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Supplementary Material

An Integration of UPLC-Q-TOF-MS, GC-MS, Electronic Nose, Electronic Tongue, and Molecular Docking for the Study of the Chemical Properties and Flavor Profiles of *Moringa oleifera* Leaves

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Figure Captions:

Figure S1. Technical roadmap of main research content.

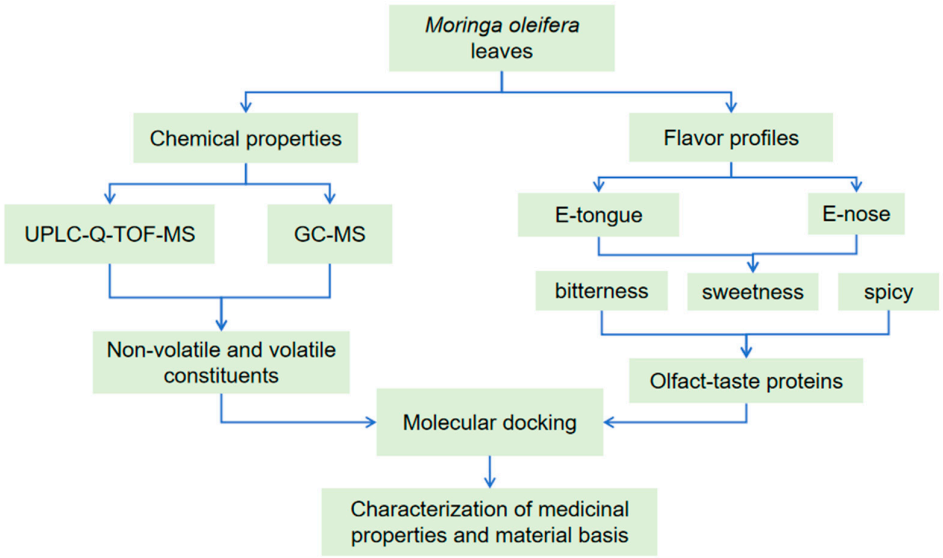


Figure S1. Technical roadmap of main research content.

Table Captions:

Table S1. Taste receptor protein and ligand information table of molecular docking.

Table S2. Binding results of the T2R10 receptor protein with corresponding ligands.

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Table S1. Taste receptor protein and ligand information table of molecular docking.

Name	Classification	Docking center（X, Y, Z）	Connection dimension	Docking ligand
T2R10	bitter taste receptors	（1.22, −1.805, −4.037）	60 × 60 × 70	16 non-volatile compounds identified by LC-MS*
T2R14	bitter taste receptors	（1.301, −1.632, −3.904）	60 × 60 × 70	
T2R38	bitter taste receptors	（1.778, −1.486, −3.292）	60 × 60 × 70	
T1R2	sweet taste receptors	（8.953, 5.817, −8.681）	100 × 100 × 100	
T1R3	sweet taste receptors	（−19.577, −0.779, 14.799）	100 × 100 × 100	
TRPV1	pungent taste receptors	（−22.725, 1.796, 15.633）	80 × 80 × 80	
OR7D4	pungent taste receptors	（2.018, 0.313, 1.684）	70 × 70 × 80	19 volatile compounds identified by GC-MS#

*: malic acid, adenosine, 4-O-(α-*L*-rhamnosyloxy)-benzyl glucosinolate, 4-O-(α-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer I, 4-O-(α-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅱ, 4-O-(α-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅲ, vicenin-2, vitexin, isoquercitrin, quercetin malonyl hexose, quercetin-hydroxy-methylglutaryl glycoside, quercetin acetyl glycoside, astragalin, kaempferol malonyl hexose, kaempferol-hydroxy-methylglutaryl glycoside, kaempferol acetyl glycoside.

#: hexanal, furfural, 2-Hexenal, benzaldehyde, isopropyl n-amyl ketone, phenyl acetaldehyde, linalyl oxide, nonanal, phenylacetonitrile, 2,3-Dihydro-2,2,6-trimethylbenzaldehyde, pelargonic acid, geranyl acetone, damascenone, β-ionone, palmitic acid, n-heneicosane, n-eicosane, n-pentacosane, oleamide.

Table S2. Binding results of the T2R10 receptor protein with corresponding ligands.

