Supplementary file 1

Boutalaka et al., ***BioImpacts.*** 2026;16:31007
doi: 10.34172/bi.31007
https://bi.tbzmed.ac.ir/

Moroccan virgin olive oil triterpenes: HPLC-DAD-ELSD profiling and computational investigation of anti-diabetic potential

Meryem Boutalaka[1], Noureddine Ouazzani[2], Mohamed Ouabane[1], Panagiotis Stathopoulos[3], Abdelkrim Guendouzi[4], Hamid Maghat[1], Alexios-Leandros Skaltsounis[3], Tahar Lakhlifi[1], Mohammed Bouachrine[1*]

[1]Department of Chemistry, Molecular Chemistry and Natural Substances Laboratory, Faculty of Science, University of Moulay Ismail, Meknes, Morocco

[2]Agro-pôle Olivier, National School of Agriculture of Meknes, BP S/40 Meknes, Morocco

[3]Department of Pharmacognosy and Natural Products Chemistry, Faculty of Pharmacy, University of Athens, 15771 Athens, Greece

[4]Department of Chemistry, Laboratory of Chemistry, Synthesis, Properties and Applications, Faculty of Science, University of Saida, Saida, Algeria

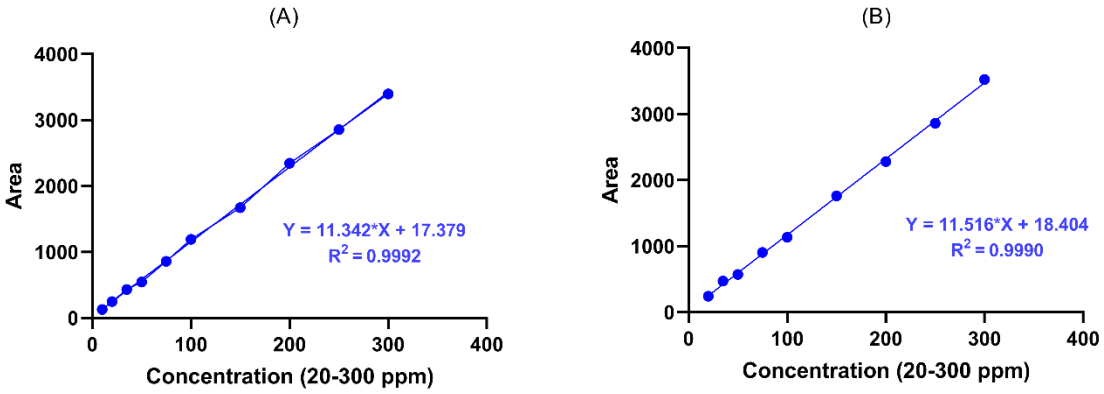

Fig. S1. Calibration Curves of Maslinic Acid (A) and Oleanolic Acid (B)

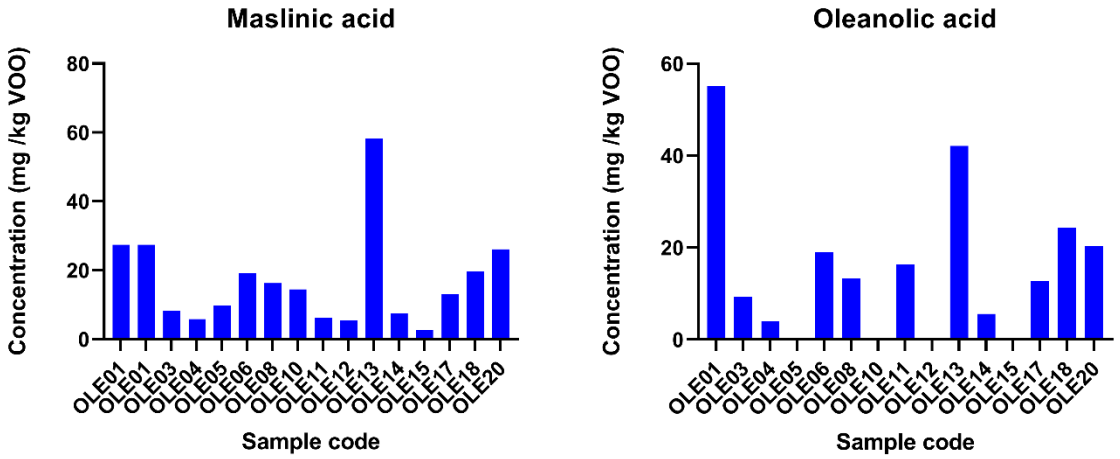

Fig. S2. Concentrations of Maslinic Acid and Oleanolic Acid in Moroccan Virgin Olive Oil Samples (mg/kg VOO)

