

Supporting Information for

**Fine tuning through valence bond tautomerization of ancillary ligand in ruthenium(II) arene complex for better anticancer activity and enzyme inhibition property**

Poulami Mandal,<sup>a</sup> Novina Malviya,<sup>a</sup> M. Fátima C. Guedes da Silva,<sup>b</sup> Sandeep Singh Dhankhar,<sup>c</sup> C. M. Nagaraja,<sup>c</sup> Shaikh M Mobin,<sup>a,d</sup> Suman Mukhopadhyay<sup>\*,a,d</sup>

<sup>a</sup> Department of Chemistry, School of Basic Sciences, Indian Institute of Technology Indore, Indore 453552, India.

<sup>b</sup> Centro de Química Estrutural, Complexo I, Instituto Superior Técnico, Technical University of Lisbon, Avenida Rovisco Pais, 1049-001, Lisbon, Portugal

<sup>c</sup> Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar 140001, Punjab, India

<sup>d</sup> Centre for Bioscience and Biomedical Engineering (BSBE), Indian Institute of Technology Indore, Indore 453552, India.

Tel : +91 731 2438 705 Fax: +91 731 2361 482 E-mail: [suman@iiti.ac.in](mailto:suman@iiti.ac.in)

Table of Contents

<sup>1</sup> H NMR spectra of Complex 2 .....	S1
<sup>13</sup> NMR spectra of Complex 2.....	S2
<sup>31</sup> P NMR spectra of Complex 2.....	S3
ESI- Mass spectrum of Complex 2.....	S4
<sup>1</sup> H NMR spectra of Complex 4 .....	S5

$^{13}$ NMR spectra of Complex 4.....	S6
$^{31}$ P NMR spectra of Complex 4.....	S7
ESI- Mass spectrum of Complex 4.....	S8
$^1$ H NMR spectra of Complex 5 .....	S9
ESI- Mass spectrum of Complex 5.....	S10
$^1$ H NMR spectra of Complex 6 .....	S11
$^{13}$ NMR spectra of Complex 6.....	S12
$^{31}$ P NMR spectra of Complex 6.....	S13
ESI- Mass spectrum of Complex 6.....	S14
$^1$ H NMR spectra of Complex 7 .....	S15
ESI- Mass spectrum of Complex 7.....	S16
$^1$ H NMR spectra of Complex 8 .....	S17
$^{13}$ NMR spectra of Complex 8.....	S18
$^{31}$ P NMR spectra of Complex 8.....	S19
ESI- Mass spectrum of Complex 8.....	S20

