Name: ______________________________ BAE 587 Hwk#2 – due Sep 8th, 2022 by midnight

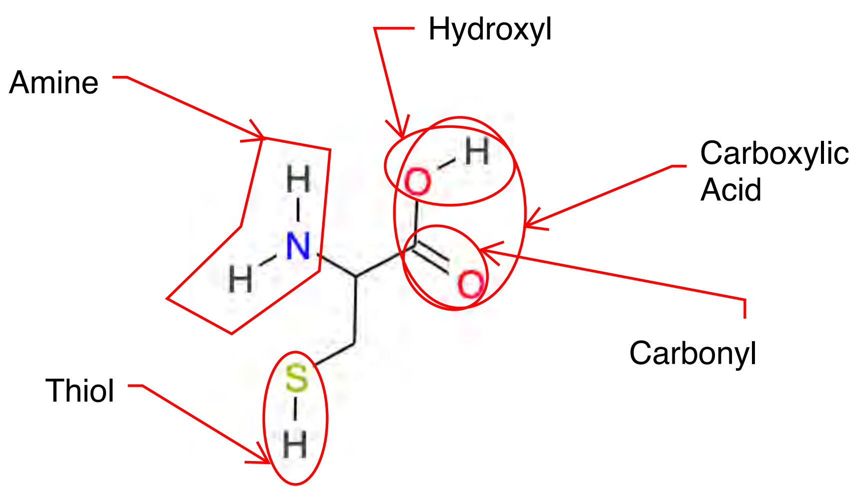
BAE 587:– Homework #2

Part 1

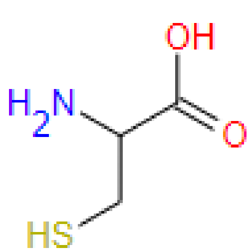
Goal: recognize skeletal and bulk formulae, identify functional groups, be able to draw organic molecules using a free organic chemistry software.

For this part you will be asked to use the JSME software available on the left side of the screen at https://peter-ertl.com/jsme/JSME_2017-02-26/JSME_autoresize.html. To learn how to use the software, watch these videos https://youtu.be/W7VTSlk0BAg and https://youtu.be/Eqx94Dybs14. You may also use this site https://wikipedia.cheminfo.org/ to verify your molecule and find its name.

2.1 identify in the molecule below, the **amine**, the **thiol**, the **carbonyl**, the **hydroxyl**, and the **carboxylic acid** functional groups. For that, you circle the group, point an arrow to it and the name of the functional group at the base of the arrow. It is possible that some groups be part of another group (see figure 3.11 at https://francoisbirgand.github.io/BAE-587/functional-groups.html#fig:FGsynthesis) (5 points)



Draw this molecule in JSME, make a screen shot copy and paste it below, and give it its name. If you are not sure, get its SMILES code and find its name on the web. Give it its compact formula (i.e., $C_xH_yO_zN_aS_b$; remember carbons and hydrogen are often implied). What general molecular family does this molecule belong to? (8 points)



Cysteine:
$C_3H_7NO_2S$

Molecular Family:
Amino Acid (Protein)

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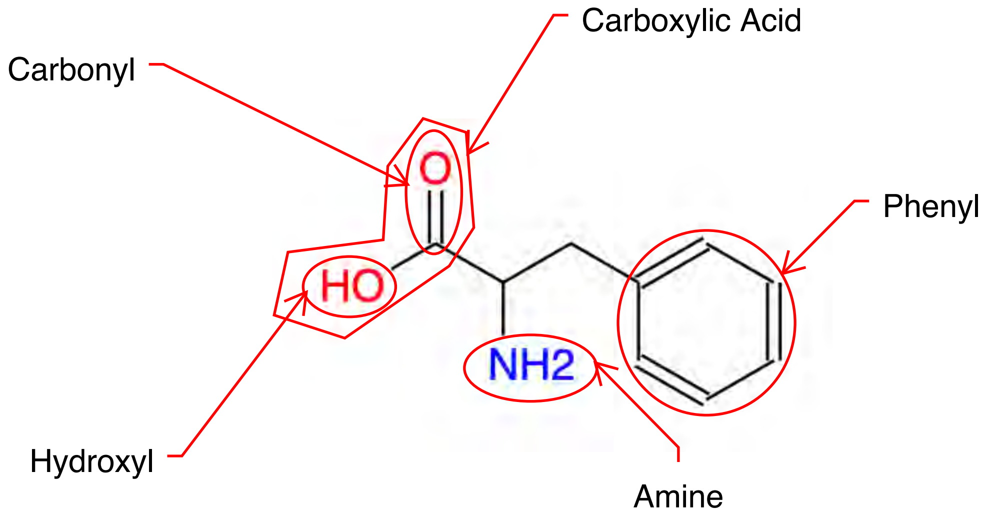
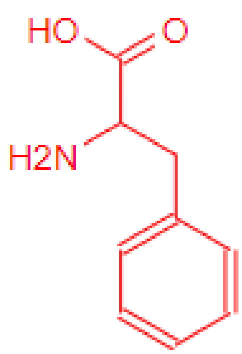
2.2. identify in the molecule below, the **amine**, the **carbonyl**, the **hydroxyl**, the **carboxylic acid**, and the **phenyl** functional groups. For that, you circle the group, point an arrow to it and the name of the functional group at the base of the arrow. (5 points)



