Supplementary Material

Exploring Molecular Heteroencoders with Latent Space Arithmetic: Atomic Descriptors and Molecular Operators

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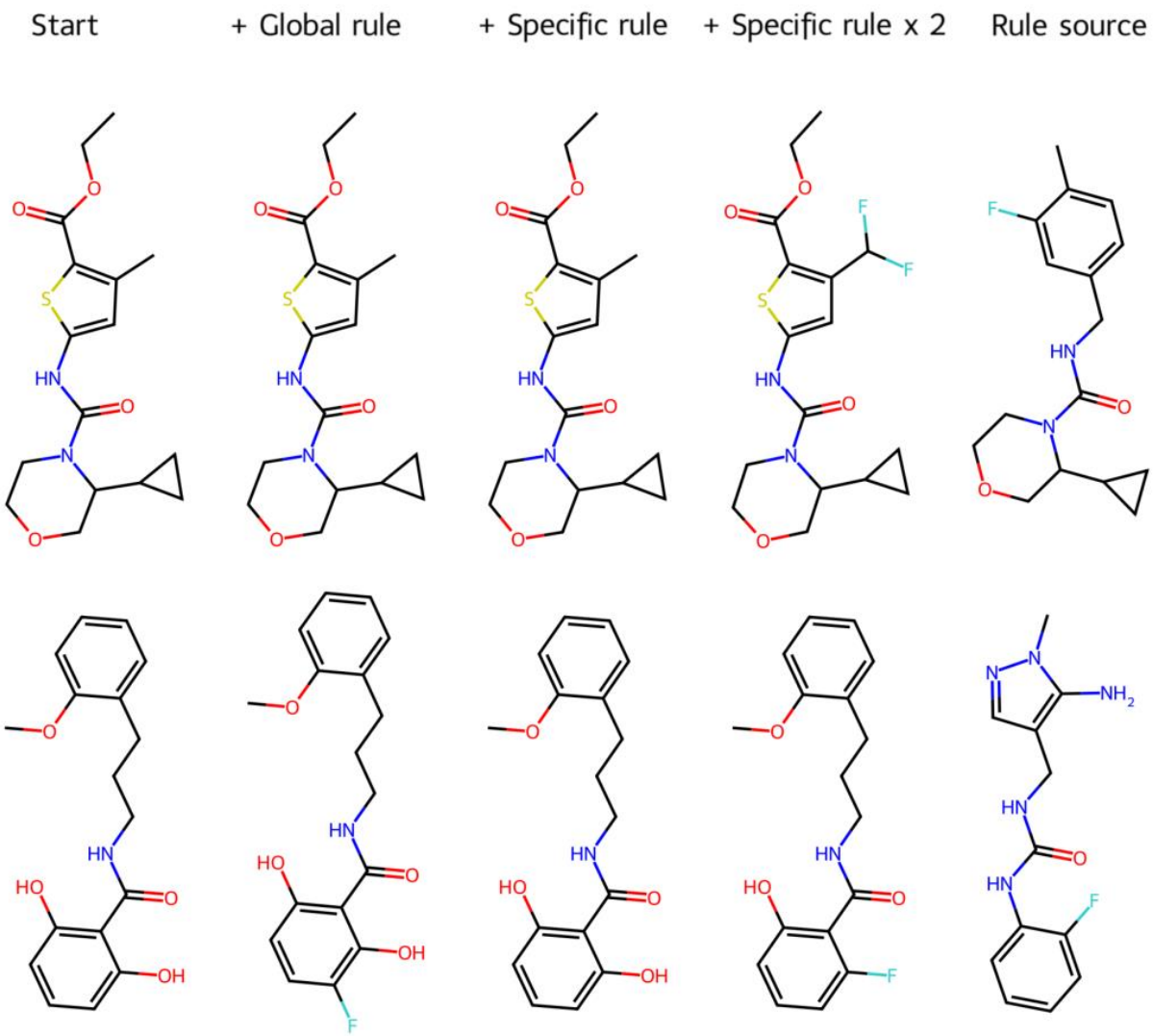
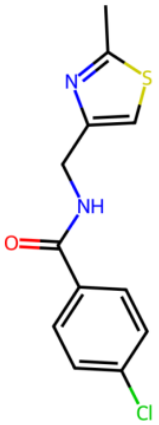
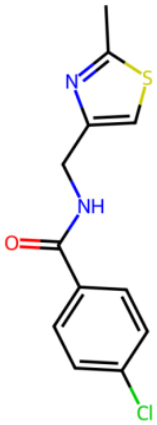
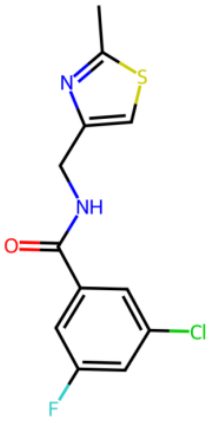
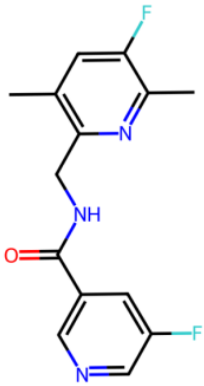
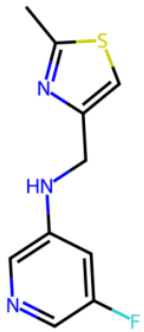
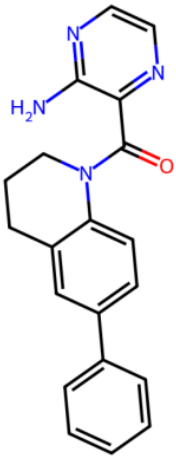
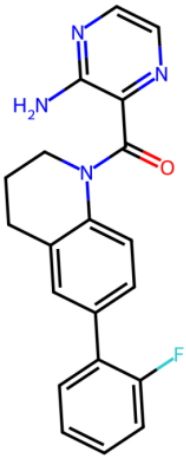
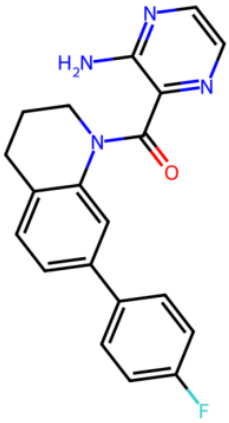
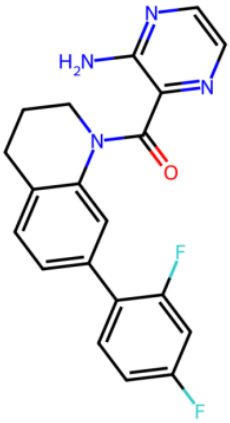
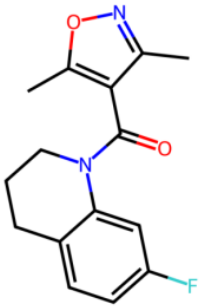
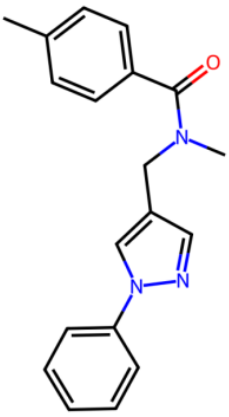
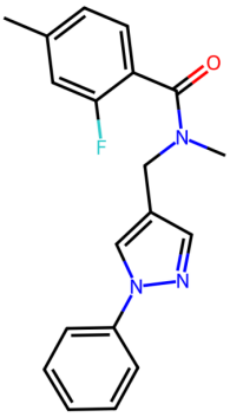
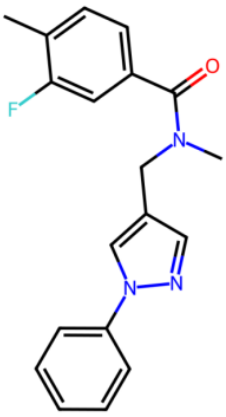
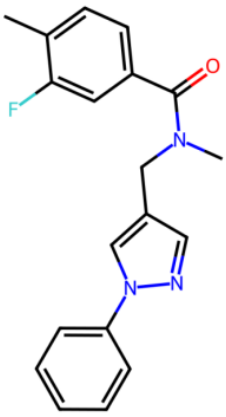
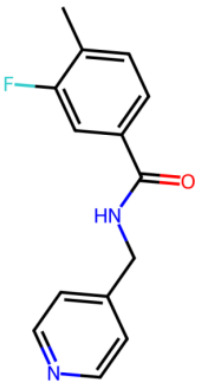
