



“Profiling of the oil of the Egyptian cultivar of sesame ‘Giza 32’ using LC-MS-based untargeted metabolomics”

**Reham Hassan Mekky, Essam Abdel-Sattar, Antonio Segura-Carretero and
María del Mar Contreras**



Outline

- **Introduction**
- **Aim of work**
- **Materials and methods**
 - Recovery of the oil phenolic-rich fraction from SG32 seeds
 - Untargeted Metabolic Profiling of the phenolic fraction SG32 oil by RP-HPLC-DAD-QTOF-MS and MS/MS
- **Results**
 - RP-HPLC-DAD-QTOF-MS and MS/MS Characterization of SG32 oil
 - Comparison between SG32 oil and cake
- **Conclusion**
- **References**



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Introduction

- Sesame (*Sesamum indicum* L.) is an oil crop whose cultivation is distributed all over the world. Its use dates since Ancient Egypt where it was used in soothing asthma [1-2].



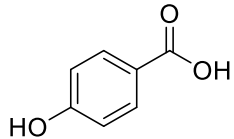
Sesamum indicum L.



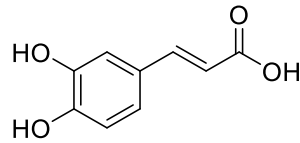
<http://ancientomnivore.com/eat-like-an-ancient-egyptian/>

Introduction

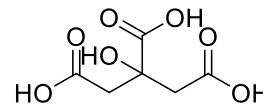
Reported Phytoconstituents in *S. indicum* (Selection)



