7.6 Hz, ArH, H-4), 7.56 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 7.61-7.68 (m, 2H, ArH, H-3, H-1), 8.03 (s, 1H, ArH, H-10), 8.31 (d, 1H, *J* = 7.2 Hz, H-9); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.1 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 85.3 (ArCH, C-f, *p*-cymene), 86.0 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.5 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 120.0 (ArCH, C-1), 121.8 (ArCH, C-4), 122.5 (ArCH, C-3), 124.0 (ArCH, C-9), 126.7 (ArC, C-13), 130.1 (ArC, C-2), 137.0 (ArCH, C-11), 140.7 (ArC, C-5), 141.2 (ArC, C-6), 141.4 (ArC, C-7), 141.8 (ArCH, C-10), 149.3 (ArC, C-12), 152.0 (ArC, C-8); ESI-MS (CH_3OH): m/z 611.97 [M-Cl]$^+$.

[(*η*^{6}-*p*-cymene)Ru-2-(6-bromopyridin-2-yl)-5-methoxy-1H-benzo[d]imidazole]Cl (5e):

49.5 mg (0.081 mmol, 45 %); *Mr* ($C_{23}H_{24}N_3OBrCl_2Ru$) = 610.34 g/mol; Anal. calcd for $C_{23}H_{24}BrCl_2N_3ORu$ (%): C 45.26, H 3.96, N 6.88. Found: C 45.01, H 3.77, N 7.02.; Mp: 222-224°C decomp.; R_f (100% ethyl acetate): 0.30; Mp: 231-232°C; R_f (100% ethyl acetate): 0.06;IR (cm^{-1}): υ 3445, 3126, 3048, 2958, 1694, 1600, 1457, 1425, 1324, 990, 744; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.87 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-j), 0.92 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-i), 2.32 (s, *p*-cymCH_3, H-a), 2.82-2.89 (m, 1H, *p*-cym CH, H-h), 3.86 (s, 3H, -OMe, H-13), 5.28 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.41 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.78 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-d), 6.02 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-c), 7.04 (d, 1H, *J* = 7.2 Hz, ArH, H-2), 7.36 (s, 1H, ArH, H-4), 7.43 (d, 1H, *J* = 8.8 Hz, ArH, H-11), 7.69 (d, 1H, *J* = 8.0 Hz, ArH, H-1), 7.82-7.88 (m, 2H, H-9, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ (solubility problem); ESI-MS (CH_3OH): m/z 573.98 [M-Cl]$^+$

[(*η*^{6}-*p*-cymene)Ru-2-(6-bromopyridin-2-yl)-6-methoxy-1H-benzo[d]imidazole]Cl (5e′): 53.0 mg (0.087 mmol, 48 %); *Mr* ($C_{23}H_{24}N_3OBrCl_2Ru$) = 610.34 g/mol; Anal. calcd for $C_{23}H_{24}BrCl_2N_3ORu$ (%): C 45.26, H 3.96, N 6.88. Found: C 45.12, H 3.72, N 7.04.; Mp: 222-224°C decomp.; R_f (100% ethyl acetate): 0.34; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, 6H, *J* = 6.8 Hz, *p*-cymCH_3, H-i, H-j), 2.32 (s, *p*-cymCH_3, H-a), 2.83 (sept, 1H, *p*-cym CH, H-h), 3.86 (s, 3H, -OMe, H-13), 5.28 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.41 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.78 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-d), 6.02 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-c), 7.04 (d, 1H, *J* = 7.2 Hz, ArH, H-3), 7.36 (s, 1H, ArH, H-1), 7.44 (d, 1H, *J* = 8.8 Hz, ArH, H-11), 7.68 (d, 1H, *J* = 8.0 Hz, ArH, H-4), 7.83-7.88 (m, 2H, H-9, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ (solubility problem); ESI-MS (CH_3OH): m/z 573.98 [M-Cl]$^+$.

[(η^6-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-5-nitro-1H-benzo[d]imidazole}]Cl (5f):

49.00 mg (0.078 mmol, 48 %); *Mr* ($C_{23}H_{21}N_3BrCl_2F_3Ru$) = 625.31 g/mol; Anal. calcd for $C_{22}H_{21}N_4O_2BrCl_2Ru$ (%): C 42.26, H 3.38, N 8.96. Found: C 42.54, H 3.59, N 8.63.; Mp: 222-224°C decomp.; R_f (100% ethyl acetate): 0.26; Mp: 226-228°C; R_f (100% ethyl acetate): 0.17; IR (cm^{-1}): υ 3444, 3043, 2962, 1601, 1455, 1417, 1324, 995, 742;; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.77 (d, 3H, *J* = 8.0 Hz, *p*-cymCH_3, H-j), 0.80 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-i), 2.32 (s, *p*-cymCH_3, H-a), 2.45 (brs, 1H, *p*-*p*-cym CH, H-h), 5.62 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.67 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.76 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-d), 5.96 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-c), 7.51 (d, 1H, *J* = 8.8 Hz, ArH, H-11), 7.67 (d, 2H, *J* = 7.2 Hz, ArH, H-10, H-1), 8.13 (d, 1H, *J* = 9.2 Hz, ArH, H-2), 8.34 (d, 1H, *J* = 6.8 Hz, ArH, H-9), 8.68 (s, 1H, H-4); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.8 (Me, C-j, *p*-cymene), 21.9 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 85.1 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.5 (ArCH, C-c, *p*-cymene), 100.5 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 119.0 (ArCH, C-4), 119.5 (ArCH, C-1), 120.3 (ArCH, C-2), 122.1 (ArCH, C-9), 130.5 (ArCH, C-11), 138.7 (ArC, C-6), 141.5 (ArCH, C-10), 141.9 (ArC, C-7), 143.7 (ArC, C-12), 148.9 (ArC, C-3), 153.8 (ArC, C-5), 162.7 (ArC, C-8); ESI-MS (CH_3OH): m/z 588.96 $[M-Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-6-nitro-1H-benzo[d]imidazole}]Cl (5f´): 43.89 mg (0.070 mmol, 43 %); *Mr* ($C_{23}H_{21}N_3BrCl_2F_3Ru$) = 625.31 g/mol; Anal. calcd for $C_{22}H_{21}N_4O_2BrCl_2Ru$ (%): C 42.26, H 3.38, N 8.96. Found: C 42.51, H 3.54, N 8.75.; Mp: 226-228°C decomp.; R_f (100% ethyl acetate): 0.14; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.83 (d, 3H, *J* = 13.6 Hz, *p*-cymCH_3, H-j), 0.87 (d, 3H, *J* = 6.4 Hz, *p*-cymCH_3, H-i), 2.39 (s, *p*-cymCH_3, H-a), 2.54 (brs, 1H, *p*-*p*-cym CH, H-h), 5.67 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.77 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.82 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-d), 5.87 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-c), 7.56 (d, 1H, *J* = 5.2 Hz, ArH, H-11), 7.73 (t, 2H, *J* = 7.2 Hz, ArH, H-10, H-4), 8.15-8.20 (m, 1H, ArH, H-3), 8.39 (d, 1H, *J* = 6.8 Hz, ArH, H-9), 8.50 (s, 1H, H-1); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 24.4 (Me, C-i, *p*-cymene), 30.5 (CH, C-h, *p*-cymene), 84.9 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.9 (ArCH, C-c, *p*-cymene), 100.7 (ArC, C-g, *p*-cymene), 107.0 (ArC, C-b, *p*-cymene), 114.8 (ArCH, C-1), 118.5 (ArCH, C-4), 121.9 (ArCH, C-3), 123.7 (ArCH, C-9), 127.2 (ArCH, C-11), 130.3 (ArC, C-5), 135.9 (ArCH, C-10), 139.4 (ArC, C-7), 150.3 (ArC, C-12), 154.2 (ArC, C-2), 156.4 (ArC, C-6), 161.1 (ArC, C-8); ESI-MS (CH_3OH): m/z 588.96 $[M-Cl]^+$.

2-(6-bromopyridin-2-yl)benzo[d]thiazole (3g): Yield: 90%, R_f (25% ethyl acetate in hexane): 0.6; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.38 (t, 1H, *J* = 7.6 Hz, ArH), 7.44 (t, 1H, *J* = 8.0 Hz, ArH), 7.50 (d, 1H, *J* = 7.6 Hz, ArH), 7.64 (t, 1H, *J* = 7.6 Hz, ArH), 7.90 (d, 1H, *J* = 8.0 Hz, ArH), 8.03 (d, 1H, *J* = 8.0 Hz, ArH), 8.26 (d, 1H, *J* = 7.6 Hz, ArH); LC-MS (CH_3OH): m/z 290.95 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)benzo[d]thiazole}]·Cl (5g): 108.55 mg (0.18 mmol, 91 %); *Mr* ($C_{22}H_{21}N_2SBrCl_2Ru$) = 597.36 g/mol; Anal. calcd for $C_{22}H_{21}N_2SBrCl_2Ru$ (%): C 44.23, H 3.54, N 4.69. Found: C 44.65, H 3.79, N 4.27.; Mp: 230-232°C decomp.; R_f (100% ethyl acetate): 0.30; IR (cm^{-1}): υ 3382, 3046, 2945, 1616, 1514, 1417, 1365, 945, 824, 742; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 1.27 (d, 6H, *J* = 6.0 Hz, *p*-cym CH_3, H-i, H-j), 2.15 (s, 3H, *p*-cym CH_3, H-a), 2.88-2.95 (m, 1H, *p*-cym CH, H-h), 5.34 (d, 2H, *J* = 5.6 Hz, *p*-cym ArH, H-e, H-f), 5.48 (d, 2H, *J* = 6.0 Hz, *p*-cym ArH, H-c, H-d), 7.44 (t, 1H, *J* = 7.6 Hz, ArH, H-2), 7.49-7.54 (m, 1H, ArH, H-3), 7.56 (d, 1H, *J* = 8.0 Hz, ArH, H-11), 7.70 (t, *J* = 8.0 Hz, 1H, ArH, H-4), 7.96 (d, 1H, *J* = 8.0 Hz, ArH, H-1), 8.1 (d, 1H, *J* = 7.6 Hz, ArH, H-10), 8.32 (d, 1H, *J* = 8.0 Hz, H-9);

^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.7 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 85.1 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.5 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 120.3 (ArCH, C-1), 123.2 (ArCH, C-4), 123.9 (ArCH, C-9), 126.6 (ArCH, C-2), 126.8 (ArCH, C-3), 127.4 (ArCH, C-11), 130.8 (ArC, C-5), 135.9 (ArCH, C-10), 141.6 (ArC, C-12), 151.9 (ArC, C-7), 154.1 (ArC, C-6), 167.3 (ArC, C-8);ESI-MS (CH_3OH): m/z 561 $[M-Cl]^+$

[(*η*^{6}-*p*-cymene)RuCl{2-(6-bromopyridin-2-yl)-5 chlorobenzo[d]thiazole}]Cl (5h): 88.4 mg (0.14 mmol, 90 %); *Mr* ($C_{22}H_{20}N_2SBrCl_3Ru$) = 621.80 g/mol; Anal. calcd for $C_{22}H_{20}N_2SBrCl_3Ru$ (%): C 41.82, H 3.19, N 4.43. Found: C 41.59, H 3.49, N 4.18; Mp: 232-234°C decomp.; R_f (100% ethyl acetate): 0.34; IR (cm^{-1}): υ 3384, 3044, 2965, 1616, 1592, 1417, 1370, 945, 827, 752;^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.22 (d, 6H, *J* = 6.8 Hz, *p*-cym CH_3, H-i, H-j), 2.09 (s, 3H, *p*-cym CH_3, H-a), 2.82-2.91 (m, 1H, *p*-cym CH, H-h), 5.28 (d, 2H, *J* = 5.6 Hz, *p*-cym ArH, H-e, H-f), 5.41 (d, 2H, *J* = 5.6 Hz, *p*-cym ArH, H-c, H-d), 7.34-7.36 (m, 1H, ArH, H-2), 7.52 (d, 1H, *J* = 8.0 Hz, ArH, H-11), 7.65 (t, 1H, *J* = 7.6 Hz, ArH, H-1), 7.81 (d, 1H, *J* = 8.4 Hz, ArH, H-10), 8.0 (brs, 1H, ArH, H-9), 8.24 (d, 1H, *J* = 7.6 Hz, ArH, H-4); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.6 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 85.3 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.8 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 120.5 (ArCH, C-4), 123.3 (ArCH, C-1), 124.8 (ArCH, C-9), 126.9 (ArCH, C-2), 131.2 (ArCH, C-11), 132.2 (ArC, C-3), 134.7 (ArC, C-5), 141.7 (ArCH, C-10), 143.9 (ArC, C-12), 148.1 (ArC, C-7), 154.9 (ArC, C-6), 158.3 (ArC, C-8); ESI-MS (CH_3OH): m/z 594.89 $[M-Cl]^+$.