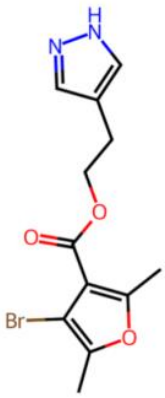
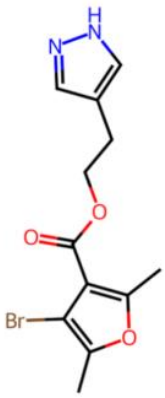
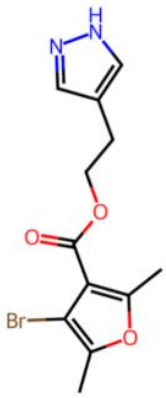
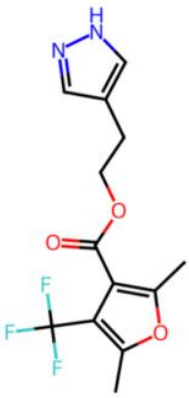
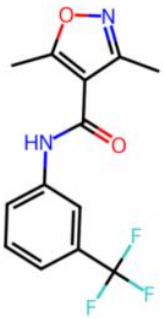
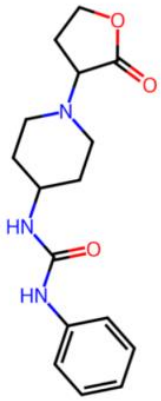
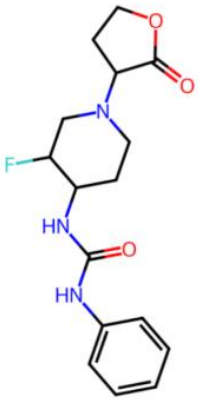
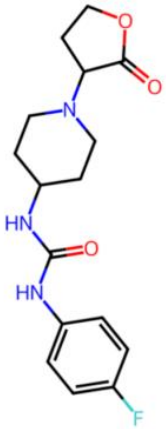
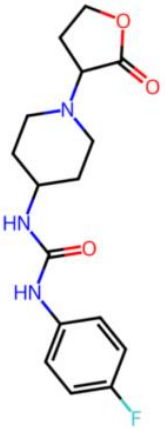
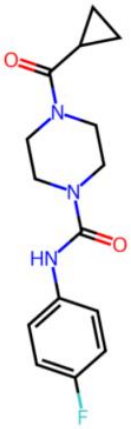
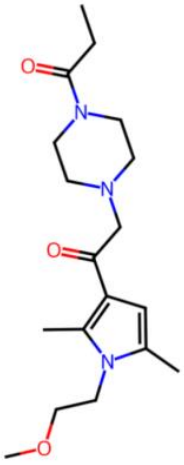
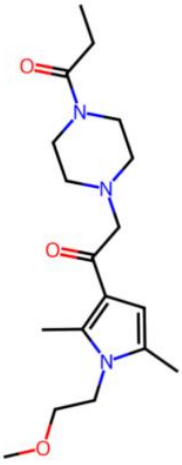
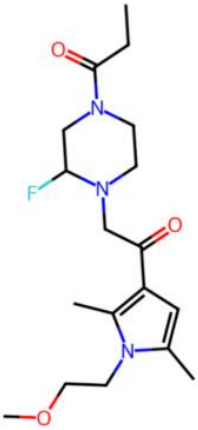
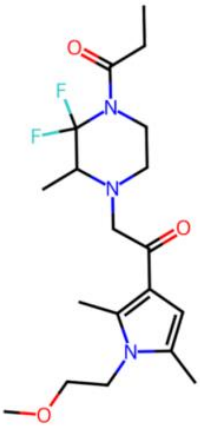
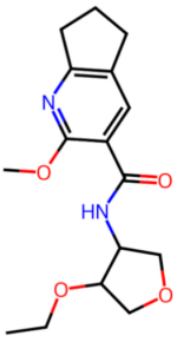
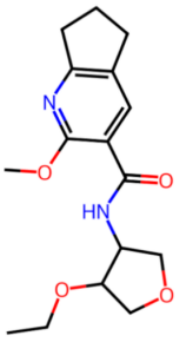
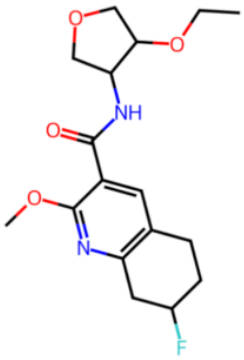
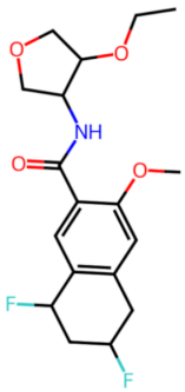
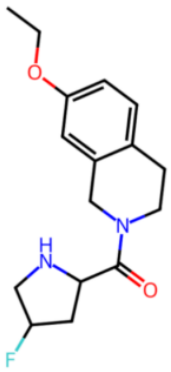
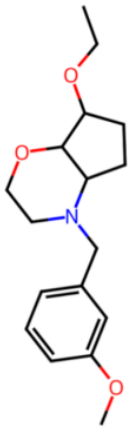
