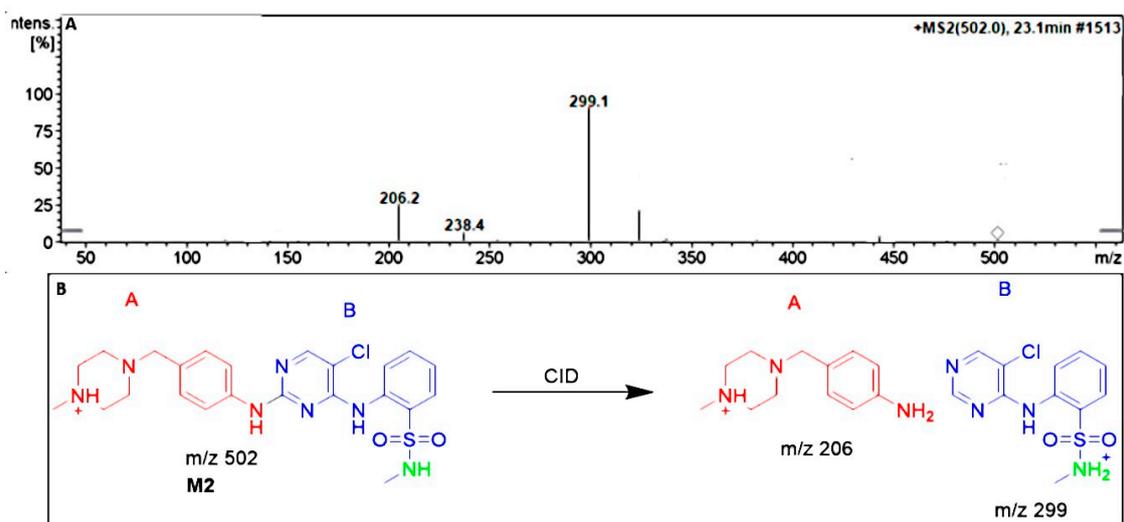


## Supplementary data

### 1. *In vitro* drug metabolism of DMB

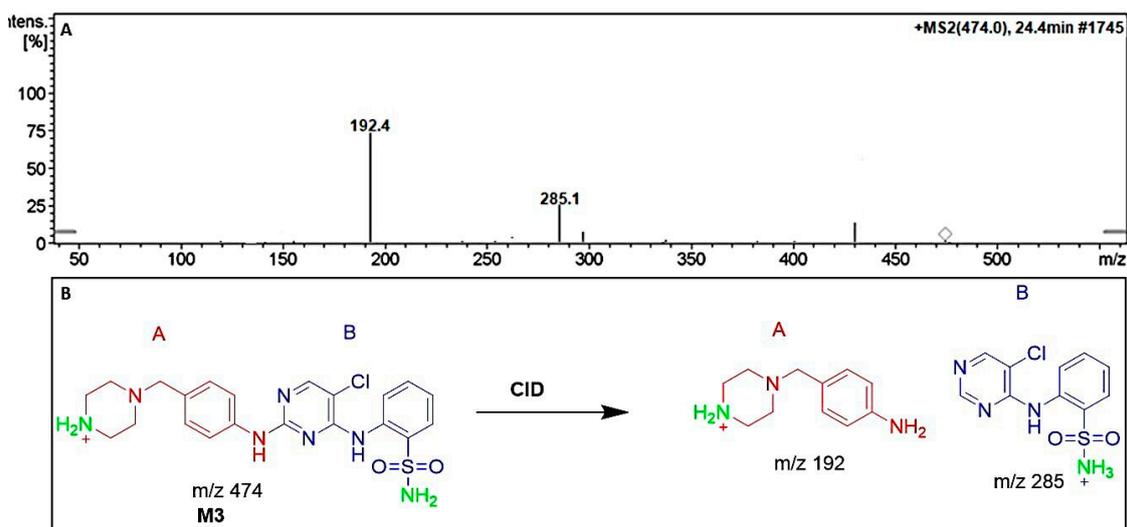
#### 1.1. Identification of dubermatinib *in vitro* phase I metabolites

