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Molecular-Level Insights into Quercetin and Caffeic Acid Extraction Using Choline Chloride–Glycerol Deep Eutectic Solvent: A Quantum Mechanical Approach

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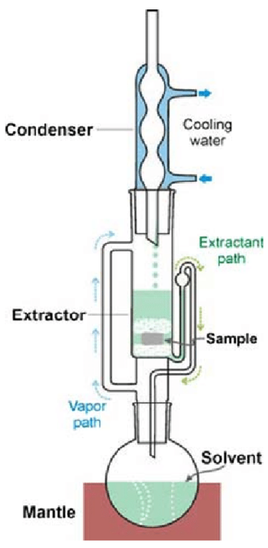
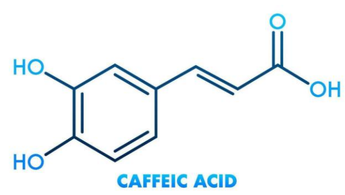
INTRODUCTION & AIM

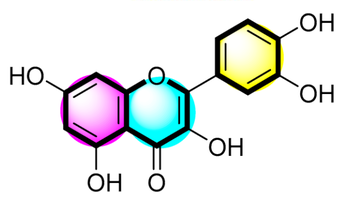


Extraction Setup

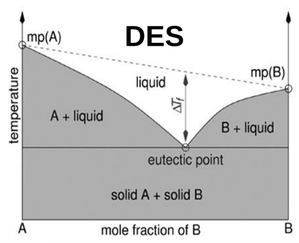
- Quercetin (QUE) and caffeic acid (CAF) are valuable bioactive compounds with health benefits [1,2].
- Efficient and sustainable extraction methods [3] are essential for their recovery.
- Deep eutectic solvents (DES), like choline chloride–glycerol (CLC-GLY), offer a green alternative to conventional solvents.



CAFFEIC ACID



Quercetin

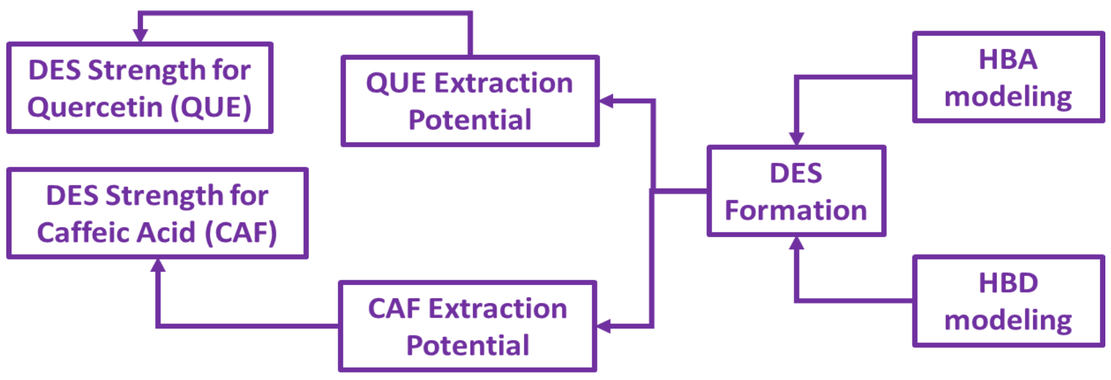


Aim of Study:

To investigate, using quantum mechanical (DFT) calculations, the molecular interactions between quercetin and caffeic acid with choline chloride–glycerol DES, and to assess its extraction efficiency compared to conventional solvent (ethanol – ETOH).

METHOD

Study Flow deployed in the Computational Study



Computational Resource:

Student Spartan v9

Computational Detail:

Density Functional Theory (DFT) [4] and compare its extraction potential with ethanol. All calculations were carried out using the wB97X-D functional, which accounts for dispersion corrections, starting from PM3-optimized geometries. A dual basis set (6-31G(d)/3-21G*) was employed in the gas phase.

RESULTS & DISCUSSION

- Choline chloride is a better acceptor (more reactive, less stable).
- Glycerol and choline chloride form a stable DES with a formation energy of -1.48 eV.

