Project Notes:

Project Title: Computationally Modeling the Ability of Cyclodextrins to Bind Short-Chain PFAS
Name: Lydia Metcalf

Note Well: There are NO SHORT-cuts to reading journal articles and taking notes from them. Comprehension is paramount. You will most likely need to read it several times, so set aside enough time in your schedule.

Contents:

Knowledge Gaps:

This list provides a brief overview of the major knowledge gaps for this project, how they were resolved and where to find the information.

Knowledge Gap	Resolved By	Information is located	Date resolved
What pharmaceutical contaminants currently pose the biggest threat to aquatic environments?	Background research (PFAS)		
How to use a molecular docking program?	Contacting chemists in the field (Dr. Alexander MacKerell, Dr. Matthew Metcalf)		
Which PFAS are the most impactful and what are their effects?	Background research		

Literature Search Parameters:

These searches were performed between (Start Date of reading) and XX/XX/2019.
List of keywords and databases used during this project.

Database/search engine	Keywords	Summary of search

Tags:

Tag Name	

Article #0 Notes: Title

Article notes should be on separate sheets

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Source Title	
Source citation (APA Format)	
Original URL	
Source type	
Keywords	
#Tags	
Summary of key points + notes (include methodology)	
Research Question/Problem/ Need	
Important Figures	
VOCAB: (w/definition)	
Cited references to follow up on	
Follow up Questions	

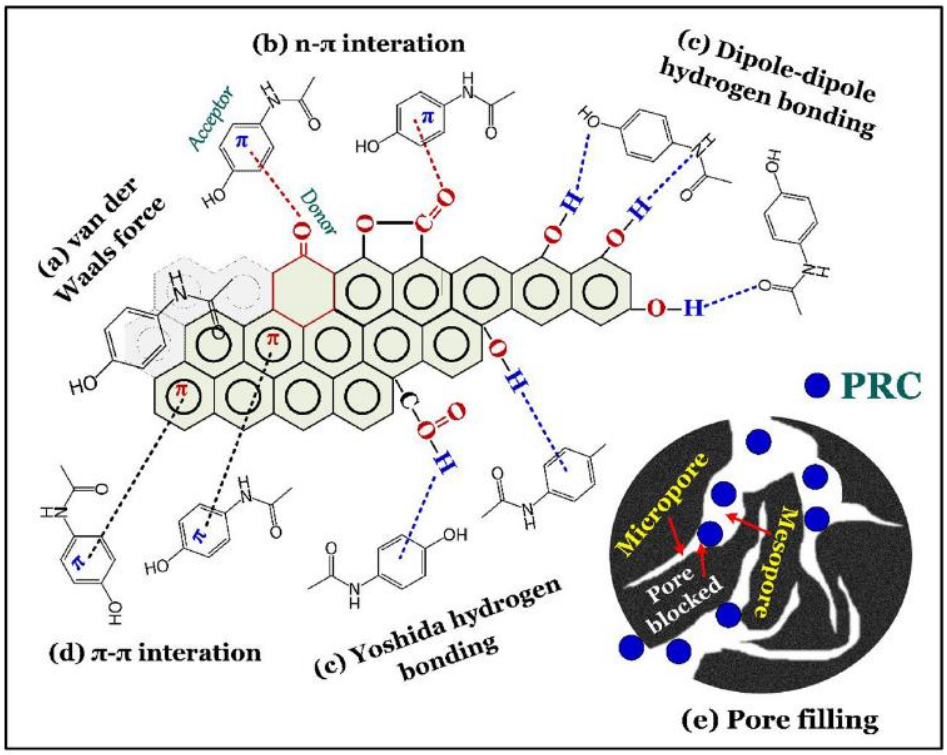
Article #1 Notes: The impact of tetracycline pollution on the aquatic environment and removal strategies.

