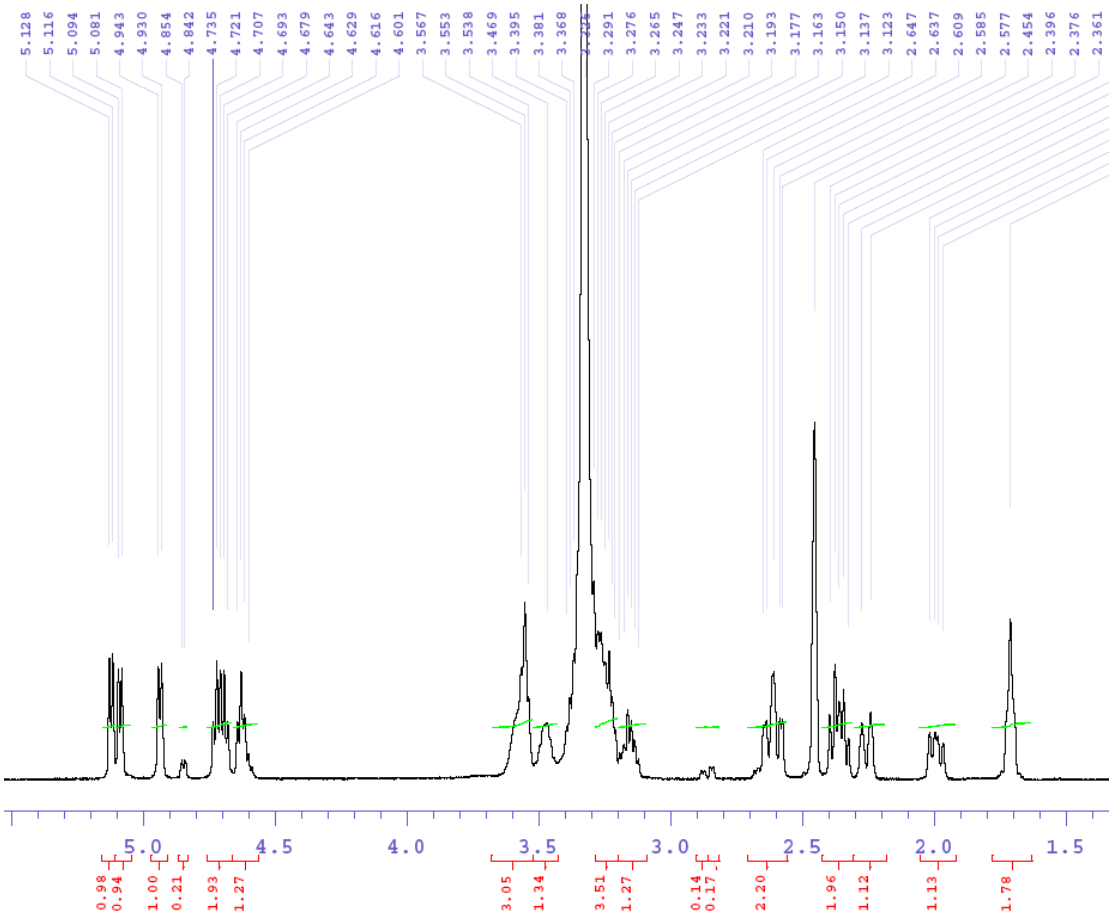
# Electronic supplementary information

## 1. Figures