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	Donor \ Receptor conflict
1	malic acid	−4.9*	ASN31、SER41、GLY44、ASN281			CYS35
2	adenosine	−6.6	GLU246、LYS174、SER85	ILE147、LEU177、VAL89、TRP162		LYS174
3	4-O-(*α*-*L*-rhamnosyloxy)-benzyl glucosinolate	−7.4	ASP34、SER41、GLY44、TYR116、ASN281	CYS35		
4	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer I	−6.7	LYS109、SER282、ASN281、SER41	PHE113、LYS283、CYS35		
5	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅱ	−6.5	GLY91	PHE56、PHE87、TYR83、LEU80、ILE60、TRP59		
6	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅲ	−6.2	SER53	PHE56、PHE87、ILE60、TRP59		
7	vicenin-2	−6.7	SER53、PHE98、GLY49	ILE90、ILE60、PHE56		
8	vitexin	−7	HIS203、GLY280	VAL228、ALA225	LYS224	
9	isoquercitrin	−7.2	SER53、ILE90、GLY91、SER94	ILE133、ILE52		
10	quercetin malonyl hexose	−6.9	SER94、PHE87	ILE90、ILE60、PHE87		GLY91
11	quercetin-hydroxy-methylglutaryl glycoside	−7.1	ILE133、GLY91、SER53	ILE52、ILE60、PHE56		
12	quercetin acetyl glycoside	−7.1	SER53、PHE56	ILE60、PHE87、ILE90		ILE61
13	astragalin	−7.3	LYS224、TYR106	ILE110、LYS224、TYR106LYS224、		SER282
14	kaempferol malonyl hexose	−6.6	GLY25、GLY28、ILE52、TRP59	VAL21、TRP59		
15	kaempferol-hydroxy-methylglutaryl glycoside	−7.4	LYS285、LYS224、SER282、	MET207、LYS224、HIS203、LYS224		GLY280

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	Donor \ Receptor conflict
16	kaempferol acetyl glycoside	−10.3	HIS203、GLY280 TYR239、LYS155、GLY242	TYR239、LEU259、TRP88、LEU259、TRP88		LYS174

* : Indicates binding energy > −5.0 kcal / mol

Table S3. Binding results of the T2R14 receptor protein with corresponding ligands.

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	Donor \ Receptor conflict
1	malic acid	−5.2	SER246、SER250、LEU257、SER254			
2	adenosine	−6.9	ASN157、SER250、SER246、GLU259、LEU257	ILE262		
3	4-O-(*α*-*L*-rhamnosyloxy)-benzyl glucosinolate	−6.8	ARG288、GLY283、LYS285、ARG209、HIS208、ALA112、LYS211	MET212、HIS208	LYS285、ARG209、HIS208	HIS208
4	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer I	−6.9	GLY38、SER42、ASP45、LYS110、GLY283、HIS208、LYS285、ARG209	PHE114	HIS208、LYS285、ARG209	HIS208
5	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅱ	−6.5	LYS110、ARG228、ALA112、HIS208	PHE114、TYR107、ILE111		HIS208
6	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅲ	−8.6	ASN157、SER167、PHE172、SER250、GLU255	PHE175		
7	vicenin-2	−8.0	ARG160、ASN260	LYS6、TYR159、PHE9、ILE5		
8	vitexin	−10.2	ASN157、SER265、THR86	ILE148、TRP89、PHE247		
9	isoquercitrin	−8.4	SER250	PHE175、ILE148、TRP89		
10	quercetin malonyl hexose	−6.9	LYS110、ASN284、LYS285、ARG209、ARG228、HIS208	PHE114、LYS285		
11	quercetin-hydroxy-methylglutaryl glycoside	−6.7	TYR159、LYS163、ARG160、ARG161	PHE9、ILE5、LYS6、TYR159		
12	quercetin acetyl glycoside	−7.3	LYS163、ASN260、LYS6	TYR159、LYS6、ILE5、PHE9		
13	astragalin	−8.5	SER167、ASP168	PHE247、LEU178、TRP89		
14	kaempferol malonyl hexose	–7	LYS163、ARG160、ARG161	PHE9、LYS6、ILE5、TYR159	LYS6	
15	kaempferol-hydroxy-methylglutaryl glycoside	−7.1	TYR159、LYS6、LYS163、ARG160	ILE5、PHE9、TYR159、LYS6		

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	Donor \ Receptor conflict
16	kaempferol acetyl glycoside	−7.4	ASN260、PHE9、LYS163	PHE9、LYS6、TYR159、ILE5		

Table S4. Binding results of the T2R38 receptor protein with corresponding ligands.

