

SNS COLLEGE OF PHARMACY AND HEALTH SCIENCES



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Coimbatore -641035*

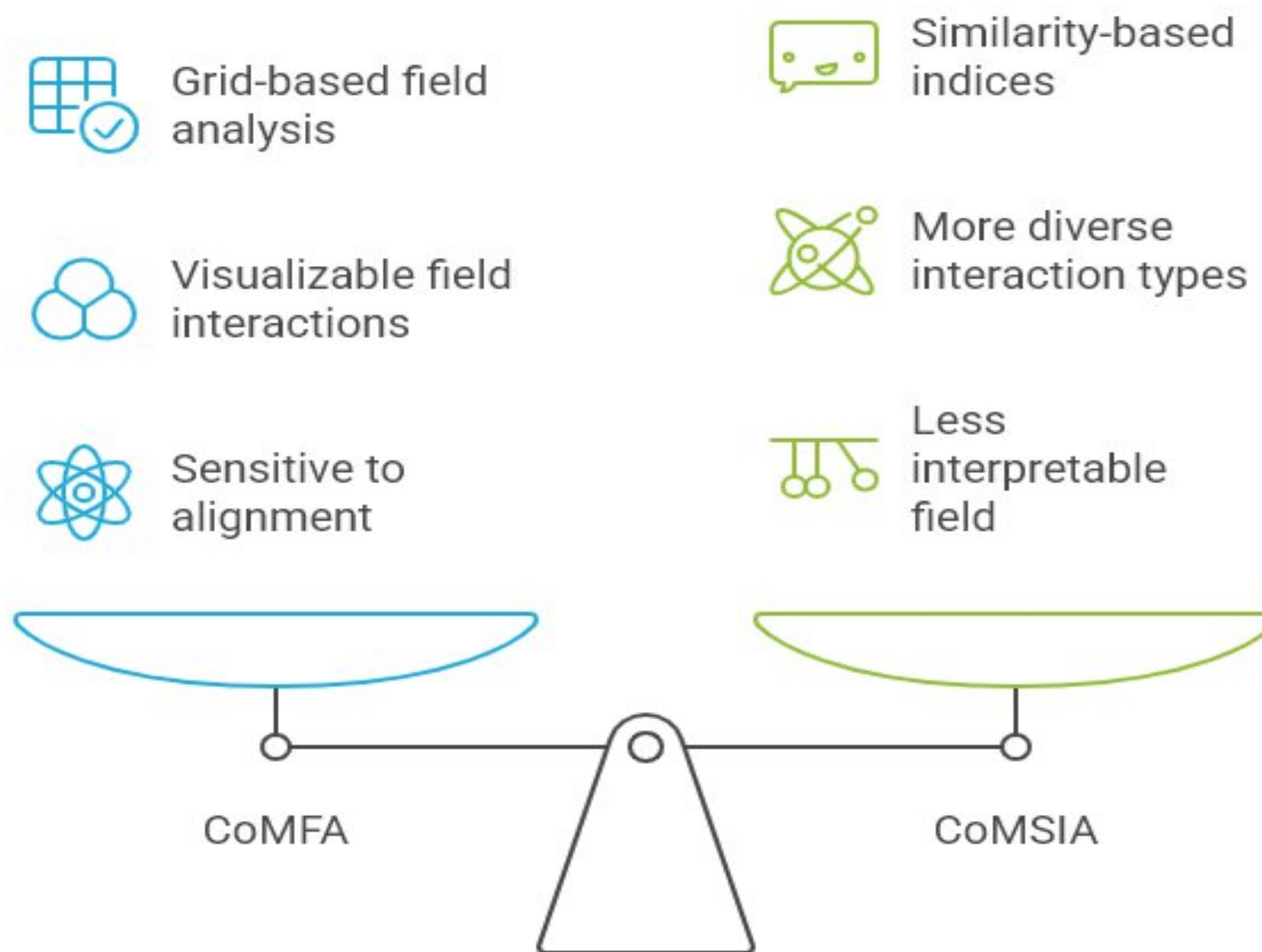
COURSE NAME : COMPUTER AIDED DRUG DESIGN(BP 807 ET)

