

# Supporting Information

## Photooxidative Dehydrogenation of Chiral Ir (III) Amino Acid Complexes Based on $[\Lambda\text{-Ir(ppy)}_2(\text{MeCN})_2](\text{PF}_6)$

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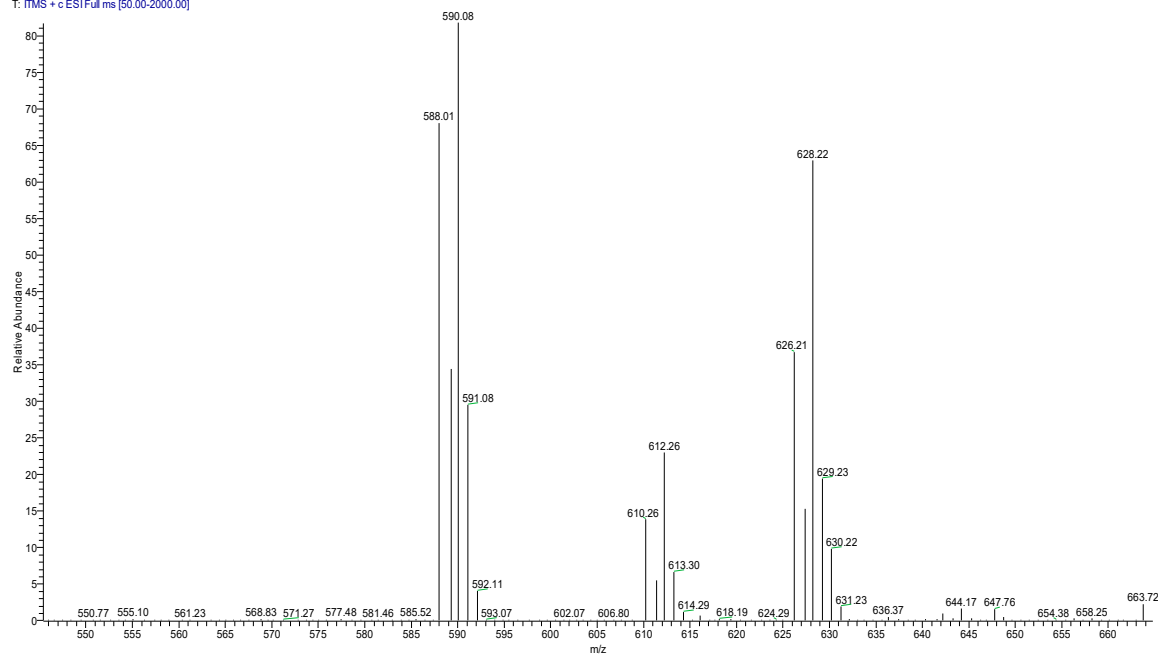
**Table S1.** Bond lengths (Å) and bond angles (°) for Complexes  $\Lambda\text{-[Ir(ppy)}_2(\text{D-Thr})]\cdot\text{CH}_3\text{OH}$  and  $\Lambda\text{-[Ir(ppy)}_2(\text{Thr-2H})]$

$\Lambda\text{-[Ir(ppy)}_2(\text{D-Thr})]\cdot\text{CH}_3\text{OH}$					
Ir1-C11	2.016(6)	Ir1-C22	2.001(5)	Ir1-N1	2.058(4)
Ir1-N2	2.047(4)	Ir1-N3	2.183(5)	Ir1-O1	2.181(4)
C23-O1	1.275(7)	C23-O2	1.237(7)	C23-C24	1.536(8)
<b>C24-N3</b>	<b>1.485(7)</b>	C24-C25	1.532(8)	C25-O3	1.429(7)
C25-C26	1.499(9)				
C22-Ir1-C11	92.6(2)	C22-Ir1-N2	80.8(2)	C11-Ir1-N2	94.7(2)
C22-Ir1-N1	97.3(2)	C11-Ir1-N1	80.6(2)	N2-Ir1-N3	86.09(18)
N2-Ir1-N1	174.85(18)	N2-Ir1-O1	95.64(17)	N1-Ir1-N3	98.81(18)
C22-Ir1-O1	170.41(18)	N1-Ir1-O1	87.02(17)	O1-Ir1-N3	77.44(17)
C11-Ir1-O1	96.63(19)	C22-Ir1-N3	93.4(2)	C11-Ir1-N3	174.1(2)

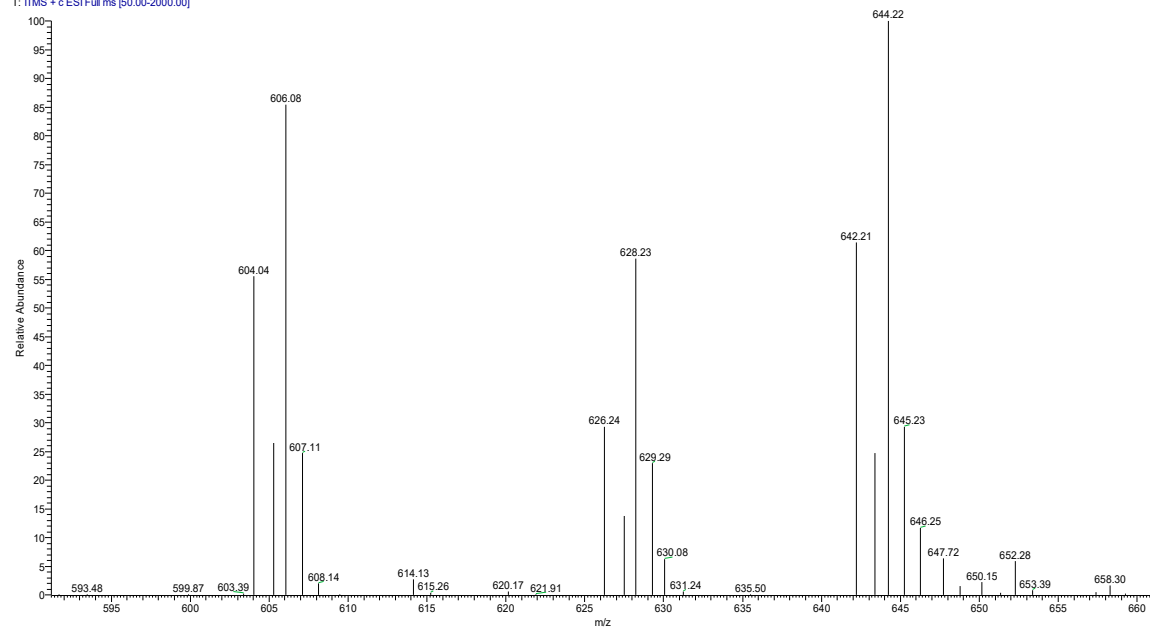
$\Lambda\text{-[Ir(ppy)}_2(\text{Thr-2H})]$					
Ir1-C11	2.038(7)	Ir1-C22	2.014(7)	Ir1-N1	2.051(6)
Ir1-N2	2.049(6)	Ir1-N3	2.115(5)	Ir1-O1	2.194(5)
C23-O1	1.300(8)	C23-O2	1.227(9)	C23-C24	1.518(9)
<b>C24-N3</b>	<b>1.261(9)</b>	C24-C25	1.507(9)	C25-O3	1.420(8)
C25-C26	1.539(12)				
C22-Ir1-C11	92.9(3)	C11-Ir1-N1	80.3(3)	N2-Ir1-N3	89.2(2)
C22-Ir1-N2	81.0(3)	N2-Ir1-N1	175.0(2)	N1-Ir1-N3	95.1(2)
C11-Ir1-N2	95.9(3)	C22-Ir1-N3	95.5(3)	C22-Ir1-O1	169.0(2)
C22-Ir1-N1	95.9(3)	C11-Ir1-N3	170.8(3)	C11-Ir1-O1	97.2(2)
N2-Ir1-O1	93.6(2)	N1-Ir1-O1	90.1(2)	N3-Ir1-O1	74.7(2)