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	Donor \ Receptor conflict
1	malic acid	−4.5*	SER194、SER159			SER259
2	adenosine	−6.1	ILE296、SER248	LEU121、LYS120		
3	4-O-(*α*-*L*-rhamnosyloxy)-benzyl glucosinolate	−6.3	LYS303、ASN301、ASP54、SER51	PHE128	LYS303	GLN48、ARG47
4	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer I	−6.8	ARG47、SER51、ASP54、LYS120、ARG305、LYS244、GLY300	ARG47	LYS244、GLY300	
5	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅱ	−6.4	ASN301、GLY300、LYS120、PHE124、LEU121	LYS303、LYS120、PHE124、LEU121	HIS223	HIS223
6	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅲ	−6.5	ASN89、TRP160、VAL159	PHE162、PHE163、TYR92		
7	vicenin-2	−6.4	ASN179、GLN82、ASN177、ARG15	TYR12		
8	vitexin	−6.8	GLU240、LYS244、ARG305	PHE124、LYS120、PHE121	LYS120	
9	isoquercitrin	−6.8	THR79、ARG15、ASN177	ARG15、THR169		GLN82
10	quercetin malonyl hexose	−6.7	SER299、LYS247、ARG305、GLY300	LYS247、LYS244、ILE296		
11	quercetin-hydroxy-methylglutaryl glycoside	−7.7	LYS120、HIS223、GLY300、SER2488、LYS244	LYS244、PHE124		
12	quercetin acetyl glycoside	−6.9	ASN178、ARG15、ASN177	ARG15、THR169		GLN82
13	astragalin	−6.8	ASN177、GLN82	ARG15、THR169		ARG15
14	kaempferol malonyl hexose	−6.8	THR79、SER11、GLN82、ASN177	ARG15、THR169		
15	kaempferol-hydroxy-methylglutaryl glycoside	−6.5	LYS244、GLY300、LYS120	LEU121、THR117、LYS303、ALA302	LYS120	
16	kaempferol acetyl glycoside	−6.9	ARG15、ASN178、GLN82、ASN177	ARG15、THR169		GLN82

* : Indicates binding energy > −5.0 kcal / mol

Table S5. Binding results of the T1R2 receptor protein with corresponding ligands.

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	π-Sulfur interaction	Donor \ Receptor conflict
1	malic acid	−5.5	TRP455、GLN452、GLN454、SER482、THR321				GLN452
2	adenosine	−6.6	GLU97、GLN361	TYR357、TYR28			SER25、TYR113
3	4-O-(*α*-*L*-rhamnosyloxy)-benzyl glucosinolate	−8.2	VAL66、LYS65、ASP307、ASP278、VAL64、HIS283	LEU243、TYR282			
4	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer I	−7.2	TYR113、GLN361、SER25、SER356	PHE27、PRO343			
5	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅱ	−8.0	GLU97、TYR113、TYR357、GLN361	PHE27	ARG352	TYR28、TYR357	
6	4-O-(*α*-*L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅲ	−7.1	GLU63、LYS65、ASN44、ASN248、MET45、HIS283、VAL64	TYR282、LEU243、TYR282			VAL64
7	vicenin-2	−7.4	ASN460、PHE462、LEU379、GLN328、VAL330、SER329、HIS434		GLU449		ARG381、HIS447
8	vitexin	−8.1	ASP307、HIS283	LEU279、TYR282、VAL309	GLU63		ASN312
9	isoquercitrin	−8.7	ASN24、SER25、SER356、SRG352、SER354	PRO349、TYR28			
10	quercetin malonyl hexose	−7.5	THR485、HIS484、TRP453、TRP455、				

