Supporting Information

Luminescent anticancer Ruthenium(II)-*p*-cymene complexes of extended imidazophenanthroline ligands: synthesis, structure, reactivity, biomolecular interaction and live cell imaging‡

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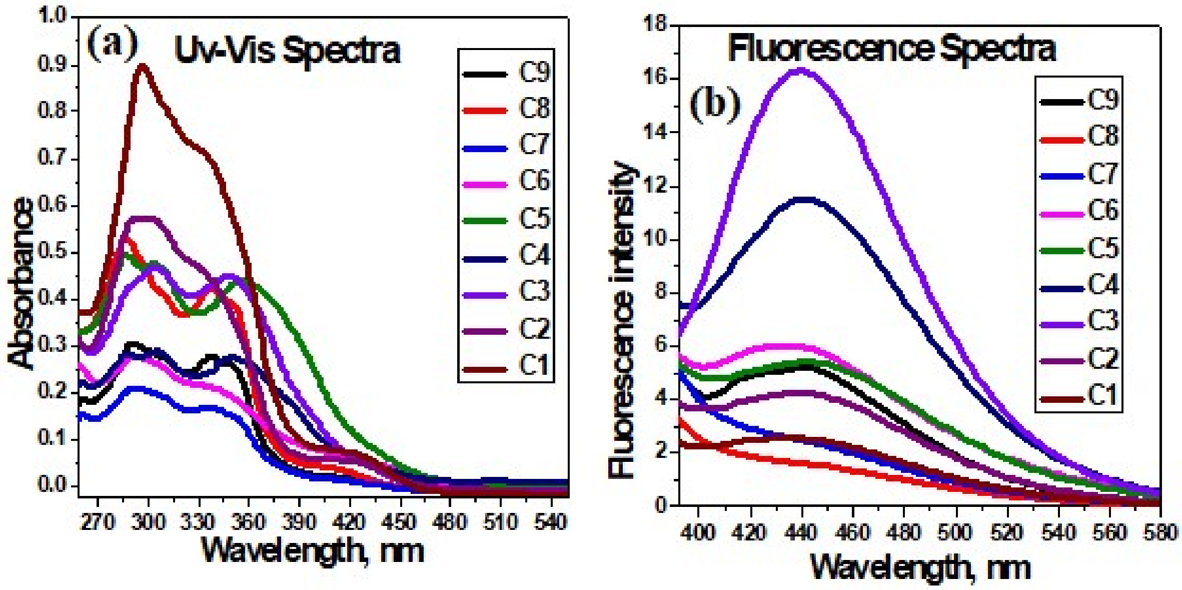
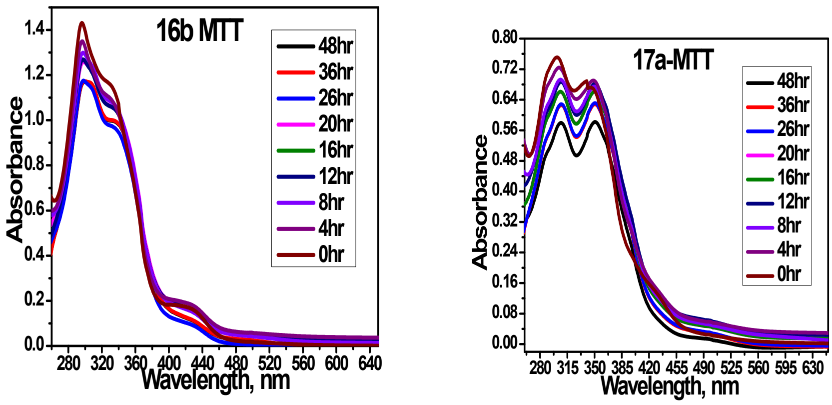


Figure S1: (a) UV-Vis Spectra and (b) Fluorescence spectra

C1: 16a, C2: 16b, C3: 17a, C4: 17b, C5: 17c, C6: 17d, C7: 19a, C8: 19b, C9: 19c



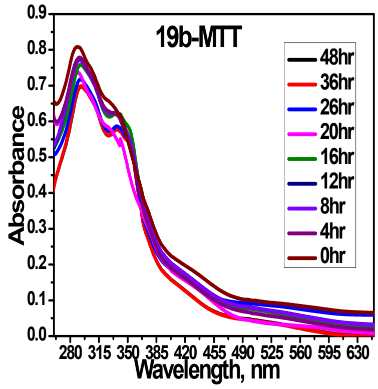
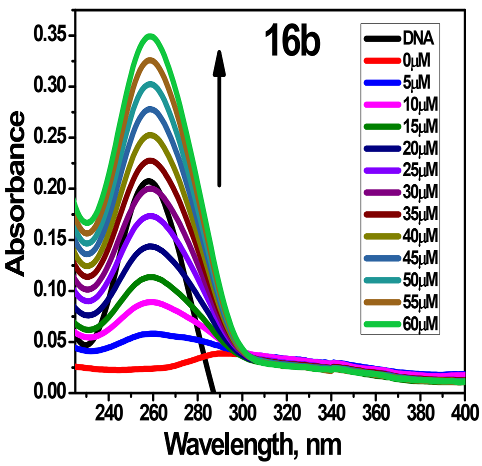
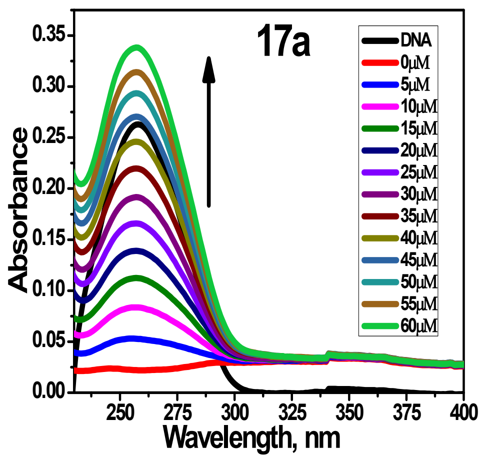


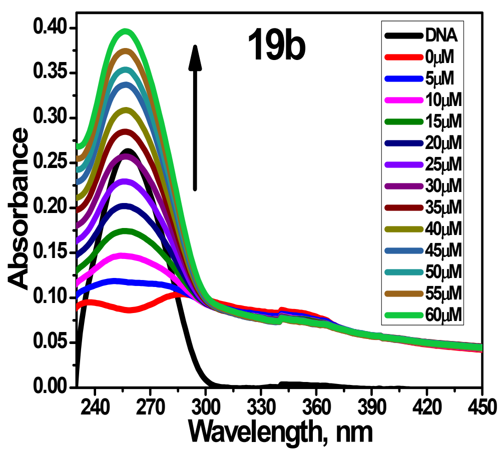
Figure S2: Stability study of Ru (II)-arene complexes (a) **16b**, (b) **17a** and (c) **19a** in 1% DMSO-PBS medium.



(a)

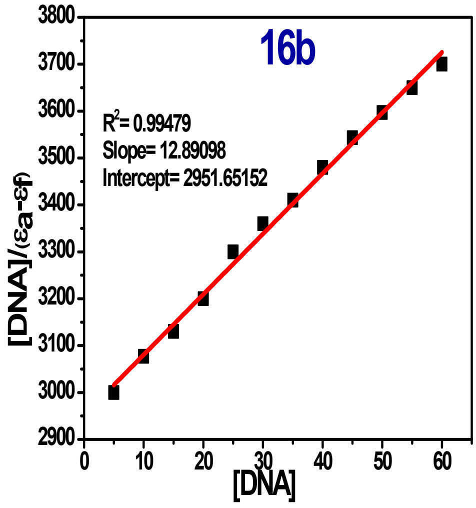


(b)

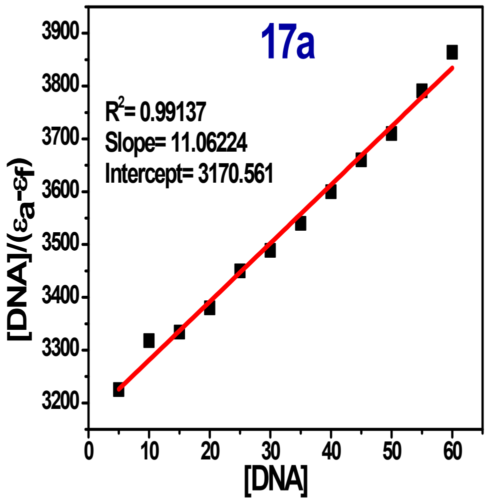


(c)

Figure S3. Absorption spectral traces for complexes (a) **16b**, (b) **17a** and (c) **19b** in 5 mM Tris-HCl-NaCl buffer with increasing concentration of CT-DNA.



(a)



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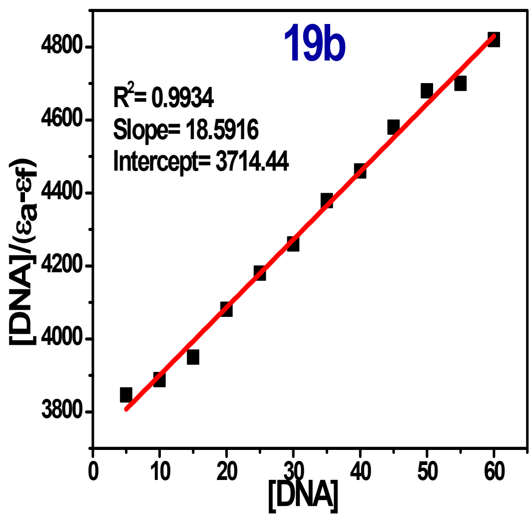
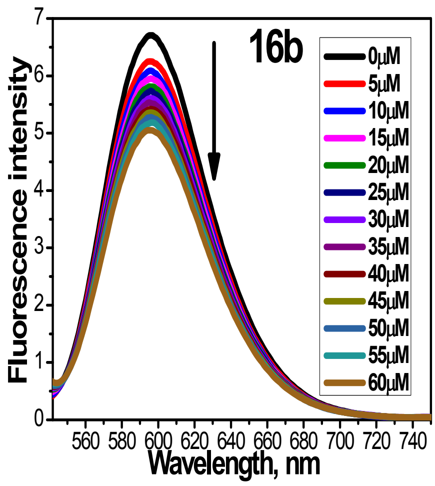
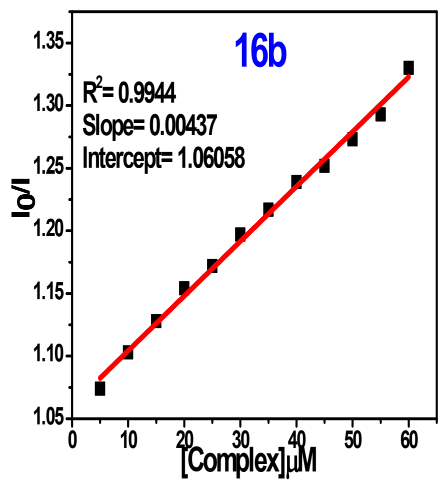


(c)

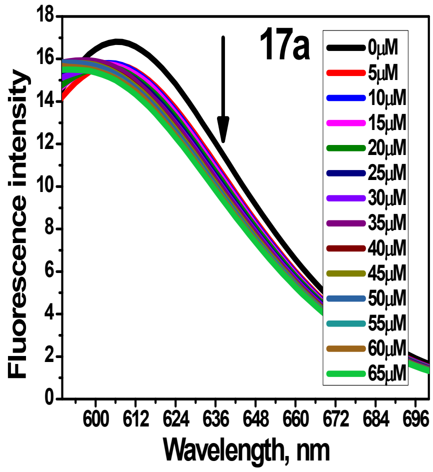
Figure S4: [DNA]/(ε_a-ε_f) vs. [DNA] linear plots of complex 16b, 17a and 19b.


16b
Fluorescence intensity
Wavelength, nm
0μM
5μM
10μM
15μM
20μM
25μM
30μM
35μM
40μM
45μM
50μM
55μM
60μM

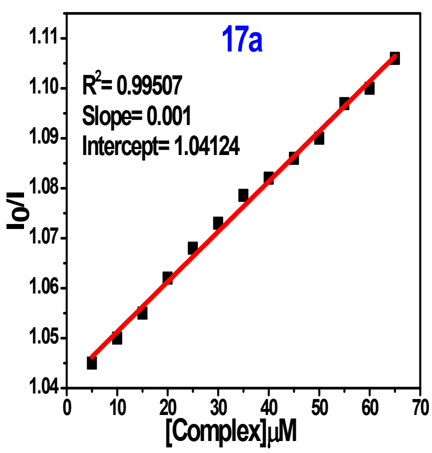
(a)


16b
R²= 0.9944
Slope= 0.00437
Intercept= 1.06058
Io/I
[Complex]μM

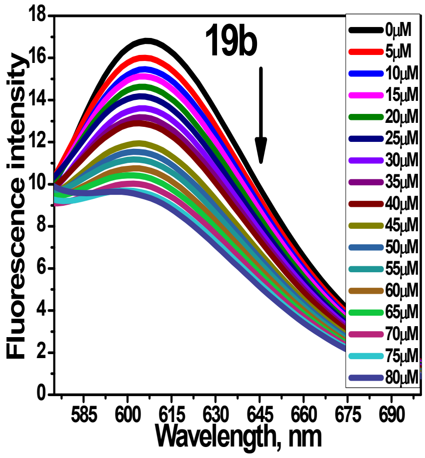
(b)


17a
Fluorescence intensity
Wavelength, nm
0μM
5μM
10μM
15μM
20μM
25μM
30μM
35μM
40μM
45μM
50μM
55μM
60μM
65μM

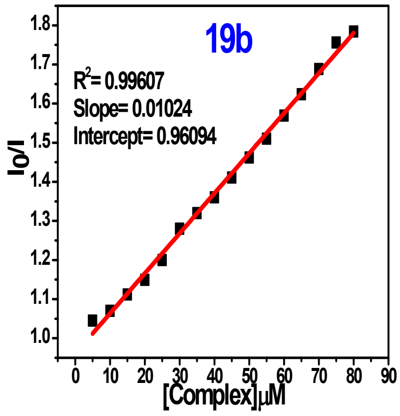
(c)


17a
R²= 0.99507
Slope= 0.001
Intercept= 1.04124
Io/I
[Complex]μM

(d)



(e)



(f)

Figure S5: Fluorescence spectra of EtBr-DNA of (a) 16b, (c) 17a and (e) 19a with increase in concentration of the complexes in 5 mM Tris-HCl /NaCl buffer of pH 7.2 at 298 K and the respective Stern-Volmer plots of I_0/I vs. complex (a) 16b, (c) 17a and (e) 19b.

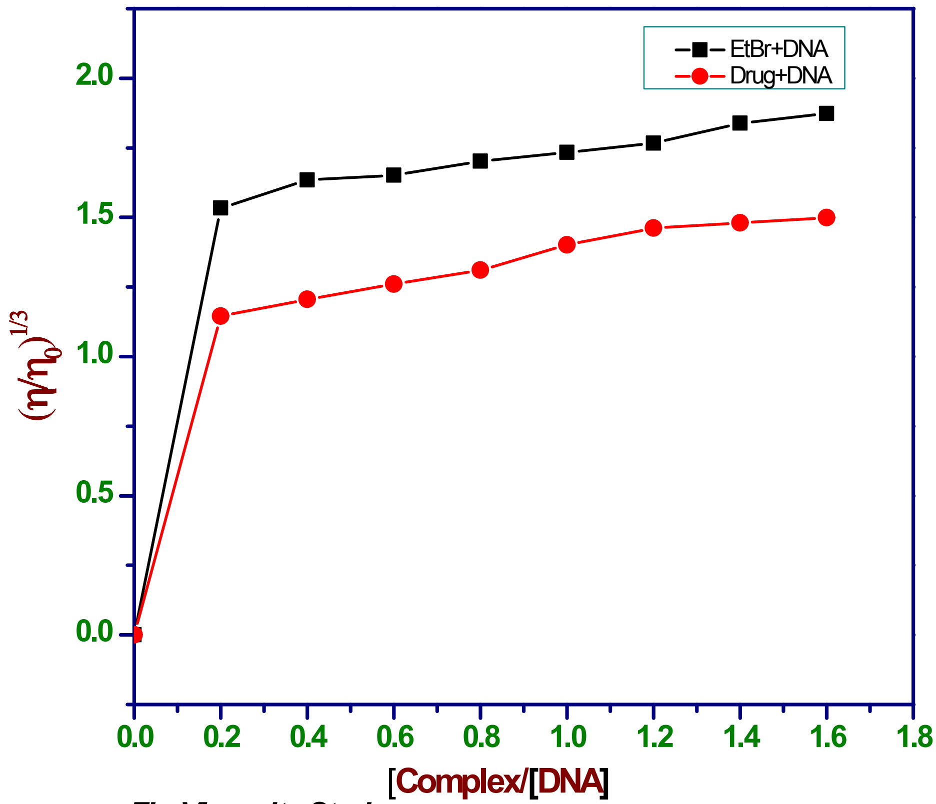
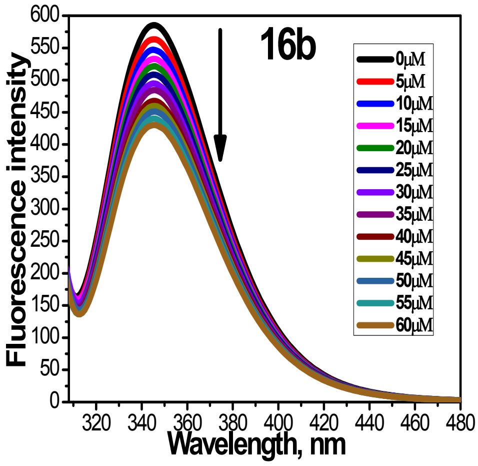
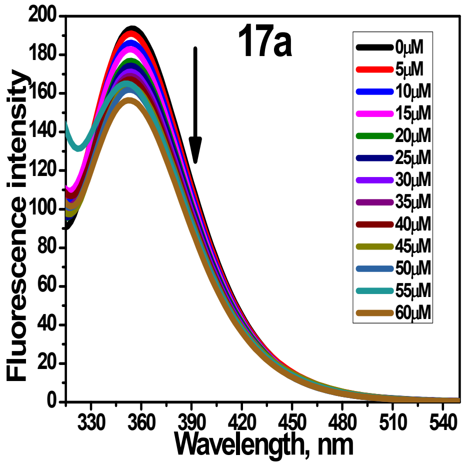


Fig:Viscosity Study

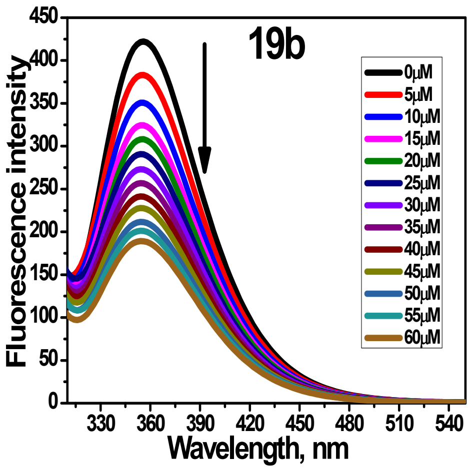
Fig. S6 Viscosity study of compound 16b with DNA



(a)



(b)



(c)

Figure S7: Fluorescence quenching of BSA on addition of complexes (a) 16b, (b) 17a and (c) 19c with increasing concentration of the complexes in 5 mM TrisHCl/NaCl buffer.

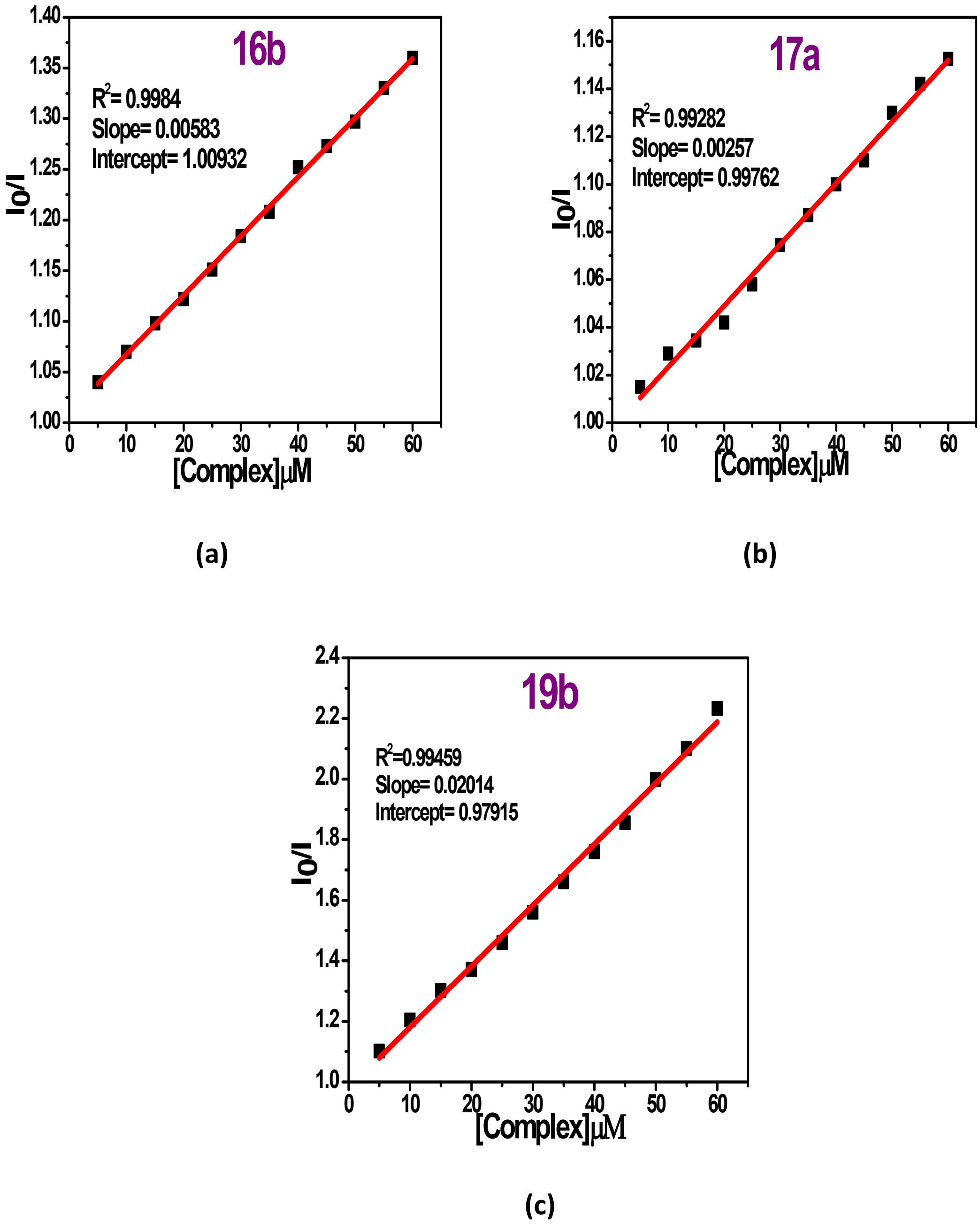
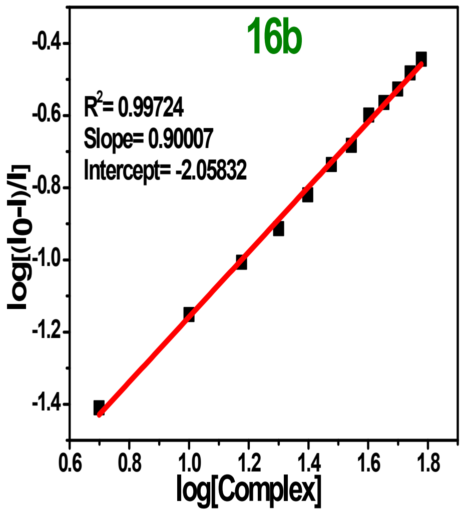
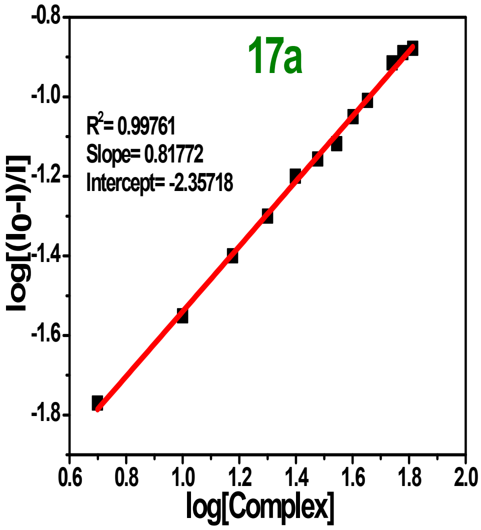


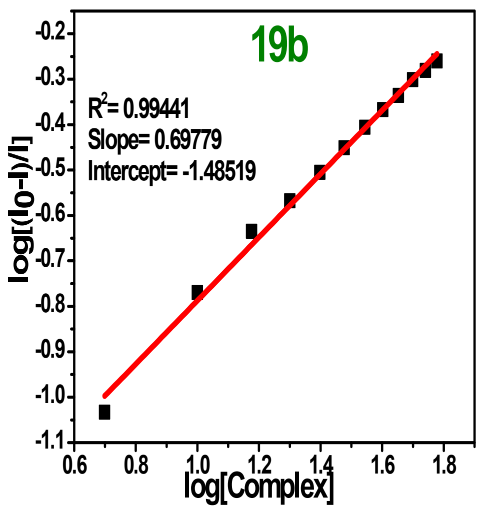
Figure S8: Plot ofI_0/I vs. concentrations of complexes (a) 16b, (b) 17a and (c) 19c.



(a)

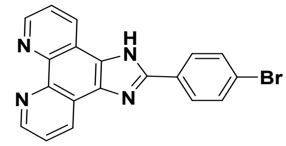


(b)

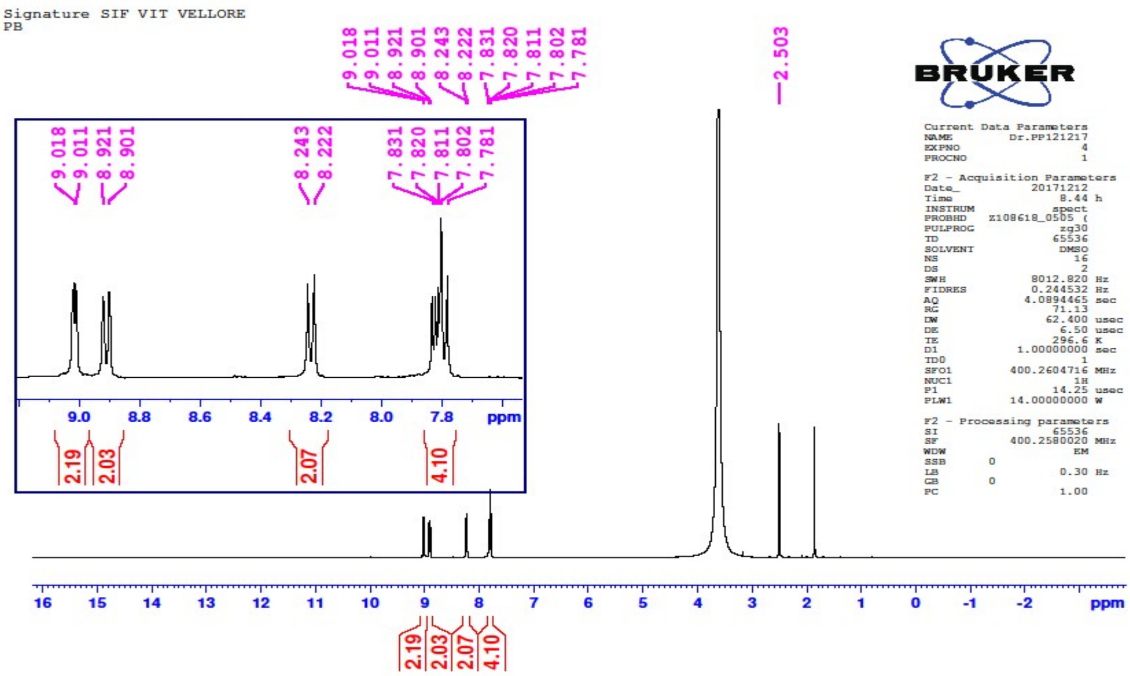


(c)

Figure S9: Scatchard plot of log([I_0-I]/I) vs. log[complex] for BSA in the presence of complexes (a) 16b, (b) 17a and (c) 19c.