2-(1H-benzo[d]imidazol-2-yl)quinoline (10a): Yield: 94%, R_f (25% ethylacetate in hexane): 0.33; IR (cm^{-1}): υ 2158, 1589, 1500, 1442, 1328, 943, 833, 742; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.54 (d, 1H, *J* = 8.0 Hz, $ArCH_3$), 7.73 (d, 6H, *J* = 8.0 Hz, $ArCH_3$), 7.92 (t, 1H, *J* = 6.0 Hz, $ArCH_3$), 8.39-8.45 (m, 2H, $ArCH_3$), 10.00 (s, 1H, ArNH); ESI-MS (CH_3OH): m/z 246.10 $[M+H]^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11a):

122.4 mg (0.22 mmol, 96 %); *Mr* ($C_{26}H_{25}N_3Cl_2Ru$) = 551.47 g/mol; Anal. calcd for $C_{26}H_{25}N_3Cl_2Ru$ (%): C 56.63, H 4.57, N 7.62. Found: C 56.34, H 4.28, N 7.94.; Mp: 228-230°C decomp. ; R_f (100% ethyl acetate): 0.31; IR (cm^{-1}): υ 3441, 3055, 2926, 1593, 1504, 1469, 1425, 1327, 1142, 825, 748;^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.68 (d, 3H, *J* = 6.4 Hz, *p*-cymCH_3, H-j), 0.71 (d, 3H, *J* = 6.8 Hz, *p*-cym CH_3, H-i), 2.28 (s, 3H, *p*-cym CH_3, H-a), 2.79-2.85 (m, 1H, *p*-cym CH, H-h), 6.08 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 6.23 (d, 1H, *J* = 6.0 Hz, *p*-cym ArCH), 6.28-6.32 (m, 2H, *p*-cym ArH, H-c, H-d), 7.61-7.63 (m, 2H, Ar H, H-2, H-3), 7.89 (d, 1H, *J* = 6.8 Hz, ArH, H-1), 7.95 (t, 1H, *J* = 7.6 Hz, ArH, H-4), 8.15-8.18 (m, 2H, ArH, H-12, H-13), 8.28 (d, 1H, *J* = 8.0 Hz, ArH, H-9), 8.65 (d, 1H, *J* = 8.4 Hz, ArH, H-14), 8.82 (d, 1H, *J* = 8.8 Hz, Ar H, H-11), 8.96 (d, 1H, *J* = 8.4 Hz, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.9 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.1 (Me, C-i, *p*-cymene), 30.7 (CH, C-h, *p*-cymene), 84.1 (ArCH, C-f, *p*-cymene), 85.6 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.5 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 115.1 (ArCH, C-4), 118.4 (ArCH, C-1), 119.2 (ArCH, C-9), 125.6 (ArCH, C-3), 126.6 (ArCH, C-2), 129.3 (ArC, C-15), 129.7 (ArCH, C-12), 129.8 (ArCH, C-11), 130.2 (ArCH, C-14), 130.5 (ArCH, C-13), 133.6 (ArCH, C-10), 138.1 (ArC, C-6), 141.8 (ArC, C-5), 142.5 (ArC, C-7), 148.9 (ArC, C-16), 151.1 (ArC, C-8); ESI-MS (CH_3OH): m/z 516.08 $[M-Cl]^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(5-chloro-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11b): 51.4 mg (0.088 mmol, 50 %); *Mr* ($C_{26}H_{24}N_3Cl_3Ru$) = 585.92 g/mol; Anal. calcd for $C_{26}H_{24}N_3Cl_3Ru$ (%):

C 53.30, H 4.13, N 7.17. Found: C 53.02, H 4.32, N 7.36.; Mp: 226-228°C decomp; R_f (100% ethyl acetate): 0.29; IR (cm^{-1}): υ 3443, 3105, 2916, 1594, 1504, 1468, 1428, 1326, 1147, 826, 748; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.72 (dd, 6H, J_1= 6.8 Hz, J_2 = 2.8 Hz, *p*-cymCH_3, H-i, H-j), 2.29 (s, 3H, *p*-cym CH_3, H-a), 3.24 (brs, 1H, *p*-cym CH, H-h), 5.51 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.61 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.66 (brs, 2H, *p*-cym ArH, H-c, H-d), 7.54 (d, 1H, *J* = 8.8 Hz, ArH, H-2), 7.61 (t, 1H, *J* = 8.0 Hz, ArH, H-1), 7.77 (s, 1H, ArH, H-9), 7.81-7.87 (m, 3H, ArH, H-12, H-13, H-14), 8.25 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 8.39 (d, 1H, *J* = 8.4 Hz, ArH, H-4), 8.78 (d, 1H, *J* = 8.8 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.5 (Me, C-j, *p*-cymene), 21.9 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 84.2 (ArCH, C-f, *p*-cymene), 85.8 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 102.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 117.0 (ArCH, C-4), 119.2 (ArCH, C-1), 119.6 (ArCH, C-9), 120.6 (ArCH, C-2), 128.4 (ArC, C-15), 129.5 (ArCH, C-12), 129.8 (ArCH, C-11), 129.9 (ArCH, C-14), 130.1 (ArC, C-3), 130.9 (ArCH, C-13), 133.7 (ArC, C-5), 141.8 (ArCH, C-10), 141.9 (ArC, C-6), 145.1 (ArC, C-7), 149.0 (ArC, C-16), 154.7 (ArC, C-8); ESI-MS (CH_3OH): m/z 550.00 $[M\text{-}Cl]^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(6-chloro-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11b´): 46.2 mg (0.079 mmol, 45 %); *Mr* ($C_{26}H_{24}N_3Cl_3Ru$) = 585.92 g/mol; Anal. calcd for $C_{26}H_{24}N_3Cl_3Ru$ (%): C 53.30, H 4.13, N 7.17. Found: C 53.05, H 4.36, N 7.32.; Mp: 227-230°C decomp.; R_f (100% ethyl acetate): 0.26; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.74 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-j), 0.80 (d, 3H, *J* = 6.8 Hz*p*-cymCH_3, H-i), 2.21 (brs, 1H, *p*-cym CH, H-h), 2.29 (s, 3H, *p*-cym CH_3, H-a), 5.41 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.69-5.74 (m, 3H, *p*-cym ArH, H-c, H-d, H-e), 7.38-7.44 (m, 2H, *J* = ArH, H-3, H-4), 7.64-7.72 (m, 3H, ArH, H-9, H-12, H-13), 7.93 (d, 2H, *J* = 7.2 Hz, ArH, H-11, H-14), 8.45 (d, 1H, *J* = 8.4 Hz, ArH, H-1), 8.68-8.70 (m, 1H, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.1 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 84.1 (ArCH, C-f, *p*-cymene), 85.7 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.5 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 116.8 (ArCH, C-1), 118.1 (ArCH, C-4), 119.5 (ArCH, C-9), 122.5 (ArCH, C-3), 128.4 (ArCH, C-11), 129.4 (ArCH, C-15), 129.7 (ArCH, C-12), 129.9 (ArC, C-14), 130.0 (ArC, C-2), 133.6 (ArC, C-13), 137.8 (ArC, C-6), 141.8 (ArCH, C-10), 141.9 (ArC, C-5), 144.9 (ArC, C-7), 148.9 (ArC, C-16), 152.0 (ArC, C-8); ESI-MS (CH_3OH): m/z 550.00 $[M\text{-}Cl]^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(5-(trifluoromethyl)-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11d): 46.6 mg (0.075 mmol, 53 %); *Mr* ($C_{27}H_{24}N_3Cl_2F_3Ru$) = 619.47 g/mol; Anal. calcd for $C_{27}H_{24}N_3Cl_2F_3Ru$ (%): C 52.35, H 3.90, N 6.78. Found: C 52.70, H 4.34, N 6.38.; Mp: 230-232°C decomp.; R_f (100% ethyl acetate): 0.23; IR (cm^{-1}): υ 3442, 3057, 2921, 1591, 1500, 1469, 1427, 1317, 1142, 1045, 829, 745; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.72 (d, 6H, *J* = 7.2 Hz, H-i, H-j), 2.26 (brs, 1H, *p*-cym CH, H-h), 2.30 (s, 3H, *p*-cym CH_3, H-a), 5.53 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.61 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.67 (brs, 2H, *p*-cym ArH, H-c, H-d), 7.45 (d, 1H, *J* = 8.4 Hz, ArH, H-9), 7.63 (d, 1H, *J* = 7.2 Hz, ArH, H-1), 7.69 (d, 1H, *J* = 8.4 Hz, ArH, H-2), 7.83-7.89 (m, 2H, ArH, H-12, H-13), 8.09 (s, 1H, ArH, H-4), 8.28 (d, 1H, *J* = 8.4 Hz, ArH, H-14), 8.43 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 8.80 (d, 1H, *J* = 8.8 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.3 (Me, C-i, *p*-cymene), 30.5 (CH, C-h, *p*-cymene), 83.9 (ArCH, C-f, *p*-cymene), 85.1 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 112.8 (ArCH, C-4), 114.6 (ArCH, C-1), 117.6 (ArCH, C-2), 118.9 (ArC, C-17), 120.3 (ArC, C-3), 127.7 (ArC, C-15), 129.1 (ArCH, C-12), 129.6 (ArCH, C-11), 129.8 (ArCH, C-14), 130.5 (ArCH, C-13), 133.5 (ArCH, C-10), 135.3 (ArC, C-6), 141.6 (ArC, C-7), 148.9 (ArC, C-5), 155.1 (ArC, C-16), 161.9 (ArC, C-8); ESI-MS (CH_3OH): m/z 584.06 $[M\text{-}Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-(trifluoromethyl)-1H-benzo[d]imidazol-2-yl)quinolone}]·Cl (11d´): 36.9 mg (0.059 mmol, 42 %); *Mr* ($C_{27}H_{24}N_3Cl_2F_3Ru$) = 619.47 g/mol; Anal. calcd for $C_{27}H_{24}N_3Cl_2F_3Ru$ (%): C 52.35, H 3.90, N 6.78. Found: C 52.65, H 4.26, N 6.52.; Mp: 226-228°C decomp.; R_f (100% ethyl acetate): 0.21; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.74 (d, 6H, *J* = 6.8 Hz, H-i, H-j), 2.26 (brs, 1H, *p*-cym CH, H-h), 2.30 (s, 3H, *p*-cym CH_3, H-a), 5.55 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.61 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.68 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, H-c, H-d), 7.43 (d, 1H, *J* = 8.4 Hz, ArH, H-4), 7.62-7.70 (m, 2H, ArH, H-1, H-3), 7.85-7.89 (m, 3H, ArH, H-9, H-12, H-13), 8.29 (d, 1H, *J* = 8.8 Hz, ArH, H-14), 8.44 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 8.81 (d, 1H, *J* = 8.4 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 19.0 (Me, C-a, *p*-cymene), 21.7 (Me, C-j, *p*-cymene), 22.2 (Me, C-i, *p*-cymene), 30.8 (CH, C-h, *p*-cymene), 84.2 (ArCH, C-f, *p*-cymene), 85.1 (ArCH, C-e, *p*-cymene), 86.0 (ArCH, C-d, *p*-cymene), 86.9 (ArCH, C-c, *p*-cymene), 100.7 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 112.8 (ArCH, C-1), 115.1 (ArCH, C-4), 119.4 (ArCH, C-3), 119.8 (ArC, C-17), 122.1 (ArC, C-2), 125.6 (ArC, C-15), 129.4 (ArCH, C-12), 129.7 (ArCH, C-11), 129.9 (ArCH, C-14), 133.7 (ArCH, C-13), 141.9 (ArCH, C-10), 144.3 (ArC, C-5), 149.1 (ArC, C-7), 156.7 (ArC, C-16), 162.3 (ArC, C-8); ESI-MS (CH_3OH): m/z 584.06 [M-Cl]$^+$.

[(η^6-*p*-cymene)RuCl{2-(5-methoxy-1H-benzo[d]imidazol-2-yl)quinolone}]·Cl (11e): 49.5 mg (0.085 mmol, 47 %); *Mr* ($C_{27}H_{27}N_3OCl_2Ru$) = 581.50 g/mol; Anal. calcd for $C_{27}H_{27}N_3OCl_2Ru$ (%): C 55.77, H 4.68, N 7.23. Found: C 55.39, H 4.31, N 7.58.; Mp: 228-230°C decomp.; R_f (100% ethyl acetate): 0.32; IR (cm^{-1}): υ 3451, 3045, 2928, 1596, 1504, 1459, 1415, 1347, 1142, 829, 748; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.76 (d, 6H, *J* = 6.8 Hz, H-i, H-j), 2.11 (brs, 1H, *p*-cym CH, H-h), 2.26 (s, 3H, *p*-cym CH_3, H-a), 3.92 (s, 3H, -OMe, H-17), 5.52 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.58 (d, 1H, *J* = 6.4 Hz, *p*-cym ArH, H-e), 5.64 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-d), 5.70 (d, 1H, *J* = 5.2 Hz, *p*-cym ArH, H-c), 7.58 (d, 2H, *J* = 8.0 Hz, ArH, H-2, H-4), 7.69 (d, 1H, *J* = 8.8 Hz, ArH, H-9), 7.78-7.83 (m, 3H, ArH, H-1, H-12, H-13), 8.18 (d, 1H, *J* = 8.4 Hz, ArH, H-14), 8.34 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 8.77 (d, 1H, *J* = 8.4 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.3 (Me, C-i, *p*-cymene), 30.9 (CH, C-h, *p*-cymene), 57.4 (OMe, C-17), 85.3 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.5 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 111.2 (ArCH, C-4), 114.8 (ArCH, C-2), 118.5 (ArCH, C-1), 122.5 (ArCH, C-9), 125.5 (ArC, C-15), 126.7 (ArCH, C-12), 129.4 (ArCH, C-11), 133.1 (ArCH, C-14), 135.3 (ArCH, C-13), 141.9 (ArC, C-5), 142.1 (ArCH, C-10), 148.8 (ArC, C-6), 149.5 (ArC, C-7), 150.4 (ArC, C-16), 157.4 (ArC, C-3), 163.7 (ArC, C-8); ESI-MS (CH_3OH): m/z 546.09 [M-Cl]$^+$.

