Supplementary tables

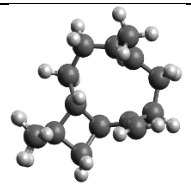
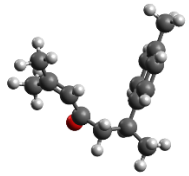
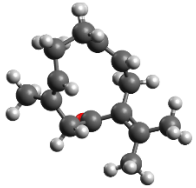
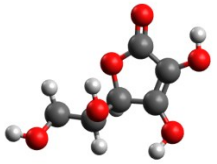
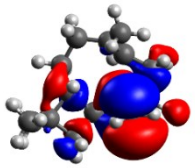
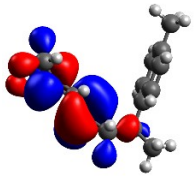
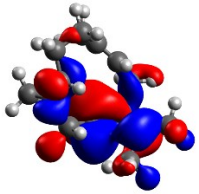
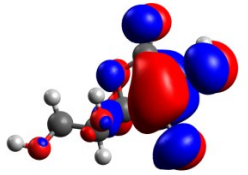
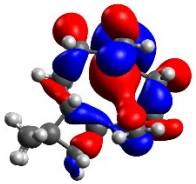
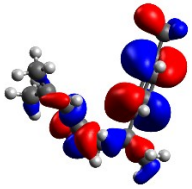
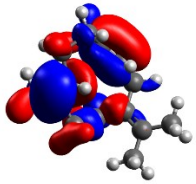
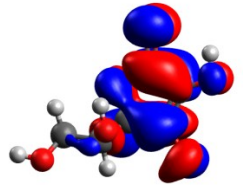
Table S1. ADME/Toxicity predicted profile of top-hit *Curcuma amada* derived phytochemicals

Properties	**β-Caryophyllene**	**ar-Turmerone**	**Germacrone**	**Ascorbic acid**
ABSORPTION				
Water solubility (log mol/L)	-5.555	-4.454	-4.298	-1.556
Caco2 permeability (log Papp in 10-6 cm/s)	1.423	1.458	1.434	-0.255
Intestinal absorption (human) (% Absorbed)	94.845	94.489	95.515	39.154
Skin permeability (log Kp)	-1.58	-1.557	-1.922	-2.955
P-Glycoprotein substrate	No	No	No	No
P-Glycoprotein I inhibitor	No	No	No	No
P-Glycoprotein II inhibitor	No	No	No	No
DISTRIBUTION				
VDss (human, log L/kg)	0.652	0.621	0.292	0.218
Fraction unbound (human) (Fu)	0.263	0.102	0.356	0.825
BBB permeability (log BB)	0.733	0.512	0.526	-0.985
CNS permeability (log PS)	-2.172	-1.771	-2.48	-3.217
METABOLISM				
CYP2D6 substrate	No	No	No	No
CYP3A4 substrate	No	No	No	No
CYP1A2 inhibitor	No	Yes	No	No
CYP2C19 inhibitor	No	No	No	No
CYP2C9 inhibitor	No	No	No	No

CYP2D6 inhibitor	No	No	No	No
CYP3A4 inhibitor	No	No	No	No
EXCRETION				
Total clearance (log ml/min/kg)	1.088	0.295	1.416	0.631
Renal OCT2 substrate	No	No	No	No
TOXICITY				
AMES toxicity	No	No	No	No
hERG I inhibitor	No	No	No	No
hERG II inhibitor	No	No	No	No
Hepatotoxicity	No	No	No	No

