Supplementary Information

for

The design, synthesis and biological evaluation of novel thiamin diphosphate analog inhibitors against pyruvate dehydrogenase multienzyme complex E1 from *Escherichia coli*

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1. The copies of all NMR spectra of the compounds

\[ ^{13}\text{C NMR of 4a in DMSO-d6} \]

\[ ^{1}H \text{ NMR of 4a in DMSO-d6} \]
$^{13}$C NMR of 4b in DMSO-$d_6$

$^1$H NMR of 4b in DMSO-$d_6$
$^{13}$C NMR of 4c in DMSO-$d_6$

1H NMR of 4c in DMSO-$d_6$
$^{13}$C NMR of 4d in DMSO-$d_6$


$^1$H NMR of 4d in DMSO-$d_6$
$^{13}$C NMR of 4e in DMSO-d$_6$

$^1$H NMR of 4e in DMSO-d$_6$
$^{13}$C NMR of 4f in DMSO-d6

$^1$H NMR of 4f in DMSO-d6
$^{13}$C NMR of 4g in DMSO-d6

$^1$H NMR of 4g in DMSO-d6
$^{13}$C NMR of $4h$ in DMSO-\textit{d6}

$^1$H NMR of $4h$ in DMSO-\textit{d6}
$^{13}$C NMR of 4i in DMSO-$d_6$

$^1$H NMR of 4i in DMSO-$d_6$
$^{13}$C NMR of 4j in DMSO-$d_6$

$^1$H NMR of 4j in DMSO-$d_6$
$^{13}$C NMR of 4k in DMSO-d6

$^1$H NMR of 4k in DMSO-d6
$^{13}$C NMR of 4I in DMSO-$d_6$

$^1$H NMR of 4I in DMSO-$d_6$
2. The representative figures for the dose-response effect of all applicable assays
Figure 4f: Inhibitory rate (%) vs. Concentration (µM)

Figure 4g: Inhibitory rate (%) vs. Concentration (µM)

Figure 4h: Inhibitory rate (%) vs. Concentration (µM)