[(η^6-*p*-cymene)RuCl{2-(6-methoxy-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11e´): 52.6 mg (0.090 mmol, 50 %); *Mr* ($C_{27}H_{27}N_3OCl_2Ru$) = 581.50 g/mol, Anal. calcd for $C_{27}H_{27}N_3OCl_2Ru$ (%): C 55.77, H 4.68, N 7.23. Found: C 55.42, H 4.43, N 7.44.;Mp: 229-231°C decomp.; R_f (100% ethyl acetate): 0.35; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.72 (dd, 6H, *J1* = 6.8 Hz, *J2* = 2.8 Hz, H-i, H-j), 2.04-2.13 (m, 1H, *p*-cym CH, H-h), 2.28 (s, 3H, *p*-cym CH_3, H-a), 3.84 (s, 3H, OMe, H-17), 5.52 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.59 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.64-5.69 (m, 2H, *p*-cym ArH, H-c, H-d), 7.25 (brs, 1H, ArH, H-1), 7.50-7.58 (m, 2H, ArH, H-3, H-4), 7.69 (d, 1H, *J* = 8.8 Hz, ArH, H-9), 7.78-7.83 (m, 2H, ArH, H-12, H-13), 8.16-8.19 (m, 1H, ArH, H-14), 8.32-8.35 (m, 1H, ArH, H-11), 8.75 (d, 1H, *J* = 8.4 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.2 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 57.8 (OMe, C-17), 84.1 (ArCH, C-f, *p*-cymene), 85.2 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 112.3 (ArCH, C-1), 115.3 (ArCH, C-3), 119.6 (ArCH, C-4), 123.0 (ArC, C-9), 128.4 (ArC, C-15), 129.5 (ArCH, C-12), 129.8 (ArCH, C-11), 130.0 (ArCH, C-14), 133.7 (ArCH, C-13), 141.8 (ArC, C-6), 141.9 (ArC,

C-10), 145.3 (ArC, C-5), 149.0 (ArC, C-7), 154.6 (ArC, C-16), 158.0 (ArCH, C-2), 164.3 (ArC, C-8); ESI-MS (CH_3OH): m/z 546.09 $[M-Cl]^+$

[(η^6-*p*-cymene)RuCl{2-(5-nitro-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11f): 49.6 mg (0.083 mmol, 51 %); *Mr* ($C_{26}H_{24}N_4O_2Cl_2Ru$) = 596.47 g/mol; Anal. calcd for $C_{26}H_{24}N_4O_2Cl_2Ru$ (%): C 52.35, H 4.06, N 9.39. Found: C 52.66, H 4.38, N 9.58.; Mp: 237-240°C decomp.; R_f (100% ethyl acetate): 0.21; IR (cm^{-1}): υ 3448, 3052 2916, 1594, 1505, 1467, 1424, 1329, 1141, 827, 748; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.74 (dd, 6H, J_1= 6.8 Hz, *J2* = 2.8 Hz, H-i, H-j), 2.05-2.11 (m, 1H, *p*-cym CH, H-h), 2.33 (s, 3H, *p*-cym CH_3, H-a), 5.53 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.62 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.66 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-d), 5.68 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-c), 7.62-7.69 (m, 2H, ArH, H-1, H-9), 7.85-7.92 (m, 2H, ArH, H-12, H-13), 8.17 (d, 1H, *J* = 10.8 Hz, ArH, H-14), 8.33 (d, 1H, *J* = 8.4 Hz, ArH, H-2), 8.45 (d, 1H, *J* = 8.0 Hz, ArH, H-4), 8.74 (brs, 1H, ArH, H-11), 8.81 (d, 1H, *J* = 8.4 Hz, H-10); ^{13}C NMR (100 MHz, DMSO-d^6): δ 18.8 (Me, C-a, *p*-cymene), 21.5 (Me, C-j, *p*-cymene), 22.2 (Me, C-i, *p*-cymene), 30.7 (CH, C-h, *p*-cymene), 84.4 (ArCH, C-f, *p*-cymene), 85.7 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.7 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 113.6 (ArCH, C-4), 117.6 (ArCH, C-1), 119.7 (ArCH, C-2), 122.8 (ArCH, C-9), 126.6 (ArC, C-15), 129.3 (ArCH, C-12), 129.5 (ArCH, C-11), 129.7 (ArCH, C-14), 129.8 (ArCH, C-13), 133.4 (ArCH, C-10), 136.9 (ArC, C-6), 141.6 (ArC, C-7), 144.3 (ArC, C-3), 148.9 (ArC, C-5), 154.3 (ArC, C-16), 164.9 (ArC, C-8); ESI-MS (CH_3OH): m/z 561.06 $[M-Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-nitro-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11f´): 41.9 mg (0.070 mmol, 43 %); *Mr* ($C_{26}H_{24}N_4O_2Cl_2Ru$) = 596.47 g/mol; Anal. calcd for $C_{26}H_{24}N_4O_2Cl_2Ru$ (%): C 52.35, H 4.06, N 9.39. Found: C 52.61, H 4.32, N 9.52.;Mp: 234-238°C decomp.; R_f (100% ethyl acetate): 0.17; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.74 (d, 6H, *J* = 6.8 Hz, H-i, H-j), 2.09-2.13 (m, 1H, *p*-cym CH, H-h), 2.36 (s, 3H, *p*-cym CH_3, H-a), 5.62 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.65 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.71 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-d), 5.79 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-c), 7.65-7.69 (m, 1H, ArH, H-4), 7.81 (d, 1H, *J* = 9.2 Hz, ArH, H-14), 7.87-7.92 (m, 2H, H-12, H-13), 8.13 (d, 1H, *J* = 11.2 Hz, ArH, H-3), 8.33 (d, 1H, *J* = 8.4 Hz, ArH, H-9), 8.45 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 8.58 (brs, 1H, ArH, H-1), 8.81 (d, 1H, *J* = 8.4 Hz, H-10); ^{13}C NMR (100 MHz, DMSO-d^6): δ 18.9 (Me, C-a, *p*-cymene), 21.6 (Me, C-j, *p*-cymene), 22.3 (Me, C-i, *p*-cymene), 30.8 (CH, C-h, *p*-cymene), 84.5 (ArCH, C-f, *p*-cymene), 85.8 (ArCH, C-e, *p*-cymene), 86.1 (ArCH, C-d, *p*-cymene), 86.9 (ArCH, C-c, *p*-cymene), 100.7 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 113.7 (ArCH, C-1), 117.6 (ArCH, C-4), 119.8 (ArCH, C-3), 122.9 (ArCH, C-9), 126.7 (ArC, C-15), 129.4 (ArCH, C-12), 129.6 (ArCH, C-11), 129.8 (ArCH, C-14), 129.9 (ArCH, C-13), 133.5 (ArCH, C-10), 138.8 (ArC, C-5), 141.7 (ArC, C-7), 144.4 (ArC, C-2), 149.1 (ArC, C-6), 154.3 (ArC, C-16), 165.0 (ArC, C-8); ESI-MS (CH_3OH): m/z 561.06 $[M-Cl]^+$.

5-chloro-2-(quinolin-2-yl)benzo[d]thiazole (10h): Yield: 94%, R_f (25% ethyl acetate in Hexane): 0.35; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.42 (d, *J* = 8.4 Hz, 1H, ArH), 7.60-7.64 (m, 1H, ArCH), 7.76-7.80 (m, 1H, ArH), 7.88 (t, *J* = 8 Hz, 2H, ArH), 8.11 (s, 1H, ArH), 8.19 (d, *J* = 8 Hz, 1H, ArH), 8.32 (d, *J* = 8.4 Hz, 1H, ArH), 8.47 (d, *J* = 8.4 Hz, 1H, ArH); ESI-MS (CH_3OH): m/z 297.02 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{5-chloro-2-(quinolin-2-yl)benzo[d]thiazole}]Cl (11h): 88.7 mg (0.147 mmol, 94 %); *Mr* ($C_{26}H_{23}N_2SCl_3Ru$) = 602.97 g/mol; Anal. calcd for $C_{26}H_{23}N_2SCl_3Ru$ (%): C 51.79, H 3.84, N 4.65. Found: C 52.18, H 4.36, N 4.88.; Mp: 222-224°C decomp.; R_f (100% ethyl acetate): 0.25; IR (cm^{-1}): υ 3381, 3051, 2924, 1614, 1591, 1516, 1425, 1371, 1095, 925, 827, 763; ^1H NMR (400 MHz, DMSO-d^6): δ (ppm) 0.74 (d, 3H, *J* = 6.8 Hz, H-j), 0.81 (d, 3H, *J* =

6.8 Hz, H-i), 2.28 (s, 3H, *p*-cym CH_3, H-a), 2.79-2.85 (m, 1H, *p*-cym CH, H-h), 6.08 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 6.29-6.33 (m, 3H, *p*-cym ArH, H-c, H-d, H-e), 7.93 (d, 1H, *J* = 8.8 Hz, ArH, H-2), 8.01 (t, 1H, *J* = 7.2 Hz, ArH, H-12), 8.19 (t, 1H, *J* = 8.0 Hz, ArH, H-13), 8.35 (brs, 2H, ArH, H-1, H-9), 8.59 (d, 1H, *J* = 8.8 Hz, ArH, H-14), 8.71 (d, 1H, *J* = 8.0 Hz, ArH, H-11), 8.81 (d, 1H, *J* = 8.8 Hz, H-4), 8.98 (d, 1H, *J* = 8.4 Hz, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.6 (Me, C-a, *p*-cymene), 21.4 (Me, C-j, *p*-cymene), 22.3 (Me, C-i, *p*-cymene), 30.7 (CH, C-h, *p*-cymene), 82.1 (ArCH, C-f, *p*-cymene), 84.3 (ArCH, C-e, *p*-cymene), 85.6 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 104.9 (ArC, C-b, *p*-cymene), 121.6 (ArCH, C-1), 122.1 (ArCH, C-4), 127.1 (ArCH, C-2), 129.6 (ArCH, C-9), 126.8 (ArC, C-15), 129.9 (ArCH, C-12), 130.9 (ArCH, C-11), 132.9 (ArC, C-3), 134.2 (ArCH, C-14), 134.8 (ArCH, C-13), 142.3 (ArCH, C-10), 149.3 (ArC, C-6), 151.4 (ArC, C-16), 151.8 (ArC, C-5), 161.6 (ArC, C-7), 168.0 (ArC, C-8); ESI-MS (CH_3OH): m/z 567.00 [M-Cl]$^+$

[(*η*^{6}-*p*-cymene)RuCl{2-(5,6-dimethyl-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11i): 103.2 mg (0.178 mmol, 97 %); *Mr* ($C_{28}H_{29}N_3Cl_2Ru$) = 579.52 g/mol; Anal. calcd for $C_{28}H_{29}N_3Cl_2Ru$ (%): C 58.03, H 5.04, N 7.25. Found: C 58.38, H 5.32, N 7.48.; Mp: 234-236°C decomp.; R_f (100% ethyl acetate): 0.33; IR (cm^{-1}): υ 3446, 3052, 2928, 1598, 1500, 1462, 1429, 1333, 1157, 828, 756; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.80 (d, 6H, *J* = 6.8 Hz, *p*-cym CH_3, H-i, H-j), 2.11 (brs, 1H, *p*-cym CH, H-h), 2.30 (s, 6H, *p*-cym CH_3, H-a), 2.36 (s, 3H, Me, H-18), 2.42 (s, 3H, Me, H-17), 5.51 (d, 1H, *J* = 5.2 Hz, *p*-cym ArH, H-f), 5.60 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-e), 5.68 (brs, 2H, *p*-cym ArH, H-c, H-d), 7.38 (s, 1H, ArH, H-9), 7.56 (brs, 2H, ArH, H-1, H-4), 7.77-7.83 (m, 2H, ArH, H-12, H-13), 8.17 (d, 1H, *J* = 8.0 Hz, ArH, H-14), 8.36 (d, 1H, *J* = 8.0 Hz, ArH, H-11), 8.77 (d, 1H, *J* = 8.8 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 14.6 (Me, C-18), 15.6 (Me, C-17), 18.9 (Me, C-a, *p*-cymene), 21.6 (Me, C-j, *p*-cymene), 22.2 (Me, C-i, *p*-cymene), 31.1 (CH, C-h, *p*-cymene), 85.2 (ArCH, C-f, *p*-cymene), 85.8 (ArCH, C-e, *p*-cymene), 87.2 (ArCH, C-d, *p*-cymene), 87.4 (ArCH, C-c, *p*-cymene), 105.4 (ArC, C-g, *p*-cymene), 105.6 (ArC, C-b, *p*-cymene), 117.6 (ArCH, C-4), 119.9 (ArCH, C-1), 124.8 (ArCH, C-9), 125.6 (ArC, C-15), 126.6 (ArCH, C-12), 129.3 (ArCH, C-11), 129.7 (ArCH, C-14), 129.8 (ArCH, C-13), 130.8 (ArC, C-3), 133.9 (ArC, C-2), 140.1 (ArC, C-6), 141.5 (ArC, C-5), 147.6 (ArCH, C-10), 148.8 (ArC, C-7), 156.1 (ArC, C-16), 171.9 (ArC, C-8); ESI-MS (CH_3OH): m/z 544.11 [M-Cl]$^+$.

[(*η*^{6}-*p*-cymene)RuCl{2-(5,6-dichloro-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11j): 83.2 mg (0.134 mmol, 95 %); *Mr* ($C_{26}H_{23}N_3Cl_4Ru$) = 620.36 g/mol; Anal. calcd for $C_{26}H_{23}N_3Cl_4Ru$ (%): C 50.34, H 3.74, N 6.77. Found: C 50.73, H 3.45, N 7.14.; Mp: 232-234°C decomp.;R_f (100% ethyl acetate): 0.28; IR (cm^{-1}): υ 3445, 3058, 2934, 1599, 1501, 1479, 1421, 1326, 1140, 815, 746; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.63 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-j), 0.73 (d, 3H, *J* = 6.8 Hz, *p*-cymCH_3, H-i), 2.29 (s, 3H, *p*-cym CH_3, H-a), 2.79-2.85 (m, 1H, *p*-cym CH, H-h), 6.07 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 6.29 (d, 2H, *J* = 6.0 Hz, *p*-cym ArH, H-d, H-e), 6.40 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-c), 7.96 (t, 1H, *J* = 7.2 Hz, ArH, H-9), 8.16-8.19 (m, 2H, ArH, H-13, H-12), 8.28 (d, 1H, *J* = 8.0 Hz, ArH, H-14), 8.33 (s, 1H, ArH, H-11), 8.68 (d, 1H, *J* = 8.4 Hz, ArH, H-1), 8.81 (d, 1H, *J* = 8.8 Hz, ArH, H-4), 8.97 (d, 1H, *J* = 8.4 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.9 (Me, C-a, *p*-cymene), 21.5 (Me, C-j, *p*-cymene), 22.3 (Me, C-i, *p*-cymene), 30.6 (CH, C-h, *p*-cymene), 83.7 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.1 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 102.8 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 116.7 (ArCH, C-1), 119.3 (ArCH, C-4), 119.6 (ArCH, C-9), 128.4 (ArC, C-15), 129.0 (ArCH, C-12), 129.5 (ArCH, C-11), 129.7 (ArC, C-3), 129.8 (ArC, C-2), 130.1 (ArCH, C-14), 133.8 (ArCH, C-13), 135.6 (ArCH, C-10), 141.8 (ArC, C-6), 141.9 (ArC, C-5), 148.2 (ArC, C-7), 149.0 (ArC, C-16), 153.5 (ArC, C-8); ESI-MS (CH_3OH): m/z 584.00 [M-Cl]$^+$.

