Supplementary Material

Highly Enantioselective Epoxidation of Olefins by H_2O_2 Catalyzed by a Non-heme Fe(II) Catalyst of a Chiral Tetradentate Ligand

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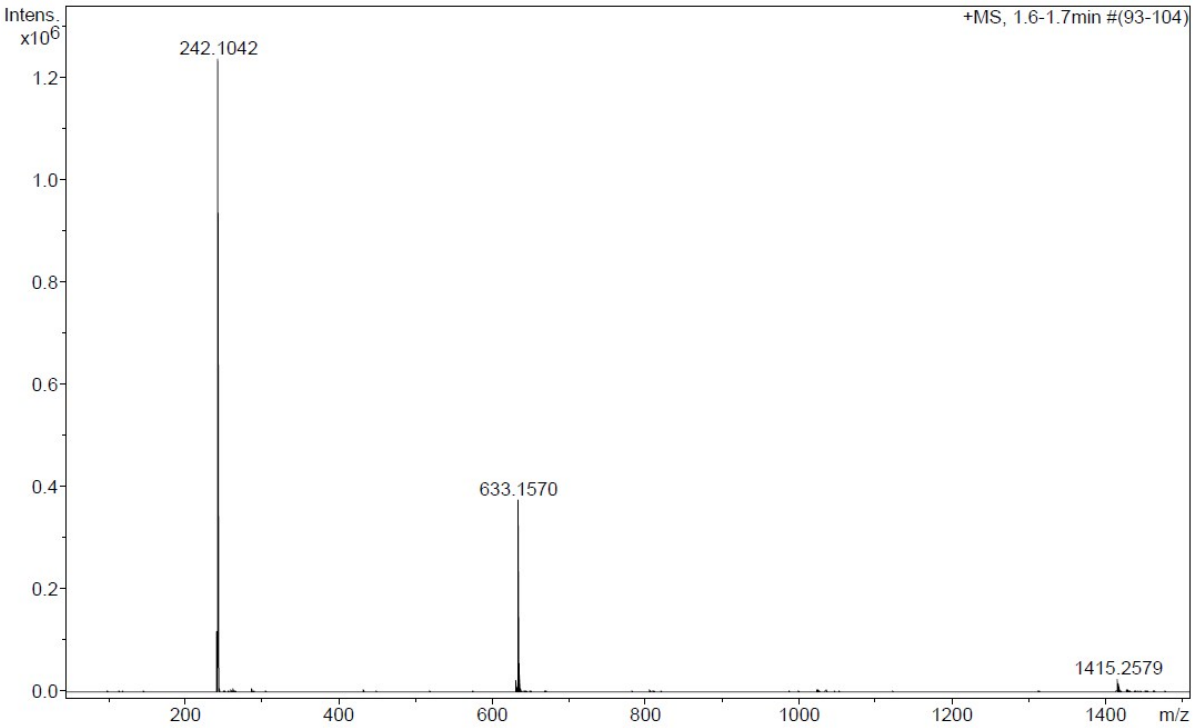


Figure S1. The HRMS of complex $\mathbf{1}^{\mathbf{OTf}}$ in CH_3CN.

