Supplementary Information

In silico Investigation of Oxypeucedanin Hydrate from Traditional Chinese Medicine as a Potential PSAT1 Inhibitor in Early-Stage Ovarian Cancer

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Pharmacokinetics and interaction fingerprints studies

Table S1. The pharmacokinetic properties of PMP, OPH, and GGC (isomer 1), compared against QikProp standard values, highlighting their drug-like characteristics

Descriptor	Standard	GGC (Isomer 1)	OPH	PMP
No. stars	0-5	1	0	1
No. amine	0-1	1	0	1
No. amidine	0	0	0	0
No. acid	0-1	2	0	2
No. amide	0-1	1	0	0
No. rotor	0-15	9	6	8
No. rtvFG	0-2	1	1	1
CNS	−2 (inactive), +2 (active)	−2	−1	−2
mol_MW	130.0-725.0	250.269	304.299	248.175
Dipole	1.0-12.5	2.165	8.291	11.483
SASA	300.01000.0	481.946	505.800	430.266
FOSA	0.0-750.0	130.723	158.267	152.739
FISA	7.0-330.0	278.354	139.755	217.911
PISA	0.0-450.0	0	207.779	56.088
WPSA	0.0-175.0	72.869	0	3.528
Volume	500.0-2000.0	787.661	896.638	721.818
donorHB	0.0-6.0	4.25	2	5
accptHB	2.0-20.0	6.250	6.200	7.750
dip^2/V	0.0-0.13	0.006	0.077	0.183
ACxDN^.5/SA	0.0-0.05	0.027	0.017	0.040
Glob	0.75-0.95	0.856	0.889	0.904
QPpolrz	13.0-70.0	19.589	27.861	18.132
QPlogPC16	4.0-18.0	8.853	9.588	8.166
QPlogPoct	8.0-35.0	16.231	16.302	19.638

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Table S1. The pharmacokinetic properties of PMP, OPH, and GGC (Isomer 1), compared against QikProp standard values, highlighting their drug-like characteristics (cont.)

Descriptor	Standard	GGC (Isomer 1)	OPH	PMP
QPlogPw	4.0-45.0	15.318	11.013	15.811
Jm	–	0.001	1.540	0.019
QPlogPo/w	−2.0-6.5	–2.342	1.571	–2.281
QPlogS	−6.5-0.5	–0.391	–2.509	–0.489
CIQPlogS	−6.5-0.5	–0.187	–3.734	–0.743
QPlogHERG	concern below −5	0.399	–4.318	–0.457
QPPCaco	< 25 poor, > 500 great	0.215	468.389	1.360
QPlogBB	−3.0-1.2	–1.935	–0.977	–1.287
QPPMDCK	< 25 poor, > 500 great	0.425	217.929	0.738
QPlogKp	−8.0-−1.0	–7.848	–2.787	–6.633
IP / eV	7.9-10.5	9.772	8.950	8.791
EA / eV	−0.9-1.7	0.317	0.916	0.135
No. metab	1-8	6	4	7
QPlogKhsa	−1.5-1.5	–1.419	–0.31	–1.198
Human oral absorption	–	1	3	1
Percent human oral Absorption	> 80% is high, < 25% is poor	1.272	83.941	15.977
SAfluorine	0.0-100.0	0	0	0
SAamideO	0.0-35.0	28.707	0	0
PSA	7.0-200.0	158.146	93.395	120.027
No. NandO	2-15	7	6	7
RuleOfFive	maximum is 4	0	0	0
No. ringatoms	–	0	13	6
No. in34	–	0	0	0
No. in56	–	0	13	6
No. noncon	–	0	0	0
No. nonHatm	–	16	22	16
RuleOfThree	maximum is 3	1	0	2

#stars, number of properties outside the recommended range for drug-likeness; No. amine, number of amine groups; No. amide, number of amide groups; No. acid, number of acidic groups; No. rotor, number of rotatable bonds; No. rtvFG, number of reactive functional groups; CNS, central nervous system activity prediction; mol_MW, molecular weight; Dipole, dipole moment; SASA, solvent-accessible surface area; FOSA, hydrophobic component of SASA; FISA, hydrophilic component of SASA; PISA, π-component of SASA; WPSA, weakly polar component of SASA; Volume, molecular volume; donorHB, number of hydrogen bond donors; acceptHB, number of hydrogen bond acceptors; dip^2/V, dipole moment squared divided by molecular volume; $ACxDN^2.5/SA$, amphiphilic moment descriptor; Glob, molecular globularity; QPpolrz, predicted polarizability; QPlogPC16, predicted hexadecane/gas partition coefficient; QPlogPct, predicted protein-cyclohexane partition coefficient; QPlogPw, predicted water/gas partition coefficient; QPlogPo/w, predicted octanol/water partition coefficient; QPlogS, predicted aqueous solubility; CIQPlogS, conformation-independent predicted solubility; QPlogHERG, predicted HERG K^+ channel inhibition; QPpCaco, predicted Caco-2 cell permeability; QPlogBB, predicted brain/blood partition coefficient; QPPMDCK, predicted MDCK cell permeability; QPlogKp, predicted skin permeability; IP, ionization potential; EA, electron affinity; No. metab, number of likely metabolic reactions; Human oral absorption, qualitative prediction of oral absorption; Percent human oral absorption, quantitative prediction of oral absorption; SAfluorine, fluorine-containing surface area; SAamideO, amide oxygen surface area; PSA, polar surface area; No. NandO, number of nitrogen and oxygen atoms; RuleOfFive, Lipinski's rule-of-five compliance; No. ringatoms, number of atoms in ring systems; No. in34, number of atoms in 3- or 4-membered rings; No. in56, number of atoms in 5- or 6-membered rings; No. noncon, number of non-conjugated ring atoms; No. nonHatm, number of non-hydrogen atoms; RuleOfThree, compliance with fragment-based rule-of-three.

Molecular mechanics and MM/GBSA studies

Table S2. Showing various energies computed during the MM/GBSA computations

Metric	PMP	GGC (Isomer 1)	OPH
Number of structures	1001	1001	1001
dG Average / (kcal mol^{-1})	–48.079	–40.732	–63.877
dG standard deviation	3.282	3.428	5.198
dG Range / (kcal mol^{-1})	–56.547 to –37.377	–51.206 to –28.331	–81.246 to -41.247
dG(NS) average / (kcal mol^{-1})	–51.189	–44.493	–67.724
dG(NS) standard deviation	3.094	3.706	5.429
dG(NS) range / (kcal mol^{-1})	–59.882 to –40.193	–56.054 to –29.499	–84.904 to –43.113
dG(Complex) average / (kcal mol^{-1})	–21297.068	–21235.733	–21248.135
dG(Complex) standard Deviation	88.471	81.193	94.629
dG(Complex) range / (kcal mol^{-1})	–21538.852 to –20955.712	–21475.287 to –20889.007	–21534.511 to –20978.727
Number of frames processed	1001	1001	1001
Number of output structures	1001	1001	1001

PMP: pyridoxamine phosphate; GGC: gamma-glutamyl cysteine; OPH: oxypeucedanin hydrate; dG: binding free energy; NS: non solvated.