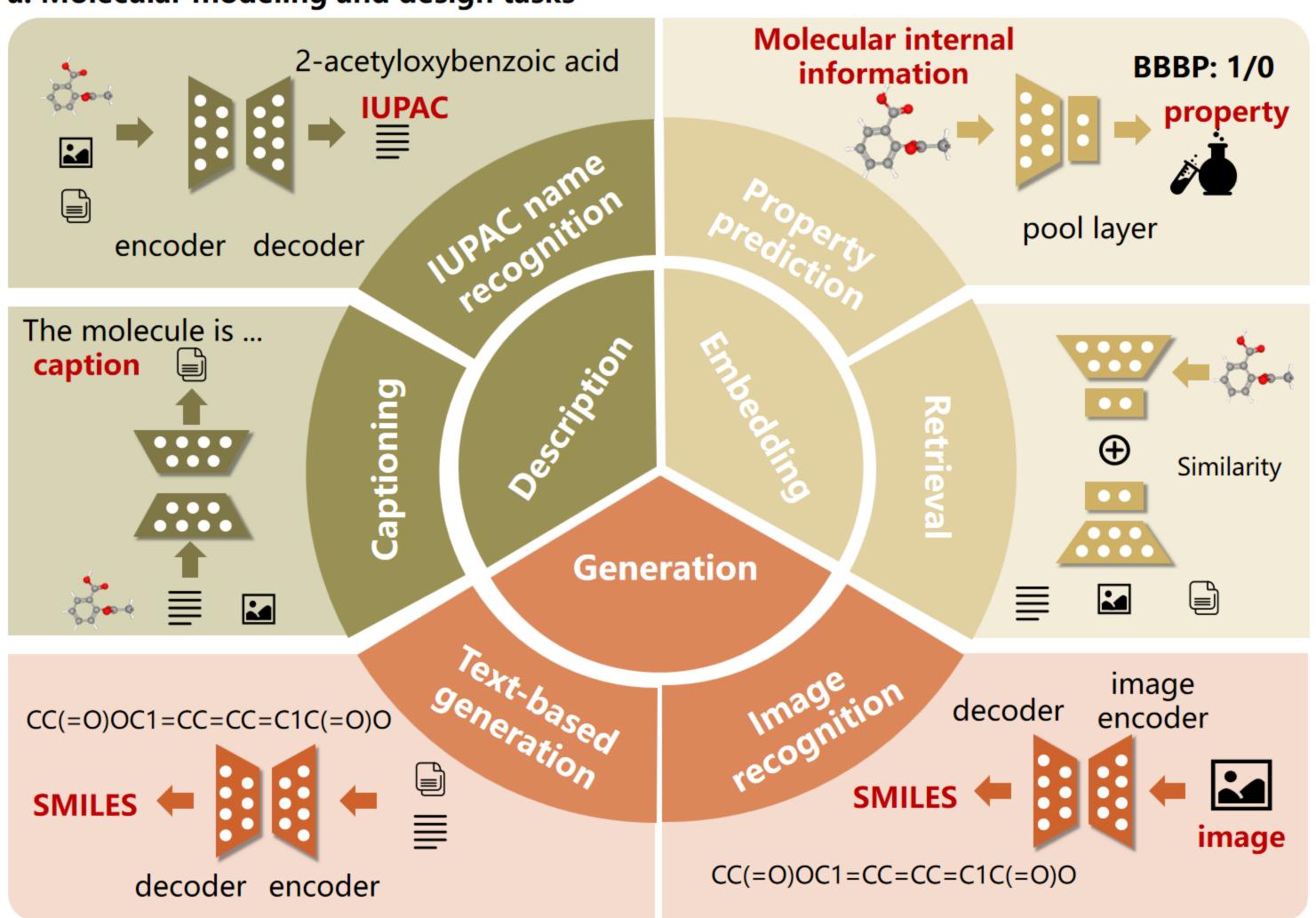
## a. Molecular modeling and design tasks



## b. The processes of tasks

Tasks with Their Inputs and Outputs									
		graph	SMILES	InChl	SELFIES	caption	IUPAC	property	image
Internal information	graph		•	•	•	14	24	3	•
	SMILES	0		0	•	14	24	3	0
	InChl	•	7		•	14	24	3	•
	SELFIES	0	0	0		14	24	3	0
External information	caption	9	5	9	9		2	8	9
	IUPAC	9	5	9	9	14		8	9
	property	9	9	9	9	9	9		9
	image	9	46	9	9	14	24	8	

- Molecule captioning
- 2 IUPAC name recognition
- 8 Property prediction
- 4 Molecular retrieval
- 6 Molecule generation
- 6 Image recognition
- **7** Tasks achievable through tools
- 8 Limitations due to data availability
- Tasks beyond our scope