Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Identification, screening and taste mechanisms analysis of two novel umami pentapeptides derived from myosin heavy chain of Atlantic cod (*Gadus morhua*)

Supplementary Fig. S1: Profile of the peptides identified from the myosin heavy chain fast skeletal muscle [*Gadus morhua*].

Supplementary Fig. S2: Primary structures, and optimal 3D-conformation of the umami peptides LVDKL and ESKIL docked with T1R1/T1R3. (A) The peptide LVDKL; (B) The peptide ESKIL.

Supplementary Table S1: Recognition threshold values and sensory description of the umami peptides LVDKL and ESKIL.

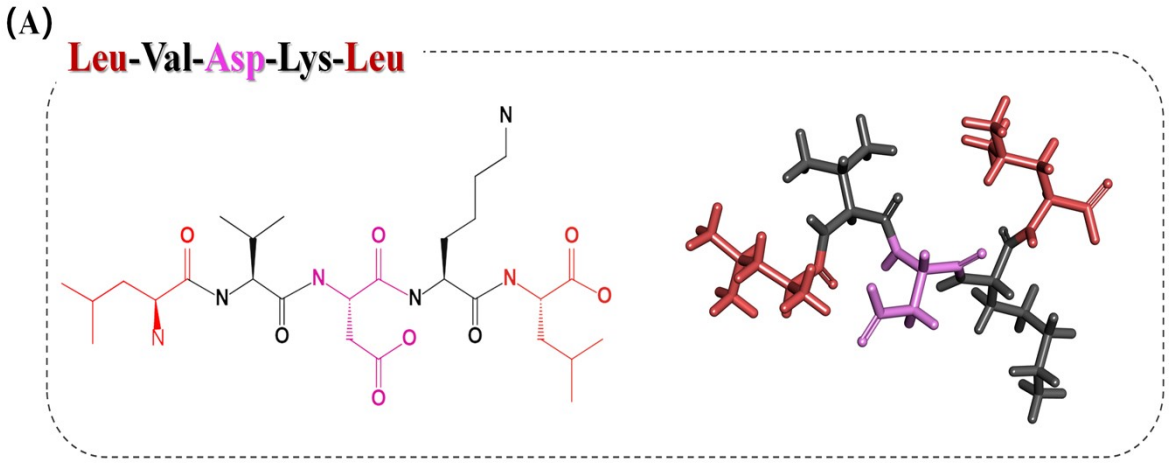
Supplementary Table S2: The interaction between the umami peptides LVDKL and ESKIL with the T1R1/T1R3 simulated by molecular docking.

Supplementary Table S3: *In silico* prediction of properties of the umami peptides LVDKL and ESKIL.

Figure S1.


