Supplementary file

Quantification of olaparib in the human liver microsomes using ultra-fast UPLC-MS/MS quantitative approach: In-vitro and in-silico metabolic stability assessment

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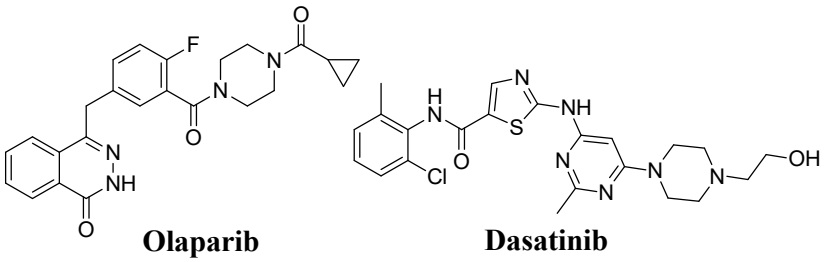
Figures:



Olaparib Molecular Weight: 434.46

Dasatinib Molecular Weight: 488.01

Fig. S1. The chemical structure of olaparib and dasatinib (IS).

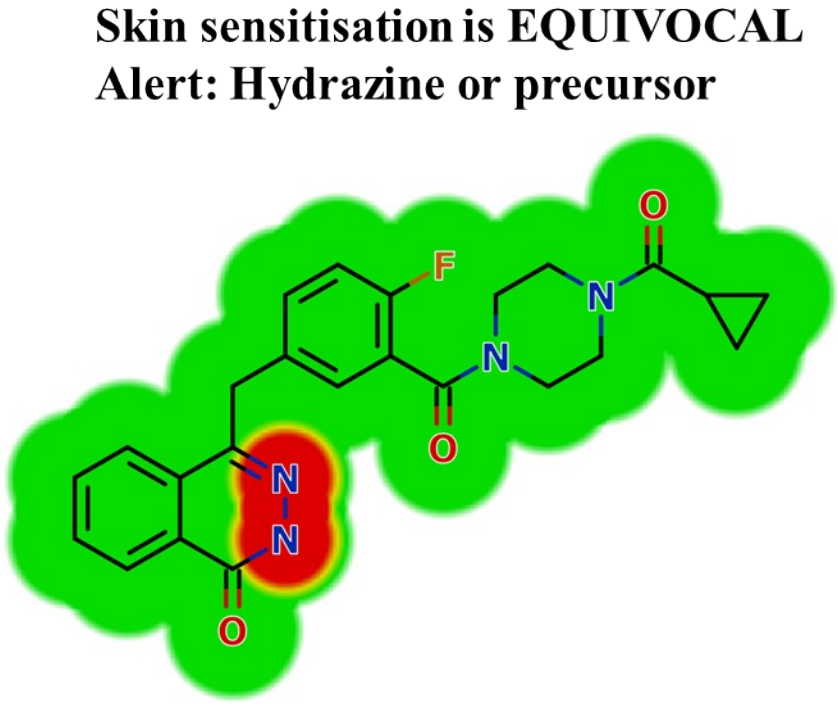


Fig. 2. The structural in-silico toxic alarms of OLA were tested utilizing the DEREK software that painted in red color.