20220420\_220421165741 #563-680 RT: 1.94-2.34 AV: 118 NL: 2.25E4  
T: ITMS + c ESI Full ms [50.00-2000.00]

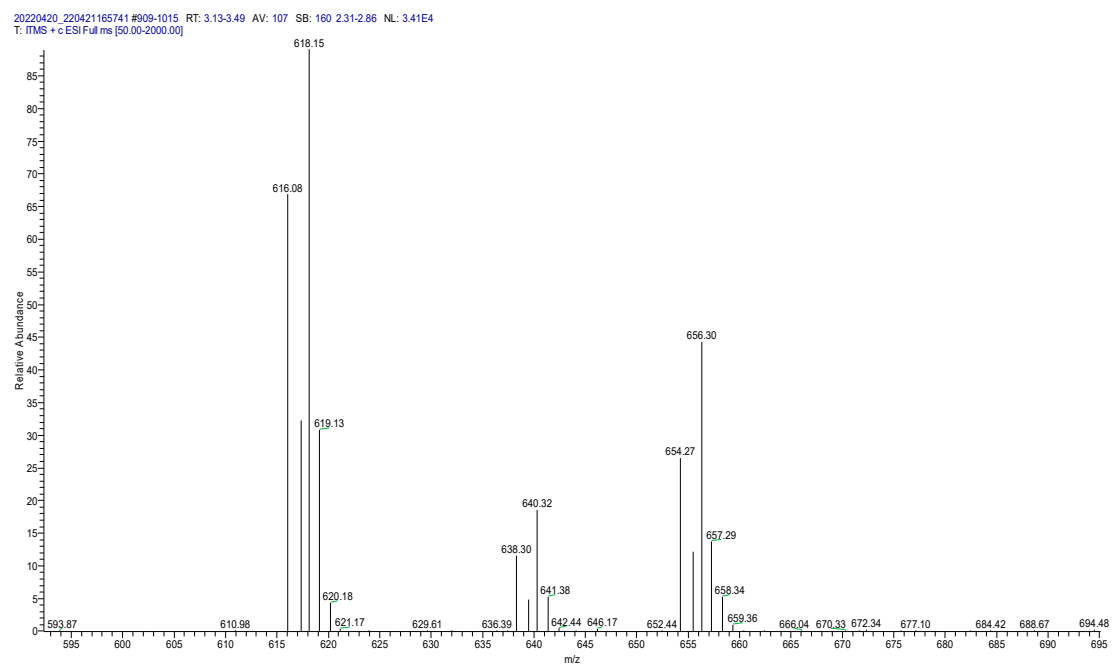


**Figure S1.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(L/D-Ala)]

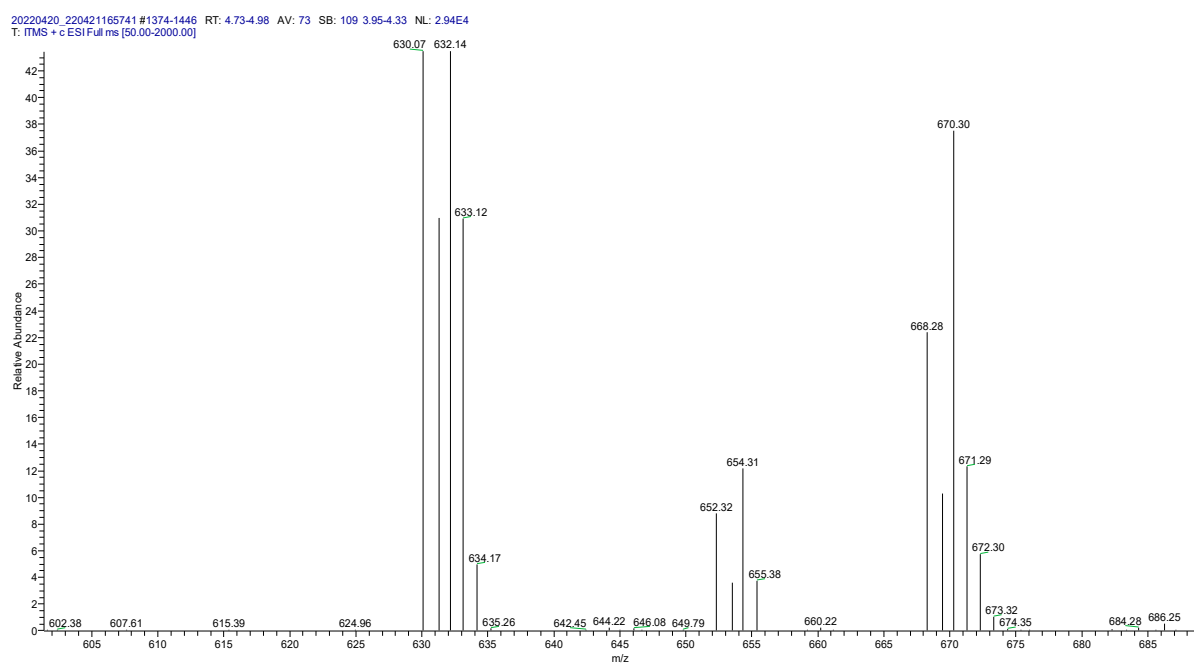
20220420\_220421165741 #2293-2378 RT: 7.90-8.19 AV: 86 SB: 141 5.53-6.01 NL: 1.06E4  
T: ITMS + c ESI Full ms [50.00-2000.00]



