## **SUPPLEMENTARY DATA**

Bisubstrate analogue inhibitors of 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase: New lead exhibits a distinct binding mode

Genbin Shi <sup>a</sup>, Gary Shaw <sup>a</sup>, Yue Li <sup>b</sup>, Yan Wu <sup>b</sup>, Honggao Yan <sup>b</sup>, and Xinhua Ji <sup>a,\*</sup>

<sup>a</sup> Macromolecular Crystallography Laboratory, National Cancer Institute, Frederick, MD

21702, USA

<sup>b</sup> Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI 48824, USA

\* Corresponding author. Tel: +1 (301) 846-5035; Fax: +1 (301) 846-6073.

E-mail address: <u>jix@mail.nih.gov</u> (X. Ji).

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## **Table of Contents**

| Figure S1. IR Spectrum of Compound 3  |
|---|
| Figure S2. IR Spectrum of Compound 4 ····· S4   |
| Figure S3. IR Spectrum of Compound 9  |
| <b>Figure S4.</b> <sup>1</sup> H NMR Spectrum of Compound <b>3</b> at 400 MHz in CD <sub>3</sub> OD S6        |
| Figure S5. <sup>13</sup> C NMR Spectrum of Compound 3 at 100 MHz in CD <sub>3</sub> OD S7                     |
| <b>Figure S6.</b> <sup>1</sup> H NMR Spectrum of Compound <b>4</b> at 400 MHz in CD <sub>3</sub> OD S8        |
| <b>Figure S7.</b> <sup>13</sup> C NMR Spectrum of Compound <b>4</b> at 100 MHz in CD <sub>3</sub> OD S9       |
| <b>Figure S8.</b> <sup>1</sup> H NMR Spectrum of Compound <b>9</b> at 400 MHz in CD <sub>3</sub> OD S10       |
| <b>Figure S9.</b> <sup>13</sup> C NMR Spectrum of Compound <b>9</b> at 100 MHz in DMSO- <b>d</b> <sub>6</sub> |

Figure S1. IR Spectrum of Compound 3

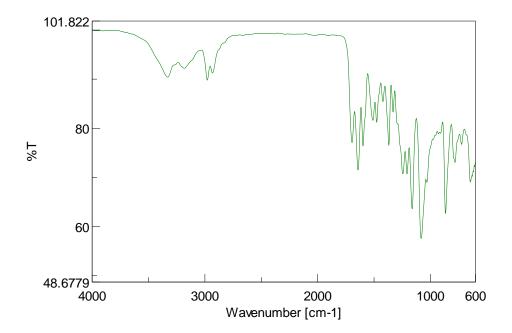


Figure S2. IR Spectrum of Compound 4

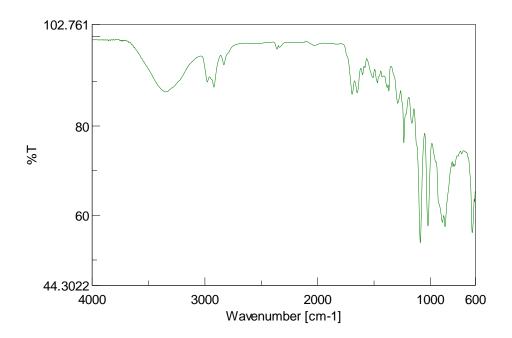


Figure S3. IR Spectrum of Compound 9

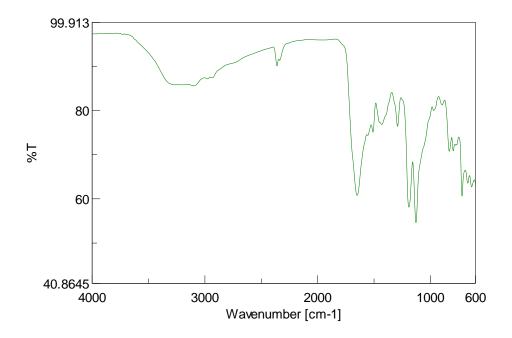
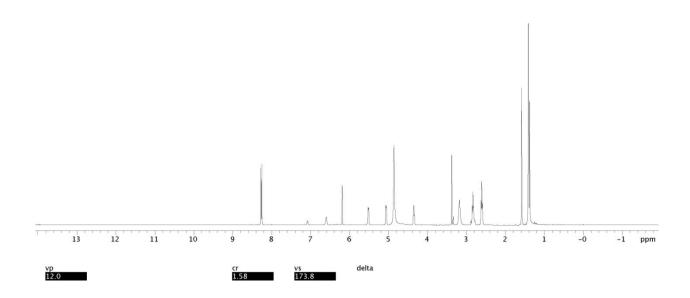