##### 1.1.1. Identification of the DMB M2 metabolites



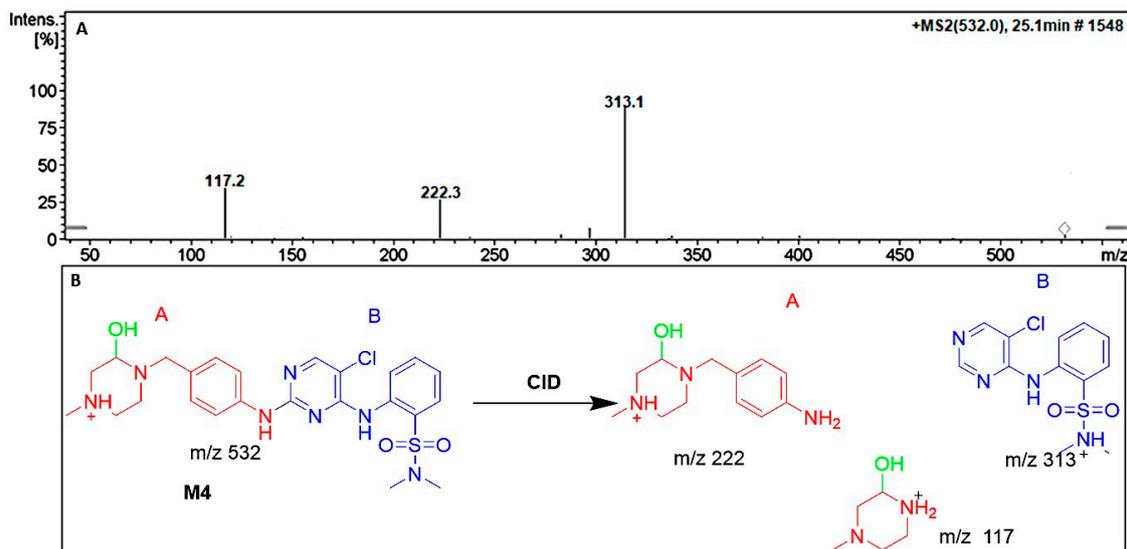
**Figure S1.** Positive ion MS/MS mass spectrum of M2 at 23.1 min (A). Proposed structural formulas of M2 and corresponding MS/MS fragments (B).

##### 1.1.2. Identification of the DMB M3 metabolite



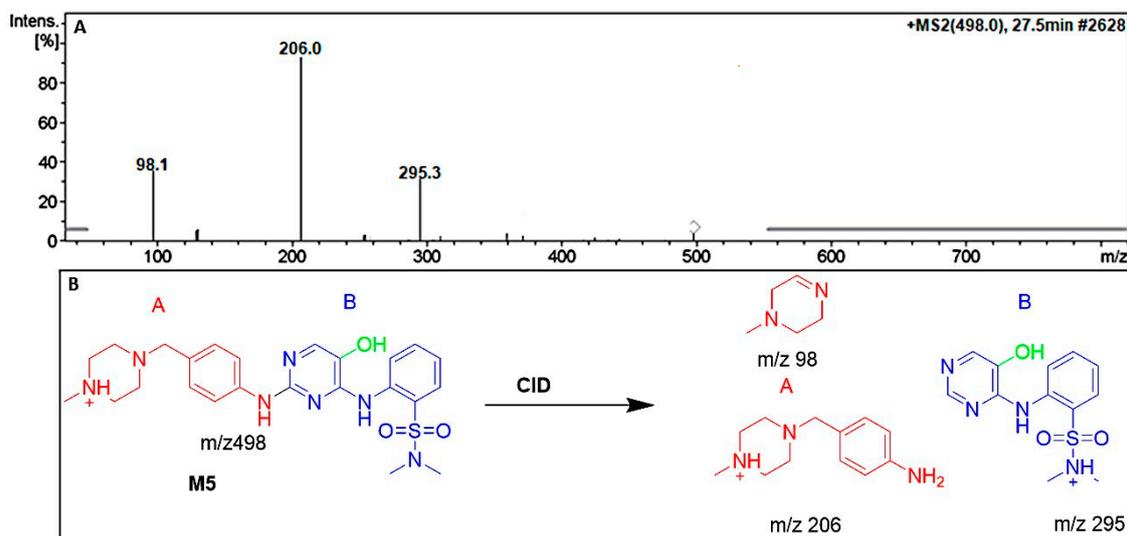
**Figure S2.** Positive ion MS/MS mass spectrum of M3 at 24.4 min (A). Proposed structural formulas of M3 and corresponding MS/MS fragments (B).