**Figure S2.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(L/D-Ser)]

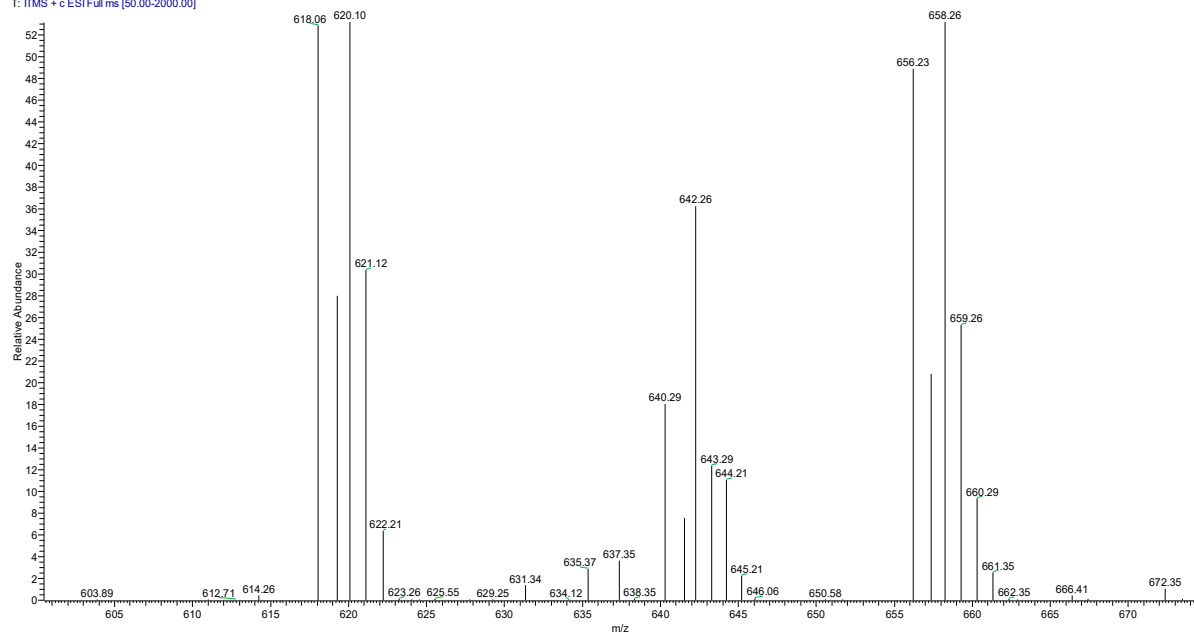


**Figure S3.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Val)]



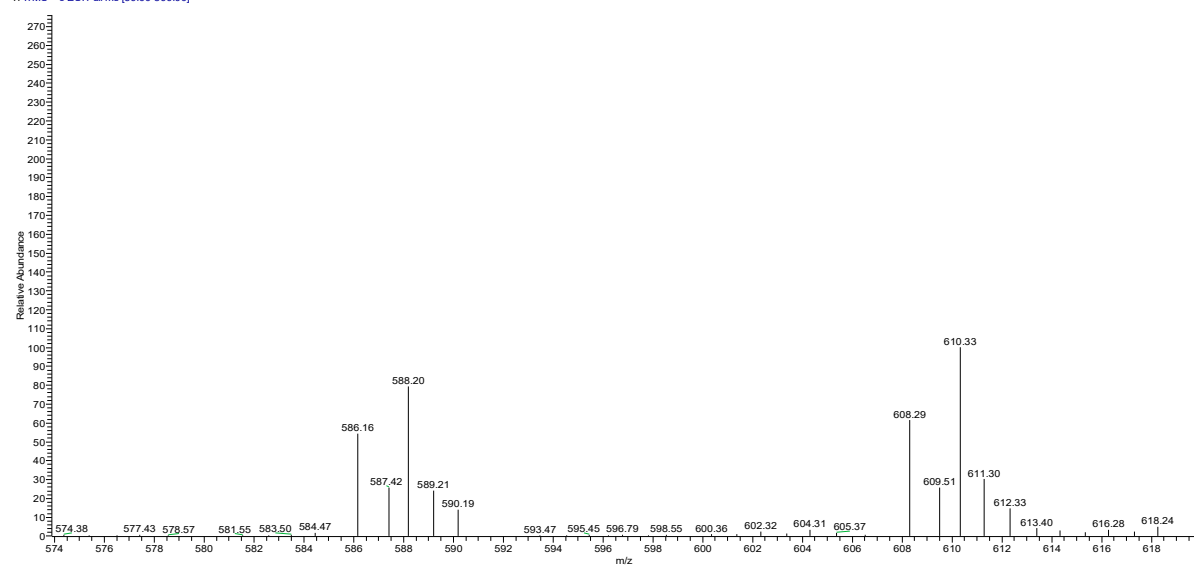
**Figure S4.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Leu)]

20220420\_220421165741 #1811-1934 RT: 6.24-6.66 AV: 124 SB: 141 5.53-6.01 NL: 1.33E4  
T: ITMS + c ESI Full ms [50.00-2000.00]



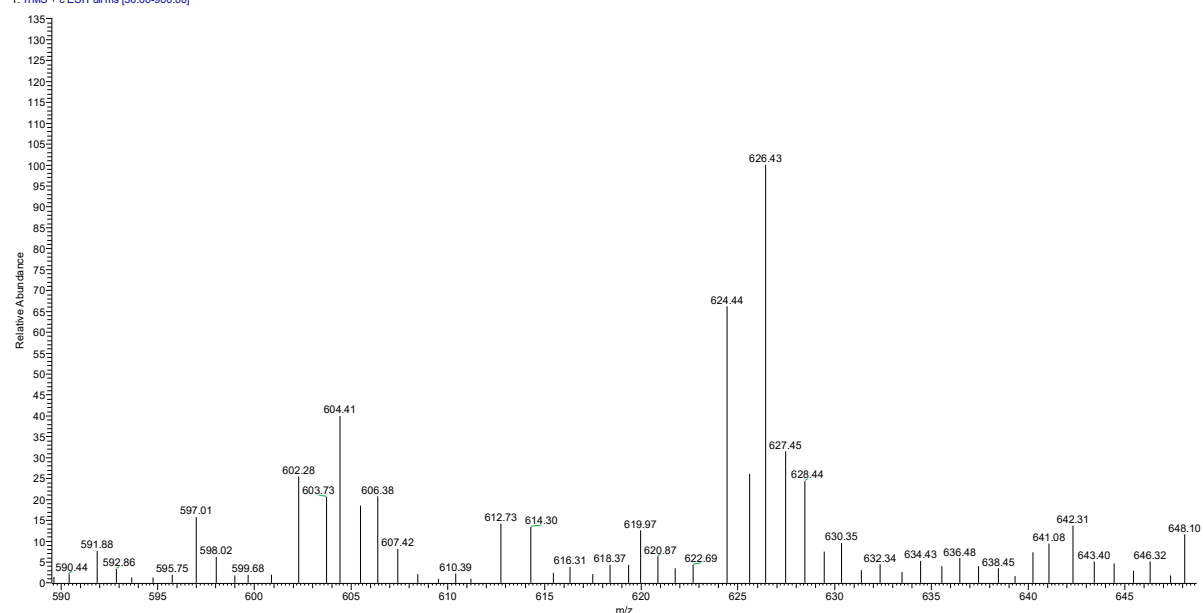
**Figure S5.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Thr)]

2022\_220401142757 #356-496 RT: 0.80-1.11 AV: 141 SB: 158 0.06-0.42 NL: 4.29E4  
T: ITMS + c ESI Full ms [50.00-800.00]



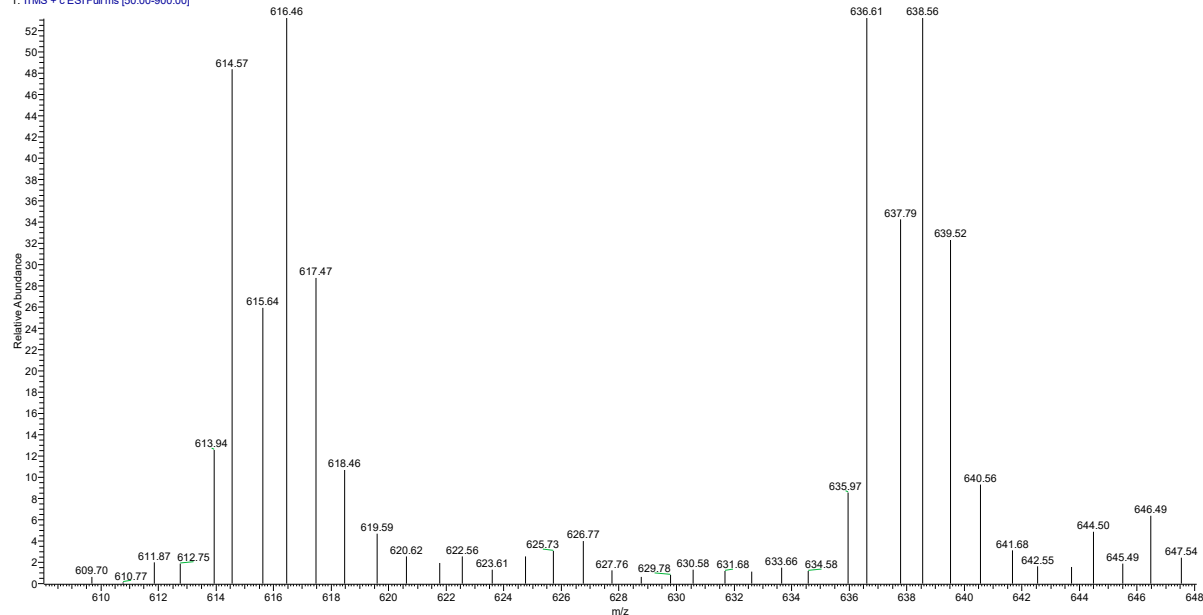
**Figure S6.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(Ala-2H)]

20220325\_220326155300 #725 RT: 5.41 AV: 1 NL: 6.20E4  
T: ITMS + c ESI Full ms [50.00-900.00]



