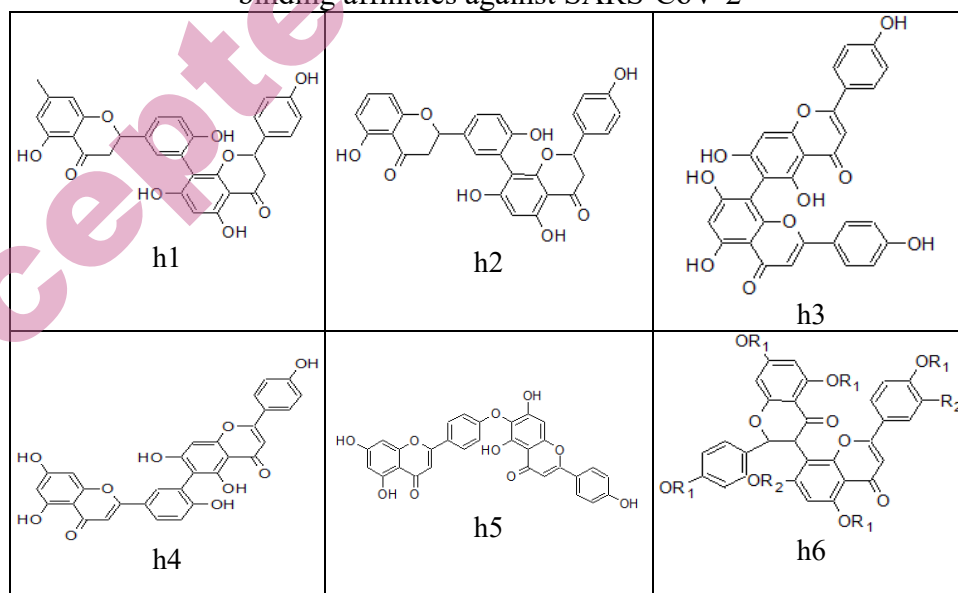


SUPPLEMENTARY MATERIAL TO
Exploring the efficacy of natural compounds against SARS-CoV-2: A synergistic approach integrating molecular docking and dynamic simulation