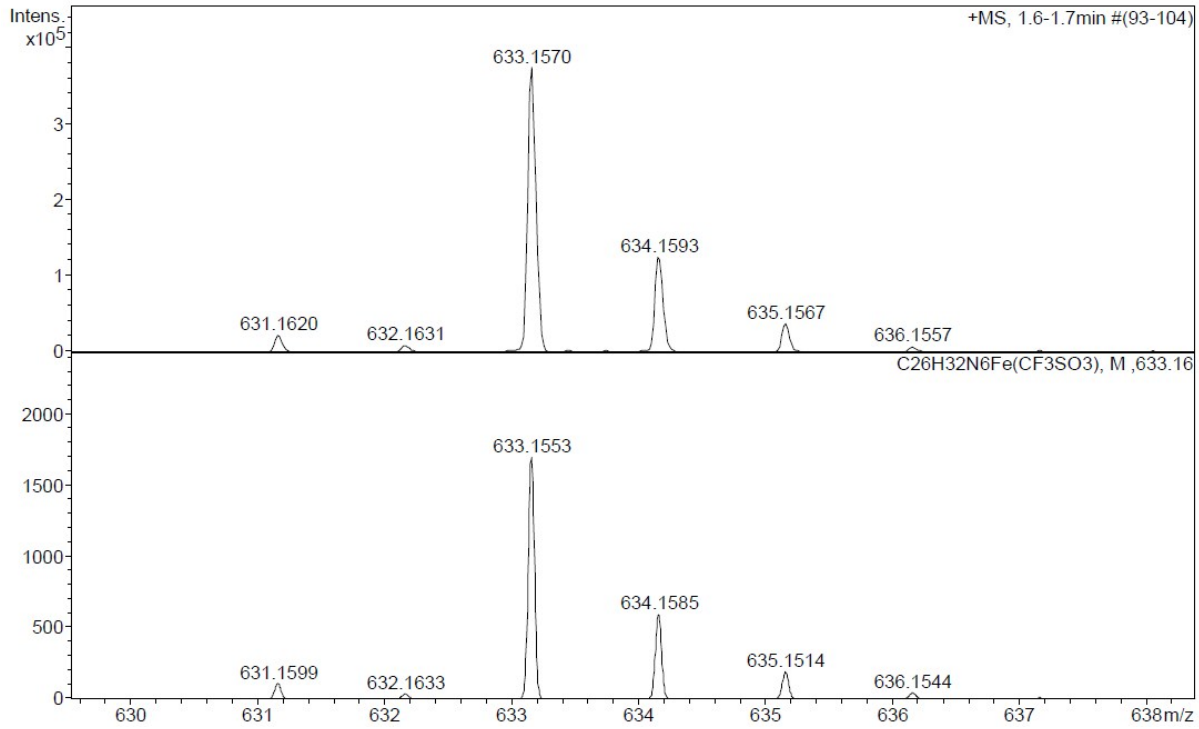


Figure S2. The experimental (top) and simulated (bottom) isotopic distribution patters for $[Fe^{II}(\boldsymbol{S,S}\text{-}^{PDBz}\mathbf{L})(CF_3SO_3)]^+$.

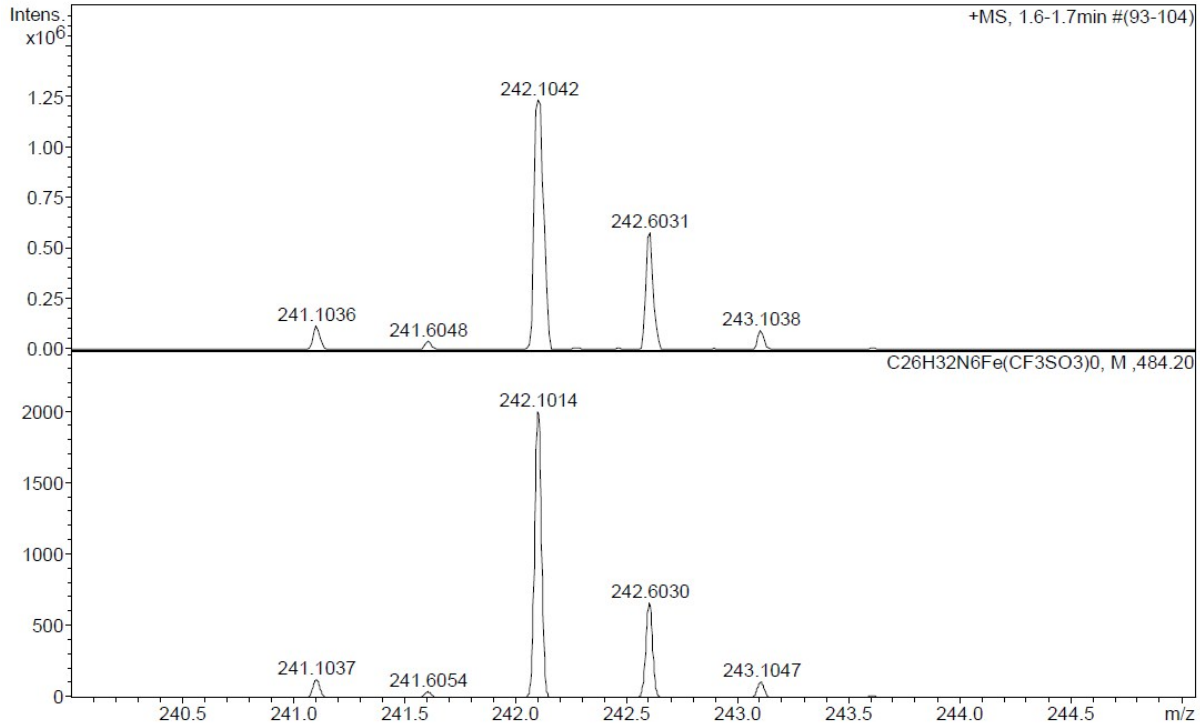


Figure S3. The experimental (top) and simulated (bottom) isotopic distribution patters for $[Fe^{II}(\boldsymbol{S,S}\text{-}^{PDBz}\mathbf{L})]^{2+}$.