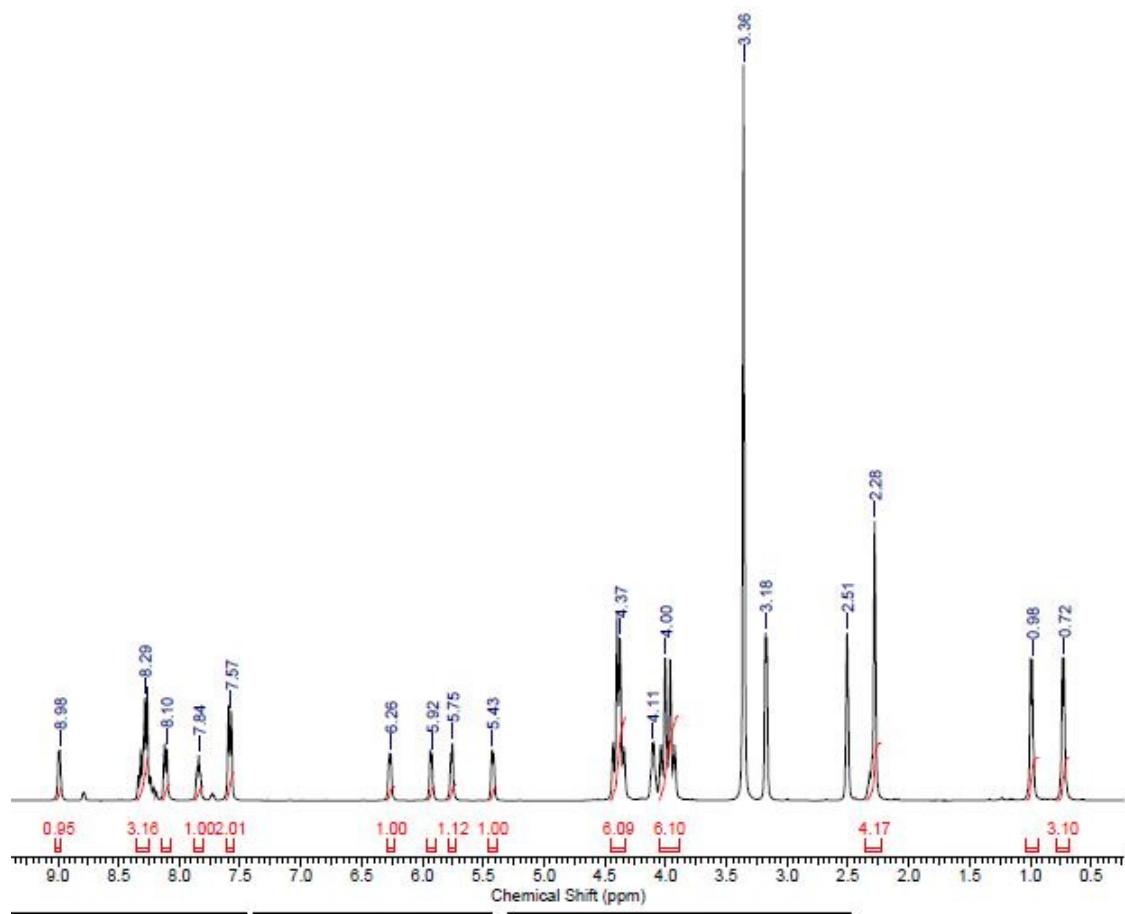


Fig S1: <sup>1</sup>H NMR Spectra of Complex 2

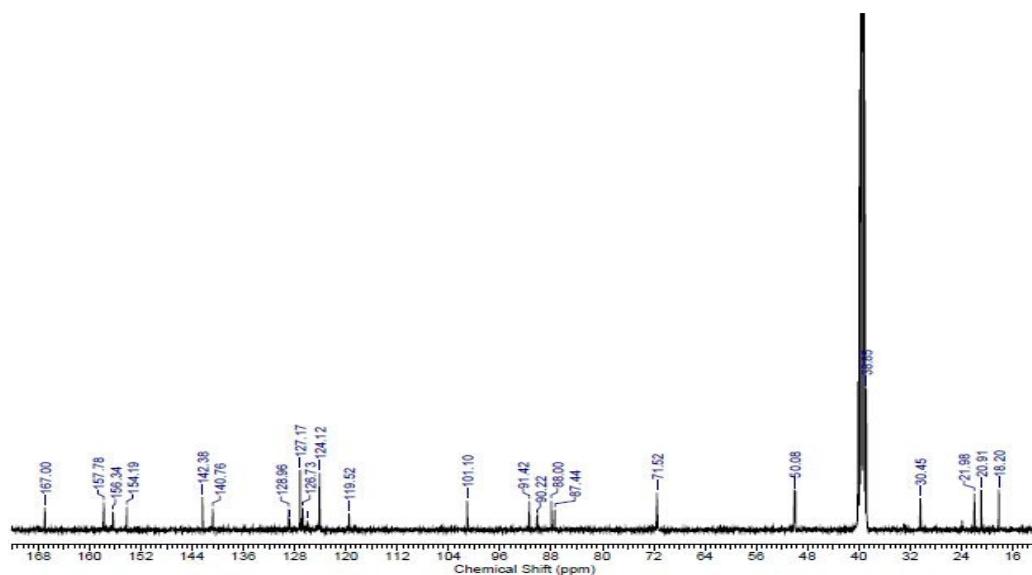


Fig S2: <sup>13</sup>C NMR Spectra of Complex 2

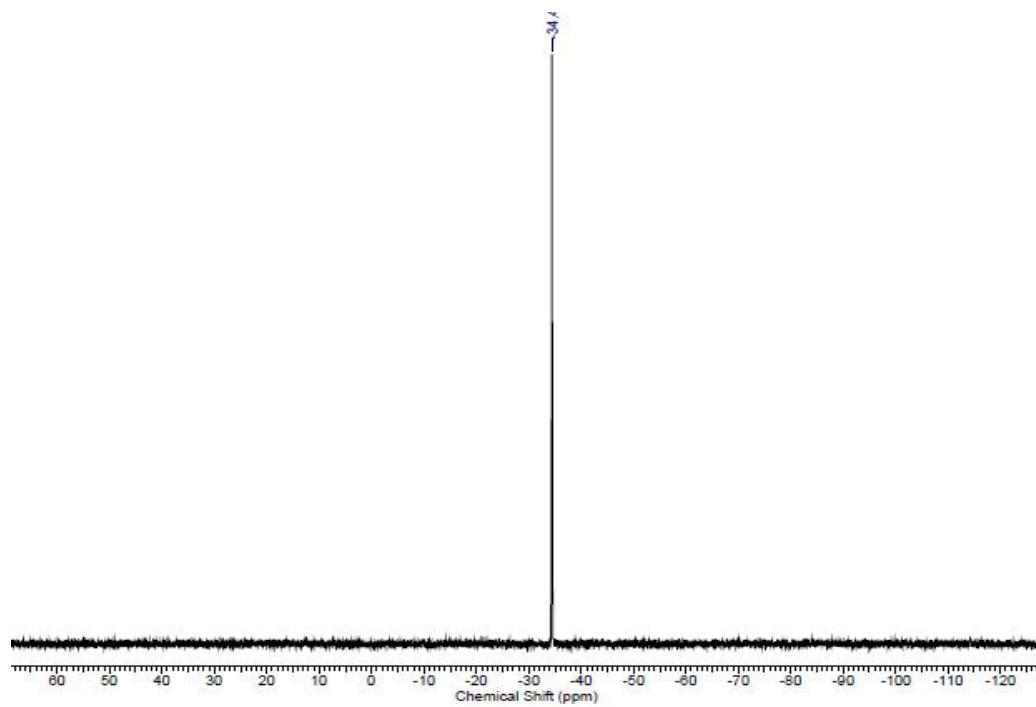


Fig S3:  $^{31}\text{P}$  NMR Spectra of Complex 2

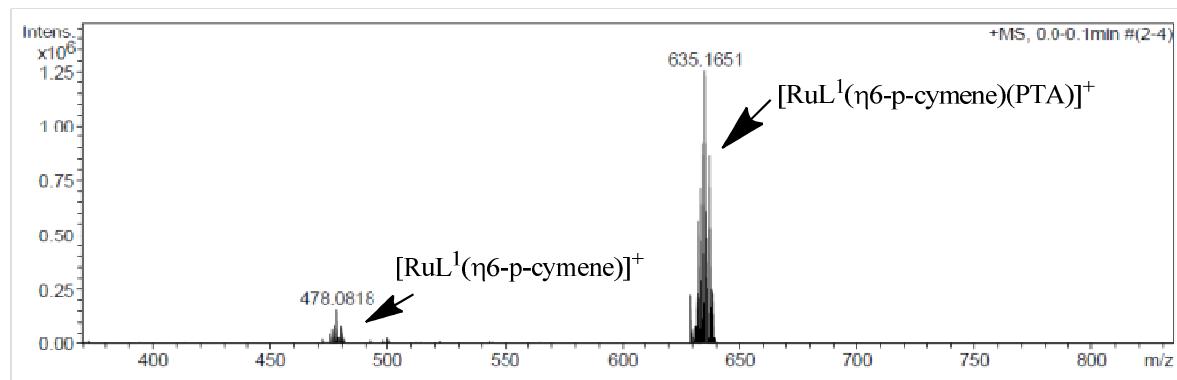


Fig S4: ESI-MS Spectra of Complex 2  $[\text{RuL}^1(\eta^6\text{-p-cymene})(\text{PTA})]^+$