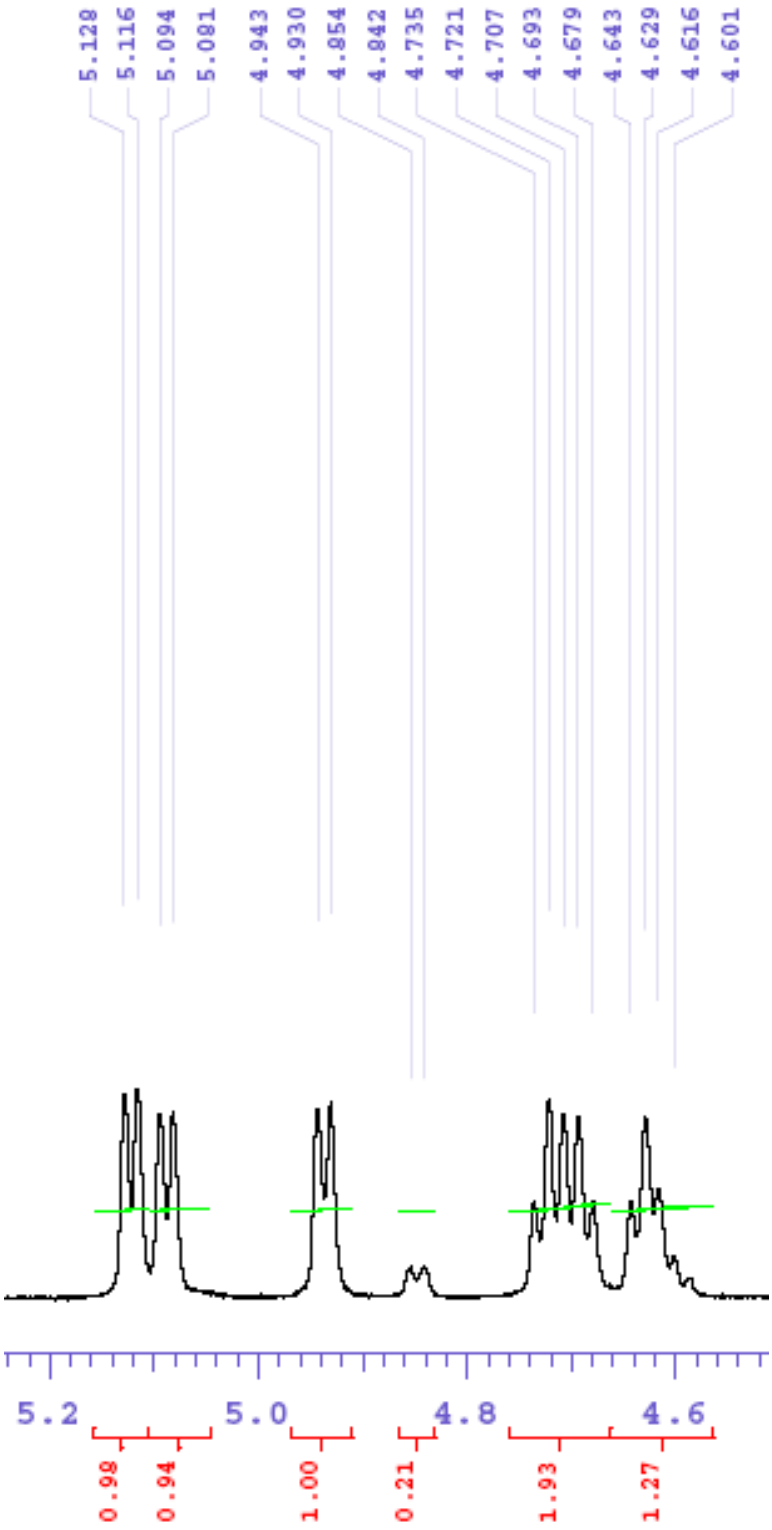
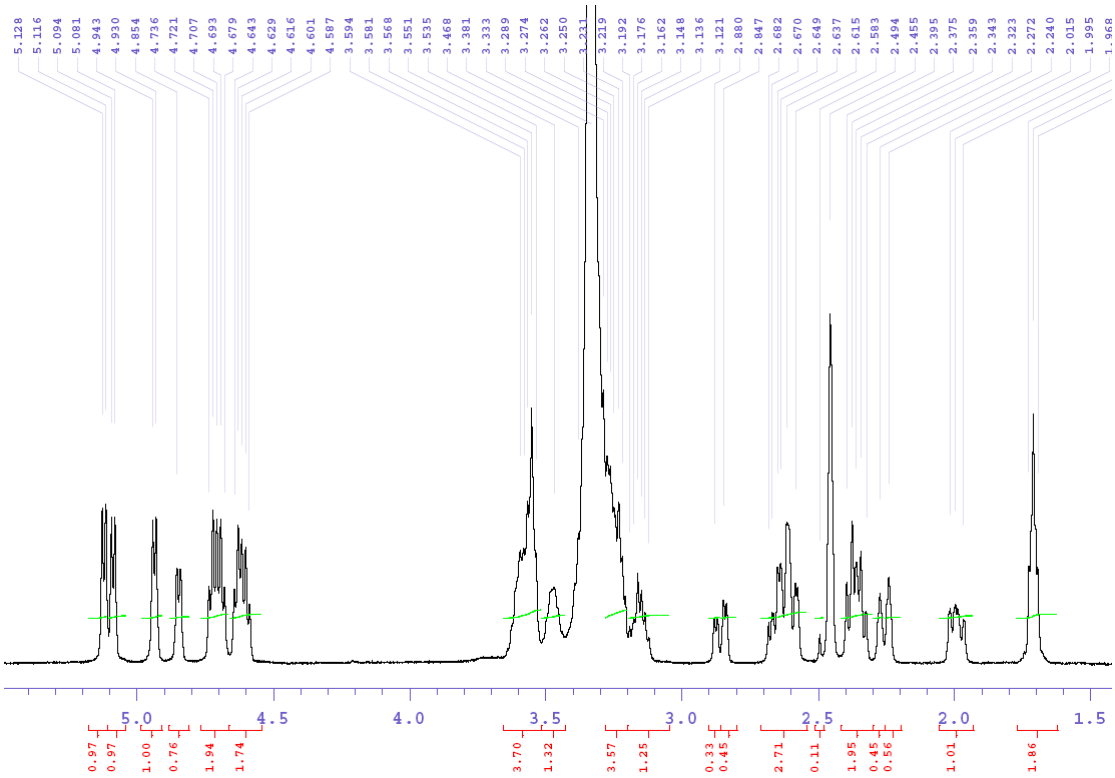