VIII SEM / IV YEAR

TOPIC: CoMFA AND CoMSIA

COMPARISON OF coMFA AND coMSIA

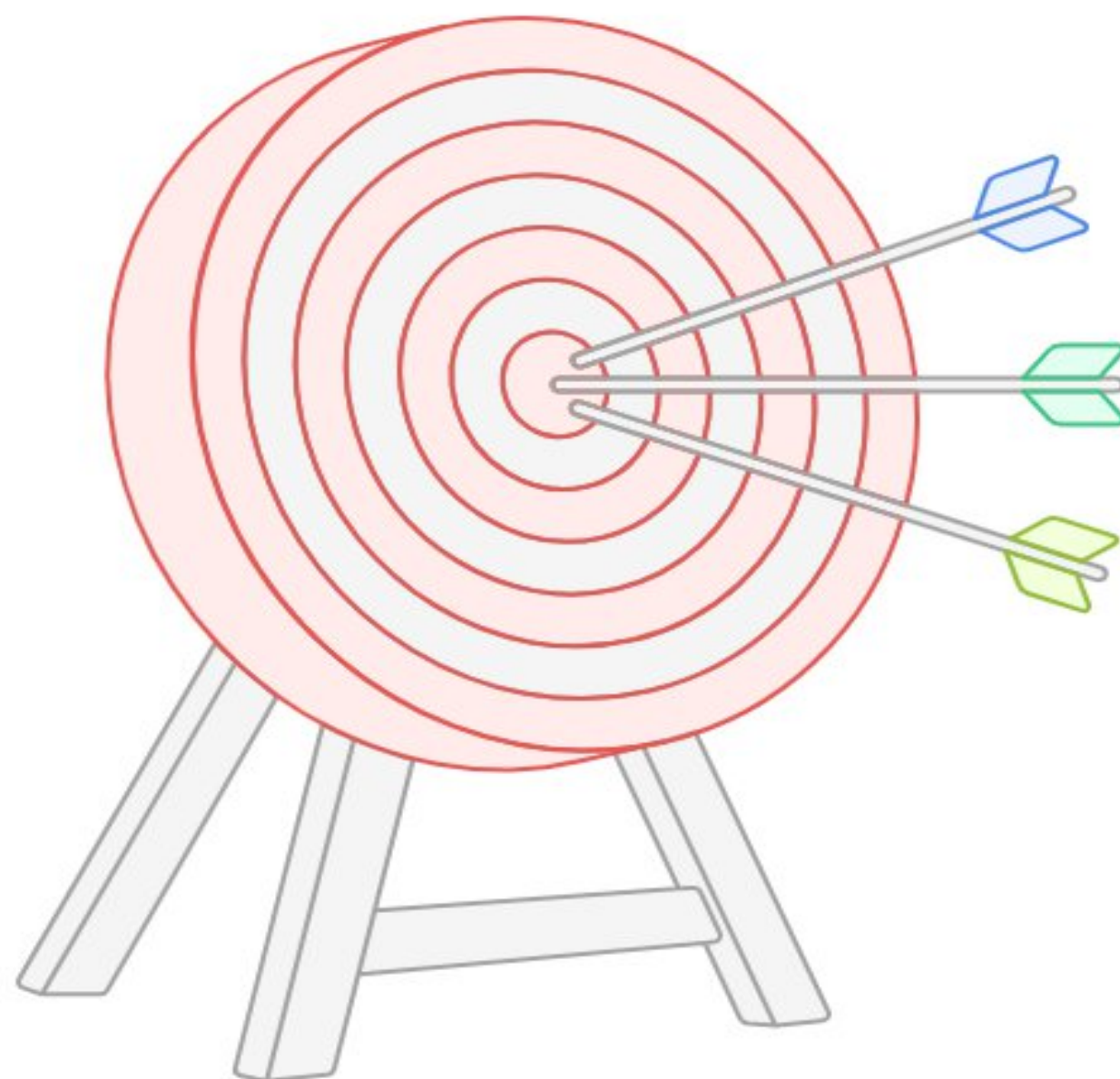
Comparing CoMFA and CoMSIA for 3D-QSAR



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CoMFA AND COMSIA ANALYSIS

3D-QSAR in Drug Discovery



3D-QSAR

Core method for structure-activity relationships



CoMFA

Field-based analysis for molecular interactions



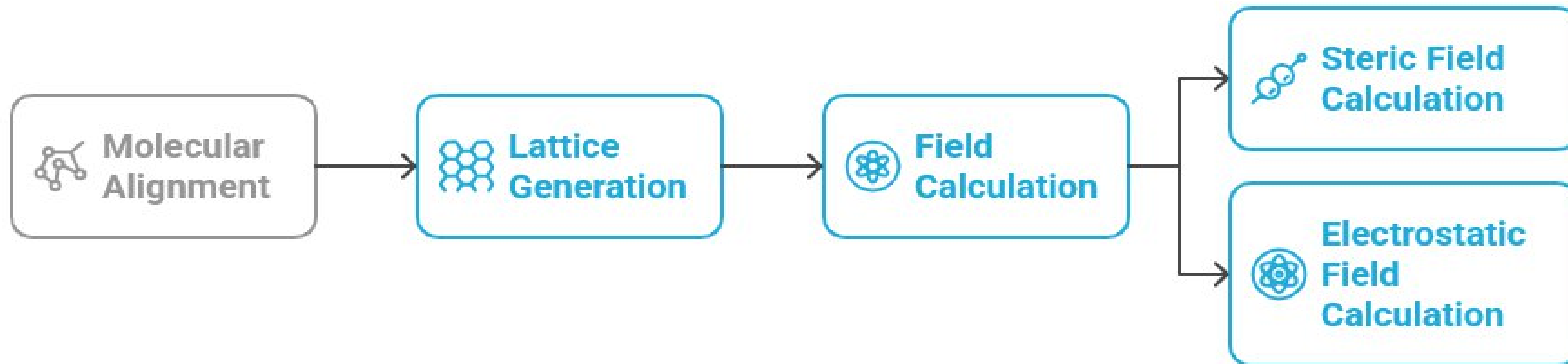
CoMSIA

Similarity-based analysis for molecular properties

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FIELD CALCULATION

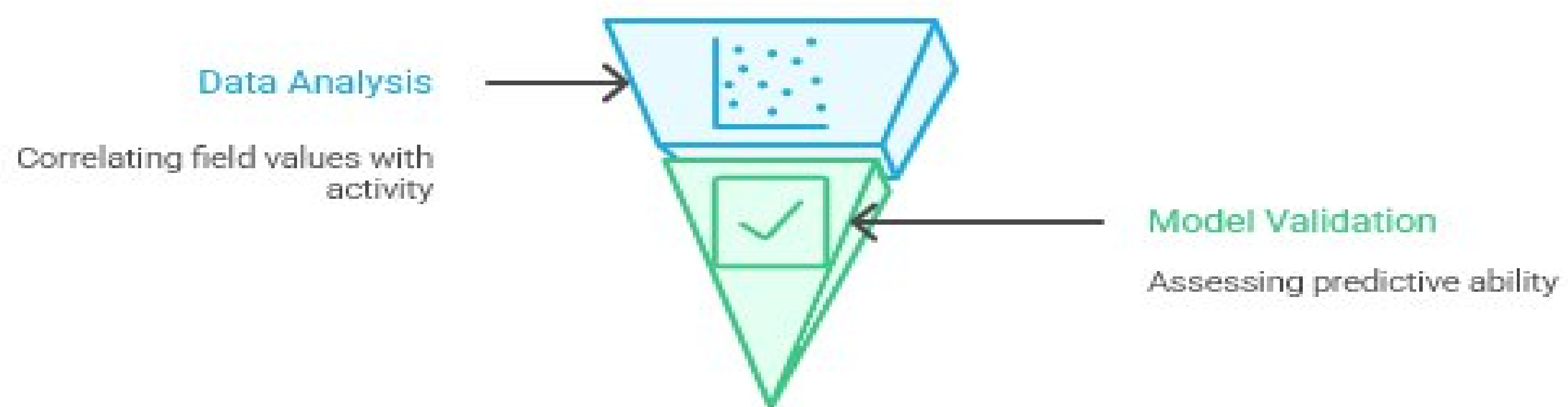
CoMFA Field Calculation Process



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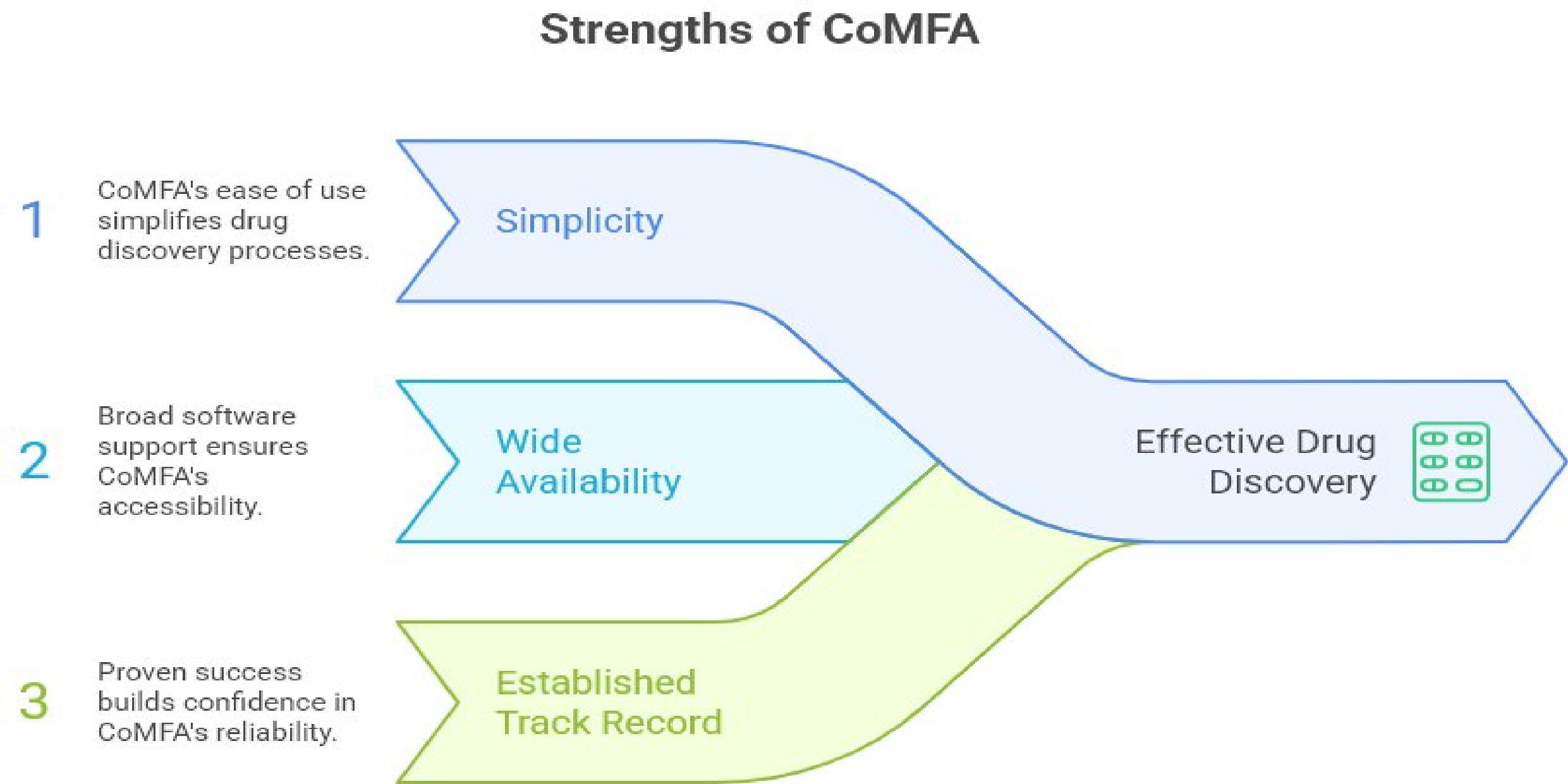
DEVELOPMENT PROCESS