Source Title	The impact of tetracycline pollution on the aquatic environment and removal strategies.
Source citation (APA Format)	Amangelsin, Y., Semenova, Y., Dadar, M., Aljofan, M., & Bjørklund, G. (2023). The impact of tetracycline pollution on the aquatic environment and removal strategies. *Antibiotics*, *12*(3), 440. https://doi.org/10.3390/antibiotics12030440
Original URL	https://doi.org/10.3390/antibiotics12030440
Source type	Journal Article
Keywords	tetracycline; tetracycline consumption; aquatic environment; tetracycline pollution; oxidative stress
#Tags	#Removal
Summary of key points + notes (include methodology)	Tetracycline is a widely used antibiotic both for therapeutic purposes and agriculture/aquaculture, but due to poor wastewater treatment practices causing antibiotic contamination, it is having a negative effect on the aquatic environment. Tetracycline is both very stable in the environment and poorly metabolized in the human body, meaning that effective methods of removal from water sources are necessary. Some methods that have been tested include adsorption, photodegradation, physico-chemical methods such as sonolysis, and biodegradation.
Research Question/Problem/ Need	What are methods of effectively removing tetracycline contamination from water sources?
Important Figures	None
VOCAB: (w/definition)	Biochars: carbon-based adsorbents from biomass sources
Cited references to follow up on	Chang, J., Shen, Z., Hu, X., Schulman, E., Cui, C., Guo, Q., & Tian, H. (2020). Adsorption of tetracycline by shrimp shell waste from aqueous solutions: adsorption isotherm, kinetics modeling, and mechanism. *ACS omega*, *5*(7), 3467-3477.
Follow up Questions	-How do microorganisms used for biodegradation interact with the existing microbiome? -How can the formation of more dangerous byproducts be prevented in the

	degradation of tetracycline? -The adsorption method of removal creates waste; how can this waste be properly treated and managed to avoid repeated contamination of the water source?

Article #2 Notes: Innovative spherical biochar for pharmaceutical removal from water: Insight into adsorption mechanism.

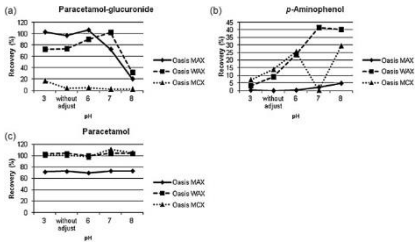
Source citation (APA Format)	Tran, H. N., Tomul, F., Ha, N. T. H., Nguyen, D. T., Lima, E. C., Le, G. T., Chang, C., Masindi, V., & Woo, S. H. (2020). Innovative spherical biochar for pharmaceutical removal from water: Insight into adsorption mechanism. *Journal of hazardous materials*, *394*, 122255. https://doi.org/10.1016/j.jhazmat.2020.122255
Original URL	https://www.sciencedirect.com/science/article/pii/S0304389420302430
Source type	Journal Article
Keywords	Emerging contaminant, Paracetamol, Biochar, Carbon sphere, Adsorption mechanism, Green material
#Tags	#Introduction #Removal
Summary of key points + notes (include methodology)	Both non-spherical and spherical biochars were prepared and analyzed by various methods (XPS, XRD, Raman spectroscopy) to determine their differences and compositions. Then, the two were tested as adsorbents of paracetamol in solution. It was concluded that both biochars were effective at adsorbing paracetamol in a wide range of conditions, but especially the spherical biochar. Significant adsorption mechanisms included pi-pi in both, pore filling in non-spherical biochar, and hydrogen bonding in spherical biochar.
Research Question/Problem/ Need	What are the applications of biochars in the adsorption of paracetamol?

Important Figures	
VOCAB: (w/definition)	XRD technique: X-ray diffraction analysis, used to gain information about the crystal properties of a substance and its components
Cited references to follow up on	Binh, Q. A., & Kajitvichyanukul, P. (2019). Adsorption mechanism of dichlorvos onto coconut fibre biochar: the significant dependence of H-bonding and the pore-filling mechanism. *Water Science and Technology*, *79*(5), 866-876.
Follow up Questions	What other pharmaceuticals can be adsorbed by such biochars? What drawbacks exist to the use of biochars instead of other adsorbents? What changes are necessary to use these in a device to treat real water contamination? How can non-spherical biochars be made more efficient?

Article #3 Notes: Interaction of Phospholipid, Cholesterol, Beta-Carotene, and Vitamin C Molecules in Liposome-Based Drug Delivery Systems: An In Silico Study.