(η^6-*p*-cymene)RuCl{2-(5-fluoro-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11k): 55.31 mg (0.097 mmol, 49 %); *Mr* ($C_{26}H_{24}N_3FCl_2Ru$) = 569.46 g/mol; Anal. calcd for $C_{26}H_{24}N_3FCl_2Ru$ (%): C 54.84, H 4.25, N 7.38. Found: C 54.36, H 4.59, N 7.73.; Mp: 234-236°C decomp.; R_f (100% ethyl acetate): 0.25; IR (cm^{-1}): υ 3445, 3055, 2929, 1587, 1509, 1459, 1425, 1410, 1327, 1142, 1065, 827, 748; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.73 (d, 3H, *J* = 2.8 Hz, *p*-cymCH_3, H-j), 0.78 (d, 3H, *J* = 2.8 Hz, *p*-cymCH_3, H-i), 2.21 (brs, 1H, *p*-cym CH, H-h), 2.27 (s, 3H, *p*-cym CH_3, H-a), 5.62 (brs, 1H, *p*-cym ArH, H-f), 5.73 (brs, 3H, *p*-cym ArH, H-c, H-d, H-e), 7.33-7.41 (m, 2H, *J* = ArH, H-2, H-4), 7.64-7.70 (m, 3H, ArH, H-1, H-12, H-13), 7.88 (d, 2H, *J* = 8.0 Hz, ArH, H-9, H-14), 8.41 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 9.23 (d, 1H, *J* = 8.0 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-d^6): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.2 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 84.1 (ArCH, C-f, *p*-cymene), 85.7 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 116.9 (ArCH, C-2), 119.3 (ArCH, C-1), 122.6 (ArCH, C-4), 129.3 (ArCH, C-9), 129.4 (ArC, C-15), 129.7 (ArCH, C-12), 129.8 (ArCH, C-11), 129.9 (ArCH, C-14), 133.7 (ArCH, C-13), 139.2 (ArC, C-5), 141.9 (ArCH, C-10), 148.4 (ArC, C-6), 148.9 (ArC, C-7), 152.3 (ArC, C-16), 159.9 (ArC, C-3), 162.4 (ArC, C-8); ESI-MS (CH_3OH): m/z 534.10 $[M\text{-}Cl]^+$.

(η^6-*p*-cymene)RuCl{2-(6-fluoro-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11k'): 53.1 mg (0.093 mmol, 47 %); *Mr* ($C_{26}H_{24}N_3FCl_2Ru$) = 569.46 g/mol; Anal. calcd for $C_{26}H_{24}N_3FCl_2Ru$ (%): C 54.84, H 4.25, N 7.38. Found: C 54.51, H 4.52, N 7.66.;Mp: 234-236°C decomp.; R_f (100% ethyl acetate): 0.23; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.73 (brs, 3H, *p*-cymCH_3, H-j), 0.78 (brs, 3H, *p*-cymCH_3, H-i), 2.27 (s, 3H, *p*-cym CH_3, H-a), 2.83 (sept, 1H, *J* = 6.8 Hz, *p*-cym CH, H-h), 5.62 (brs, 1H, *p*-cym ArH, H-f), 5.73-5.81 (m, 3H, *p*-cym ArH, H-c, H-d, H-e), 7.32-7.41 (m, 2H, *J* = ArH, H-1, H-3), 7.64-7.73 (m, 3H, ArH, H-4, H-9, H-12), 7.88 (d, 2H, *J* = 8.0 Hz, ArH, H-13, H-14), 8.41 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 9.23 (d, 1H, *J* = 8.0 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-d^6): δ 18.4 (Me, C-a, *p*-cymene), 21.7 (Me, C-j, *p*-cymene), 22.2 (Me, C-i, *p*-cymene), 30.5 (CH, C-h, *p*-cymene), 84.1 (ArCH, C-f, *p*-cymene), 85.7 (ArCH, C-e, *p*-cymene), 86.0 (ArCH, C-d, *p*-cymene), 86.9 (ArCH, C-c, *p*-cymene), 100.7(ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 116.8 (ArCH, C-1), 119.3 (ArCH, C-3), 122.4 (ArCH, C-4), 129.3 (ArCH, C-9), 129.4 (ArC, C-15), 129.7 (ArCH, C-12), 129.8 (ArCH, C-11), 129.9 (ArCH, C-14), 133.8 (ArCH, C-13), 139.2 (ArC, C-6), 141.9 (ArCH, C-10), 148.4 (ArC, C-5), 149.0 (ArC, C-7), 152.5 (ArC, C-16), 160.0 (ArC, C-2), 162.5 (ArC, C-8); ESI-MS (CH_3OH): m/z 534.10 $[M\text{-}Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(5-bromo-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11l): 40.4 mg (0.064 mmol, 48 %); *Mr* ($C_{26}H_{24}N_3BrCl_2Ru$) = 630.37 g/mol; Anal. calcd for $C_{26}H_{24}N_3BrCl_2Ru$ (%): C 49.54, H 3.84, N 6.67. Found: C 49.21, H 4.26, N 6.23.; Mp: 232-234°C decomp.; R_f (100% ethyl acetate): 0.27; IR (cm^{-1}): υ 3444, 3045, 2927, 1591, 1506, 1467, 1416, 1325, 1144, 827, 746; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.71 (d, 3H, *J* = 7.6 Hz, *p*-cymCH_3, H-j), 0.72 (d, 3H, *J* = 7.6 Hz, *p*-cymCH_3, H-i), 2.21-2.26 (m, 1H, *p*-cym CH, H-h), 2.30 (s, 3H, *p*-cym CH_3, H-a), 5.51 (d, 1H, *J* = 5.6 Hz, *p*-cym ArH, H-f), 5.60 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.66 (brs, 2H, *p*-cym ArH, H-c, H-d), 7.32 (d, 1H, *J* = 8.0 Hz, ArH, H-2), 7.50 (d, 1H, *J* = 8.8 Hz, ArH, H-1), 7.62 (t, 1H, *J* = 7.2 Hz, ArH, H-9), 7.83-7.88 (m, 2H, ArH, H-12, H-13), 7.94 (s, 1H, ArH, H-4), 8.25 (d, 1H, *J* = 8.4 Hz, ArH, H-14), 8.39 (d, 1H, *J* = 8.8 Hz, ArH, H-11), 8.78 (d, 1H, *J* = 8.4 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-d^6): δ 18.9 (Me, C-a, *p*-cymene), 21.6 (Me, C-j, *p*-cymene), 22.1 (Me, C-i, *p*-cymene), 30.7 (CH, C-h, *p*-cymene), 83.5 (ArCH, C-f, *p*-cymene), 84.8 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.5 (ArC, C-g, *p*-cymene), 106.8 (ArC, C-b, *p*-cymene), 113.9 (ArCH, C-1), 116.1 (ArCH, C-4), 119.8 (ArC, C-3), 120.1 (ArCH, C-9), 128.3 (ArC, C-15), 129.3 (ArCH, C-2), 129.7 (ArCH, C-12), 129.8 (ArC, C-11), 130.3 (ArCH, C-14), 133.6 (ArCH, C-13), 136.2 (ArCH,

C-10), 141.8 (ArC, C-5), 141.9 (ArC, C-6), 143.9 (ArC, C-7), 148.9 (ArC, C-16), 163.8 (ArC, C-8); ESI-MS (CH_3OH): m/z 593.99 $[M\text{-}Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-bromo-1H-benzo[d]imidazol-2-yl)quinolone}]Cl (11l´): 39.6 mg (0.063 mmol, 47 %); *Mr* ($C_{26}H_{24}N_3BrCl_2Ru$) = 630.37 g/mol; Anal. calcd for $C_{26}H_{24}N_3BrCl_2Ru$ (%): C 49.54, H 3.84, N 6.67. Found: C 49.30, H 4.12, N 6.43.;Mp: 231-232°C decomp.; R_f (100% ethyl acetate): 0.24; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.72 (d, 6H, *J* = 6.8 Hz, H-l, H-j), 2.02-2.09 (m, 1H, *p*-cym CH, H-h), 2.33 (s, 3H, *p*-cym CH_3, H-a), 5.52 (d, 1H, *J* = 4.0 Hz, *p*-cym ArH, H-f), 5.62 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.67 (d, 1H, *J* = 9.4 Hz, *p*-cym ArH, H-d), 5.69 (brs, 1H, *p*-cym ArH, H-c), 7.30 (t, 1H, *J* = 8.8 Hz, ArH, H-3), 7.61 (d, 1H, *J* = 7.2 Hz, ArH, H-4), 7.67 (d, 1H, *J* = 9.2 Hz, ArH, H-9), 7.81-7.87 (m, 2H, ArH, H-12, H-13), 7.94 (s, 1H, ArH, H-1), 8.25 (d, 1H, *J* = 8.4 Hz, ArH, H-14), 8.39 (d, 1H, *J* = 8.4 Hz, ArH, H-11), 8.79 (d, 1H, *J* = 8.8 Hz, ArH, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 19.0 (Me, C-a, *p*-cymene), 21.7 (Me, C-j, *p*-cymene), 22.2 (Me, C-i, *p*-cymene), 30.8 (CH, C-h, *p*-cymene), 84.1 (ArCH, C-f, *p*-cymene), 84.9 (ArCH, C-e, *p*-cymene), 86.1 (ArCH, C-d, *p*-cymene), 86.9 (ArCH, C-c, *p*-cymene), 100.8 (ArC, C-g, *p*-cymene), 107.2 (ArC, C-b, *p*-cymene), 113.9 (ArCH, C-4), 117.7 (ArCH, C-1), 119.9 (ArC, C-2), 120.0 (ArCH, C-9), 120.2 (ArC, C-15), 129.4 (ArCH, C-3), 129.8 (ArCH, C-12), 129.9 (ArCH, C-11), 130.4 (ArCH, C-14), 137.8 (ArCH, C-13), 141.9 (ArCH, C-10), 142.0 (ArC, C-6), 144.0 (ArC, C-5), 149.1 (ArC, C-7), 152.8 (ArC, C-16), 164.0 (ArC, C-8); ESI-MS (CH_3OH): m/z 593.99 $[M\text{-}Cl]^+$.

[(η^6-*p*-cymene)RuCl{2-(quinolin-2-yl)benzo[d]oxazole}]Cl (11m): 121.5 mg (0.219 mmol, 96 %); *Mr* ($C_{26}H_{24}N_2OCl_2Ru$) = 552.46 g/mol; Anal. calcd for $C_{26}H_{24}N_2OCl_2Ru$ (%): C 56.53, H 4.38, N 5.07. Found: C 56.85, H 4.56, N 5.39.; Mp: 224-226°C decomp.; R_f (100% ethyl acetate): 0.30; IR (cm^{-1}): υ 3351, 3054, 2927, 1600, 1592, 1526, 1427, 1375, 925, 827, 763; ^{1}H NMR (400 MHz, DMSO-*d*^{6}): δ (ppm) 0.76 (d, 3H, *J* = 6.8 Hz, H-j), 0.89 (d, 3H, *J* = 6.8 Hz, H-i), 2.18 (s, 3H, *p*-cym CH_3, H-a), 2.28-2.35 (m, 1H, *p*-cym CH, H-h), 5.17 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.74 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-e), 5.90 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-d), 6.09 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-c), 7.38 (t, 1H, *J* = 7.6 Hz, ArH, H-4), 7.81 (d, 1H, *J* = 8.0 Hz, ArH, H-1, H-9), 8.02 (t, 1H, *J* = 7.2 Hz, ArH, H-12), 8.18 (t, 1H, *J* = 8.0 Hz, ArH, H-3), 8.31 (d, 1H, *J* = 8.0 Hz, ArH, H-2), 8.39 (d, 1H, *J* = 8.0 Hz, ArH, H-13), 8.74 (d, 1H, *J* = 8.4 Hz, H-14), 8.92 (d, 1H, *J* = 8.0 Hz, H-11), 9.18 (s, 1H, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.9 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 22.1 (Me, C-i, *p*-cymene), 30.7 (CH, C-h, *p*-cymene), 83.8 (ArCH, C-f, *p*-cymene), 84.9 (ArCH, C-e, *p*-cymene), 85.9 (ArCH, C-d, *p*-cymene), 86.8 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 116.9 (ArCH, C-1), 117.8 (ArCH, C-4), 119.3 (ArCH, C-9), 122.8 (ArCH, C-2), 123.6 (ArCH, C-3), 127.5 (ArC, C-15), 128.6 (ArCH, C-12), 129.4 (ArCH, C-11), 129.6 (ArCH, C-14), 129.8 (ArCH, C-13), 133.6 (ArCH, C-10), 141.7 (ArC, C-6), 145.9 (ArC, C-16), 148.9 (ArC, C-5), 151.2 (ArC, C-7), 161.2 (ArC, C-8); ESI-MS (CH_3OH): m/z m/z 517.06 $[M\text{-}Cl]^+$.

[(η^6-*p*-cymene)RuCl{5-bromo-2-(quinolin-2-yl)benzo[d]oxazole}]Cl (11n): 79.7 mg (0.126 mmol, 95 %); *Mr* ($C_{26}H_{24}N_2OCl_2Ru$) = 631.35 g/mol; Anal. calcd for $C_{26}H_{23}N_2OBrCl_2Ru$ (%): C 49.46, H 3.67, N 4.44. Found: C 49.68, H 3.91, N 4.81.; Mp: 226-228°C decomp.; R_f (100% ethyl acetate): 0.24; IR (cm^{-1}): υ 3354, 3057, 2928, 1611, 1594, 1516, 1425, 1368, 925, 827, 753; ^{1}H NMR (400 MHz, DMSO-*d*^{6}): δ (ppm) 0.82 (d, 3H, *J* = 6.8 Hz, H-j), 0.89 (d, 3H, *J* = 6.8 Hz, H-i), 2.09 (s, 3H, *p*-cym CH_3, H-a), 2.29-2.37 (m, 1H, *p*-cym CH, H-h), 5.76 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-f), 5.80 (d, 2H, *J* = 5.2 Hz, *p*-cym ArH, H-d, H-e), 5.88 (d, 1H, *J* = 6.0 Hz, *p*-cym ArH, H-c), 7.55 (d, 1H, *J* = 8.8 Hz, ArH, H-4), 7.98 (s, 1H, ArH, H-2), 8.03 (t, 1H, *J* = 7.6 Hz, ArH, H-9), 8.18 (t, 1H, *J* = 7.6 Hz, ArH, H-1), 8.31 (d, 1H, *J* = 8.0 Hz, ArH, H-12), 8.41 (d, 1H, *J* = 8.0 Hz, ArH, H-13), 8.73 (d, 1H, *J* = 8.8 Hz, H-14), 8.93 (d, 1H, *J* = 8.0 Hz, H-11), 9.19 (s, 1H, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.7 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-

cymene), 22.1 (Me, C-i, *p*-cymene), 30.4 (CH, C-h, *p*-cymene), 84.9 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.3 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 110.3 (ArCH, C-1), 119.7 (ArCH, C-9), 120.8 (ArCH, C-3), 123.6 (ArCH, C-4), 125.0 (ArCH, C-15), 127.8 (ArCH, C-12), 129.8 (ArCH, C-2), 131.0 (ArCH, C-11), 133.3 (ArC, C-14), 135.0 (ArCH, C-13), 149.1 (ArC, C-10), 147.2 (ArC, C-6), 148.9 (ArC, C-16), 155.8 (ArC, C-5), 170.8 (ArC, C-7), 172.8 (ArC, C-8); ESI-MS (CH_3OH): m/z 594.97 $[M\text{-}Cl]^+$.