CoMFA Model Development Process



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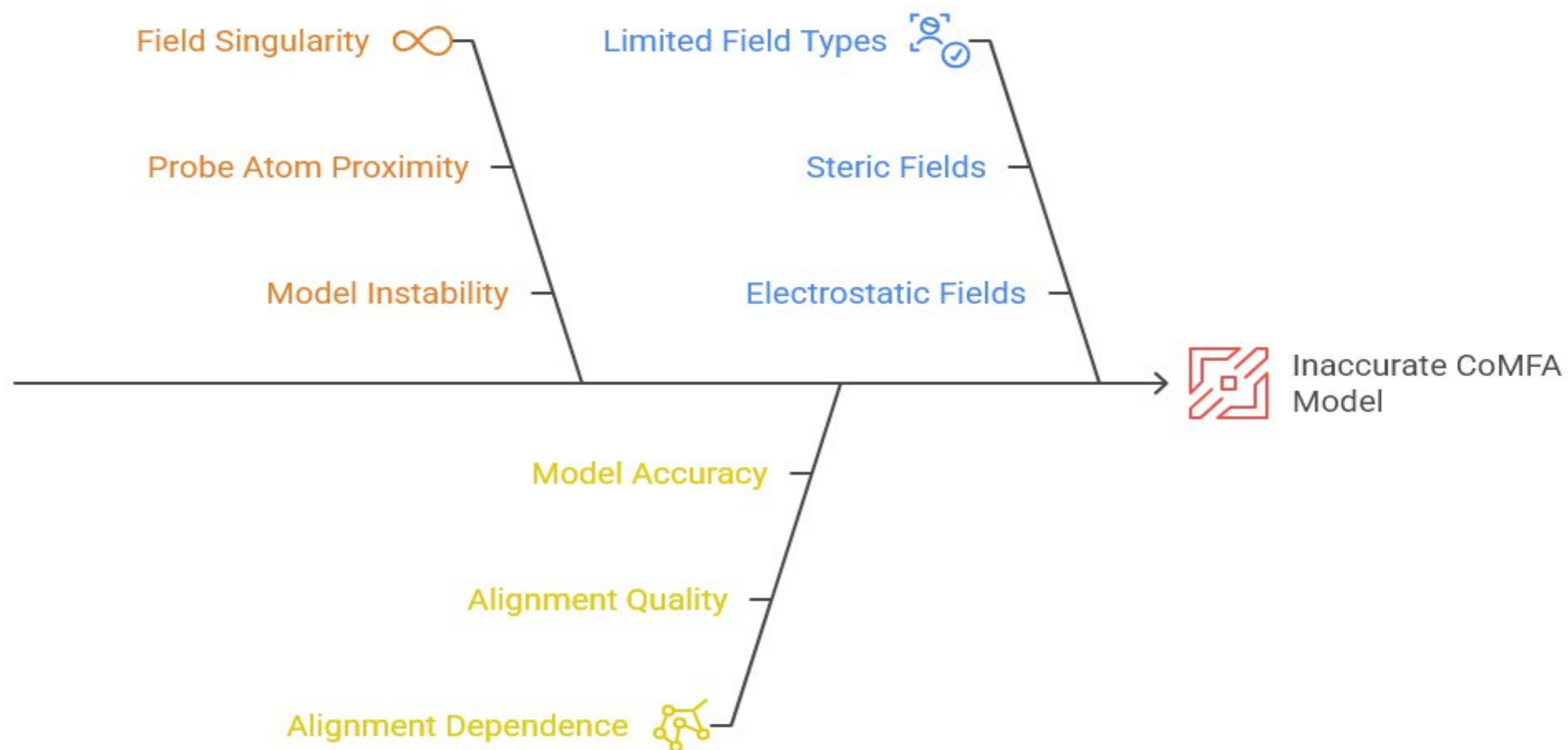
STRENGTHS OF CoMFA



