Chemical compositions and experimental and computational modeling of anticancer effects of cnidocyte venoms of jellyfish *Cassiopea andromeda* and *Catostylus mosaicus* on human adenocarcinoma A549 cells

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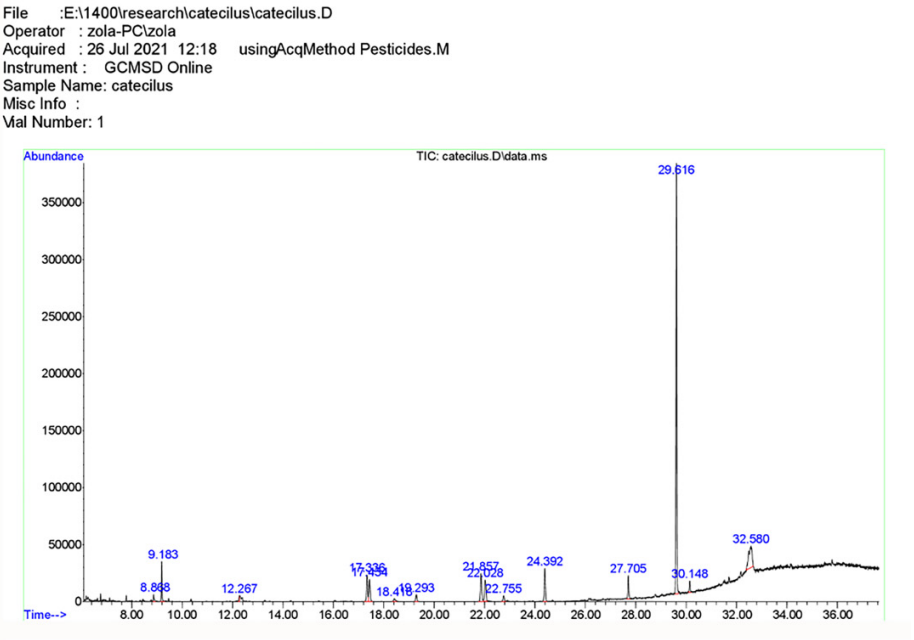
C. andromeda



C. mosaicus

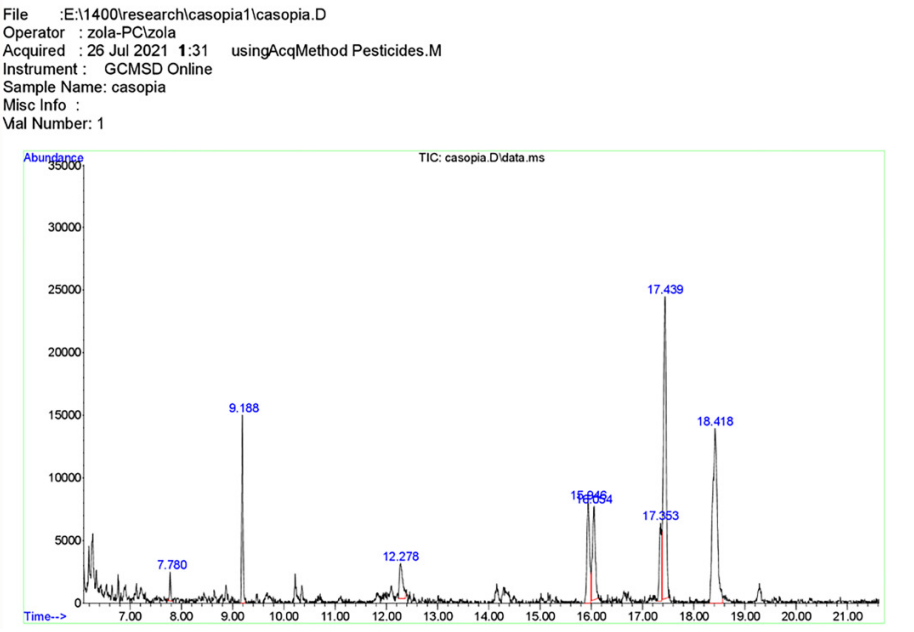


Figure S1.
GC-MS chromatogram of the venom of *Cassiopea andromeda* and Catostylus *mosaicus*