Fig. S1 $^{1}$H NMR of complex **1** with relatively lesser ee isomer.


5.128
5.116
5.094
5.081
4.943
4.930
4.854
4.736
4.721
4.707
4.693
4.679
4.643
4.629
4.616
4.601
4.587
3.594
3.581
3.568
3.551
3.535
3.468
3.381
3.333
3.289
3.274
3.262
3.250
3.231
3.219
3.192
3.176
3.162
3.148
3.136
3.121
2.880
2.847
2.682
2.670
2.649
2.637
2.615
2.583
2.494
2.455
2.395
2.375
2.359
2.343
2.323
2.272
2.240
2.015
1.995
1.968
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
0.97
0.97
1.00
0.76
1.94
1.74
3.70
1.32
3.57
1.25
0.33
0.45
2.71
0.11
1.95
0.45
0.56
1.01
1.86

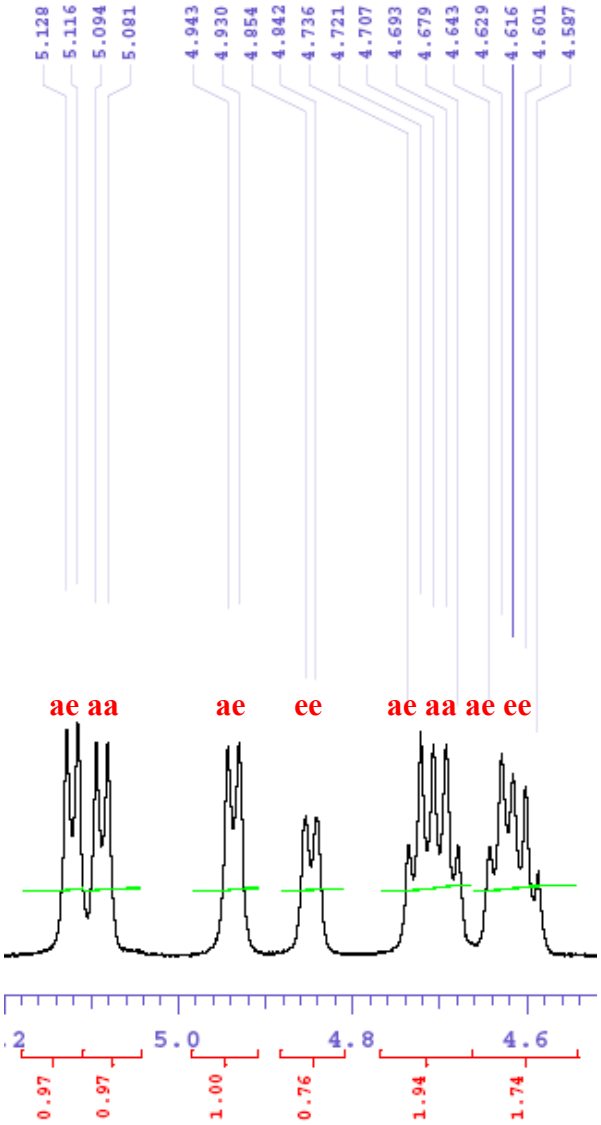



Fig. S2 $^{1}$H NMR of complex **1** with relatively more ee isomer.