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CHALLENGES OF CoMFA

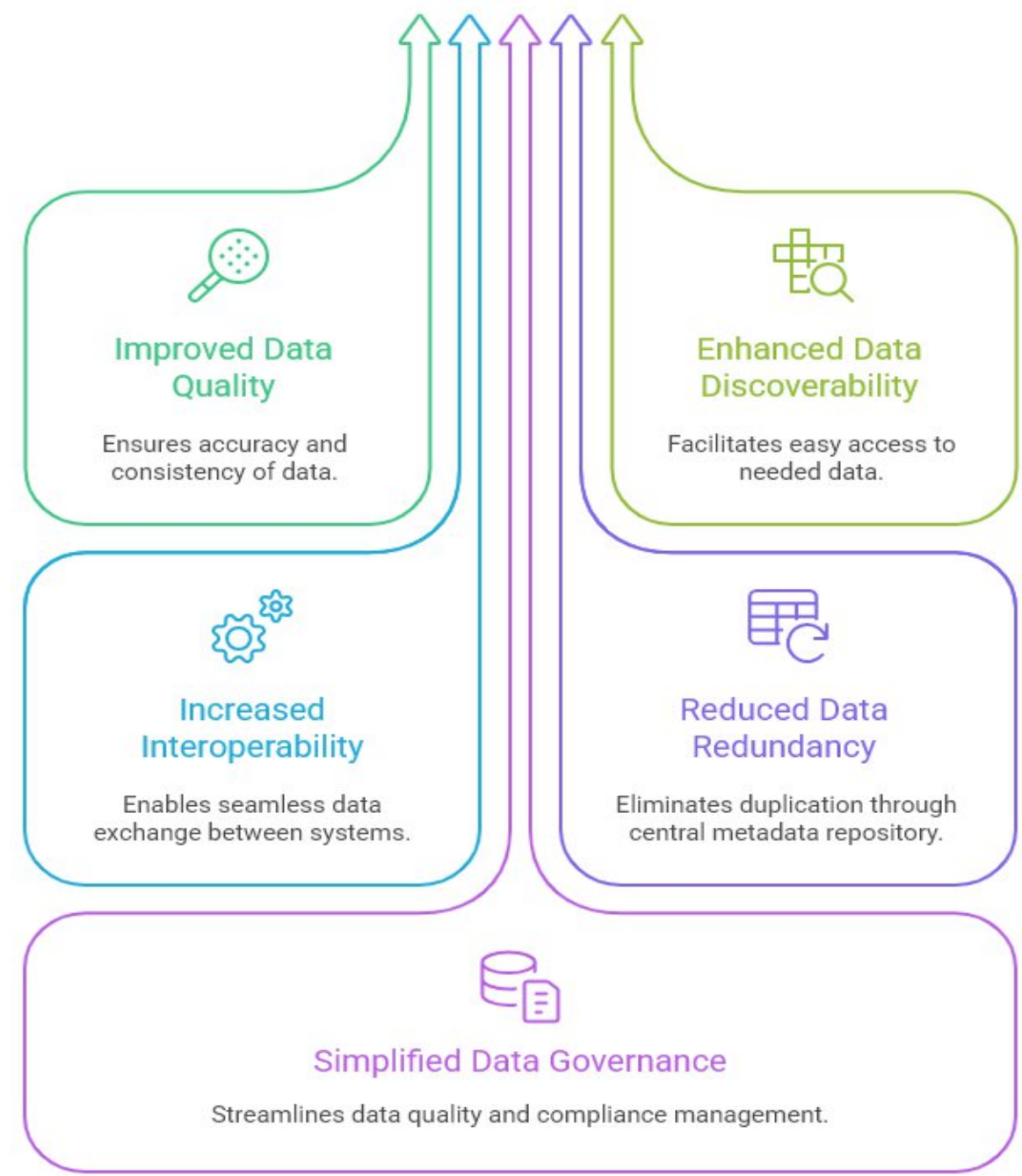
Challenges in CoMFA Model Accuracy



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CoMFA MANAGEMENT ADVANTAGES

COMFA's Data Management Advantages

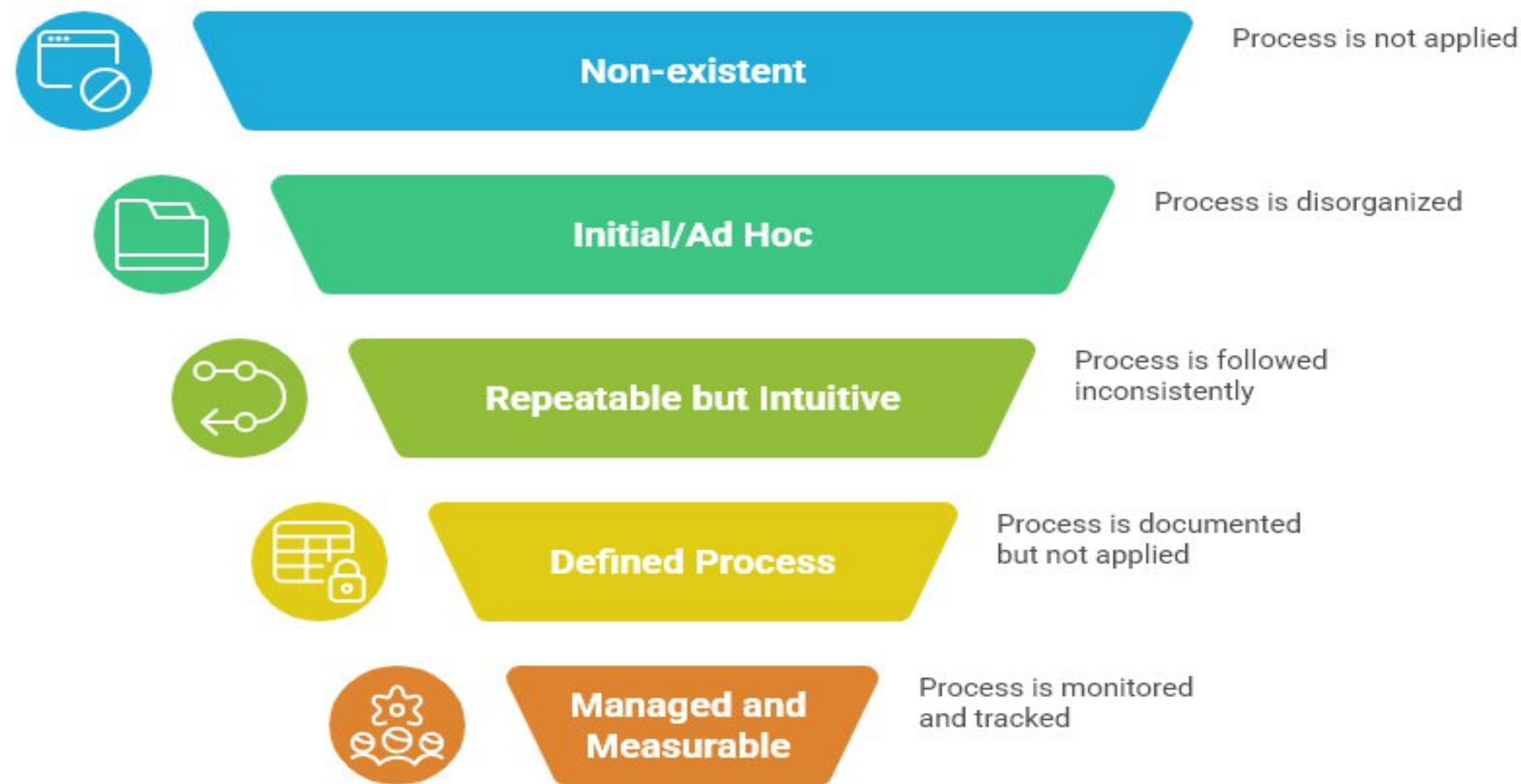


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CoMFA MATURITY PROCESS



COMFA Maturity Process



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COMFA's Core Functions



Metadata Standardization

Enforces common metadata schemas and vocabularies.



Metadata Discovery

Enables easy access to relevant metadata.



Metadata Interoperability

Facilitates metadata exchange between systems.



Metadata Governance

Ensures metadata quality and consistency.



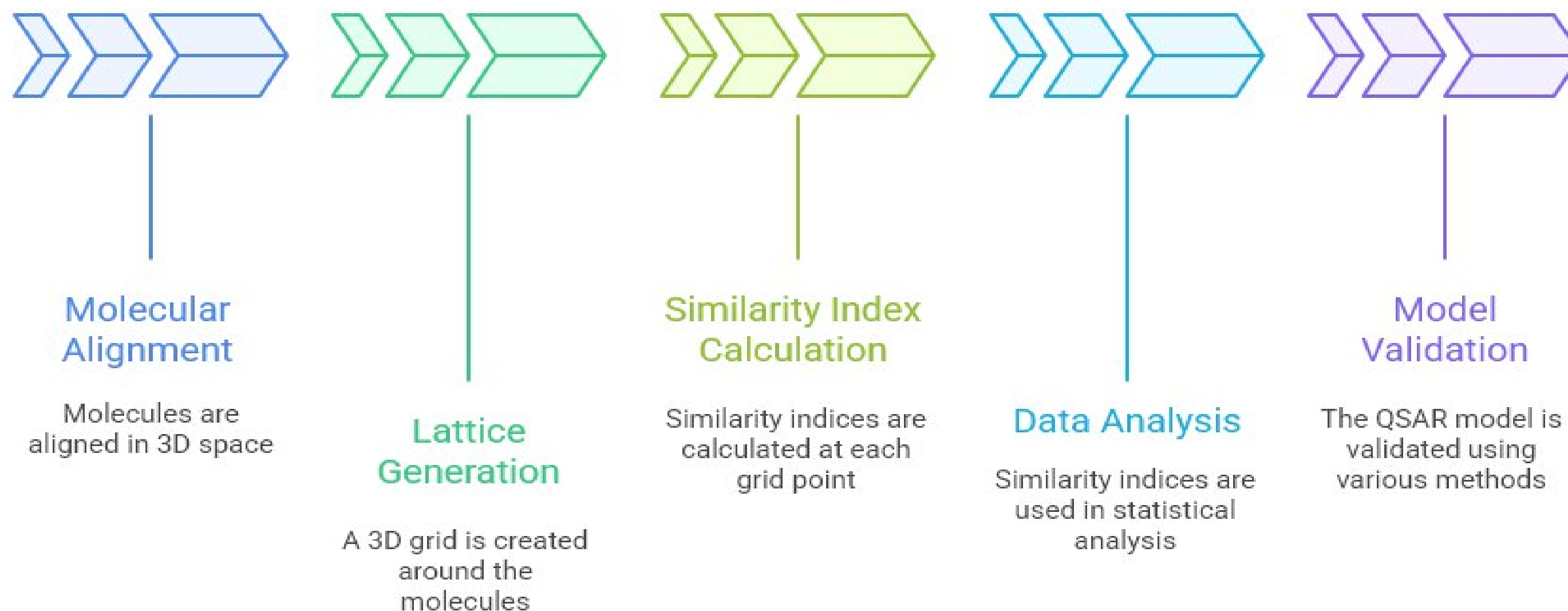
Metadata Lineage Tracking

Tracks the origin and history of metadata.