Characterization data for some Suzuki coupled ligand [7(g1-g3, Ia-I9)] and their corresponding ruthenium(II)-*p*-cymene complexes [8(g1-g3, Ia-I9)]

2-(6-(4-methoxyphenyl)pyridin-2-yl)benzo[d]thiazole (7g1): Yield: 95%, R_f (16.5% ethyl acetate in hexane): 0.37; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 3.89 (s, 3H, OCH_3), 7.05 (d, *J* = 8 Hz, 2H, ArCH), 7.42 (t, 1H, *J* = 8 Hz, ArCH), 7.51 (t, 1H, *J* = 8 Hz, ArCH), 7.77 (d, 1H, *J* = 8 Hz, ArCH), 7.86 (t, 1H, *J* = 8 Hz, ArCH), 7.96 (d, 1H, *J* = 8 Hz, ArCH), 8.11 (t, 3H,*J* = 8 Hz, ArCH), 8.23 (d, 1H, *J* = 8 Hz, ArCH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4 (OCH_3), 114.2, 118.1, 120.8, 121.9, 123.5, 125.5, 126.1, 128.2, 130.8, 132.1, 136.4, 137.7, 150.9, 154.4, 156.7, 160.9, 170.4; LC-MS (CH_3OH): m/z 319.08 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-(4-methoxyphenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8g1): 54.7 mg (0.075 mmol, 95 %); *Mr* ($C_{29}H_{28}N_2OPSClF_6Ru$) = 734.10 g/mol; Anal. calcd for $C_{29}H_{28}N_2OPSClF_6Ru$ (%): C 47.45, H 3.84, N 3.82 Found: C 47.78, H 3.57, N 4.18.; Mp: 240-242°C decomp.; R_f (100% ethyl acetate): 0.28; IR (cm^{-1}): υ 3051, 2941, 1697, 1600, 1554, 1406, 1327, 1176, 1072, 929, 829, 744; ^1H NMR (400 MHz, DMSO-*d6*): δ (ppm) 0.63-0.69 (m, 6H, H-i, H-j), 2.13 (s, 3H, *p*-cym CH_3, H-a), 2.78-2.85 (m, 1H, *p*-cym CH, H-h), 3.93 (s, 3H, -OMe, H-19), 5.75 (d, 1H, *J* = 6.4 Hz, *p*-cym ArH, H-f), 5.80 (d, 1H, *J* = 6.4 Hz, *p*-cym ArH, H-e), 6.06 (brs, 2H, *p*-cym ArH, H-c, H-d), 7.26 (d, 2H, *J* = 8.8 Hz, H-15, H-16), 7.83 (t, 1H, *J* = 7.2 Hz, ArH, H-2), 7.89 (t, 1H, *J* = 7.2 Hz, ArH, H-3), 7.96 (d, 1H, *J* = 7.2 Hz, ArH, H-9), 8.09-8.11 (m, 2H, ArH, H-4, H-10), 8.29 (d, 1H, *J* = 8.0 Hz, ArH, H-11), 8.38 (t, 1H, *J* = 7.6 Hz, ArH, H-18), 8.48 (d, 1H, *J* = 7.6 Hz, H-14), 8.65 (d, 1H, *J* = 7.6 Hz, H-1); ^{13}C NMR (DMSO-*d*^{6},100 MHz): δ 18.6 (Me, C-a, *p*-cymene), 21.7 (Me, C-j, *p*-cymene), 24.4 (Me, C-i, *p*-cymene), 31.1 (CH, C-h, *p*-cymene), 56.1 (OMe, C-19), 85.4 (ArCH, C-f, *p*-cymene), 86.0 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 86.9 (ArCH, C-c, *p*-cymene), 102.4 (ArC, C-g, *p*-cymene), 105.4 (ArC, C-b, *p*-cymene), 114.8 (ArCH, C-15), 118.5 (ArCH, C-17), 121.9 (ArCH, C-9), 123.1 (ArCH, C-11), 123.6 (ArCH, C-4), 123.6 (ArCH, C-2), 124.9 (ArCH, C-1), 126.5 (ArCH, C-3), 128.5 (ArC, C-13), 130.3 (ArCH, C-14), 133.1 (ArCH, C-18), 135.9 (ArCH, C-10), 141.1 (ArC, C-7), 150.3 (ArC, C-6), 154.2 (ArC, C-8), 156.4 (ArC, C-12), 161.1 (ArC, C-16); ^{31}P NMR (162 MHz, DMSO-*d*^{6}): δ(ppm) (-153.01)-(-135.45) (m, 1P, PF_6); ^{19}F NMR (376 MHz, DMSO-*d*^{6}): δ(ppm) = -71.02, -69.13 (6F, PF_6); ESI-MS (CH_3OH): m/z 589.06 $[M\text{-}Cl]^+$.

2-(6-(4-formylphenyl)pyridin-2-yl)benzo[d]thiazole (7g2): Yield: 95%, R_f (16.5% ethyl acetate in hexane): 0.31; IR (cm^{-1}): υ 3350, 3049, 2850, 1687, 1674, 1587, 1562, 1506, 1427, 1315, 1211, 1149, 1078, 989, 796, 752; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.45 (d, 1H, *J* = 8 Hz, ArCH), 7.52 (t,1H, *J* = 8 Hz, ArCH), 7.91-7.99 (m, 3H, ArCH), 8.04 (d, 2H, *J* = 8 Hz, ArCH), 8.11 (d, 1H, *J* = 8 Hz, ArCH), 8.32-8.38 (m, 3H, ArCH), 10.11 (s, 1H, ArCHO); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.34, 122.03, 122.28, 123.69, 125.81, 126.35, 127.50, 130.25, 136.32, 136.75, 138.15, 143.69, 151.49, 154.36, 155.44, 169.56, 191.97 (CHO); ESI-MS (CH_3OH): m/z 317.09 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-(4-formylphenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8g2): 53.8 mg (0.073 mmol, 93 %); *Mr* ($C_{29}H_{26}N_2OPSClF_6Ru$) = 732.08 g/mol; Anal. calcd for

$C_{29}H_{26}N_2OPSClF_6Ru$ (%): C 47.58, H 3.58, N 3.83 Found: C 47.79, H 3.89, N 4.18.; Mp: 241-243°C decomp.; R_f (100% ethyl acetate): 0.23; IR (cm^{-1}): υ 3124, 3045, 2835, 1695, 1600, 1564, 1404, 1330, 1182, 831, 761; ^1H NMR (400 MHz, DMSO): δ(ppm) Solubility problem; ^{31}P NMR (162 MHz, $CDCl_3$): δ(ppm) = (-153.26)-(-135.66) (m, 1P, PF_6). ^{19}F NMR (376 MHz, $CDCl_3$): δ(ppm) = -73.38, -71.49 (6F, PF_6); ESI-MS (CH_3OH): m/z 587.05 $[M-Cl]^+$.

2-(6-(4-acetylphenyl)pyridin-2-yl)benzo[d]thiazole (7g3): Yield: 90%, R_f (16.5% ethyl acetate in hexane): 0.18; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.66 (s, 3H, $COCH_3$), 7.43 (t, 1H, *J* = 7.6 Hz, ArCH), 7.51 (t,1H, *J* = 7.6 Hz, ArCH), 7.70 (d, 1H, *J* = 8 Hz, ArCH), 7.87 (d, 1H, *J* = 8 Hz, ArCH), 7.91-7.97 (m, 2H, ArCH), 8.04 (d, 1H, *J* = 8 Hz, ArCH), 8.09 (d, 2H, *J* = 8 Hz, ArCH), 8.24 (d, 1H, *J* = 8 Hz, ArCH), 8.33 (d, 1H, *J* = 7.6 Hz, ArCH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.75 (Acetyl CH_3), 119.71, 122.00, 122.06, 123.66, 125.74, 126.30, 127.05, 128.88, 136.35, 136.60, 137.58, 138.03, 142.35, 144.33, 151.39, 154.38, 155.63, 169.68, 197.74 (C=O); ESI-MS (CH_3OH): m/z 331.08 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{2-(6-(4-acetylphenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8g3): 41.25 mg (0.07 mmol, 93 %); *Mr* ($C_{30}H_{28}N_2OPSClF_6Ru$) = 746.11 g/mol; Anal. calcd for $C_{30}H_{28}N_2OPSClF_6Ru$ (%): C 48.29, H 3.78, N 3.75 Found: C 47.60, H 4.22, N 3.58. N 4.38.; Mp: 242-244°C decomp.; R_f (100% ethyl acetate): 0.24; IR (cm^{-1}): υ 3302, 1670, 1600, 1419, 1267, 993, 839, 758; ^1H NMR (400 MHz, DMSO-*d6*): δ (ppm) 1.18 (d, 6H, *J* = 7.2 Hz, H-i, H-j), 2.4 (s, 3H, *p*-cym CH_3, H-a), 2.74 (s, 3H, $COCH_3$, H-20), 2.78-2.89 (m, 1H, *p*-cym CH, H-h), 3.93 (s, 3H, -OMe, H-19), 5.76 (d, 2H, *J* = 6.0 Hz, *p*-cym ArH, H-e, H-f), 5.80 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, H-c, H-d), 7.62 (d, 1H, *J* = 6.8 Hz, H-2), 7.90 (d, 2H, *J* = 7.2 Hz, ArH, H-3, H-9), 8.06 (t, 2H, *J* = 10.4 Hz, ArH, H-4, H-10), 8.29 (t, 3H, *J* = 10.0 Hz, ArH, H-1, H-11, H-14), 8.44-8.51 (m, 2H, ArH, H-13, H-17), 8.73 (d, 1H, *J* = 8.0 Hz, ArH, H-18); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): (solubility problem); ^{31}P NMR (400 MHz, DMSO): ^{31}P NMR (162 MHz, DMSO-*d*^{6}): δ(ppm) (-157.39)-(-131.04) (m, 1P, PF_6). ^{19}F NMR (376 MHz, DMSO-*d*^{6}): δ(ppm) -71.03, -69.15 (6F, PF_6); ESI-MS (CH_3OH): m/z 601.06 $[M-Cl]^+$.

5-chloro-2-(6-phenylpyridin-2-yl)benzo[d]thiazole (7l1): Yield: 92%, R_f (20% ethyl acetate in hexane): 0.55; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.39 (d, 1H, *J* = 8 Hz, ArCH), 7.48 (t, 1H, *J* = 7.2 Hz, ArCH), 7.53 (t, 2H, *J* = 7.6 Hz, ArCH), 7.86 (d, 2H, *J* = 8 Hz, ArCH), 7.92 (t, 1H, *J* = 7.6 Hz, ArCH), 8.08 (s, 1H, ArCH), 8.15 (d, 2H, *J* = 7.6 Hz, ArCH), 8.26 (d, 1H, *J* = 7.6 Hz, ArCH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 118.99, 121.98, 122.72, 123.32, 126.07, 126.93, 128.90, 129.61, 132.18, 134.65, 137.96, 138.06, 150.68, 155.24, 157.09, 172.10; ESI-MS (CH_3OH): m/z 323.03 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{5-chloro-2-(6-phenylpyridin-2-yl)benzo[d]thiazole}]PF_6 (8l1): 54.5 mg (0.074 mmol, 95 %); *Mr* ($C_{28}H_{25}N_2PSCl_2F_6Ru$) = 738.52 g/mol; Anal. calcd for $C_{28}H_{25}N_2PSCl_2F_6Ru$ (%): C 45.54, H 3.41, N 3.79 Found: C 45.80, H 3.70, N 4.08.; Mp: 245-247°C decomp.; R_f (100% ethyl acetate): 0.23; IR (cm^{-1}): υ 3306, 3078, 1672, 1600, 1429, 1269, 996, 829, 758; ^1H NMR (400 MHz, DMSO-*d6*): δ (ppm) 0.65 (brs, 6H, H-i, H-j), 2.07 (s, 3H, *p*-cym CH_3, H-a), 3.16 (brs, 1H, *p*-cym CH, H-h), 5.69 (brs, 4H, *p*-cym ArH, H-c, H-d, H-e, H-f), 7.71-7.77 (m, 3H, H-15, H-16, H-17), 7.88 (dd, 1H, *J1* = 8.8 Hz, *J2* = 1.6 Hz, ArH, H-2), 8.01 (d, 1H, *J* = 7.6 Hz, ArH, H-9), 8.09-8.12 (m, 3H, ArH, H-4, H-10, H-11), 8.41 (t, 1H, *J* = 7.6 Hz, ArH, H-18), 8.48 (d, 1H, *J* = 8.8 Hz, ArH, H-14), 8.68 (d, 1H, *J* = 7.6 Hz, H-1); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): (solubility problem); ^{31}P NMR (162 MHz, DMSO-*d*^{6}): δ(ppm) (-157.43)-(-135.48) (m, 1P, PF_6); ^{19}F NMR (376 MHz, $CDCl_3$): δ(ppm) -73.65, -71.75 (6F, PF_6); ESI-MS (CH_3OH): m/z 593.02 $[M-Cl]^+$.