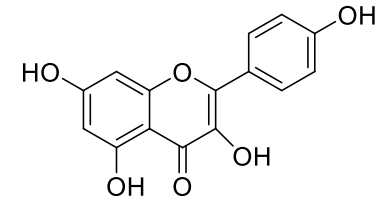
p-hydroxybenzoic acid



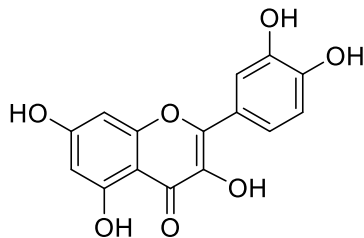
Caffeic acid



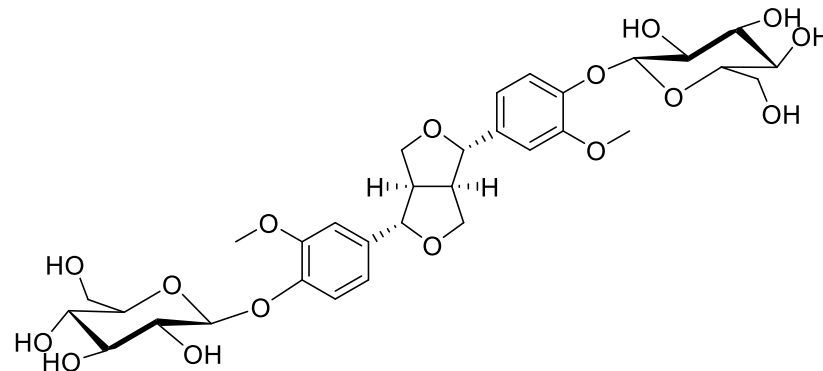
Citric acid



Kaempferol



Quercetin

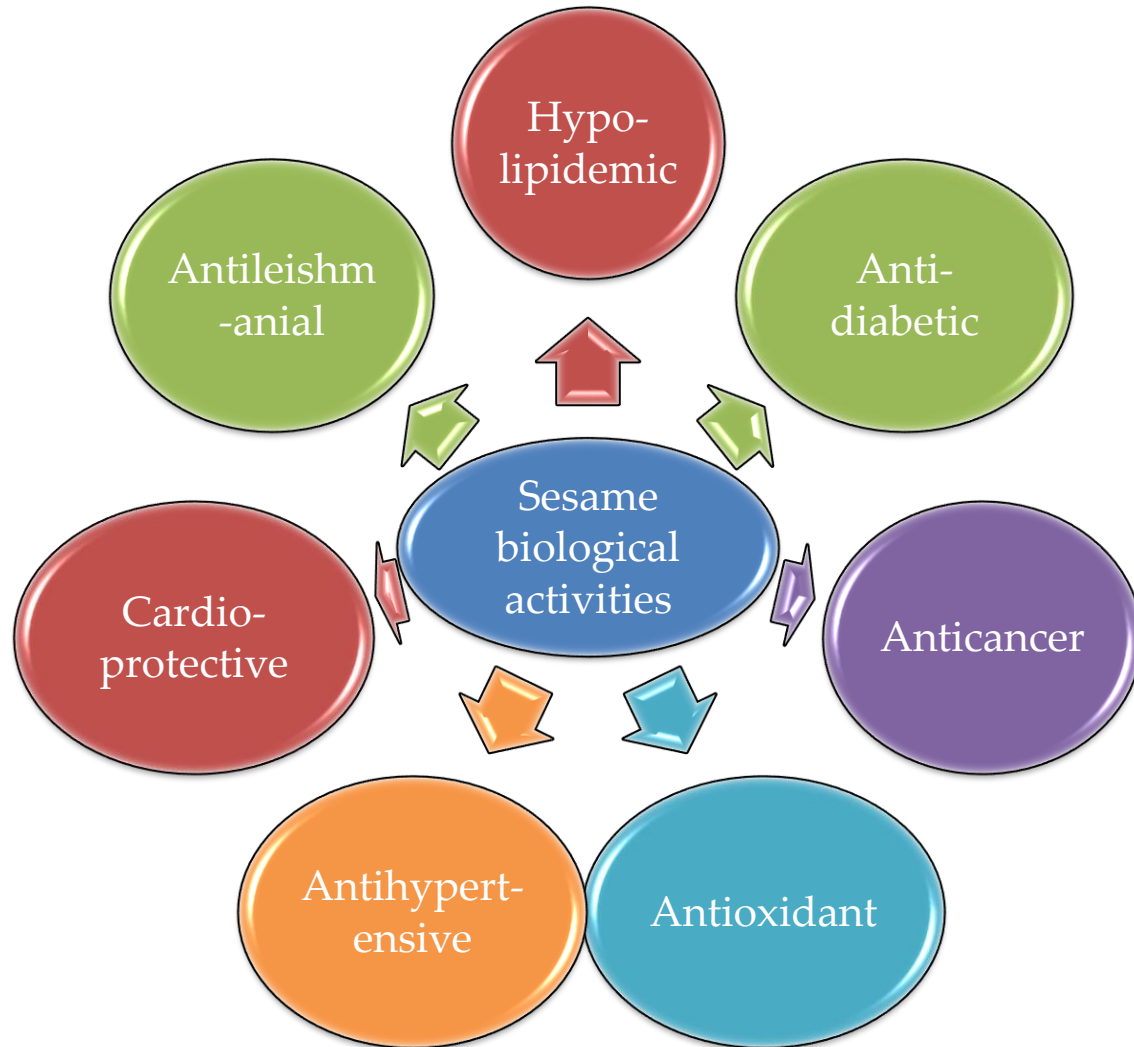


Pinoresinol diglucoside



Introduction

Reported biological activities in *S. indicum* (Selection)



[3]



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Aim of Work

1

- Performing untargeted profiling of SG 32 oil

2

- Comparing the phenolic composition of the sesame oil was with the cake counterpart.



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Material and methods

Recovery of the oil phenolic-rich fraction from SG32 seeds



Sesame Seeds
'Giza 32'
SG32

- 1) Homogenized in 10 mL *n*-hexane
- 2) Stirring 30 min
- 3) Centrifugation 5 min, 8000 rpm

Pellet
(Sesame Cake)

Supernatant

4) Evaporation

Sesame Oil

- 5) Reconstitution in hexane
- 6) Liquid-liquid extraction with (MeOH:H₂O, 80:20) × 3

RP-HPLC-
DAD-
QTOF-MS
& MS/MS

Material and methods

Untargeted Metabolic Profiling of the phenolic fraction SG32 oil by
RP-HPLC-DAD-QTOF-MS and MS/MS



Agilent 1200 series rapid resolution equipped with a diode array detector and A 6540 Agilent Ultra-High-Definition Accurate-Mass Q-TOF LC/MS (equipped with an ESI interface).