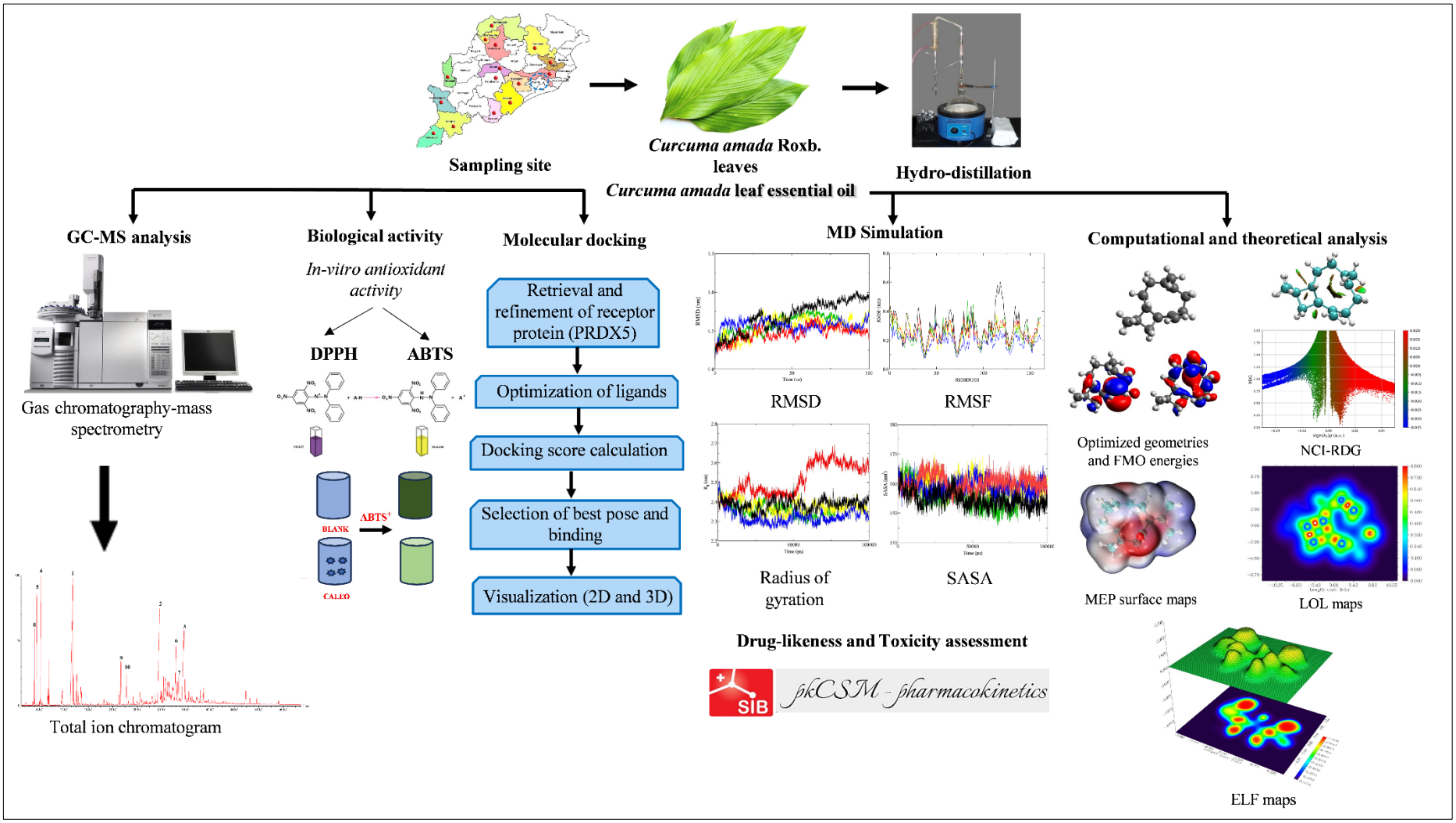
Caco2: human colorectal adenocarcinoma epithelial cells, VDss: Volume of distribution, BBB: Blood brain barrier, CNS: Central nervous system, Renal OCT2: Renal uptake transporters include organic cation transporter 2, and hERG: Human ether-a-go-go-related gene.

Table S2. The DFT optimized geometries, frontier molecular orbital (HOMO/LUMO) energy diagram and calculated values of quantum chemical parameters for the selected compounds of *Curcuma amada* leaf essential oil (a) β-caryophyllene (b) ar-Turmerone and (c) Germacrone and (d) Ascorbic acid (standard) at B3LYP function, 6-31G (d) basis set.

Parameters	B3LYP/6-31G (d) (eV)			
	β-Caryophyllene	ar-Turmerone	Germacrone	Ascorbic acid
Optimized structure				
LUMO				
HOMO				
E_{LUMO}	0.529	-1.317	-0.796	-0.851
E_{HOMO}	-5.950	-6.177	-5.875	-6.23
ΔE	6.479	4.86	5.079	5.379
A	-0.529	1.317	0.796	0.851
I	5.950	6.177	5.875	6.23
χ	2.710	3.747	3.335	3.54
μ	-2.710	-3.747	-3.335	-3.54
η	3.239	2.430	2.539	2.689
S	0.308	0.411	0.393	0.371
ω	1.133	2.888	2.190	2.33

LUMO: Lowest unoccupied molecular orbital, HOMO: Highest occupied molecular orbital, ELUMO: Energy of LUMO, EHOMO: Energy of HOMO, ΔE: Energy gap between HOMO and LUMO, A: Electron affinity, I: Ionisation energy, χ: Electronegativity, μ: Chemical potential, η: Chemical hardness, S: Chemical softness, and ω: Electrophilicity index.

Supplementary Figure



Supplementary Figure SF1. Detailed workflow of the study.