

# CHARACTERIZATION OF STARCH-BASED BIOPLASTICS

## (AMYLOSE/AMYLOPECTIN) AS AN ALTERNATIVE TO NON-RENEWABLE MATERIALS THROUGH MD AND MQ SIMULATIONS.

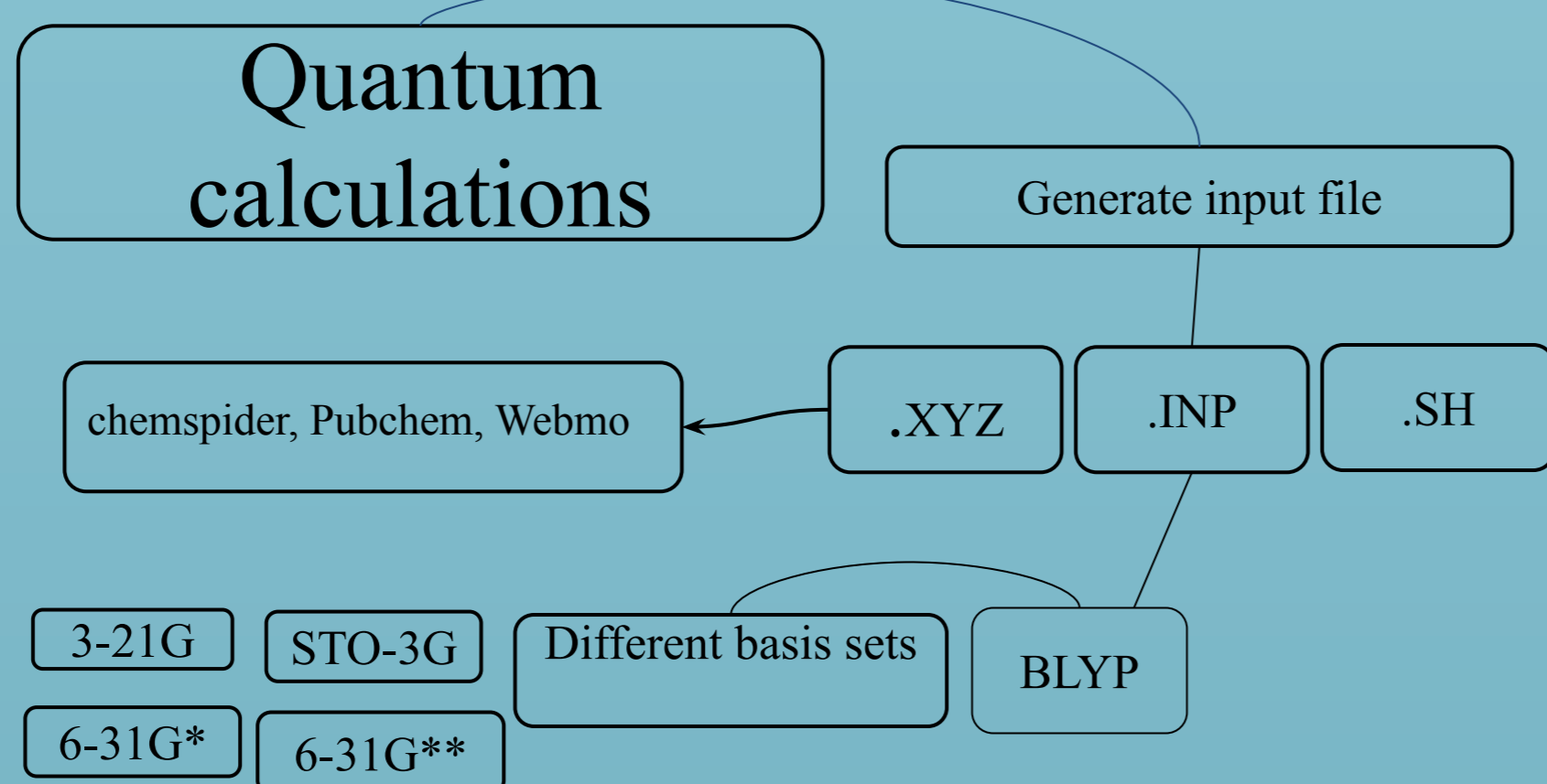
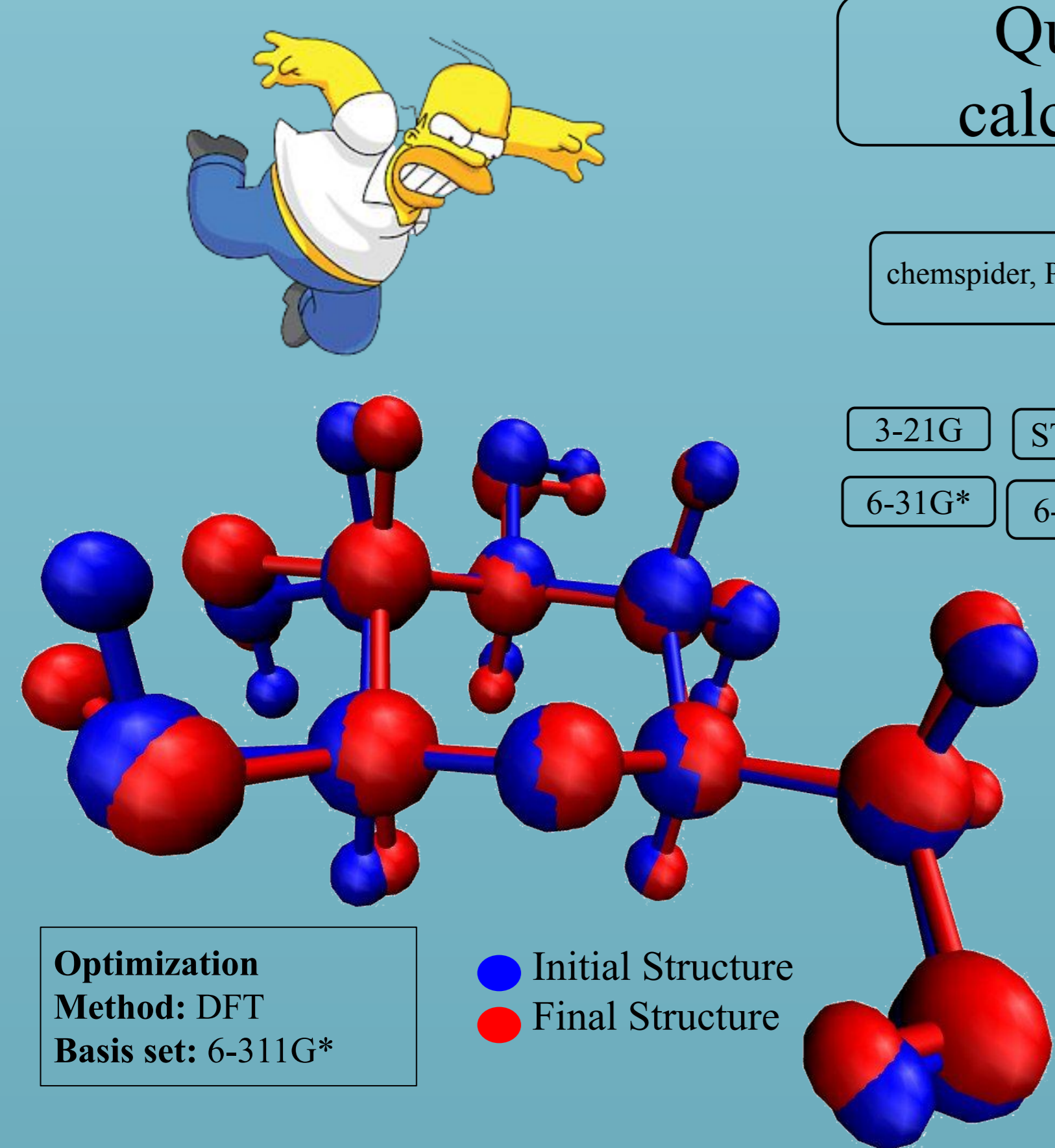