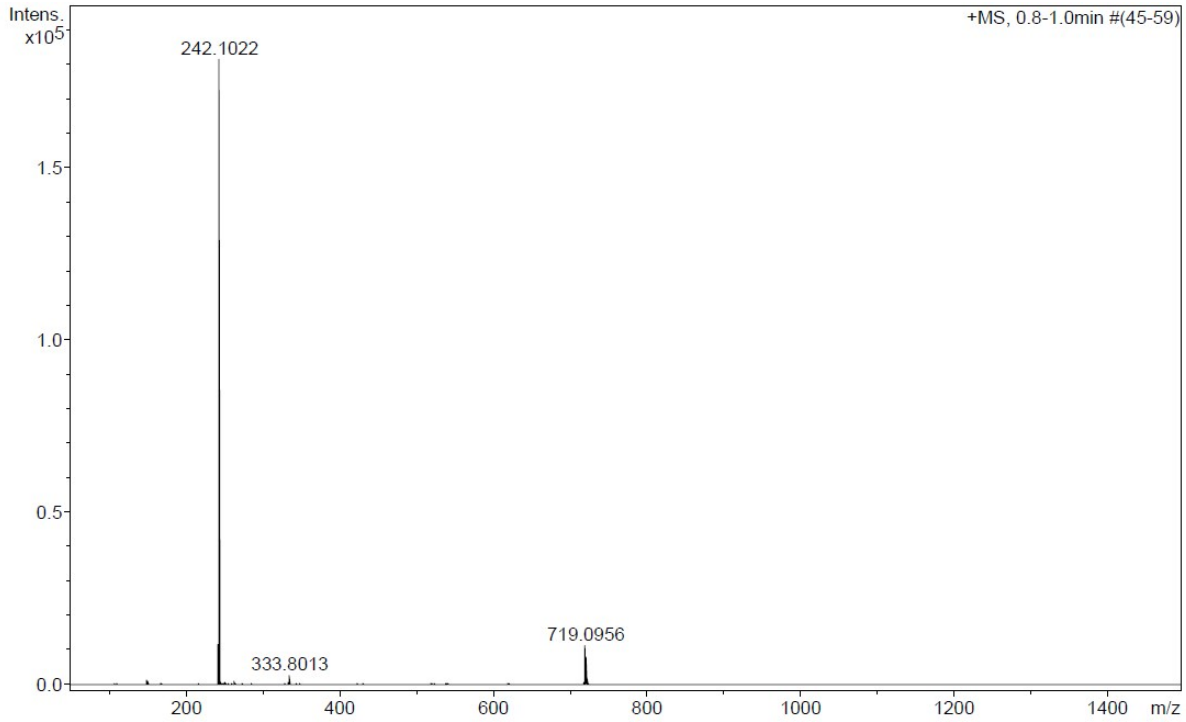


Figure S4. The HRMS of complex **1**$^{\mathbf{SbF6}}$ in CH_3CN.

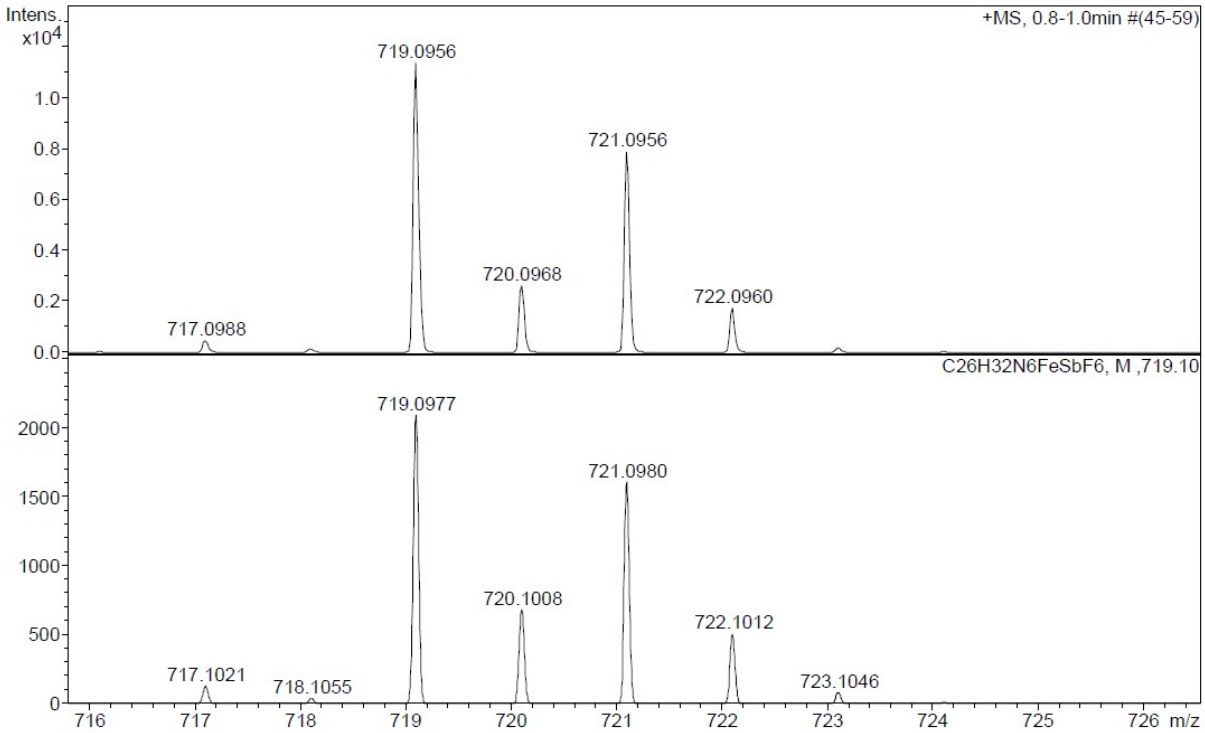


Figure S5. The experimental (top) and simulated (bottom) isotopic distribution patters for $[Fe^{II}(\boldsymbol{S,S}\text{-}^{PDBz}\mathbf{L})(SbF_6)]^+$.

