Electronic supplementary information

1. Figures

![Graph or diagram from the document]
Fig. S1 $^1$H NMR of complex 1 with relatively lesser ee isomer.
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$_2$O.

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 °C 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$^{-1}$. 

QSG-7701
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 °C.

<table>
<thead>
<tr>
<th>Complex 1 (mol L&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>0.011</th>
<th>0.011</th>
<th>0.011</th>
<th>0.011</th>
<th>0.011</th>
</tr>
</thead>
<tbody>
<tr>
<td>CysA (mol L&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td>0.034</td>
<td>0.069</td>
<td>0.138</td>
<td>0.207</td>
<td>0.276</td>
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<tr>
<td>$k_{obs}$</td>
<td>0.011</td>
<td>0.062</td>
<td>0.11</td>
<td>0.19</td>
<td>0.24</td>
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<tr>
<td>$k$</td>
<td>0.32</td>
<td>0.9</td>
<td>0.78</td>
<td>0.9</td>
<td>0.87</td>
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<tr>
<td>$t_{1/2}$ (min)</td>
<td>63.0</td>
<td>11.1</td>
<td>6.4</td>
<td>3.7</td>
<td>2.9</td>
</tr>
<tr>
<td>Time for complete decomposition (min)&lt;sup&gt;a&lt;/sup&gt;</td>
<td>400</td>
<td>280</td>
<td>200</td>
<td>180</td>
<td>100</td>
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</table>

<sup>a</sup>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.

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<th>Con.</th>
<th>HepG2</th>
<th>SD</th>
<th>QSG-7701</th>
<th>SD</th>
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<td>90</td>
<td>27.0</td>
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<td>80</td>
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<td>91.6</td>
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<tr>
<td>50</td>
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<td>94</td>
<td>1.7</td>
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<td>1.4</td>
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<td>1.5</td>
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<td>1.4</td>
<td>99.9</td>
<td>2.6</td>
</tr>
<tr>
<td>0 (control)</td>
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<td>1.4</td>
<td>100.0</td>
<td>0.4</td>
</tr>
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</table>

*a For each concentration, 6-fold of CysA is presented.*