**Annotation Benchmarking**

**Chemical Reaction Figures**

**Models:**

* AI4Chem/ChemVLM-8B
* GPT-4 turbo-2024-04-09

**Input prompt:**

* You are a chemical annotation assistant. Analyze chemical reaction images, and annotate all relevant information such as reactants, products, catalysts, conditions, and mechanisms. Don't include any reactions or formulas in your annotations. Explain what they mean and serve for. Ensure chemical accuracy, use standard conventions, and maintain completeness and clarity in the annotations.

**Sample document:**

* ChemBioChem - 2020 - Norvaiša - Porphyrins as Colorimetric and Photometric Biosensors in Modern Bioanalytical Systems.pdf

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| **Num** | **Chemical Reaction Figures** | **AI4Chem/ChemVLM-8B** | **GPT-4 turbo-2024-04-09** |
| 1 |  | In this image, we see a chemical reaction pathway involving the synthesis of metalloporphyrins. The process is divided into two main steps: Type 1 and Type 2.  ### Step-by-Step Analysis:  #### \*\*Type I\*\*  The first step involves synthesizing free base nonplanar porphyrin from an amine compound (NH). This intermediate will be used in subsequent reactions to form other complexes.  - Reactants:  - NH  - Products/Intermediates:  Free base nonplannar porpyhrin  #### \*\*Analyte Preparation\*\*  This stage prepares analytes for further analysis or use as catalysts/reporter units by introducing specific functional groups such as stars (\*), hexagons (=), etc., which are essential components within these molecules that can interact with metals later on during catalysis processes.  #### \*\*Catalyst Introduction & Recognition Unit Formation\*\*  Next comes the formation of recognition reporter unit using various building blocks like red star symbols representing different parts of the molecule structure needed at each position depending upon their functionality required downstream applications e.g., binding sites for substrates or inhibitors; fluorescent moieties if it's meant for sensing purposes.  Finally,  - Catalytic Complex Synthesis occurs where metallocorophyrin forms through coordination between central metal ion M+3 and nitrogen atoms present around its periphery - essentially completing our desired product after all transformations have taken place successfully without any side products interfering negatively throughout entire synthetic route depicted here visually via diagrammatic representation provided above! | The image you provided illustrates a schematic representation of a Type 2 sensor system based on porphyrin structures. This system is designed to detect specific analytes (molecules of interest) through a change in the structure or properties of the sensor, which is then reported visually or through another detectable change.  ### Components of the System:  1. \*\*Recognition and Reporter Unit:\*\*  - This unit is depicted as a star-shaped symbol in red, which represents a free base nonplanar porphyrin. Porphyrins are a group of heterocyclic macrocycle organic compounds, which are often used in sensor applications due to their ability to interact with various analytes through mechanisms such as coordination or electronic effects.  2. \*\*Analyte:\*\*  - Represented by various shapes and colors (yellow star, blue star, green diamond), these are the target molecules that the sensor aims to detect. The interaction between the analyte and the porphyrin causes a change in the sensor, triggering the reporting mechanism.  3. \*\*Metalloporphyrin:\*\*  - This is a modified version of the porphyrin where a metal ion (M^n+) is coordinated in the center of the porphyrin ring (shown with a grey circle in the center of the porphyrin structure). The presence of the metal ion often enhances the sensitivity and selectivity of the porphyrin towards specific analytes.  ### Mechanism of Action:  - The sensor system operates by undergoing a structural or electronic change upon interaction with an analyte. This change can affect the optical properties of the porphyrin, such as its absorbance or fluorescence, which serves as the basis for the detection and reporting of the presence of the analyte.  - The diagram shows a transformation from a non-metalated porphyrin to a metalloporphyrin upon interaction with an analyte, suggesting that the analyte may facilitate or trigger the metalation process, or that the metalation enhances the interaction with the analyte.  ### Purpose and Application:  - Such sensor systems are valuable in environmental monitoring, medical diagnostics, and industrial processes where specific detection of chemicals or biological molecules is required.  - The ability to tailor the porphyrin structure and the metal center allows for customization of the sensor to detect a wide range of analytes with high specificity and sensitivity.  This type of sensor system exemplifies the integration of chemical recognition elements with signal transduction mechanisms, enabling the direct and selective detection of target molecules in complex mixtures. |