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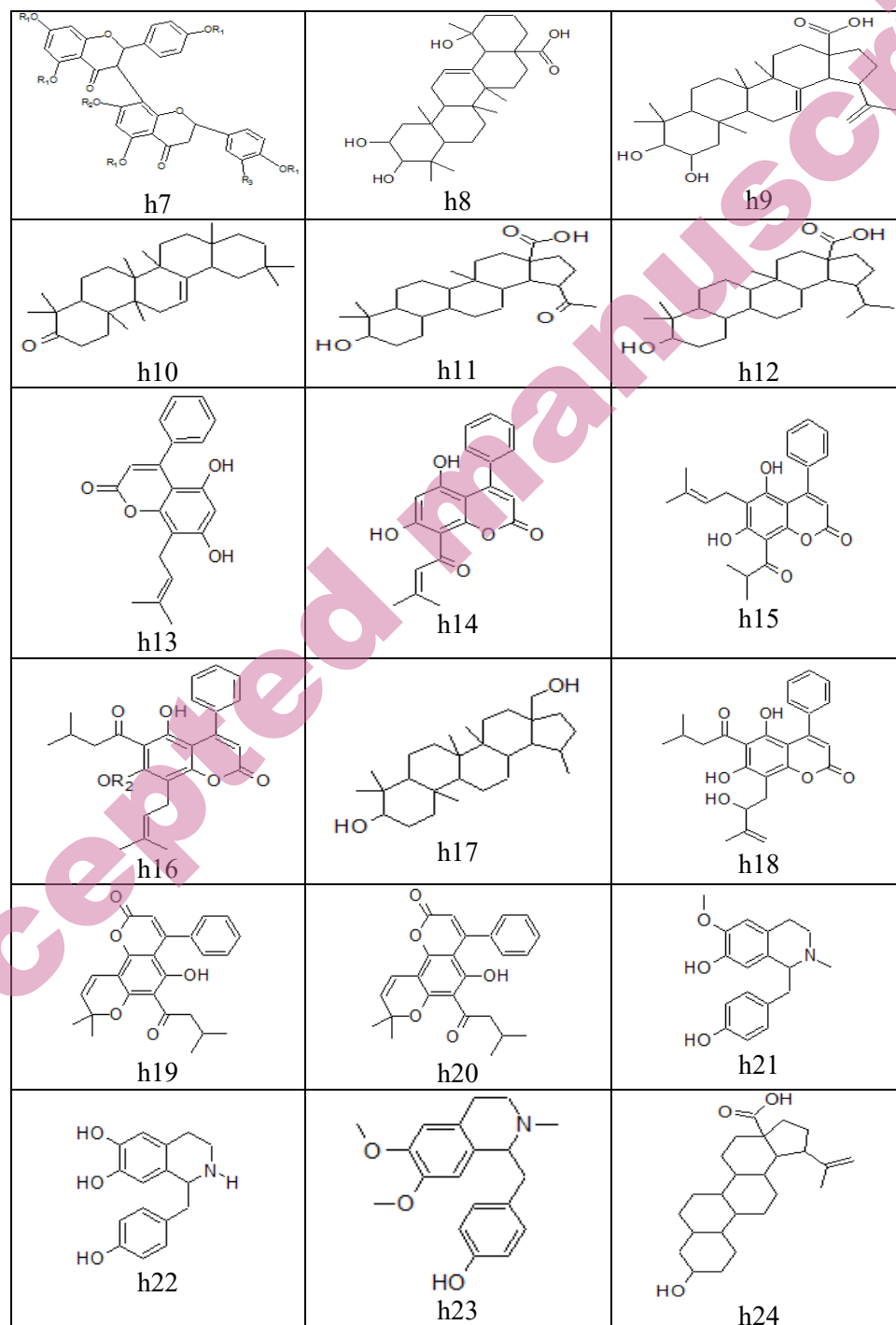
¹University of Sciences and Technologies of Oran (USTO), Laboratory of Process Engineering and Environment, BP 1503 Oran 31000, Algeria, ²Biskra University, LMCE Laboratory, Department of Matter Sciences, Biskra, Algeria, ³Hassan II University of Casablanca, Laboratory of Analytical and Molecular Chemistry, Casablanca, Morocco, and ⁴University of Lucknow, Department of Physics, 226007 Lucknow, India.

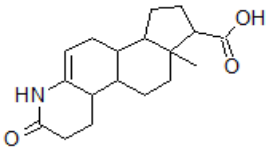
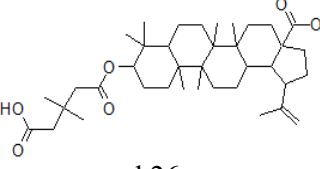
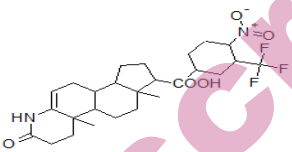
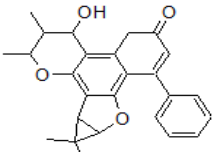
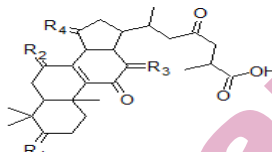
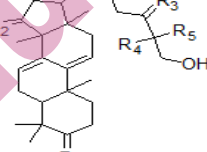
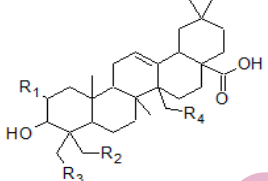
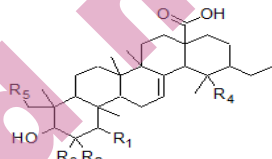
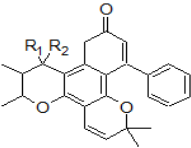
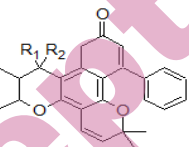
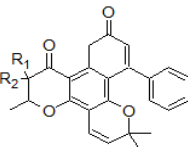
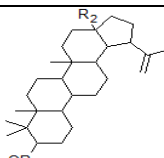
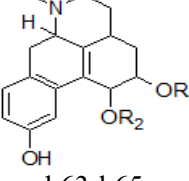
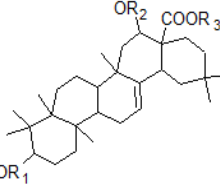
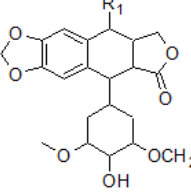
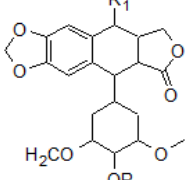
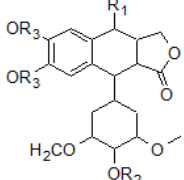
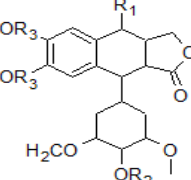
Figure S1: Antiviral natural products h1–h18 with significant binding affinities against SARS-CoV-2