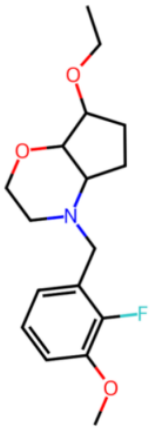
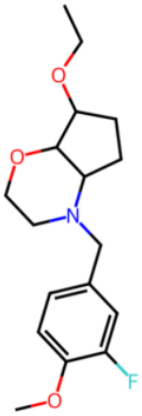
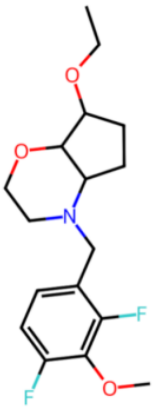
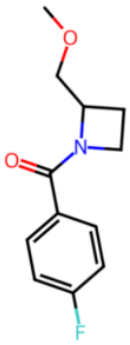
Figure S1: Examples of molecules transformed by H→F LSV molecular operators (each example includes the starting molecule (Start), the molecule obtained with the global rule (+ Global rule), the molecule obtained with the specific rule (+ Specific rule), the molecule obtained with the specific rule multiplied by 2 (+ Specific rule × 2), and the most similar molecule that was used to build the specific rule (Rule source).



Start	+ Global rule	+ Specific rule	+ Specific rule x 2	Rule source
				
				
				

Start	+ Global rule	+ Specific rule	+ Specific rule x 2	Rule source
				
				
				

Start	+ Global rule	+ Specific rule	+ Specific rule x 2	Rule source