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MassHunter
Workstation Software

Qualitative Analysis

Version B.06.00

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Results and discussion

RP-HPLC-DAD-QTOF-MS and MS/MS Characterization of SG32 oil

Phenolic compounds characterized in the oil of Egyptian cultivar of Sesame 'Giza 32':															
	RT (min)	Experimental m/z [M+H] ⁺	Theoretical mass (M)	Molecular formula	Error (ppm)	Error (mDa)	Score	Main fragments	DBE	UV (nm)	Proposed compound	Subclass	Species	Family	Reference
63	21.32	463.0883	464.09548	C ₂₁ H ₂₀ O ₁₂	98.82	-0.02	-0.01	301.0324, 300.0248 271.0223, 255.0276, 178.9974, 151.0027, 136.0172, 135.0447	12	250, 352	Quercetin 3-O-β-D-glucopyranoside*	Flavonol	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	Mekky et al 2015/ Mekky et al 2019

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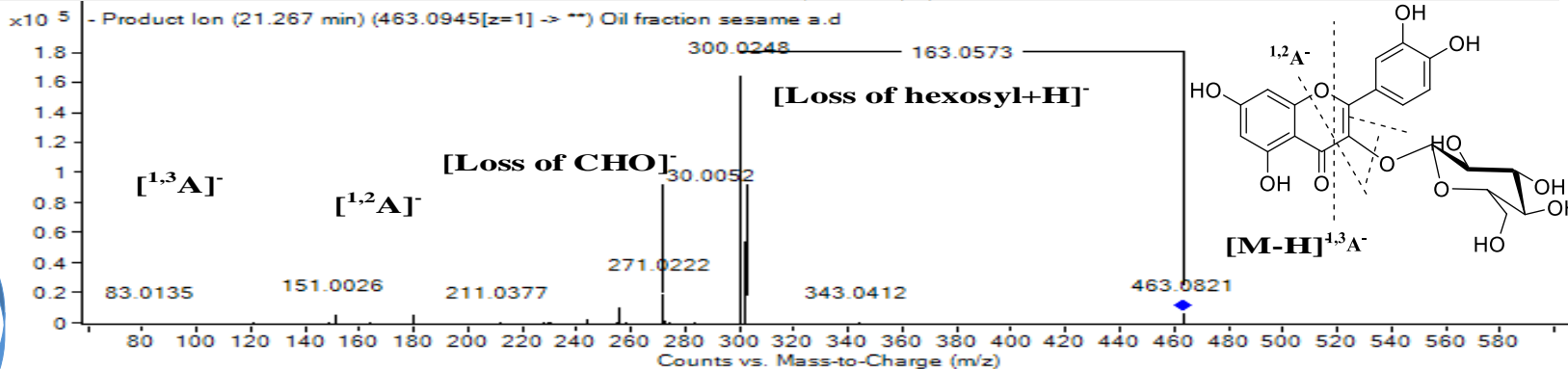
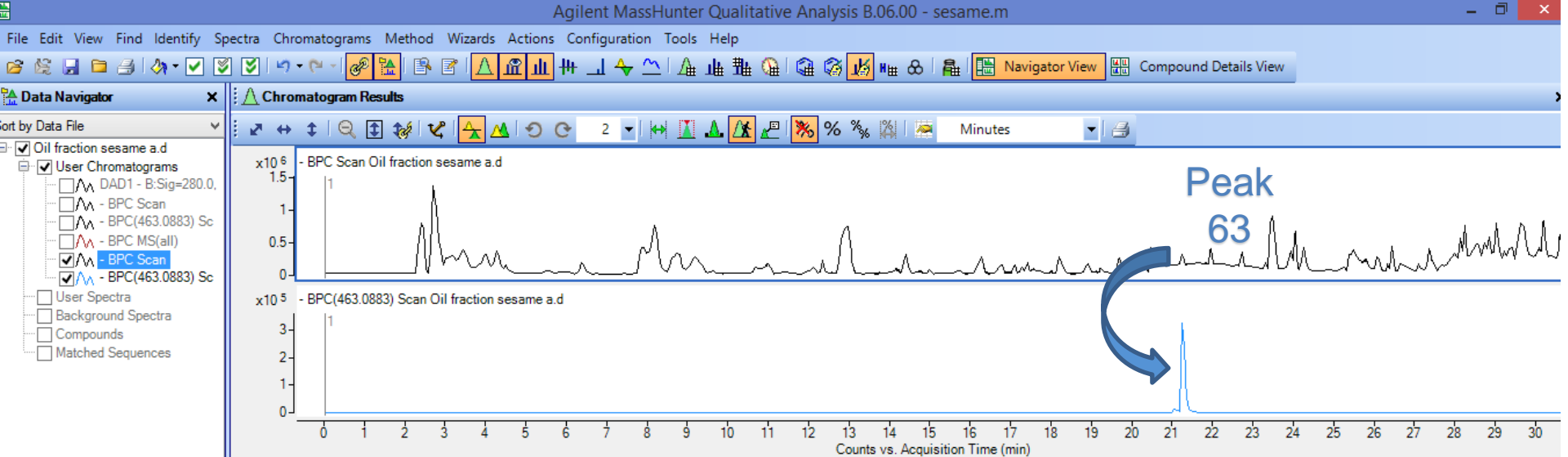