Table 1. DES Formation mechanism

Specie	HOMO	LUMO	E Gap	Interaction E-Gap		Formation energy (eV)
				HBA LUMO	HBA HOMO	
HBA	-7.90	2.65	10.55	10.55	10.55	-1.48
HBD	-9.90	3.61	13.51	12.55	11.52	

Table 2. Molecular properties

Species	HOMO	LUMO	E Gap	CAF IEG		QUE IEG	
				HBA LUMO	HBA HOMO	HBA LUMO	HBA HOMO
CAF	-8.69	-0.65	8.04	8.04	8.04	8.41	8.52
QUE	-9.17	-0.28	8.89	8.52	8.41	8.89	8.89
CLC-GLY	-9.00	2.19	11.19	8.35	10.88	8.72	11.36
ETOH	-9.78	4.28	14.06	9.13	12.97	9.50	13.45

- CLC–GLY (11.19 eV) has a lower energy gap than ethanol (14.06 eV), so it's more reactive but less stable.
- CLC–GLY showed better interaction with both CAF and QUE compared to the use of ethanol.
- CLC–GLY shows stronger binding with caffeic acid (–1.12 eV) and quercetin (–0.96 eV) than ethanol (–0.33 eV, –0.30 eV).
- CLC–GLY indicates better extraction potential than ethanol.

Table 3. Bioactive compounds extractive potential of the different solvents

Species	CAF Binding energy (eV)	QUE Binding energy (eV)
CLC-GLY	-1.12	-0.96
ETOH	-0.33	-0.30

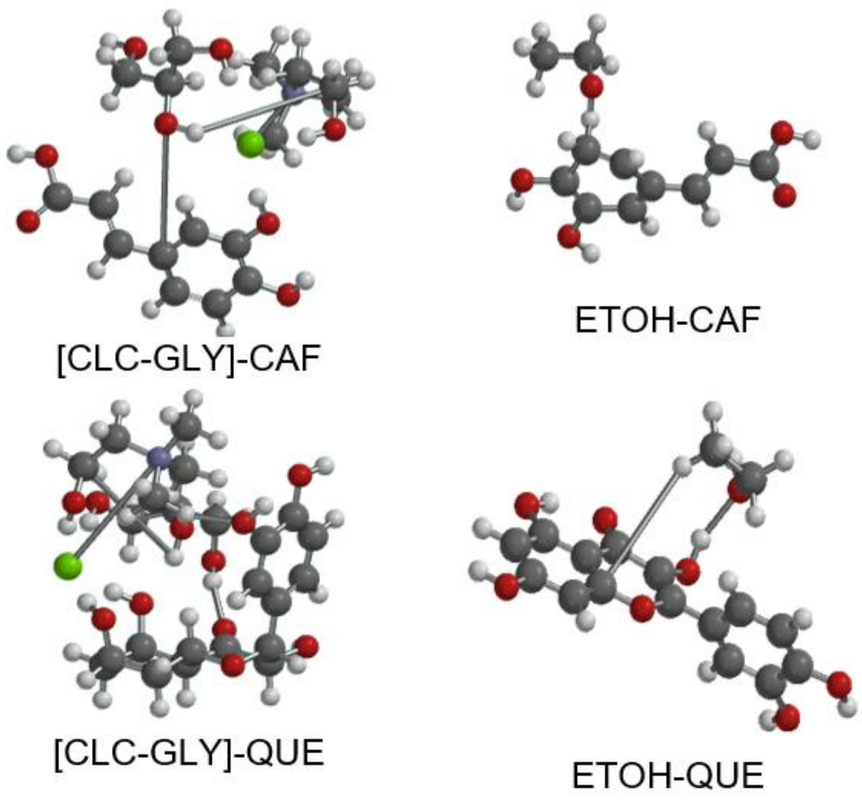


Figure 1 Molecular structure of CAF and QUE with the different solvents

CONCLUSION

- CLC–GLY showed stronger binding with quercetin and caffeic acid than ethanol, indicating better extraction performance.
- Higher reactivity and green nature make CLC–GLY, a promising solvent for sustainable pharmaceutical use.

ACKNOWLEDGEMENT

Spartan Student

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[2] Ming Z. (2021). *Horticulturae* 7(11):491.
[3] Magdalena R. (2021). *Scientific Technical Review* 71(2):41.
[4] Kyle et al. (2014). *Journal of Chemical Education* 91(12):2116-2123