(a) ^{1}H- NMR



(b) ^{13}C- NMR

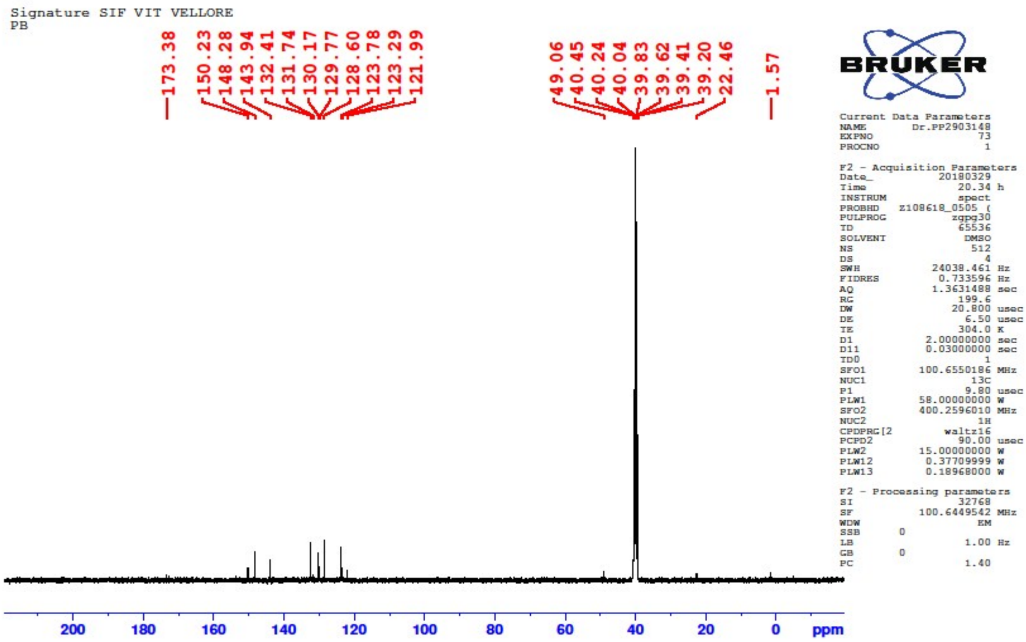
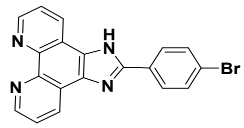
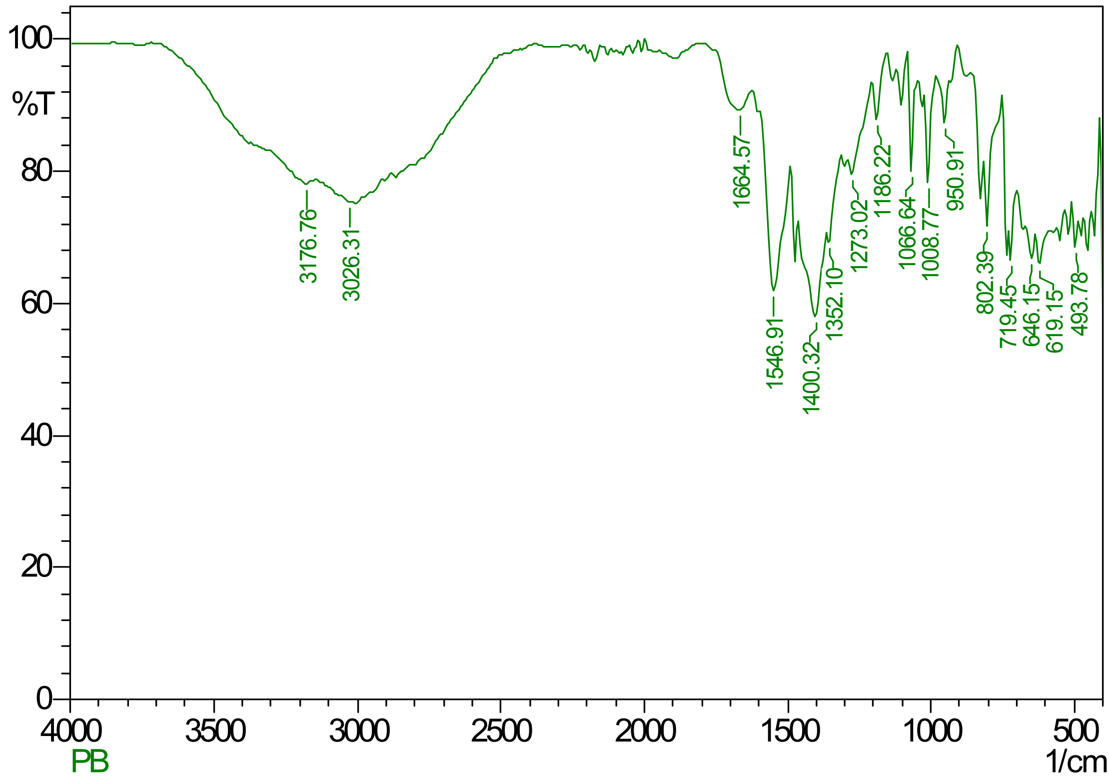


Figure S10: (a) ^{1}H-NMR and (b) ^{13}C-NMR of 10



(a) IR Spectra



(b) LC-MS spectra

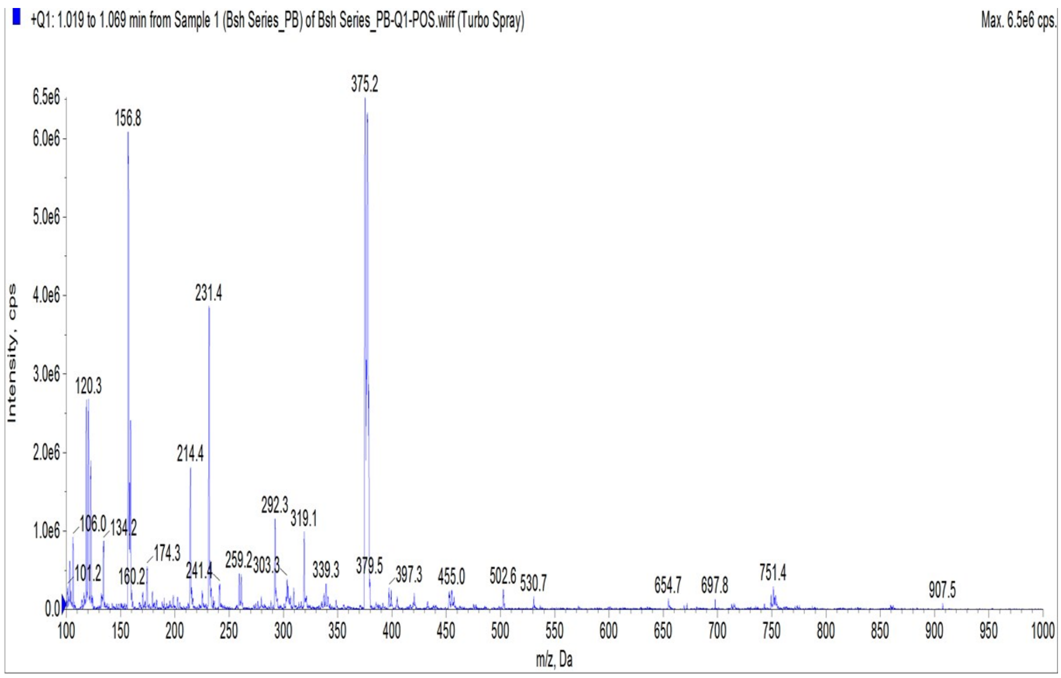
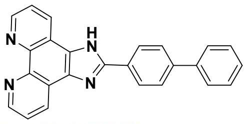
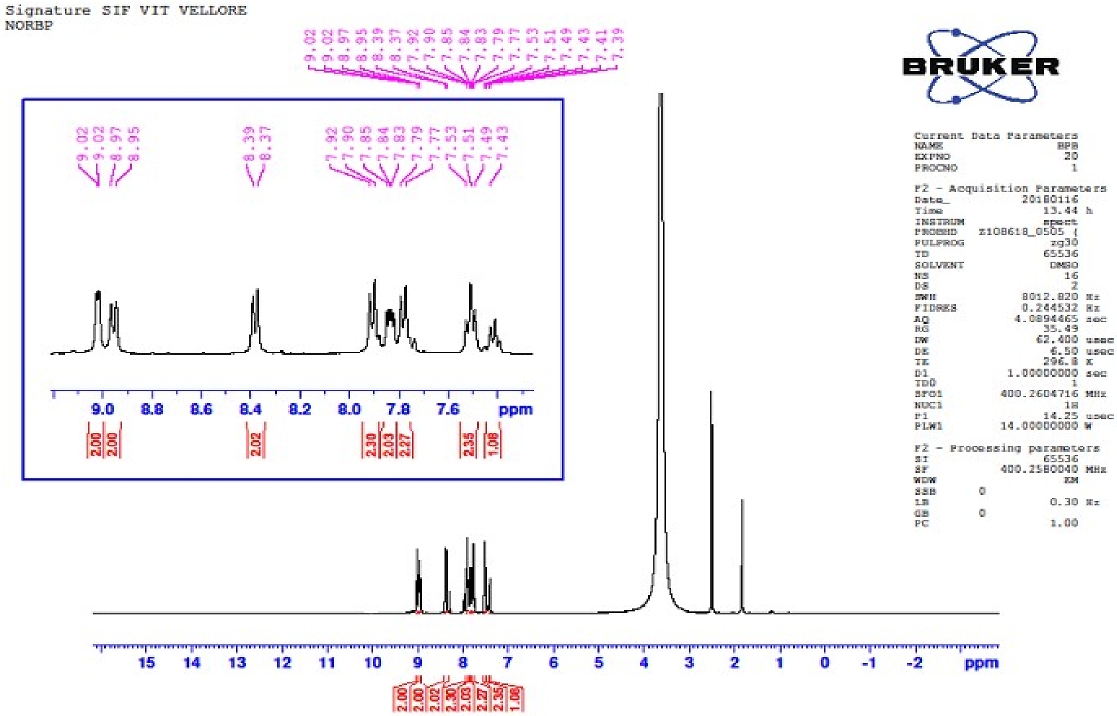


Figure S11: (a) IR Spectra and (b) LC-MS Spectra of 10



(a)



(b) ^{13}C-NMR

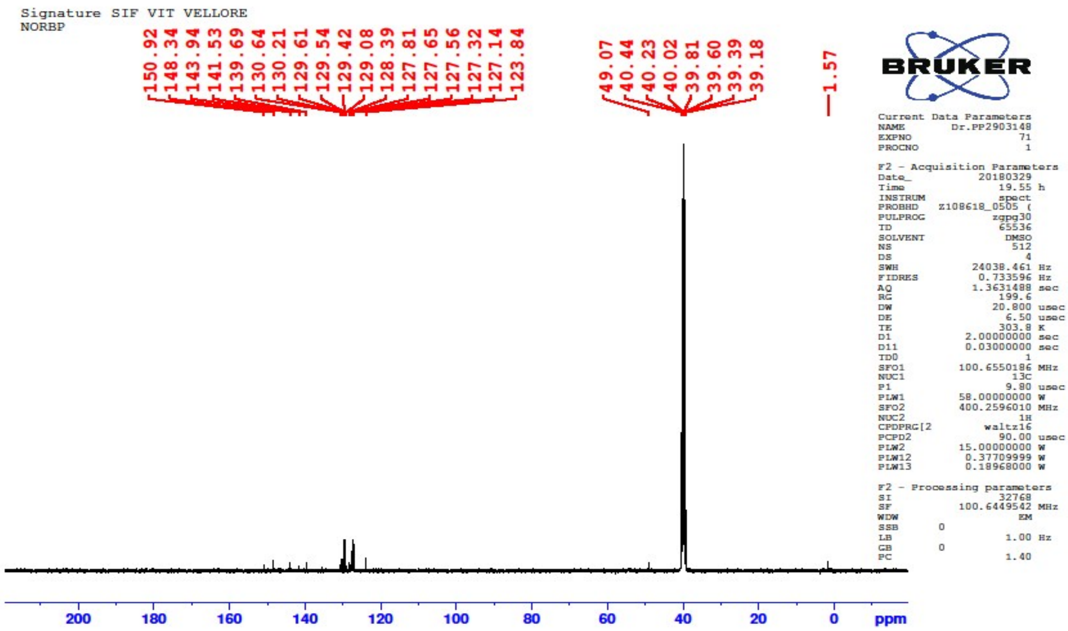
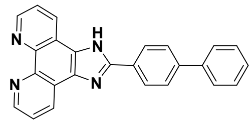
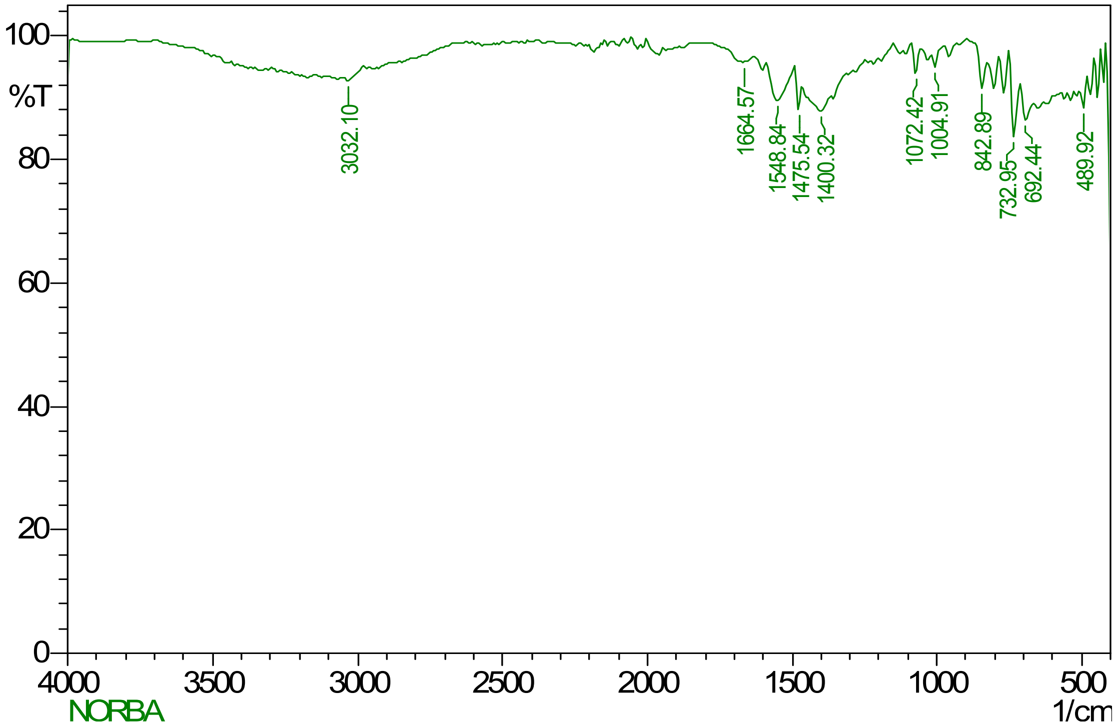


Figure S12: (a) ^{1}H-NMR and (b) ^{13}C-NMR of 12a



(a) Spectra



(b) LC-MS Spectra

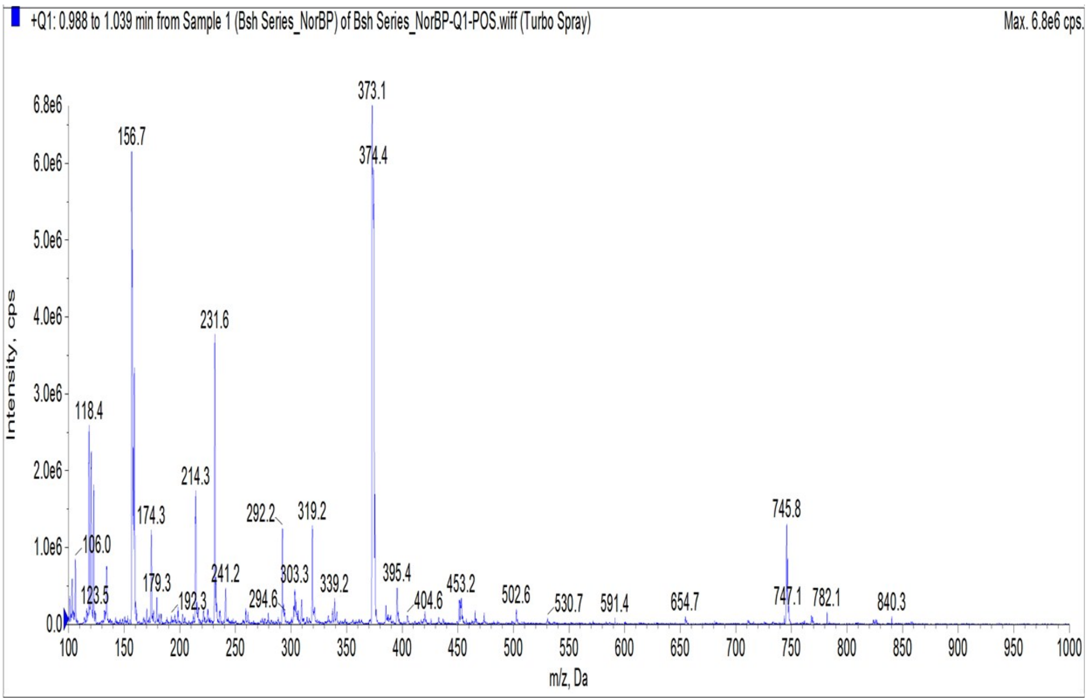
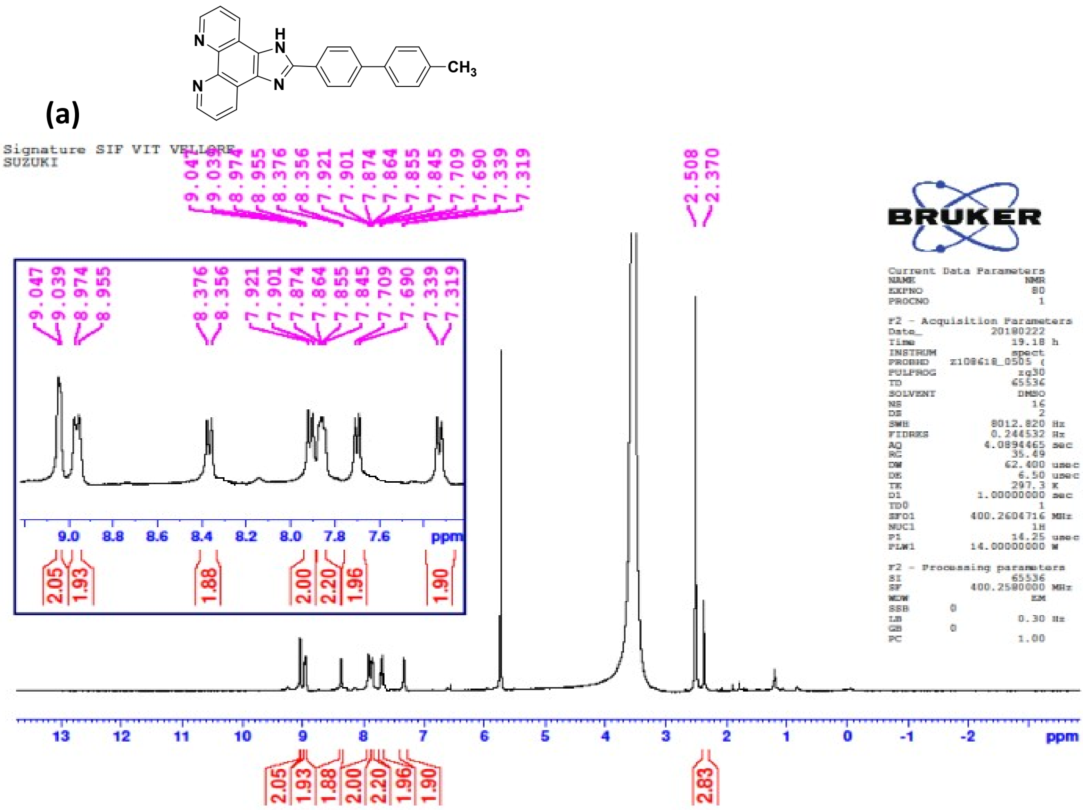


Figure S13: (a) IR Spectra and (b) LC-MS Spectra of 12a

(a)



(b) IR Spectra

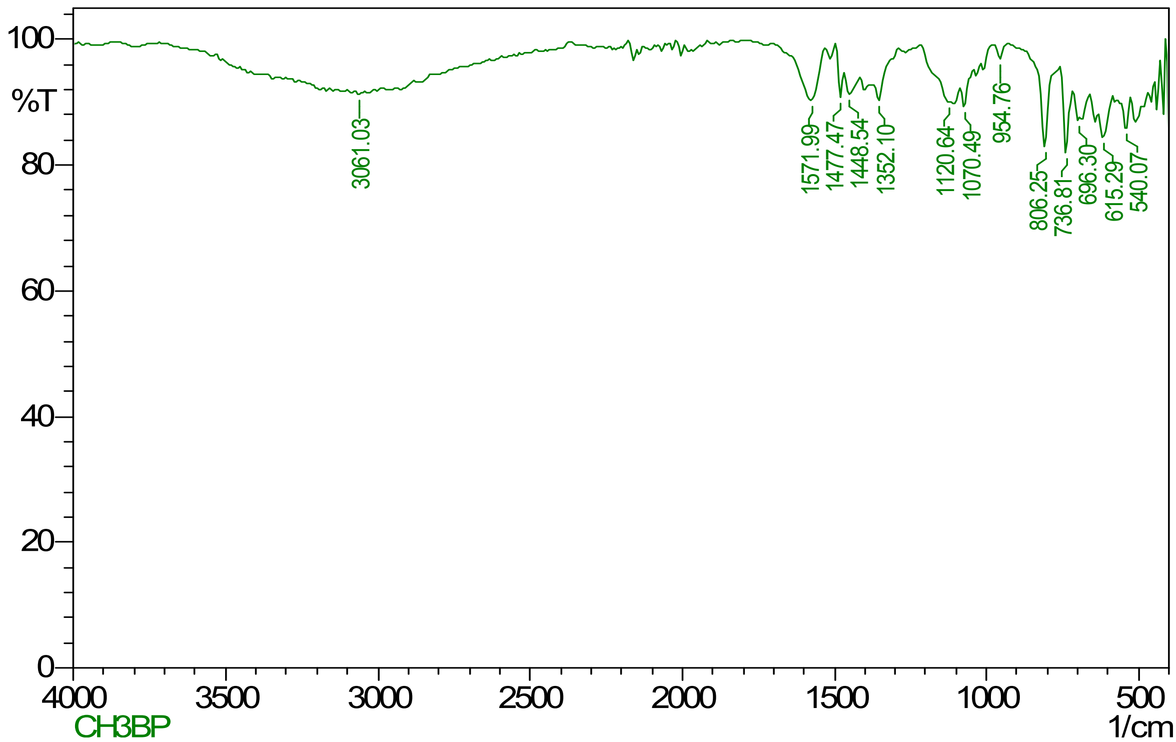
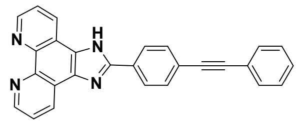
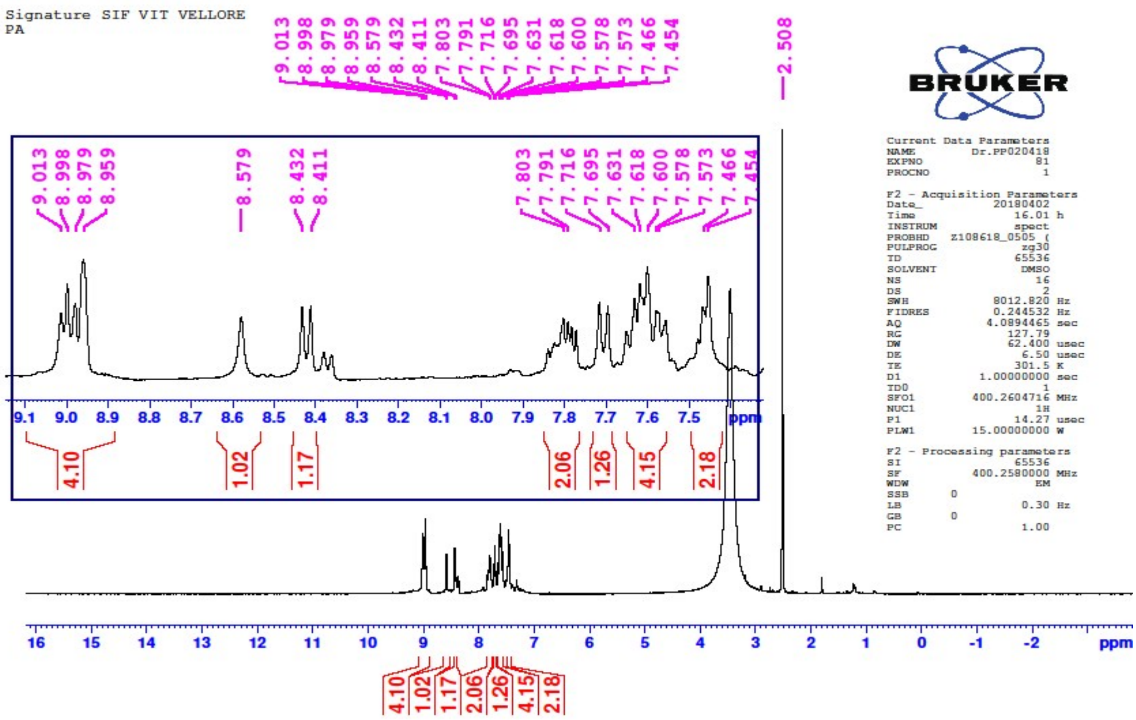


Figure S14: (a) ^{1}H-NMR and (b) IR Spectra of 12b



(a) ^{1}H-NMR



(b) ^{13}C-NMR

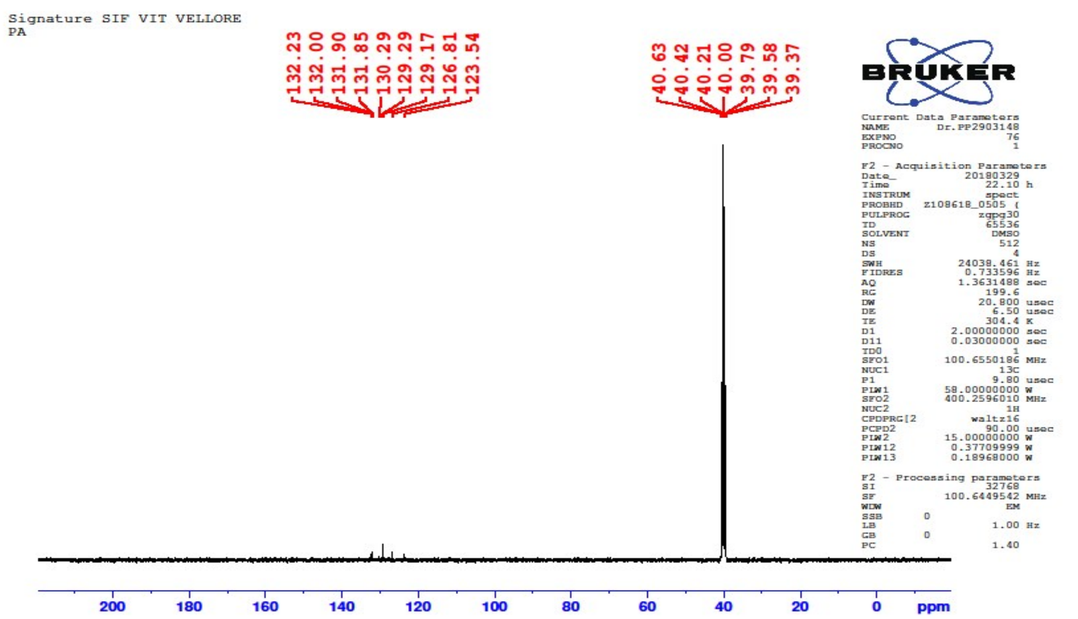
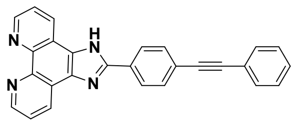


Figure S15: (a) ^{1}H-NMR and (b) ^{13}C-NMR Spectra of 14a

(a) IR Spectra



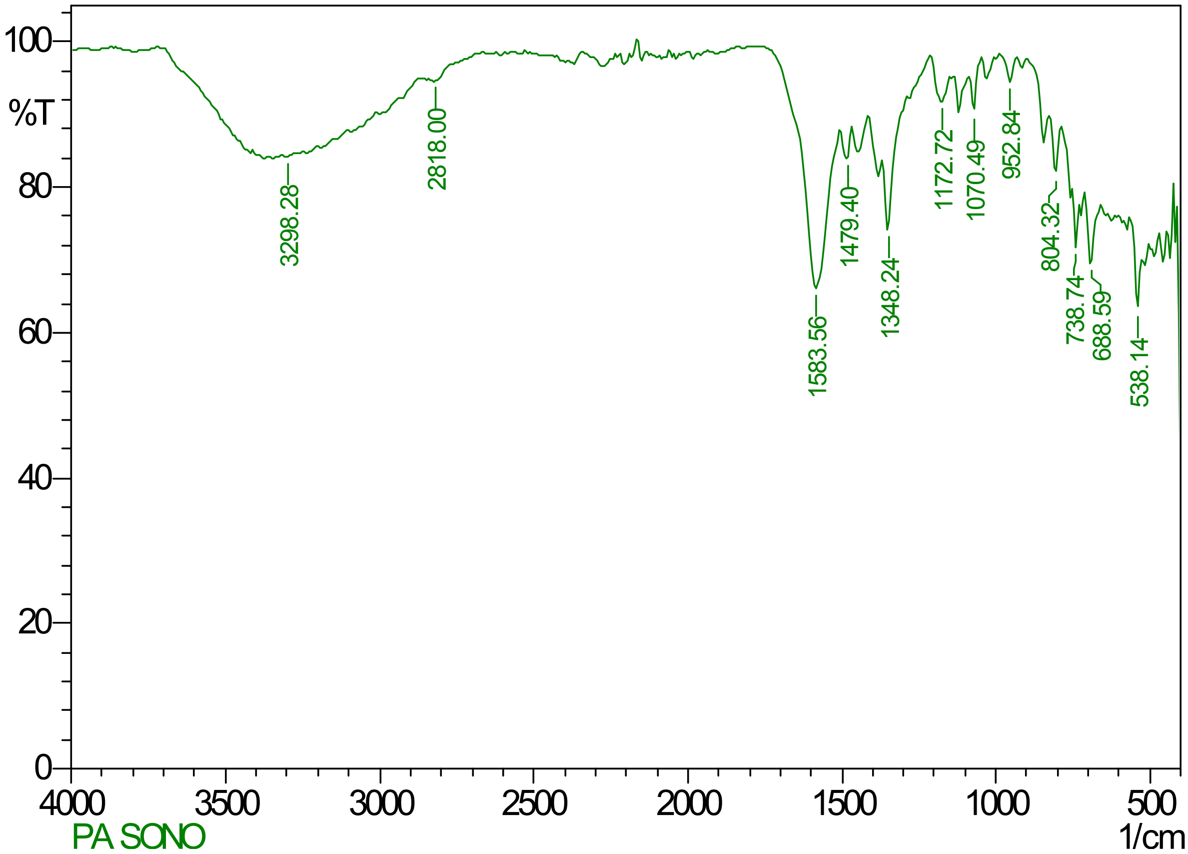
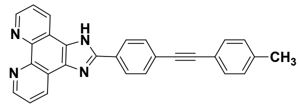
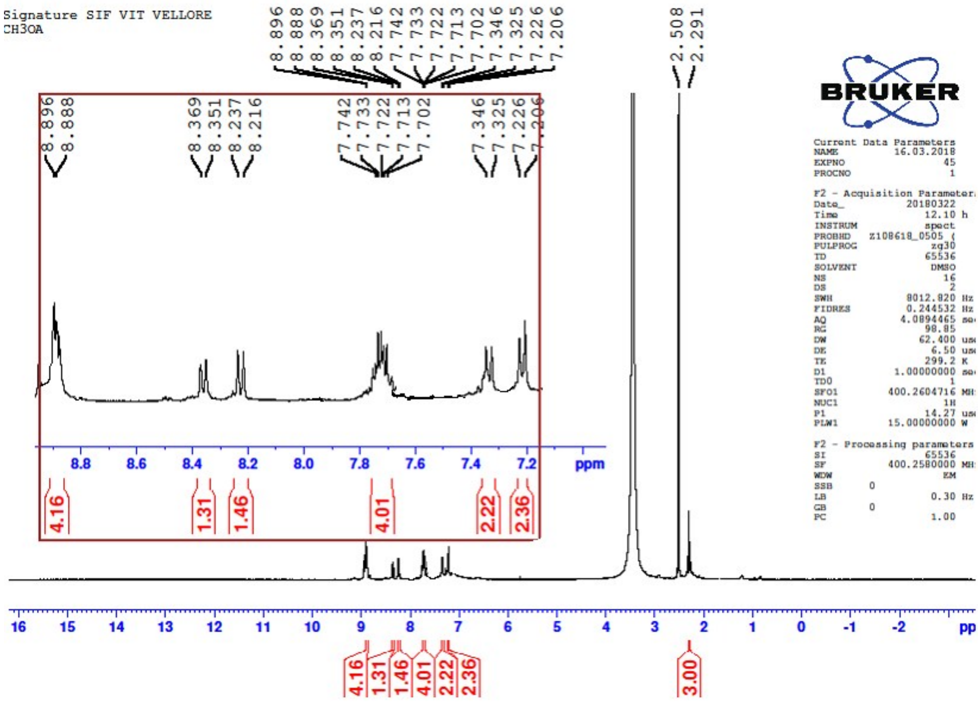