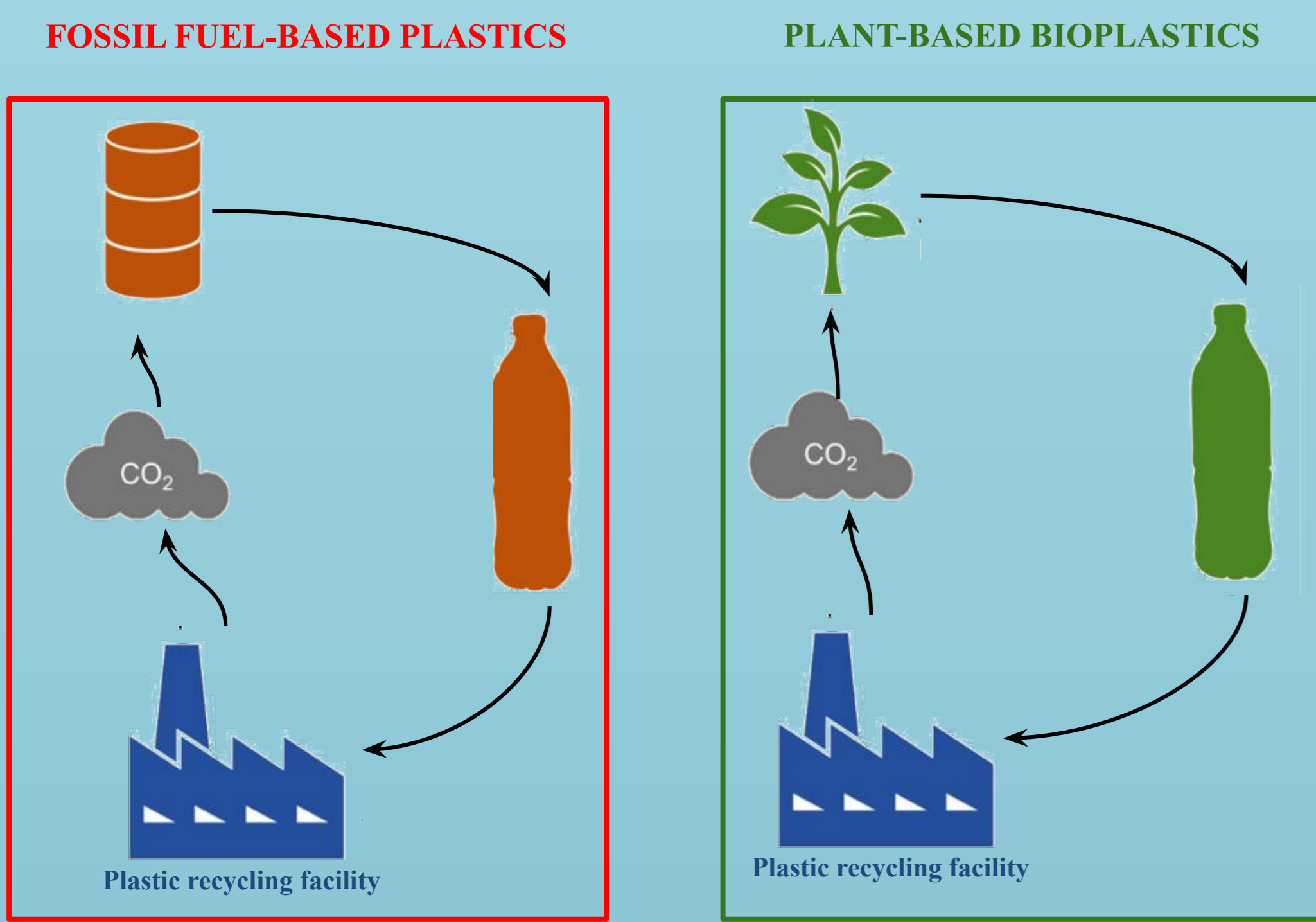
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### PLASTIC PROBLEMATIC & ALTERNATIVES