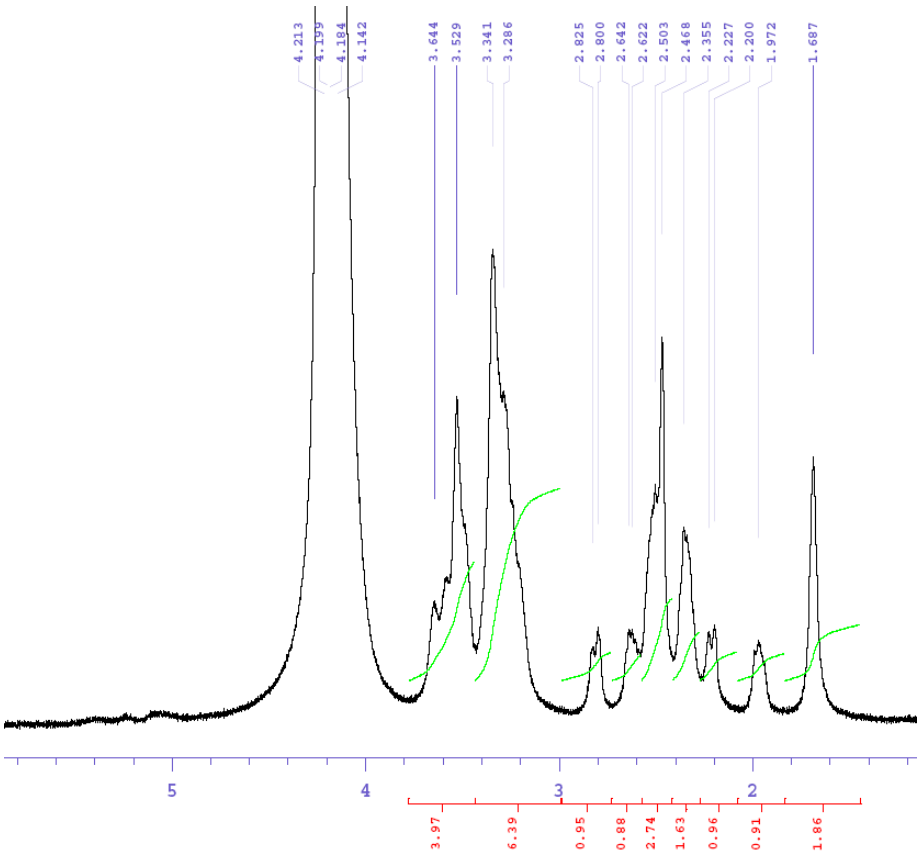



Fig. S3 Identifying the signals of OH groups of complex 1 by addition of $D_2O$.

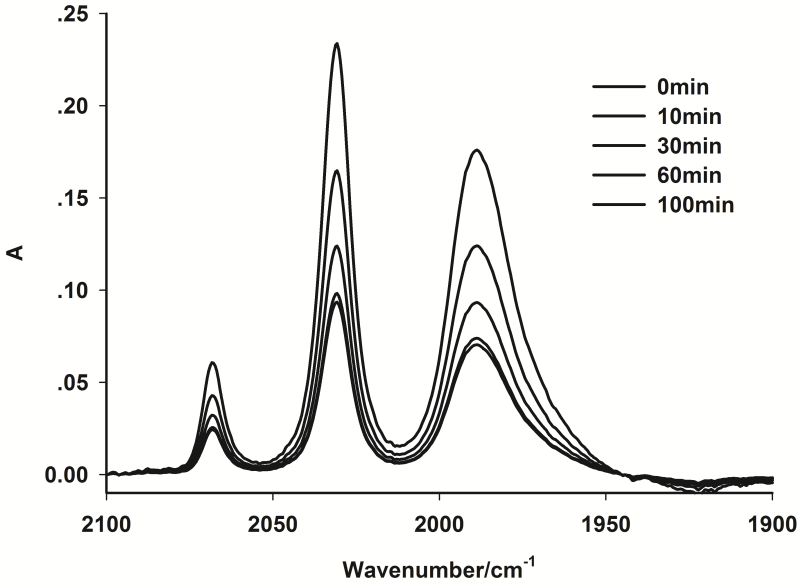



Fig. S4 Spectral variation of complex 1 (C = 4.0 mmol $L^{-1}$) with its reaction of dithionite (C = 40 mmol $L^{-1}$) in DMSO at 37 ℃ under inert atmosphere.