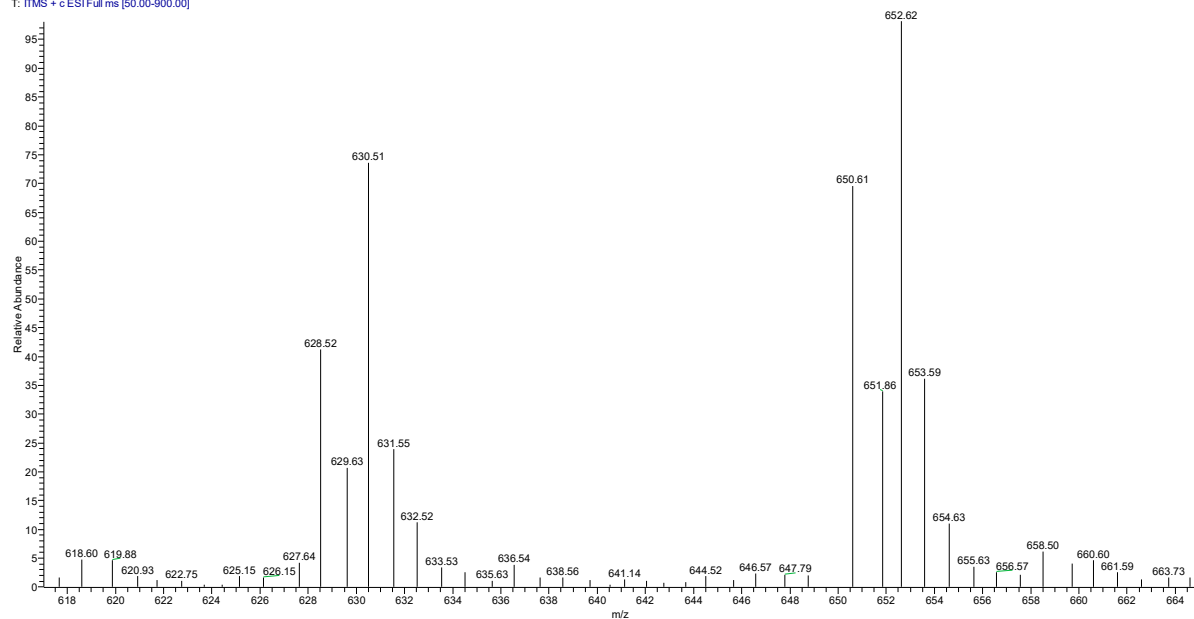
**Figure S7.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(Ser-2H)]

20220325\_220326155300 #118 RT: 0.91 AV: 1 NL: 8.47E4  
T: ITMS + c ESI Full ms [50.00-900.00]



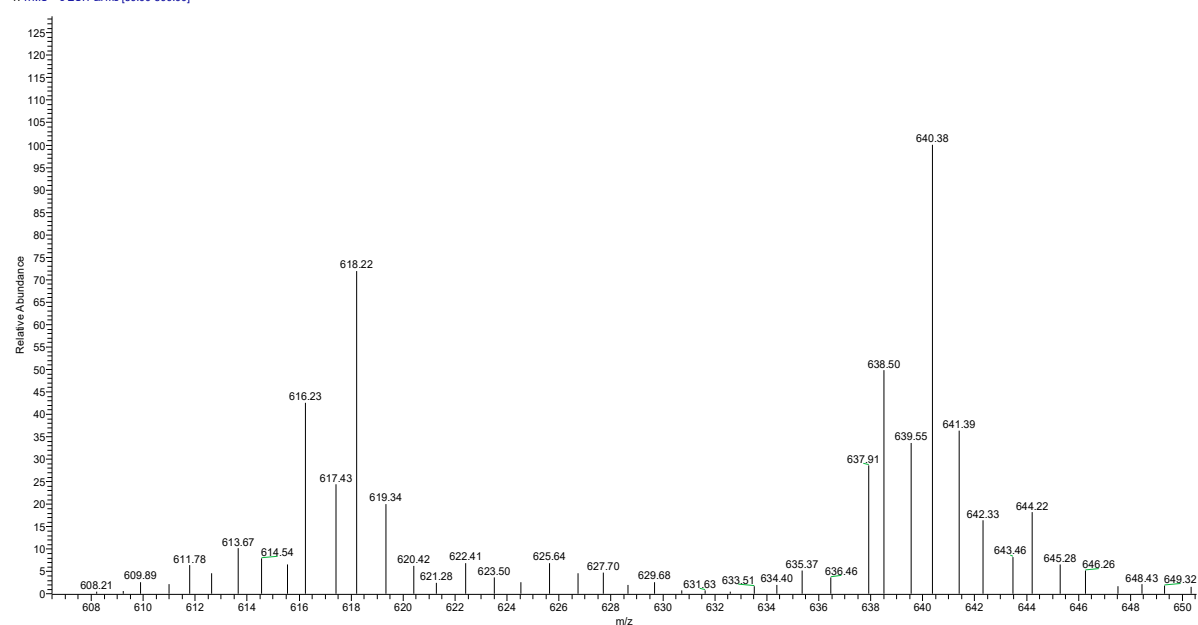
**Figure S8.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(Val-2H)]

20220325\_220326155300 #325 RT: 2.42 AV: 1 NL: 8.70E4  
T: ITMS + c ESI Full ms [50.00-900.00]

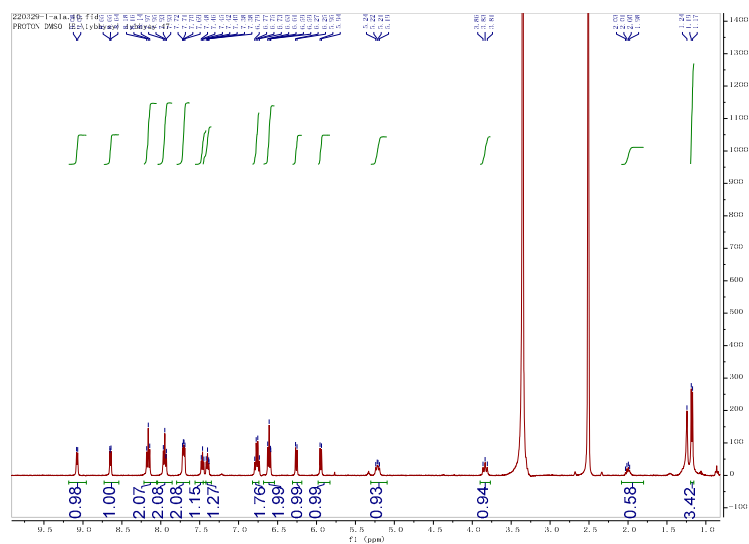


**Figure S9.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(Leu-2H)]

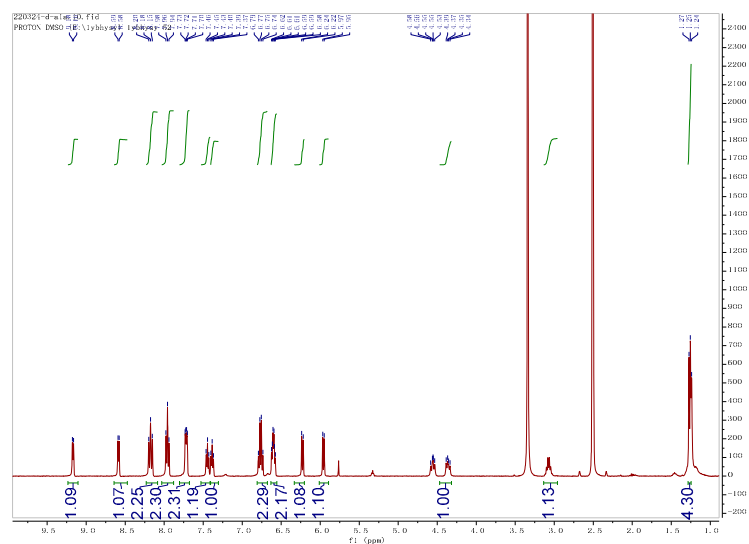
xiaopu\_220402190806 #338 RT: 0.76 AV: 1 SB: 127 0.02-0.16 , 1.18-1.32 NL: 6.00E4  
T: ITMS + c ESI Full ms [50.00-800.00]