Figure S4. <sup>1</sup>H NMR Spectrum of Compound 3 at 400 MHz in CD<sub>3</sub>OD



**Figure S5.** <sup>13</sup>C NMR Spectrum of Compound **3** at 100 MHz in CD<sub>3</sub>OD

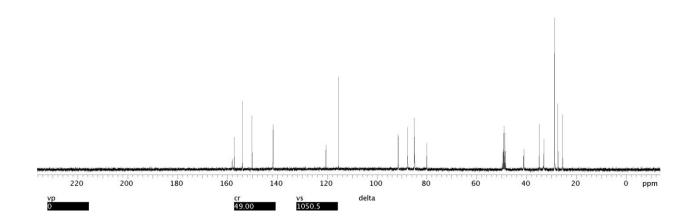
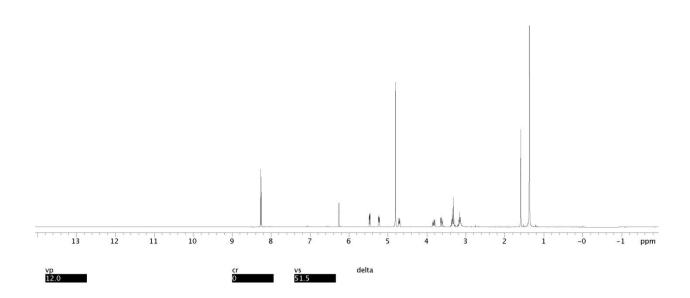


Figure S6. <sup>1</sup>H NMR Spectrum of Compound 4 at 400 MHz in CD<sub>3</sub>OD



**Figure S7.** <sup>13</sup>C NMR Spectrum of Compound **4** at 100 MHz in CD<sub>3</sub>OD

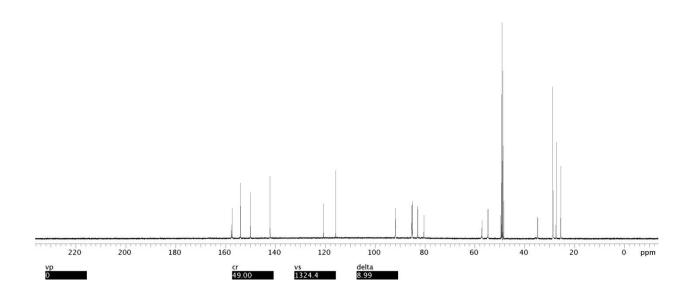
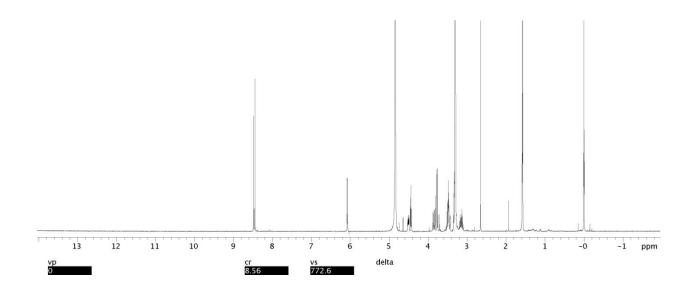


Figure S8. <sup>1</sup>H NMR Spectrum of Compound 9 at 400 MHz in CD<sub>3</sub>OD



**Figure S9.**  $^{13}$ C NMR Spectrum of Compound **9** at 100 MHz in DMSO- $\mathbf{d}_6$ 