DIFERENCE OF POSITION IN GLUCOSE (Ams)

	C0-C1	H0-O	O-C	C1-C2	C2-C3	C3-C4	03-H6
TZVP	1.523	0.973	1.973	1.547	1.537	1.532	0.975
cc-pVDZ	1.527	0.978	1.959	1.548	1.537	1.532	0.980
cc-pVTZ	1.523	0.971	1.969	1.545	1.535	1.530	0.973
cc-pVQZ	1.523	0.969	1.972	1.546	1.536	1.531	0.972

DIFERENCE OF POSITION IN GLUCOSE (Ams)

	C0-C1	H0-O	O-C	C1-C2	C2-C3	C3-C4	03-H6
3.61G	1.524	0.990	2.021	1.548	1.538	1.532	0.991
6-31G*	1.529	0.976	1.959	1.551	1.540	1.534	0.978
6-311G**	1.523	0.974	1.967	1.547	1.536	1.530	0.975

### Bonding & Non-bonding Interactions

**Bonding interactions**  
Bond Potential (Harmonic Potential)

$$V(r_{ij}) = \frac{1}{2}K_{ij}(r_{ij} - r_{0ij})^2$$

Angle Bending Potential (Harmonic Potential)

$$V(r_{ijk}) = \frac{1}{2}K_{ijk}(r_{ijk} - r_{0ijk})^2$$

Dihedral Potential (Torsion Angle Potential)

$$V_{id}(ijkl) = \frac{1}{2}k_{ijkl}(r_{ijkl} - r_{0ijkl})^2$$

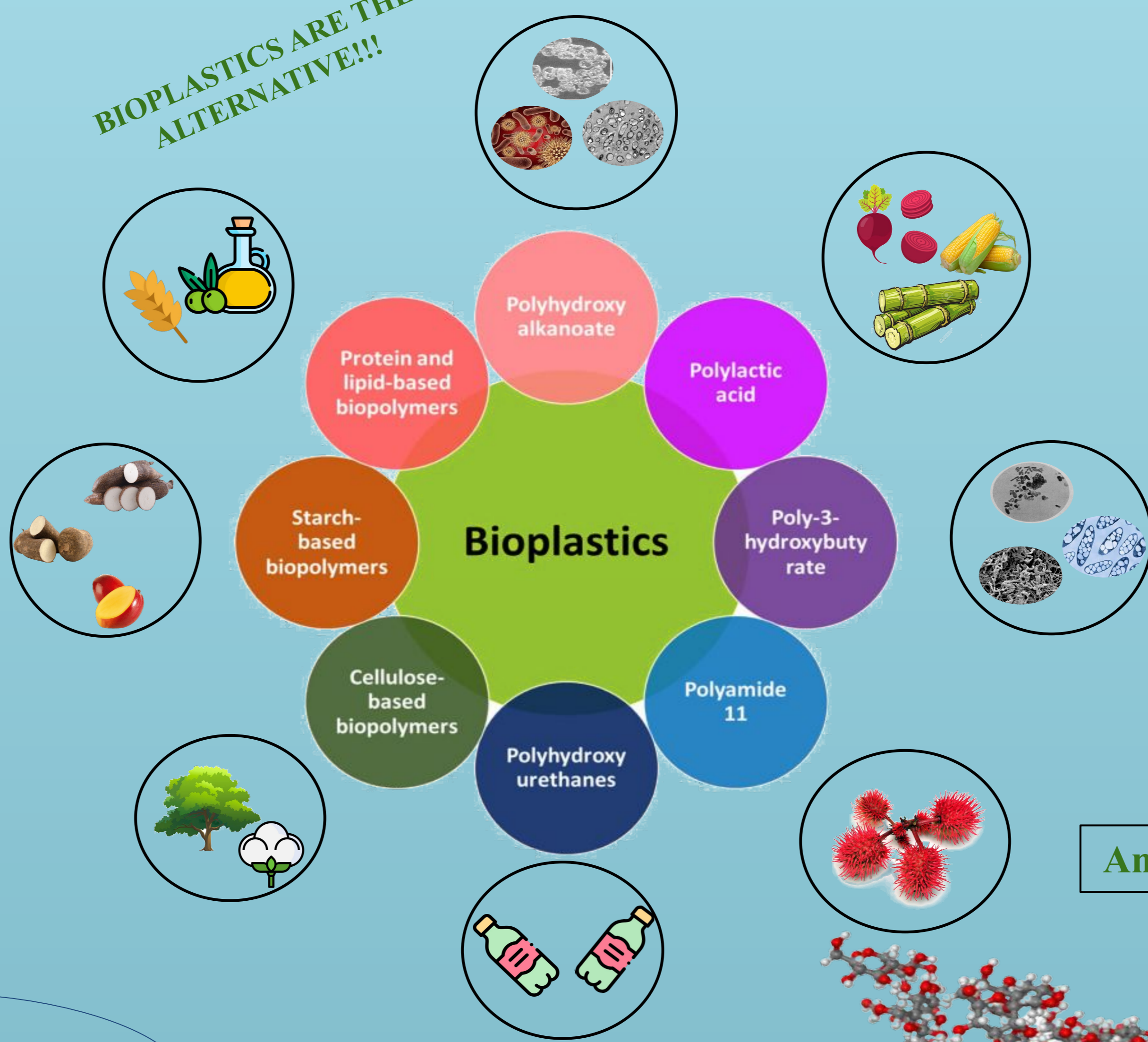
**Non-bonding interactions**  
Electrostatic Interaction

$$(F) = k \frac{q1^+q1^-}{r^2}$$

Lennard-Jones Potential (12-6)