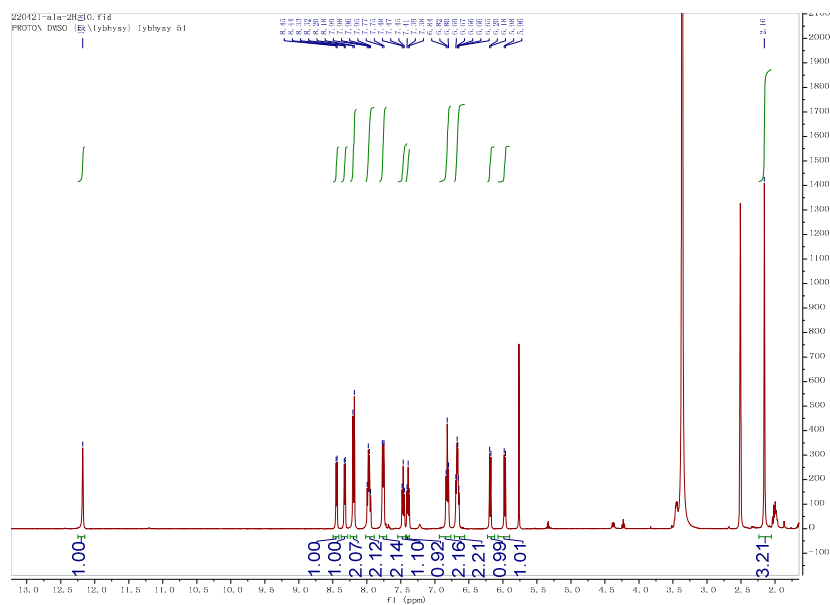
**Figure S10.** ESI-MS characterization of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(Thr-2H)]



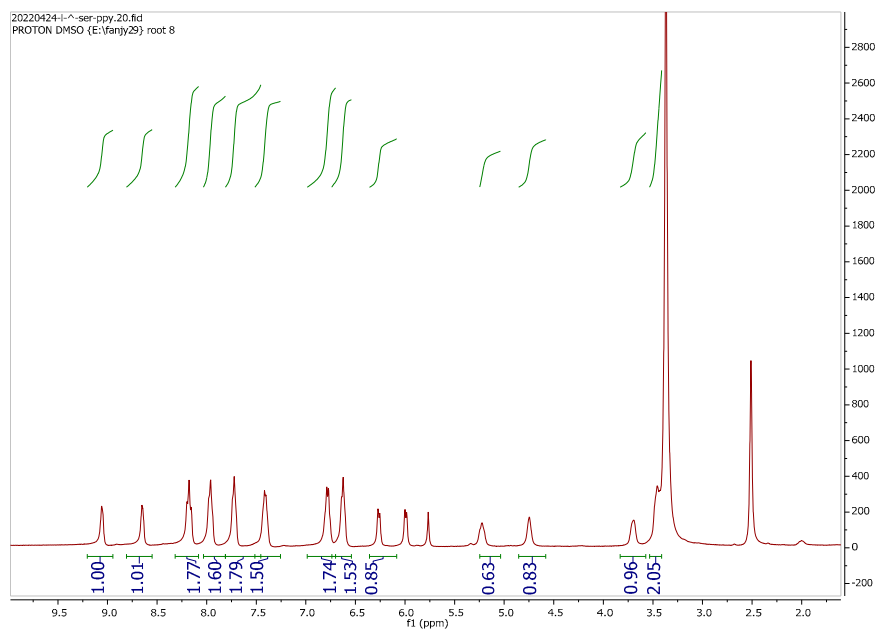
**Figure S11.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{L-Ala})]$



