Article

# PSMA-Oriented Target Delivery of Novel Anticancer Prodrugs: Design, Synthesis, and Biological Evaluations of Oligopeptide-Camptothecin Conjugates

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## Supplementary Data



Figure S1: The structure of HT-A.







Figure S3: The <sup>13</sup>C-NMR of **HT-A**.



Figure S4: The HRMS of **HT-A**.







Figure S6: The <sup>1</sup>H-NMR of **HT-B**.











Figure S9: The structure of HT-C.









Figure S11: The <sup>13</sup>C-NMR of **HT-C**.



Figure S12: The HRMS of **HT-C**.











Figure S15: The <sup>13</sup>C-NMR of **HT-D**.



#### Figure S16: The HRMS of HT-D.



Figure S17: The structure of **HT-E**.







Figure S19: The <sup>13</sup>C-NMR of **HT-E**.



Figure S20: The HRMS of **HT-E**.



HT-F









Figure S21: The <sup>13</sup>C-NMR of HT-F.



#### Figure S22: The HRMS of HT-F.





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Figure S24: The <sup>1</sup>H-NMR of **HT-I**.











Figure S27: The structure of **HT-J**.







Figure S29: The <sup>13</sup>C-NMR of **HT-J**.



Figure S30: The HRMS of HT-J.



Figure S31: The structure of CPT-A-L<sub>2</sub>.



Figure S32: The <sup>1</sup>H-NMR of **CPT-A-L**<sub>2</sub>.







Figure S34: The HRMS of **CPT-A-L**<sub>2</sub>.



Figure S35: The structure of CPT-B-L<sub>2</sub>.



Figure S36: The <sup>1</sup>H-NMR of **CPT-B-L**<sub>2</sub>.



Figure S37: The <sup>13</sup>C-NMR of **CPT-B-L**<sub>2</sub>.



### Figure S38: The HRMS of CPT-B-L<sub>2</sub>.



Figure S39: The structure of  $CPTD-HT-J-L_2$ .



Figure S40: The <sup>1</sup>H-NMR of **CPT-HT-J-L**<sub>2</sub>.











Figure S43: The structure of CPT-HT-J-ZL<sub>2</sub>.







Figure S45: The  ${}^{13}$ C-NMR of **CPT-HT-J-ZL**<sub>2</sub>.



Figure S46: The HRMS of  $CPT-HT-J-ZL_2$ .







Figure S48: The <sup>1</sup>H-NMR of **CPT-A-L**<sub>4</sub>.











Figure S51: The structure of **CPT-B-L**<sub>4</sub>.







Figure S53: The <sup>13</sup>C-NMR of **CPT-B-L**<sub>4</sub>.



#### Figure S54: The HRMS of CPT-B-L4.



Figure S55: The structure of CPT-HT-J-L4.





Figure S56: The <sup>1</sup>H-NMR of CPT-HT-J-L<sub>4</sub>.











Figure S59: The structure of CPT-HT-J-ZL<sub>4</sub>.



Figure S60: The <sup>1</sup>H-NMR of **CPT-HT-J-ZL**<sub>4</sub>.



Figure S61: The  ${}^{13}$ C-NMR of **CPT-HT-J-ZL**<sub>4</sub>.



### Figure S62: The HRMS of CPT-HT-J-ZL<sub>4</sub>.







Figure S64: The <sup>1</sup>H-NMR of **CPT-A-L**<sub>6</sub>.







Figure S66: The HRMS of **CPT-A-L**<sub>6</sub>.



Figure S67: The structure of CPT-B-L<sub>6</sub>.



Figure S68: The <sup>1</sup>H-NMR of **CPT-B-L**<sub>6</sub>.



Figure S69: The <sup>13</sup>C-NMR of **CPT-B-L**<sub>6</sub>.



Figure S70: The HRMS of  $\ensuremath{CPT-B-L_6}$ .







Figure S72: The <sup>1</sup>H-NMR of **CPT-HT-J-L**<sub>6</sub>.











Figure S75: The structure of CPT-HT-J-ZL<sub>6</sub>.

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Figure S77: The <sup>13</sup>C-NMR of **CPT-HT-J-ZL**<sub>6</sub>.



### Figure78: The HRMS of CPT-HT-J-ZL<sub>6</sub>.



### Figure S79: The structure of $CPT-A-L_{12}$ .



Figure S80: The <sup>1</sup>H-NMR of **CPT-A-L**<sub>12</sub>.



Figure S81: The <sup>13</sup>C-NMR of **CPT-A-L**<sub>12</sub>.



Figure S82: The HRMS of CPT-A-L<sub>12</sub>.



Figure S83: The structure of **CPT-B-L**<sub>12</sub>.



Figure S84: The <sup>1</sup>H-NMR of **CPT-B-L**<sub>12</sub>.



Figure S85: The <sup>13</sup>C-NMR of **CPT-B-L**<sub>12</sub>.



Figure S86: The HRMS of **CPT-B-L**<sub>12</sub>.



Figure S87: The structure of CPT-HT-J-L<sub>12</sub>.



Figure S88: The <sup>1</sup>H-NMR of CPT-HT-J-L<sub>12</sub>.



Figure S89: The  $^{\rm 13}C\text{-}NMR$  of  $\textbf{CPT-HT-J-ZL}_{12}.$ 







Figure S91: The structure of  $CPT-HT-J-ZL_{12}$ .







Figure S93: The <sup>13</sup>C-NMR of **CPT-HT-J-ZL**<sub>12</sub>.



#### Figure S94: The HRMS of CPT-HT-J-ZL<sub>12</sub>.



















Figure S99: The structure of CPT-D-GL<sub>2</sub>.





Figure S101: The <sup>13</sup>C-NMR of **CPT-D-GL**<sub>2</sub>.



### Figure S102: The structure of CPT-C-GL<sub>4</sub>.

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Figure S103: The <sup>1</sup>H-NMR of **CPT-C-GL**<sub>4</sub>.



Figure S104: The <sup>13</sup>C-NMR of **CPT-C-GL**<sub>4</sub>.



Figure S105: The structure of **CPT-D-GL**<sub>4</sub>.



Figure S106: The <sup>1</sup>H-NMR of **CPT-D-GL**<sub>4</sub>.



Figure S107: The <sup>13</sup>C-NMR of **CPT-D-GL**<sub>4</sub>.



Figure S108: The HRMS of CPT-D-GL4.







Figure S110: The <sup>1</sup>H-NMR of **CPT-C-GL**<sub>6</sub>.







Figure S112: The HRMS of CPT-C-GL<sub>6</sub>.



Figure S113: The structure of **CPT-D-GL**<sub>6</sub>.



Figure S114: The <sup>1</sup>H-NMR of CPT-D-GL<sub>6</sub>.



Figure S113: The <sup>13</sup>C-NMR of CPT-D-GL<sub>6</sub>.







Figure S115: The structure of  $CPT-C-GL_{12}$ .





Figure S117: The <sup>13</sup>C-NMR of **CPT-C-GL**<sub>12</sub>.



Figure S118: The HRMS of **CPT-C-GL**<sub>12</sub>.



Figure S119: The structure of **CPT-D-GL**<sub>12</sub>.



Figure S120: The <sup>1</sup>H-NMR of **CPT-D-GL**<sub>12</sub>.



Figure S121: The <sup>13</sup>C-NMR of **CPT-D-GL**<sub>12</sub>.



Figure S122: The HRMS of CPT-D-GL<sub>12</sub>.