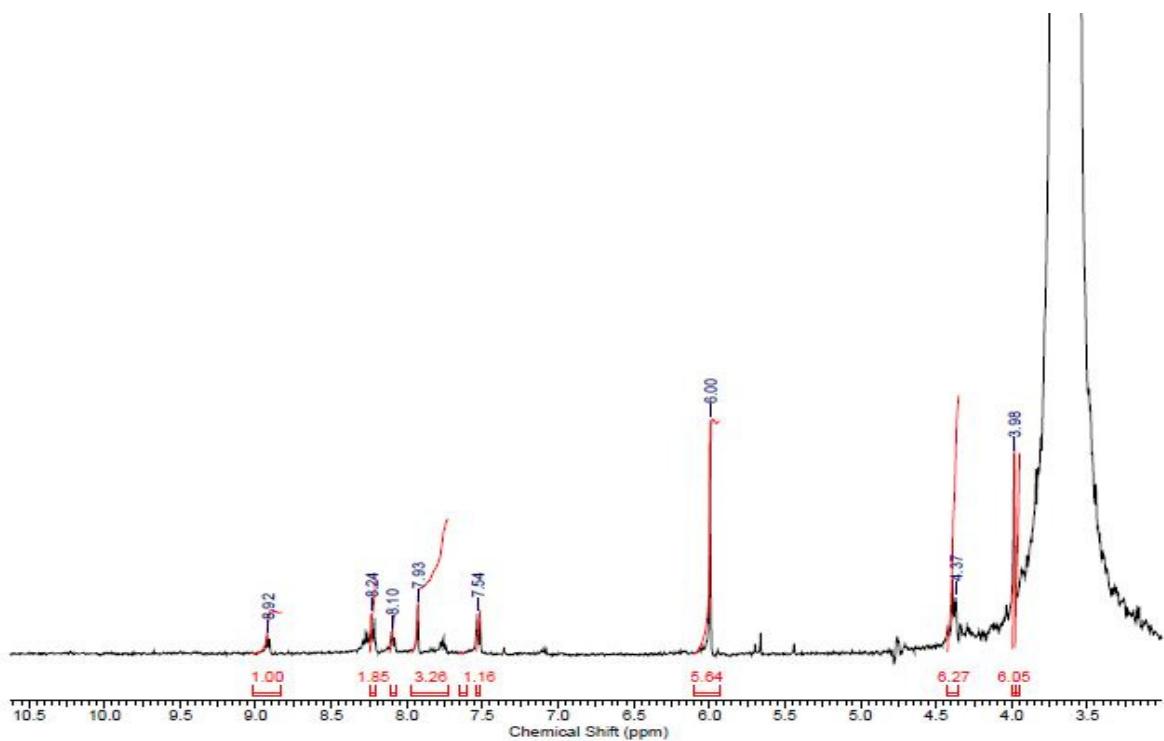


Fig S5: <sup>1</sup>H NMR Spectra of Complex 4

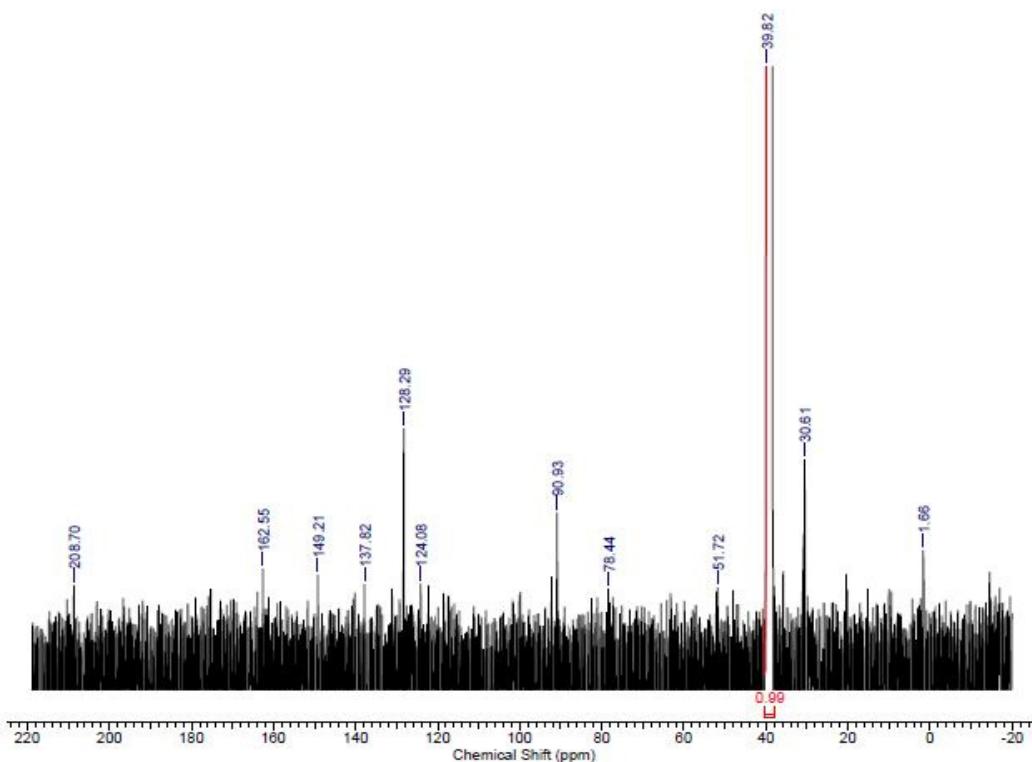


Fig S6: <sup>13</sup>C NMR Spectra of Complex 4

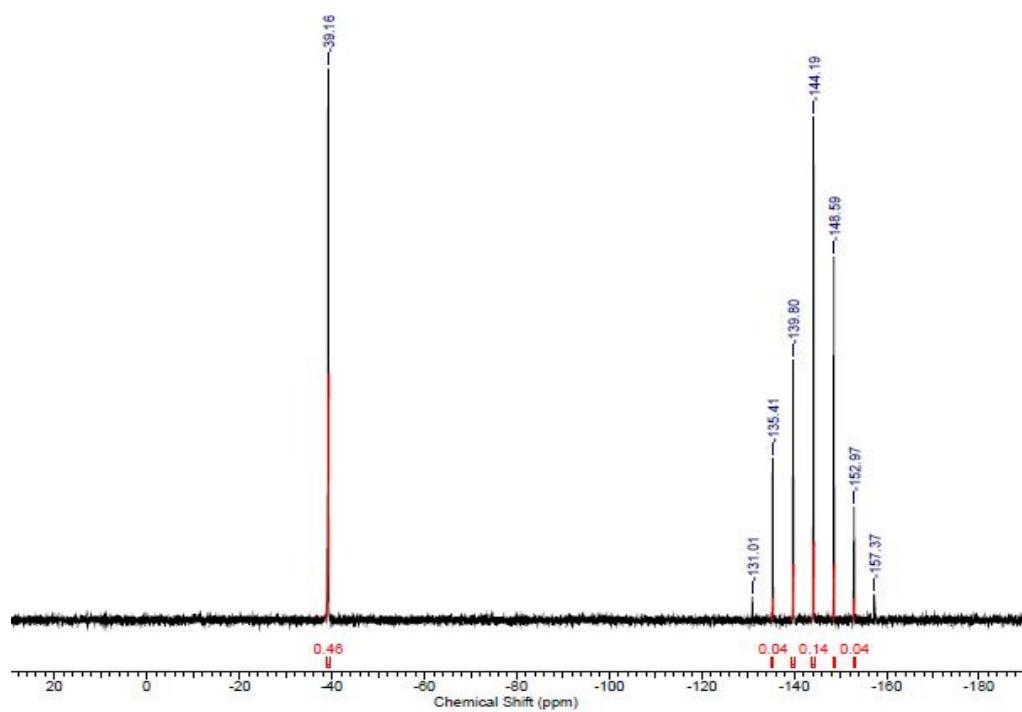


Fig S7:  $^{31}\text{P}$  NMR of Complex 4

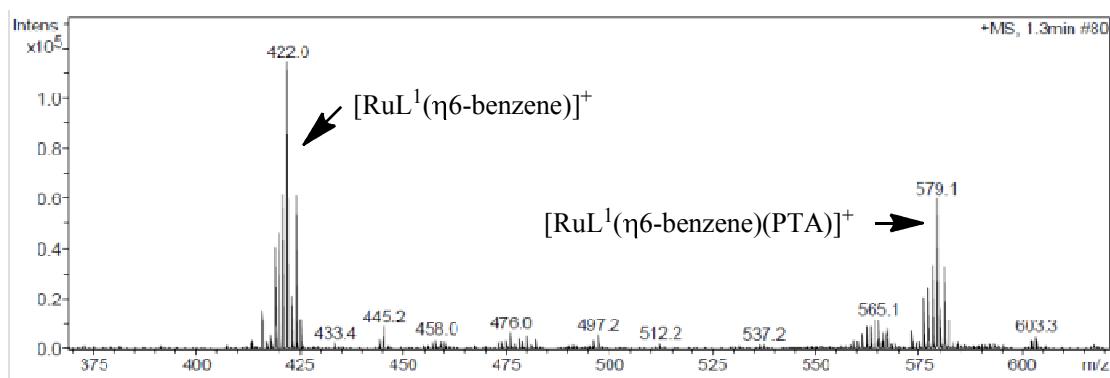


Fig S8: ESI-MS Spectra of Complex 4  $[\text{RuL}^1(\eta^6\text{-benzene})(\text{PTA})]^+$