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CoMSIA METHODOLOGY

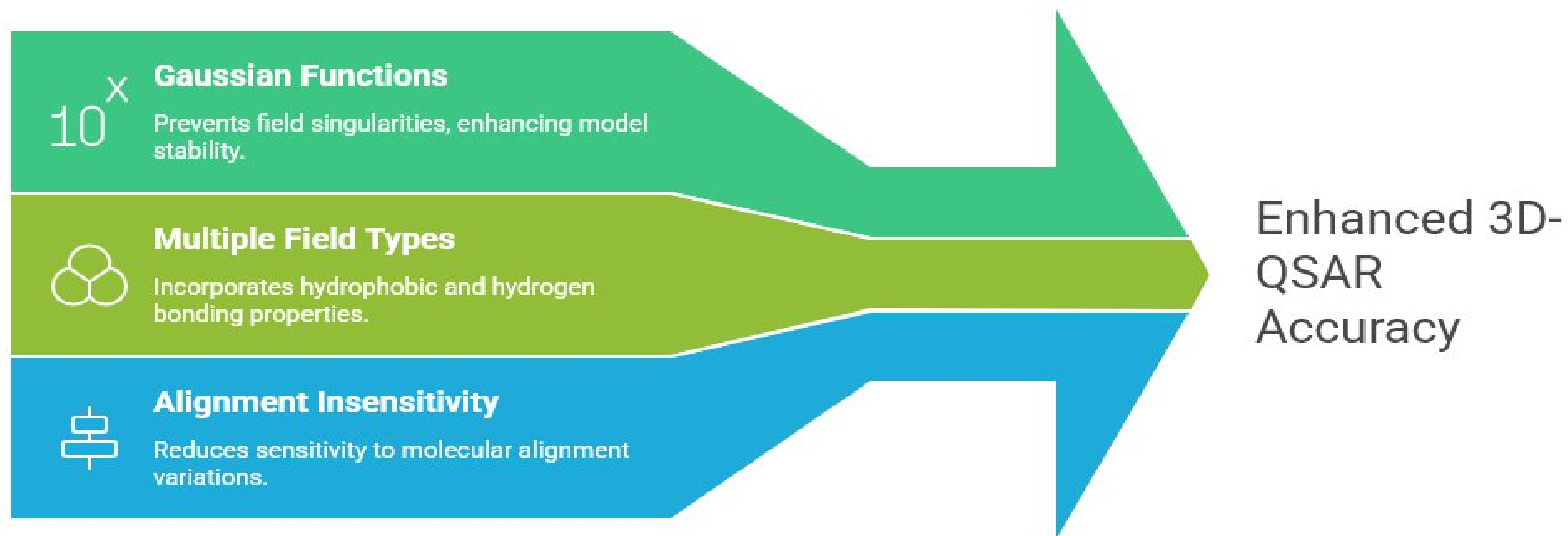
CoMSIA Methodology



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CoMSIA ADVANTAGES

COMSIA's Advantages



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BALANCING CAPACITY

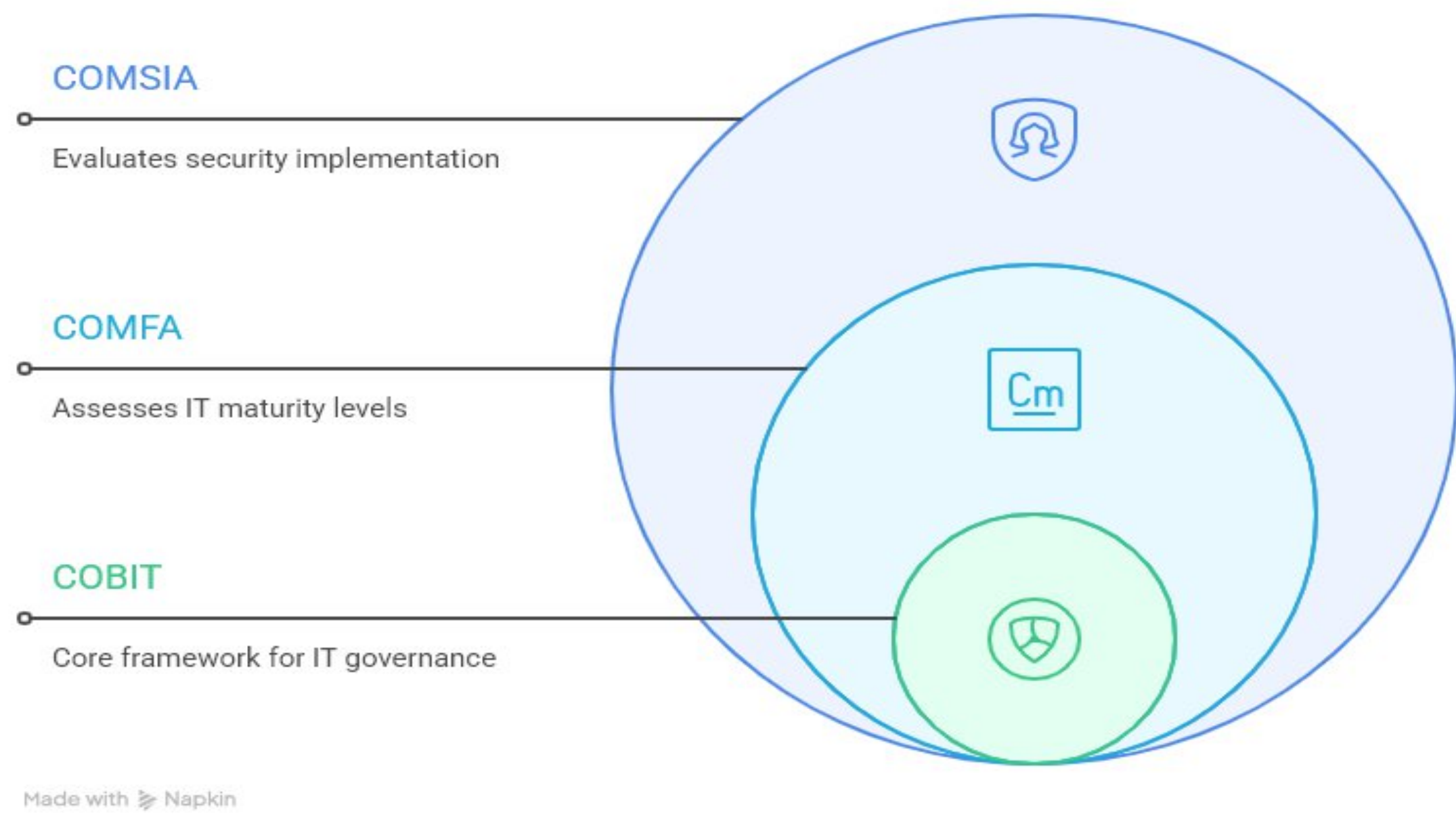
Balancing Complexity and Cost in 3D-QSAR