Table S1.
GC-MS-detected compounds in the venom of *Cassiopea andromeda*

Compounds	Formula	Effects	MW	RT	Abundance ratio (%)	Cancer/Cell line	References
Ethaneperoxoic acid, 1-cyano-1-[2-(2-phenyl-1,3-dioxolan-2-yl)ethyl]pentyl ester	C19H25NO5	Anticancer Antimicrobial Anti-inflammatory	347.4	15.94	1.098	MCF-7	[1-3]
Dibutyl phthalate	C16H22O4	Anticancer Antimicrobial Induce apoptosis Induce inflammation Induce oxidative stress	278.34	18.41	3.153	Brain Breast Lung Prostate Bladder	[4-6]
9,12-Octadecadienoic acid, methyl ester	C19H34O2	Anticancer Antioxidant Antimicrobial Anti-inflammatory	294.5	21.86	4.852	B16 Eca-109 BGC823 HeLa NCTC1469	[7-10]
6-Octadecenoic acid, methyl ester, (Z)-	C19H36O2	Antioxidant Antimicrobial Antiviral	296.5	22.03	3.575	NA	[11-13]
Heptadecane,2,6,10,14-Tetramethyl-	C21H44	Anticancer Antioxidant	296.6	24.4	0.775	LnCap 22RV1 MDA-MB-231 MCF7	[14]
1-Hexadecyne	C16H30	Antimicrobial	222.41	26.13	0.451	NA	[15]

Nonadecane	C19H40	Antioxidant Anti-inflammatory	268.5	27.7	1.176	NA	[16]
Batilol	C21H44O3	Anticancer Anti-inflammatory	344.6	30.14	0.506	Leukemia	[17,18]
2-Bromononane	C9H19Br	NA	207.15	7.78	0.123	NA	NA
Tetradecanoic acid, 12-methyl-, methyl ester, (S)-	C16H32O2	NA	256.42	22.77	0.880	NA	NA
Androst-11-en-17-one, 3-formyloxy-, (3a',5a')-	C20H28O3	NA	316.4	31.14	4.701	NA	NA
Pseduosarsasapogenin-5,20-dien	C27H42O3	NA	414.6	32.6	29.621	NA	NA
1,3-Dioxolane-2-heptanenitrile, alpha-methyl-e-oxo-2-phenyl-	C17H21NO3	NA	287.35	16.05	0.998	NA	NA
Aspidofractinine-3-methanol, (2a',3a',5a')-	C22H28N2O2	NA	352.5	29.62	42.856	NA	NA
1,4,5,6-Tetrahydrocyclopentapyrazole-3-carboxylic acid, (1-adamantan-1-ylethylidene)hydrazide	C19H26N4O	NA	326.4	9.18	0.927	NA	NA
3β-hydroxyallobetulane	C30H50O2	NA	442.7	17.43	3.165	NA	NA
3-oxo-18-nor-ent-ros-4-ene-15β,16-acetonide	C22H34O3	NA	346.5	17.35	0.687	NA	NA
Cholestan-22(26)-isoepoxy	C27H42O1	NA	414.6	12.27	0.457	NA	NA

Table S2.
GC-MS-detected compounds in the venom of *Catostylus mosaicus*

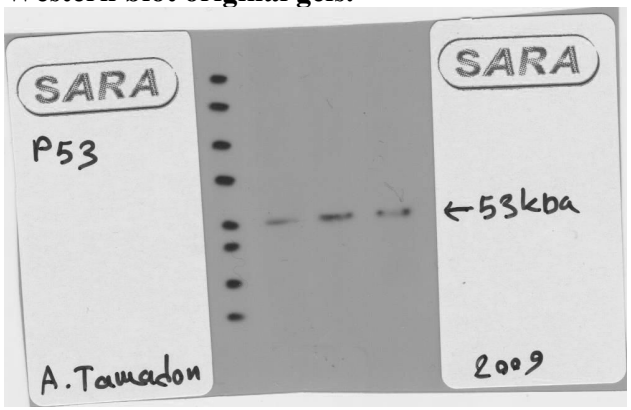
Compounds	Formula	Effects	MW	RT	Abundance ratio (%)	Cancer/Cancer cell line	References
Citrinin	C13H14O5	Anticancer Antioxidant Antimicrobial Anti-inflammatory Induce apoptosis Induce oxidative stress Antiviral	250.25	17.33	4.402	MCF-7 LNCaP LU-1 KB	[19-24]
Dibutyl phthalate	C16H22O4	Anticancer Antimicrobial Induce apoptosis Induce inflammation Induce oxidative stress	278.34	18.41	0.746	Brain Breast Lung Prostate Bladder	[4-6]
Eicosane	C20H42	Anticancer Antimicrobial Anti-inflammatory Antiviral	282.5	19.29	1.269	HeLa MCF7 SGC-7901	[25-29]
9,12-Octadecadienoic acid, methyl ester	C19H34O2	Anticancer Antioxidant Antimicrobial	294.5	21.85	5.552	B16 Eca-109 BGC823 HeLa NCTC1469	[7-10]