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 h25	 h26	 h27
 h28	 h29-32	 h33-36
 h37-h40	 h41-h47	 h48-h50
 h51-h53	 h54-h55	 h56-h62
 h63-h65	 h66-h70	 h71-h77
 h78-h80	 h81-h87	 h88-h94

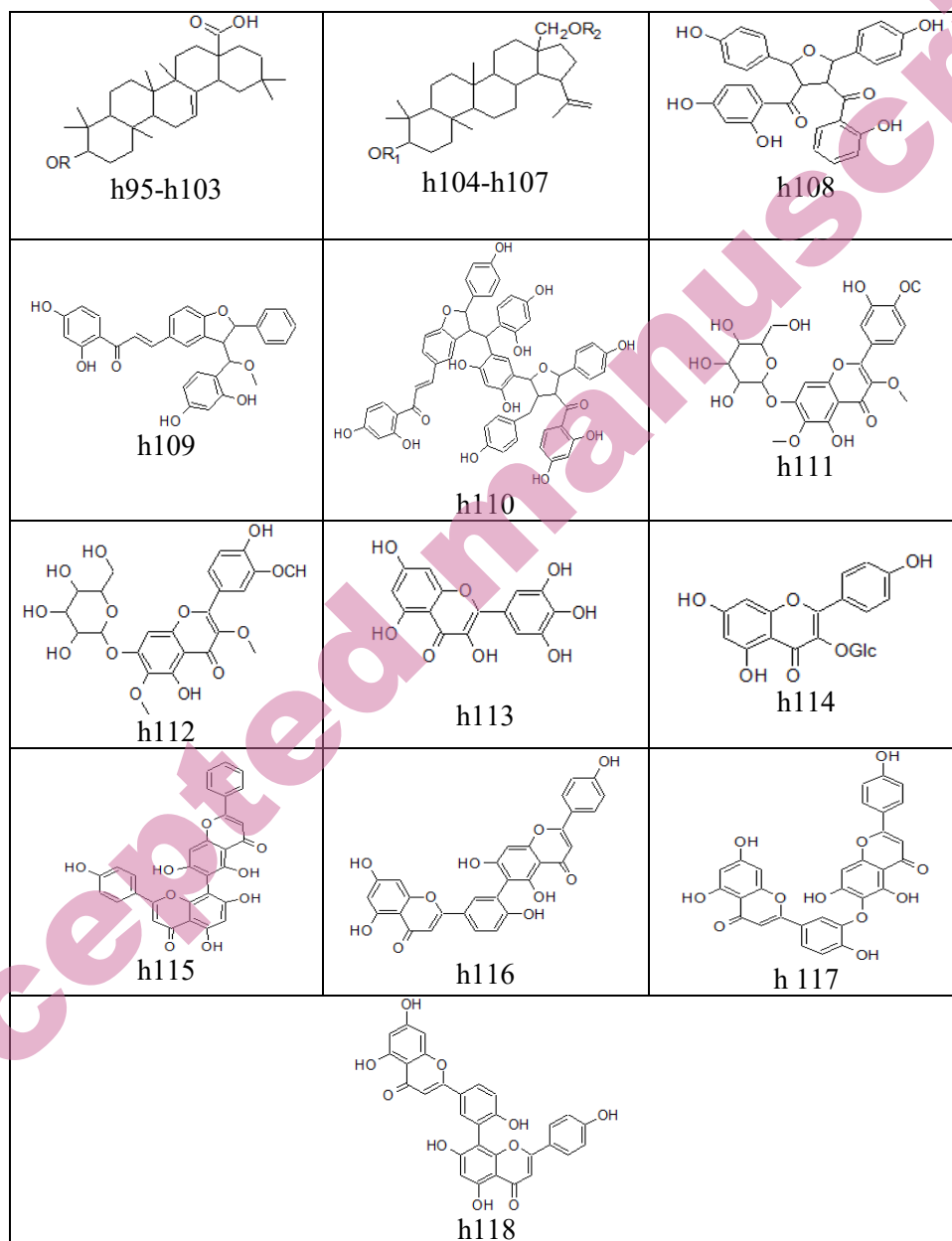
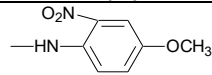
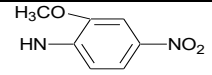
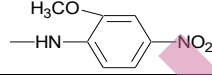
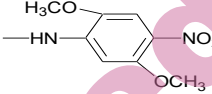
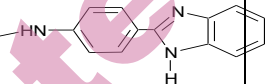
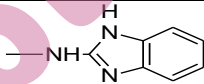
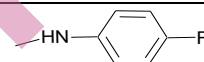
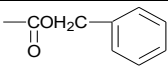
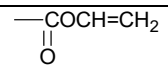
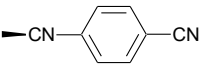
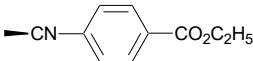
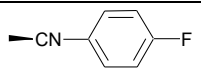