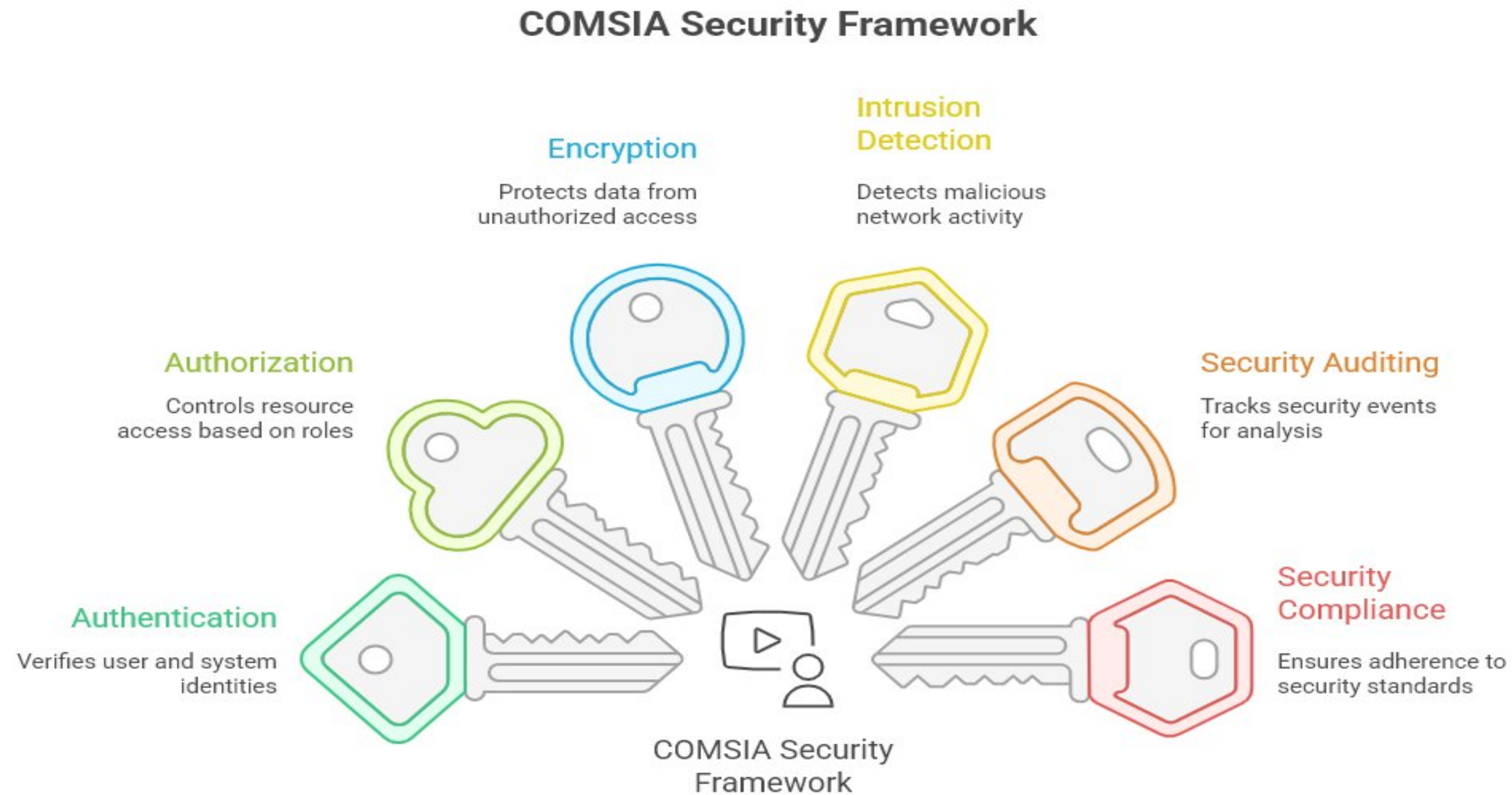
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CoMFA CoMSIA ASSESSMENT CONCEPTS