6-Octadecenoic acid, methyl ester, (Z)-	C19H36O2	Anti-inflammatory Antioxidant Antimicrobial	296.5	22.03	4.480	NA	[11-13]
Heptadecane,2,6,10,14-Tetramethyl-	C21H44	Anticancer Antioxidant	296.6	24.4	5.221	LnCap 22RV1 MDA-MB-231 MCF7	[14]
Nonadecane	C19H40	Antioxidant Anti-inflammatory	268.5	27.7	3.297	NA	[16]
Batilol	C21H44O3	Anticancer Anti-inflammatory	344.6	30.14	1.397	Leukemia	[17,18]
Decane, 1-bromo-2-methyl-	C11H23Br	NA	235.20	8.86	0.791	NA	NA
3β-hydroxyallobetulane	C30H50O2	NA	442.7	17.43	3.961	NA	NA
Aspidofractinine-3-methanol, (2a',3a',5a')-	C22H28N2O2	NA	352.5	29.62	52.603	NA	NA
Tetradecanoic acid, 12-methyl-, methyl ester, (S)-	C16H32O2	NA	256.42	22.76	1.145	NA	NA
1,4,5,6-Tetrahydrocyclopentapyrazole-3-carboxylic acid, (1-adamantan-1-ylethylidene)hydrazide	C19H26N4O	NA	326.4	9.18	3.912	NA	NA
Cholestan-22(26)-isoepoxy	C27H42O1	NA	414.6	12.26	0.609	NA	NA
Pseduosarsasapogenin-5,20-dien	C27H42O3	NA	414.6	32.6	10.616	NA	NA

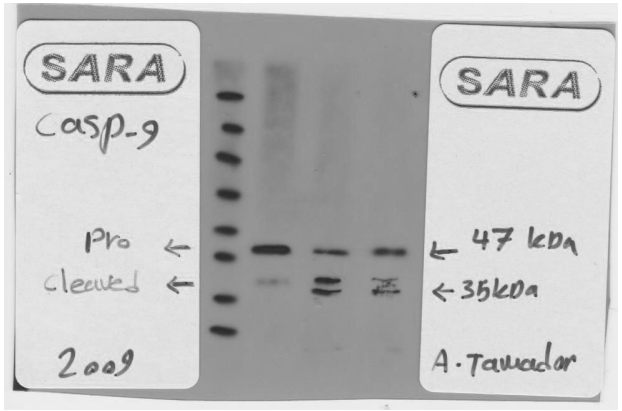
Table S3.
Receptors involve in the apoptosis of cells of human pulmonary adenocarcinoma cells (A59).

Receptor	**Type of effect on the apoptosis in A549 cells**	**Ref.**
Fas receptor	Activation	[30]
TNF receptor-1(TNF-R1)	Activation	[30]
Death receptor 4 (DR4 or TRAIL-RI)	Activation	[31]
Insulin-like growth factor 1 receptor (IGF1R)	Activation	[32]
Peroxisome proliferator-activated receptor-γ (PPAR-γ)	Activation	[33]
Caspase-8	Activation	[34]
Caspase-3	Activation	
Caspase-9	Activation	
Caspase-7	Activation	[35]
Cannabinoid receptor type 1 (CB1)	Activation	[36]
Cannabinoid receptor type 2 (CB2)		
Toll-like receptor 4 (TLR4)	Activation	[37]
Toll-like receptor 9 (TLR9)	Activation	[38]
Blockade of Endothelial protein C receptor (EPCR)	Inhibition	[39]
Metabotropic glutamate receptors (mGluRs)	Activation	[40]
Prostaglandin D2 (PGD2) receptor	Activation	[41]
Transforming Growth Factor Beta Receptor 2 (TGFBR2)	Activation	[42]

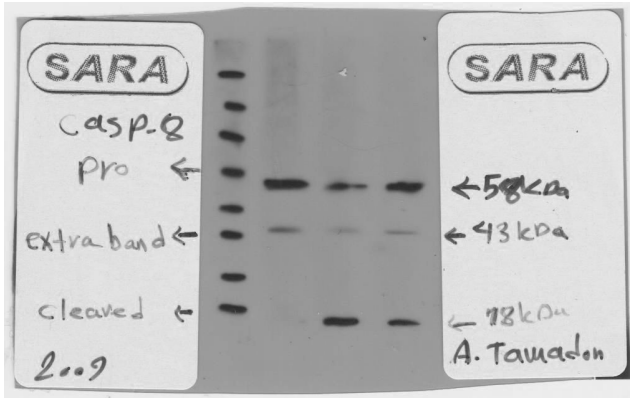
Western blot original gels.