Figure S16: (a) IR Spectra of 14a



(a) ^{1}H-NMR



(b) ^{13}C-NMR

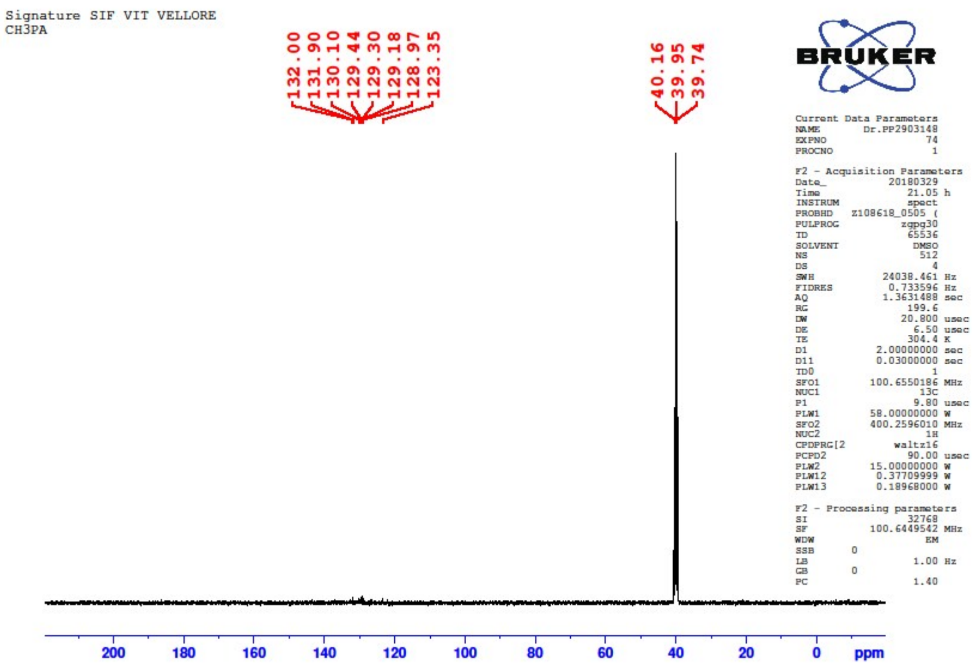
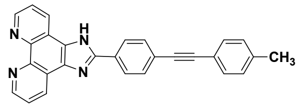


Figure S17: (a) ^{1}H-NMR and (b) ^{13}C-NMR Spectra of 14b

(a) IR Spectra



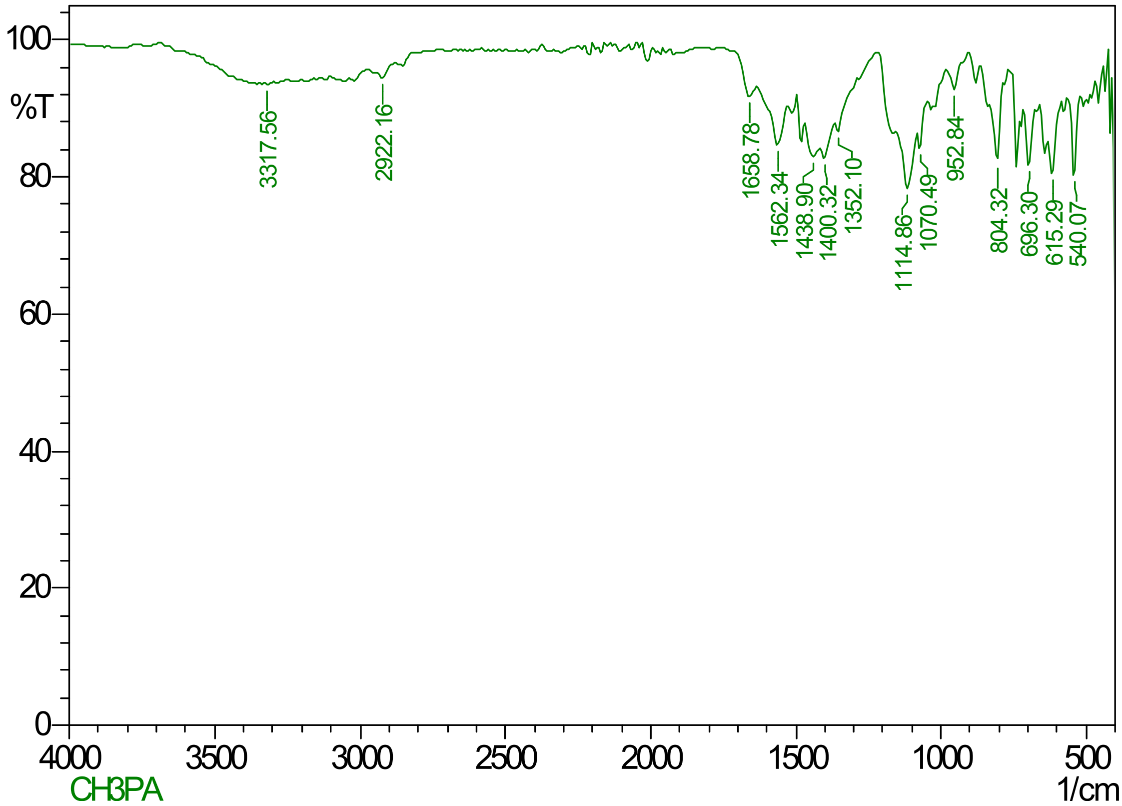
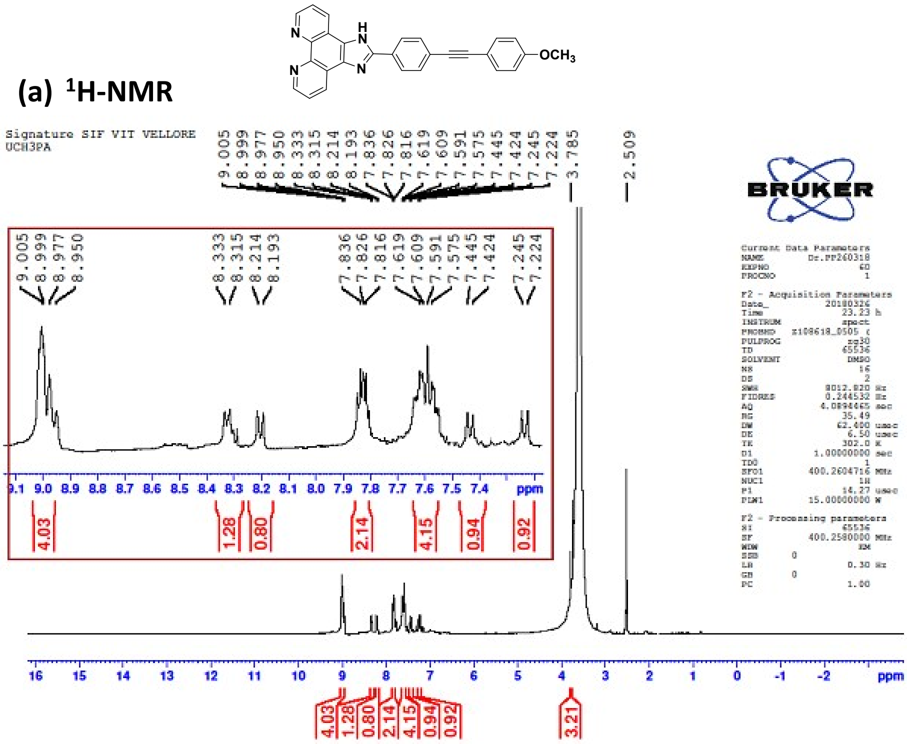


Figure S18: (a) IR Spectra of 14b

(a) ^{1}H-NMR



(b) ^{13}C-NMR

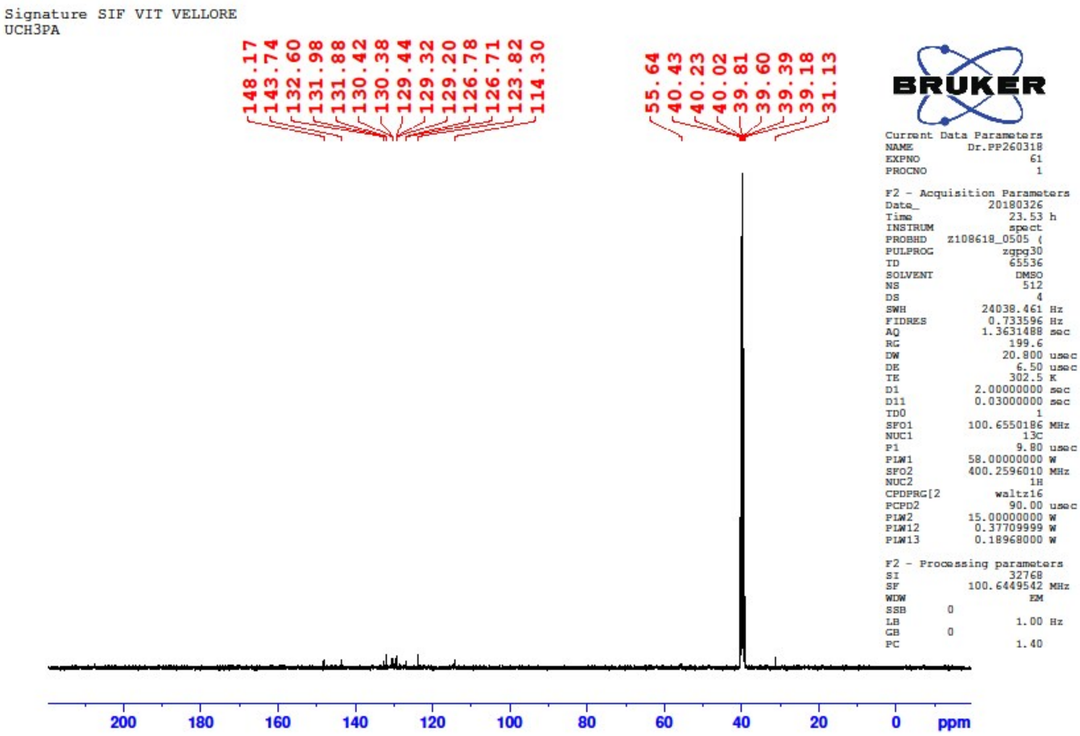
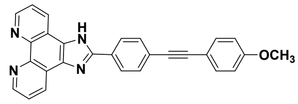


Figure S19: (a) ^{1}H-NMR and (b) ^{13}C-NMR Spectra of 14c

(a) IR Spectra



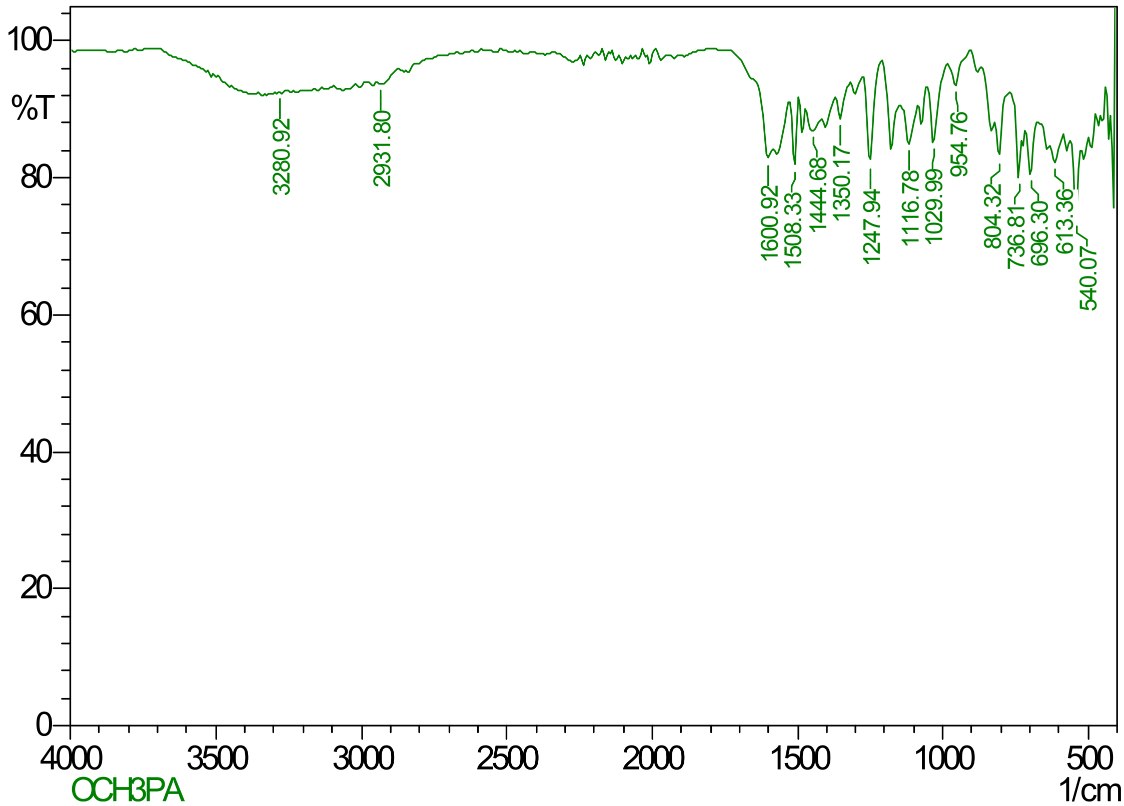
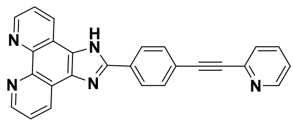
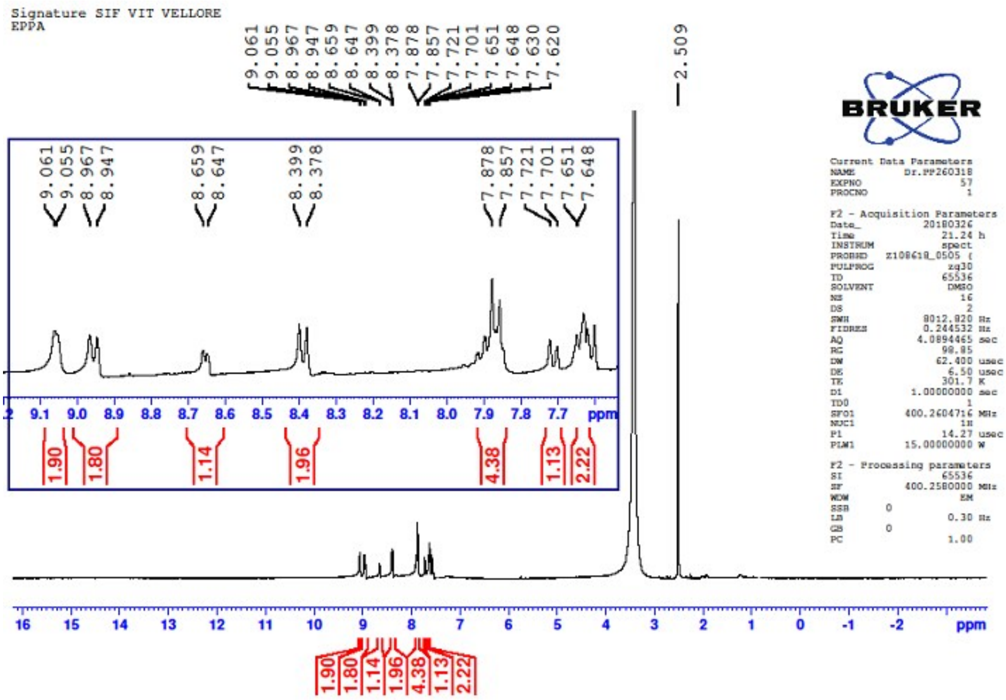


Figure S20: (a) IR Spectra of 14c



(a) ^{1}H-NMR



(b) ^{13}C-NMR

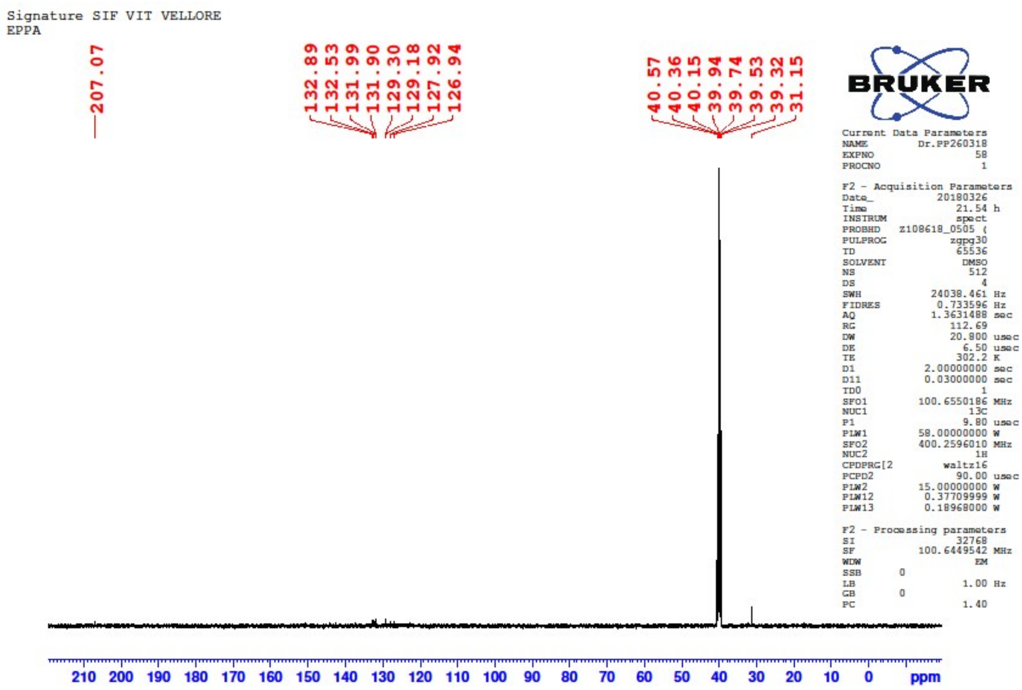
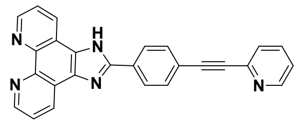


Figure S21: (a) ^{1}H-NMR and (b) ^{13}C-NMR Spectra of 14d



(a) IR Spectra

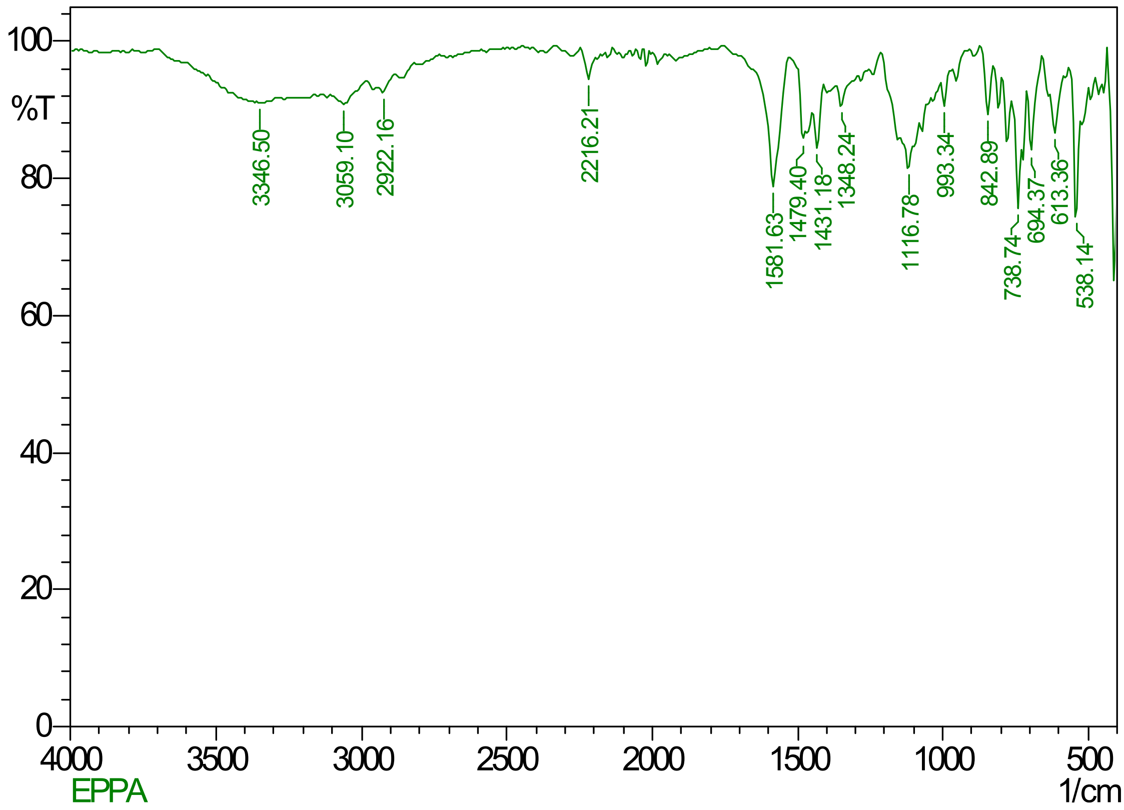
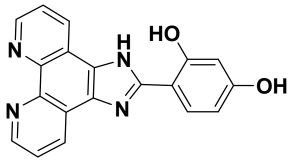
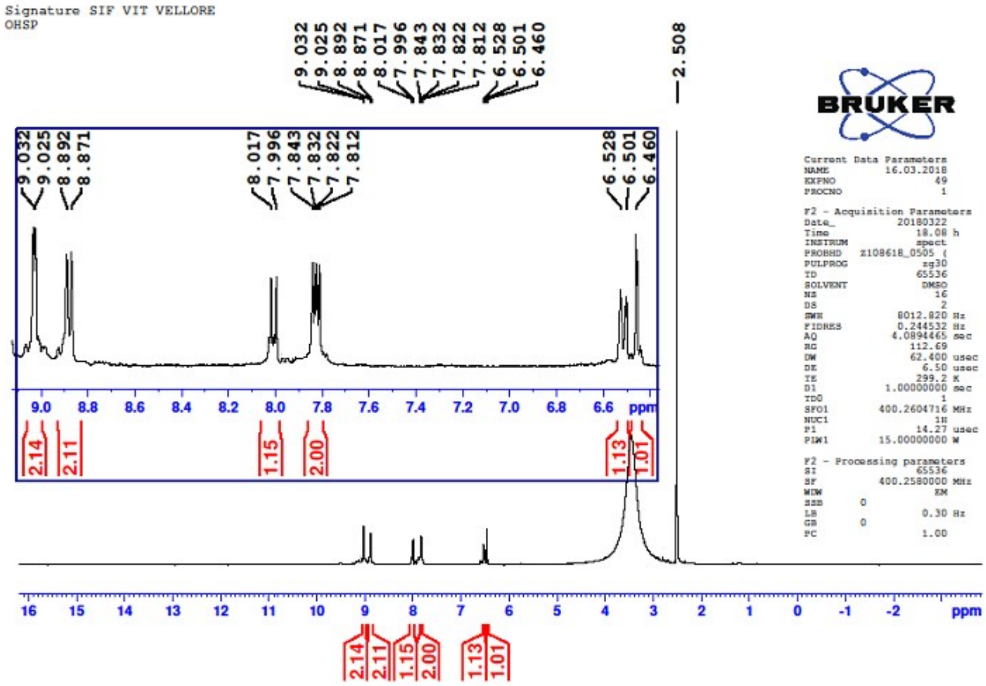


Figure S22: (a) IR Spectra of 14d



(a) ¹H-NMR



(b) IR Spectra

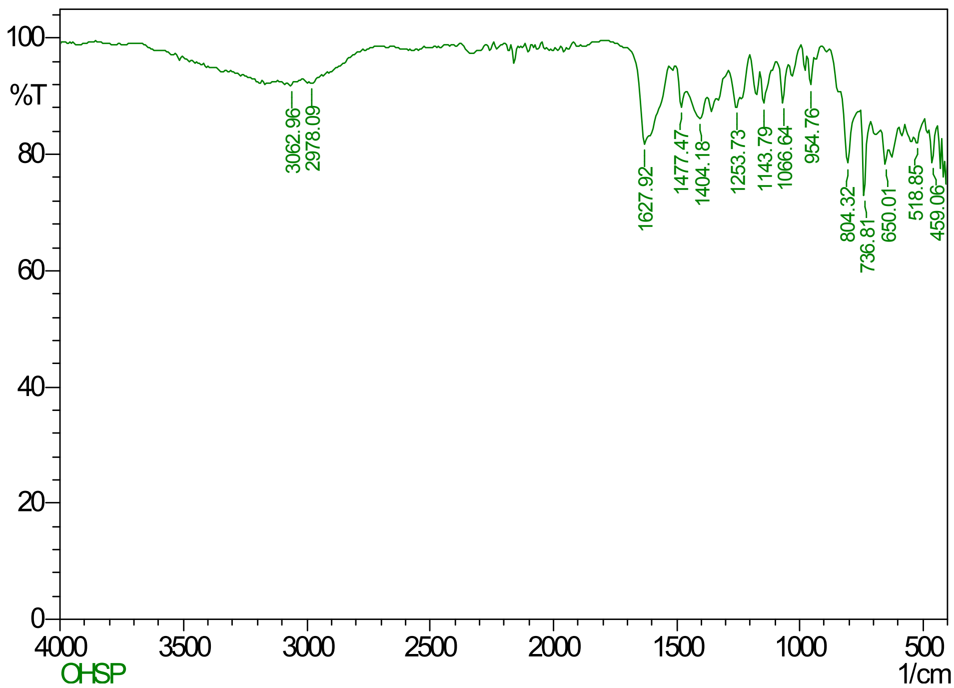
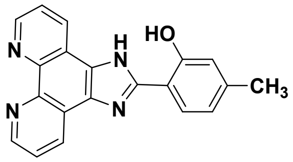
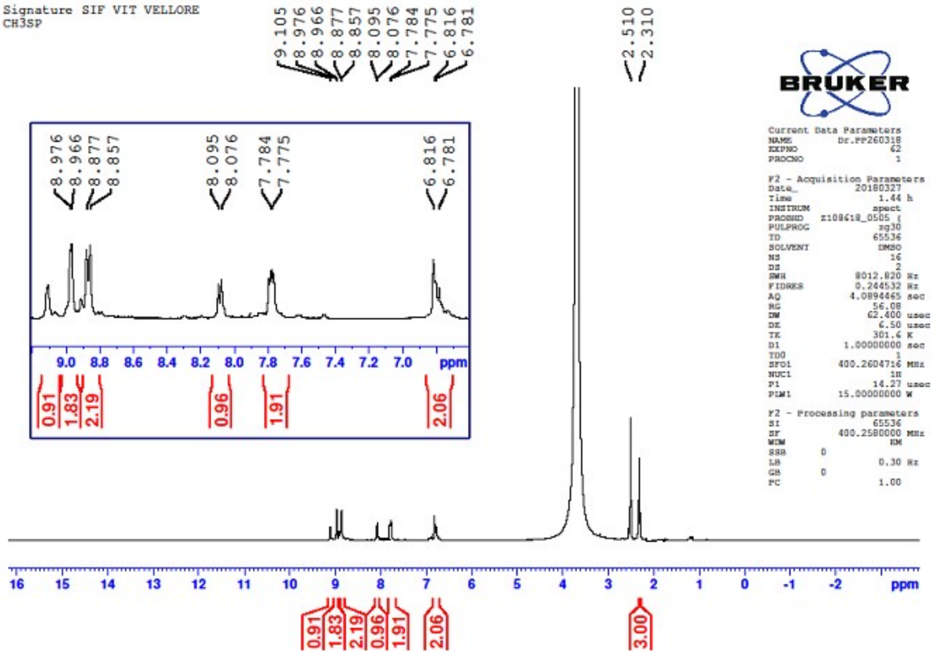


