

## Supporting Information

### Structure-based discovery of pyrazolobenzothiazine derivatives as inhibitors of hepatitis C virus replication

*Maria Letizia Barreca,<sup>\*,†</sup> Giuseppe Manfroni,<sup>\*,†</sup> Pieter Leyssen,<sup>‡</sup> Johan Winquist,<sup>#</sup> Neerja Kaushik-Basu,<sup>§</sup> Jan Paeshuyse,<sup>‡</sup> Ramalingam Krishnan,<sup>§</sup> Nunzio Iraci,<sup>†</sup> Stefano Sabatini,<sup>†</sup> Oriana Tabarrini,<sup>†</sup> Amartya Basu,<sup>§</sup> U. Helena Danielson,<sup>#</sup> Johan Neyts,<sup>‡</sup> and Violetta Cecchetti<sup>†</sup>*

<sup>†</sup>Dipartimento di Chimica e Tecnologia del Farmaco, Sezione di Chimica Farmaceutica II, Università degli Studi di Perugia, Via del Liceo 1, 06123 Perugia, Italy

<sup>‡</sup>Rega Institute for Medical Research, Katholieke Universiteit Leuven, B-3000 Leuven, Belgium

<sup>#</sup>Department of Chemistry – BMC, Uppsala University, Box 576, SE-751 23 Uppsala, Sweden.

<sup>§</sup>Department of Biochemistry and Molecular Biology UMDNJ-New Jersey Medical School 185 South Orange Avenue, New Jersey 07103, USA

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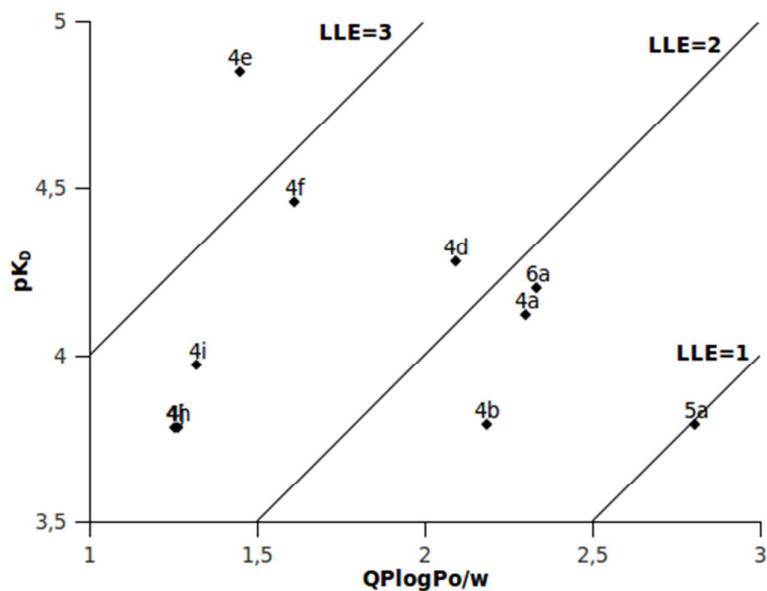
**Plot of calculated logP versus pIC<sub>50</sub>.....S3**

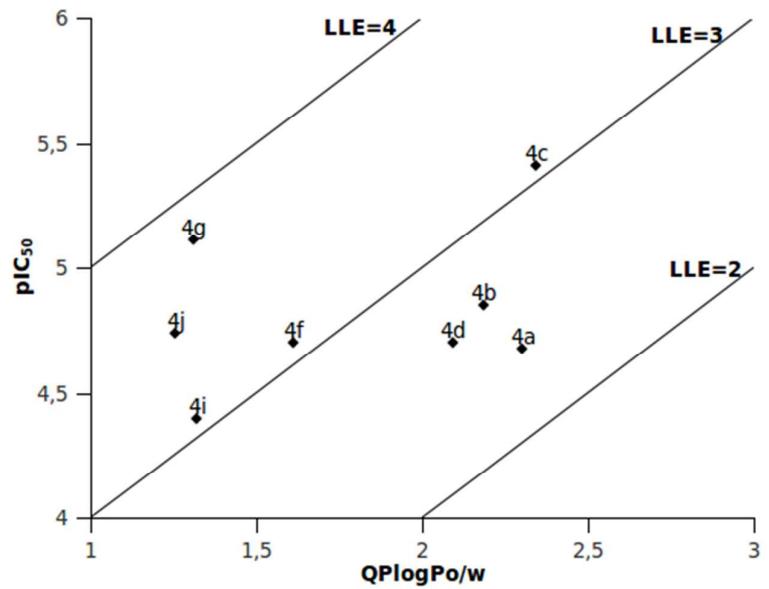
**Table S1**

Values of  $pK_D$ ,  $pIC_{50}$  and  $\log P$  calculated using the program QikProp (descriptor QPlogPo/w) for compounds **4a-j**, **5a**, and **6a**

cpds	$pK_D$	$pIC_{50}$	QPlogPo/w
<b>4a</b>	4.12	4.68	2.30
<b>4b</b>	3.79	4.85	2.18
<b>4c</b>	-	5.41	2.34
<b>4d</b>	4.28	4.70	2.09
<b>4e</b>	4.85	-	1.45
<b>4f</b>	4.46	4.70	1.61
<b>4g</b>	-	5.11	1.31
<b>4h</b>	3.79	-	1.27
<b>4i</b>	3.97	4.40	1.32
<b>4j</b>	3.78	4.74	1.26
<b>5a</b>	3.79	-	2.81
<b>6a</b>	4.20	-	2.33

Plots of QPlogPo/w versus  $pK_D$  (Figure S1) and  $pIC_{50}$  (Figure S2). Diagonal lines represent area of identical LLE values.

**Figure S1.** Calculated  $\log P$  vs  $pK_D$ .



**Figure S2.** Calculated logP vs pIC<sub>50</sub>.