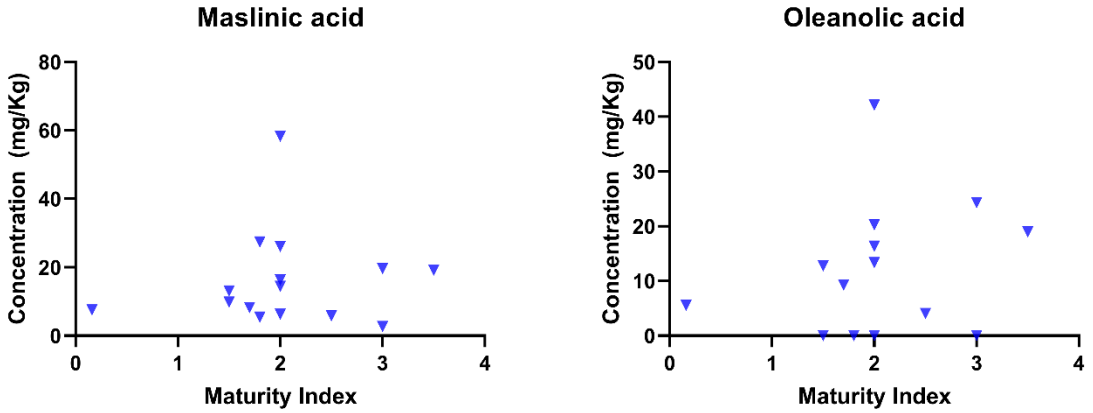

Fig. S3. Variation in Maslinic Acid and Oleanolic Acid Concentrations with Maturity Index in Virgin Olive Oil

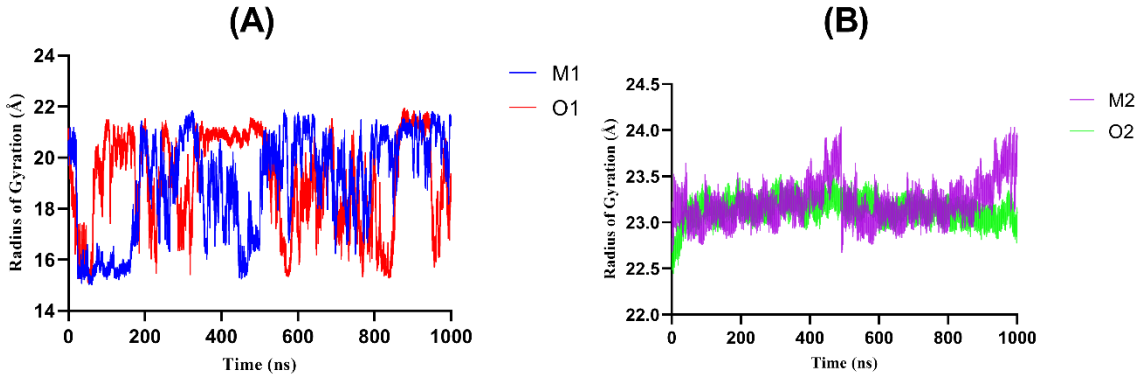

Fig. S4. Radius of Gyration (Rg) vs. Time for Protein–Ligand Complexes M1, M2, O1, and O2 with α-Amylase (A) and α-Glucosidase (B)