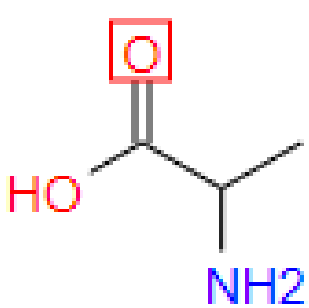
Draw this molecule in JSME, make a screen shot copy, trim it to leave just the molecule, and paste it below, and give it its name. Give it its compact formula (i.e., $C_xH_yO_zN_aS_b$; remember carbons and hydrogen are often implied). What general molecular family does this molecule belong to? Draw on JSME the common structure between this and the previous molecule, and copy/paste it (10 points)



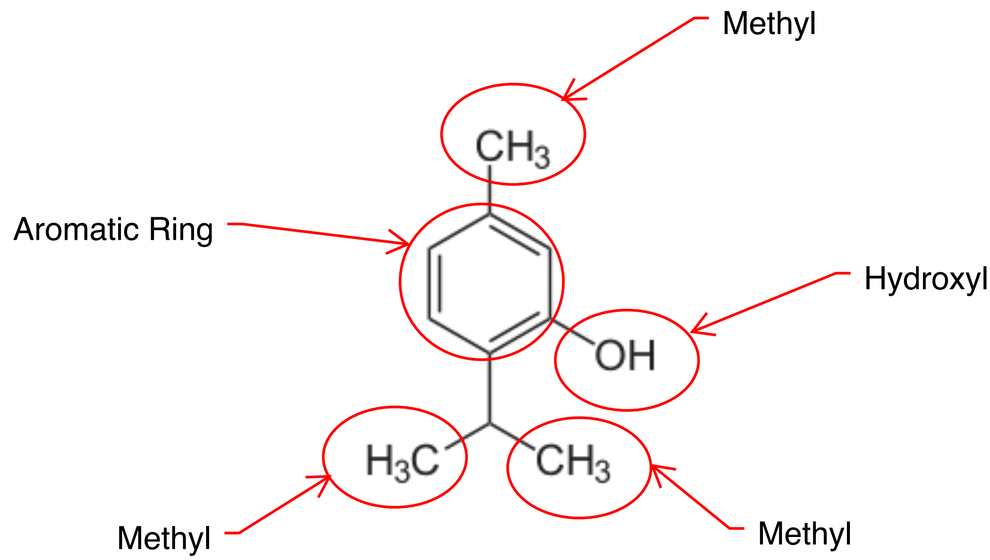
Phenylalanine:
$C_9H_{11}NO_2$

Molecular Family: Amino Acid (Protein)

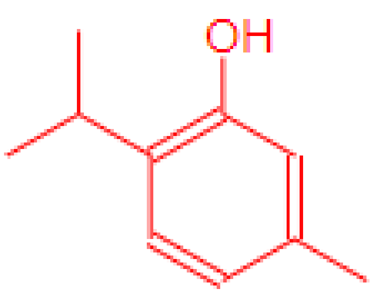
Similar Structure: Alanine



2.3. identify in the molecule below, the **methyl**, and the **hydroxyl** functional groups, as well as the **aromatic ring**. For that, you circle the group, point an arrow to it and the name of the functional group at the base of the arrow. (5 points)