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Method Explorer: work...

Identify Compounds

Search Database

Search Accurate Mass...

Generate Formulas

Compound Automati...

Worklist Automation

Export

Method Editor: Generate Formulas

Generate Formulas from Compound

Allowed Species [Limits] [Change State] [Fragment Formulas]

Charge carrier to be assumed if not known

Positive ions: [electron] [+H] [+Na] [+K] [+NH4] [+2H5] [+C3H5]

Negative ions: [electron] [-H] [-Cl] [-Br] [-COOH] [-CF3COOH] [-CH2COOH]

MS ion electron state: allow both even and odd

Group hits with same formula (but different charge carriers)

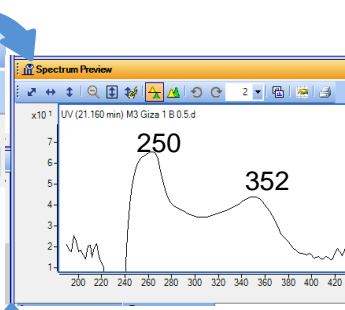
Elements and limits

Element	Minimum	Maximum
C	3	60
H	0	120
O	0	30
N	0	0
S	0	0

Spectrum Identification Results: - Scan (21.242 min)

Automatically Show Columns

Score (MFG)	Diff (ppm)	m/z	Formula	Species	Score	ID Source	Diff (mDa)	RT	Mass (MFG)
99	0.27	463.08803	C21 H20 O12	(M-H)-	99	MFG	0.13		464.09548