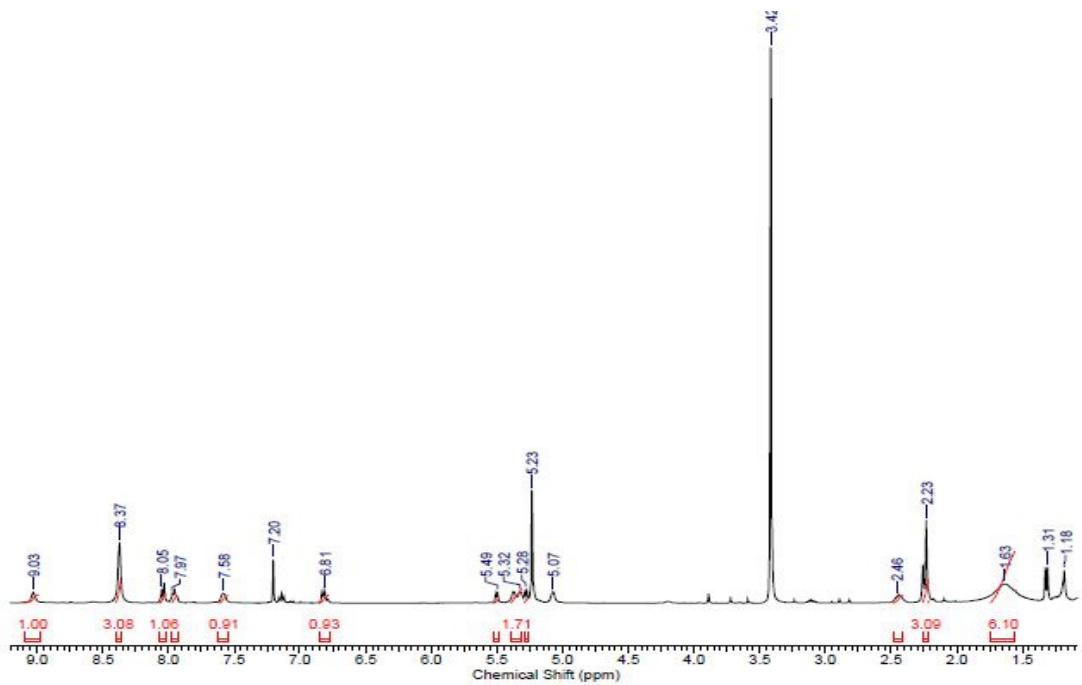


Fig S9:  $^1\text{H}$  NMR of Complex **5**

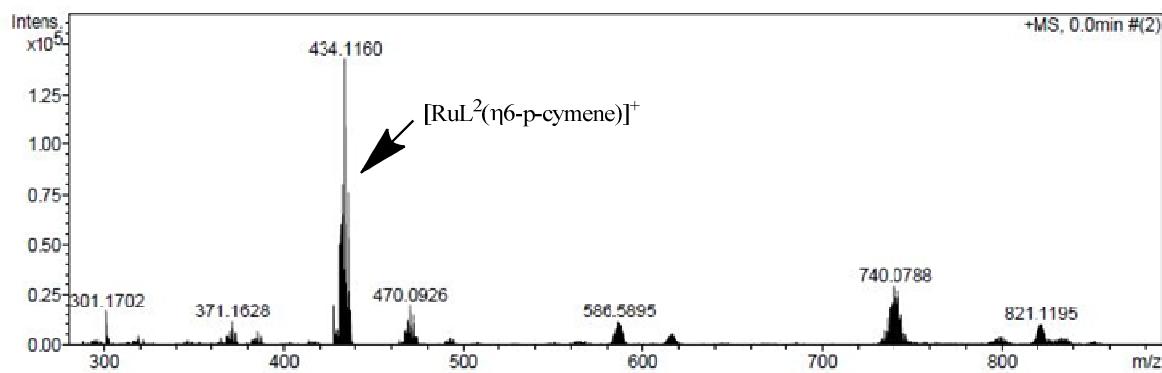


Fig S10: ESI-MS Spectra of Complex **5**  $[\text{RuL}^2(\eta^6\text{-p-cymene})]^+$