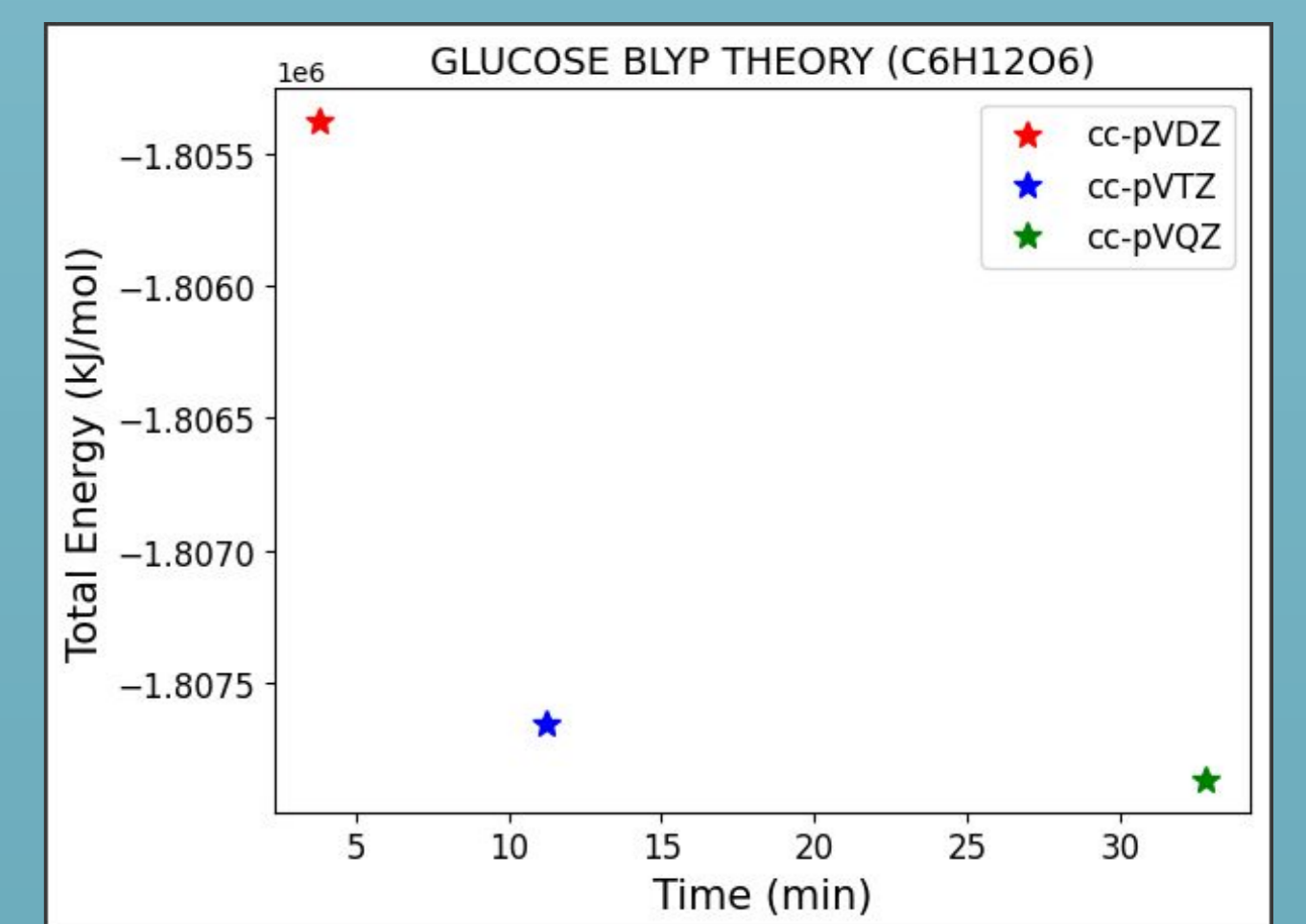
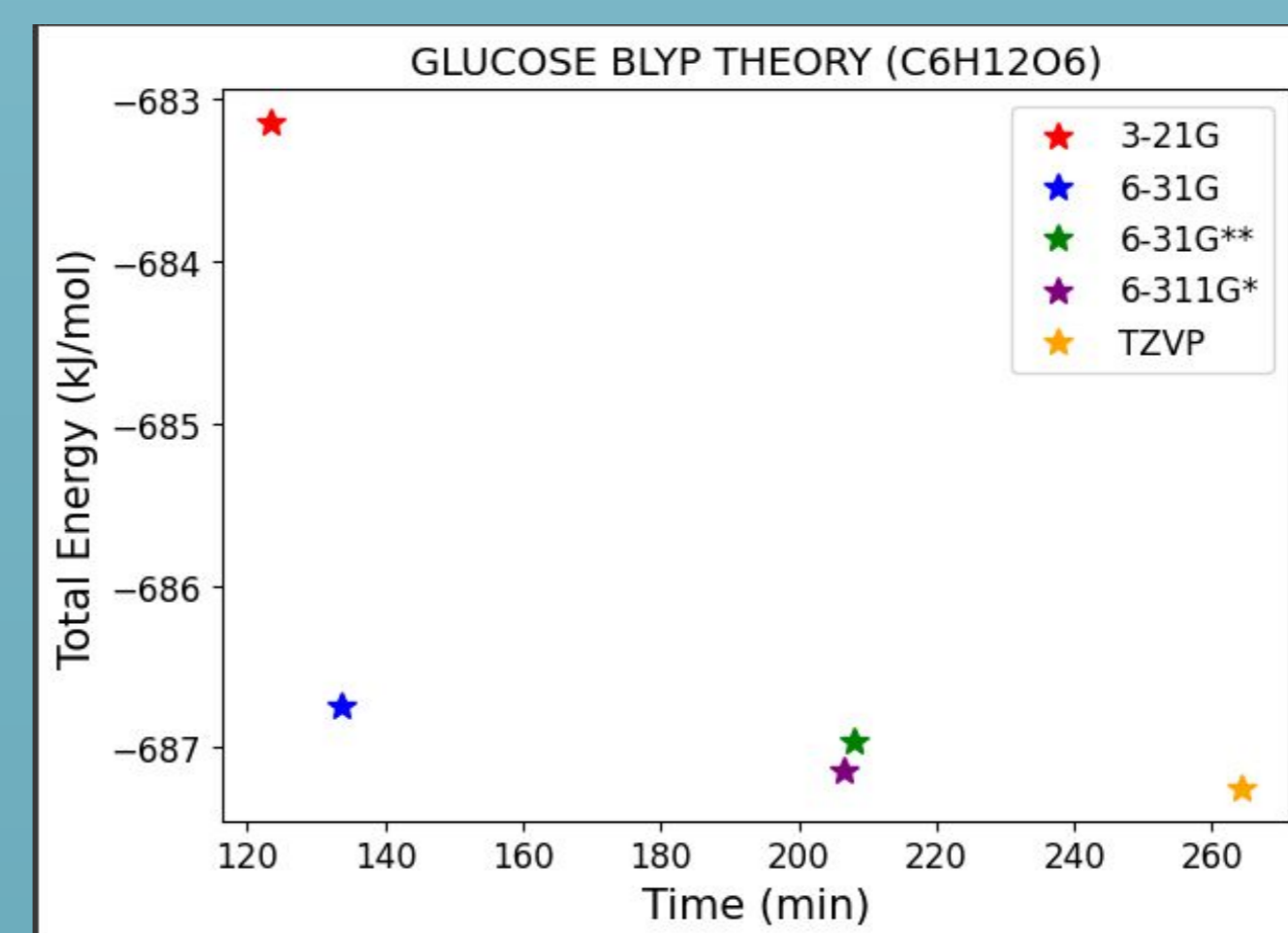