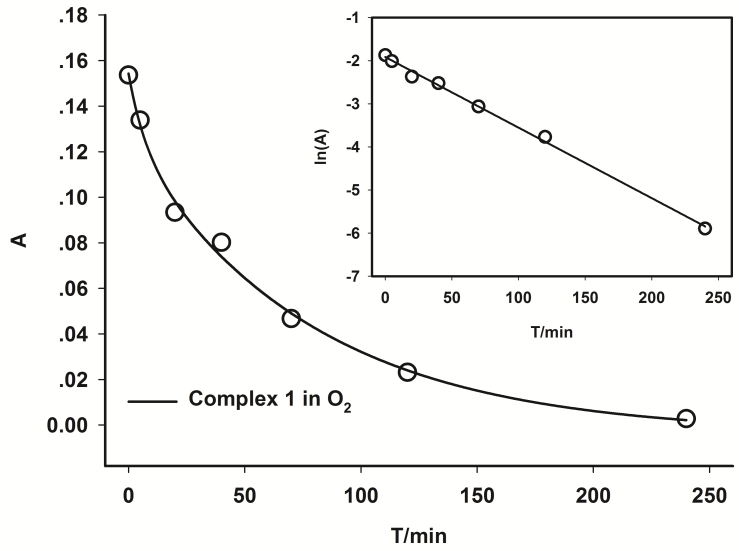
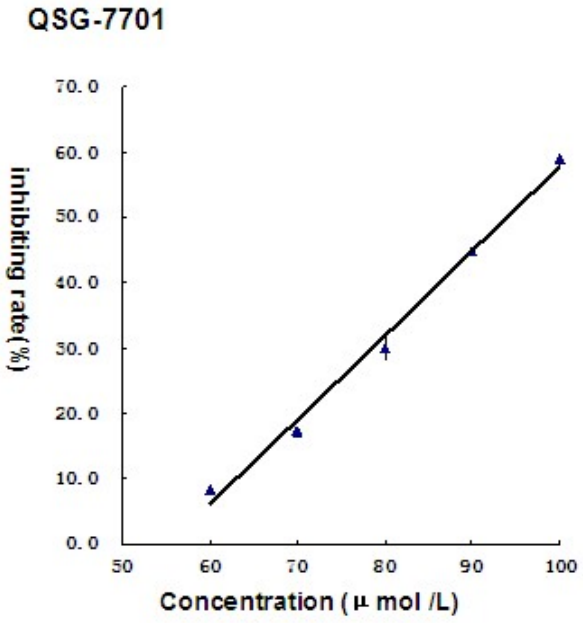



Fig. S5 Plot of the concentrations of complex **1** against reaction time ([**CysA**] = 0.069 mol $L^{-1}$, [**1**] = 0.011 mol $L^{-1}$) and its logarithmic plot (inset) in $O_2$. Please note that the absorbance used for the kinetic analysis was at 2068 $cm^{-1}$.