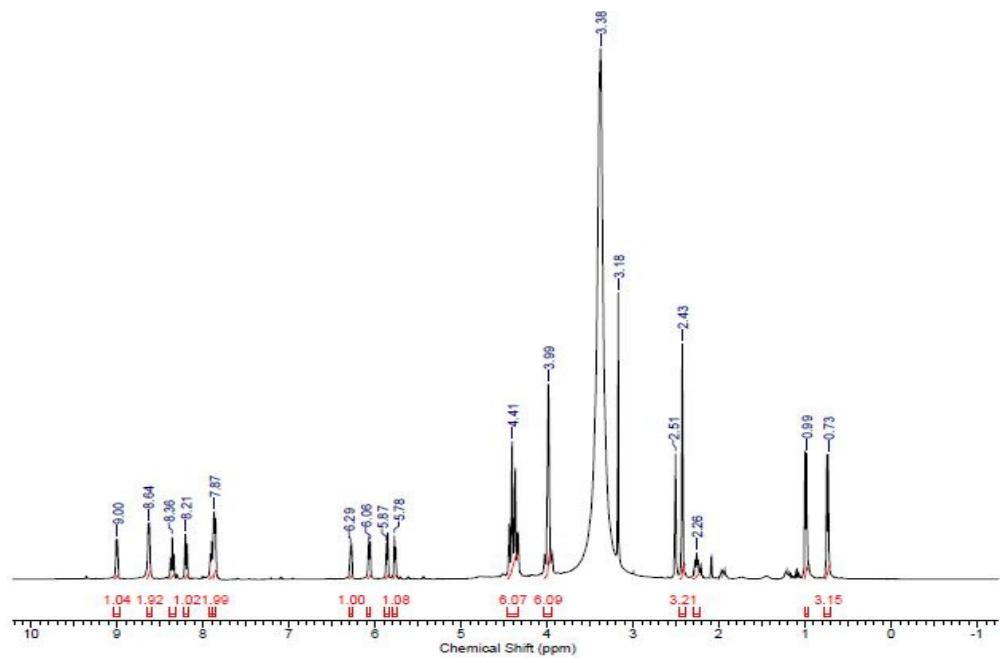


Fig S11: <sup>1</sup>H NMR of Complex 6

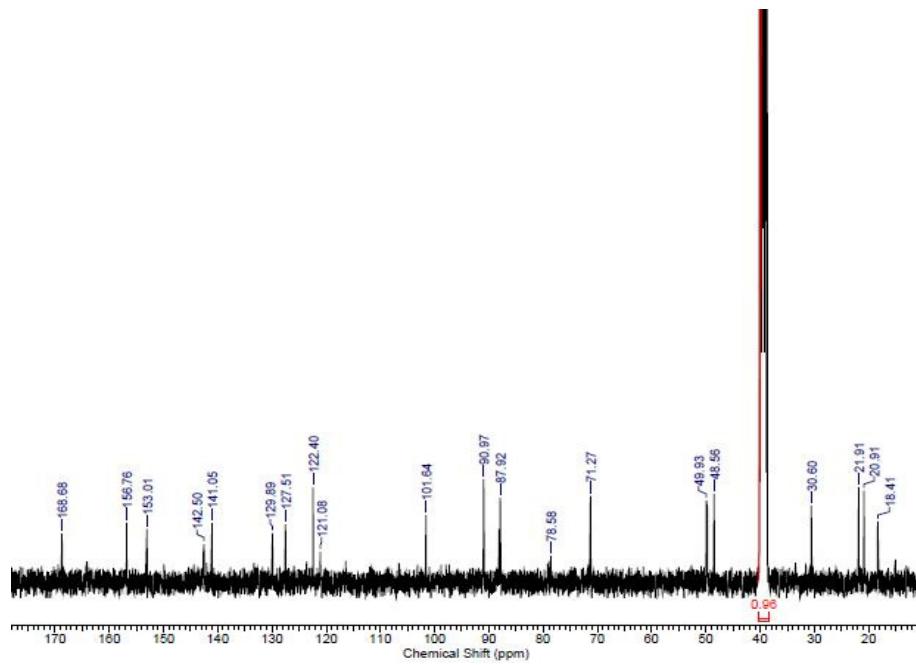


Fig S12: <sup>13</sup>C NMR of Complex 6

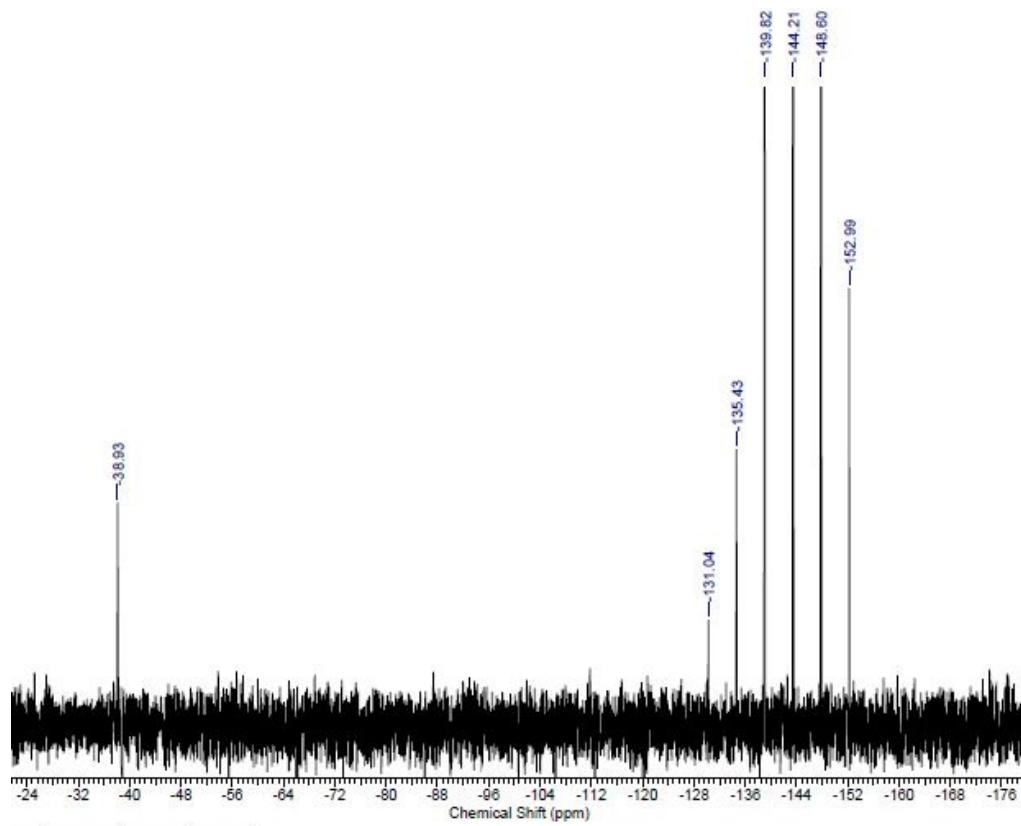


Fig S13:  $^{31}\text{P}$  NMR of Complex **6**

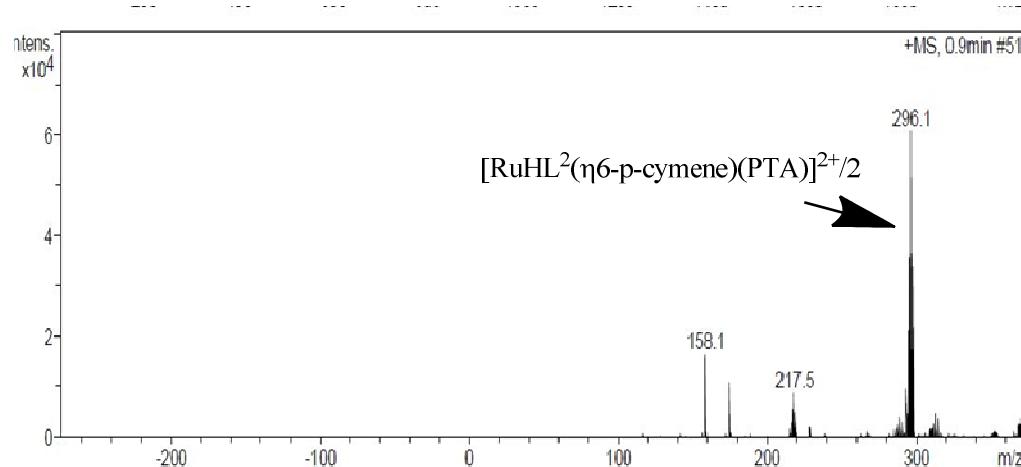


Fig S14: ESI-MS Spectra of Complex **6**  $[\text{RuHL}^2(\eta^6\text{-p-cymene})(\text{PTA})]^{2+}/2$