Figure S23: (a) ¹H-NMR and (b) IR Spectra of 18a



(a) ^{1}H-NMR



(b) ^{13}C-NMR

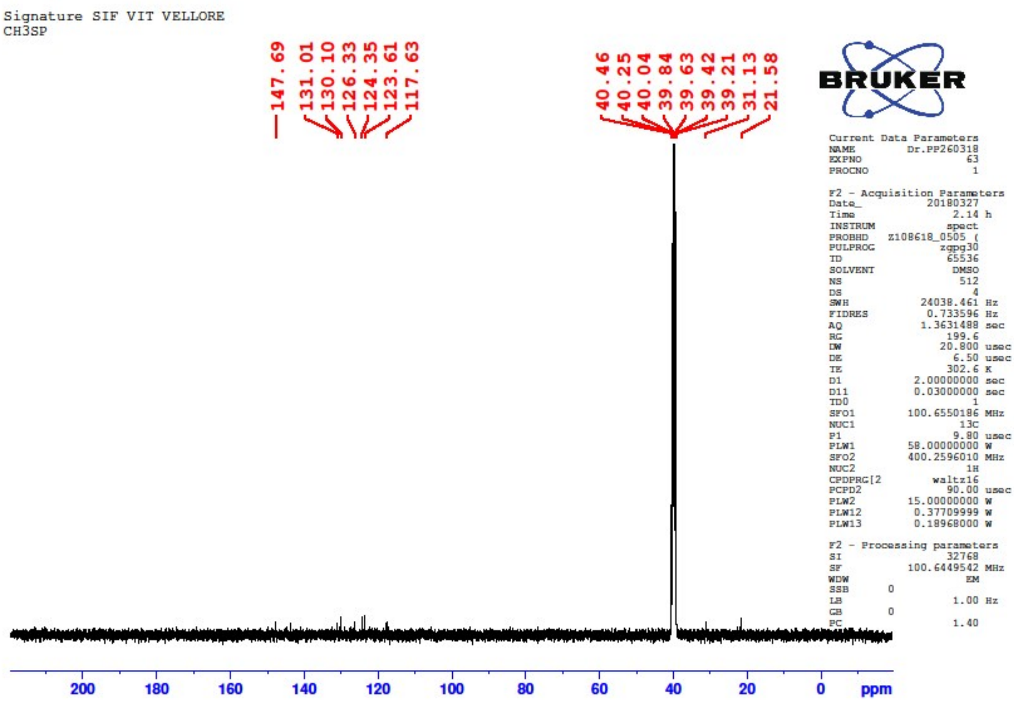


Figure S24: (a) ^{1}H-NMR and (b) ^{13}C-NMR Spectra of 18b

(a) IR Spectra

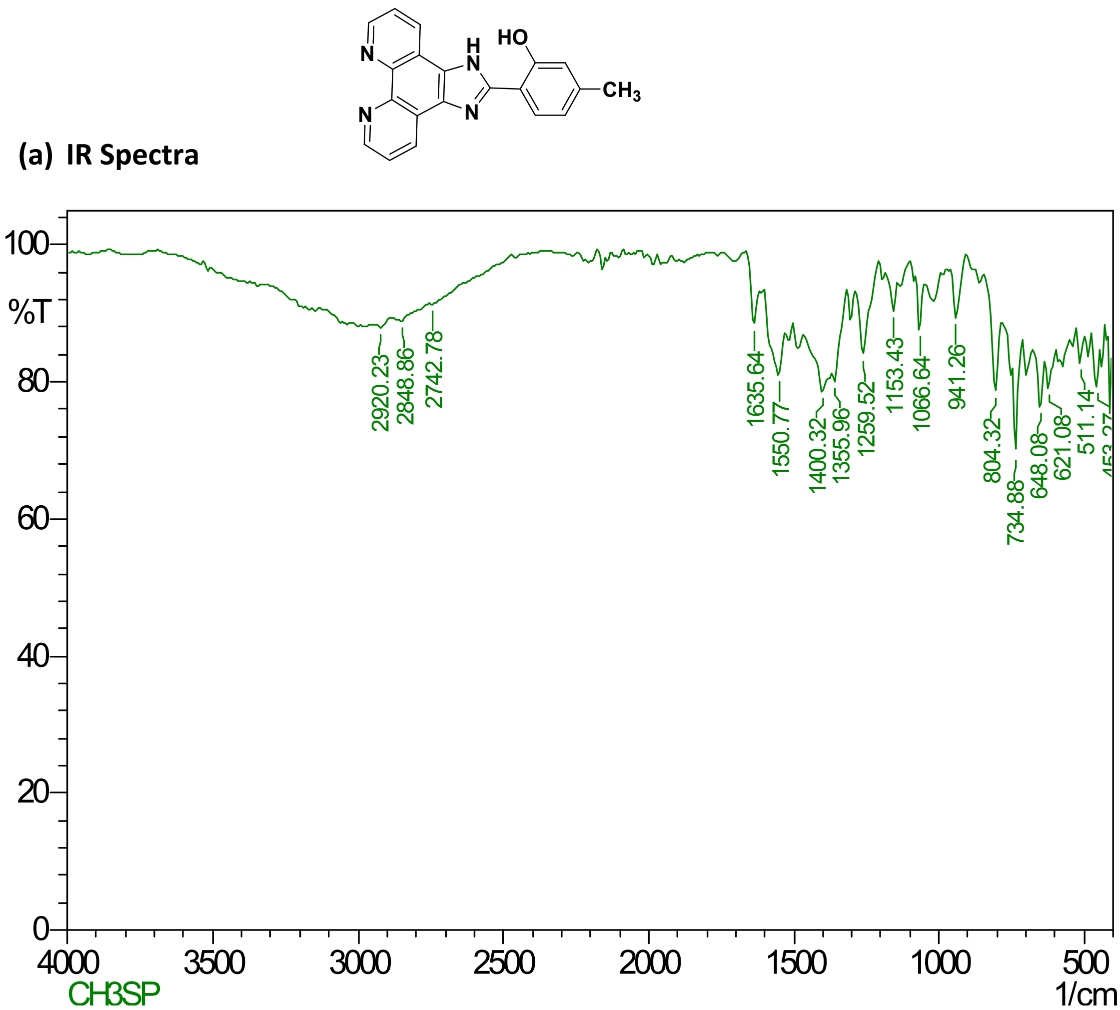
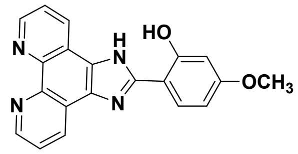
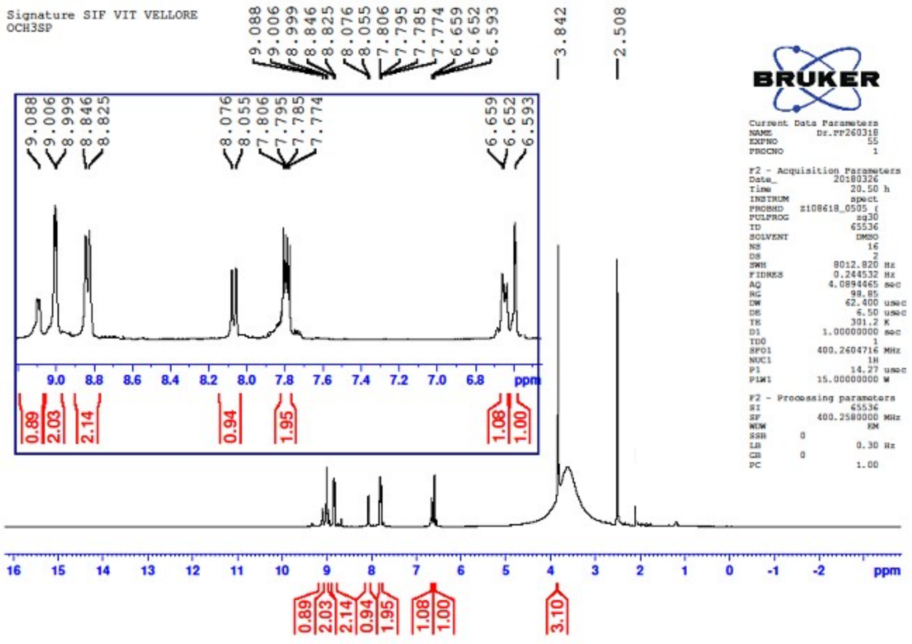


Figure S25: (a) IR Spectra of 18b



(a) ^{1}H-NMR



(b) ^{13}C-NMR

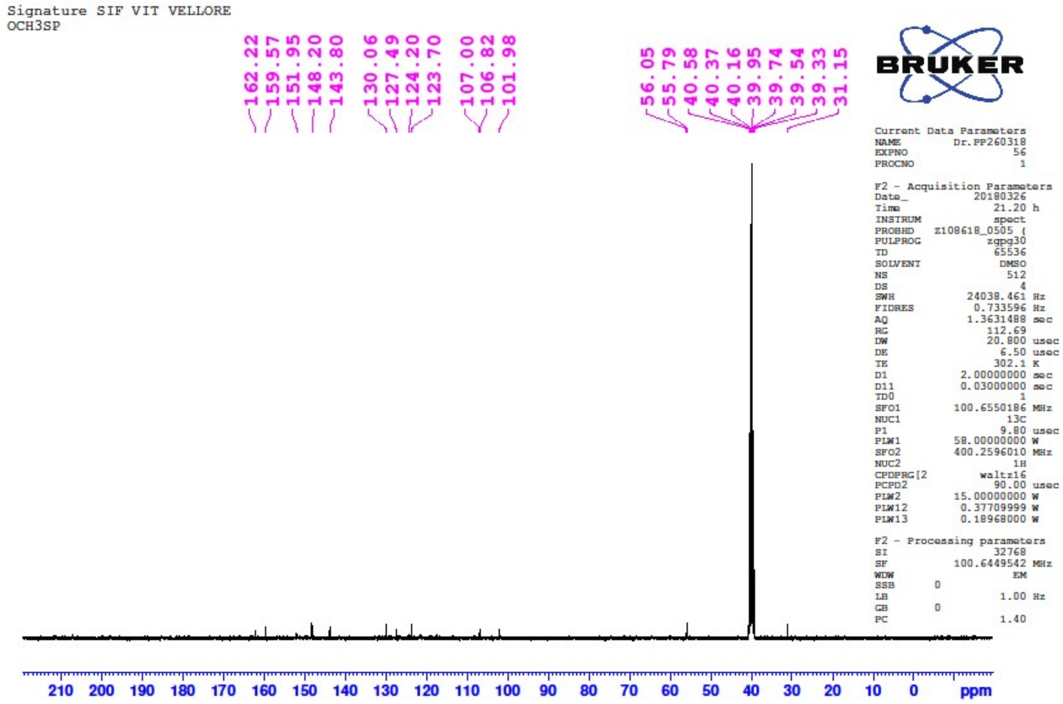
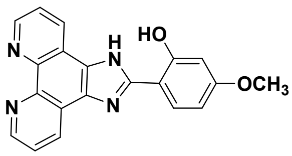


Figure S26: (a) ^{1}H-NMR and (b) ^{13}C-NMR Spectra of 18c



(a) IR Spectra

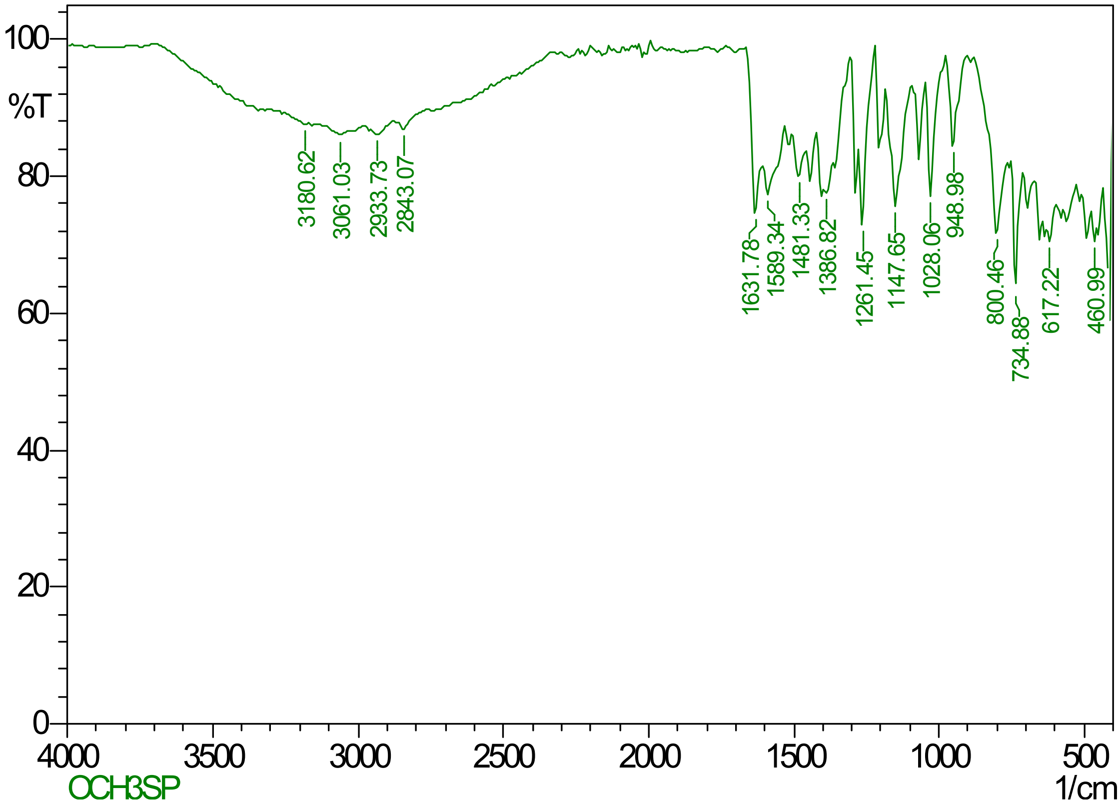
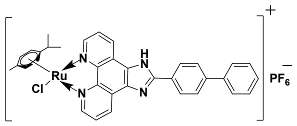
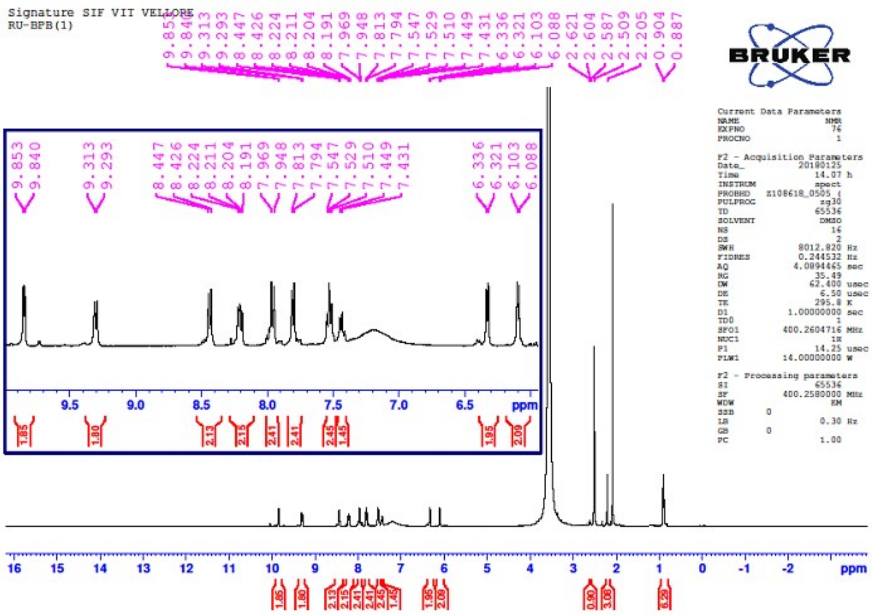


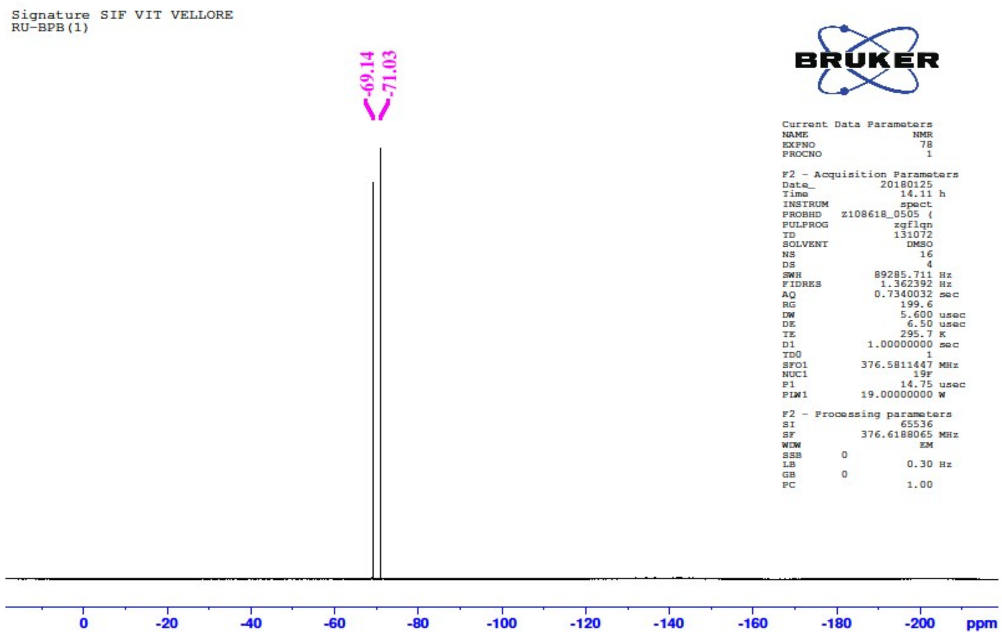
Figure S27: (a) IR Spectra of 18c



(a) ^{1}H-NMR



(b) ^{19}F-NMR



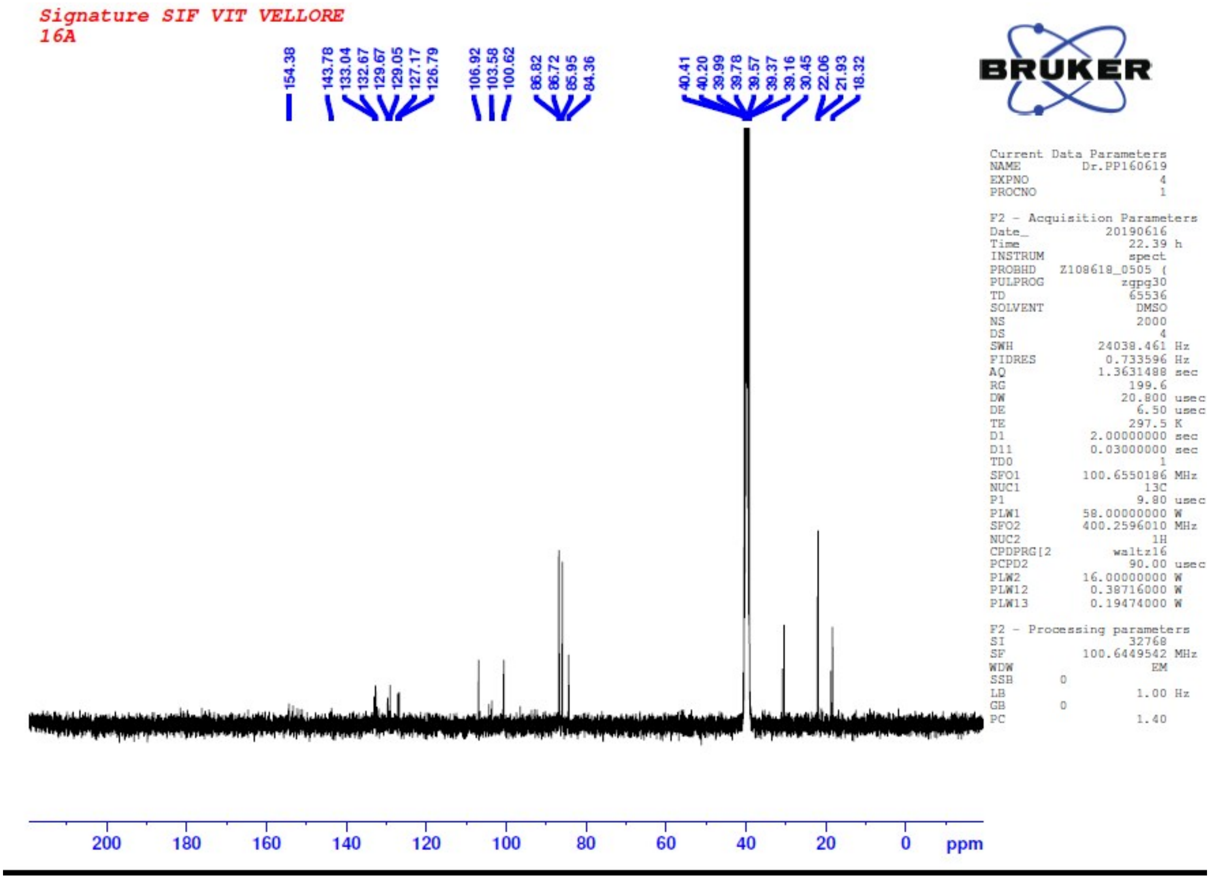
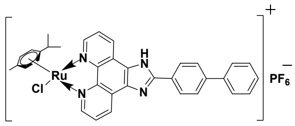
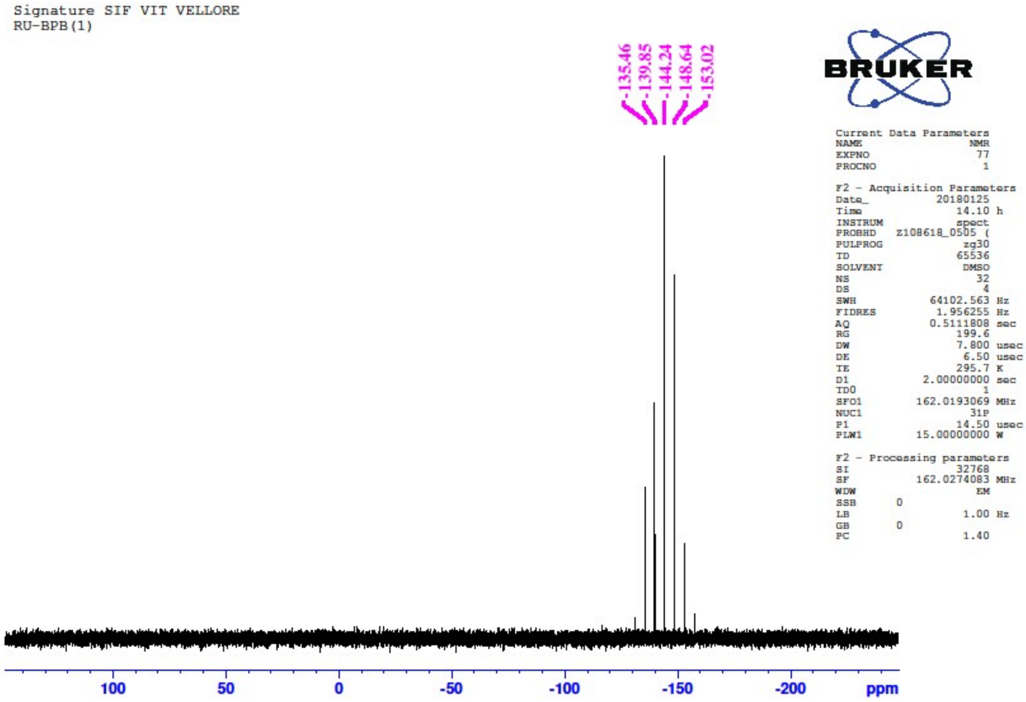


Figure S28: (a) ^{1}H-NMR (b) ^{19}F-NMR (c) ^{13}C NMR Spectra of 16a



(a) ^{31}P-NMR



(b) IR Spectra

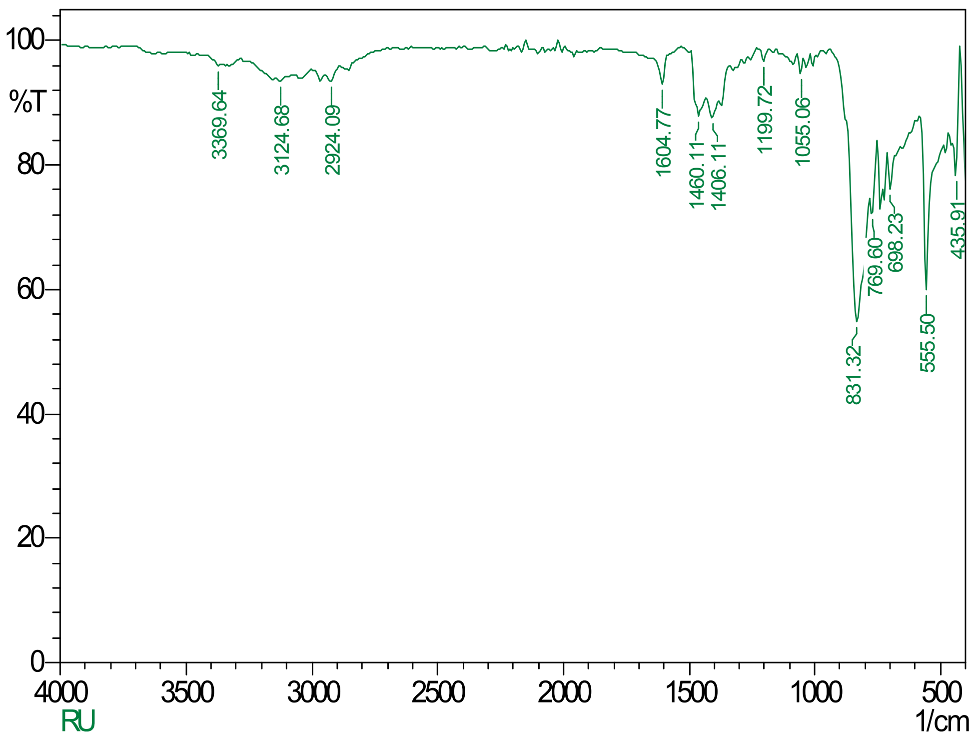
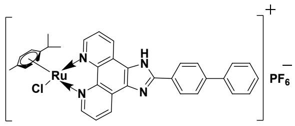


Figure S29: (a) ^{31}P-NMR (b) IR Spectra of16a



(a) LC-MS Spectra

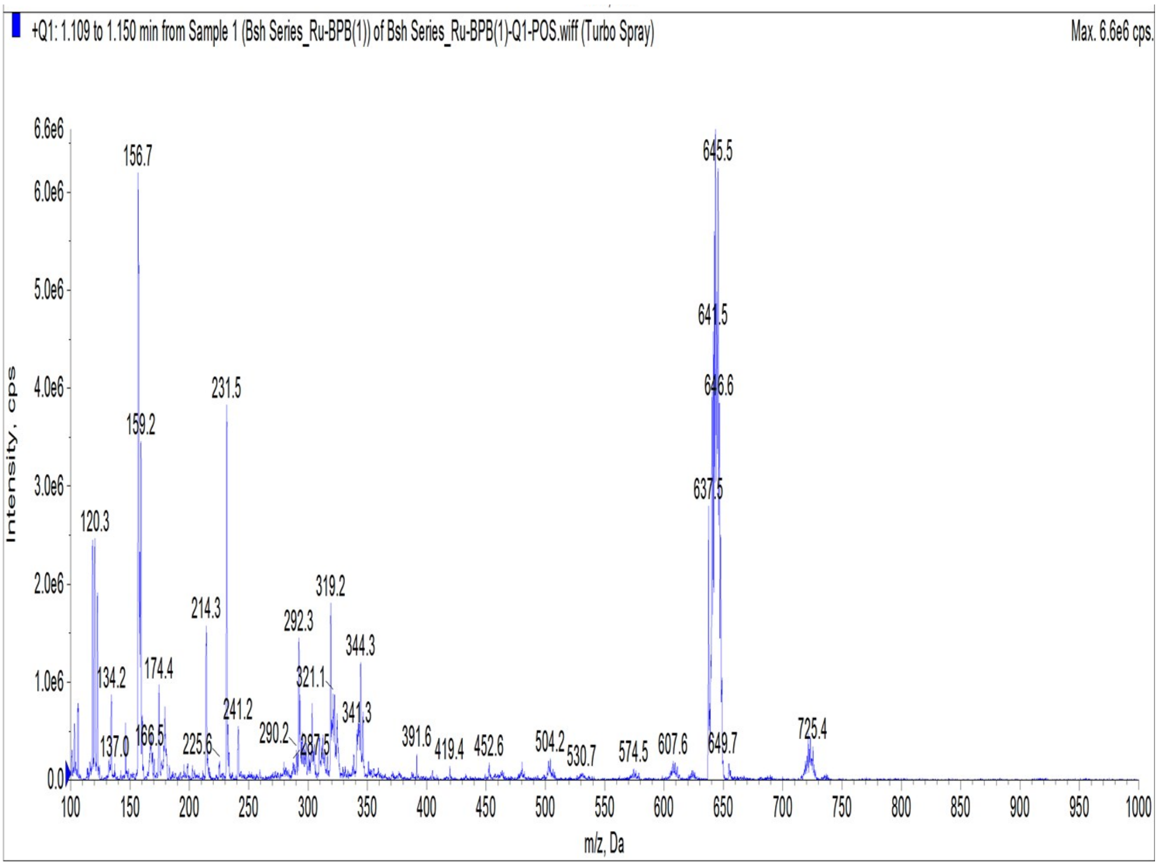
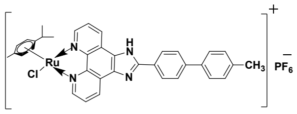
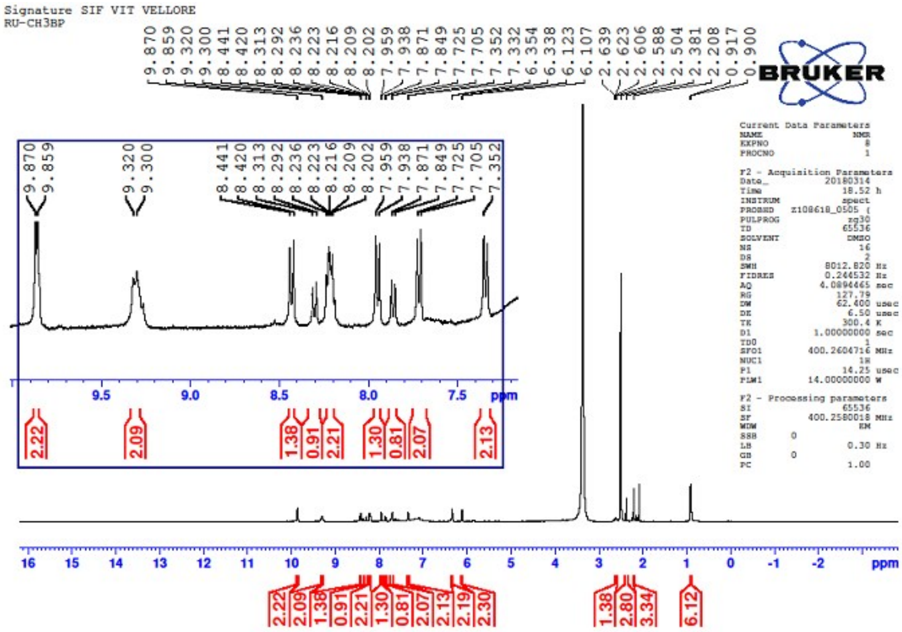