5-chloro-2-(6-(4-formylphenyl)pyridin-2-yl)benzo[d]thiazole (7l2): Yield: 91%, R_f (20% ethyl acetate in hexane): 0.26; IR (cm^{-1}): υ 3055, 2845, 1693, 1604, 1573, 1452, 1427, 1301, 1209, 1161, 1068, 987, 794; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.40 (d, 1H, *J* = 8 Hz, ArCH), 7.87 (d, 1H, *J* = 8 Hz, ArCH), 7.93-7.99 (m, 2H, ArCH), 8.03 (d, 2H, *J* = 8 Hz, ArCH), 8.08 (s, 1H, ArCH), 8.32 (t, 3H, *J* = 8 Hz, ArCH), 10.11 (s, 1H, CHO); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.57, 120.03, 122.55, 122.73, 123.43, 126.27, 127.47, 129.94, 130.24, 132.32, 134.50, 136.83, 138.23, 143.50, 151.09, 155.19, 155.50, 171.40, 191.89 (CHO); ESI-MS (CH_3OH): m/z 351.03 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{5-chloro-2-(6-(4-formylphenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8l2):

51.3 mg (0.067 mmol, 94 %); *Mr* ($C_{29}H_{25}N_2OPSCl_2F_6Ru$) = 766.53 g/mol; Anal. calcd for $C_{29}H_{25}N_2OPSCl_2F_6Ru$ (%): C 45.44, H 3.29, N 3.65 Found: C 45.72, H 3.57, N 3.80.; Mp: 242-244°C decomp.; R_f (100% ethyl acetate): 0.21; IR (cm^{-1}): υ 3105, 2972, 1697, 1600, 1431, 1408, 1327, 1209, 1176, 1072, 929, 829, 742, 555; ^{1}H NMR (400 MHz, DMSO-*d6*): δ (ppm) 0.69 (d, 6H, *J* = 16.4 Hz, H-i, H-j), 2.08 (s, 3H, *p*-cym CH_3, H-a), 2.79-2.84 (m, 1H, *p*-cym CH, H-h), 5.76-5.82 (m, 3H, *p*-cym ArH, H-d, H-e, H-f), 6.13 (brs, 1H, *p*-cym ArH, H-c), 7.93 (d, 1H, *J* = 5.6 Hz, H-2), 8.10 (t, 1H, *J* = 8.0 Hz, ArH, H-10), 8.15 (brs, 1H, ArH, H-9), 8.22-8.25 (m, 2H, ArH, H-1, H-11), 8.36 (d, 1H, *J* = 8.4 Hz, ArH, H-17), 8.43-8.50 (m, 2H, ArH, H-14, H-15), 8.55 (d, 1H, *J* = 8.8 Hz, H-4), 8.78 (d, 1H, *J* = 7.6 Hz, H-18); ^{13}C NMR (100 MHz, DMSO-d^6): (solubility problem); ^{31}P NMR (DMSO-*d6,* 162 MHz): δ(ppm) (-153.01)-(-131.06) (m, 1P, PF_6); ^{19}F NMR (376 MHz, DMSO-d^6): δ(ppm) -71.03, -69.14 (6F, PF_6); ESI-MS (CH_3OH): m/z 621.01 $[M-Cl]^+$.

5-chloro-2-(6-(4-acetylphenyl)pyridin-2-yl)benzo[d]thiazole (7l3): Yield: 96%, R_f (20% ethyl acetate in hexane): 0.21; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.67 (s, 3H, $COCH_3$) 7.39 (d, 1H, *J* = 8 Hz, ArCH), 7.70 (d, 1H, *J* = 8 Hz, ArCH), 7.85-7.94 (m, 3H, ArCH), 8.03-8.10 (m, 3H, ArCH), 8.22 (d, 1H, *J* = 7.6 Hz, ArCH), 8.30 (d, 1H, *J* = 7.6 Hz, ArCH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.82 (Acetyl CH_3), 119.83, 122.42, 122.74, 123.39, 126.23, 127.06, 127.46, 128.93, 129.03, 132.30, 134.59, 137.60, 138.18, 142.21, 150.98, 155.18, 155.71, 171.57, 197.83 (C=O); ESI-MS (CH_3OH): m/z 365.04 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{5-chloro-2-(6-(4-acetylphenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8l3):

49.7 mg (0.064 mmol, 93 %); *Mr* ($C_{30}H_{27}N_2OPSCl_2F_6Ru$) = 780.55 g/mol; Anal. calcd for $C_{30}H_{27}N_2OPSCl_2F_6Ru$ (%): C 46.16, H 3.49, N 3.59 Found: C 46.41, H 3.77, N 3.85.; Mp: 235-237°C decomp.; R_f (100% ethyl acetate): 0.22; IR (cm^{-1}): υ 2972, 1687, 1600, 1402, 1263, 1226, 1182, 1072, 927, 833, 744, 555; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.61 (d, 3H, *J* = 6.8 Hz, H-j), 0.87 (d, 3H, *J* = 6.8 Hz, H-i), 2.11 (s, 3H, *p*-cym CH_3, H-a), 2.33-2.38 (m, 1H, *p*-cym CH, H-h), 2.69 (3H, -$COCH_3$, H-20), 5.40-5.46 (m, 2H, *p*-cym ArH, H-e, H-f), 5.58 (d, 2H, *J* = 6.0 Hz, *p*-cym ArH, H-c, H-d), 7.66 (d, 2H, *J* = 7.2 Hz, H-2, H-9), 7.78-7.81 (m, 1H, ArH, H-10), 7.96 (brs, 1H, ArH, H-1), 8.01 (t, 2H, *J* = 8.4 Hz, ArH, H-11, H-17), 8.22-8.24 (m, 4H, ArH, H-4, H-14, H-15, H-18); ^{13}C NMR (100 MHz, DMSO-d^6): (solubility problem); ^{31}P NMR (DMSO-d^6*,* 162 MHz): δ(ppm) (-157.40)-(-135.45) (m, 1P, PF_6); ^{19}F NMR (DMSO-d^6*,* 376 MHz): δ(ppm) -71.03, -69.15 (6F, PF_6); ESI-MS (CH_3OH): m/z 635.03 $[M-Cl]^+$.

5-chloro-2-(6-(4-chlorophenyl)pyridin-2-yl)benzo[d]thiazole (7l4): Yield: 95%; R_f (20% ethyl acetate in hexane): 0.47; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.39 (d, 1H, *J* = 8 Hz,

ArCH), 7.49 (d, 2H, *J* = 8.8 Hz, ArCH), 7.80-7.87 (q, 2H, ArCH), 7.91 (t, 1H, *J* = 8 Hz, ArCH), 8.05 (m, 3H, ArCH), 8.26 (d, 1H, *J* = 8 Hz, ArCH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.24, 121.67, 122.69, 123.37, 126.15, 128.17, 129.06, 132.25, 134.60, 135.78, 136.48, 138.07, 150.80, 155.22, 155.87, 171.72; ESI-MS (CH_3OH): m/z 356.99 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{5-chloro-2-(6-(4-chlorophenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8l4): 55.85 mg (0.072 mmol, 93 %); *Mr* ($C_{28}H_{24}N_2PSCl_3F_6Ru$) = 772.96 g/mol; Anal. calcd for $C_{28}H_{24}N_2PSCl_3F_6Ru$ (%): C 43.51, H 3.13, N 3.62 Found: C 43.81, H 3.40, N 3.86.; Mp: 237-239°C decomp.; R_f (100% ethyl acetate): 0.25; IR (cm^{-1}): υ 2974, 1737, 1597, 1487, 1406, 1325, 1276, 1182, 1093, 833, 808, 555; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 1.27 (d, 6H, *J* = 6.8 Hz, *p*-cym CH_3, H-i, H-j), 2.14 (s, 3H, *p*-cym CH_3, H-a), 2.89 (sept, 1H, *J* = 6.8 Hz, *p*-cym CH, H-h), 5.34 (d, 2H, *J* = 5.6 Hz, *p*-cym ArH, H-e H-f), 5.46 (d, 2H, *J* = 5.6 Hz, *p*-cym ArH, H-c, H-d), 7.49 (d, *J* = 8.4 Hz, 1H, ArH, H-15), 7.65 (brs, 3H, ArH, H-2, H-9, H-17), 7.82-7.88 (m, 2H, ArH, H-1, H-10), 7.98 (s, 1H, ArH, H-11), 8.08 (d, 1H, *J* = 8.0 Hz, ArH, H-4), 8.28 (d, 2H, *J* = 7.2 Hz, ArH, H-14, H-18); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): (solubility problem); ^{31}P NMR (162 MHz, DMSO-*d*^{6}): δ(ppm) (-157.40)-(-135.45) (m, 1P, PF_6); ^{19}F NMR (376 MHz, DMSO-*d*^{6}): δ(ppm) = -71.05, -69.15 (6F, PF_6); ESI-MS (CH_3OH): m/z 626.98 $[M-Cl]^+$.

5-chloro-2-(6-(4-fluorophenyl)pyridin-2-yl)benzo[d]thiazole (7l5): Yield: 95%, R_f (20% ethyl acetate in hexane): 0.15; ^{1}H NMR (100 MHz, $CDCl_3$): δ (ppm) 7.21 (t, 2H, *J* = 8.8 Hz, ArH), 7.39 (d, 1H, *J* = 8.4 Hz, ArH), 7.81 (d, 1H, *J* = 7.6 Hz, ArH), 7.85-7.93 (m, 2H, ArH), 8.08 (s, 1H, ArH), 8.12-8.15 (m, 2H, ArH), 8.26 (d, 1H, *J* = 7.6 Hz, ArH); ^{13}C NMR (400 MHz, $CDCl_3$): δ 115.7, 115.9, 118.9, 121.6, 122.7, 123.4, 126.1, 128.7, 128.8, 132.2, 134.2, 134.2, 134.6, 138.0, 150.7, 155.2, 156.1, 171.8; ^{19}F NMR (400 MHz, $CDCl_3$): δ(ppm) = -112.00 (s, 1F); LC-MS (CH_3OH): m/z 341.02 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{5-chloro-2-(6-(4-fluorophenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8l5):

50.5 mg (0.067 mmol, 92 %); *Mr* ($C_{28}H_{24}N_2PSCl_2F_7Ru$) = 756.51 g/mol; Anal. calcd for $C_{28}H_{24}N_2PSCl_2F_7Ru$ (%): C 44.46, H 3.20, N 3.70 Found: C 44.71, H 3.48, N 4.06.; Mp: 236-238°C decomp.; R_f (100% ethyl acetate): 0.24; IR (cm^{-1}): υ 2976, 1736, 1599, 1477, 1406, 1327, 1274, 1181, 1094, 836, 808, 555; ^{1}H NMR (400 MHz, DMSO): δ (ppm) solubility problem; ^{13}C NMR (100 MHz, DMSO-*d*^{6}): (solubility problem); ^{31}P NMR (162 MHz, DMSO-*d*^{6}): δ(ppm) (-157.38)-(-135.43) (m, 1P, PF_6); ^{19}F NMR (376 MHz, DMSO-*d*^{6}): δ(ppm) -79.76, -77.23 (1F), -71.04, -69.15 (6F, PF_6); LC-MS (CH_3OH): m/z 611.01 $[M-Cl]^+$.

5-chloro-2-(6-(4-(trifluoromethyl)phenyl)pyridin-2-yl)benzo[d]thiazole (7l6): Yield: 92%, R_f (16.5% ethyl acetate in hexane): 0.42; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.39 (d, 1H, *J* = 8.4 Hz, ArH), 7.64 (t, 1H, *J* = 8 Hz, ArH), 7.72 (d, 1H, *J* = 7.6 Hz, ArH), 7.85-7.88 (m, 2H, ArH), 7.95 (t, 1H, *J* = 8 Hz, ArH), 8.07 (s, 1H, ArH), 8.31 (brs, 2H, ArH), 8.39 (s, 1H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.7, 121.9, 122.7, 123.4, 123.7, 123.8, 126.2, 129.4, 130.1, 131.2, 131.5, 132.3, 134.6, 138.2, 138.8, 150.8, 155.2, 155.4, 171.5; ^{19}F NMR (376 MHz, $CDCl_3$): δ(ppm) -62.63 (s, 3F); LC-MS (CH_3OH): m/z 391.02 $[M+H]^+$

[(η^6-*p*-cymene)RuCl{5-chloro-2-(6-(4-(trifluoromethyl)phenyl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8l6):

48.5 mg (0.06 mmol, 94 %); *Mr* ($C_{29}H_{24}N_2PSCl_2F_9Ru$) = 806.51 g/mol; Anal. calcd for $C_{29}H_{24}N_2PSCl_2F_9Ru$ (%): C 43.19, H 3.00, N 3.47 Found: C 43.51, H 3.34, N 3.27.; R_f (100%

ethyl acetate): 0.20; Mp: 239-241°C decomp.; IR (cm^{-1}): υ 3120, 3041, 2972, 1598, 1552, 1406, 1313, 1226, 1124, 1072, 929, 831, 758, 555; ^{1}H NMR (400 MHz, DMSO-*d6*): δ (ppm) 1.18 (d, 6H, *J* = 6.8 Hz, H-i, H-j), 2.08 (s, 3H, *p*-cym CH_3, H-a), 2.79-2.86 (m, 1H, *p*-cym CH, H-h), 5.77 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, H-e, H-f), 5.81 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, H-c, H-d), 7.56-7.59 (m, 1H, H-10), 7.87 (d, 1H, *J* = 8.0 Hz, ArH, H-2), 7.92 (d, 1H, *J* = 8.8 Hz, ArH, H-9), 7.99 (t, 1H, *J* = 8.0 Hz, ArH, H-17), 8.15(brs, 1H, ArH, H-15), 8.21 (brs, 1H, H-1), 8.32 (d, 1H, *J* = 7.6 Hz, H-11), 8.47 (d, 1H, *J* = 8.0 Hz, H-14), 8.56 (d, 1H, *J* = 8.4 Hz, H-18), 8.79 (d, 1H, *J* = 8.0 Hz, H-4); ^{13}C NMR (100 MHz, DMSO-*d6*): (solubility problem); ^{31}P NMR (162 MHz, DMSO-*d6*): δ(ppm) (-157.39)-(-131.04) (m, 1P, PF_6); ^{19}F NMR (376 MHz, DMSO-*d6*): δ(ppm) = -71.04, -69.15 (6F, PF_6), -60.68 (s, 3F, CF_3); ESI-MS (CH_3OH): m/z 661.01 $[M-Cl]^+$.