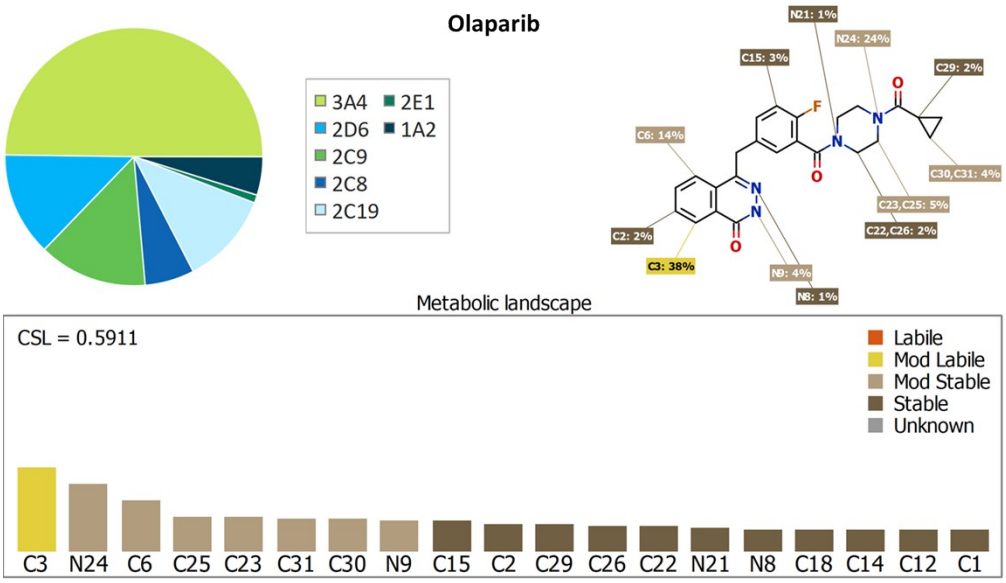


Fig. S3. The metabolic lability data revealed CSL mark at 0.5911 that designates that low susceptibility of OLA to metabolism (more stable). The outcomes were estimated applying the WhichP450 module.