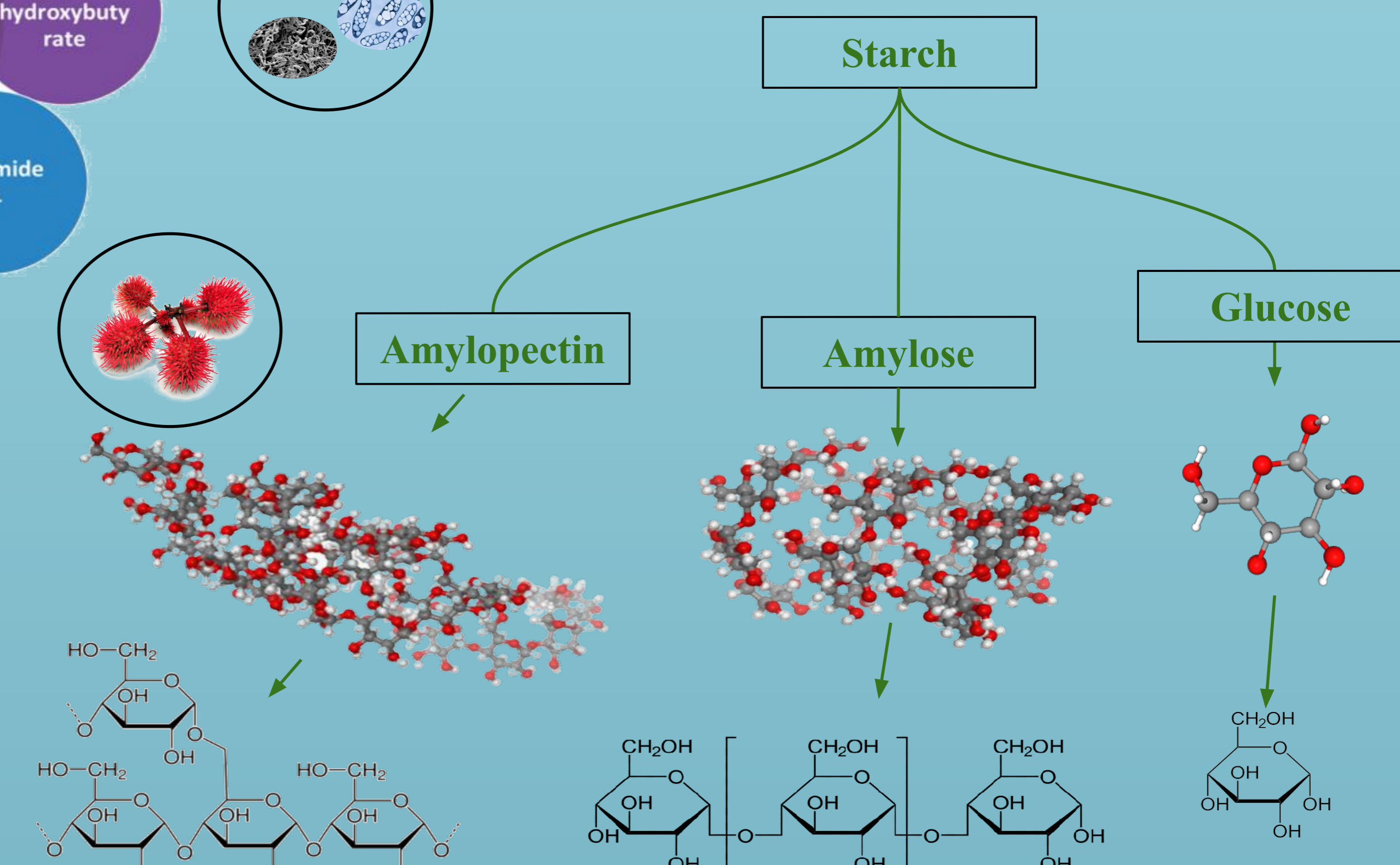
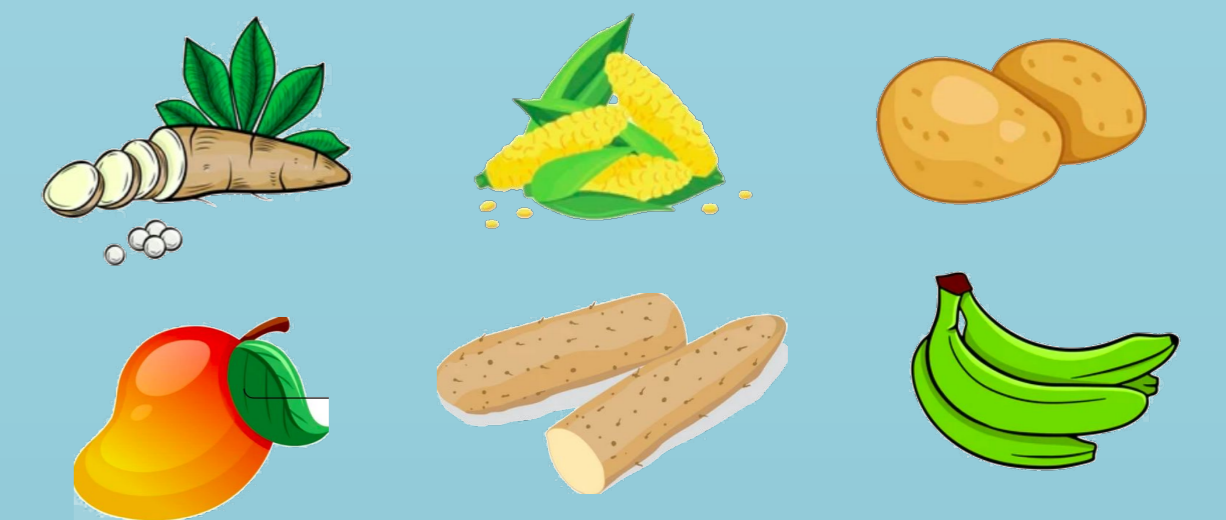
$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