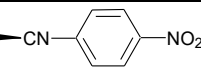
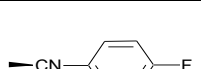
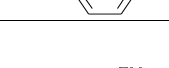
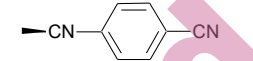
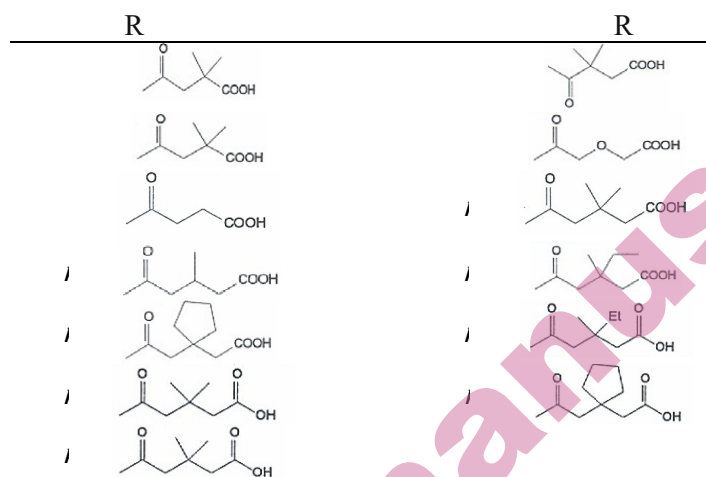


Table S1 : Functional group

	R1	R2	R3	R4	R5
h29		O			-
h30				O	-
h31	O	O		O	-
h32			O	O	-
h33		H ₂		OH	CH ₃
h34	O		CH ₃	CH ₃	CH ₂ O H
h35	O	H ₂	CH ₃	CH ₃	CH ₂ O H
h36	O	H ₂		OH	CH ₃
h37	H	H	H	H	-
h38	OH	H	OH	H	-
h39	OH	OH	H	H	-
h40	H	H	H	OH	-
h41	H	H	H	OH	H
h42	H	H	H	H	H
h43	H	OH	H	H	H
h44	H	OH	H	H	OH
h45	H	OH	OH	OH	H
h46	H	OH	OH	OH	H
h47	OH	OH	OH	OH	H
h48,h51	H	OH	-	-	-
h49,h52	OH	H	-	-	-
h50,h53	H	OAc	-	-	-
h54	Me	H	-	-	-
h55	H	Me	-	-	-
h56	H	COOH	-	-	-
h57	H	CH ₂ OH	-	-	-
h58	H	COOCH ₂ COOCH ₃	-	-	-
h59	Ac	COOH	-	-	-