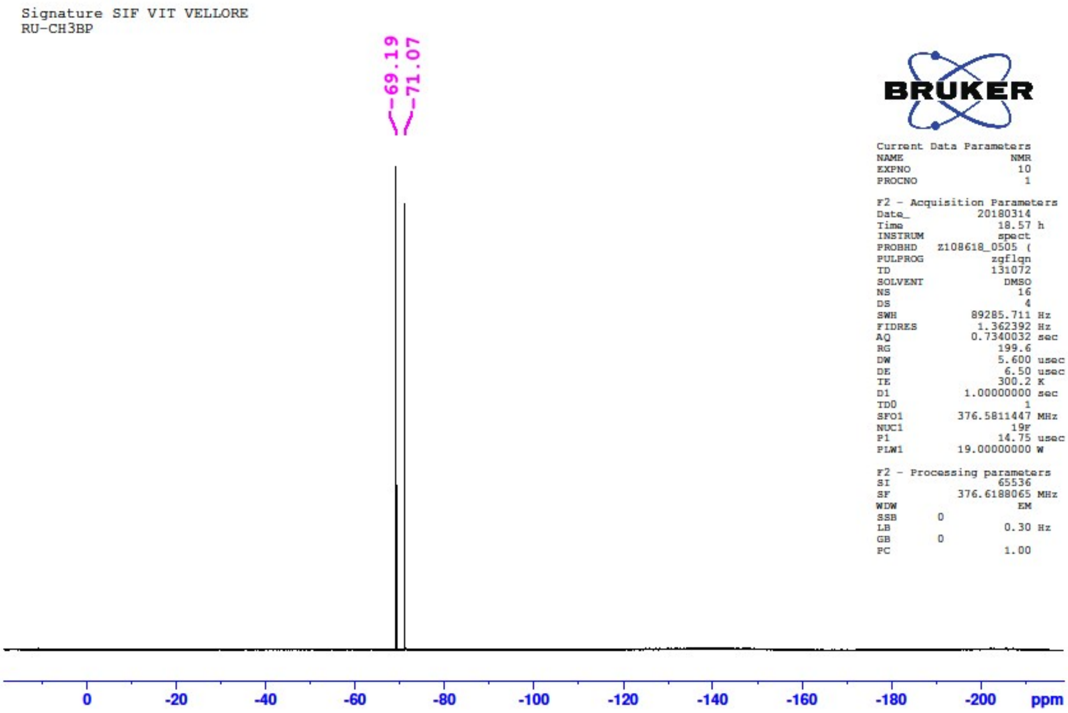
Figure S30: (a) LC-MS Spectra of 16a



(a) ^{1}H-NMR



(b) ^{19}F-NMR



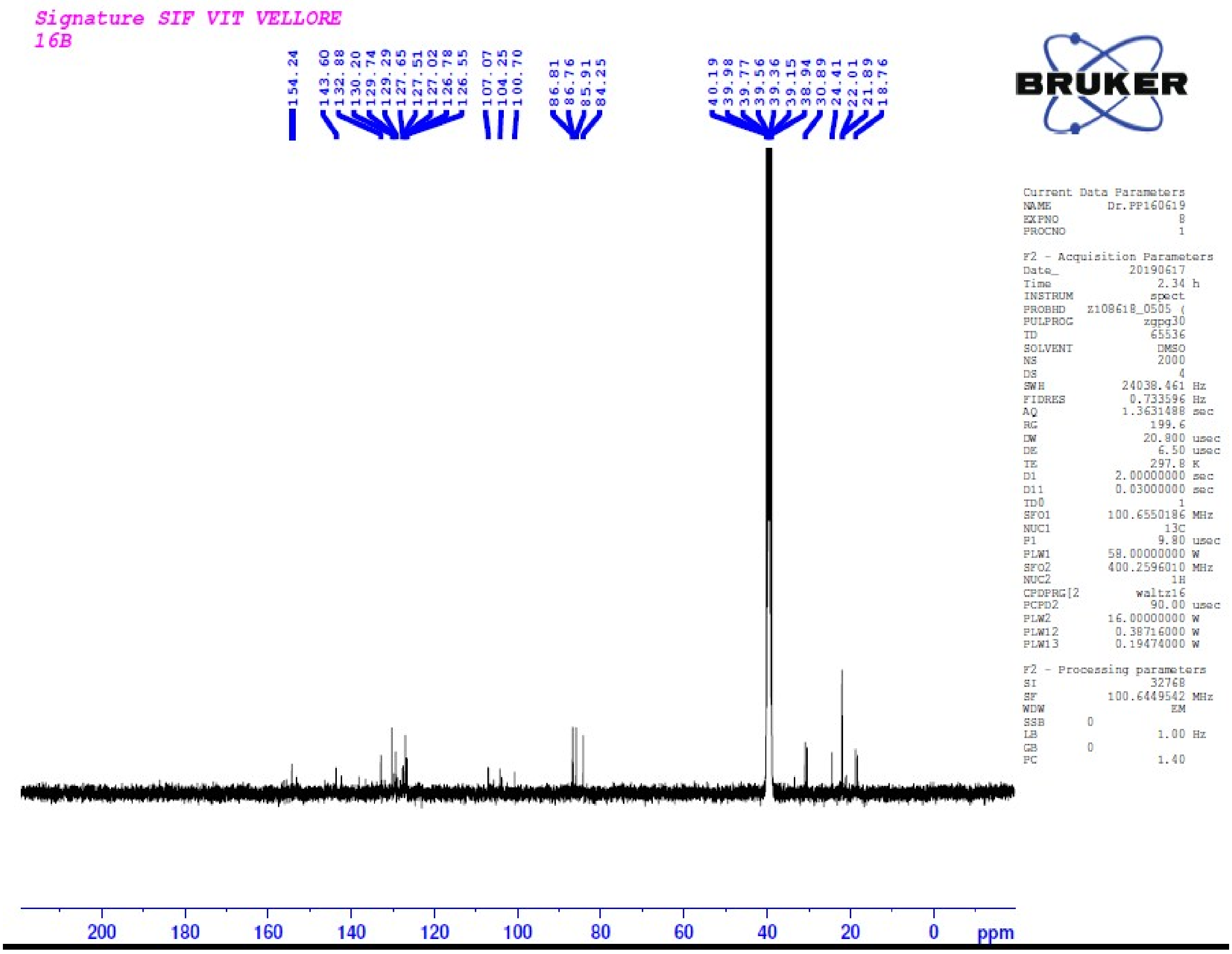
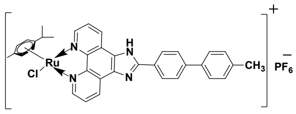
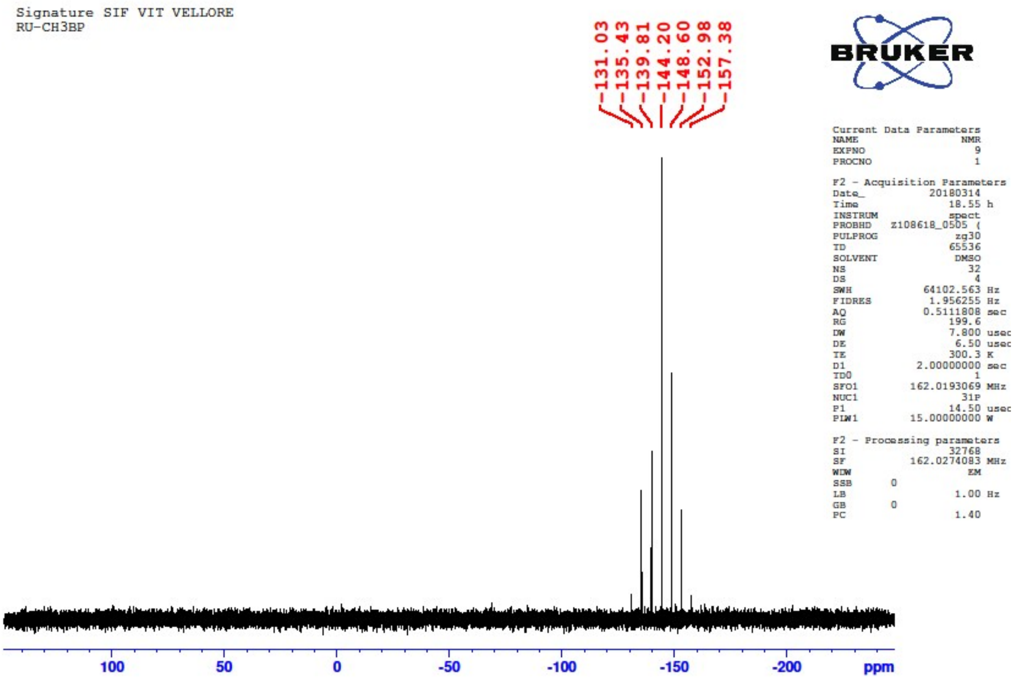


Figure S31: (a) ^{1}H-NMR and (b) ^{19}F-NMR (c) ^{13}C-NMR Spectra of 16b

(a) ^{31}P-NMR





(b) IR Spectra

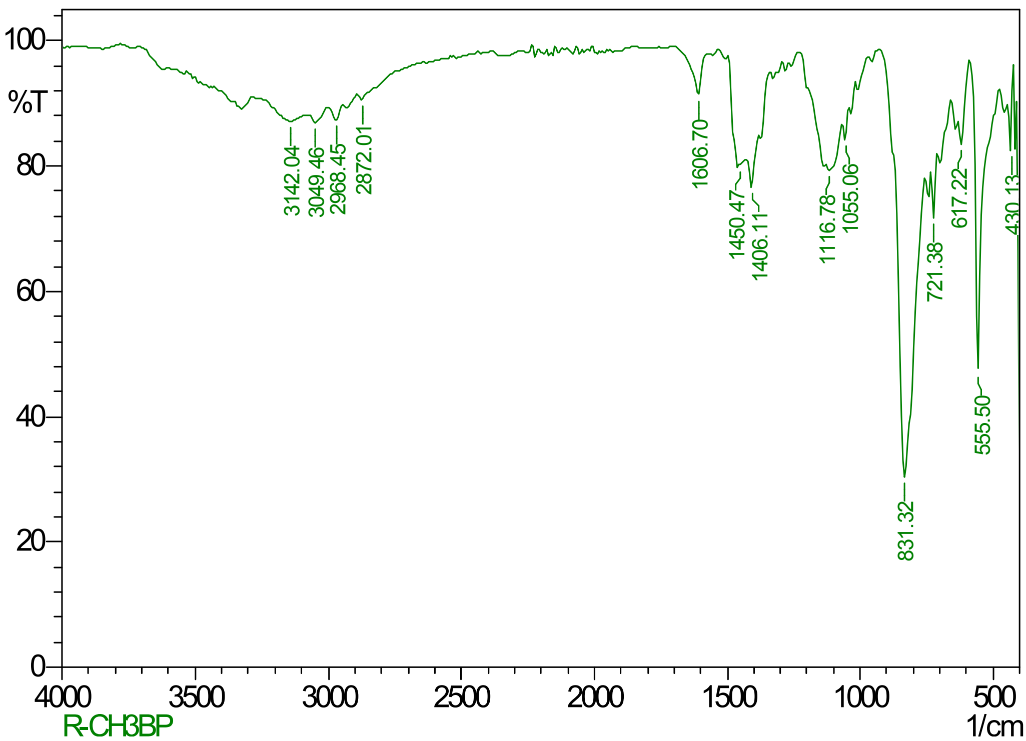
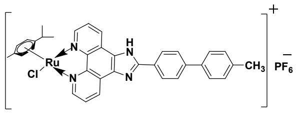


Figure S32: (a) ^{31}P-NMR (b) IR Spectra of 16b

(a) LC-MS Spectra



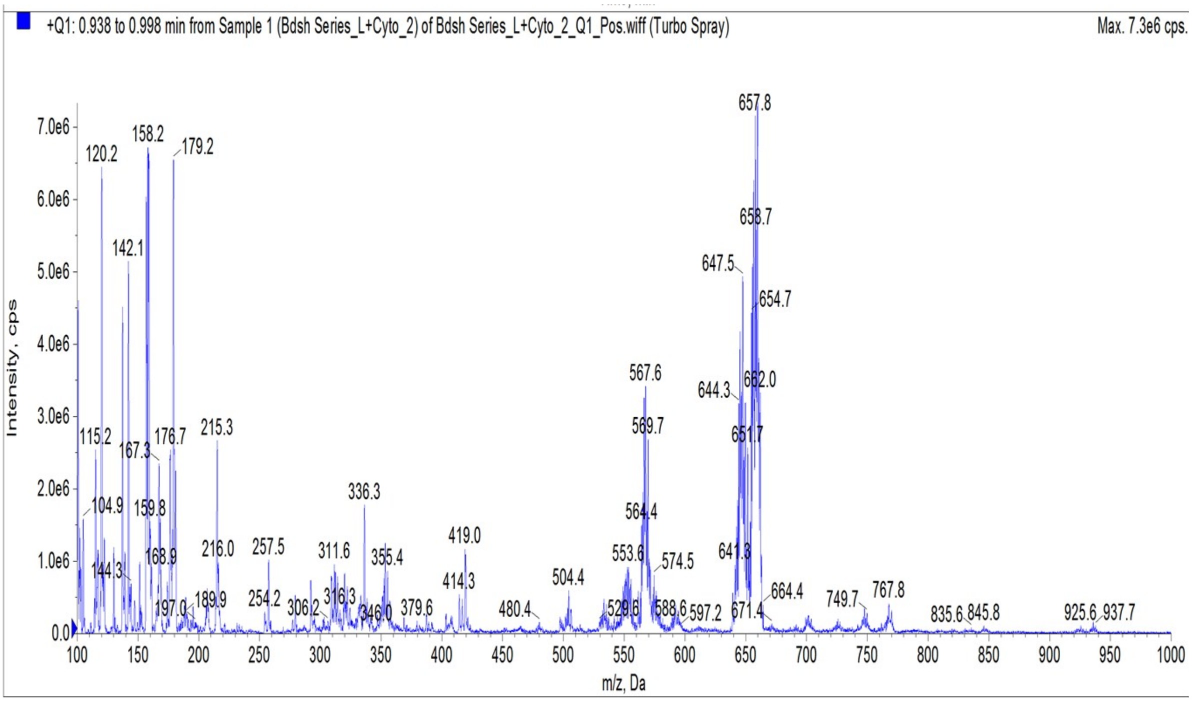
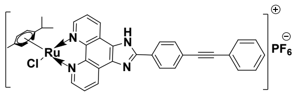
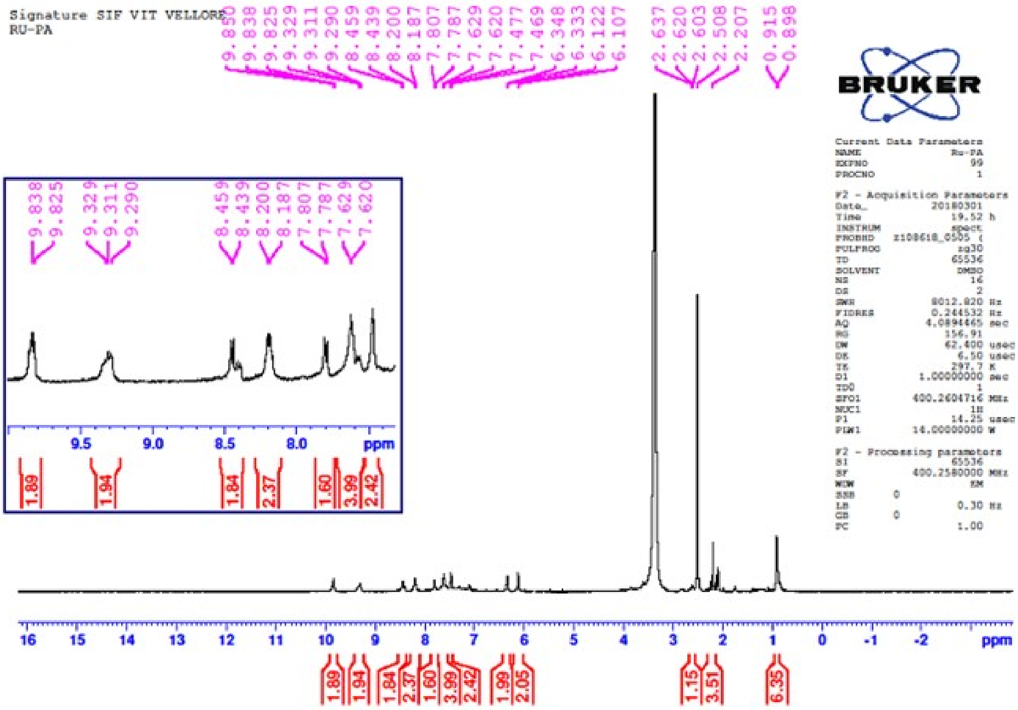


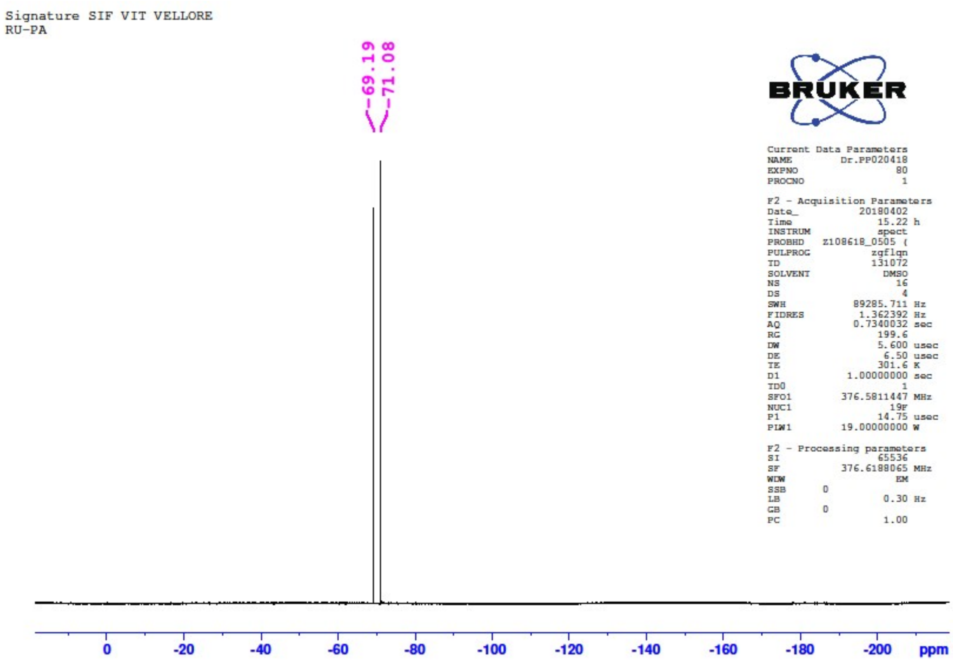
Figure S33: (a) LC-MS Spectra of 16b



(a) ^{1}H-NMR



(b) ^{19}F-NMR



(C)

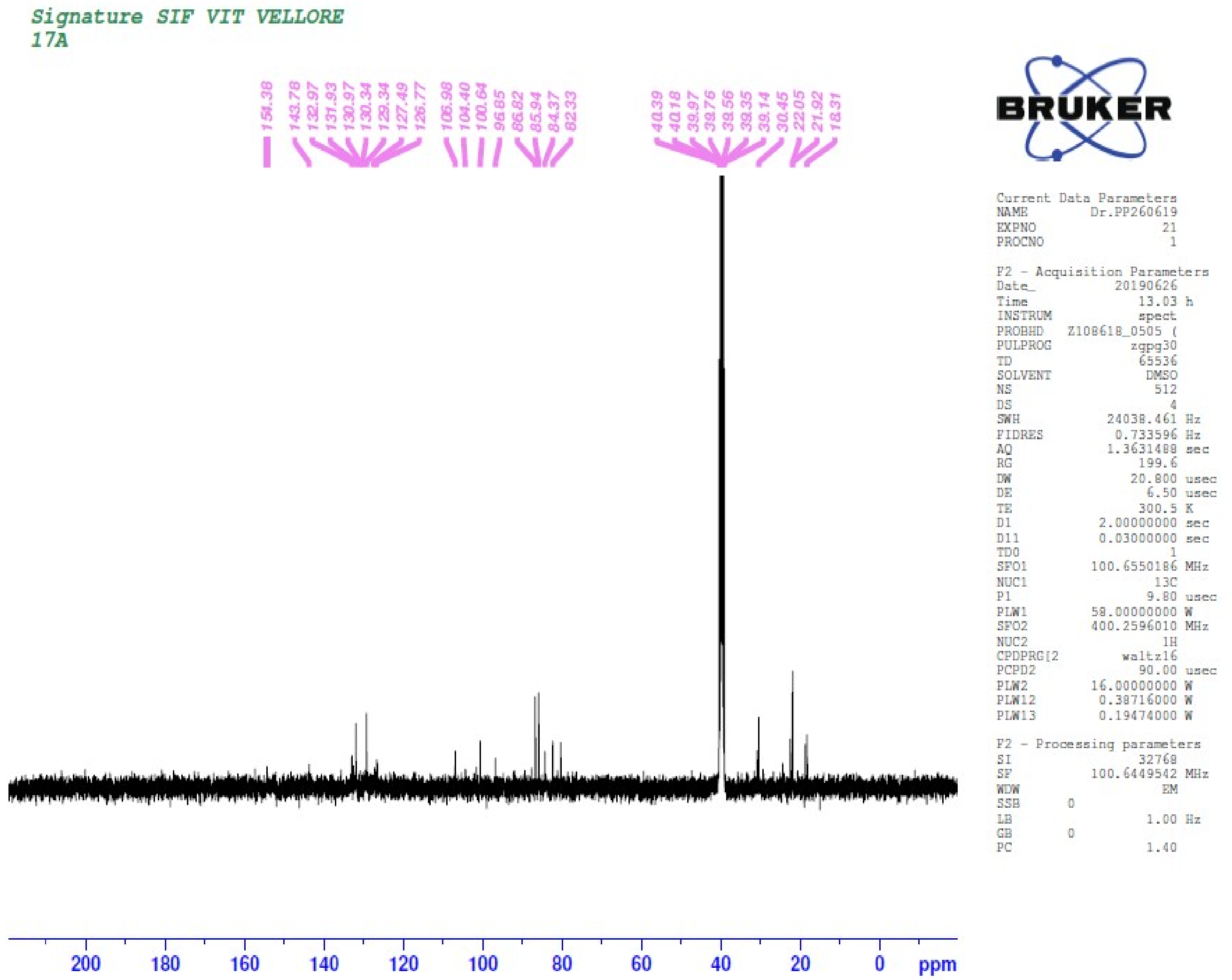
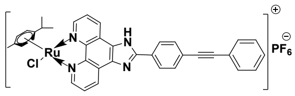
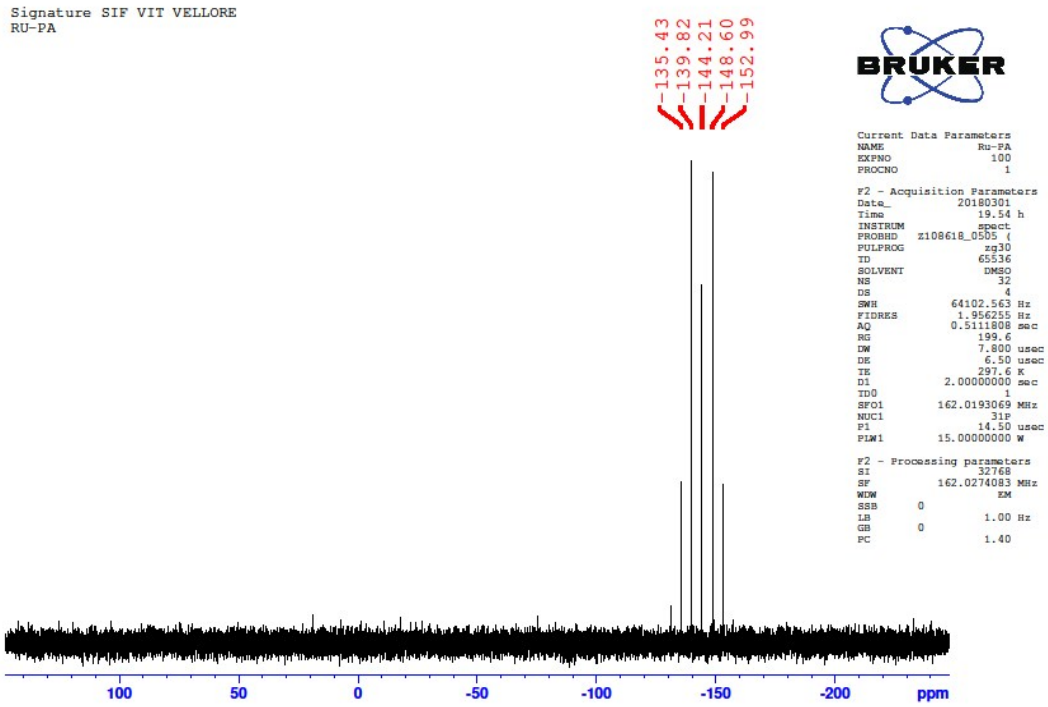


Figure S34: (a) ^{1}H-NMR (b) ^{19}F-NMR (c) ^{13}C NMR Spectra of 17a

(a) ^{31}P-NMR





(b) IR Spectra

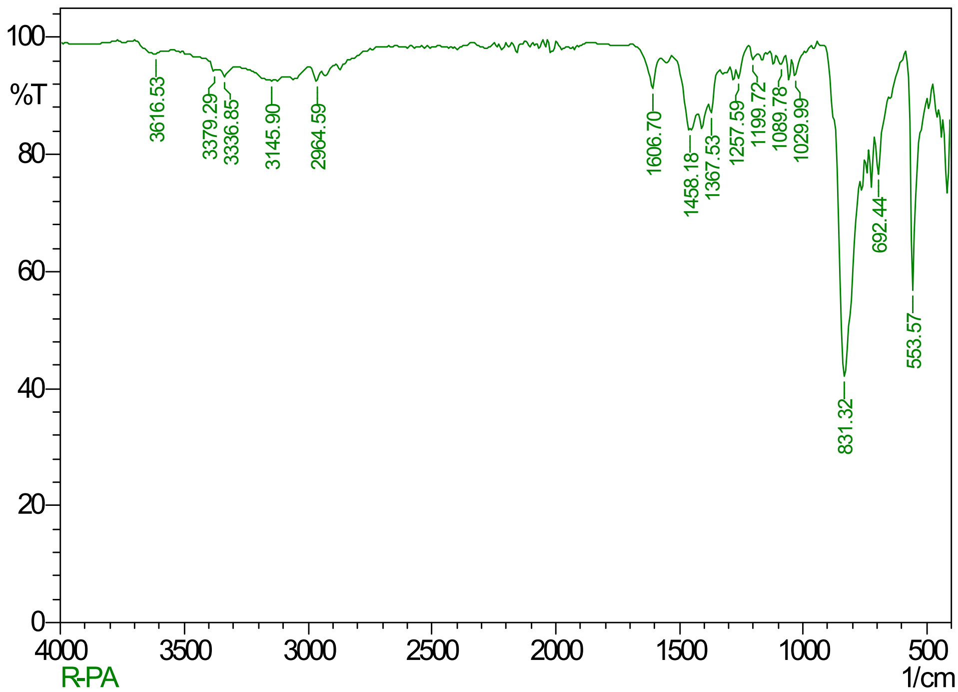
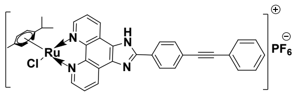


Figure S35: (a) ^{31}P-NMR (b) IR Spectra of 17a

(a) LC-MS Spectra



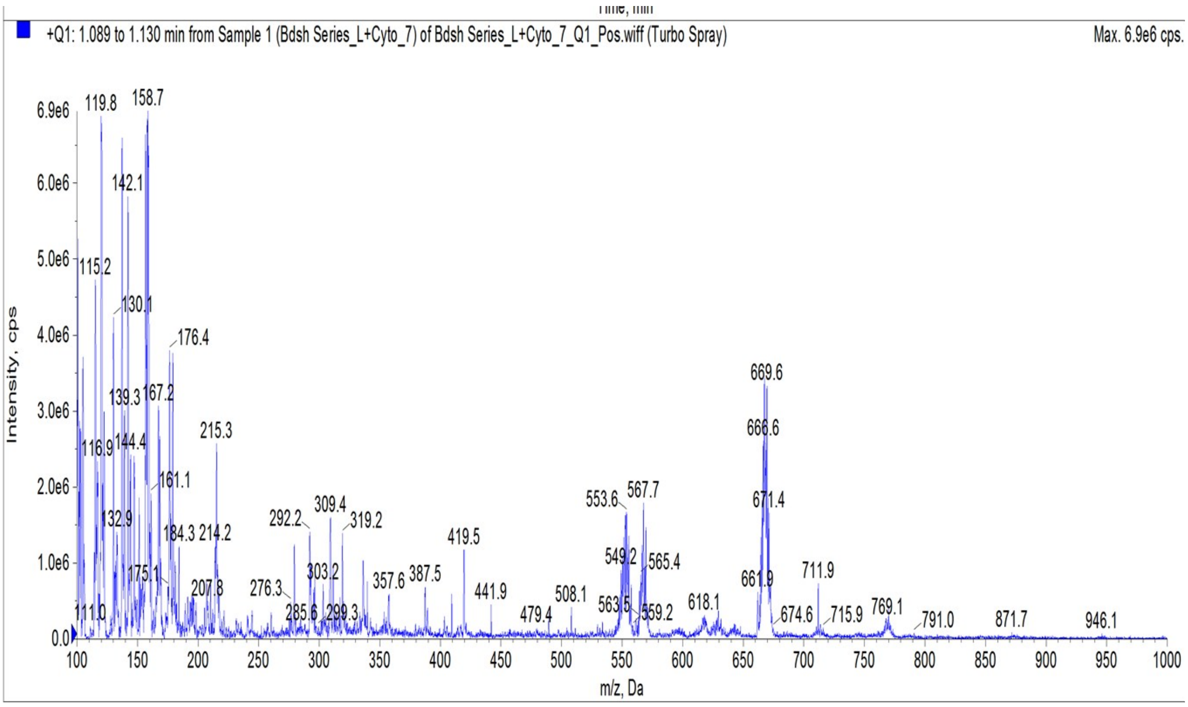
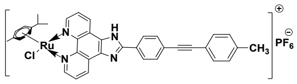
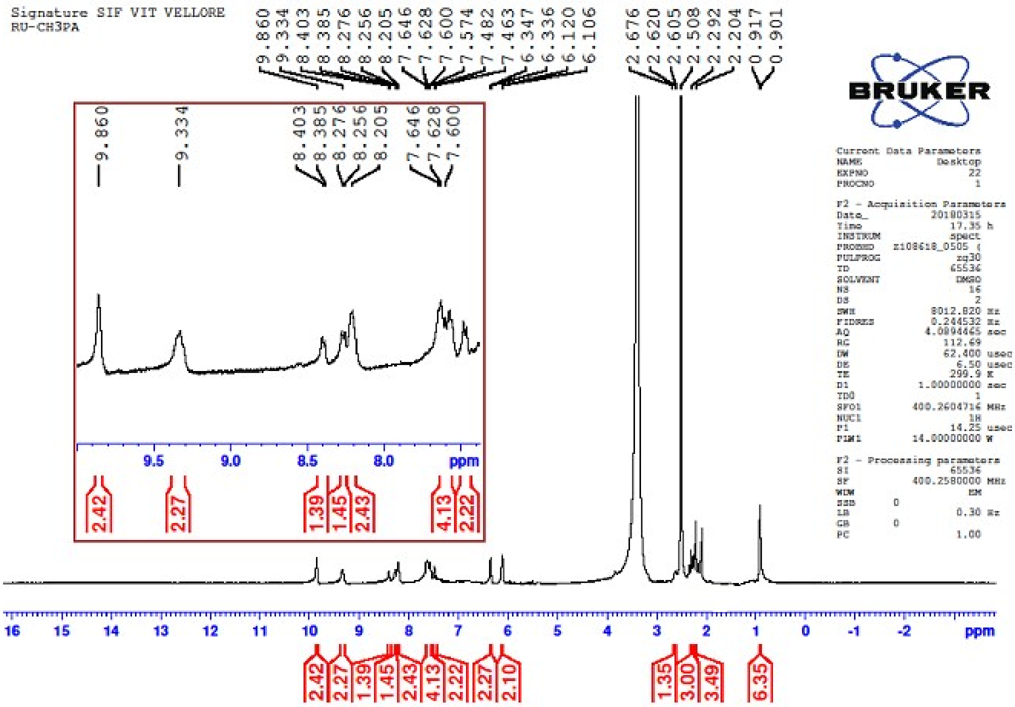


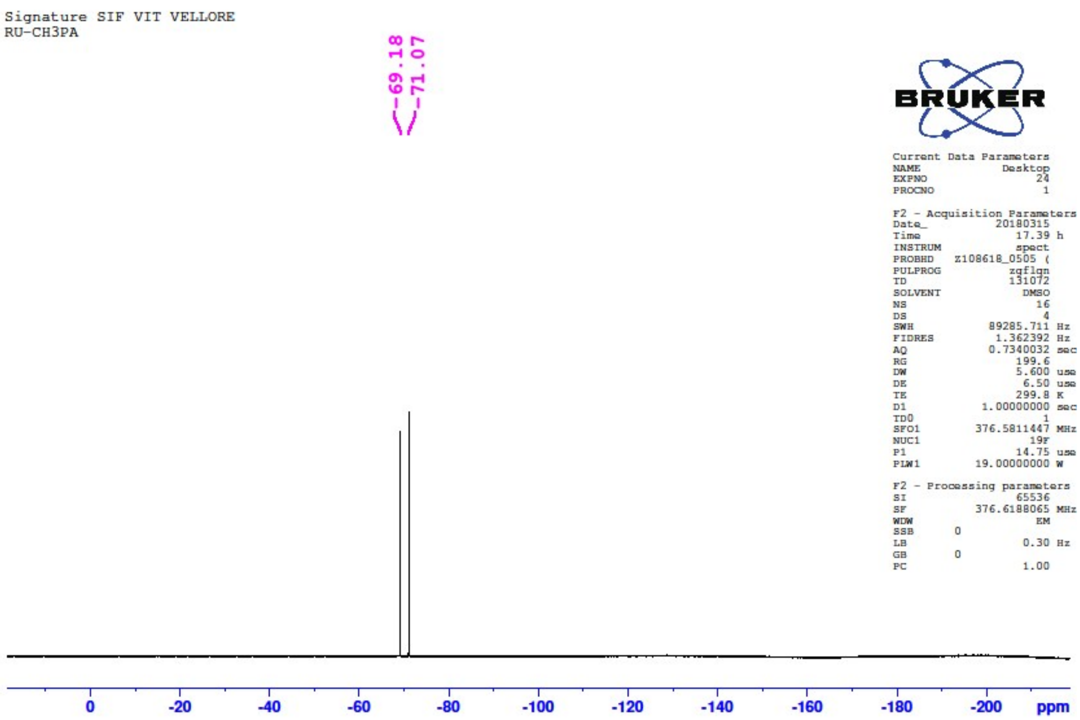
Figure S36: (a) LC-MS Spectra of 17a

(a) ^{1}H-NMR





(b) ^{19}F-NMR



(c)