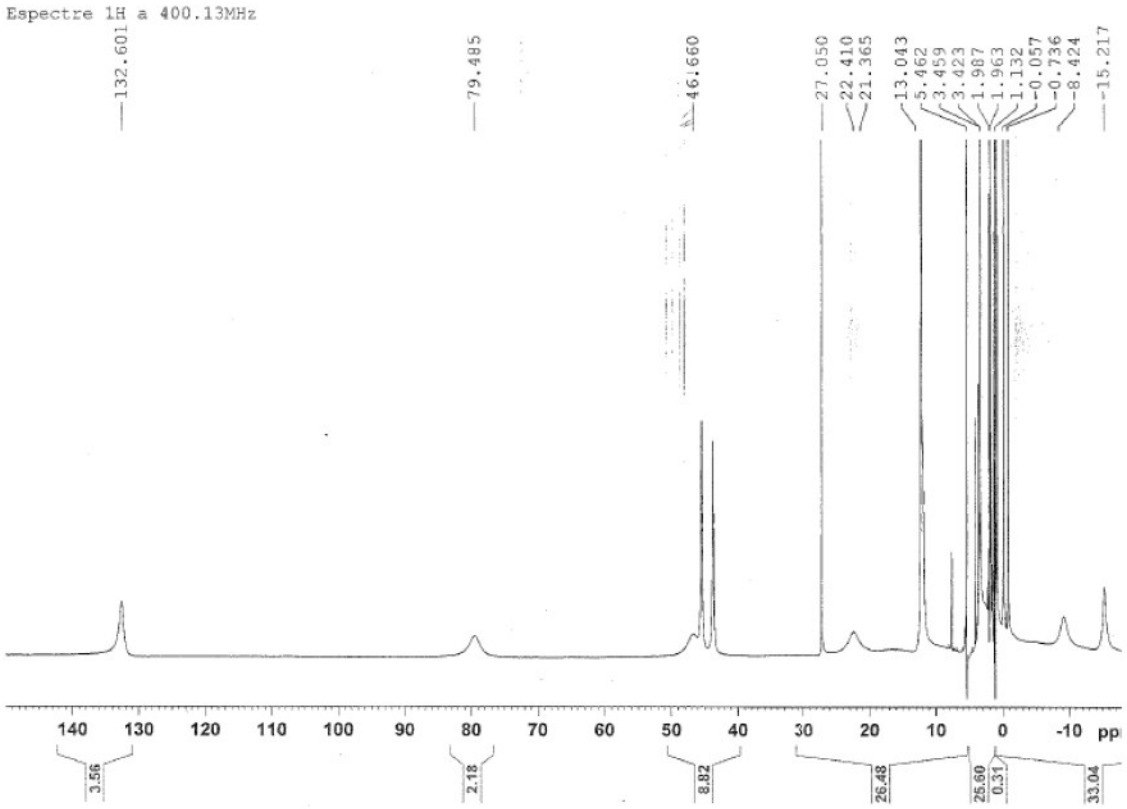


Figure S6. The ^{1}H-NMR spectrum of complex $\mathbf{1}^{OTf}$ in CD_3CN.

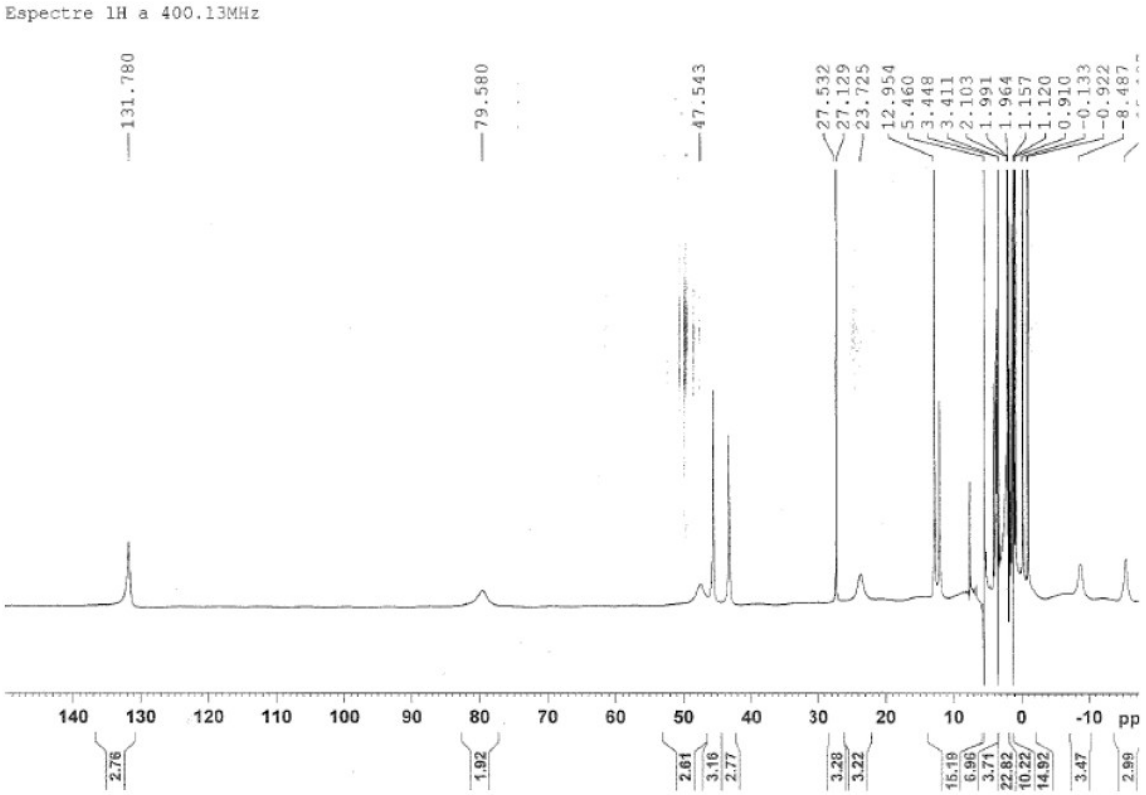


Figure S7. The ^{1}H-NMR spectrum of complex $\mathbf{1}^{\mathbf{SbF6}}$ in CD_3CN.