1 MGDGEMQCFG EAAVYLRKPE RERLEAQTSP FDAKTAFFVS EPKEMYLKGV LQSRDGGKAT VKTLCDKTLT VKEEEIYPMN
81 PPKYDKIEDM AMMTHLNEPT VLYNLKERYA AWMIYTYSGL FCVTVNPYKW LPVYDSSVVN AYRGKKRIEA PPHIFSISDN
161 AYQAMLTDRE NQSILITGES GAGKTVNTKR VIQYFATIAV SGPKKTEQVA GKMQGSLEDQ IIAANPLLEA YGNAKTVRND
241 NSSRFGKFIR IHFATSGKLA SADIETYLLE KSRVTFQLSA ERSYHIFYQL MTGHKPELID ALLITKNPFD YHMISQGEIT
321 VKSIDDVEEF IATDDAIDIL GFTADEKIGI YKLTGAVLHH GNMKFKQKQR EEQAEPDGNE EADKIGYLMG LNSADVLKAL
401 CYPRVKVGNE YVTKGQTCPQ VHNSVMALCK SVYEKMFLWM VVRINEMLDT KQPRQFFIGV LDIAGFEIFN YNSLEQLCIN
481 FTNEKLQQFF NHHMFVLEQE EYKKEGIEWE FIDFGMDLAA CIELIEKPMG IFSILEEECM FPKASDTTFK NKLHDQHLGK
561 TKAFEKPKPA KGKAEAHFSL VHYAGTVDYN ITGWLDKNKD PLNDSVIQLY QKSSVKLLAL LYASHALPDA DAASKKGAKK
641 KGGSFQTVSA LFRENLGKLM TNLRSTHPHF VRCLIPNESK TPGLMENFLV IHQLRCNGVL EGIRICRKGF PSRVLYGDFK
721 QRYKVLNASV IPEGQFIDNK KASEKLLGSI DVDSTQYKFG HTKVFFKAGL LGALEEMRDE KLAALVTLTQ ALCRGFNMRK
801 EFVKMMERRE AVFTIQYNIR SFMNVKTWPW MKVYFKIKPL LKSAETEKEM AQMKETFGKT KEDLAKALSK KKELEEKMVS
881 LLQEKNDLLL QVQSEAETLS DSEERCEGLI KSKIQLEARL KETSERLEDE EEINSELTAK KRKLEDECSE LKKDIDDLEL
961 TLAKVEKEKH ATENKVKNLT EEMSSQDEII AKLTKEKKAL QEAHQQTLDD LQAEEDKVNT LSKAKCKLEQ QVDDLEGSLE
1041 QEKKLRMDLE RAKRKLEGDL KLAQESIMDL ENDKQQSDEK IKKRDFETSQ LLNKIEDEQT LSAQFQKKIK ELQARIEELE
1121 EEIEAERAAR AKVEKQRADL SRELEEISER LEEAGGATSL QIEMNKKREA EFQKLRRDLE ESTLQHEATS AALRKKQADS
1201 VAELGEQIDN LQRVKQKLEK EKSECKMEID DLSSNMEAVA KSKANLEKLA RTLEDQLSEL KSKNDEHVRQ LNDLSVQRAR
1281 LQTENGEFGR QQEEKEALIS QLTRGKQAYT QQIEELKRHI EEEVKAKNAL AHSVQSARHD CDLLREQFEE EQEAKAELQR
1361 GMSKANSEVA QWRSKYETDA IQRTEELEEA KKKLAQRLQD AEEAVEATNS KCASLEKTKQ RLLGEVEDLM IDVERANALA
1441 ANLDKKQRNF DKVLAEWKQK YEESQAELEG AQKEARSLST EMFKLKNSYE ESLDQLETLK RENKNLQQEI SDLSEQMGET
1521 GKTIHELEKG KKTVEVEKSE LQTSLEEAEA TLEHEESKIL RVQLELTQIK GEVDRKMAEK DEEMEQIKRN SLRVIDSMQS
1601 NLDSEIRSRN DALRIKKKME GDLNEMEIQL SHANRQASEA QKQLRNVQGQ LKDAQLHLDD ALRGQEDMKE QVAMVERRNN
1681 LMLAEIEELR AALEQTERGR KVAEQELVDA SERLGLLHSQ NTSLINTKKK LETDLIQIQG EVEDTVQEAR NAEEKAKKAI
1761 TDAAMMAEEL KKEQDTSSHL ERMKKNLELT VKDLQHRLDE AESLAMKGGK KQLQKLEARV RELETECEAE QRRGSEAIKG
1841 VRKYERKVKE LSYQCDEDKK NICRLQDLVD KLQLKMKAYK RQAEESEEQA NTHLSRYRKV QHELEEAQER ADVSESQVNK
1921 LRTKSREFGK AKDAEE

Figure S2.