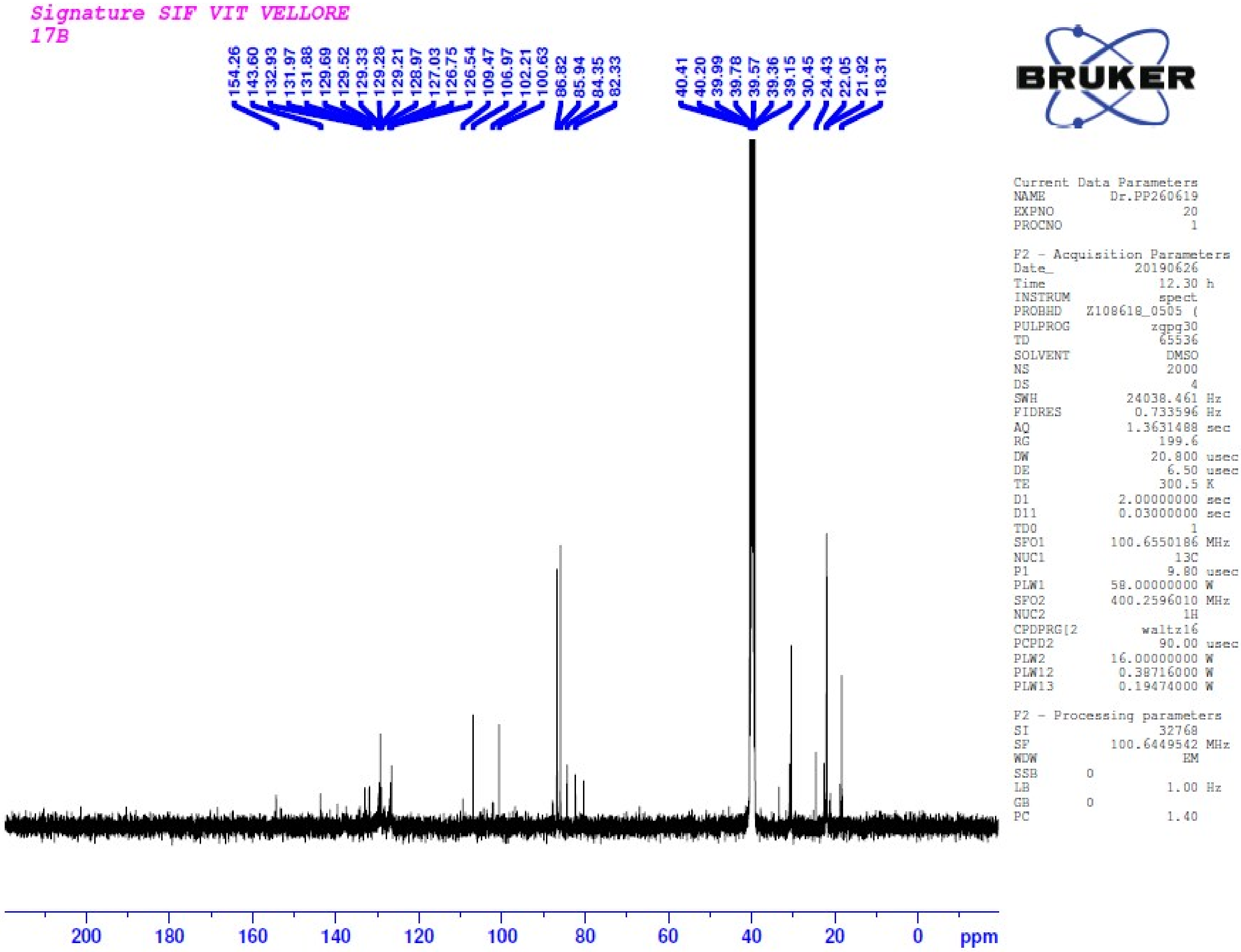
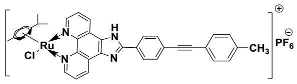
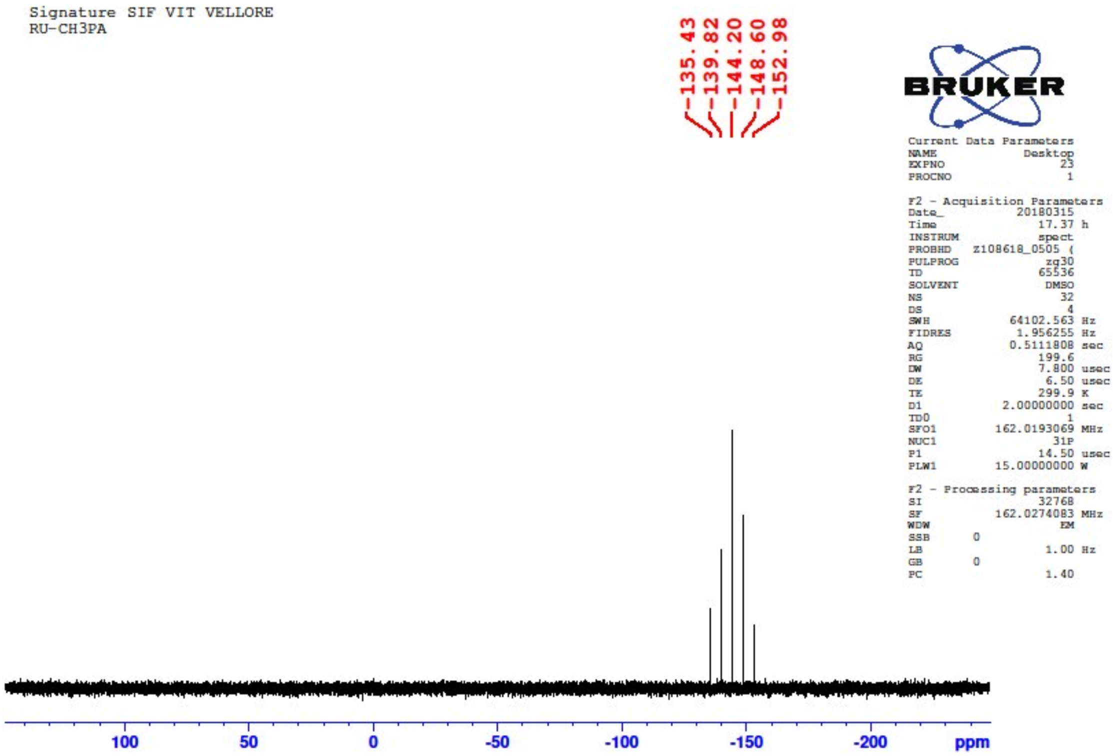


Figure S37: (a) ^{1}H-NMR (b) ^{19}F-NMR (c) ^{13}C NMR Spectra of 17b

(a) ^{31}P-NMR





(b) IR Spectra

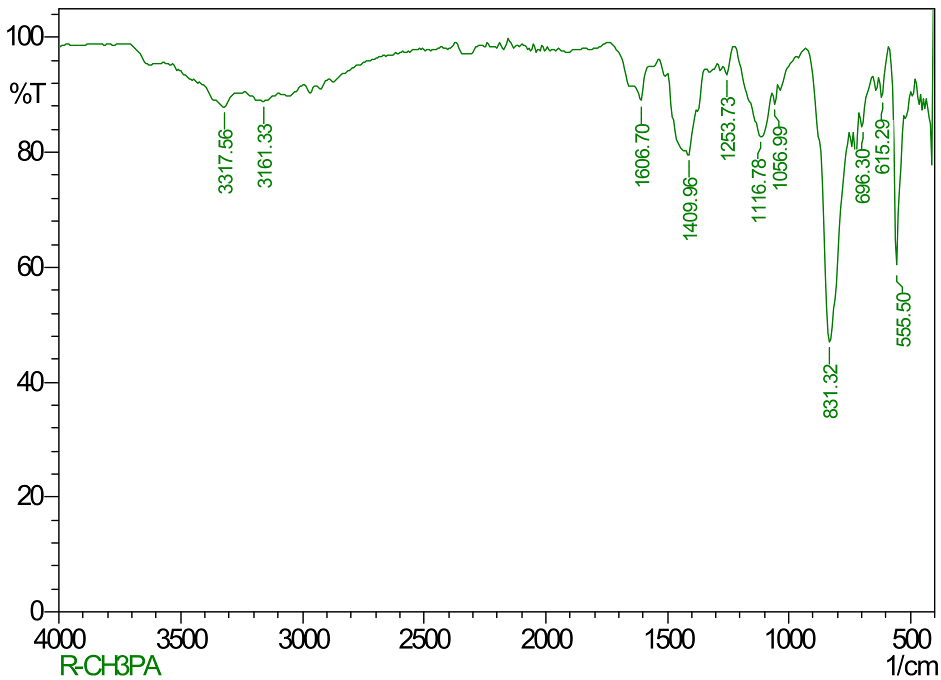
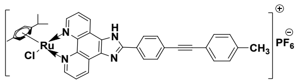


Figure S38: (a) ^{31}P-NMR (b) IR Spectra of 17b

(a) LC-MS Spectra



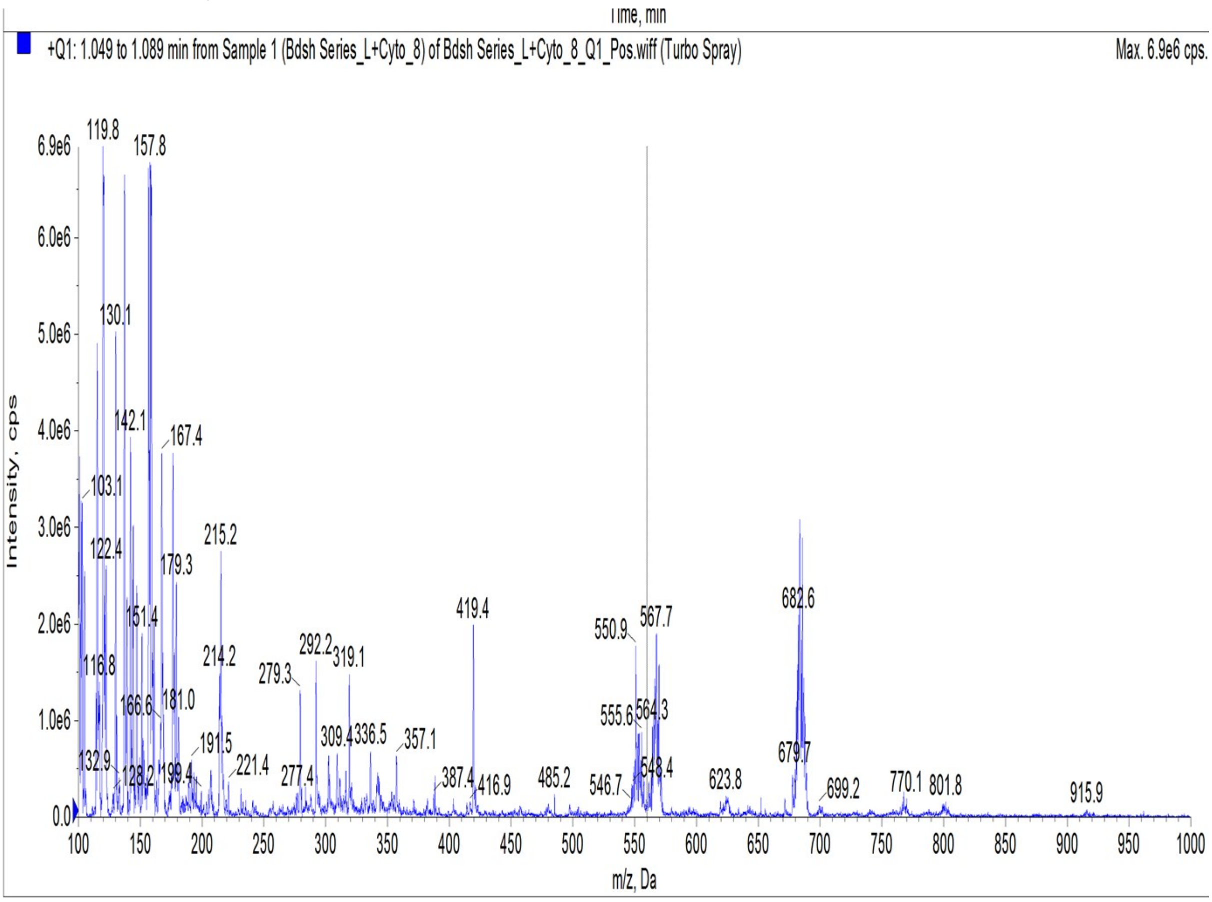
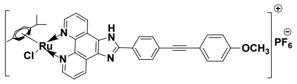
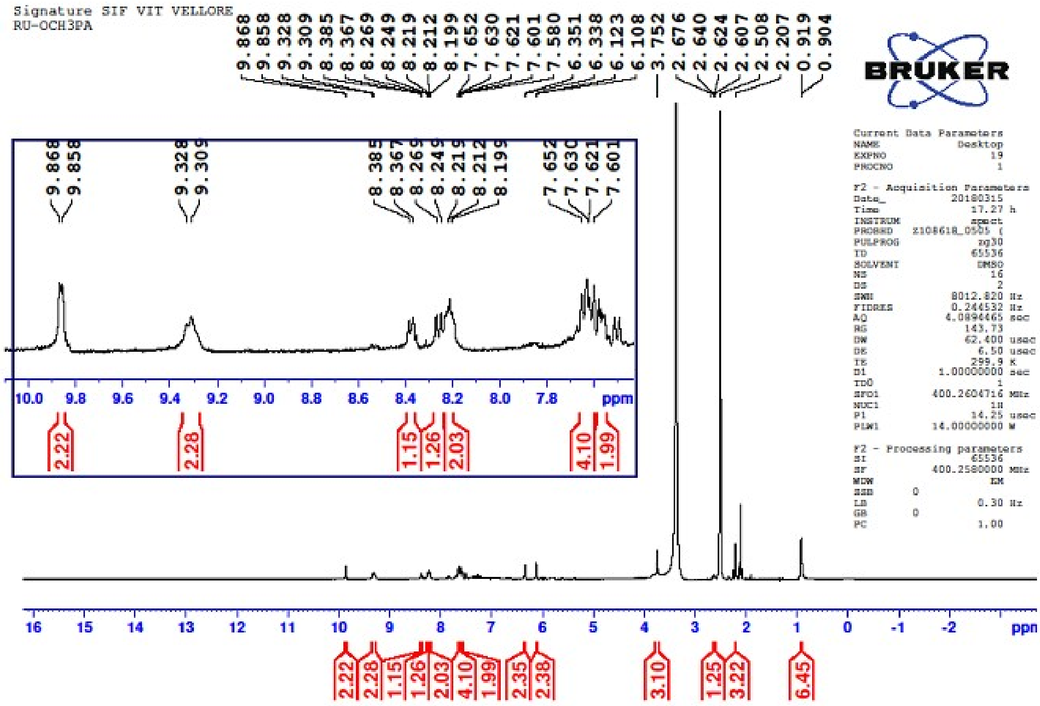


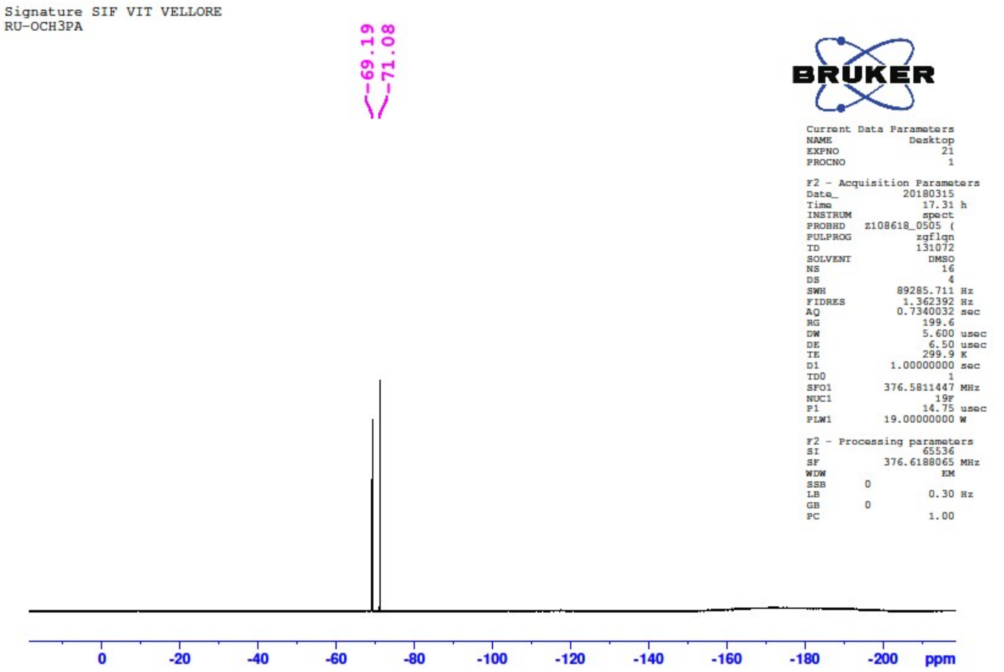
Figure S39: (a) LC-MS Spectra of 17b

(a) ^{1}H-NMR





(b) ^{19}F-NMR



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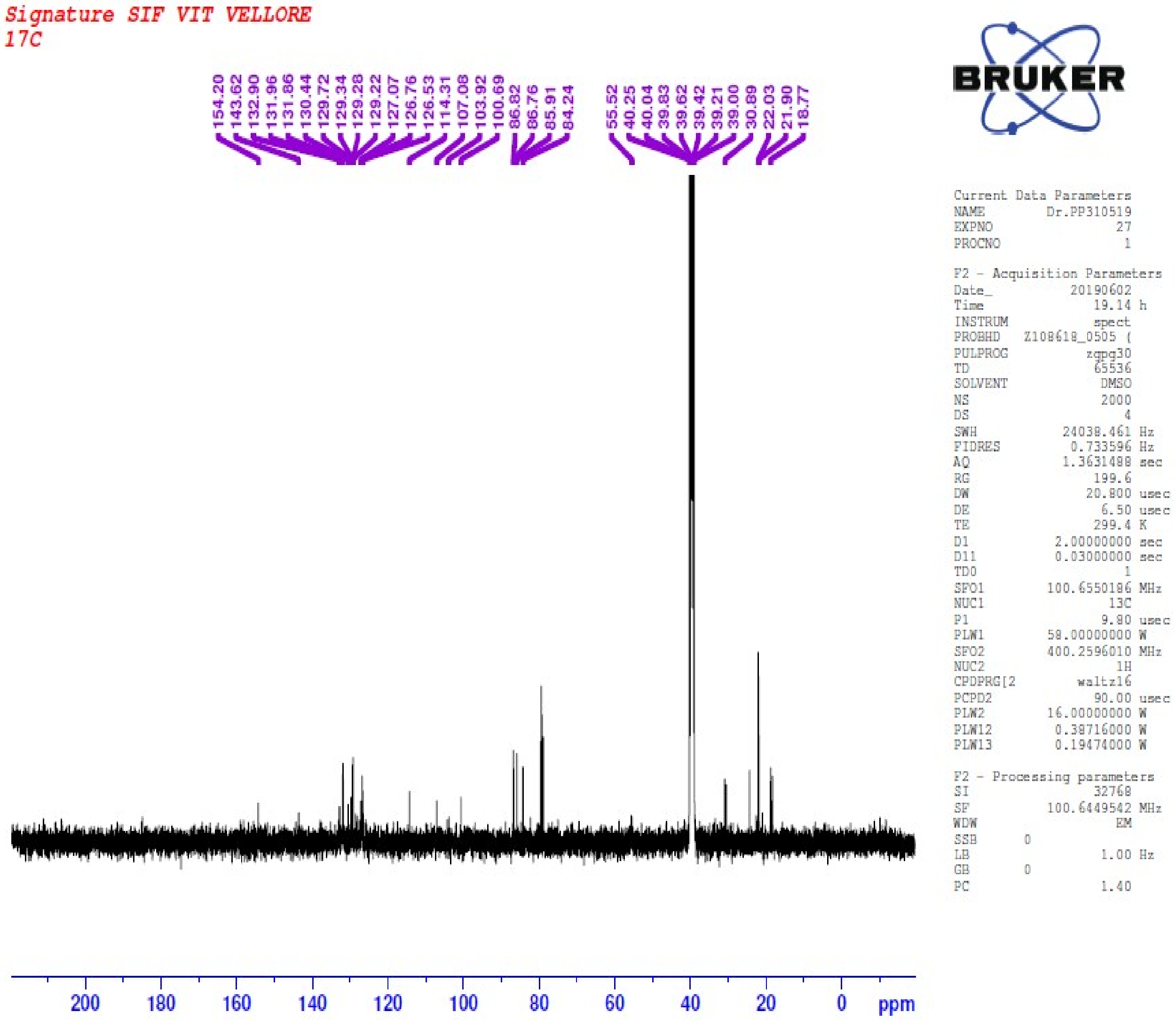

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SFO2 400.2596010 MHz
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WDW EM
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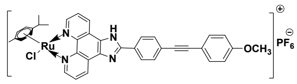
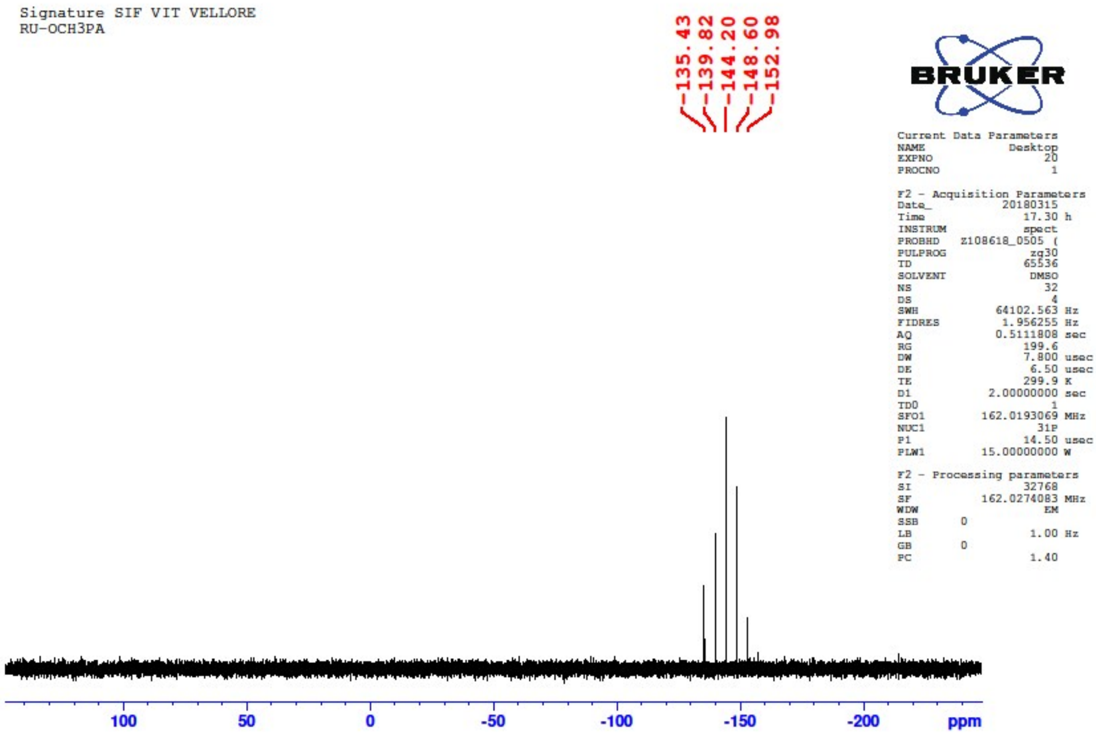
Figure S40: (a) ^{1}H-NMR (b) ^{19}F-NMR and (C) ^{13}C NMR Spectra of 17c



(a) ^{31}P-NMR



(b) IR Spectra

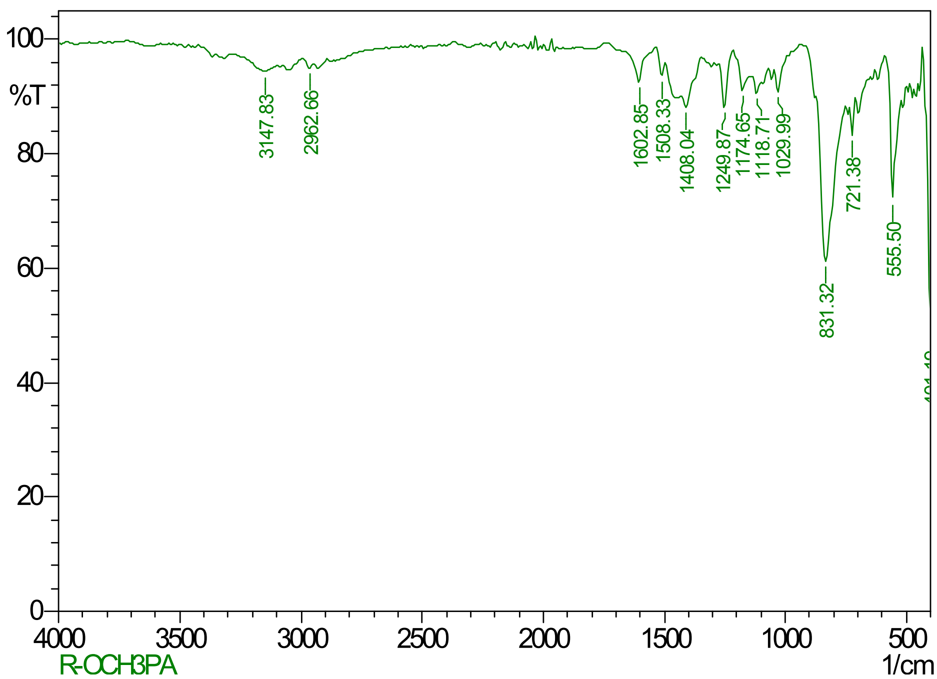
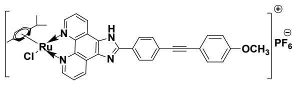


Figure S41: (a) ^{31}P-NMR (b) IR Spectra of 17c

(a) LC-MS Spectra



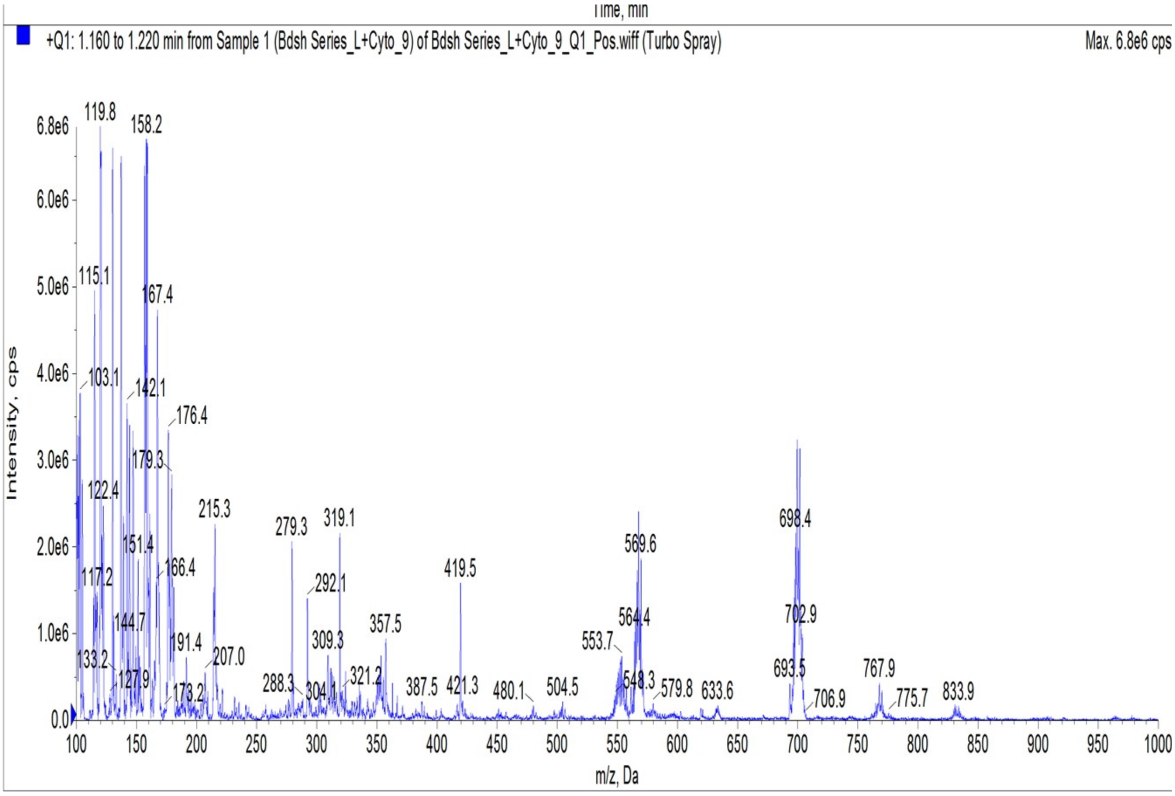
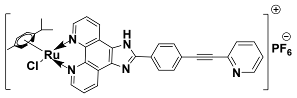
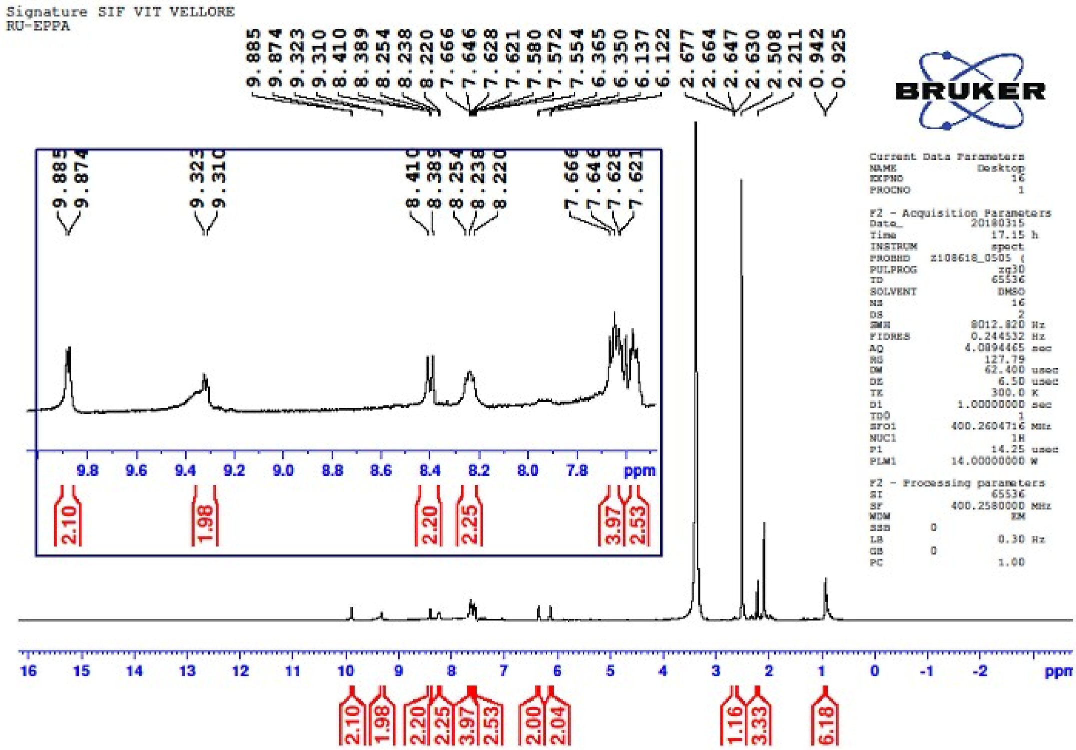