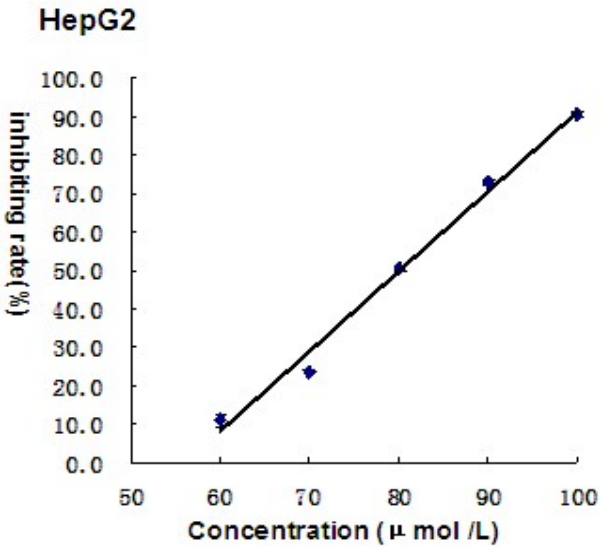
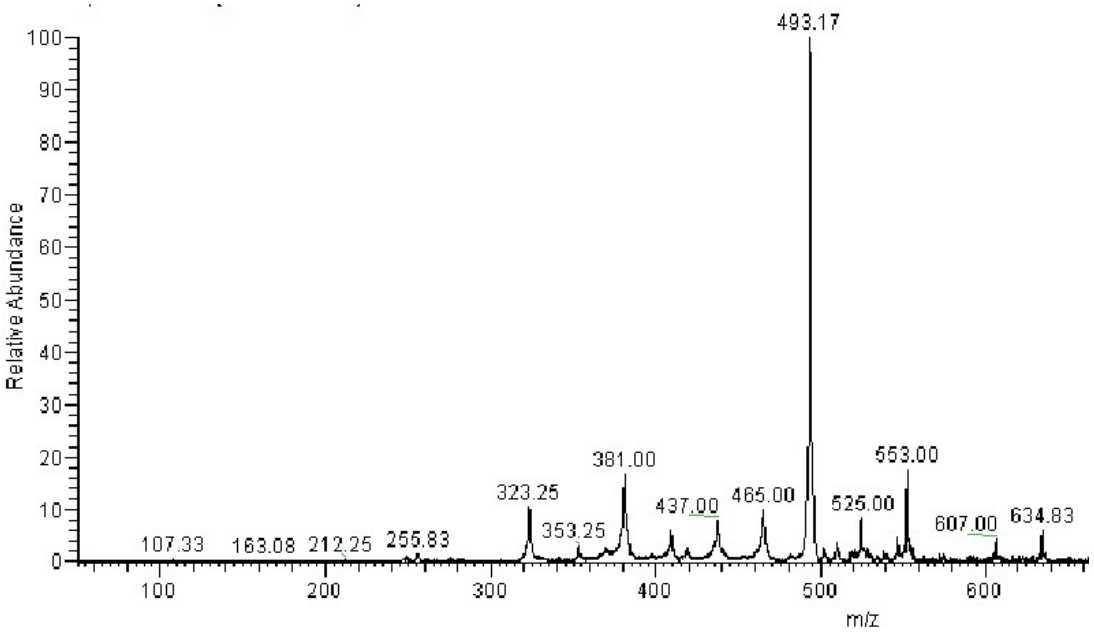



Fig. S6 Correlation plots for the estimation of $IC_{50}$ values.