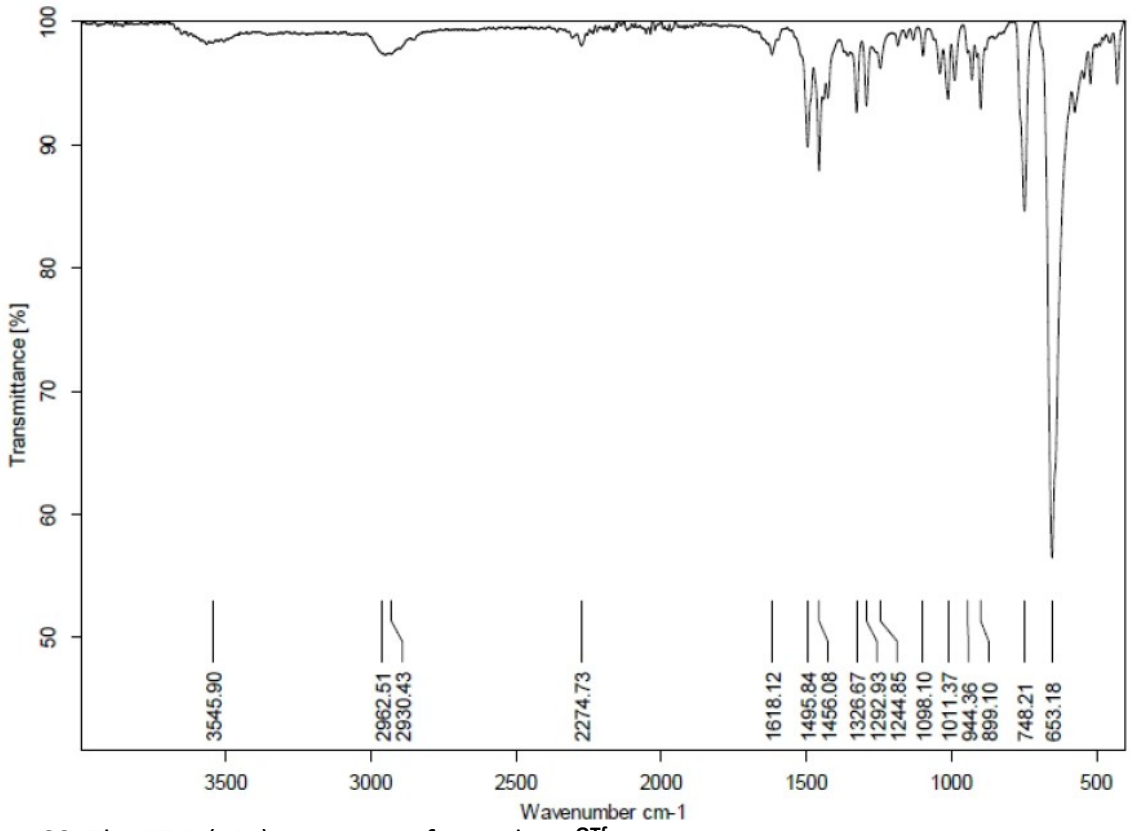


Figure S8. The FTIR (KBr) spectrum of complex $\mathbf{1}^{\mathbf{OTf}}$.