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	π-Sulfur interaction	Donor \ Receptor conflict
11	quercetin-hydroxy-methylglutaryl glycoside	−6.8	GLN454、ASP456 TRP483、HIS484、SER482、TRP455、TRP453、GLN454、ARG317				ASN488、GLY320
12	quercetin acetyl glycoside	−9.3	GLN361、SER356、GLU23	PRO28、TYR357、PRO349			
13	astragalin	−7.8	ARG317、GLN454、TRP455、GLY320、HIS484				TRP455
14	kaempferol malonyl hexose	−7.6	HIS318、HIS484、THR321、PHE322、SER482、GLN454、ASP456、ARG317				TRP455
15	kaempferol-hydroxy-methylglutaryl glycoside	−8.8	ASP26、GLU362、GLN361、ARG352	PRO349、TYR357、TYR28			ASP26
16	kaempferol acetyl glycoside	−8.1	HIS318、THR485、HIS484、THR321、PHE322、TRP455、SER482、GLN454、ASP456				TRP455

Table S6. Binding results of the T1R3 receptor protein with corresponding ligands.

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	π-Sulfur interaction	Donor \ Receptor conflict
1	malic acid	−5.2	TYR218、GLY168、SER170、SER147				SER146、SER17、GLY168
2	adenosine	−7.5	LEU331、ASN386、GLY328、GLN330	LEU331			
3	4-O-(*α-L*-rhamnosyloxy)-benzyl glucosinolate	−9	SER146、HIS278、SER276、SER170、GLY168、GLN389、ASP307	VAL277、HIS145、HIS387、TRP72			ASP216、GLY168
4	4-O-(*α-L*-acetylrhamnopyranosyloxy) -thioglucoside isomer I	−6.8	ARG327、GLN330、HIS388、ALA329、GLN326	LEU440			HIS387、GLY328
5	4-O-(*α-L*-acetylrhamnopyranosyloxy) -thioglucoside isomer Ⅱ	−7.8	PRO466、GLN330、HIS387、ASN386、ALA383、LYS457	HIS387、LEU468、VAL465	LYS457、ARG327		
6	4-O-(*α-L*-acetylrhamnopyranosyloxy) -thioglucoside isomer Ⅲ	−9.4	ASP307、ARG247、ASP216、SER276、SER146、ASN68、THR305、SER66	THR218	ASP307、ARG247	ASP216 TRP72	
7	vicenin-2	−7.9	SER276、SER146、ASN68、THR305、SER66、LEU468	MET310			
8	vitexin	−9.1	LYS457、GLN326、ARG327、ASN386、LEU385、ALS329	HIS387			

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	π-Sulfur interaction	Donor \ Receptor conflict
9	isoquercitrin	−7.9	GLN330、GLN326、LEU325、HIS388、LEU331、PHE391	LEU331	LYS457		
10	quercetin malonyl hexose	−7.1	LEU468、LYS457、ASP470、GLN330、ARG327	LEU468	LYS457		
11	quercetin-hydroxy-methylglutaryl glycoside	−7.0	ARG486、YHR489、TRP459、TRP461、HIS488、GLY319	ALA316			TRP461
12	quercetin acetyl glycoside	−8.3	GLY328、PHE391、THR390、ASN386、HIS388、HIS387、ALA383、LYS457				
13	astragalin	−7.7	ASN386、HIS388、ALA383		LYS457		HIS388、GLY328
14	kaempferol malonyl hexose	−8.3	ASN386、HIS388、LEU331、PHE391、GLY328、LYS457、ASP455				HIS388、GLY328
15	kaempferol-hydroxy-methylglutaryl glycoside	−8.4	ARG327、ASP455、HIS388、LEU385、HIS387	LEU468			
16	kaempferol acetyl glycoside	−8.6	GLN330、LYS457、LEY325、GLN326、HIS388、LEU331、PHE391	ARG327	LYS457		ASP455

Table S7. Binding results of the TRPV1 receptor protein with corresponding ligands.

