

## Supplementary Materials

### Molecular docking study and 3D-QSAR model for trans-stilbene derivatives as ligands of CYP1B1

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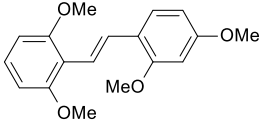
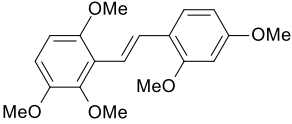
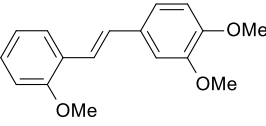
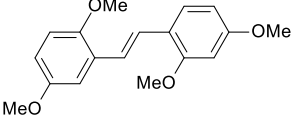
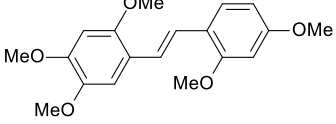
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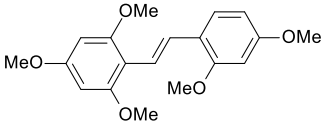
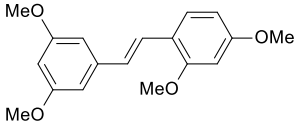
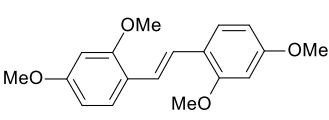
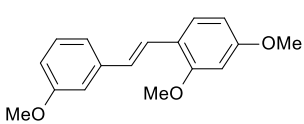
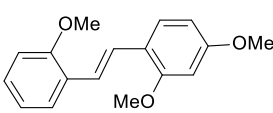
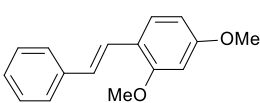
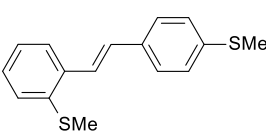
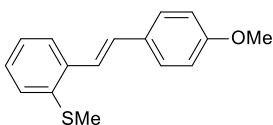
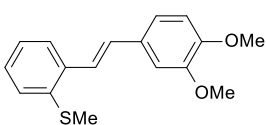
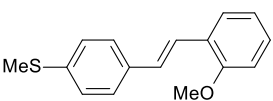
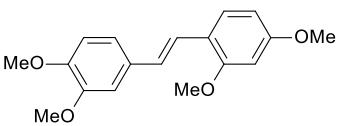
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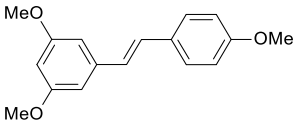
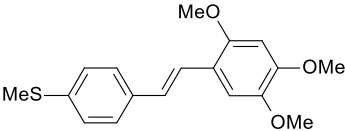
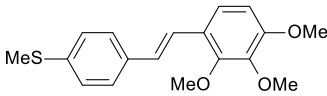
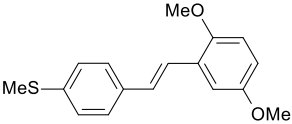
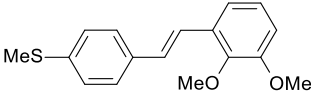
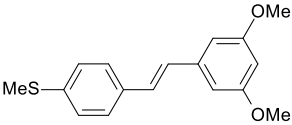
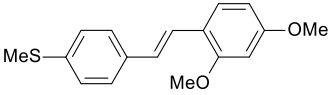
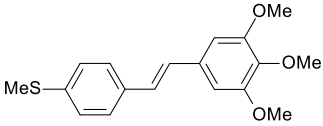
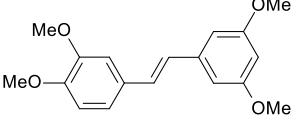
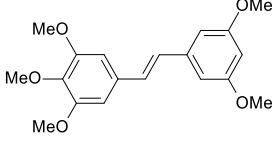
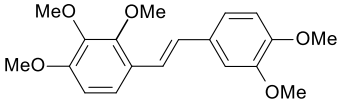
**Keywords:** cytochrome P450, CYP1B1, 3D-QSAR, trans-stilbene derivatives.

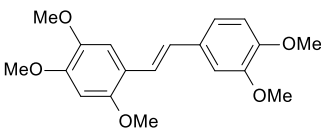
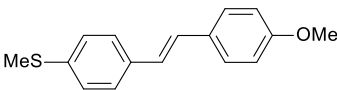
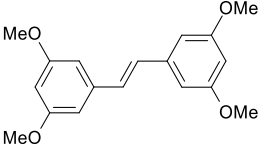
**Table S1.** Ligand orientation relative to heme.

Compound	Structure	Ring close to HEME
1		2,4-disubstituted
2		2,4-disubstituted
3		3,4-disubstituted
4		2,4-disubstituted
5		2,4-disubstituted

Compound	Structure	Ring close to HEME
6		2,4-disubstituted
7		2,4-disubstituted
8		2,4-disubstituted
9		3'-monosubstituted
10		2,4-disubstituted
<u>11</u>		unsubstituted
<u>12</u>		4'(SMe)-substituted
<u>13</u>		4'(OMe)-substituted
14		3,4-disubstituted
15		4'(SMe)-substituted
16		3,4-disubstituted

Compound	Structure	Ring close to HEME
17		4'(OMe)-substituted
18		2',3'-disubstituted
19		4'(OMe)-substituted
20		2,4-disubstituted
21		unsubstituted
22		3,4-disubstituted
<u>23</u>		3,4-disubstituted
24		3,4-disubstituted
<u>25</u>		4(SMe)-substituted
26		4(SMe)-substituted
27		3,4-disubstituted

Compound	Structure	Ring close to HEME
<u>28</u>		4'(OMe)–substituted
29		4(SMe)–substituted
30		4(SMe)–substituted
31		4(SMe)–substituted
32		4(SMe)–substituted
<u>33</u>		4(SMe)–substituted
34		4(SMe)–substituted
35		4(SMe)–substituted
36		3,4-disubstituted
<u>37</u>		3'4'5'-trisubstituted
38		3,4-disubstituted

Compound	Structure	Ring close to HEME
39		3,4-disubstituted
40		4(SMe)-substituted
41		3,5-disubstituted