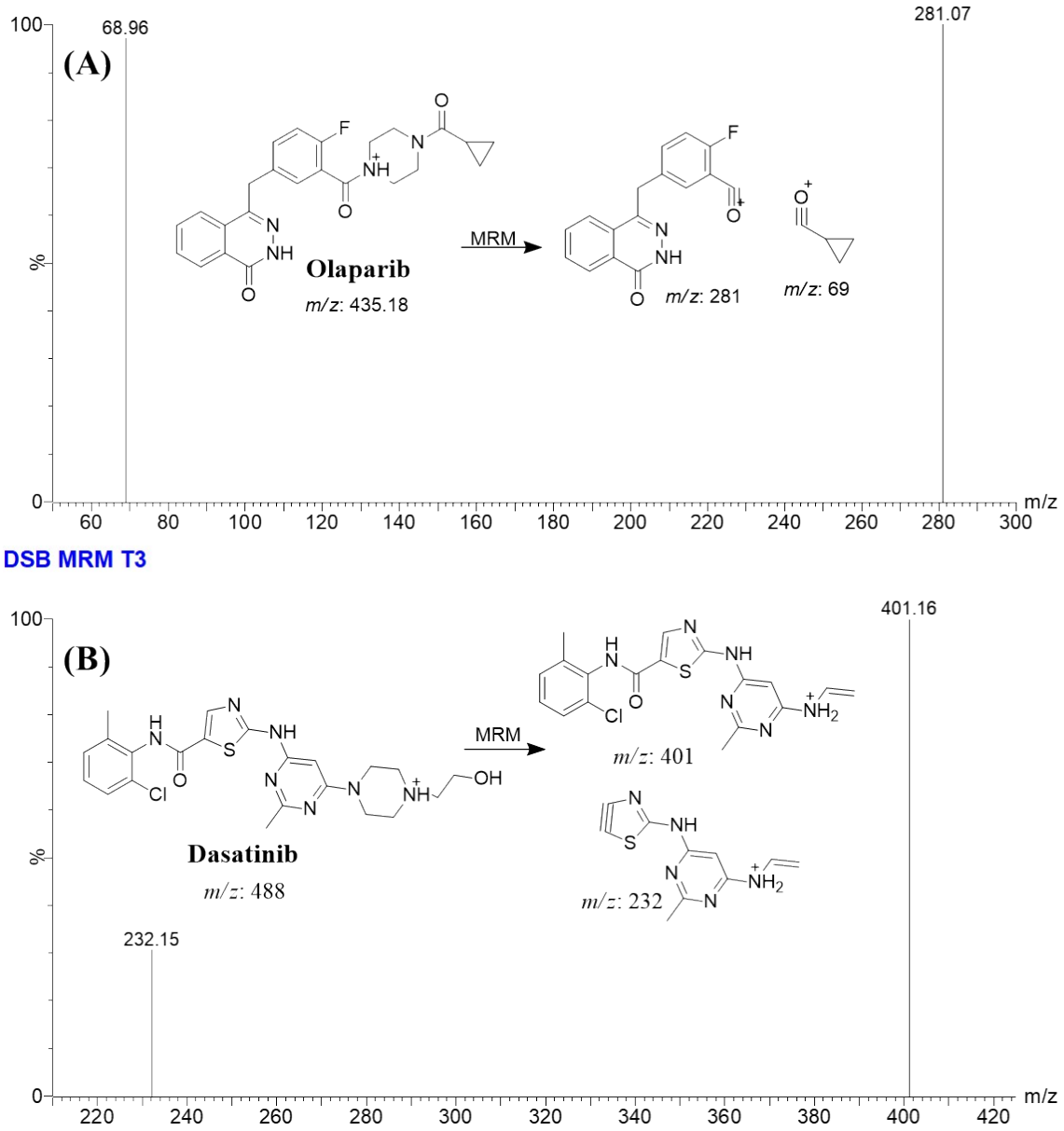


Fig. S4. MS spectra of OLA (**A**) and DSB as IS (**B**) attained applying MRM mass detector mode. The proposed dissociation behaviors are displayed.

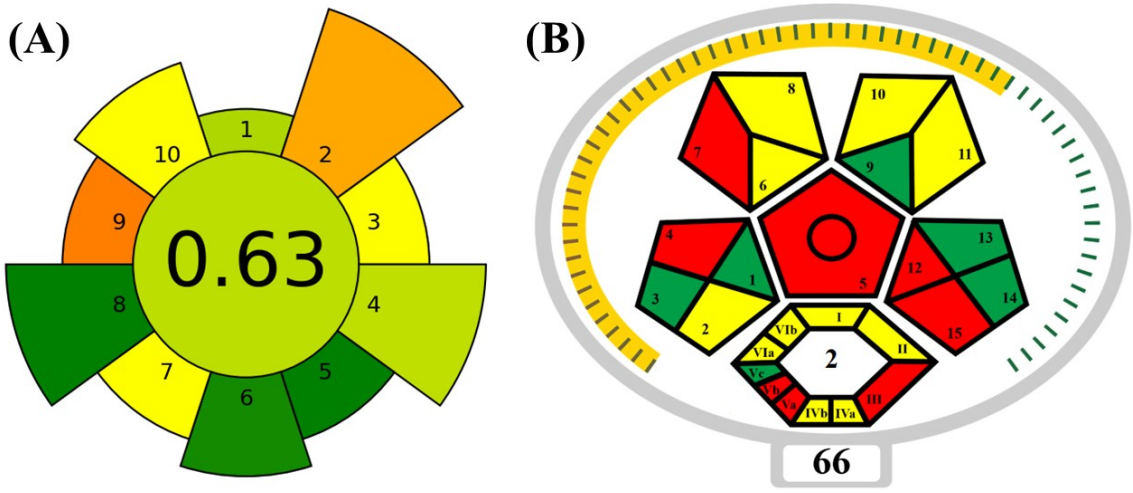


Fig. S5. The greenness evaluation results for the established technique (UPLC-MS/MS), yielding a score of 0.63 with the AGREEprep tool (**A**) and a value of 66.0 with the ComplexMoGAPI freely online software (**B**), suggesting a good greenness degree.

Tables:

Table S1. The ten features of the AGREEprep tool for the UPLC-MS/MS method.

Criterion		Mark	Weight
1	**Placement of sample preparation** Placement of sample preparation: On-line/In situ.	0.66	1
2	**Dangerous substances** Volume [mL] or mass [g] of problematic materials: 0.9.	0.33	5
3	**Resource sustainability, recycling, and reuse of resources** Materials are not environmentally friendly nor reusable, yet they are utilized multiple times.	0.5	2
4	**Waste** Volume [mL] or mass [g] of waste: 0.9.	0.63	4
5	**Economies of scale of the sample** One should select automated and miniaturized approaches.	1.0	2
6	**Sample yield** Hourly sample output: 60 units.	0.96	3
7	**Integration and automating** Number of sample preparation steps: two or fewer; level of automation: Semi-automated systems.	0.5	2
8	**Energy utilization** Estimated consumption of energy per analysis [W]: 10.	1.0	4
9	**Configuration for analysis following sample preparation** Liquid chromatography, gas chromatography with quadrupole detection, etc.	0.25	2
10	**Safety of the operator** Number of unique dangers: No hazards or absence of exposure.	0.5	3