COBIT Assessment Concepts

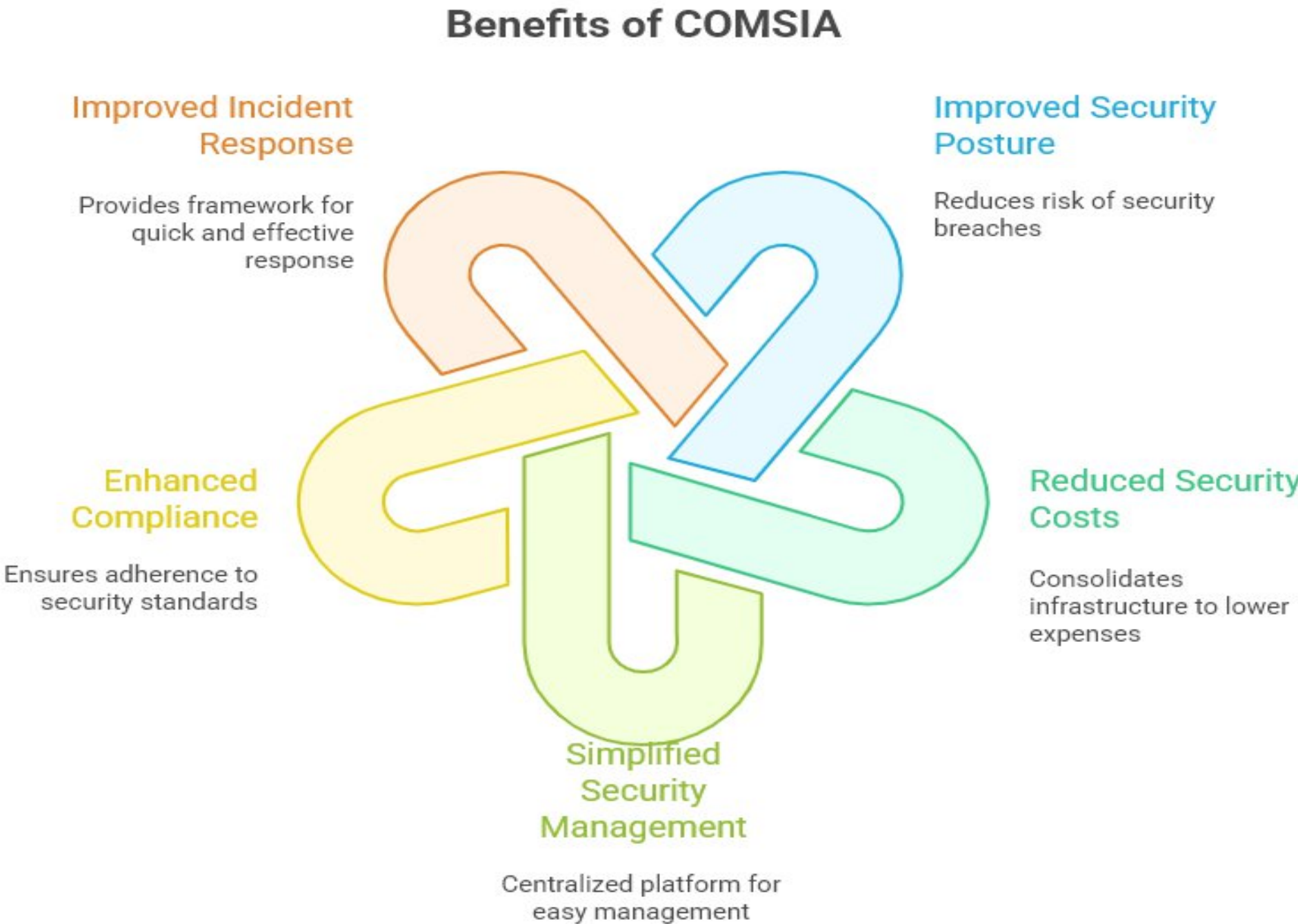



CoMSIA SECURITY CAPACITY



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BENEFITS OF CoMSIA



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FEATURES OF CoMFA VS CoMSIA

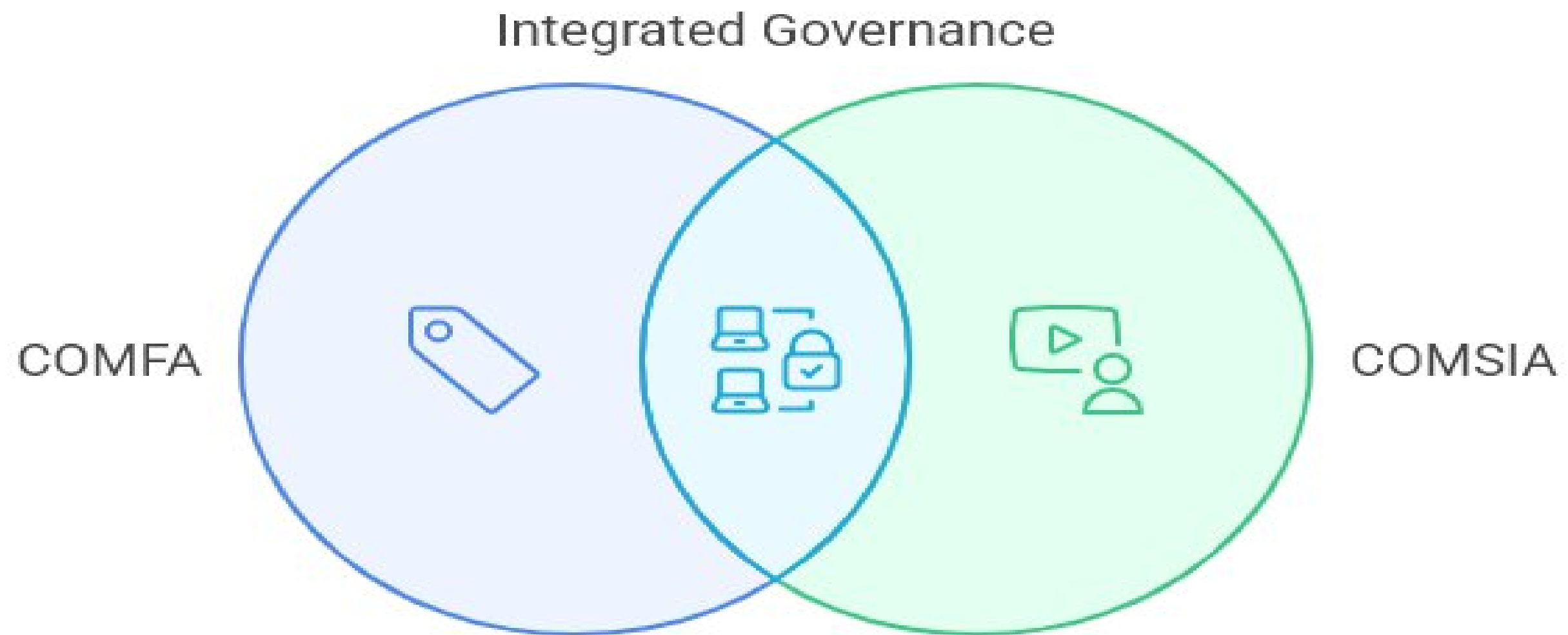
COMFA vs. COMSIA

Feature	Primary Focus	Key Components	Main Goal	Benefits
COMFA (Metadata)	Metadata Management	Metadata Registry, Repository, Services, etc.	Metadata Interoperability and Consistency	Improved Data Quality, Discoverability
COMSIA (Security)	Security Infrastructure	IAM, Cryptography, Monitoring, Vulnerability Mgmt.	Consistent and Robust Security Posture	Improved Security, Reduced Costs

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CONCLUSION

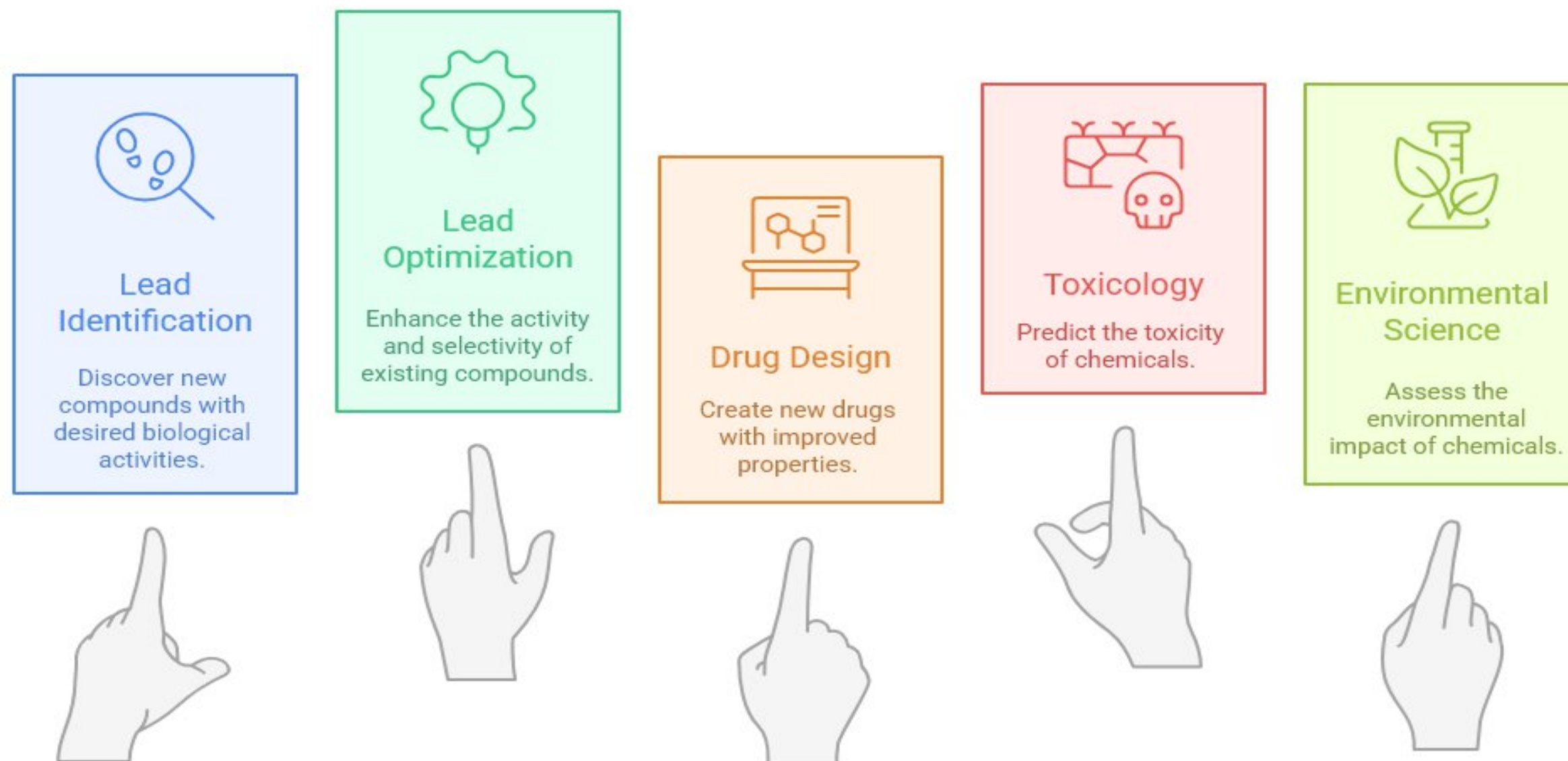
Synergy in Metadata and Security Frameworks



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APPLICATIONS OF CoMFA AND CoMSIA

How can CoMFA and CoMSIA be applied in drug discovery?



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ASSESSMENTS

1} CoMFA stands for:

- a) Comfort Formula Analysis
- b) Comfort Formula
- c) Climate Formula Assessment
- d) Combined Meteorological Factor Analysis

2}} CoMSIA is mainly used to:

- a) Measure air pollution
- b) Simulate human thermal comfort
- c) Predict rainfall
- d) Calculate wind speed



3]Which of the following is not an input parameter in COMFA?