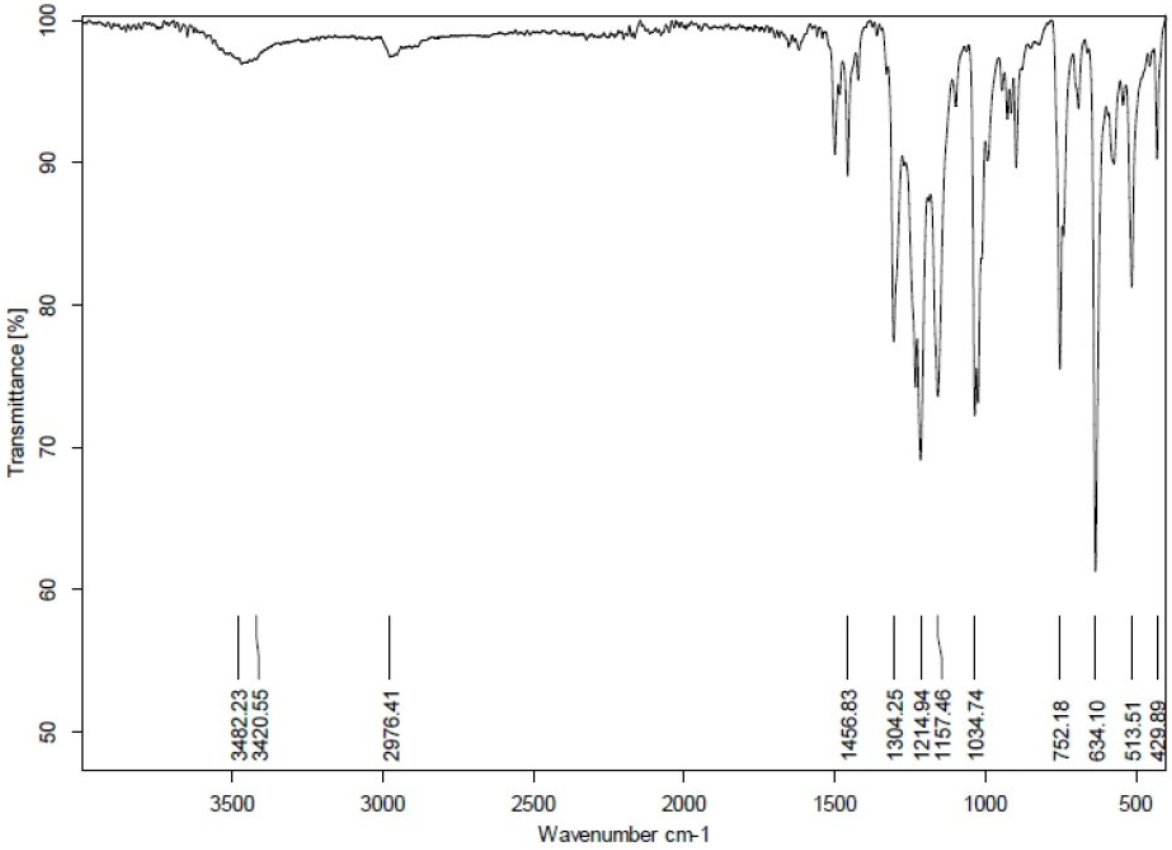
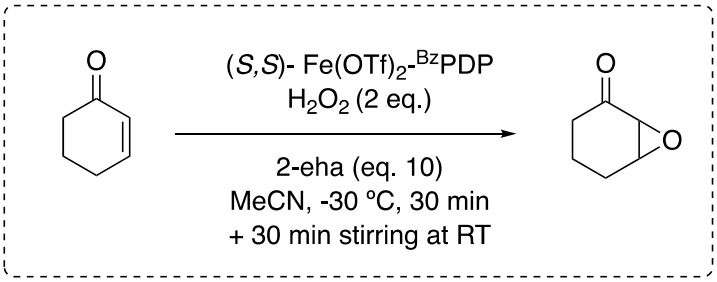


Figure S9. The FTIR (KBr) spectrum of complex $\mathbf{1}^{\mathbf{SbF6}}$.



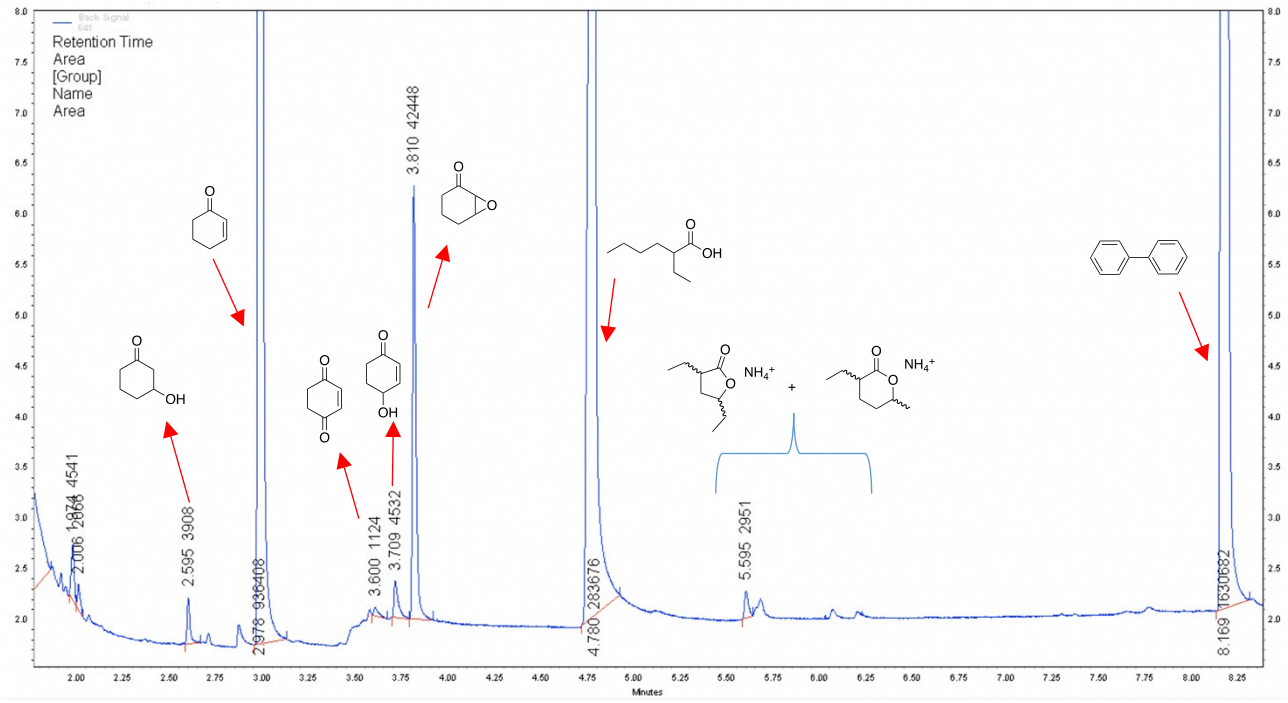


Figure S10. GC chromatogram for the oxidation of cyclohexanone by complex **1OTf** in the presence of 2-ethylhexanoic acid (eha).