BIOPLASTICS ARE THE ALTERNATIVE!!!



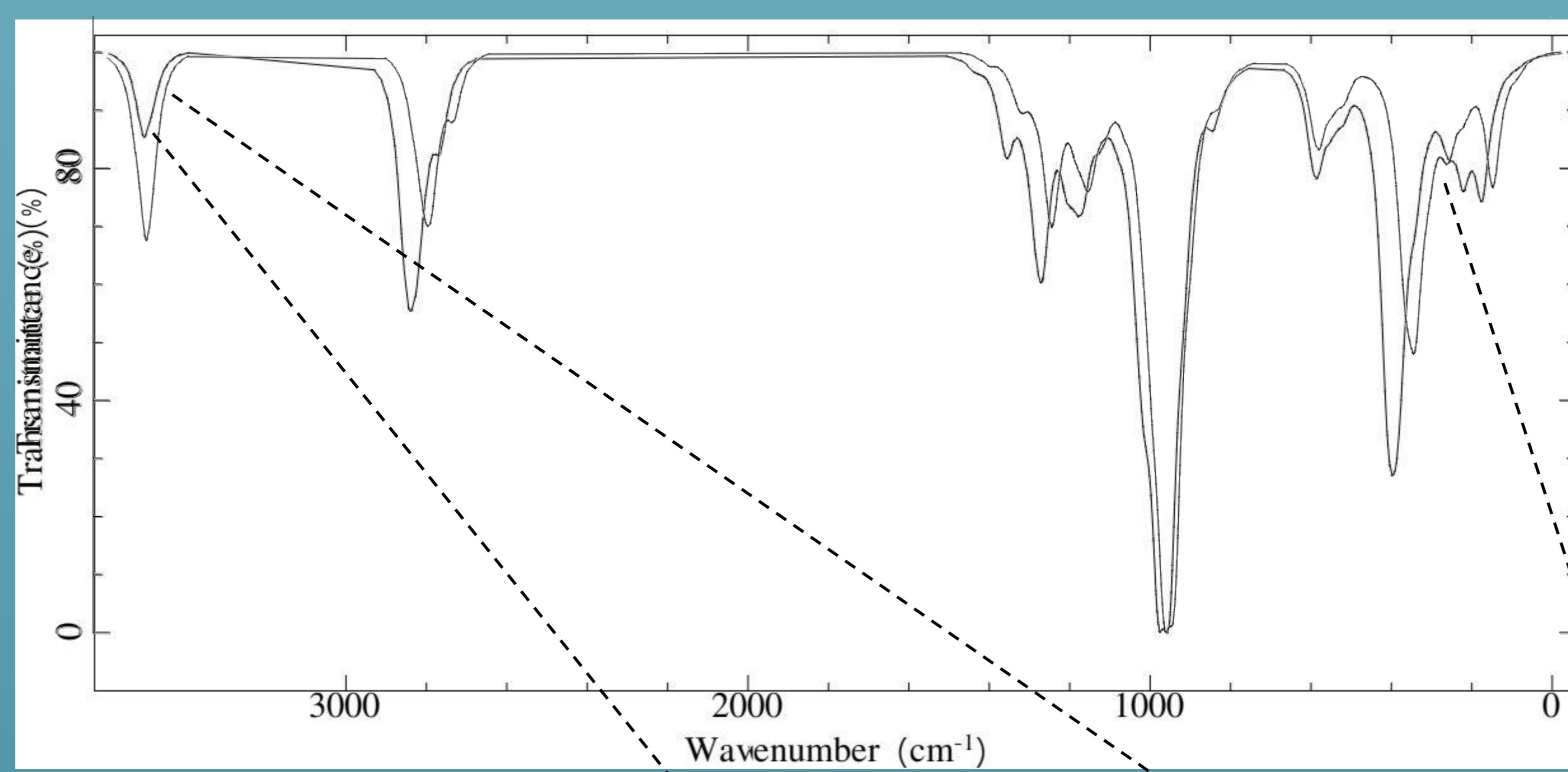
### STARCH-BASED BIOPOLYMERS

#### MAIN SOURCES OF STARCH



### OVERLAPED INFRARED SPECTRUM

BLYP Theory and 6-311g\*\* basis set vs BLYP Theory and cc-pVQZ basis set



ENERGY / TIME GLUCOSE

	cc-pVDZ/ cc-pVTZ	cc-pVTZ/ cc-pVQZ
deltaEnergy (KJ/mol)	-1142.7595	-886.59867
delta Time (min)	7.43	21.24

### Software and HPC



### Preliminary Conclusions

- The importance of carefully choosing the basis set in quantum chemistry calculations lies in considering both the accuracy of the results and the required computational time.

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### References

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