- a) Air temperature
- b) Wind speed
- c) Solar radiation
- d) Soil moisture

4]COMFA evaluates thermal comfort based on:

- a) Psychological factors
- b) Human energy balance
- c) Building materials
- d) Vegetation index

5]COMSIA differs from COMFA because it:

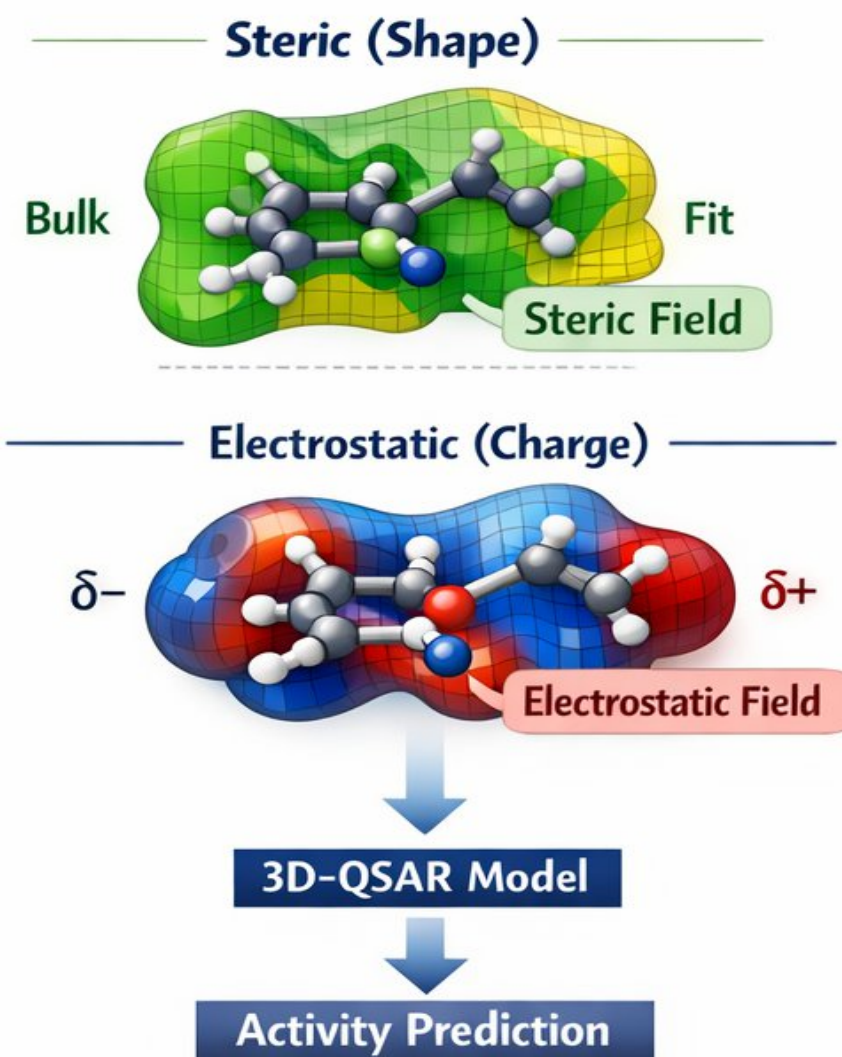
- a) Uses fewer variables
- b) Is only theoretical
- c) Uses computer-based simulation
- d) Ignores human physiology



SUMMARY

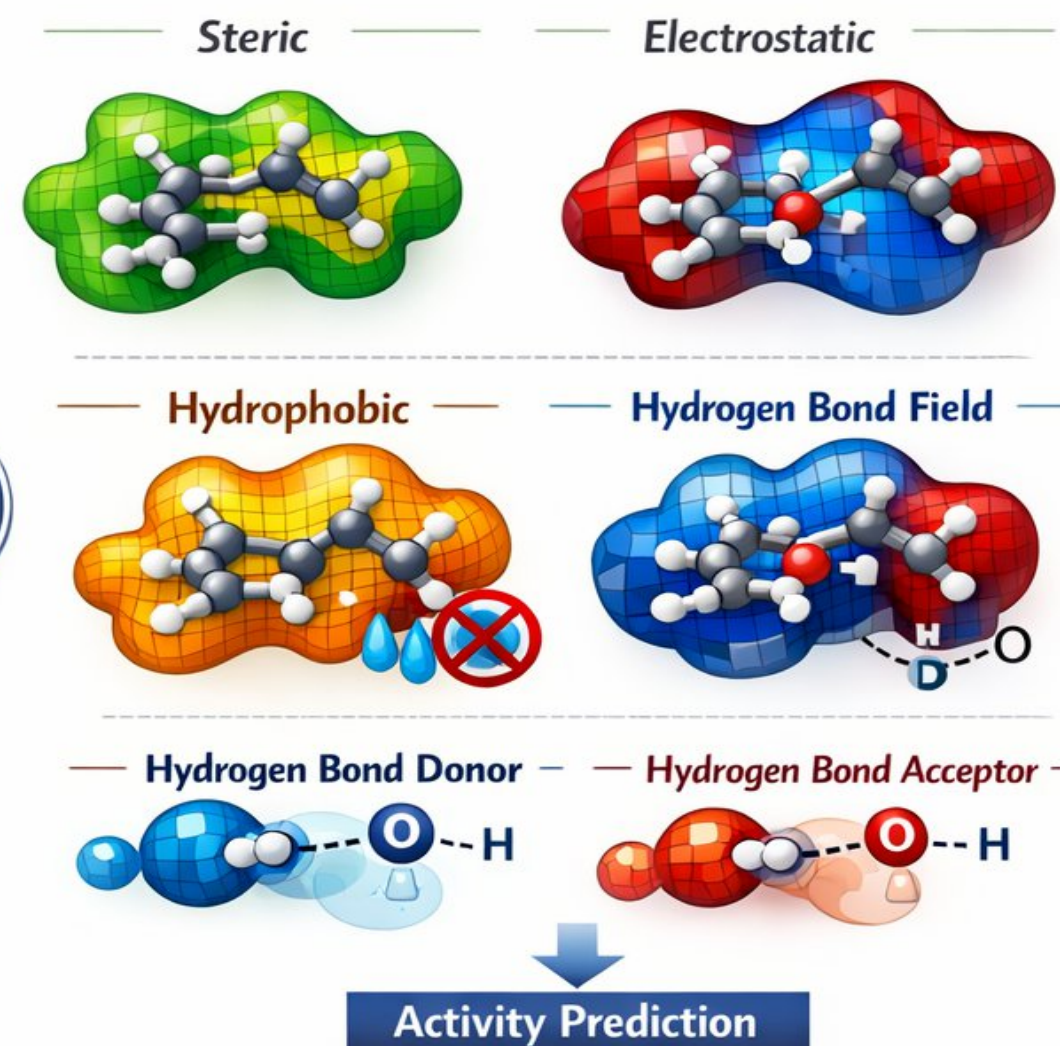
CoMFA

Comparative Molecular Field Analysis



CoMSIA

Comparative Molecular Similarity Indices Analysis



REFERENCES

1. Cramer, R. D., Patterson, D. E., & Bunce, J. D. (1988) Comparative Molecular Field Analysis (CoMFA): Effect of Shape on Binding of Steroids to Carrier Proteins.
Journal of the American Chemical Society, 110(18), 5959–5967
2. Foundational paper that introduced CoMFA. Klebe, G., Abraham, U., & Mietzner, T. (1994) Molecular Similarity Indices in a Comparative Analysis (CoMSIA) of Drug Molecules to Correlate and Predict Their Biological Activity. Journal of Medicinal Chemistry, 37(24), 4130–4146.
3. Original paper introducing CoMSIA. Kubinyi, H. (1998) 3D QSAR in Drug Design: Theory, Methods and Applications. Kluwer Academic Publishers, Dordrecht
4. Excellent theory background for both CoMFA and CoMSIA. Hansch, C., & Leo, A. (1995) Exploring QSAR: Fundamentals and Applications in Chemistry and Biology.
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5. Strong QSAR fundamentals reference. Verma, J., Khedkar, V. M., & Coutinho, E. C. (2010) 3D-QSAR in Drug Design – A Review. Current Topics in Medicinal Chemistry, 10(1), 95–115