| 2 |  | This image contains a variety of chemical reaction pathways, each involving different reactants and products. Here's an analysis with annotations for the reactions depicted:  1) TPP-DSNDA: This pathway involves using triphenylphosphine (TPP), diphosgene (DSN2A or DSN3B in this case depending on which one is used as reagent 6a/7b respectively). The product formed here includes cyclohexane rings.  2) COFss: Involves cyclotrimerization to form carbon oxide frameworks such as covalent organic framework structures containing hexagonal benzene units connected by C-C bonds via tris(4-pyridinyl)methanone ligand complexes.    3) TPY-DIBH: Tripyrrolidino borate ester derivative formation from dihydroboronic acid derivatives through condensation followed by deprotection steps including hydrolysis under basic conditions leading into further transformations like oxidation forming ketones etc., often seen at later stages within these synthetic routes  4) O-HSOCOc-cyclopenta[c]furan-N(CC)c1ccccc1-S(O)(=O)=O  The synthesis route employs sulfonamide coupling between phenol group bearing thiophenium salt intermediate & cinnamic aldehydes yielding sulfonyl substituted aromatic compounds that are useful intermediates towards various biologically active molecules  5) N-Me-TMPDPA: A method where trimethyl phosphonoacetate acts as nucleophile attacking electrophilic carbonyls resulting in methoxy-substituted acetic acids after subsequent reduction processes typically carried out over metal catalyst systems e.g Pd/C  Overall it seems there’re several distinct types of transformation occurring across multiple paths - some involve ring closures while others focus more on functional groups manipulation i.e addition/substitution/dealkylation/halogenations/sulfonation/cyclizations etc.  Please note without specific contextual information about what exactly you're looking forward to synthesize its hard to pinpoint exact mechanisms but I've tried my best based upon general knowledge related to common synthetics strategies employed during organics lab work! | The image you provided displays a collection of chemical structures, primarily focusing on various porphyrin derivatives and covalent organic frameworks (COFs). These structures are not presented in the context of specific chemical reactions but rather as individual molecules or frameworks, each with distinct chemical features and potential applications. Here’s an analysis of the types of compounds shown and their relevance:  1. \*\*Porphyrin Derivatives (Top Section)\*\*:  - \*\*Structures 1-6\*\*: These are variously substituted porphyrins, which are macrocyclic compounds typically known for their role in biological systems (e.g., heme in hemoglobin). The substitutions on the porphyrin ring can significantly alter their chemical and physical properties, making them useful in areas like catalysis, photodynamic therapy, and materials science.  - \*\*Structures (TH)₂PP, (TN₂O₂,OH₂OMe)PP, TPPP, TSPP, TCIPP, TPyP, TMPyP, TDMP₂P\*\*: These are specific types of substituted porphyrins with different functional groups that impact their solubility, electronic properties, and potential for interaction with other molecules. For example, sulfonate groups (SO₃H) enhance water solubility, which is crucial for biological applications.  2. \*\*Covalent Organic Frameworks (COFs) (Middle Section)\*\*:  - \*\*TPP-TRBE, TPyP-DBH, TAPP-TPA\*\*: These structures represent different types of COFs, which are crystalline porous polymers formed by linking organic building blocks through strong covalent bonds. COFs are noted for their high surface areas, tunable porosities, and stability, making them suitable for gas storage, catalysis, and sensing applications.  - The depicted COFs show different linking strategies and pore structures, indicated by the red and blue dots representing different atoms or connectivity points.  3. \*\*Complex Porphyrin Structures and Metal-Organic Frameworks (Bottom Section)\*\*:  - \*\*Structures 7, TPP(MN), TPP(CN)₄, TPP(PE)₈\*\*: These are more complex porphyrin derivatives or polymers, some incorporating metal centers (as indicated by "M" which typically stands for a metal such as zinc or iron). These structures can be part of larger coordination polymers or networks with applications in catalysis and materials science.  - \*\*Structure 8 and 9\*\*: These are examples of metal-organic frameworks (MOFs) or related complexes, where metals are coordinated with organic ligands to form extended networks. These are useful in applications similar to COFs but often with enhanced catalytic or electronic properties due to the presence of metal centers.  Each of these structures is a representation of how organic chemistry can be tailored to create materials with specific properties for targeted applications. The annotations do not indicate specific reactions but rather highlight the diversity and complexity of synthetic chemistry in creating functional materials. |