.**5-chloro-2-(6-(naphthalen-1-yl)pyridin-2-yl)benzo[d]thiazole (7l7):** Yield: 95%, R_f (20% ethyl acetate in hexane): 0.65; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.39 (t, 1H, *J* = 8 Hz, ArC), 7.52-7.55 (m, 2H, ArC), 7.58-7.62 (m, 1H, ArC), 7.69-7.73 (m, 2H, ArC), 7.81-7.87 (m, 1H, ArC), 7.95-8.01 (m, 3H, ArC), 8.08 (d, 1H, *J* = 12.0 Hz, ArC), 8.28-8.33 (m, 1H, ArC), 8.38 (d, 1H, *J* = 8 Hz, ArC); ^{13}C NMR (100 MHz, $CDCl_3$): δ 118.9, 119.6, 122.7, 122.8, 123.3, 123.5, 125.3, 125.6, 126.0, 126.5, 126.6, 126.9, 127.9, 128.5, 129.5, 129.9, 131.1, 132.2, 134.1, 137.3, 137.6, 139.3; LC-MS (CH_3OH): m/z 373.05 $[M+H]^+$.

[(η^6-*p*-cymene)RuCl{5-chloro-2-(6-(naphthalen-1-yl)pyridin-2-yl)benzo[d]thiazole}]PF_6 (8l7):

50.7 mg (0.064 mmol, 96 %); *Mr* ($C_{32}H_{27}N_2PSCl_2F_6Ru$) = 788.57 g/mol; Anal. calcd for $C_{32}H_{27}N_2PSCl_2F_6Ru$ (%): C 48.74, H 3.45, N 3.55 Found: C 48.97, H 3.77, N 3.16.; Mp: 240-242°C decomp. ; R_f (100% ethyl acetate): 0.27; IR (cm^{-1}): υ 3122, 3045, 2806, 1734, 1593, 1404, 1182, 1072, 925, 829, 781, 553; ^{1}H NMR (400 MHz, DMSO-*d6*): δ (ppm) 1.18 (d, 6H, *J* = 7.6 Hz, H-i, H-j), 2.07 (s, 3H, *p*-cym CH_3, H-a), 2.78-2.85 (m, 1H, *p*-cym CH, H-h), 5.75 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, H-e, H-f), 5.80 (d, 2H, *J* = 6.0 Hz, *p*-cym ArH, H-c, H-d), 7.84-7.90 (m, 2H, H-1, H-2), 7.92 (d, 1H, *J* = 5.6 Hz, ArH, H-15), 7.99 (t, 1H, *J* = 8.0 Hz, ArH, H-9), 8.06 (d, 2H, *J* = 6.8 Hz, ArH, H-1, H-10), 8.19-8.21 (m, 1H, ArH, H-11), 8.26 (d, 1H, *J* = 8.0 Hz, H-19), 8.32 (d, 1H, *J* = 7.6 Hz, H-17), 8.36 (d, 1H, *J* = 8.0 Hz, H-4), 8.47 (t, 1H, *J* = 7.6 Hz, H-18), 8.55 (d, 1H, *J* = 8.8 Hz, H-20), 8.82 (1H, d, *J* = 7.6 Hz, H-14).; ^{13}C NMR (100 MHz, DMSO-*d6*): (solubility problem); ^{31}P NMR (162 MHz, DMSO-*d6*): δ(ppm) (-157.40)-(-131.06) (m, 1P, PF_6); ^{19}F NMR (376 MHz, DMSO-*d6*): δ(ppm) -71.03, -69.14 (6F, PF_6); LC-MS (CH_3OH): m/z 643.03 $[M-Cl]^+$.

2-(6-(benzo[b]thiophen-2-yl)pyridin-2-yl)-5-chlorobenzo[d]thiazole (7l8): Yield: 90%; R_f (16.5% ethyl acetate in hexane): 0.53; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.39-7.42 (m, 3H, ArH), 7.50 (s, 1H, ArH), 7.57 (d, 1H, *J* = 7.6 Hz, ArH), 7.70 (d, 1H, *J* = 8 Hz, ArCH), 7.85 (s, 1H, ArCH), 7.87-7.90 (m, 2H, ArCH), 8.06 (s, 1H, ArCH), 8.29 (d, 1H, *J* = 7.6 Hz, ArCH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.6, 121.4, 122.2, 122.8, 123.7, 124.8, 124.9, 126.5, 128.5, 128.6, 129.9, 132.1, 132.2, 132.5, 134.6, 139.3, 141.8, 151.9, 154.9; LC-MS (CH_3OH): m/z 379.01 $[M+H]^+$.

[(η^6-*p*-cymene)Ru-2-(6-(benzo[b]thiophen-2-yl)pyridin-2-yl)-5-chlorobenzo[d]thiazole (8l8):

49.8 mg (0.063 mmol, 95 %); *Mr* ($C_{30}H_{25}N_2PS_2Cl_2F_6Ru$) = 794.60 g/mol; Anal. calcd for $C_{30}H_{25}N_2PS_2Cl_2F_6Ru$ (%): C 45.35, H 3.17, N 3.53 Found: C 45.72, H 3.48, N 3.26.; Mp: 242-244°C decomp. ; R_f (100% ethyl acetate): 0.29; IR (cm^{-1}): υ 3126, 3045, 2973, 1589, 1552,

1409, 1323, 1226, 1126, 1071, 929, 834, 768, 554; ^{1}H NMR (400 MHz, DMSO-*d6*): δ (ppm) 1.18 (d, 6H, *J* = 7.2 Hz, H-i, H-j), 2.08 (s, 3H, *p*-cym CH_3, H-a), 2.79-2.86 (m, 1H, *p*-cym CH, H-h), 5.77 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, H-e, H-f), 5.81 (d, 2H, *J* = 6.0 Hz, *p*-cym ArH, H-c, H-d), 7.57-7.59 (m, 4H, H-2, H-15, H-16, H-17), 7.87 (d, 1H, *J* = 7.6 Hz, ArH, H-1), 7.92 (t, 1H, *J* = 9.2 Hz, ArH, H-14), 8.0 (t, 1H, *J* = 8.0 Hz, ArH, H-18), 8.21-8.23 (m, 2H, ArH, H-9, H-11), 8.25 (s, 1H, H-4), 8.33 (d, 1H, *J* = 7.6 Hz, H-10); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): δ 18.3 (Me, C-a, *p*-cymene), 21.9 (Me, C-j, *p*-cymene), 24.4 (Me, C-i, *p*-cymene), 30.5 (CH, C-h, *p*-cymene), 84.8 (ArCH, C-f, *p*-cymene), 85.9 (ArCH, C-e, *p*-cymene), 86.8 (ArCH, C-d, *p*-cymene), 87.6 (ArCH, C-c, *p*-cymene), 100.6 (ArC, C-g, *p*-cymene), 106.9 (ArC, C-b, *p*-cymene), 120.4 (ArCH, C-4), 121.0 (ArCH, C-14), 122.4 (ArCH, C-18), 123.2 (ArCH, C-9), 124.7 (ArCH, C-15), 126.6 (ArCH, C-1), 126.9 (ArCH, C-11), 129.2 (ArCH, C-16), 129.2 (ArCH, C-17), 129.3 (ArCH, C-2), 131.1 (ArC, C-3), 131.8 (ArCH, C-5), 131.9 (ArC, C-20), 132.1 (ArC, C-19), 134.6 (ArCH, C-10), 141.6 (ArC, C-13), 144.8 (ArC, C-8), 151.1 (ArC, C-6), 154.9 (ArC, C-7), 169.6 (ArC, C12); ^{31}P NMR (162 MHz, DMSO-*d*^{6}): δ(ppm) = (-157.38)-(-131.03) (m, 1P, PF_6); ^{19}F NMR (376 MHz, DMSO-*d*^{6}): δ(ppm) = -71.06, -69.17 (6F, PF_6); ESI-MS (CH_3OH): m/z 648.99 $[M\text{-}Cl]^+$.

2-(6-(benzofuran-2-yl)pyridin-2-yl)-5-chlorobenzo[d]thiazole (7l9): Yield: 94%, R_f (16.5% ethyl acetate in hexane): 0.62; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.15 (s, 1H, ArCH), 7.52-7.55 (m, 1H, ArCH), 7.40 (d, 1H, *J* = 8 Hz, ArCH), 7.53-7.58 (m, 2H, ArCH), 7.62 (d, 1H, *J* = 6.8 Hz, ArCH), 7.70 (t, 1H, *J* = 7.6 Hz, ArCH), 7.86 (d, 1H, *J* = 8.4 Hz, ArCH), 7.92-8.01 (m, 1H, ArCH), 8.05 (s, 1H, ArCH), 7.29 (d, *J* = 8.0 Hz, 1H, ArCH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 103.70, 105.81, 111.29, 119.59, 121.40, 121.89, 122.81, 123.36, 123.47, 125.09, 126.48, 129.96, 132.48, 134.60, 137.97, 139.29, 141.78, 151.98, 154.96, 155.09; LC-MS (CH_3OH): m/z 363.03 $[M+H]^+$.

[(*η*^{6}-*p*-cymene)Ru-2-(6-(benzofuran-2-yl)pyridin-2-yl)-5-chlorobenzo[d]thiazole (8l9):

50.9 mg (0.065 mmol, 95 %); *Mr* ($C_{30}H_{25}N_2OPSCl_2F_6Ru$) = 778.54 g/mol; Anal. calcd for $C_{30}H_{25}N_2OPSCl_2F_6Ru$ (%): C 46.28, H 3.24, N 3.60 Found: C 46.62, H 3.71, N 3.92.; Mp: 244-246°C decomp.; R_f (100% ethyl acetate): 0.28; IR (cm^{-1}): υ 3126, 3040, 2970, 1589, 1552, 1408, 1328, 1226, 1125, 1071, 929, 834, 758, 555; ^{1}H NMR (400 MHz, DMSO-*d*^{6}): δ (ppm) 1.18 (d, 6H, *J* = 7.2 Hz, H-i, H-j), 2.08 (s, 3H, *p*-cym CH_3, H-a), 2.79-2.86 (m, 1H, *p*-cym CH, H-h), 5.77 (d, 2H, *J* = 6.4 Hz, *p*-cym ArH, H-e, H-f), 5.81 (d, 2H, *J* = 6.0 Hz, *p*-cym ArH, H-c, H-d), 7.57-7.59 (m, 2H, H-16, H-17), 7.73 (d, 1H, *J* = 8.4 Hz, H-14), 7.87 (d, 1H, *J* = 8.0 Hz, ArH, H-2), 8.01 (t, 2H, *J* = 8.0 Hz, ArH, H-15, H-18), 8.21-8.23 (m, 2H, ArH, H-1, H-10), 8.25 (s, 1H, H-4), 8.33 (d, 2H, *J* = 7.2 Hz, H-9, H-11); ^{13}C NMR (100 MHz, DMSO-*d*^{6}): Solubility problem; ^{31}P NMR (100 MHz, DMSO-*d*^{6}): δ(ppm) (-157.38)-(-135.43) (m, 1P, PF_6); ^{19}F NMR (100 MHz, DMSO-*d*^{6}): δ(ppm) = -71.06, -69.17 (6F, PF_6); LC-MS (CH_3OH): m/z 633.01 $[M\text{-}Cl]^+$.

In vitro cytotoxic activities (MTT assay)[1]

MTT assay, a standard protocol, has been used to determine the *in vitro* cytotoxicity.[2] This assay is based on the reduction of the yellow MTT tetrazolium salt (3-[4,5-dimethylthiazol-2-yl]-2,5 diphenyltetrazolium bromide) by mitochondrial dehydrogenases to form a blue MTT formazan in viable cells. Synthesized ruthenium(II)-*p*-cymene-2-aryl benzimidazole (BIZ), benzothiazole (BTZ) and benzoxazole (BOZ) scaffolds were accomplished above-mentioned to the experiment by dissolving in 0.1% DMSO followed by serial dilution with medium. Two different types of cancer cell lines i.e. human epitheloid cervix carcinoma (HeLa), human colorectal adenocarcinoma cell line (Caco-2), and one normal human embryonic kidney cells (HEK-293) were used in the assay. Nearly 1 × 10^4 cells per well for all the three cell lines were

cultured in 100 µL of a growth medium in 96-well plates and incubated at 37 °C under a 5% CO_2 atmosphere. After that the cells were treated with different concentrations of the complexes (1-200 µM) in the volume of 100 µM/well. cisplatin, chlorpromazine and RAPTA-C have been used as standard positive control drug. It was also mentioned that cells are in the control wells filled with the same volume of medium containing 0.1% DMSO. After 24 h (for HeLa and HEK-293) and 48 h (for Caco-2), the medium was superfluous and cell cultures were subjected to incubate with 100 µl MTT reagent (1 mg/ml) for 5 h at 37^o C. Then the suspension was placed on microvibrator for 10-15 min and sequentially the absorbance was recorded by the ELISA reader at λ = 570 nm. The experiment was also performed in triplicate. The data were expressed as the growth inhibition percentage calculated according to the equation: % cell viability = [OD_{sample}-OD_{blank}/$OD_{control}$-OD_{blank}] x 100, where OD_{sample} is the measured absorbance in wells containing samples, $OD_{control}$ is the absorbance measured for cells with a medium and a vehicle and $OD_{blank}$is the absorbance measured for blank well (no cells). Dose response curve was fitted in Origin 8.5 software and IC_{50} was calculated.

Conductivity measurement[1]

To confirm the interaction of the complexes with water, DMSO, GSH and CT-DNA solutions, conductivity of the prepared complexes were performed using conductivity-TDS meter-307 (Systronics, India) and cell constant 1.0 cm^{-1}.[3] Rate of conductivity was also measured in different PH medium. Time dependent Conductivity measurement was also performed.