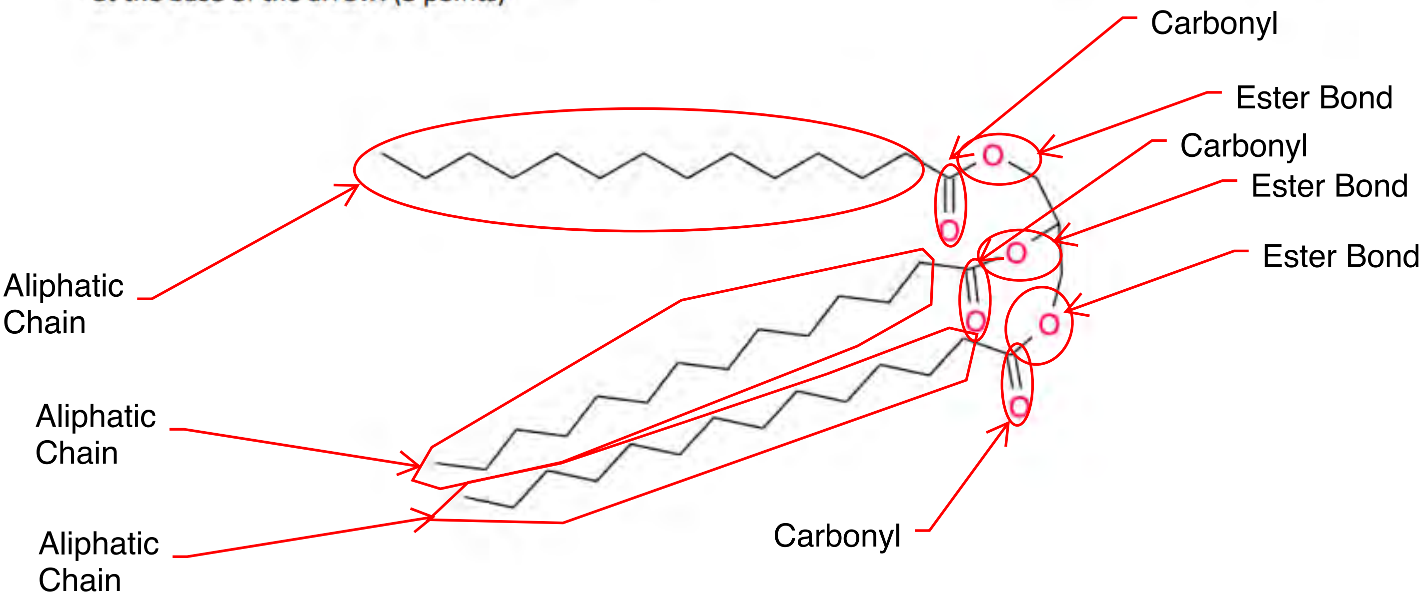
Draw this molecule in JSME, make a screen shot copy, trim it to leave just the molecule, and paste it below, and give it its name. Give it its compact formula (i.e., $C_xH_yO_zN_aS_b$; remember carbons and hydrogen are often implied). What general molecular family does this molecule belong to? (8 points)



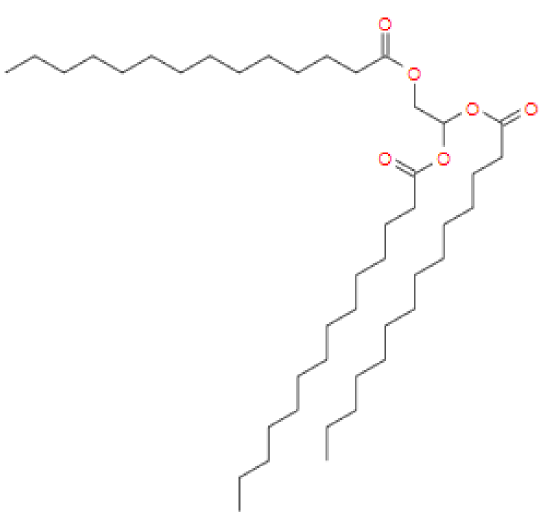
Thymol:
$C_{10}H_{14}O$

Molecular Family: Amino Carbohydrate

2.4. identify in the molecule below, the **carbonyl** functional groups, and the **ester bonds**, as well as the **aliphatic chains**. For that, you circle the group, point an arrow to it and the name of the functional group at the base of the arrow. (5 points)