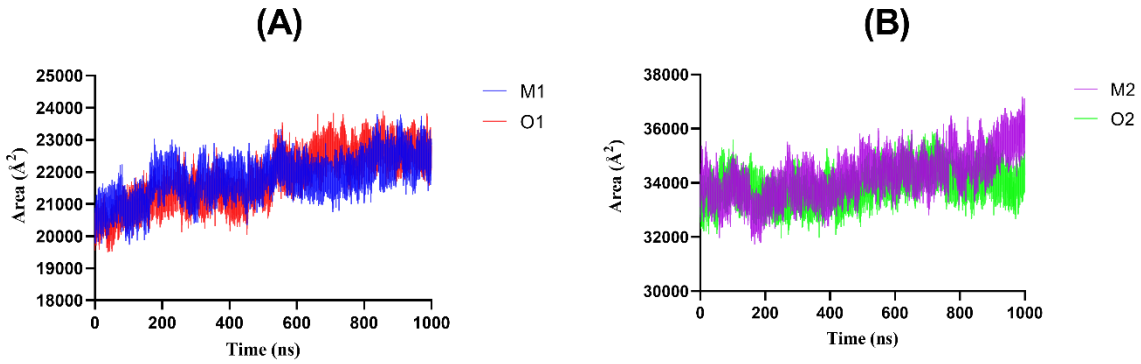

Fig. S5. Solvent Accessible Surface Area (SASA) vs. Time for Protein–Ligand Complexes M1, M2, O1, and O2 with α-Amylase (A) and α-Glucosidase (B)

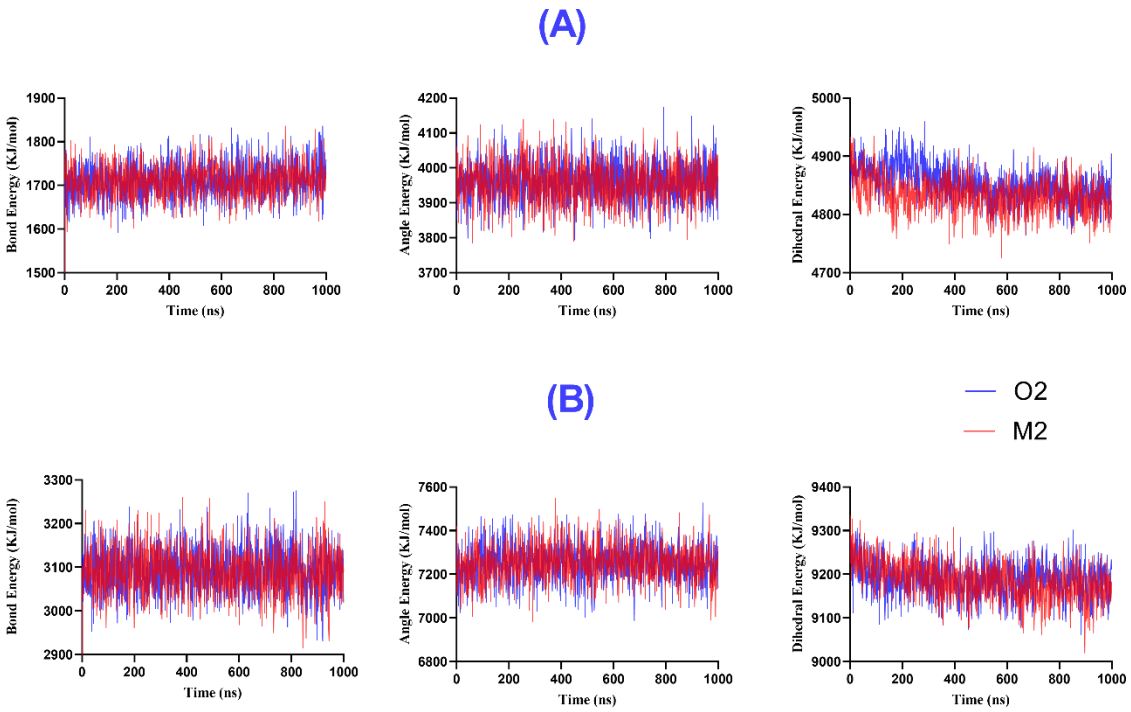

Fig. S6. Bonded Energy Components for M1, O1, M2, and O2 Complexes: (A) α-Amylase and (B) α-Glucosidase