### 1.1.3. Identification of the DMB M4 metabolite



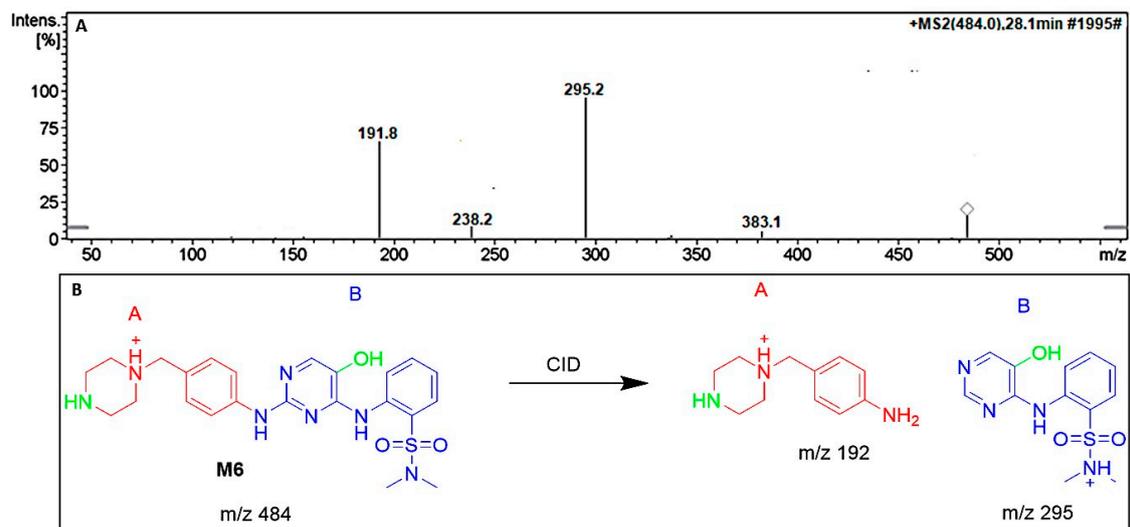
**Figure S3.** Positive ion MS/MS mass spectrum of M4 (A). Proposed structural formulas of M4 and corresponding MS/MS fragments (B).

### 1.1.4. Identification of the DMB M5 metabolite



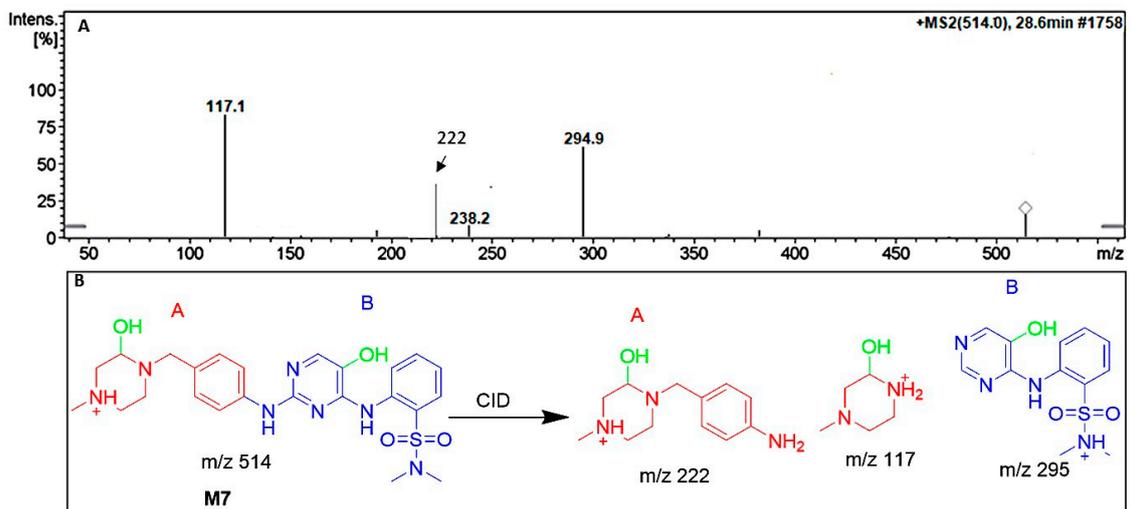
**Figure S4.** Positive ion MS/MS mass spectrum of M5 at 27.5 min (A). Proposed structural formulas of M5 and corresponding MS/MS fragments (B).

### 1.1.5. Identification of the DMB M6 metabolite



**Figure S5.** Positive ion MS/MS mass spectrum of M6 at 28.1 min (A). Proposed structural formulas of M6 and corresponding MS/MS fragments (B).

### 1.1.6. Identification of the M7 DMB metabolite



**Figure S6.** Positive ion MS/MS mass spectrum of M7 at 28.6 min. (A). Proposed structural formulas of M7 and its corresponding MS/MS fragments (B)