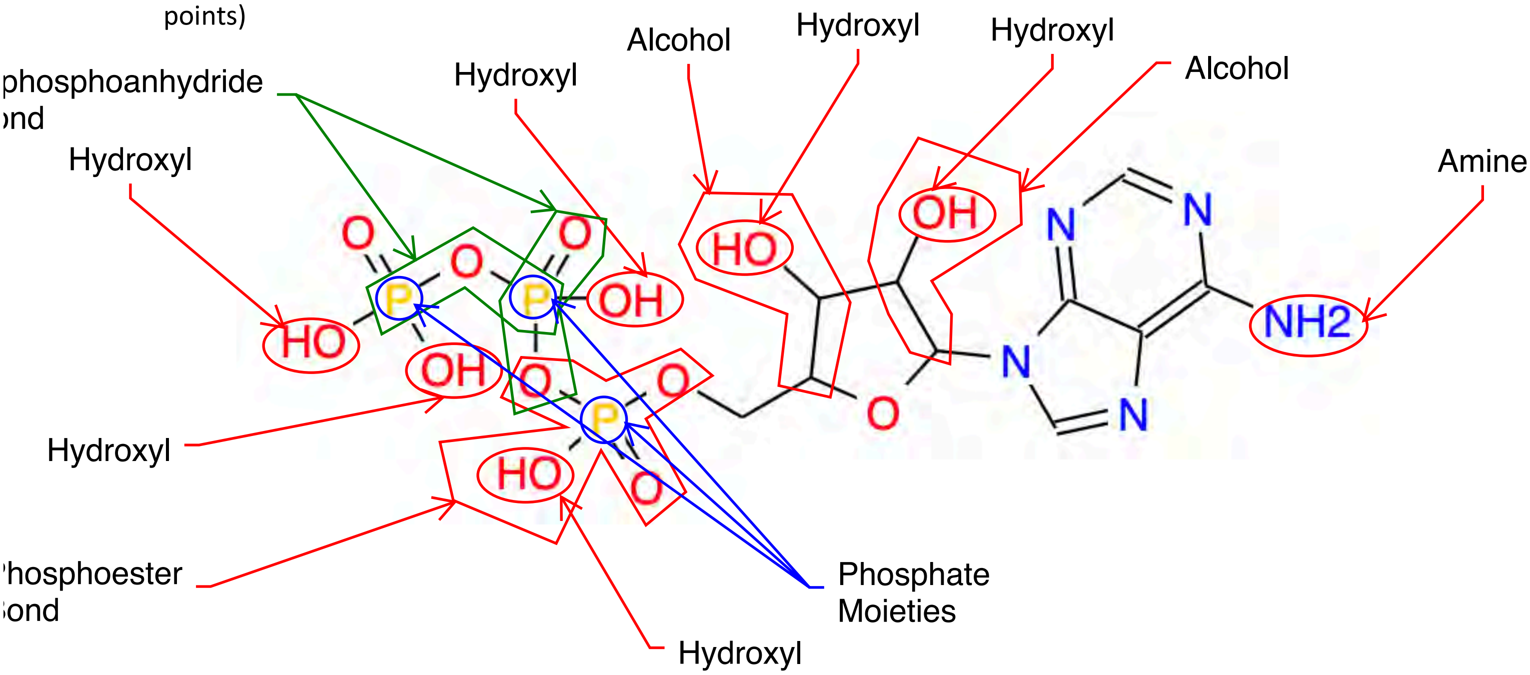
Draw this molecule in JSME, make a screen shot copy, trim it to leave just the molecule, and paste it below, and give it its name. Give it its compact formula (i.e., $C_xH_yO_zN_aS_b$; remember carbons and hydrogen are often implied). What general molecular family does this molecule belong to? (8 points)



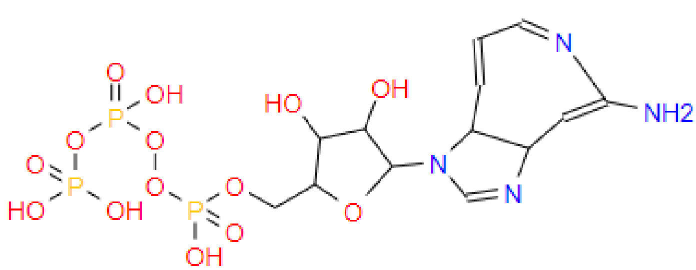
Trimyristin:
CHO_6

Molecular Family:
Lipid

2.5. identify in the molecule below, the **hydroxyl**, **alcohol**, **amine** functional groups, the **phosphoester** bond, the **diphosphoanhydride bonds**, as well as the **phosphate moieties**. For that, you circle the group and moieties, point an arrow to it and the name of the functional group at the base of the arrow. (10 points)