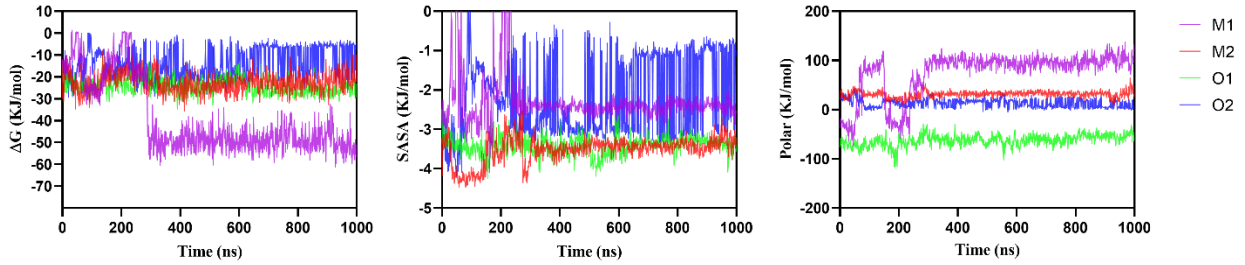

Fig. S7. Free Energy and Solvation Components (ΔG Binding, SASA, and Polar Solvation) vs. Time for Maslinic Acid and Oleanolic Acid Complexes

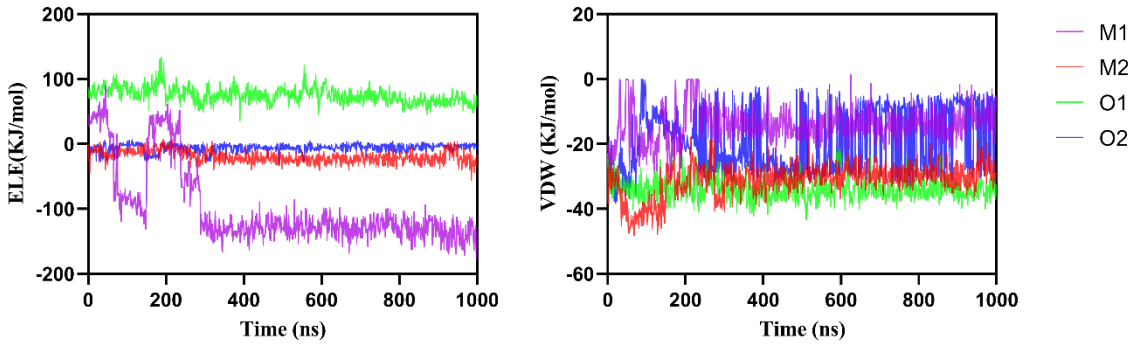

Fig. S8. Non-Bonded Energy Components (Van der Waals and Electrostatic Energy) vs. Time for Maslinic Acid and Oleanolic Acid Complexes

Table S1. Mean values of the concentration of the maslinic acid. Results are expressed in mg/Kg VOO

Sample code	HPLC-DAD-ELSD (UV 210nm)			
	7.7min Maslinic acid (y = 11,342x + 17,379)			
	RT (min)	AREA	CC (ppm)	mg /kg VOO
OLE01	7.51	314.7	26.21	27.46
OLE03	7.51	152.77	11.94	8.21
OLE04	7.51	99.33	7.23	5.85
OLE05	7.52	122.55	9.27	9.81
OLE06	7.52	188.02	15.04	19.14
OLE08	7.52	155.35	12.16	16.3
OLE10	7.53	161.51	12.71	14.46
OLE11	7.52	128.18	9.77	6.33
OLE12	7.53	66.78	4.36	5.43
OLE13	7.57	740.67	63.77	58.3
OLE14	7.53	101.85	7.45	7.54
OLE15	7.53	44.03	2.35	2.71
OLE17	7.53	183.91	14.68	13.1
OLE18	7.52	173.96	13.81	19.6
OLE20	7.52	444.31	37.64	26.07

***Rt**: Retention Time, **CC**: Concentration, **ppm**: parts per million.

Table S2. Mean values of the concentration of the Oleanolic acid. Results are expressed in mg/Kg VOO

Sample code	HPLC-DAD-ELSD (UV 210nm)			
	12.3min Oleanolic acid (y = 11,516x + 18,404)			
	RT (min)	AREA	CC (ppm)	mg /kg VOO
OLE01	11.41	623.72	52.56	55.06