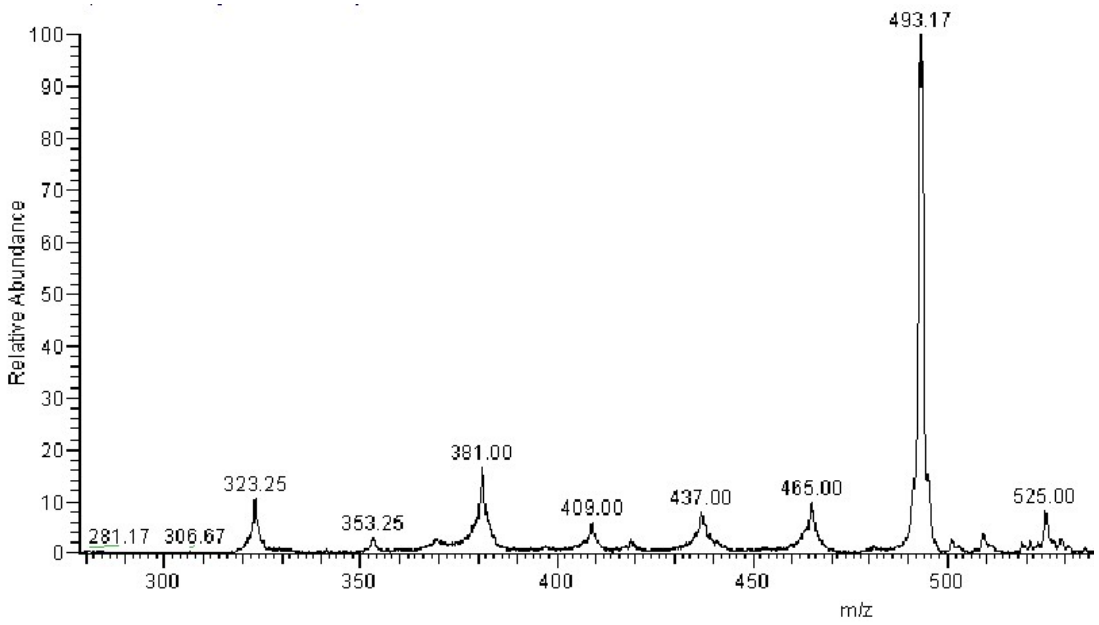
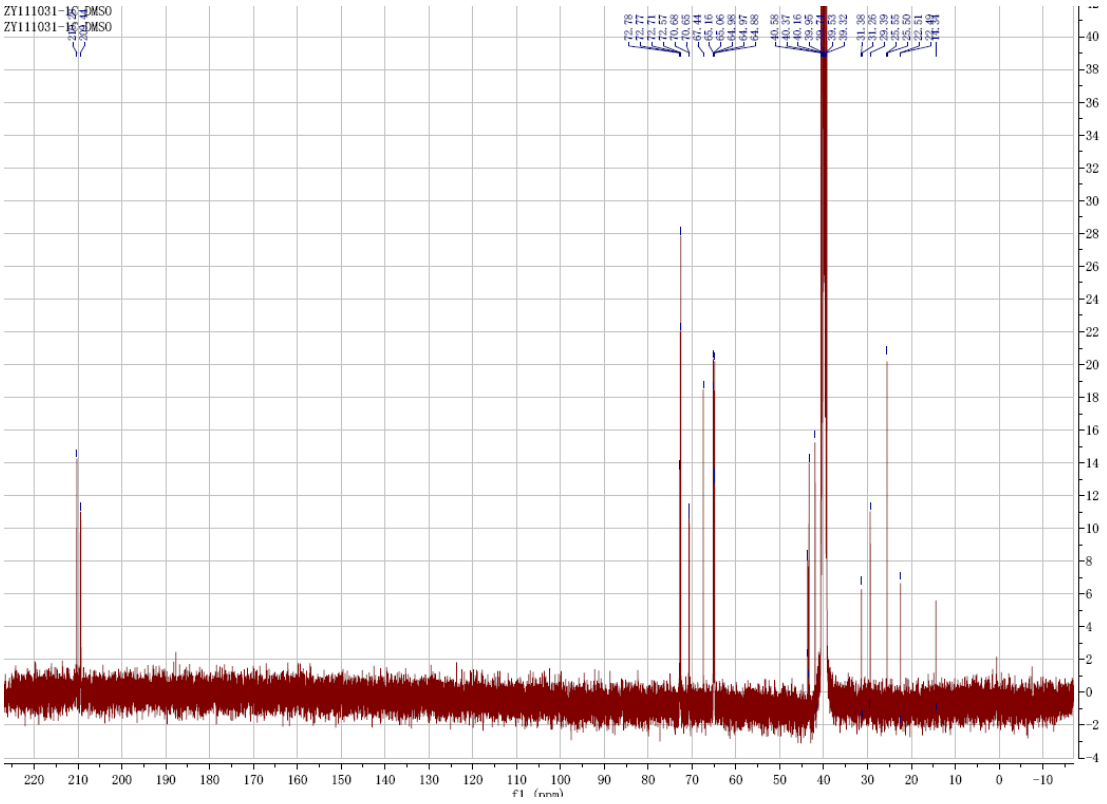



Fig. S7 Mass spectra of complex **1** (ESI, negative).