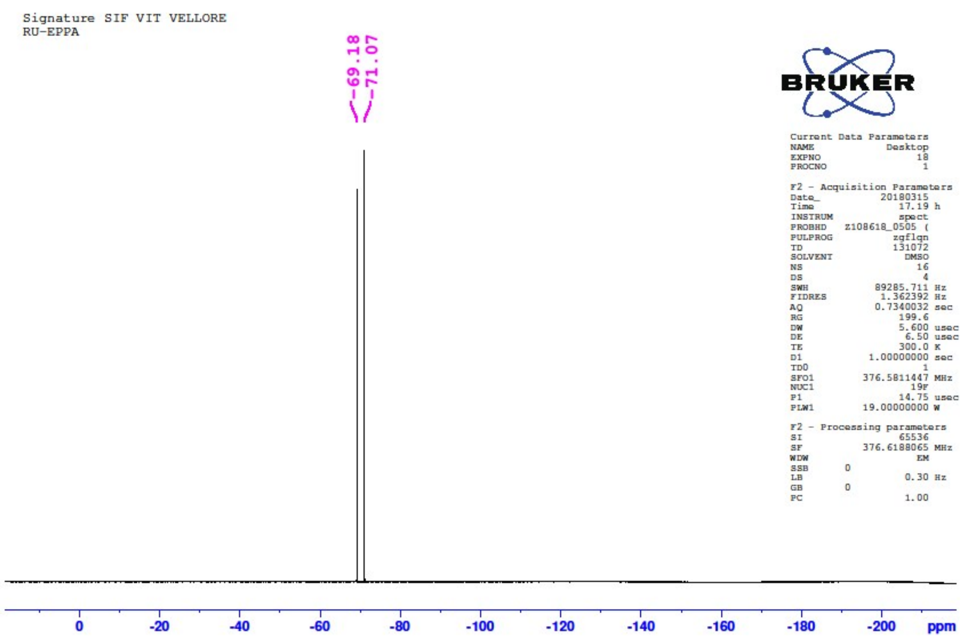
Figure S42: (a) LC-MS Spectra of 17c



(a) ^{1}H-NMR



(b) ^{19}F-NMR



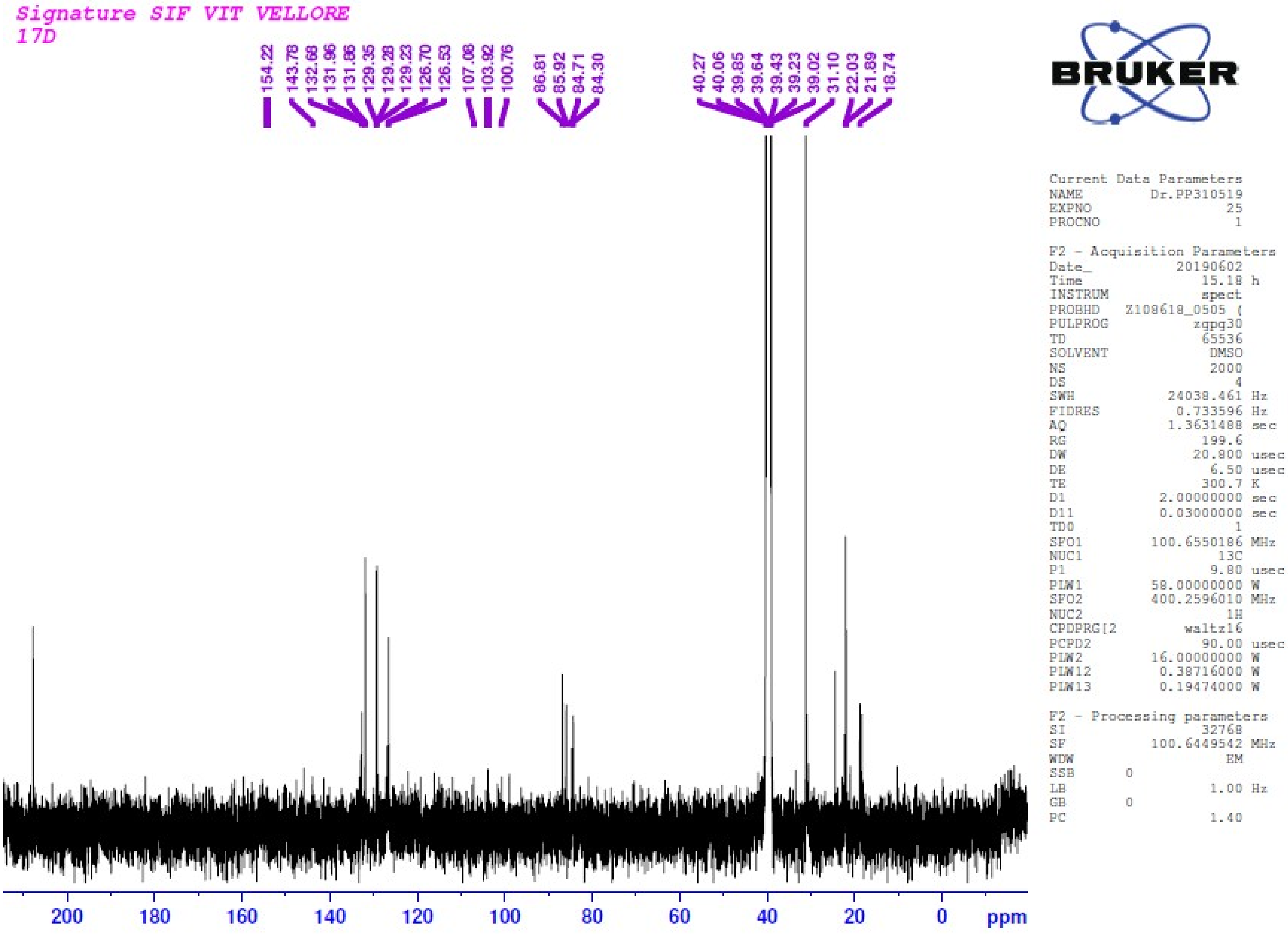
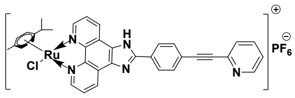
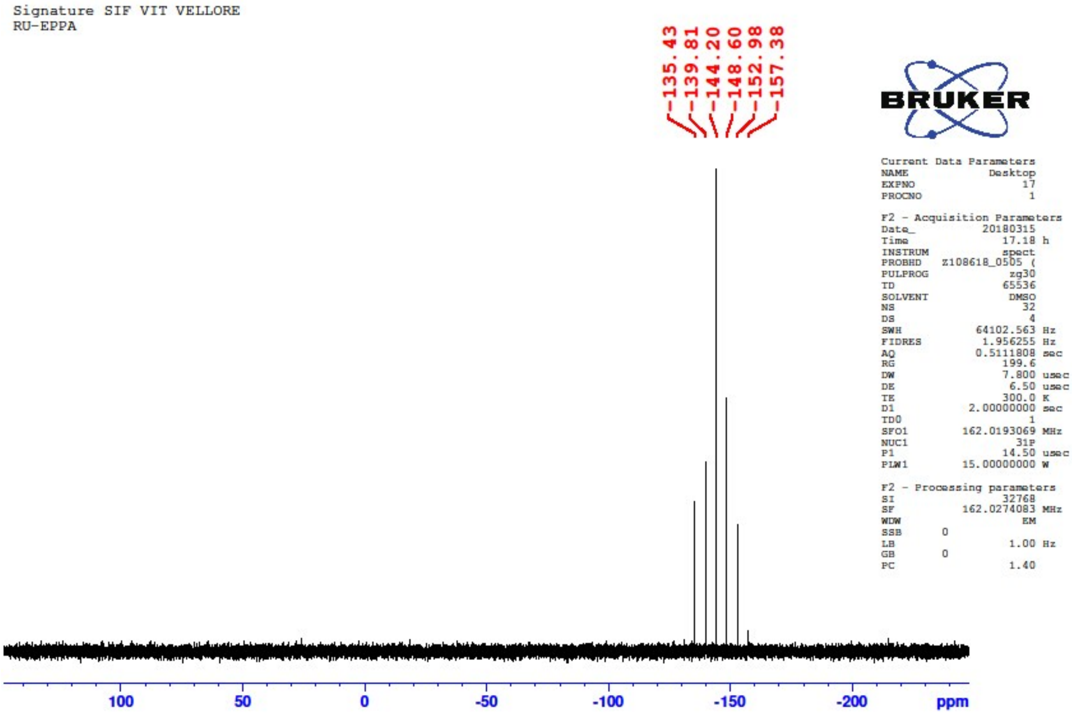


Figure S43: (a) ^{1}H-NMR (b) ^{19}F-NMR and (c) ^{13}C NMR Spectra of 17d



(a) ^{31}P-NMR



(b) IR Spectra

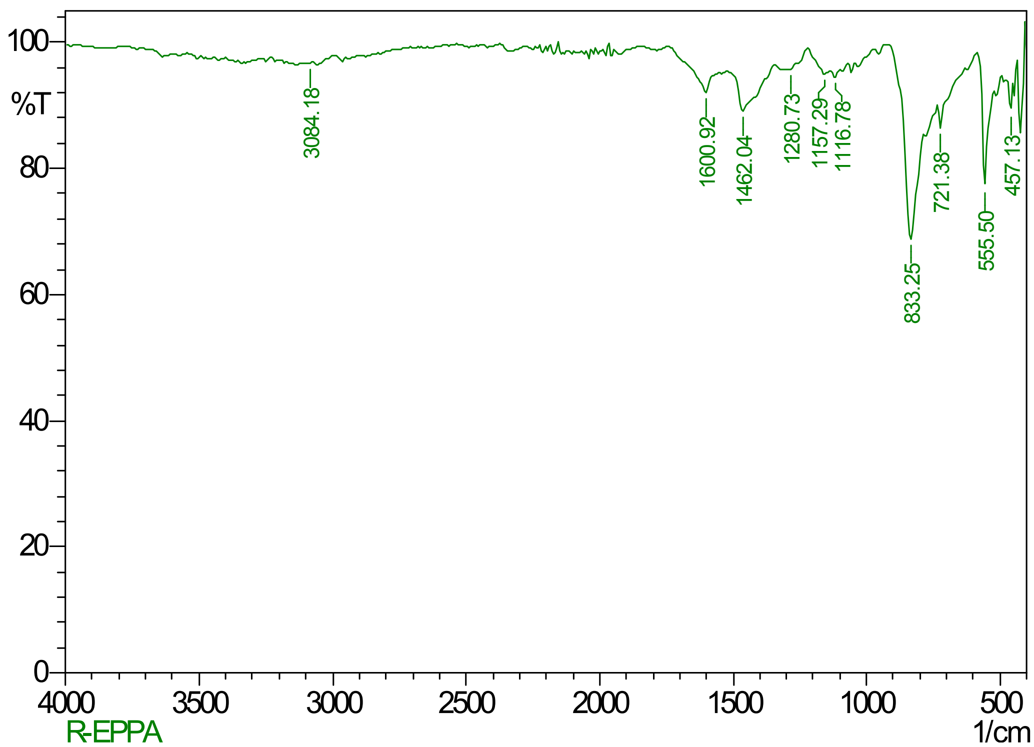
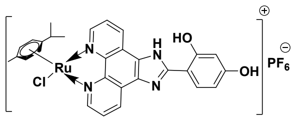
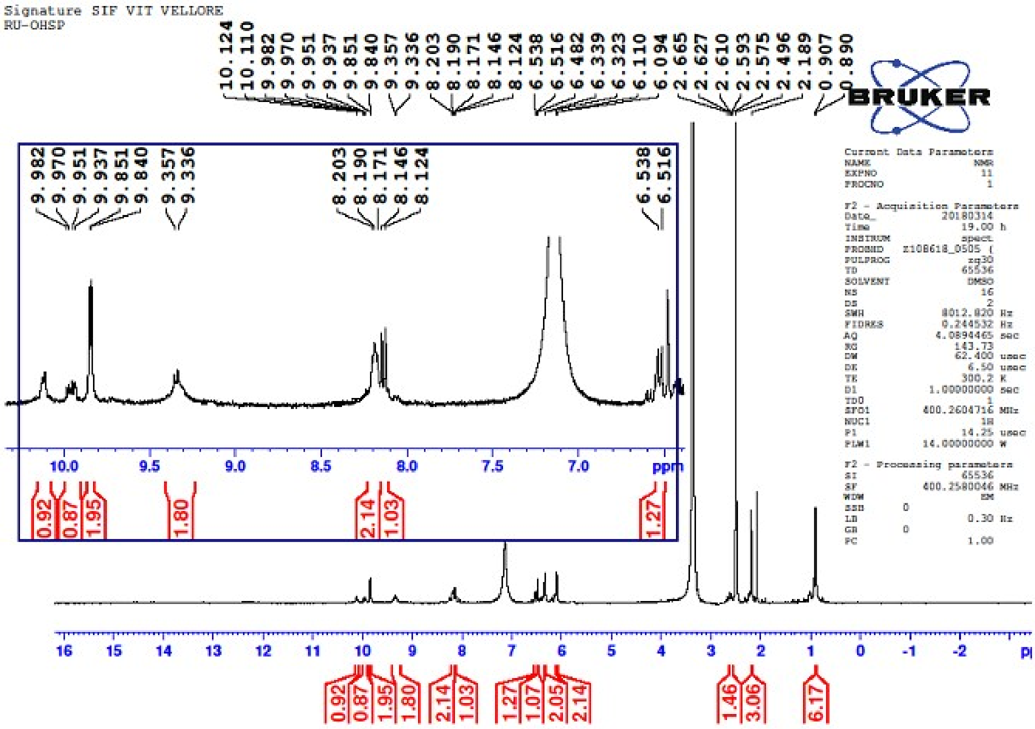


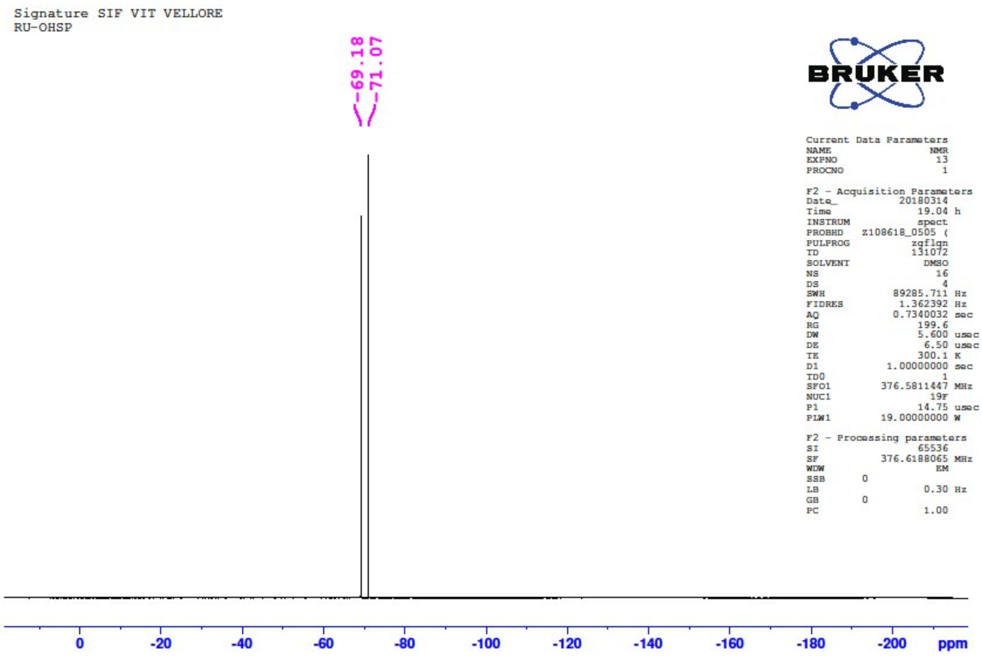
Figure S44: (a) ^{31}P-NMR (b) IR Spectra of 17d



(a) ^{1}H-NMR



(b) ^{19}F-NMR



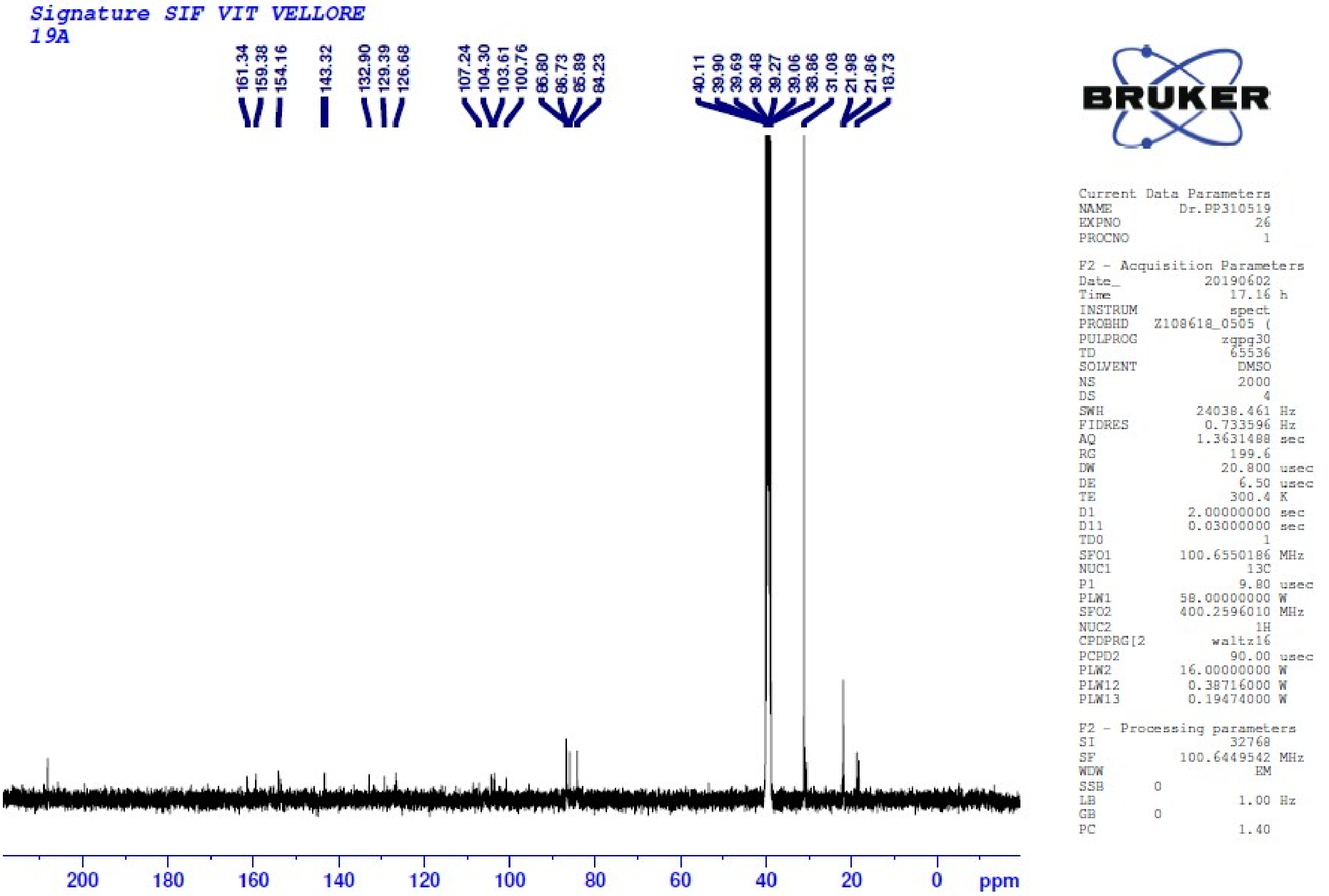
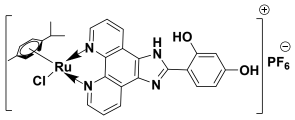
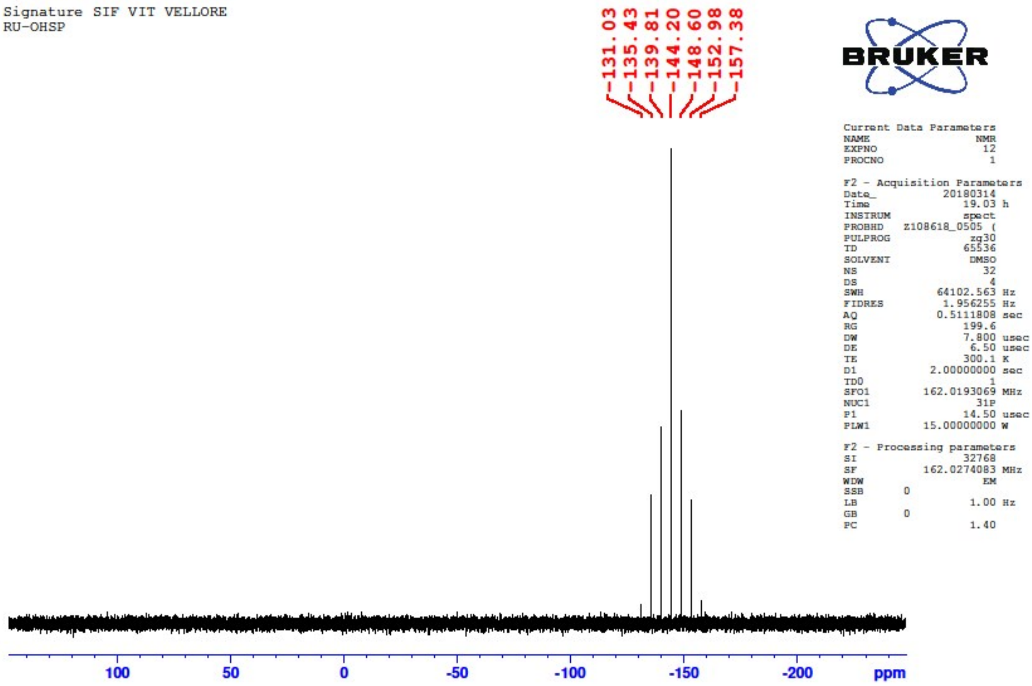


Figure S45: (a) ^{1}H-NMR (b) ^{19}F-NMR and (c) ^{13}C NMR Spectra of 19a



(a) ^{31}P-NMR



(b) IR Spectra

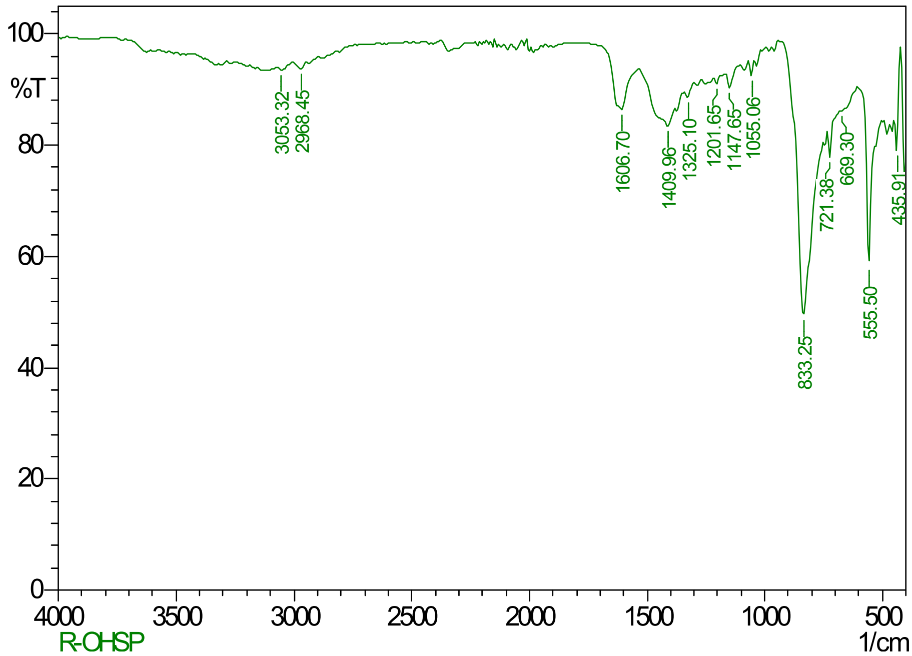
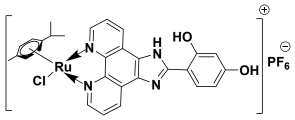


Figure S46: (a) ^{31}P-NMR (b) IR Spectra of 19a



(a) LC-MS Spectra

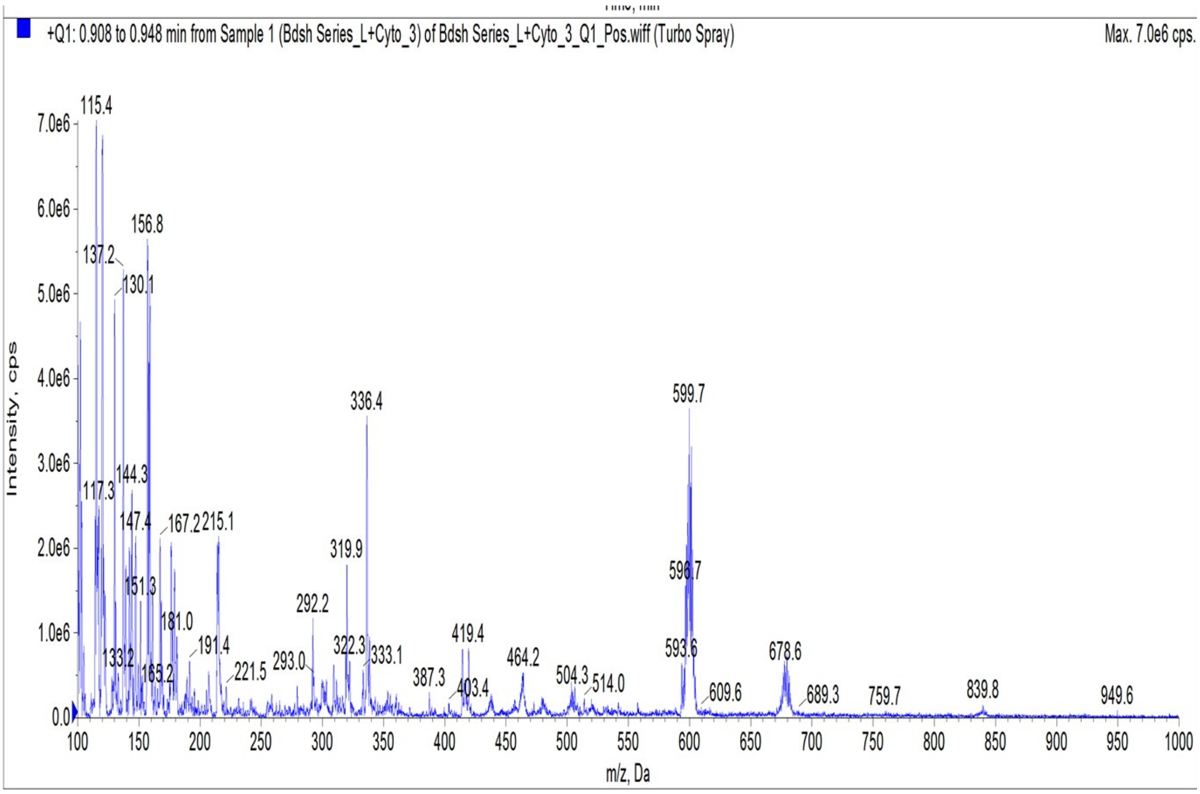
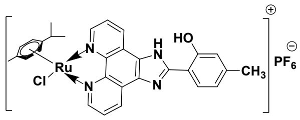
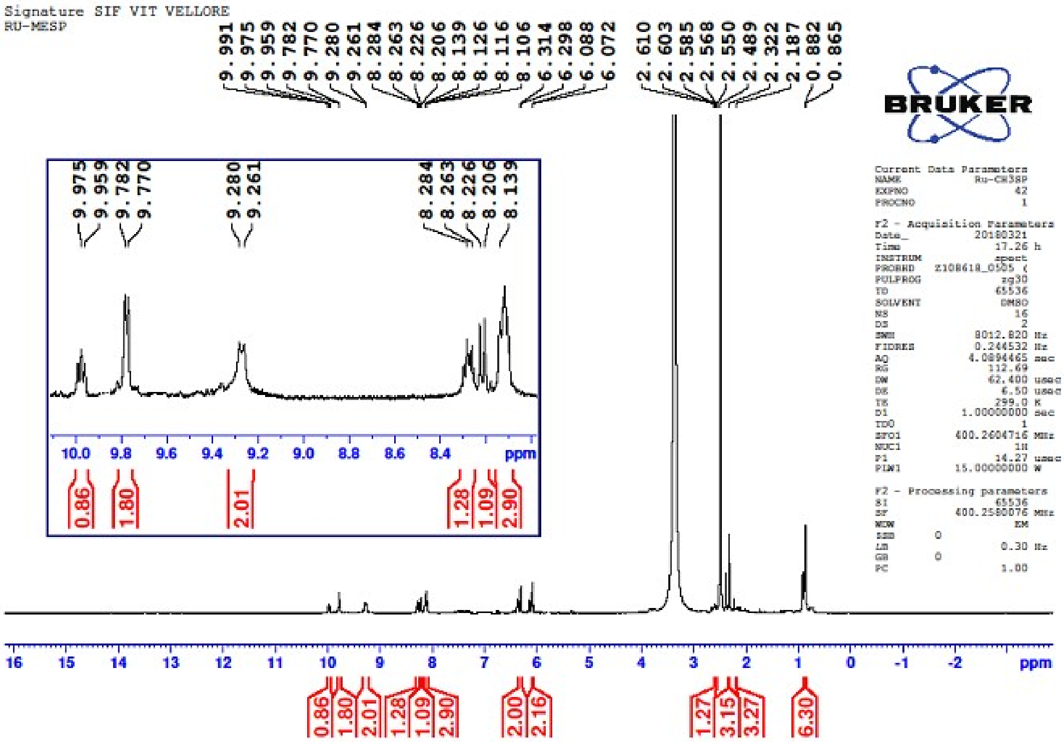