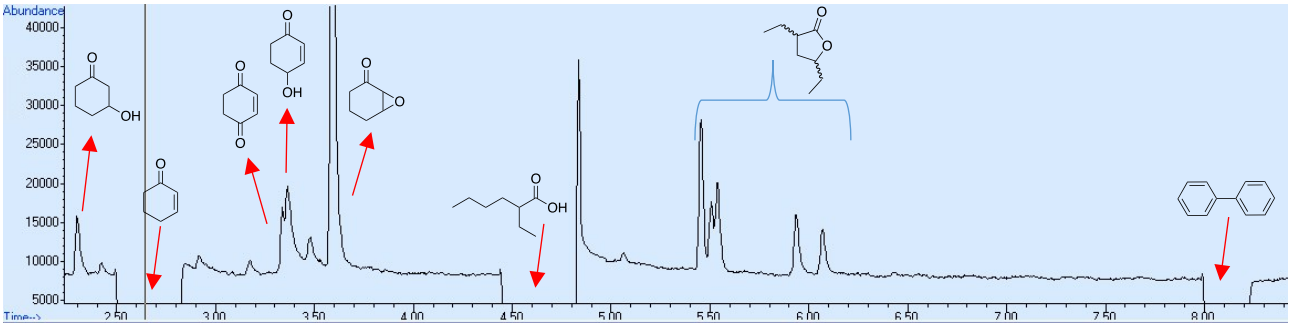
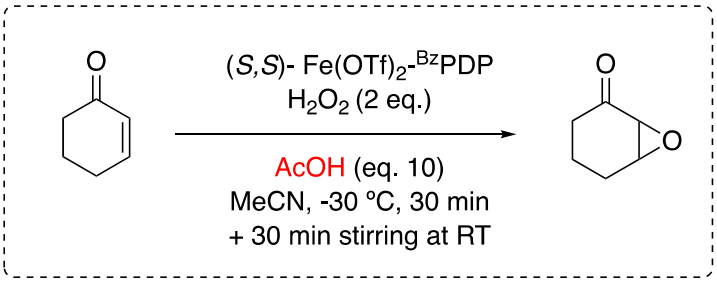


Figure S11. GC-MS chromatogram for the oxidation of cyclohexanone by complex **1**^{OTf} in the presence of 2-ethylhexanoic acid (eha). Individual mass spectra are not shown.



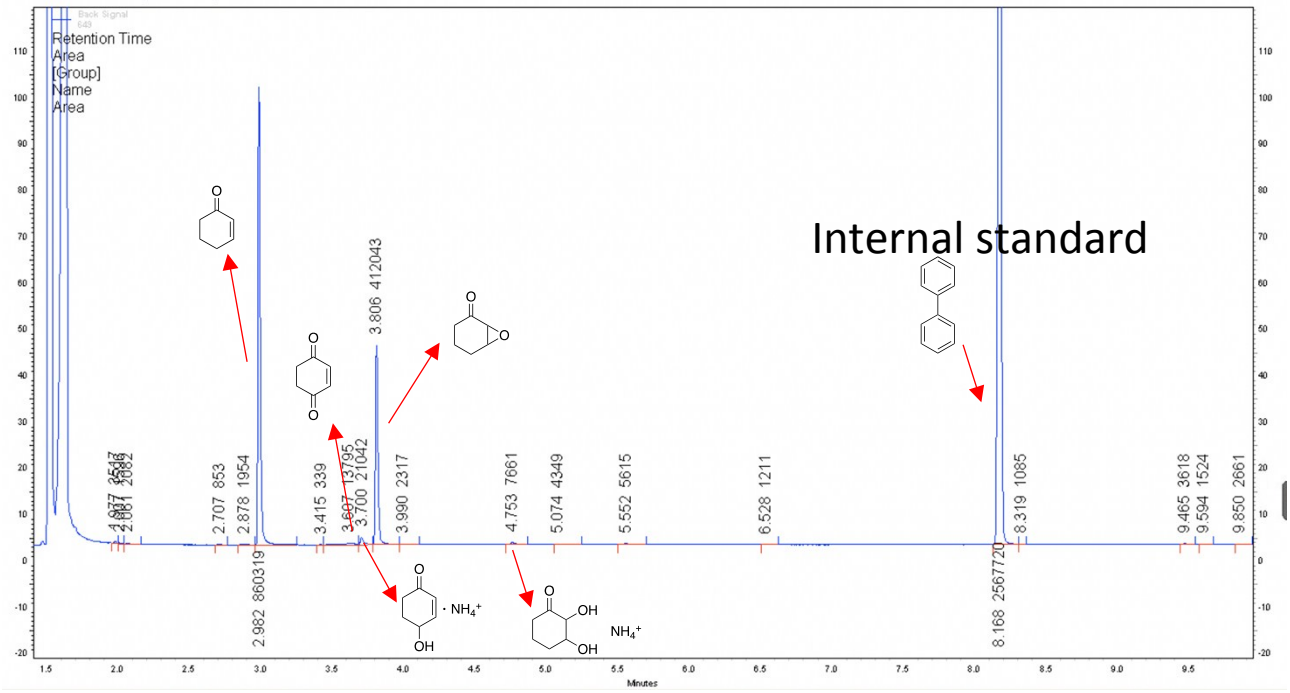


Figure S12. GC chromatogram for the oxidation of cyclohexanone by complex **1**^{OTf} in the presence of acetic acid.