OLE03	11.41	173.56	13.47	9.26
OLE04	11.4	76.47	5.04	4.08
OLE05	< LOD	< LOD	< LOD	< LOD
OLE06	11.42	190.3	14.93	18.99
OLE08	11.42	133.06	9.96	13.34
OLE10	< LOD	< LOD	< LOD	< LOD
OLE11	11.41	309.32	25.26	16.36
OLE12	< LOD	< LOD	< LOD	< LOD
OLE13	11.4	549.38	46.11	42.15
OLE14	11.42	81.88	5.51	5.58
OLE15	< LOD	< LOD	< LOD	< LOD
OLE17	11.41	183.4	14.33	12.79
OLE18	11.42	215.45	17.11	24.30
OLE20	11.41	355.22	29.25	20.25

* **LOD**: Limit of Detection, **Rt**: Retention Time, **CC**: Concentration, **ppm**: parts per million.

Table S3. Molecular Properties and Drug-Likeness Prediction of Maslinic Acid, Oleanolic Acid, and the Reference Drug Acarbose Based on Lipinski and Veber Rules

Compound	MW (<500Da)	LogP (<5)	HBD (<5)	HBA (<10)	TPSA (<140 Å^2)	SA	Lipinski	Veber
Maslinic Acid	472.70	3.38	3	4	77.76	6.22	YES	YES
Oleanolic Acid	456.70	3.94	2	3	57.53	6.08	YES	YES
Acarbose	645.60	0.17	14	19	329.01	7.25	No	No

* **MW**: Molecular Weight, **HBD**: number of hydrogen bonds donors, **LogP**: logarithm of partition coefficient of molecule between water and n-octanol, **HBA**: number of hydrogen bonds acceptors, **SA**: Synthetic Accessibility, **TPSA**: Topological Polar Surface Area.

Table S4. Docking Interactions of Maslinic Acid (**M1**, **M2**), Oleanolic Acid (**O1**, **O2**) and the reference drug Acarbose (**A1**, **A2**) with α-Amylase and α-Glucosidase Receptors

Ligand	Recepteur	Affinity (kJ/mol)	Hydrogen Bond	Hydrophobic Interaction
M1	**α-Amylase**	-41.42	Asp-197, Ser-163	Trp-59, Ile-51, Val-107, Leu-162
O1		-38.91	Asp-300, Glu-233	Trp-59, Tyr-62, His-299, Trp-58
A1		-27.61	Gly-306, Ser-163, Asp-193, Glu-233	Ile-235, His-305
M2	**α-Glucosidase**	-35.56	Glu-1284, Phe-1289, Glu-1400	Pro-1293, Pro-1329, Pro-1405
O2		-32.22	Asn-1404	Leu-1291, Ala-1296, Arg-1410, Pro-1329, Pro-1405
A2		-30.54	Gln-1254, Ser-1292, Asp-1281, Gln-1286, Asp-1357, Arg-1377	ILE-1587, Tyr-1251

Table S5. Bonded Energy Components (kJ/mol) for Complex Stability of Maslinic and Oleanolic Acid Complexes with α-Amylase and α-Glucosidase

Complex	Bond energy ± SD	Angle energy ± SD	Dihedral energy ± SD
M1	1708 ± 64.27	3958 ± 58.51	4833 ± 30.70
O1	1711 ± 66.22	3961 ± 57.44	4853 ± 31.89
M2	3088 ± 108.70	7250 ± 81.30	9185 ± 45.00
O2	3088 ± 108.70	7251 ± 82.90	9189 ± 41.29

Table S6. Validation of Calculated Binding Affinity: Correlation Between $K_i^{MM\text{-}PBSA}$ and Experimental IC_{50} Values

Complex	Ligand	Receptor	$K_i^{MM\text{-}PBSA}$ (μM)	IC_{50} (μM)
O1	Oleanolic Acid	α-Amylase	62.55	81.3
M1	Maslinic Acid		0.16	67
O2	Oleanolic Acid	α-Glucosidase	3686.47	33.5
M2	Maslinic Acid		114.42	34.5