**Figure S12.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{D-Ala})]$

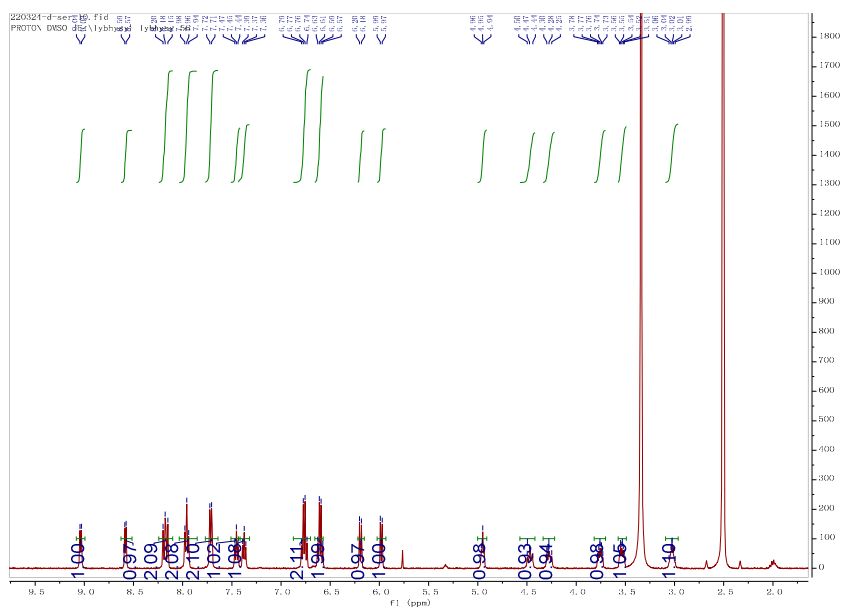


**Figure S13.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{Ala-2H})]$ .

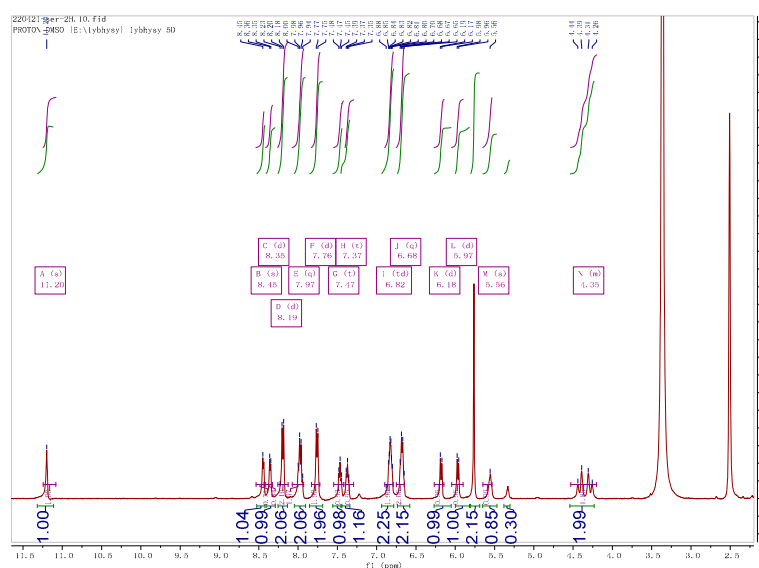


**Figure S14.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{L-Ser})]$

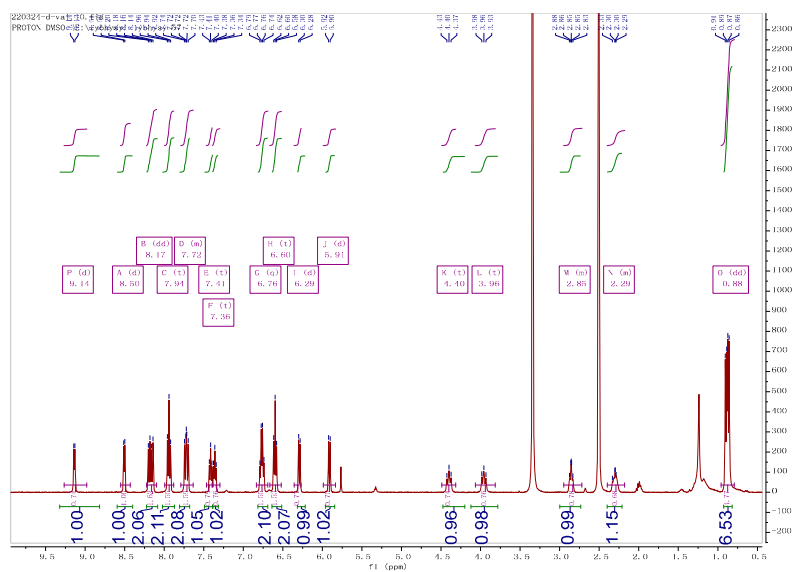




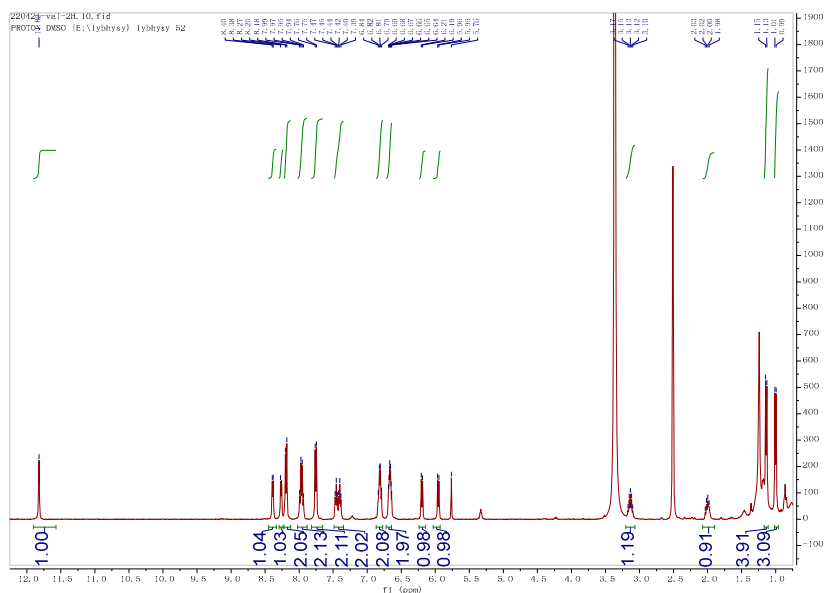
**Figure S15.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{D-Ser})]$



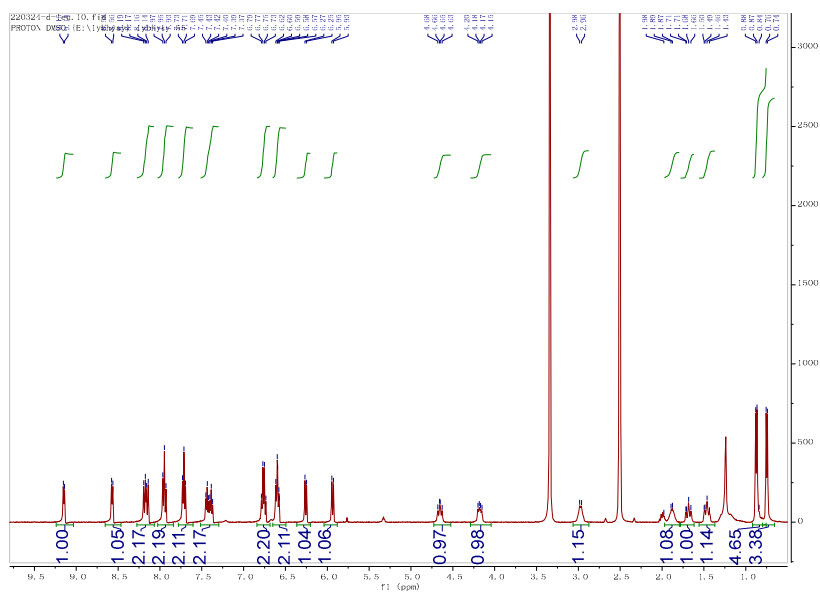
**Figure S16.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{Ser-2H})]$



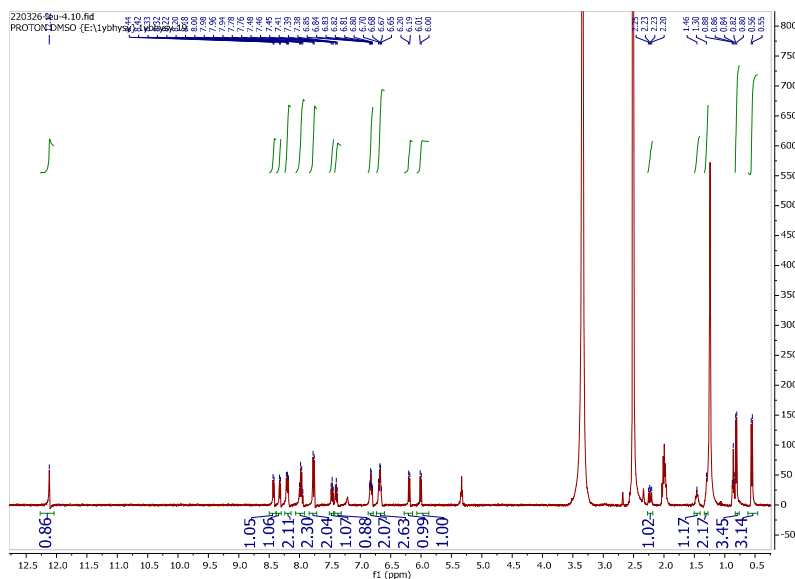
**Figure S17.** <sup>1</sup>H NMR spectrum of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Val)]



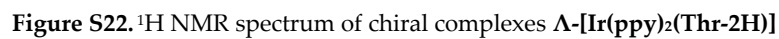
**Figure S18.** <sup>1</sup>H NMR spectrum of chiral complexes  $\Lambda$ -[Ir(ppy)<sub>2</sub>(Val-2H)]