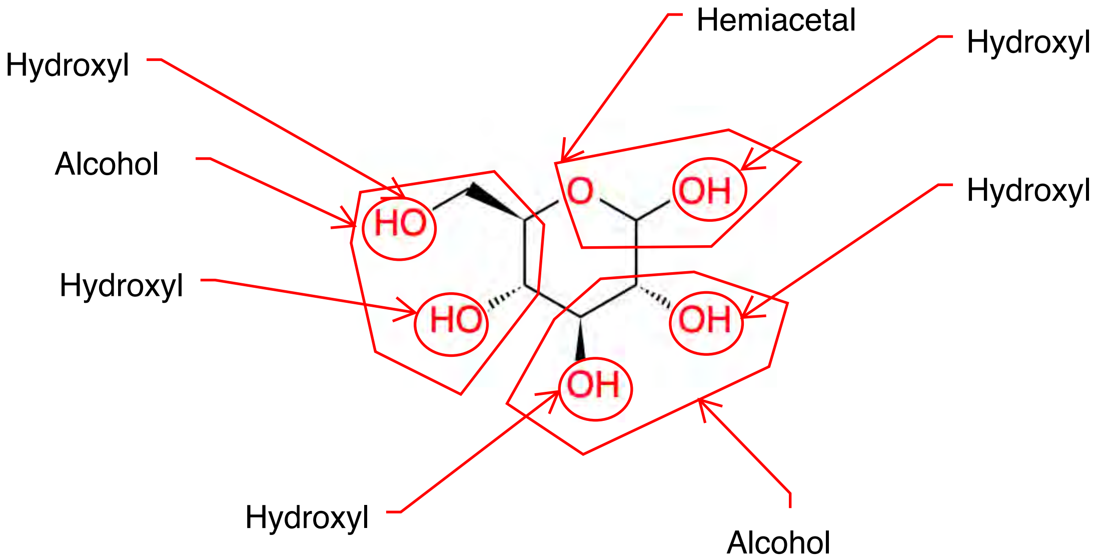
Draw this molecule in JSME, make a screen shot copy, trim it to leave just the molecule, and paste it below, and give it its name. What is the role of this molecule in cells? (5 points)



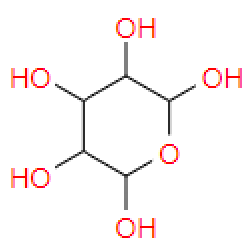
Cyclic
ADP-ribose:
CHN5O13P2

Role:
Used to form NAD+ in compliment with ADPI
Also helps with calcium signaling and muscle
contraction

2.6. identify in the molecule below, the **hydroxyl**, **alcohol** and **hemiacetal** functional groups. For that, you circle the group and moieties, point an arrow to it and the name of the functional group at the base of the arrow. (5 points)



Draw this molecule in JSME, make a screen shot copy, trim it to leave just the molecule, and paste it below, and give it its name. Give it its compact formula (i.e., $C_xH_yO_zN_aS_b$; remember carbons and hydrogen are often implied). What general molecular family does this molecule belong to? (8 points)



Xylose:
CHO5

Molecular Family:
Carbohydrate

Part 2: Using **ALL the words and expressions** given herein, answer this question: **What is aerobic respiration?** (18 points)

I expect that this will take nearly a full page of 1.5 spacing writing. Make sure you write with your best English and in logical order. There are a lot of resources available for you to take ideas in the book. The hardest part is going to be to use your own words.

1. Proton gradient,
2. oxidative phosphorylation,
3. NAD^+,
4. $FADH_2$,
5. outer membrane space,
6. electron transfer,
7. electron transfer molecule,
8. reduced state,
9. ATP,
10. ATPase,
11. Krebs cycle,
12. glycolysis,
13. glucose,
14. pyruvate,
15. CO_2,
16. Acetyl-coA,
17. CH_3-CO-COO^-,
18. dioxygen reduction,
19. proton pumps,
20. oxidized state,
21. citric acid cycle,
22. inner membrane space,
23. mitochondrion,
24. electron acceptor,
25. electron donor,
26. eukaryotic cells,
27. prokaryotic cells,
28. aerobic environment,
29. phospholipid bilayer,
30. substrate-level phosphorylation,
31. proton motive force,
32. carbon oxidation,
33. organotrophs,
34. compartment,
35. rotation,
36. nucleotide,
37. cytoplasm,
38. ADP,
39. Adenine,
40. Flavine.