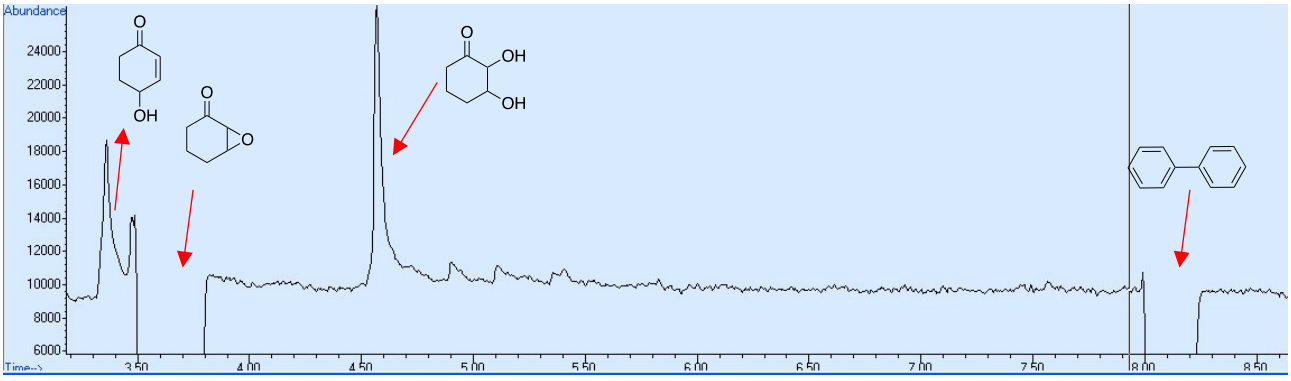
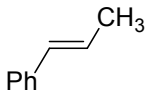
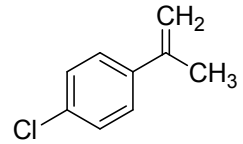
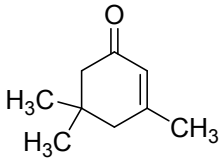
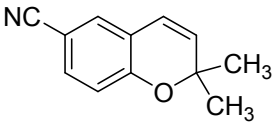
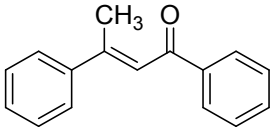


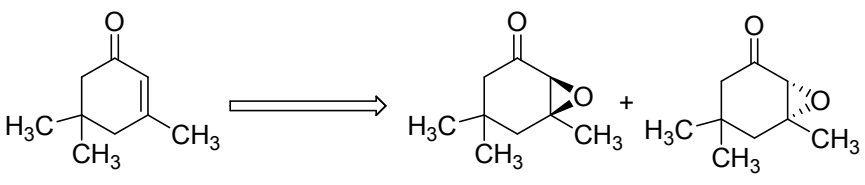
Figure S13. GC-MS chromatogram for the oxidation of cyclohexanone by complex **1**^{OTf} in the presence of acetic acid. Individual mass spectra are not shown.

Table S1. Catalytic epoxidation by complex **1**^{OTf} [a]

Substrate	CA[b] (equivalent)	Conversion of substrate	Yield of epoxide	ee (%)[c]
	EHA (1.4)	67	40	10
 4-Chloro-α-methylstyrene	EHA (1.4)	95	37	9
 Isophorone	EHA (1.4)	45	12	91
	EHA (1.4)	100	28	80
	EHA (1.4)	96	60	20

[a] Reaction conditions: see Experimental section; [b] carboxylic acid; [c] ee determined by GC.

Table S2. Catalytic epoxidation of isophorone by complex **1**^{OTf} [a]



Catalyst used (other reaction conditions)	Solvent	Temp (°C)	CA (Equivalent)	Conversion	Yield of epoxides	ee (%)
2 mol %	CH_3CN	-30	EHA (1.4)	45	12	91
4 mol %	CH_3CN	-30	EHA (1.4)	39	10	89
6 mol %	CH_3CN	-30	EHA (1.4)	40	11	90
2 mol %	CH_3CN	-30	EHA (2.8)	35	9	90
2 mol %	CH_3CN	0	EHA (1.4)	51	19	88
2 mol %	CH_3COCH_3	0	EHA (1.4)	34	8	90
2 mol %	DMF	0	EHA (1.4)	00	00	00
2 mol %	CH_3CN	0	mCPBA (1.4)	17	<1	31
2 mol %	CH_3CN	0	Peracetic acid (1.4)	16	<1	57
2 mol % catalyst (after H_2O_2 addition additional stirring for 1 h)	CH_3CN	0	EHA (0.3)	45	7	79
2 mol % catalyst (after H_2O_2 addition additional stirring for 1 h)	CH_3CN	0	EHA (1.4)	57	18	89
2 mol % catalyst (filtered through silica only)	CH_3CN	0	EHA (1.4)	54	18	93
2 mol % catalyst (filtered through alumina only)	CH_3CN	0	EHA (1.4)	61	17	89