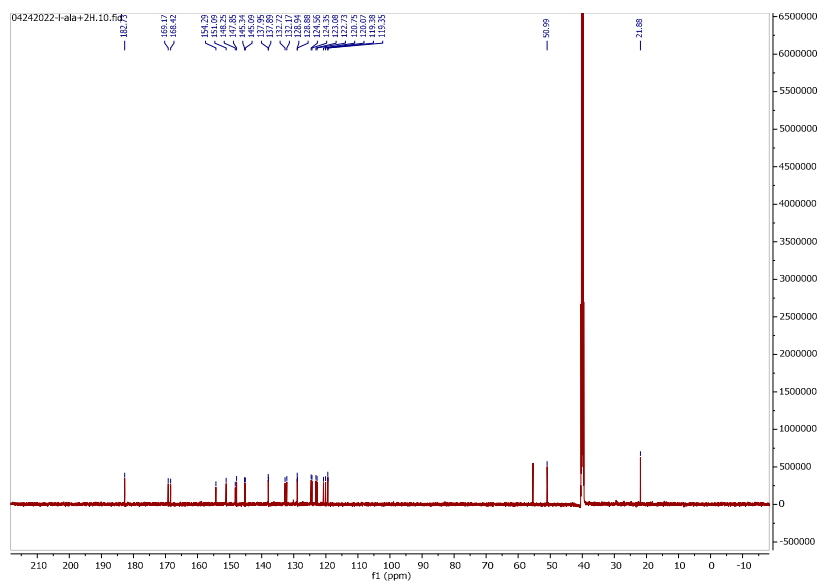


**Figure S19.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{D-Leu})]$

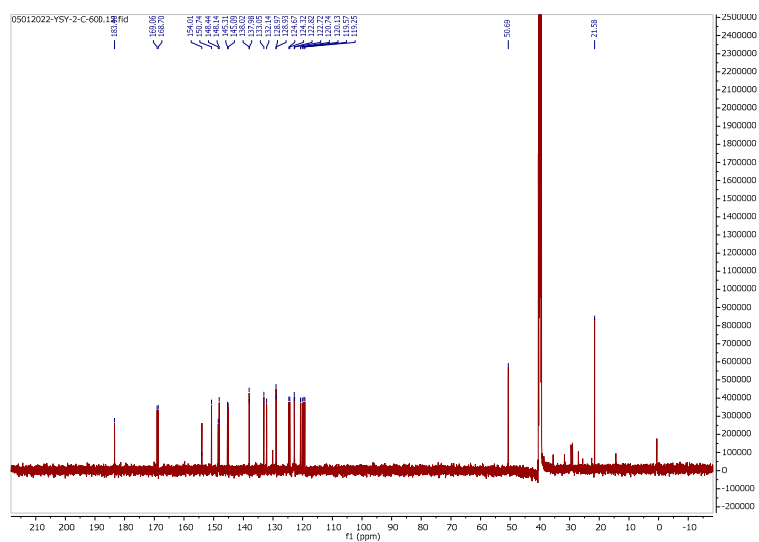


**Figure S20.**  $^1\text{H}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{Leu-2H})]$





**Figure S23.**  $^{13}\text{C}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{L-Ala})]$



**Figure S24.**  $^{13}\text{C}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{D-Ala})]$

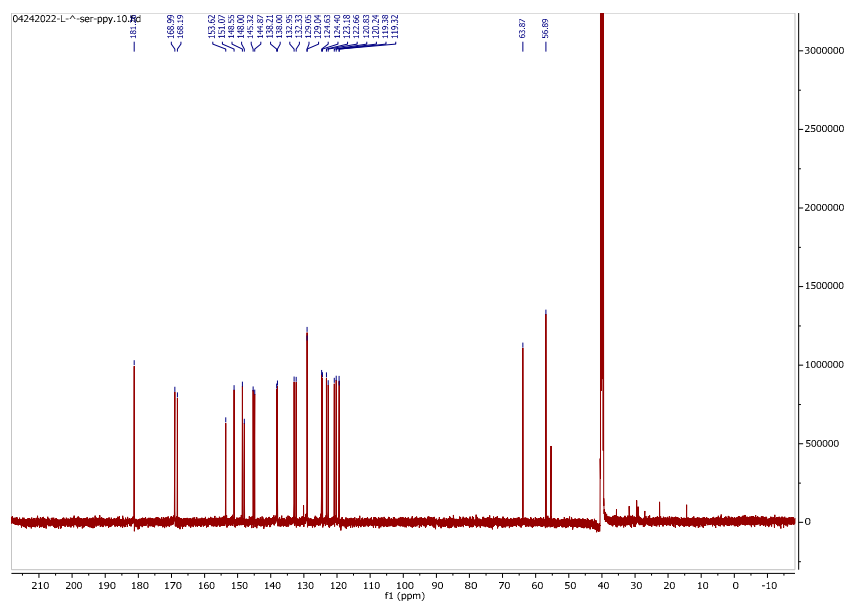


Figure S25.  $^{13}\text{C}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{L-Ser})]$

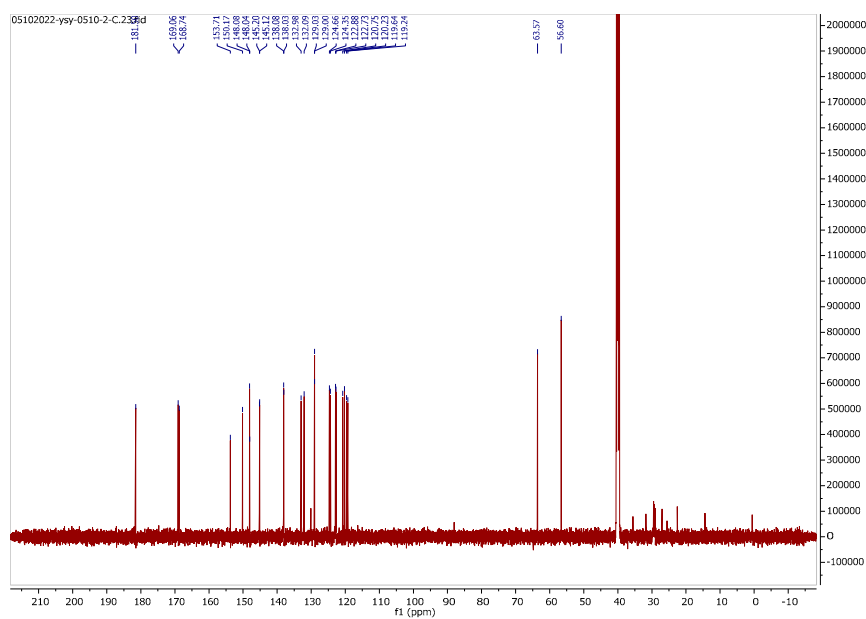


Figure S26.  $^{13}\text{C}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{D-Ser})]$

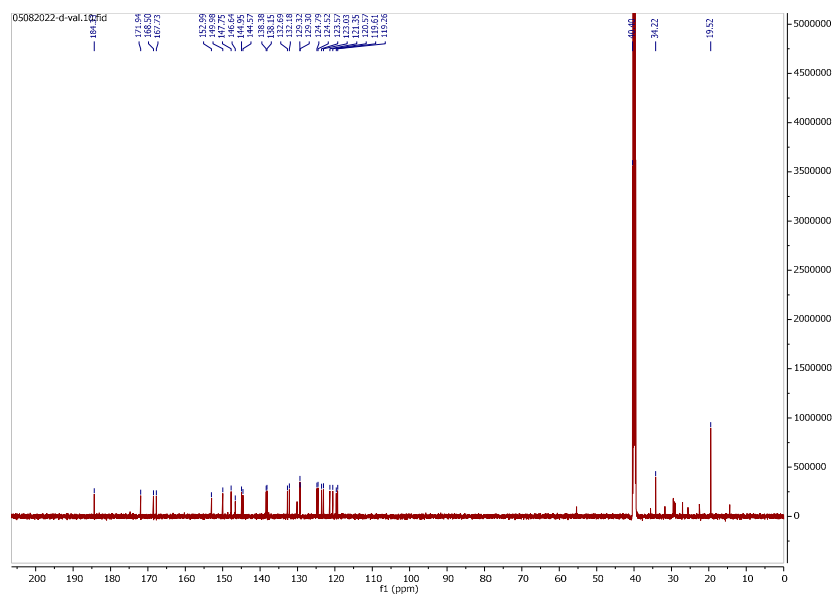


Figure S27.  $^{13}\text{C}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{D-Val})]$

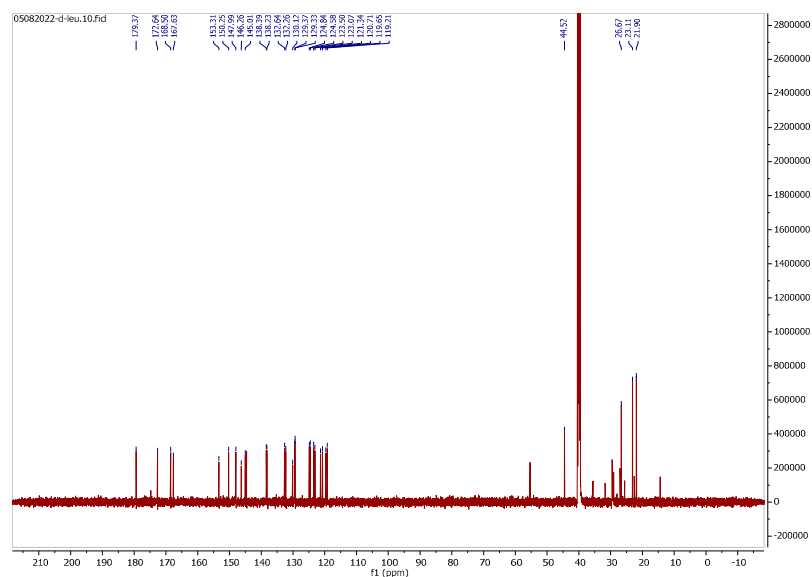
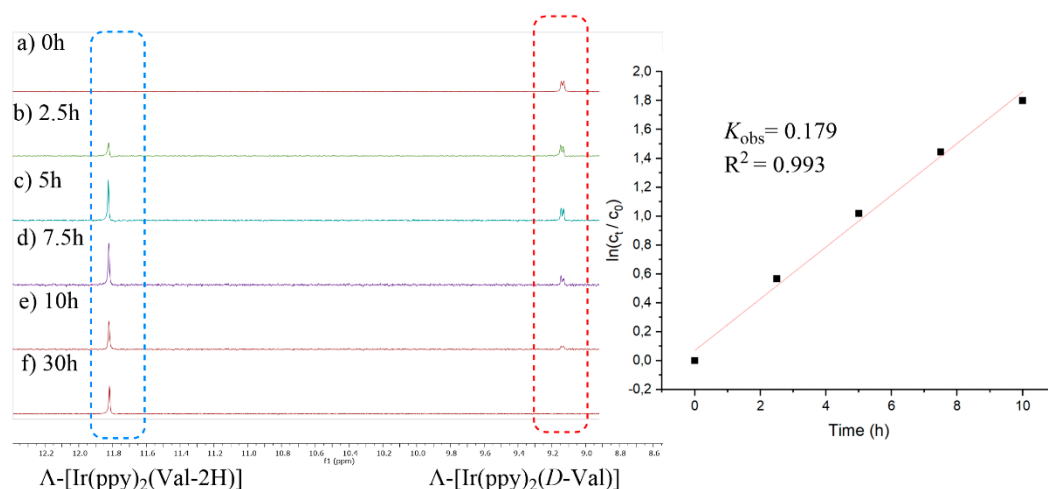