John McNulty

Aerobic respiration is a multi-step conversion process of **glucose** and oxygen into **ATP**, water and **CO_2** in an **aerobic environment** where oxygen is bountiful, and breathing is required**.** In this process, Carbon is the **electron donor**, and you will see it in it's **oxidized form CO_2** often in this description, O_2 is the universal **electron acceptor**. The special thing about respiration is the efficiency in which ATP, a molecule that we use primarily for organ function and moving any muscle in our body, is manufactured and released.

This manufacturing process takes place in our **mitochondrion,** famously tagged as the "powerhouse of the cell". It should be noted that since we use an organic molecule (carbon), we are considered organotrophs who have mitochondria in our **eukaryotic cells.** Eukaryotic cells have clearly defined boundaries on the outside and within the cell, which develop membrane-bound compartments for organelles that perform functions for the cell. The outer membrane is the overall footprint of the cell, while the inner membrane, lined with different proteins, execute a wide array of functions. Mitochondria themselves have an outer and inner membrane. The outer membrane is a protective barrier, but just within there is an **outer membrane space** that separates the mitochondria from the **cytoplasm** sandwiched between two layers of **phospholipid bilayers** that makes up the inner membrane. The **inner membrane space** has a very intricate structure in order to maximize the amount of surface area where ATP is produced. Organisms that do not have clearly defined membranes are called **prokaryotic cells** and do not rely on respiration for their main source of energy.

Once food is consumed by an organotrophic and oxygen is in the blood, respiration can begin. The sugars are broken down into glucose. An intermediate step of **glycolysis** includes the addition of a phosphate group via **substrate-level phosphorylation** to glucose in order to make ATP. Phosphorylation required the presence of **nucleotides** to accomplish this. Glucose is also broken down to make 2 molecules of **pyruvate ($CH_3(C{=}O)COOH$)**, 2 molecules of ATP and 2 molecules of water, and importantly 2 molecules of NADH. NADH and pyruvate are involved in the next step of the process called the **Krebs Cycle**, or the **citric acid cycle.**

The Krebs cycle starts with the presence of broken-down carbohydrates that help CoA react with acetyl to become **acetyl-COA**. Pyruvate helps with this complex process by giving 2 electrons to Carbon and moving to its **oxidized state.** During this operation, carbon receives electrons and transitions to a more **reduced state.** Such is a typical handoff during an **electron transfer.** The Krebs cycle includes 8 main steps, with important byproducts including (3) NADH, (1) **$FADH_2$** (2) CO_2 , 1 ATP and 3 hydrogens in their reduced state.

So far, all of this is described to set up the final stage of respiration, and the real reason you need oxygen in your cells is so that the next step can be completed.

Oxidative Phosphorylation takes place in the intermembrane space and where molecules described in the previous sections come to in order to deliver their electrons. The first step includes the two main **electron transfer molecules**, NADH and $FADH_{2\,h}$ into the mitochondria's **proton pumps** that strip it of its protons. These two molecules in their reduced form then revert back to **NAD_+** and FAD and can be used in the Krebs cycle again. The consistent delivery of these 2 molecules to proteins and molecules in the inner membrane of the mitochondria for the "harvesting" of protons make up the **electron transport**

chain that deliver protons. This harvesting of protons on one end of the intermembrane space can be described as a build up of pressure, also called a **proton gradient.**

With an abundance of protons available, the O_2 molecules in your blood which only have 6 electrons for themselves react via **dioxygen reduction** to create water. At this time there's a significant amount more protons in the intermembrane space than outside of it.

Previously used ATP, in the form of **ADP** are also abundant outside of the intermembrane space. Although used before, there is potential for them to be used for energy again. ATP is a molecule that is comprised of an , ribose, and a tri-phosphate group. The unique composition of the tri-phosphate group leads to a lot of unstable loan pairs that the oxygen it's paired to has. A lot of energy is released when this bond it broken, enough that our bodies have adapted to use it at its main source of energy. It also takes quite a bit of energy to put that bond back together, which is the reason for the storing of the protons. At the last step of oxidative phosphorylation, a protein is attached to the membrane wall whose function is to funnel the outflow of protons. Attached to it is a ADP, an "uncharged" ATP molecule which is then funneled with energy via the flow of protons, the **proton motive force** to connect it's bonds back together. The energy required to accomplish this feat is made easier by the presence of **ATPases** used by the cells. The constant flow of these protons powers the protein that hosts the reaction to **rotate** constantly, providing for a very effective ADP catching method.