h60	<chem>COC6H5</chem>	<chem>COOH</chem>	-	-	-
h61	<chem>COCH=CHCH3</chem>	<chem>COOH</chem>	-	-	-
h62	<chem>COCH2CH2COOH</chem>	<chem>COOH</chem>	-	-	-
h63	Me	OH	-	-	-
h64	Me	Me	-	-	-
h65	H	Me	-	-	-
h66	H	H	H	-	-
h67	H	H	Me	-	-
h68	Ac	H	Me	-	-
h69	Ac	Ac	H	-	-
h70	Butyryl	H	Me	-	-
h71		-	-	-	-
h72		-	-	-	-
h73		-	-	-	-
h74		-	-	-	-
h75		-	-	-	-
h76		-	-	-	-
h77		-	-	-	-
h78		-	-	-	-
h79			-	-	-
h80			-	-	-
h81		Me	H	-	-
h82		Me	Me	-	-

h83		H	Me	-	-
h84		H	Me	-	-
h85		Me	Me	-	-
h86		H	Me	-	-
h87		H	Me	-	-
h88		Me	H	-	-
h89		Me	Me	-	-
h90		H	Me	-	-
h91		H	Me	-	-
h92		Me	Me	-	-
h93		H	Me	-	-
h94		H	Me	-	-

**Table S2:** Results 6LU7 enzyme SCORE with studied ligands.

N°.Comp.	S-Score (kJ/mol)	N°.Comp.	S-Score (kJ/mol)	N°.Comp.	S-Score (kJ/mol)
h1	-30.270	h47	-26.376	h91	-32.782
h2	-32.405	h48	-18.045	h92	-30.940
h3	-33.996	h49	-27.214	h93	-32.489
h4	-29.433	h50	-27.214	h94	-32.405
h5	-30.144	h51	-28.051	h95	-23.906
h6	-32.112	h52	-8.206	h96	-24.409
h7	-34.708	h53	-26.879	h97	-25.665
h8	-22.315	h54	-28.595	h98	-25.623
h9	-23.655	h55	-28.553	h99	-10.718
h10	-22.064	h56	-22.608	h100	-25.790
h11	-14.528	h57	-23.362	h101	-24.785
h12	-23.822	h58	-26.000	h102	-25.790
h13	-27.130	h59	-25.958	h103	-8.499
h14	-25.539	h60	-25.330	h104	-26.586
h15	-30.144	h61	-23.362	h105	-25.330
h16	-31.024	h62	-22.776	h106	-27.256
h17	-22.818	h63	-25.455	h107	-26.628
h18	-30.479	h64	-25.413	h108	-31.903
h19	-29.977	h65	-25.120	h109	-33.075
h20	-30.103	h66	-21.101	h110	-40.360
h21	-26.753	h67	-20.682	h111	-30.144
h22	-25.706	h68	-23.404	h112	-28.595
h23	-25.204	h69	-25.790	h113	-23.069

h24	-22.399	h70	-26.376	h114	-30.103
h25	- 26.041	h71	-31.149	h115	-33.578
h26	-17.291	h72	-29.768	h116	-31.066
h27	-15.742	h73	-32.489	h117	-32.238
h28	-28.888	h74	-31.610	h118	-30.479
h29	-26.000	h75	-31.526	Réf (N3)	-32.615
h30	-25.916	h76	-30.061		
h31	-29.140	h77	-29.851		
h32	-6.070	h78	-30.144		
h33	-26.669	h79	-30.270		
h34	-24.618	h80	-30.270		
h35	-24.367	h81	-26.376		
h36	-26.795	h82	-27.758		
h37	-26.795	h83	-27.758		
h38	-24.450	h84	-35.336		
h39	-23.822	h85	-32.615		
h40	-22.776	h86	-31.735		
h41	-24.576	h87	-32.154		
h42	-23.278	h88	-25.874		
h43	-25.037	h89	-28.679		
h44	-25.413	h90	-33.452		