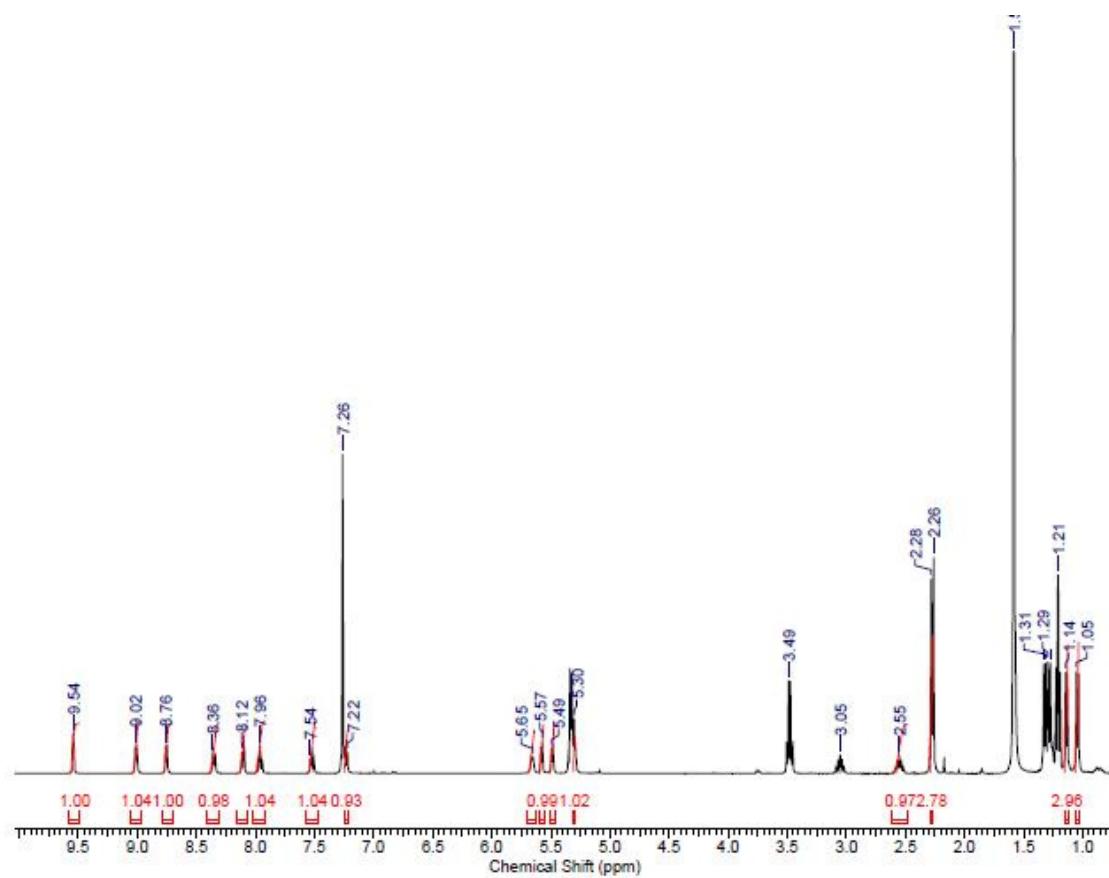


Fig S15: <sup>1</sup>H NMR of Complex 7

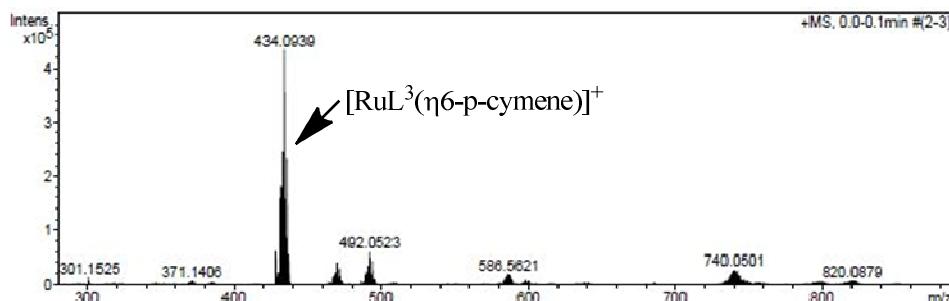


Fig S16: ESI-MS Spectra of Complex 7 [RuL<sup>3</sup>(η<sup>6</sup>-p-cymene)]<sup>+</sup>

