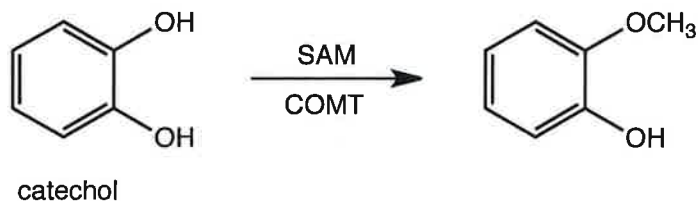


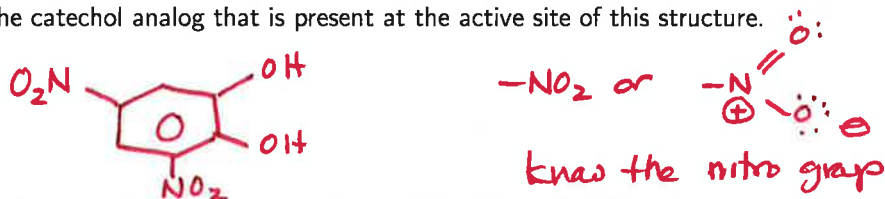
Study Question 4: Catechol O-Methyl Transferase

Go to the PDB site and fetch the entry 3BWM. This structure is catechol O-methyl transferase or COMT, an enzyme that catalyzes the addition of methyl group from SAM to catechol. Many neurotransmitters have similar structures and COMT is important in this context. The general reaction is shown below.



Go to *Presets* → *Interactive 1* to begin.

1. Give the structure of the catechol analog that is present at the active site of this structure.



2. How far is the oxygen of the catechol OH from the electrophilic CH₃ of SAM?

2.71 Å

3. What is the metal ion at the active site?

Mg²⁺

4. Give the name and number of each amino acid side chain that is coordinated to this metal.

asp 169.A asn 170.A asp 141.A

5. Besides the amino acid side chains, there is another species coordinated to the metal. What is it?

water (and the O of the catechol analog)

6. What amino acid side chain is positioned over the adenine ring (name and number)? What kind of force is acting between the two groups?

ile 91.A London forces

7. What amino acid side chain is positioned near the hydroxyls of the ribose (name and number)? What kind of force is acting between the two groups? Sketch the arrangement below.