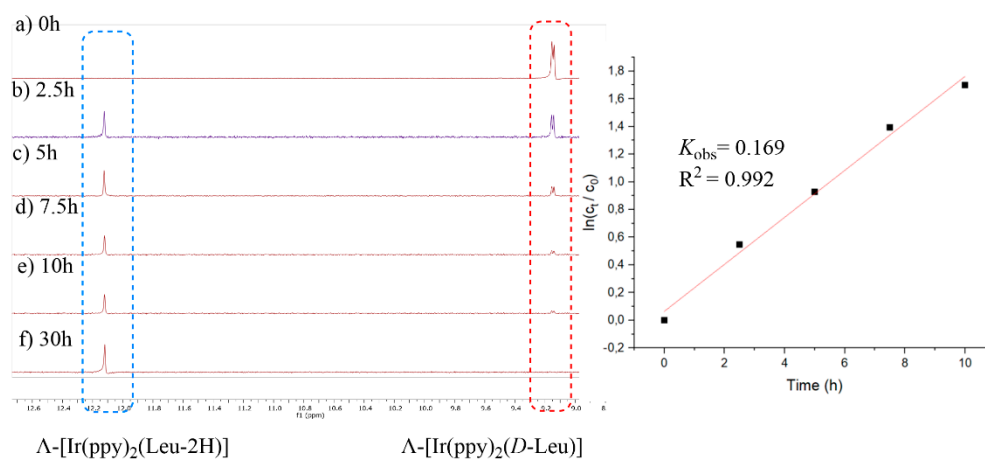
Figure S28.  $^{13}\text{C}$  NMR spectrum of chiral complexes  $\Lambda\text{-}[\text{Ir}(\text{ppy})_2(\text{D-Leu})]$



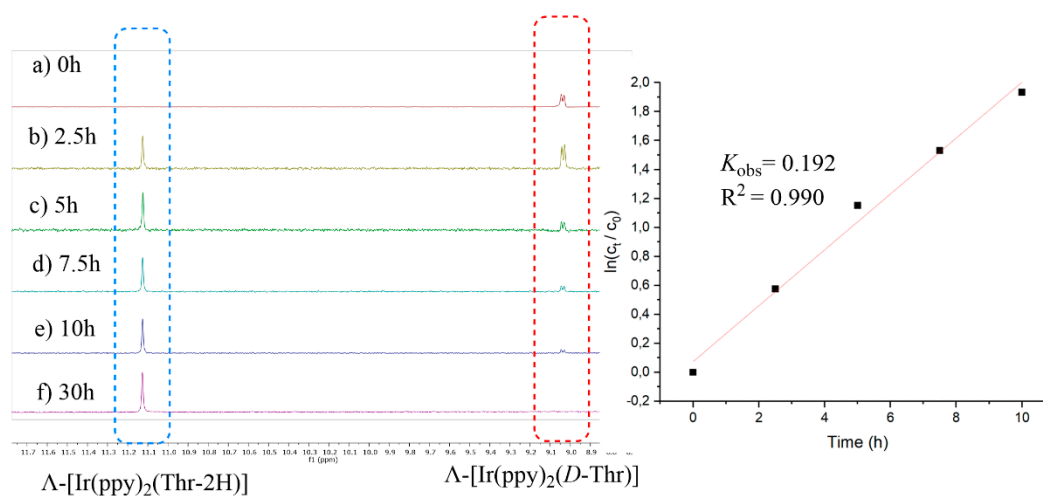




**Figure S32. (Left)** Intercept <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) spectra of dehydrogenation process of  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Val)] in different time. **(Right)** Dehydrogenation rate constant of  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Val)].



**Figure S33. (Left)** Intercept <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) spectra of dehydrogenation process of  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Leu)] in different time. **(Right)** Dehydrogenation rate constant of  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Leu)].



**Figure S34. (Left)** Intercept <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) spectra of dehydrogenation process of  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Thr)] in different time. **(Right)** Dehydrogenation rate constant of  $\Lambda$ -[Ir(ppy)<sub>2</sub>(D-Thr)].

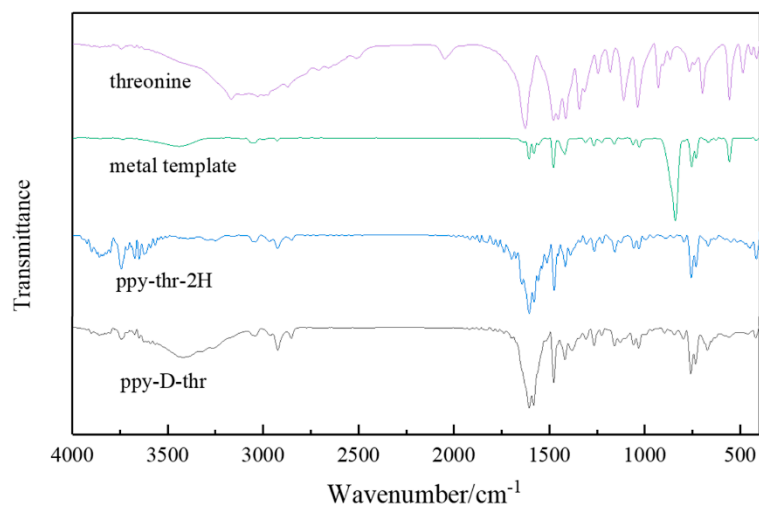


Figure S35. IR spectra of threonine,  $[\Lambda\text{-Ir(ppy)}_2(\text{MeCN})_2](\text{PF}_6)$ ,  $\Lambda\text{-Ir(ppy)}_2(\text{Thr-2H})$  and  $[\Lambda\text{-[Ir(ppy)}_2(\text{D-Thr})]$ .

$[\Lambda\text{-Ir(ppy)}_2(\text{MeCN})_2](\text{PF}_6)$ , IR: (KBr,  $\nu[\text{cm}^{-1}]$ ): 3731(w), 3438(w), 3062(w), 3046(w), 2999(w), 2928(w), 1609(w), 1582(w), 1481(m), 1421(w), 1311(w), 1268(w), 1227(w), 1162(w), 1064(w), 1031(w), 843(vs), 758(m), 735(w), 672(w), 559(w), 419(w);

Threonine, IR: (KBr,  $\nu[\text{cm}^{-1}]$ ): 3745(w), 3169(s), 3028(s), 2998(s), 2978(s), 2874(s), 2712(m), 2660(m), 2513(w), 2050(w), 1628(vs), 1481(vs), 1456(vs), 1418(vs), 1346(s), 1317(s), 1248(m), 1184(m), 1113(s), 1042(s), 932(s), 908(m), 870(w), 770(w), 744(w), 700(s), 559(s), 490(m), 445(w), 419(w);