Western blot gel P53



Western blot gel caspase-9



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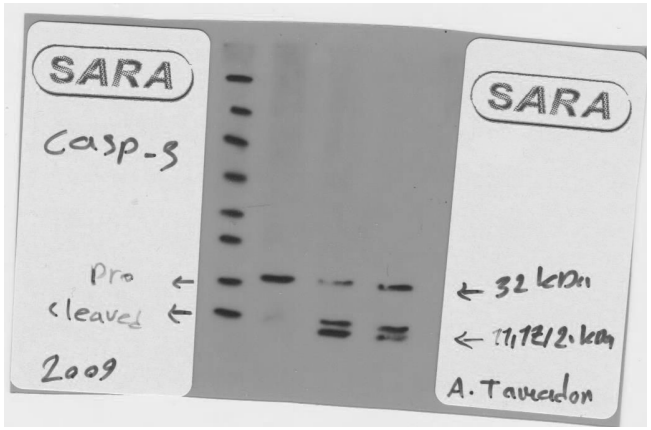

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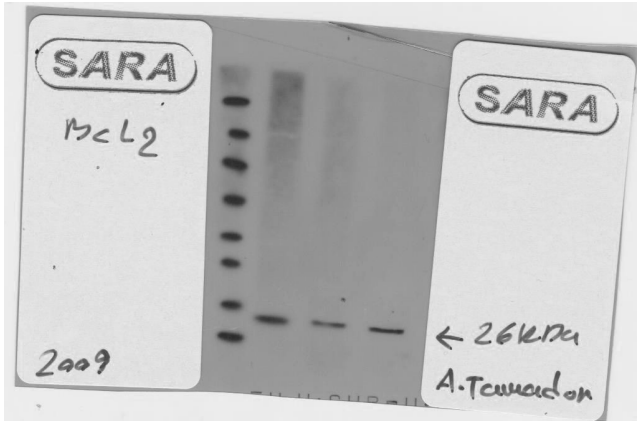
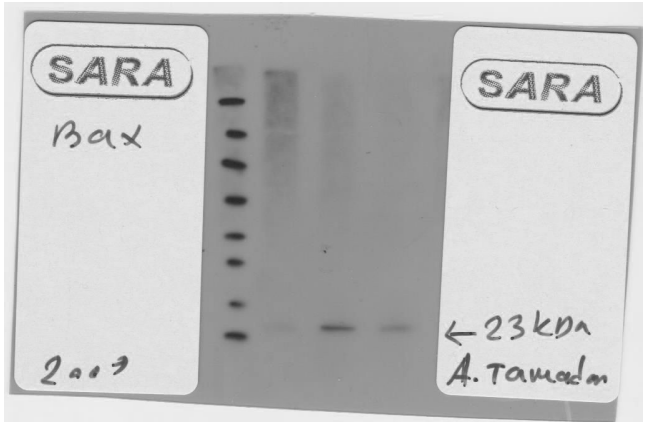
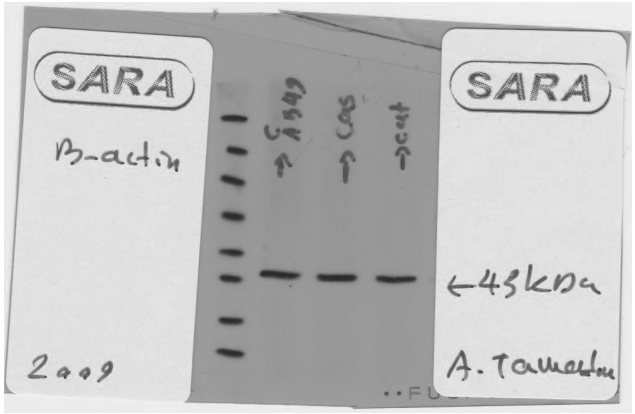


Western blot gel BCL-2



Western blot gel BAX



Western blot gel β-actin

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