Cellular imaging assay[1]

Cellular imaging study was performed by using cancerous HeLa cell line procured from NCCS. 6 well plates have been used for this study. Cultured cells with 80% confluence were taken followed by trypsinisation using 1-2 ml of 1X trypsin. Then, it was transferred to fresh 15 ml falcon tube and centrifuged for 2000 rpm for 1-5 min. DMEM fresh media (80µl) was added to the pellet formed at the bottom of the tube and the cells were seeded in 6 well plates. Subsequently, the complex **11j'** in PBS buffer was added to the well plates. After incubated for 2-4 h at 37 °C, all the wells were washed twice with PBS buffer (pH 7.4). Finally, the fluorescence images were recorded using the glass slides with an Olympus Fluorescence microscope at 480-550 nm excitations.[4]

DNA binding study[1]

The calf-thymus DNA (CT-DNA) binding tendency of the complexes was monitored by electronic spectra and competitive binding assay using a classical DNA intercalator, ethidium bromide (EtBr) by fluorescence spectroscopy.

UV–visible studies[1]

DNA binding experiments was conducted by using complex **5l** and **11c** in Tris-HCl buffer (5 mMTris-HCl in water, pH 7.4) in water medium.[5] The concentration of ct-DNA was determined from its absorbance intensity at 260 nm and its known molar absorption coefficient value 6600 M^{-1} cm^{-1}. Same concentration of DNA was taken both in the sample and reference in cuvettes. UV titration was conducted by subsequent increase of ct-DNA concentration. The sample was equilibrated with ct-DNA for about 5 min before each measurement. After that absorbance of the complex were estimated after each 5 µL addition of ct-DNA. The intrinsic DNA binding constant (K_b) was calculated using the equation (i):

$$\frac{[DNA]}{(\varepsilon_a - \varepsilon_f)} = \frac{[DNA]}{(\varepsilon_b - \varepsilon_f)} + \frac{1}{K_b(\varepsilon_a - \varepsilon_f)} (i)$$

Where [DNA] is the concentration of DNA in the base pairs, ε_a is the apparent extinction coefficient observed for the complex, ε_f corresponds to the extinction coefficient of the complex in its free form, and ε_b refers to the extinction coefficient of the complex when fully bound to DNA. Data were plotted using Origin 8.5 software to obtain the [DNA]/(ε_a-ε_f) vs. [DNA] linear plot. The ratio of the slope to intercept from the linear fit gives the value of the intrinsic binding constant (K_b).

Fluorescence study[1]

The emission property of all the synthesized complexes was investigated by using spectrofluorometric method. Fluorescence quantum yield (Φ) of all the prepared complexes performed in water solution were calculated by employing the comparative William's method which involves the use of well-characterized standard with the known quantum yield value.[6] Quinine sulfate was used as reference fluorophore excited at 350 nm and emission at 452 nm, quantum yield (Φ_R) = 0.50 in 1N H_2SO_4. The gradients of the plots are proportional to the quantum yield (Φ) of the studied system. The data obtained and quantum yield value calculated according to the equation (ii):

$$\Phi = \Phi_R \times (I_S / I_R) \times (OD_R / OD_S) \times (\eta_S / \eta_R) (ii)$$

Where, φ = Quantum yield, I = Peak Area, OD = absorbance at $\lambda_{max,}$ η = Refractive index of solvent and reference. Quinine Sulphate was used as a standard for calculating emission of quantum yield. 0.5 M H_2SO_4 was used as solvent for the standard and water for synthesized complexes.

Ethidium bromide displacement assay[1]

The ethidium bromide fluorescence displacement assay was performed to identify the mode of binding between the potent complexes with DNA.[7] The intercalation of EthB to DNA is accompanied by strong fluorescence emission owing to the formation of the EtBr-DNA complex. Once a second molecule intercalates into DNA, there is a decrease of number of binding sites on the DNA available to EtBr giving rise to reduction in the fluorescence intensity. The apparent binding constant (K_{app}) of the complex to CT-DNA was determined from the emission spectral measurements using ethidium bromide (EtBr) as a spectral probe in 5 mMTris-HCl buffer (pH 7.4). EtBr showed no apparent emission in Tris-buffer medium because of fluorescence quenching of free EthB by solvent molecules.[8] The emission intensity gets significantly enhanced due to its intercalative binding to duplex DNA. A competitive binding of the complex to DNA is found to reduce the EthB emission intensity. The relative binding propensity of the complex to DNA was estimated from the reduction of the emission intensity. The values of the apparent binding constant (K_{app}) were obtained by using the (iii) equation:

$$K_{app} \times [Complex]_{50} = K_{EtBr} \times [EtBr] (iii)$$

where K_{app} is the apparent binding constant of the complex studied, $[Complex]_{50}$ is the concentration of the complex at 50% quenching of DNA-bound ethidium bromide emission

intensity, K_{EthB} is the binding constant of the EtBr (K_{EtBr} = 1.0 x 10^7 M^{-1}), and [EtBr] is the concentration of ethidium bromide (8 μM). The Stern-Volmer quenching constant (K_{SV}) has been calculated by using Stern-Volmerequation.Stern-Volmer plots of F_0/F vs. [Complex] was prepared using the corrected fluorescence data taking into account the effect of dilution. Linear fit of the data using the equation (iv):[9]

$$I_0/I = 1 + \mathrm{K}_{SV}[Q] \quad (iv)$$

Where F_0 and F are the emission intensities of EthB-DNA in the absence and in the presence of complex of concentration [Q], gave the quenching constant (K_{SV}) using Origin Pro 8.5 software.

Protein binding studies[1]

Serum albumin proteins constitute a major component in blood plasma proteins and plays important roles in drug transport and metabolism.[10] The interaction of the drug with bovine serum albumin (BSA), a structural homolog with human serum albumin (HSA) has been studied from tryptophan emission quenching experiment. Emission intensity of BSA at λ = 340 nm decreases gradually with increasing the complex concentration, which confirms that the interaction between the complex and BSA have occurred. The complex solutions were gradually added to the solution of BSA (2 μM) in 5 mMTris-HCl/NaCl buffer (pH 7.2) and the quenching of the emission signals at 340 nm (λex = 295 nm) were recorded. The quenching constant (K_{BSA}) has been determined quantitatively by using Stern-Volmer equation. Stern-Volmer plots of F_0/F vs. [Complex] was made using the corrected fluorescence data taking into account the effect of dilution. Linear fit of the data using the equation (v):

$$I_0/I = 1 + \mathrm{K}_{BSA}[Q] = 1 + k_q\tau_0[Q] \quad (v)$$

Where, F_0 and F are the emission intensities of BSA in the absence and in the presence of quencher of concentration [Q], gave the quenching constant (K_{BSA}) using Origin Pro 8.0 software. kq is the quenching rate constant, τ_0 is the average lifetime of the tryptophan in BSA without quencher reported as 1x10^{-8} s. For such static quenching interaction, the binding constant (K) and the number of binding sites (n) can be determined according to the Scatchard equation (vi).[11]

$$\log(I_0 - I/I) = \log K + n\log[Q] \quad (vi)$$

Density functional theory

All theoretical calculations were done by using the computational code Gaussian 09W.[12] To avoid computational time and complexity, the 3D structure was calculated by applying the semi-empirical PM6 method in the gas phase. The resulting geometry were verified as minima by frequency calculation and the energy of the calculated structure was estimated by applying the time depended density functional theory (TD-DFT) method by using Becke 3-Parameter, Lee, Yang and Parr (B3LYP) functional and the 6-311G(d,p) basis set. The NBO program is embedded in Gaussian 09 package used for calculations was developed at optimized molecules by applying Hartree-Fock (HF) method using 6-311G(d,p) basis set.

MTT assay of compound 11j in HT-29

HT-29 and HeLa cells were grown in 96-well plates at 5000 cells per well. Cells were allowed to grow for 24 hours and followed by treated with the drug **11j** at different concentrations (1 µM to 15 µM). Twenty-four hours later, 10µL of 3-(4,4-dimethylthiazol-2-yl)-2,5-diph enyltetrazolium bromide (MTT) solution (5 mg/mL in PBS) was added to each well, and the plate was incubated at 37 °C for 4 hrs. Absorbance was measured on MULTISCAN sky plate reader (Thermo scientific) at a wavelength of 570 nm. The data was analysed and EC_{50} value was determined using Origin software. The cell growth/inhibition was expressed as the percentage of cell proliferation as compared to untreated control.

Morphological analysis

HT-29 cells were cultured in 6-well plate. After reaching 70% confluency, the cells were subjected to serum starvation for 6h. The cells were treated with various doses of the Drug **11j** (0, 5, 6.8 µM) for 24h. At the end of 24 hour's media was changed to fresh 10% FBS media containing Hoechst 33342 and the live cell morphology was observed under inverted microscope (Primovert, Zeiss) and the live cell images were captured using ZOE, cell imager (Bio-Rad).

Live and dead cell assay

Briefly, HT-29 cells were cultured in 6-well plate. After reaching 70% confluency, the cells were subjected to serum starvation for 6h. The cells were treated with various doses of the Complex**11j** (0, 5, 6.8 µM) for 24 h. At the end of 24 h media was changed to fresh 10% FBS media with 5 µL of 10 mM DCFDA so as to obtain a final concentration of 5 µM; 5µL of 10 mg/mL Hoechst solution (final concentration 5 µg/ml) and 200 µL of 1 mg/mL propidium iodide (final concentration 20µg/ml). Then the cells were incubated for 30 minutes in 37 °C incubator. After the completion of 30 minutes of incubation, the staining media was discarded and fresh media change was given before observation under fluorescent imager. The live cell nuclei was visible in blue (with Hoechst 33342 dye), the apoptotic cells were visible as pale blue with fragmented nuclei (with Hoechst 33342 dye) while the damaged cells were Red with PI. Captured images were then subjected to live and dead cell enumeration using ImageJ software and represented graphically.

Cell cycle analysis

For cell cycle analysis, approximately 1 million HT-29 cells were treated with the drug **11j** with concentrations 5 µM AND 6.8 µM respectively. After 24 hours of treatment, the cells were fixed with chilled 70% ethanol for 2 hours. Fixed cells were washed with PBS and stained with 500µl of the FxCycle™ PI/ RNase solution (Thermo Fisher Scientific, USA) for 30 minutes in dark. The cells were analysed using Guava EasyCyte Flow Cytometer (Millipore Sigma, USA). Untreated HT-29 cells were taken as control. Serum starvation for 6 hours was given prior to the treatment. Cell cycle data was analysed by FCS express 5.0 software (by De Novo software).

Annexin-V-FITC assay/ Apoptosis assay

Apoptosis was evaluated using PI/Annexin-V-FITC apoptosis detection kit (Invitrogen, Thermo Fisher). Briefly, cells cultured in 6 well plate were trypsinized, washed, stained with Annexin V-

FITC and PI for 15 minat room temperature in dark, and then analysed by guava easyCyte flow cytometer (Merck, Germany).This assay was repeated in 3 independent experiments and the data was analysed by FCS express 5.0 software (by De Novo software).

Statistical analysis

All the experiments were carried as biological and technical triplicates and results are presented as mean ± SD. The differences between more than two groups were analysed by two-way ANOVA. The P values of P≤0.05 (**) and P≤0.01 (***) were considered as significant. Error bar represents the ± standard error of mean by using graph pad prism software.

Author Contributions

Ashaparna Mondal and Nilmadhab Roy– Synthesis, characterization, photophysical study, DNA and BSA binding study of all the complexes

Utsav Sen - Biological evaluation of all synthesized compounds

Suban Kumar Sahoo–DFT study

Venkatesan Muthukumar–Stability study in UV and NMR

Priyankar Paira and Bipasha Bose- Manuscript preparation.

Reference and Notes:

1 (a) G. R.Jadhav, S. Sinha, M. Chhabra, P. Paira, *Bioorg. Med. Chem. Lett.*2016, **26**, 2695–2700; (b) S. K.Subran, S. Banerjee, A.Mondal, P. Paira, *New J. Chem*., 2016, **40**, 10333—10343; (c) A.Mondal, S. De, S.Maiti, B.Sarkar, A.K.Sk, R. Jacob, A. Moorthy, P. Paira, *Journal of Photochemistry & Photobiology, B: Biology*, 2018, **178**, 380–394; (d) S. De, S. Ray Chaudhuri, A. Panda, G. R. Jadhav, R. S. Kumar, P. Manohar, N. Ramesh, A. Mondal, A.Moorthy, S. Banerjee, P. Paira, A. K.SK,*New J. Chem*., 2019, **43**, 3291-3302; (e) B. Sarkar, A.Mondal, Y.Madaan, N.Roy, A. Moorthy, Y. –C.Kuo, P. Paira, *Dalton Transaction*, 2019, **48**, 12257-12271.

2 R. Menicagli, S. Samaritani, G. Signore, F. Vaglini, L. Dalla, *J. Med. Chem*. 2004, **47**, 4649–4652.

3 a) W. J. Geary, *Coord. Chem. Rev*., 1971, **7**, 81–122; (b) I. Ali, W. A. Wani, K. Saleem, *Synth. React. Inorg. Met. Org. Chem*, 2013, **43**, 1162–1170.

4 M. R. Gill, J. A. Thomas, *Chem. Soc. Rev*. 2012, **41**, 3179-3192.

5 M. Sirajuddin, S. Ali, A. Badshah, *J. Photochem. Photobio. B: Bio.*, 2013, **124**, 1–19.

6 M. S. Sani, F. Shirini, M. Abedini, M. Seddighi, *Res. Chem. Intermed*., 2016, **42**, 1091–1099.

7 S. Dasari, A. K. Patra, *Dalton Trans*. 2015, **44**, 19844-19855.

8 J. Keizer, *J. Am. Chem. Soc*., 1983, **105**, 1494–1498.

9 V. D. Suryawanshi, L. S. Walekar, A. H. Gore, P. V. Anbhule, G. B. Kolekar, *J. Pharm. Anal.* 2016, **6**, 56–63.

10 T.Nakamura, M.Oka, K. Aizawa, H.Soda, M. Fukuda, Terashi, K. Ikeda, Y. Mizuta, Y. Noguchi, Y.Kimura, T. Tsuruo, S. Kohno, *Biochem. Bioph. Res. Co*., 1999, **255**, 618-624.

11J. Liu, J. Tian, W. He, J. Xie, Z. Hu, X. Chen, *J. Pharm. Biomed. Anal*, 2004, **35**, 671-677.

12H. Tanak, *J. Mol. Struc*. 2015, **1090**, 86-92.