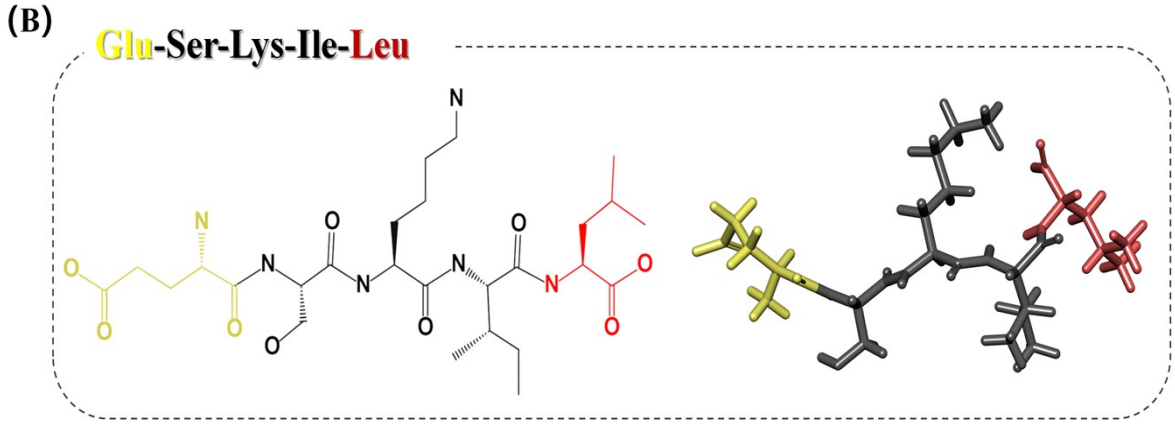


Table S1 Recognition threshold values and sensory description of the umami peptide LVDKL and ESKIL.

Peptide	Threshold value (mM)	Sensory description
LVDKL	0.427	Umami, slight sourness, and sweetness
ESKIL	0.574	Umami, bitterness, and slight sweetness

Table S2 The interaction between the umami peptide LVDKL and ESKIL with the T1R1/T1R3 simulated by molecular docking.

Peptide	Bond site	Interaction	Distance	Category
LVDKL	ARG712	B:ARG712:NH1 - LVDKL:O91	4.59276	Electrostatic
	ARG712	B:ARG712:HH12 - LVDKL:O90	2.74973	Hydrogen Bond
	HIS915	B:HIS915:HD1 - LVDKL:O91	2.66896	Hydrogen Bond
	GLN853	LVDKL:H51 - B:GLN853:O	2.59138	Hydrogen Bond
	GLN853	LVDKL:H69 - B:GLN853:OE1	1.85112	Hydrogen Bond
	ARG854	B:ARG854:HA - LVDKL:O46	2.53144	Hydrogen Bond
	GLY911	B:GLY911:HA1 - LVDKL:O47	2.5314	Hydrogen Bond
	HIS914	B:HIS914:HE1 - LVDKL:O49	2.58556	Hydrogen Bond
	ARG854	LVDKL:C12 - B:ARG854	5.16444	Hydrophobic
	LEU852	LVDKL:C28 - B:LEU852	5.20432	Hydrophobic
	LEU912	LVDKL:C81 - B:LEU912	4.48624	Hydrophobic
	LEU852	LVDKL:C85 - B:LEU852	4.68424	Hydrophobic
	PHE851	B:PHE851 - LVDKL:C12	5.10725	Hydrophobic
	PHE851	B:PHE851 - LVDKL:C32	5.01356	Hydrophobic
ESKIL	GLN853	B:GLN853:HN - ESKIL:O28	2.98375	Hydrogen Bond
	GLN853	ESKIL:H4 - B:GLN853:OE1	1.86582	Hydrogen Bond
	GLN853	ESKIL:H19 - B:GLN853:OE1	2.24902	Hydrogen Bond
	GLN853	ESKIL:H26 - B:GLN853:OE1	3.01244	Hydrogen Bond
	PRO715	B:PRO715:HD2 - ESKIL:O25	2.63504	Hydrogen Bond
	HIS914	B:HIS914:HE1 - ESKIL:O50	2.66629	Hydrogen Bond
	VAL714	ESKIL:C57 - B:VAL714	3.95501	Hydrophobic
	VAL714	ESKIL:C64 - B:VAL714	5.34317	Hydrophobic
	LEU852	ESKIL:C64 - B:LEU852	4.79617	Hydrophobic
	HIS672	B:HIS672 - ESKIL:C83	5.1179	Hydrophobic

Table S3 *In silico* prediction of properties of the umami peptide LVDKL and ESKIL.

Peptide	Human intestinal absorption (HIA)	Acute oral toxicity	Instability index	Isoelectric point	Water solubility	Net charge
LVDKL	-	III	Stable	6.63	Good water solubility	0
ESKIL	+	III	Unstable	6.85	Good water solubility	0