Quercetin 3-O-β-D-glucopyranoside

23/10/2020



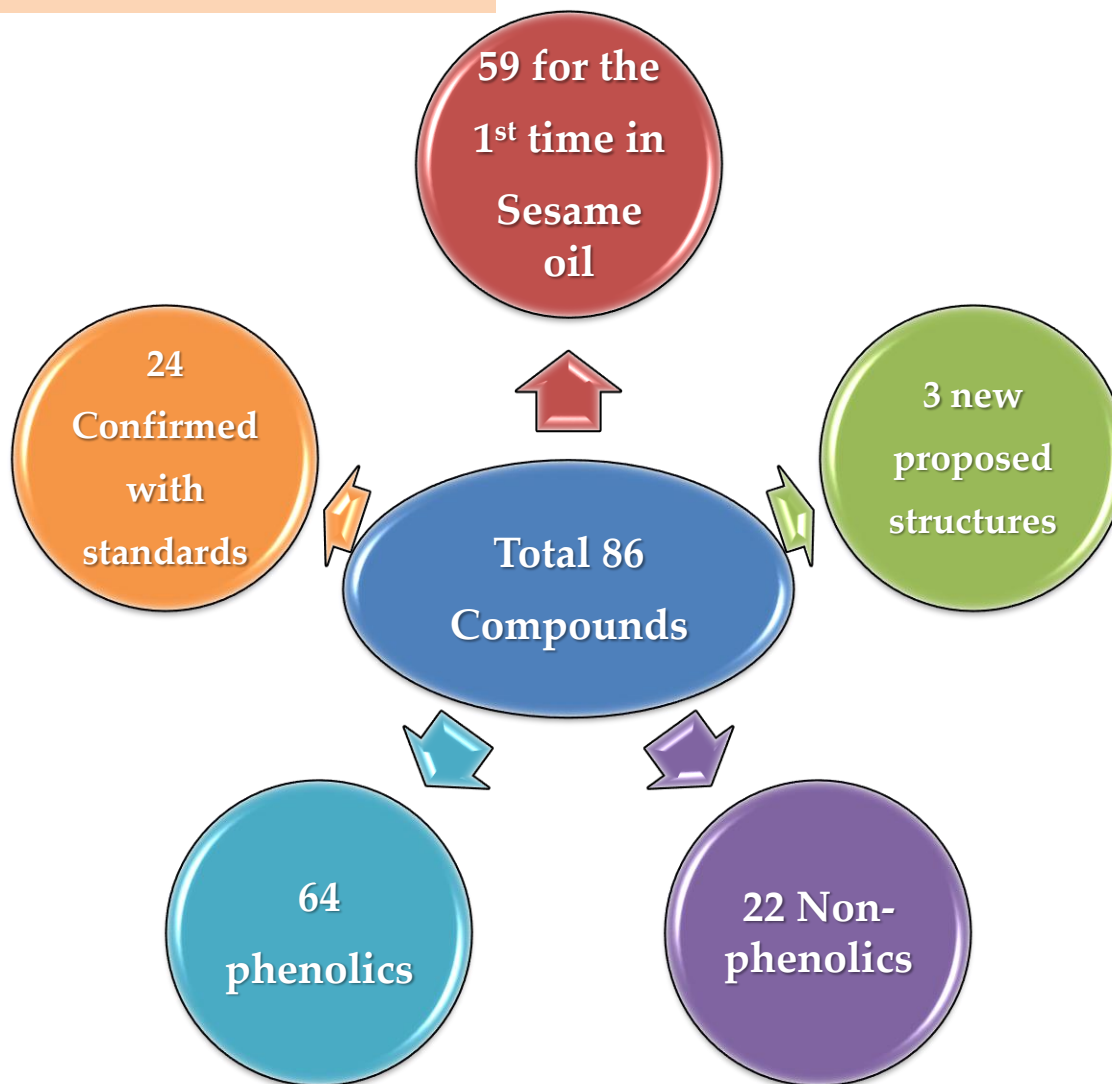
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Flavonols



The Global Number of Characterized Compounds from SG 32 Oil

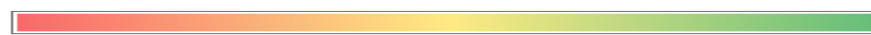
Results and discussion



Results and discussion

Classification, number of compounds found per class, and relative in sesame oil.

	Class	Number	Mean area
	Phenolic metabolites		
★	Coumarins	1	1.60E+04
	Flavonoids	19	1.48E+07
	Hydroxybenzoic acids	13	7.54E+06
	Hydroxycinnamic acids	19	9.47E+06
	Lignans	10	1.20E+07
	Phenol derivatives	1	1.43E+05
	Phenolic aldehydes	1	1.14E+05
	Non-phenolic metabolites		
	Amino acids	8	9.82E+06
★	Peptides	1	1.25E+06
	Organic acids	13	2.28E+07



Lowest value

Highest value

Comparison between Sesame Oil and Cake

Results and discussion



A Venn diagram illustrating the common metabolites between SG32 oil and SG32 cake.

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Conclusion

- The present study demonstrates the first report dealing with the metabolic profiling of sesame oil using RP-HPLC–DAD–ESI–QTOF-MS and -MS/MS.
- 86 metabolites, mainly belonging to the phenolic class were characterized.
- 64 metabolites were commonly present in both SG32 oil and cake.
- Further studies are required to trace the presence of biologically important metabolites in commercial sesame oils

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References

1. FAO-Statistics (2018). Productions, crops.
2. Aboelsoud, N.H. Herbal medicine in ancient Egypt. *Journal of Medicinal Plants Research* **2010**, 4, 082-086.
3. Lim, T. *Sesamum indicum*. In *Edible Medicinal and Non-Medicinal Plants*, Springer: 2012; Vol. 4, pp. 187-219.

Thank you!!!

Questions