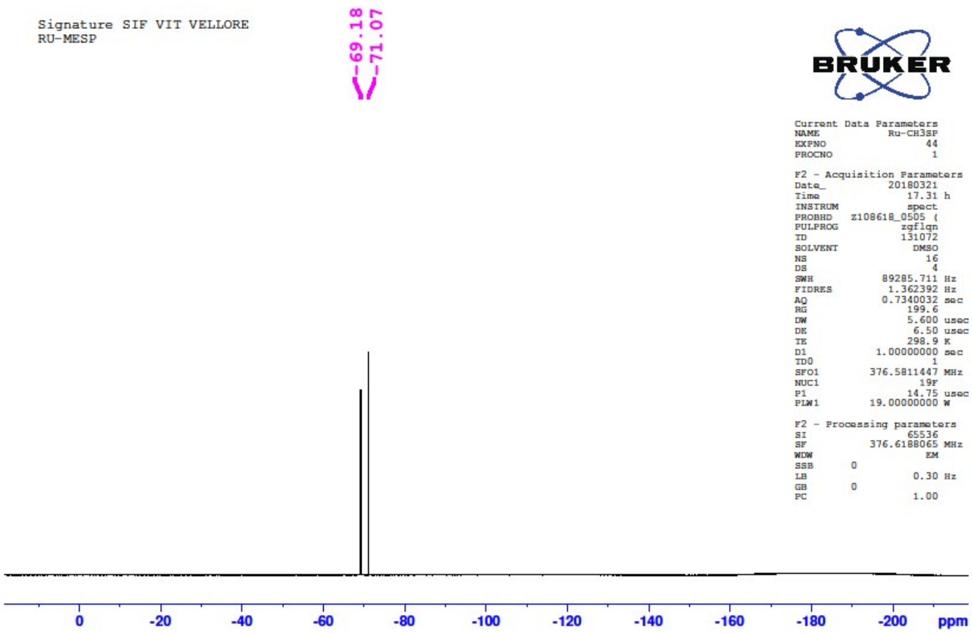
Figure S47: LC-MS Spectra of 19a



(a) ^{1}H-NMR



(b) ^{19}F-NMR



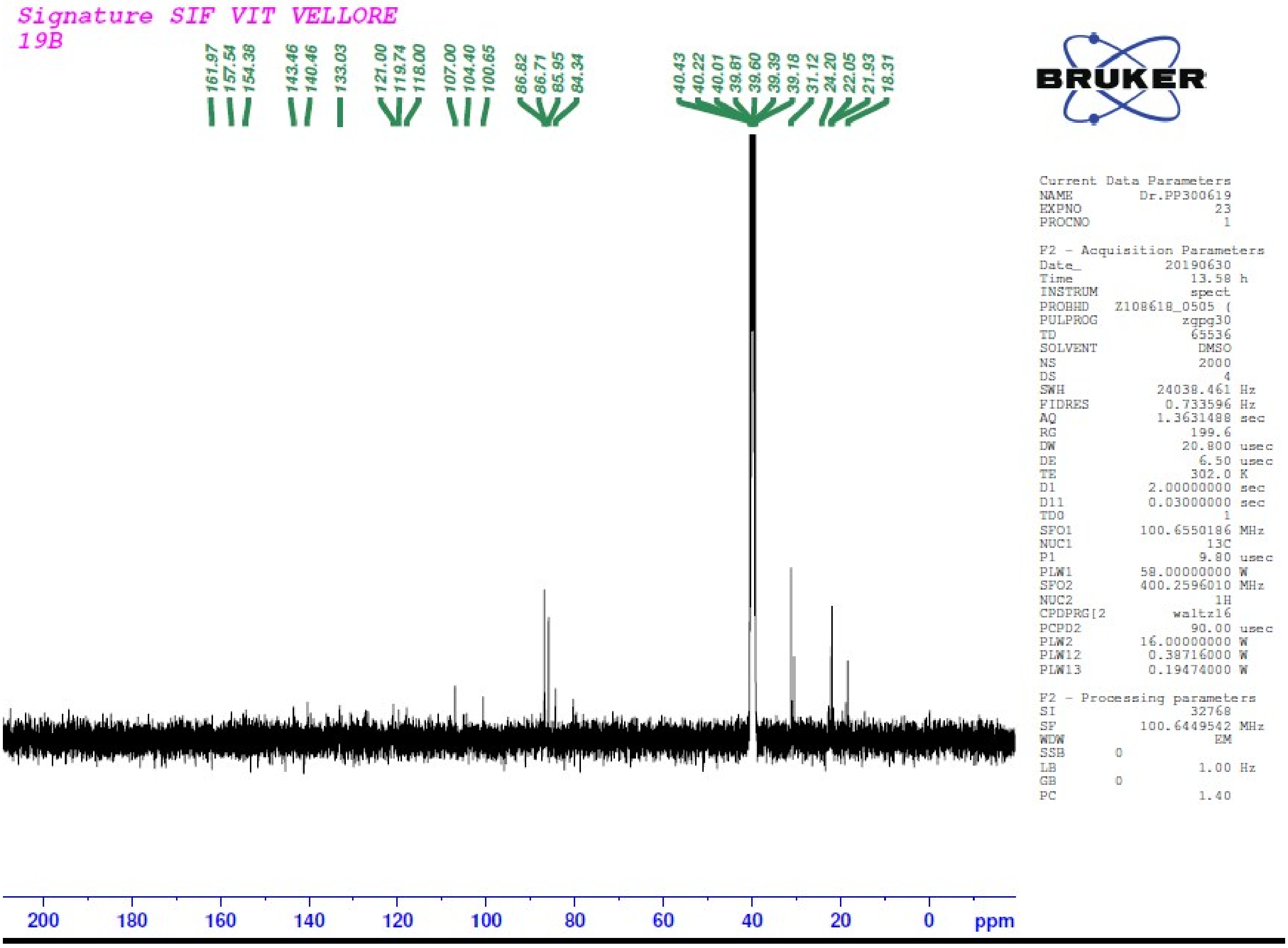
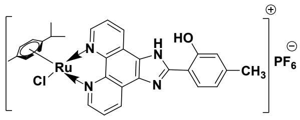
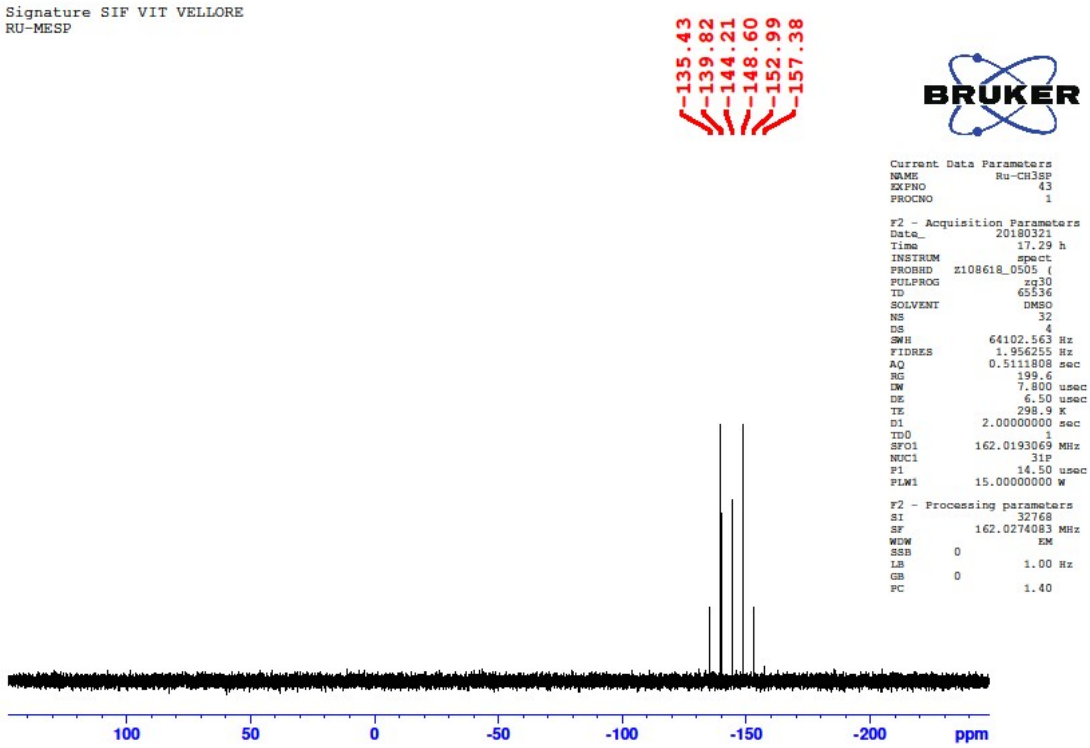


Figure S48: (a) ^{1}H-NMR (b) ^{19}F-NMR and (c) ^{13}C NMR Spectra of 19b



(a) ^{31}P-NMR



(b) IR Spectra

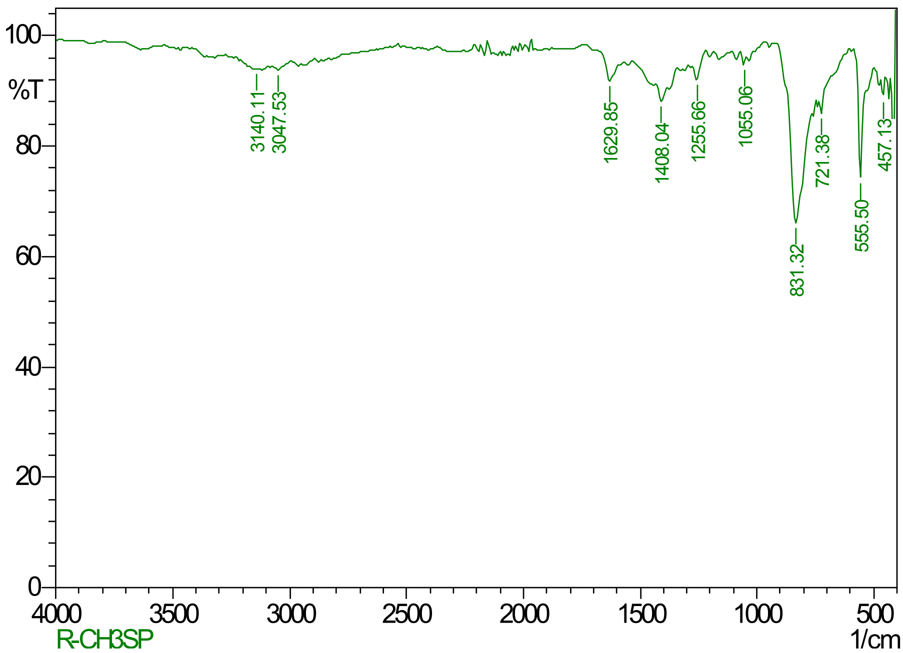
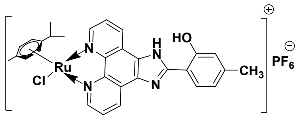


Figure S49: (a) ^{31}P-NMR (b) IR Spectra of 19b

(a) LC-MS Spectra



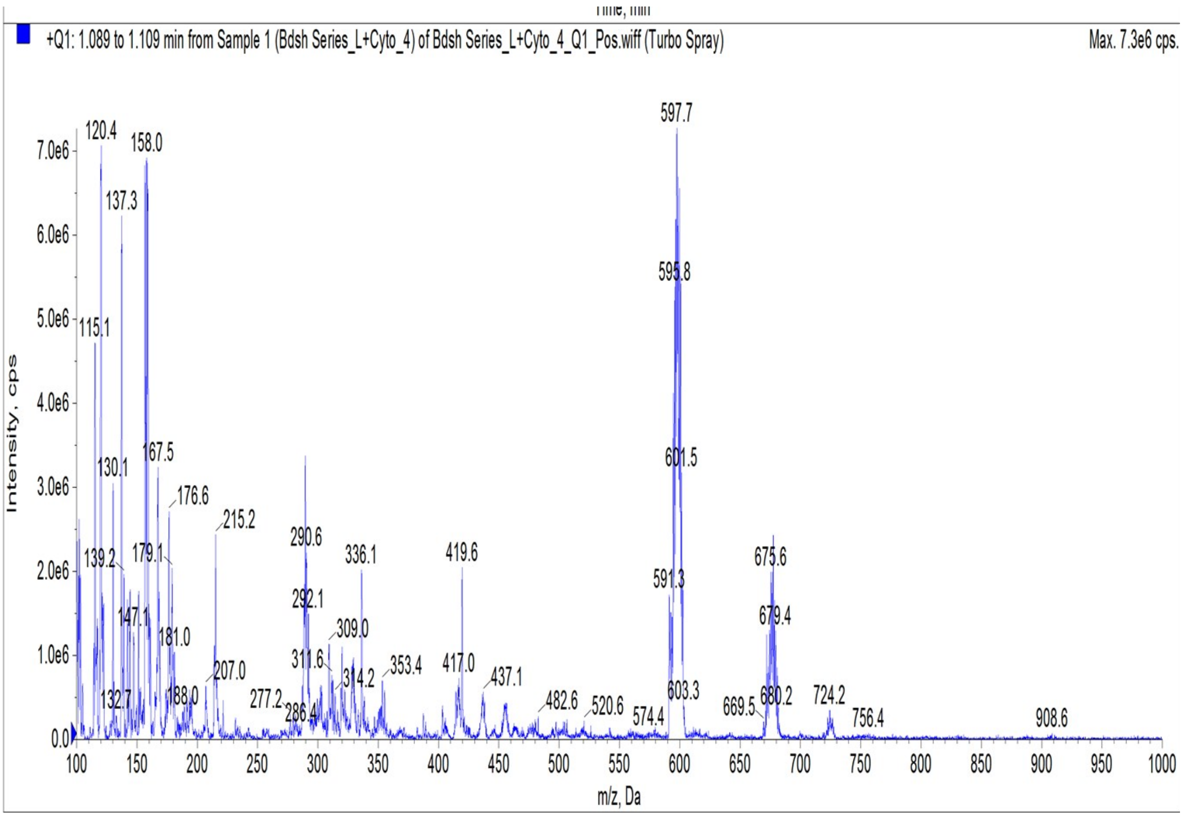
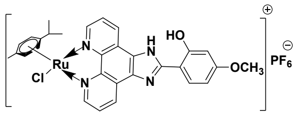
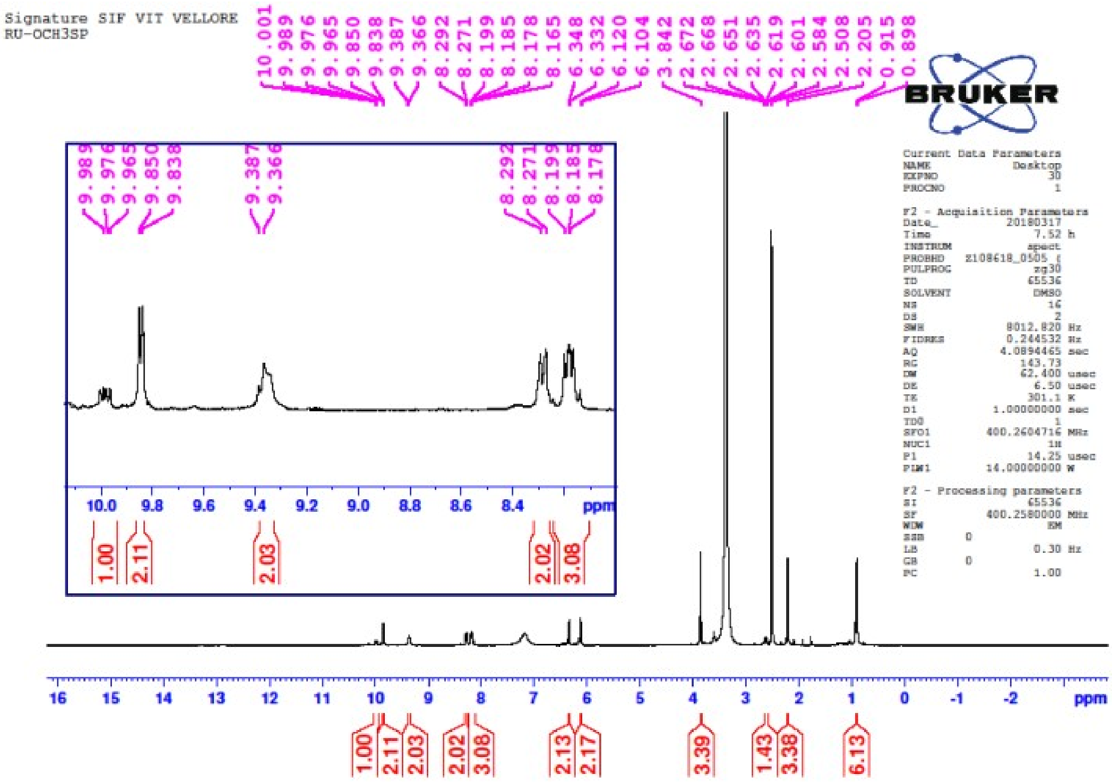


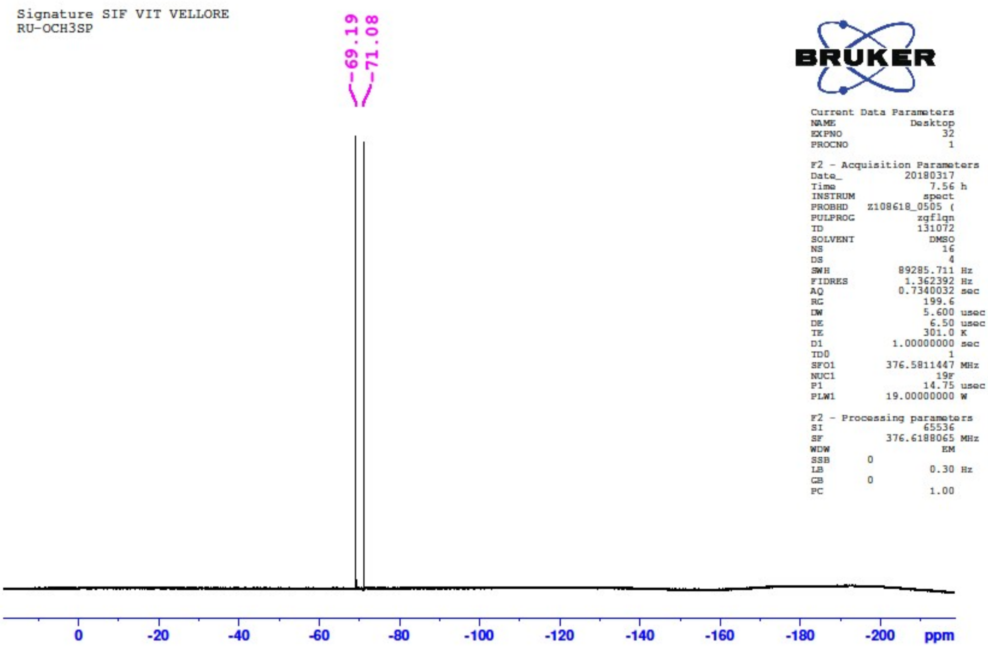
Figure S50: (a) LC-MS Spectra of 19b



(a) ^{1}H-NMR



(b) ^{19}F-NMR



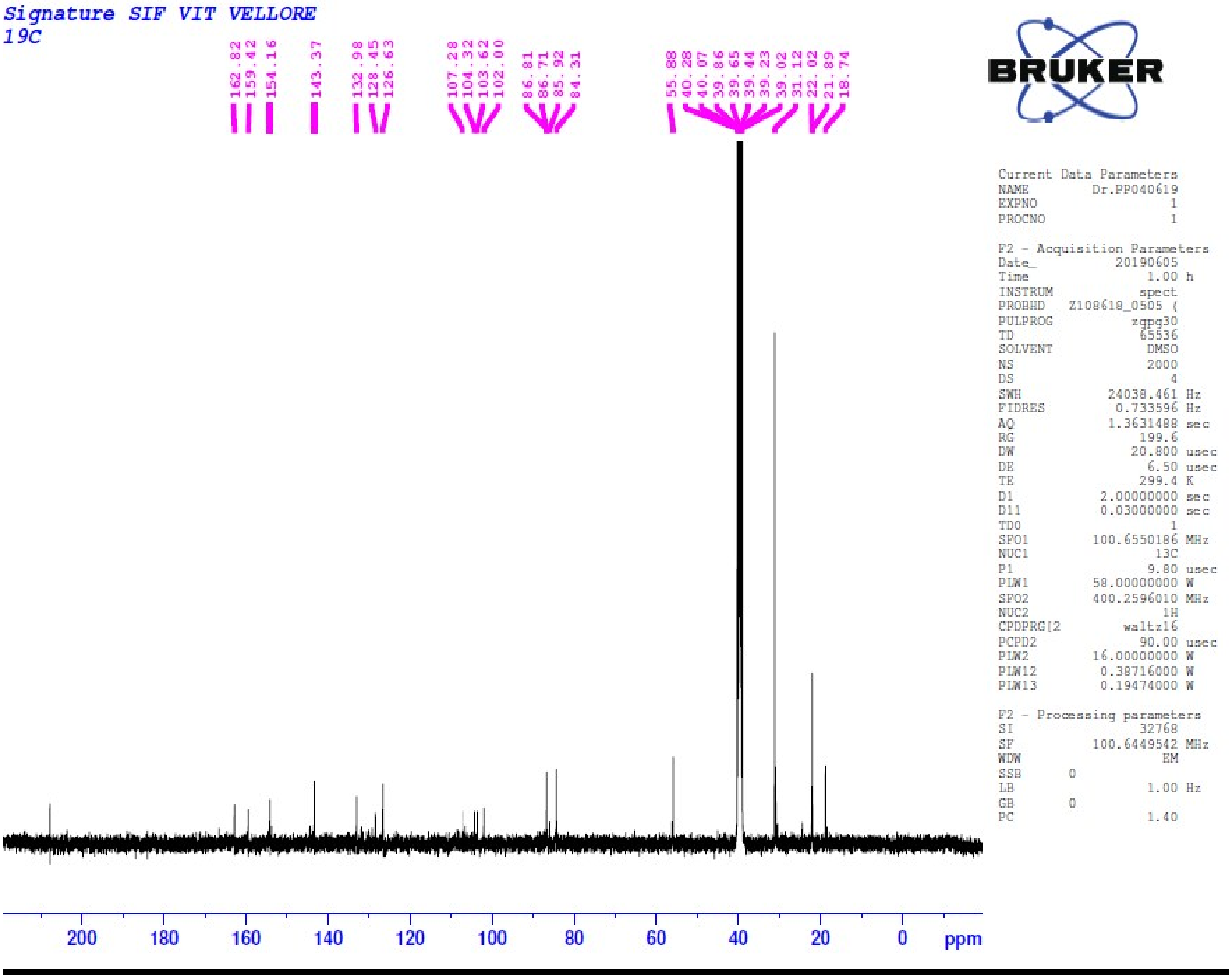
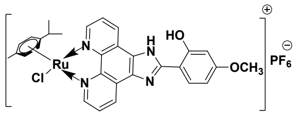
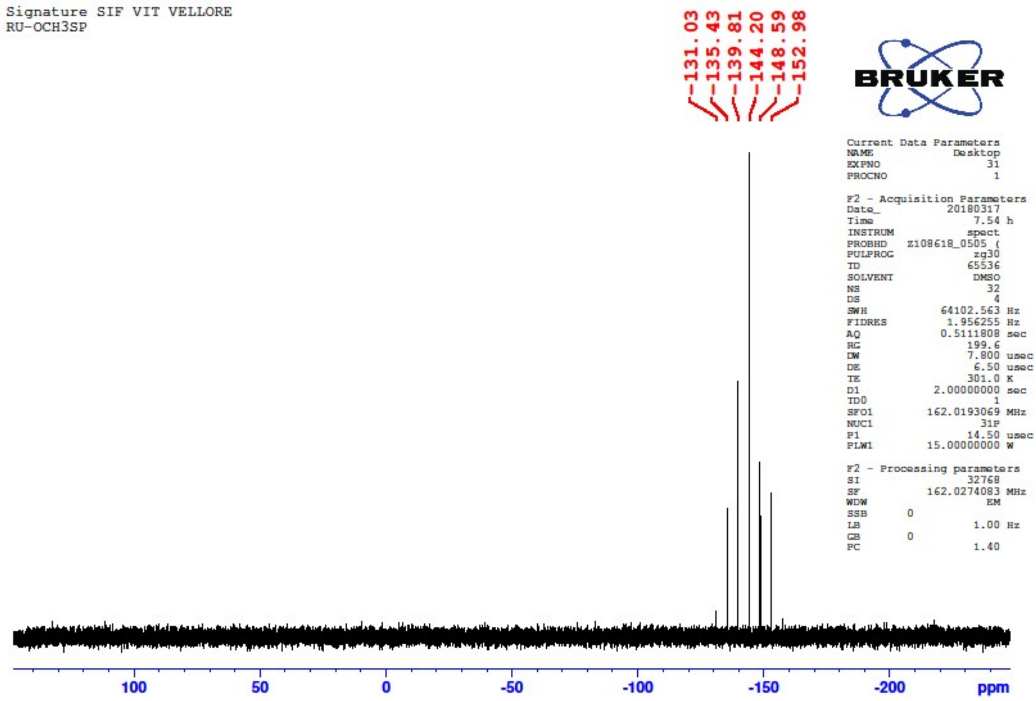


Figure S51: (a) ^{1}H-NMR (b) ^{19}F-NMR and (c) ^{13}C NMR Spectra of 19c



(a) ^{31}**P-NMR**



(b) IR Spectra

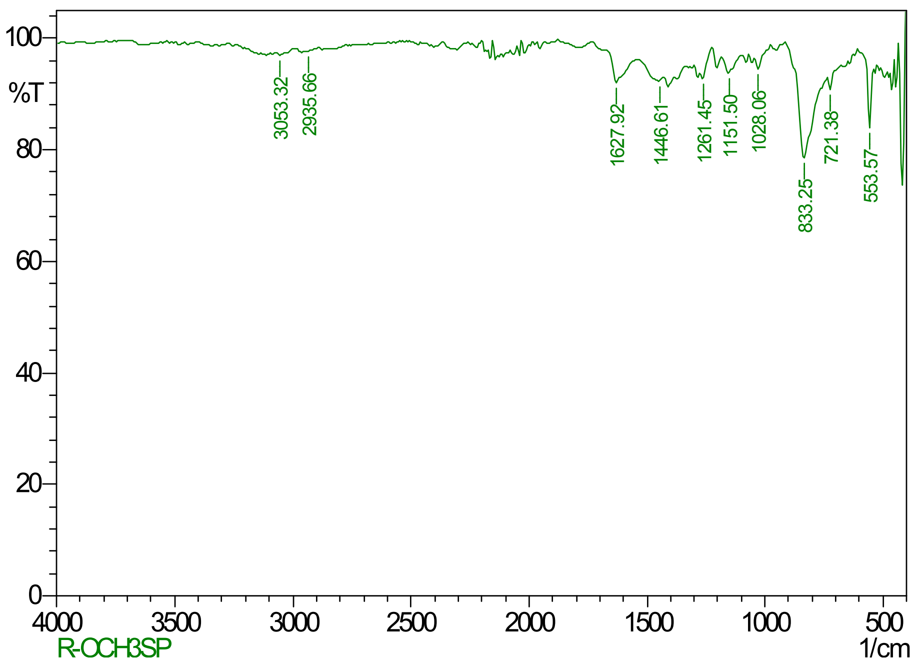
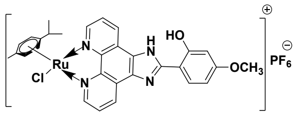


Figure S52: (a) ^{31}**P-NMR (b) IR Spectra of 19c**



(a) LC-MS Spectra

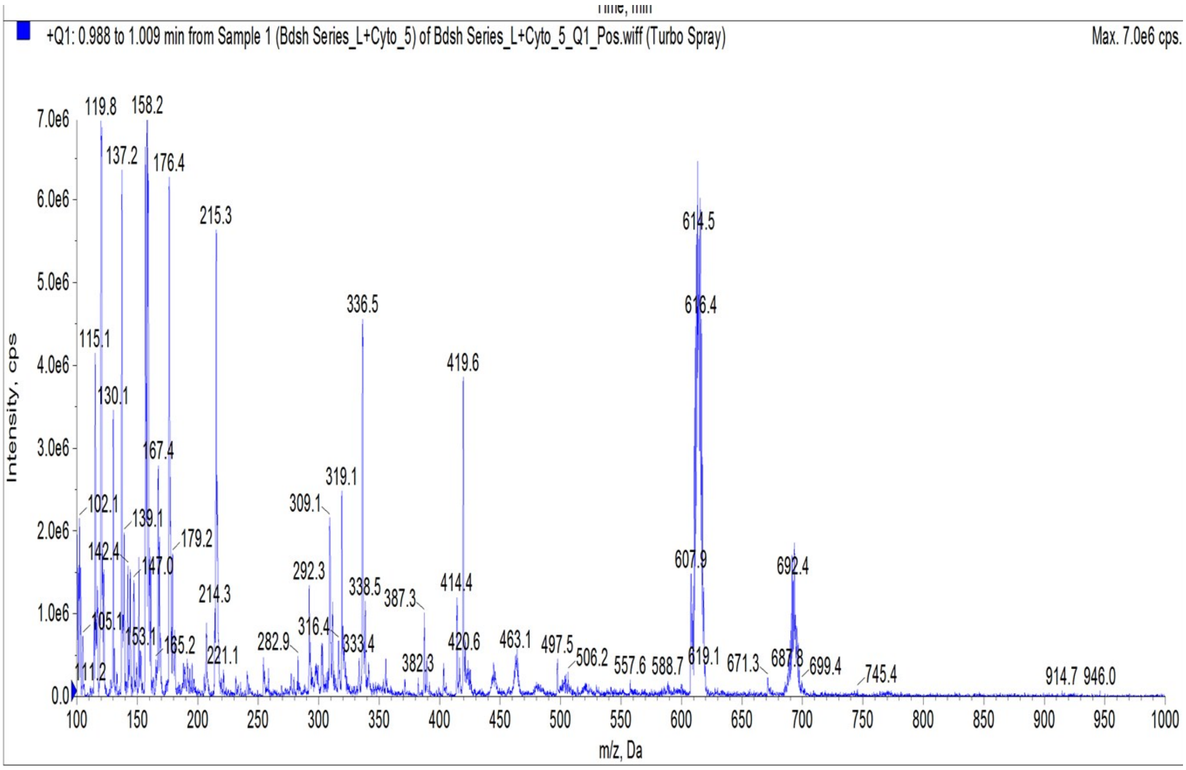


Figure S53: (a) LC-MS Spectra of 19c

Table S1 Time dependent conductance measurement

Samples	Time (h)	Conductance $\Lambda_M{}^a$ in 10% aq. DMSO
16b	0 1 6 12	160 194 300 400
17c	0 1 6 12	95 112 150 168
19c	0 1 6 12	86 105 194 220

[complex] = 3 X 10^{-5} M

Table S2 PH dependent conductivity study

Samples	PH	Conductance (Λ_M, ms) in 100% DMSO
16b	5	1.3
	4	2.6
	3	3.9
	2	4.8
	1	6.1

[16b] = 3 X 10^{-5} M

Table S3 GSH dependent conductivity study

Samples	[GSH] (10^{-4})	Conductance (Λ_M, µs) in 100% DMSO
16b	1	60
	2	65
	3	68
	4	72

	5	**75**
17c	**1**	**35**
	2	**39**
	3	**43**
	4	**48**
	5	**54**
19c	**1**	**34**
	2	**38**
	3	**42**
	4	**48**
	5	**53**

[complex] = 3 X 10^{-5} M

Table S4 conductivity study in presence of DNA

Samples	**[DNA] (10^{-6})**	**r_i = [complex]/[DNA]**	**Conductance (Λ_M, µs) in 100% DMSO**
16b	**1**	**30**	**28**
	2	**15**	**32**
	3	**10**	**34**
	4	**7.5**	**36**

[16b] = 3 X 10^{-5} M