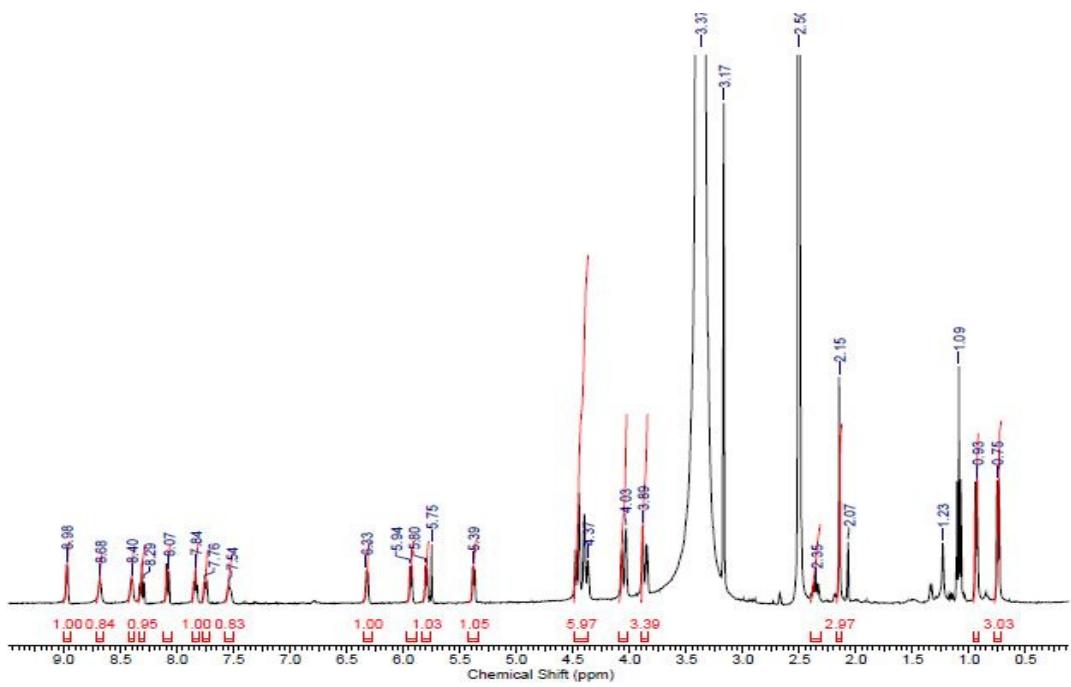


Fig S17:  $^1\text{H}$  NMR of Complex 8

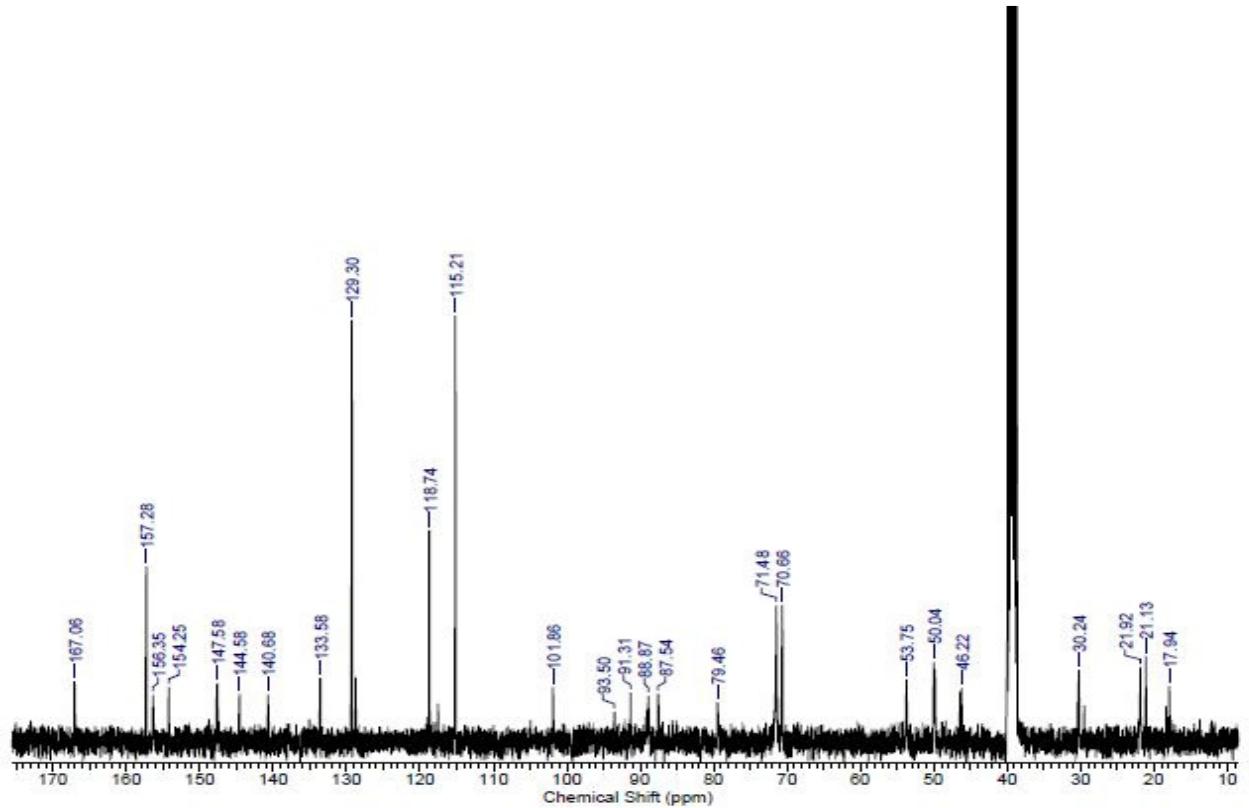


Fig S18:  $^{13}\text{C}$  NMR of Complex 8

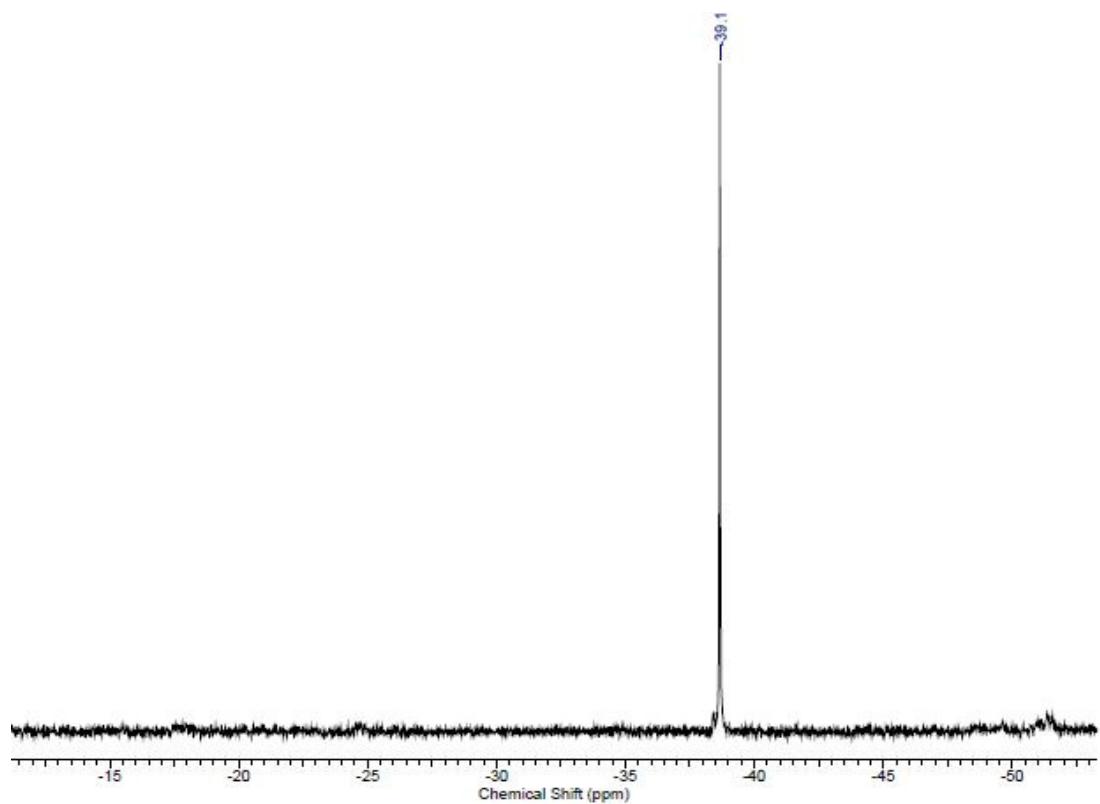


Fig S19:  $^{31}\text{P}$  NMR of Complex 8

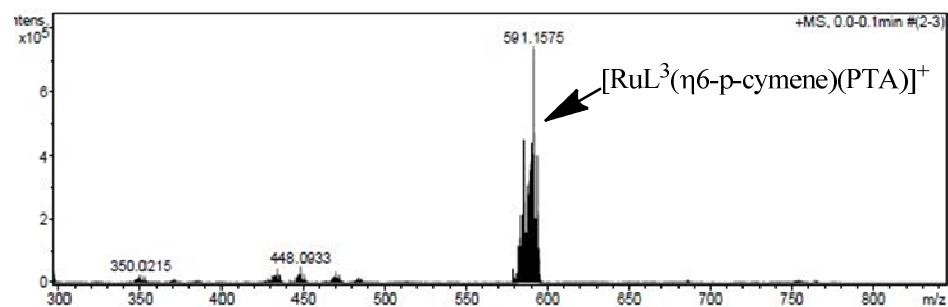


Fig S20: ESI-MS Spectra of Complex 8  $[\text{Ru L}^3(\eta^6\text{-p-cymene})(\text{PTA})]^+$