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	Donor \ Receptor conflict
1	malic acid	−4.7*	ASN438、YHR709、TYR554			
2	adenosine	−7.1	ARG491、GLN494		ARG491	
3	4-O-(*α-L*-rhamnosyloxy)-benzyl glucosinolate	−8.1	ASP708、ARG491、VAL441、TYR487	PHE488、TYR487、LEU483		
4	4-O-(*α-L*-acetylrhamnopyranosyloxy)-thioglucoside isomer I	−7.1	ASP708、SER712	LEU483、TYR487、TYR487		
5	4-O-(*α-L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅱ	−7.3	TYR455、PHE473	PHE473、ALA452、MET451	ARG474	ARG456
6	4-O-(*α-L*-acetylrhamnopyranosyloxy)-thioglucoside isomer Ⅲ	−8.3		LEU480、TYR445、TYR487、	PHE435、ARG491、TYR487、ASP708、GLY484	
7	vicenin-2	−7.9	GLU406、THR407、HIS411、GLN701、GLU570、ASN409、GLU693	ILE697、VAL508、ILE697	ASP509	
8	vitexin	−7.6	ASN438	PHE488、TYR487、VAL441		
9	isoquercitrin	−8.1	LYS711、SER510、PRO501、TYR495	TYR402、ARG499、PRO501、TYR402		
10	quercetin malonyl hexose	−7.6	VAL399、SER403、TYR495	PRO501、ARG499		GLN498
11	quercetin-hydroxy-methylglutaryl glycoside	−8.7	SER712、TYR487	PHE488、TYR487	ARG491	
12	quercetin acetyl glycoside	−9.1	ARG499、GLN498、GLN494、SER712、ASP708、LYS711、THR709	ASP708、ARG491	ARG491	

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	Electrostatic interaction	Donor \ Receptor conflict
13	astragalin	−8.8	ARG499、GLN498、ASP708、GLN494、SER712、YHR709、TYR554、LYS711	ASP708、ARG491	ARG491	
14	kaempferol malonyl hexose	−7.9	LYS711、ASN394、THR505、TYR495	PRO501、ARG499		
15	kaempferol-hydroxy-methylglutaryl glycoside	−8.9	ASN438、TYR555、SER712	VAL441		ARG491
16	kaempferol acetyl glycoside	−8.8	THR709、SER712、ARG491、TYR554、ASP708、LYS711、GLN498、GLN494、ARG499	ARG491、ASP708	ARG491	

* : Indicates binding energy > −5.0 kcal / mol

Table S8. Binding results of the OR7D4 receptor protein with corresponding ligands.

Number	Compounds	Binding energy kcal/mol	Hydrogen-bonding interaction	Hydrophobic interaction	π-Sulfur interaction
1	hexanal	−3.9*	ALA108、THR112	TYR278、PHE251	
2	furfural	−4.5*	SER18、GLN24	ILE85	MET81
3	2-Hexenal	−4*	THR112	TYR278、PHE251、TYR278	
4	benzaldehyde	−4.9*	THR112	TYR278、PHE251	
5	isopropyl n-amyl ketone	−4.5*	LEU256	TYR278、	
6	phenyl acetaldehyde	−5.3		TYR102	
7	linalyl oxide	−5.5	TYR252、LEU256	TYR252、TYR278、PHE251、ALA108、TYR278	
8	nonanal	−4.3*	THR112	TYR278、PHE251、TYR252	
9	phenylacetonitrile	−5.4	THR112	PHE251、TYR278	
10	2,3-Dihydro-2,2,6-trimethylbenzaldehyde	−5.7	THR112	TYR252、PHE251、TYR278、ALA108	
11	pelargonic acid	−5.0	ALA108	PHE251、TYR278、TYR252、ALA108	
12	geranyl acetone	−6.0	THR112、GLY109	PHE251、TYR252、TYR278、TYR278	
13	damascenone	−6.4	THR112	ALA108、TYR278、PHE251、TYR252、PHE251	
14	β-ionone	−6.9		ALA108、TYR278、PHE251、TYR252	
15	palmitic acid	−5.4	ALA108	TYR278、PHE251、TYR252	
16	n-heneicosane	−5.4		ALA108、TYR278、PHE251、TYR252、LEU206、MET105、PHE155、PRO181	
17	n-eicosane	−5.4		MET105、PHE155、TYR278、PHE251、TYR252	
18	n-pentacosane	−5.3		ALA108、TYR278、PHE251、TYR252、LEU206、MET105、PHE155、PRO181、TYR259、LEU199	
19	oleamide	−5.3	SER271	TYR278、PRO181、ALA182、PHE251、PHE251	

* : Indicates binding energy > −5.0 kcal / mol