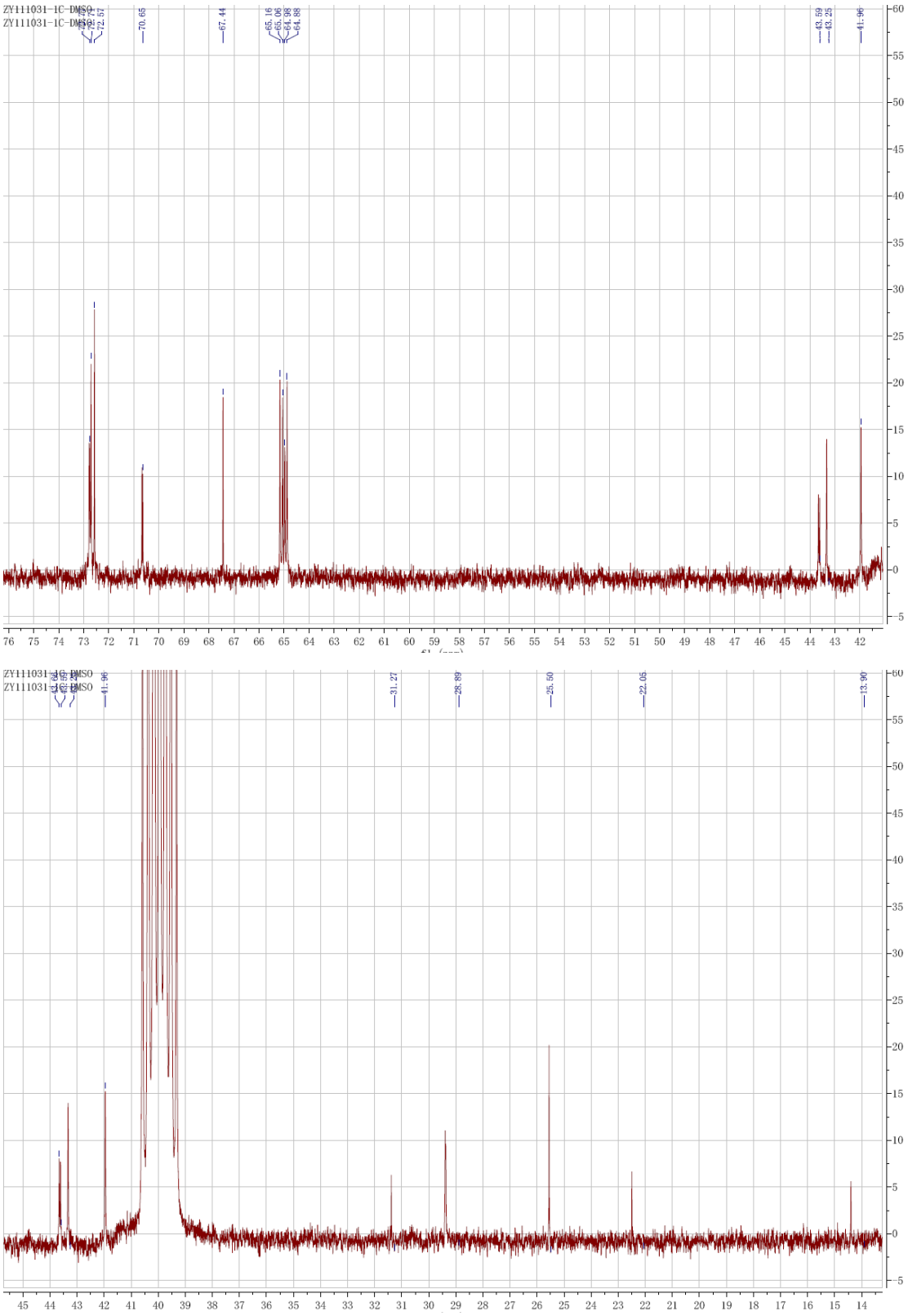



Fig. S8 $^{13}C$ NMR spectra of complex 1 (DMSO-$d_6$).

Table S1 Kinetic analysis of the substitution reaction of complex **1** by **CysA** in DMSO at 37 ℃.

| | | | | | |
|---|---|---|---|---|---|
| Complex **1** (mol $L^{-1}$) | 0.011 | 0.011 | 0.011 | 0.011 | 0.011 |
| **CysA** (mol $L^{-1}$) | 0.034 | 0.069 | 0.138 | 0.207 | 0.276 |
| $k_{obs}$ | 0.011 | 0.062 | 0.11 | 0.19 | 0.24 |
| k | 0.32 | 0.9 | 0.78 | 0.9 | 0.87 |
| $t_{1/2}$ (min) | 63.0 | 11.1 | 6.4 | 3.7 | 2.9 |
| Time for complete decomposition (min)[a] | 400 | 280 | 200 | 180 | 100 |

[a]Approximate time at which trace amount of monoiron species remained as indicated by the intensity of the infrared absorption bands.

Table S2 Cell viability at various concentration of complex **1**.

| [a]Con. | HepG2 | SD | QSG-7701 | SD |
|---|---|---|---|---|
| 100 | 9.6 | 0.7 | 41.0 | 0.7 |
| 90 | 27.0 | 0.6 | 55.1 | 0.5 |
| 80 | 49.5 | 0.6 | 70.1 | 1.9 |
| 70 | 76.3 | 0.3 | 82.8 | 0.6 |
| 60 | 89 | 1.5 | 91.6 | 0.5 |
| 50 | 113 | 1.0 | 94 | 1.7 |
| 40 | 129.4 | 0.4 | 94.4 | 0.7 |
| 30 | 140.4 | 0.4 | 95 | 1.4 |

| | | | | |
|---|---|---|---|---|
| 20 | 150.1 | 0.6 | 99 | 1.5 |
| 10 | 147 | 1.4 | 99.9 | 2.6 |
| 0 (control) | 100 | 1.4 | 100.0 | 0.4 |

[a] For each concentration, 6-folder of **CysA** is presented.