Source citation (APA Format)	Hudiyanti, D., Putri, V. N. R., Hikmahwati, Y., Christa, S. M., Siahaan, P., & Anugrah, D. S. B. (2023). Interaction of Phospholipid, Cholesterol, Beta-Carotene, and Vitamin C Molecules in Liposome-Based Drug Delivery Systems: An In Silico Study. *Advances in Pharmacological and Pharmaceutical Sciences*, *2023*(1), 4301310.
Original URL	https://onlinelibrary.wiley.com/doi/10.1155/2023/4301310#bib-0049
Source type	Journal article
Keywords	Liposomes, cholesterol, hydrogen bonding, beta-carotene, vitamin C, drug delivery
#Tags	None (not relevant to overall project)
Summary of key points + notes (include methodology)	A computational model was used to simulate the interactions between two drugs being delivered (here, beta-carotene and vitamin C) and the phospholipid bilayer used in the delivery. It was also tested how cholesterol being added to improve rigidity would interact with the various components.
Research Question/Problem/ Need	How do components of a liposome-based drug delivery system interact with one another?
Important Figures	None
VOCAB: (w/definition)	None
Cited references to follow up on	Aljoundi A., Bjij I., El Rashedy A., and Soliman M. E. S., Covalent versus non-covalent enzyme inhibition: which route should we take? A justification of the good and bad from molecular modelling perspective, *The Protein Journal*. (2020) 39, no. 2, 97–105, https://doi.org/10.1007/s10930-020-09884-2.
Follow up Questions	Would the findings be generalizable to all drugs that would be delivered with this method? How does the concentration of cholesterol affect the timing of delivery? Do the various strength IMFs (e.g. LDFs, hydrogen bonding) behave differently?

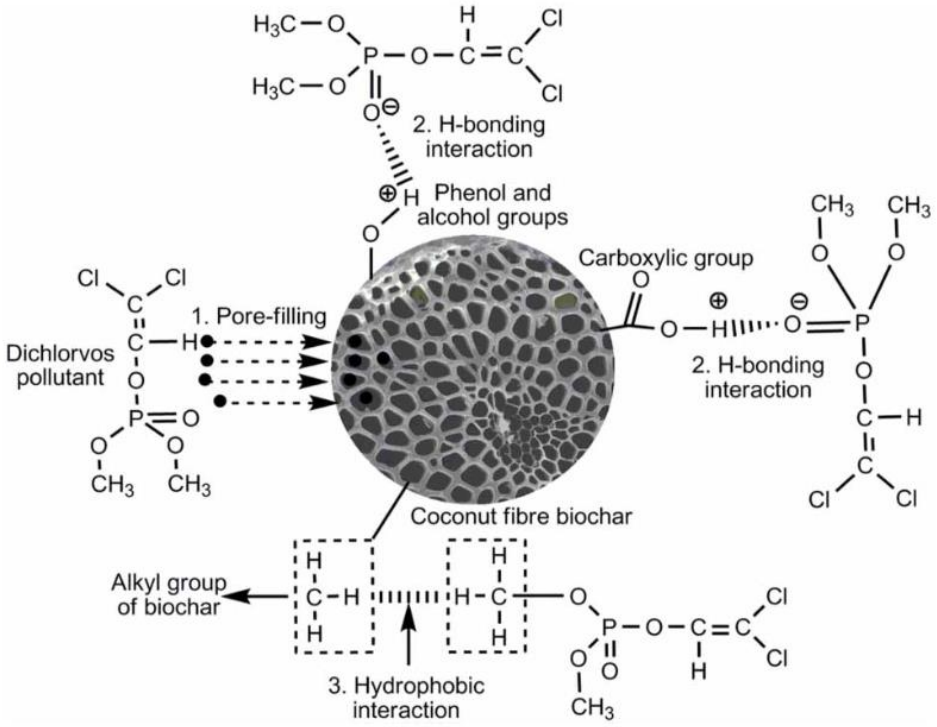
Article #4 Notes: Development of a simple analytical method for the simultaneous determination of paracetamol, paracetamol-glucuronide and p-aminophenol in river water

Source Title	Development of a simple analytical method for the simultaneous determination of paracetamol, paracetamol-glucuronide and *p*-aminophenol in river water
Source citation (APA Format)	Santos, L. H., Paíga, P., Araújo, A. N., Pena, A., Delerue-Matos, C., & Montenegro, M. C. B. (2013). Development of a simple analytical method for the simultaneous determination of paracetamol, paracetamol-glucuronide and p-aminophenol in river water. *Journal of Chromatography B*, *930*, 75-81.
Original URL	https://www.sciencedirect.com/science/article/pii/S1570023213002432
Source type	Journal article
Keywords	Paracetamol, Paracetamol-glucuronide, *p*-Aminophenol, Solid phase extraction, HPLC, River water
#Tags	#Detection
Summary of key points + notes (include methodology)	Various solid phase extraction and chromatography conditions were tested on water samples containing different concentrations of paracetamol and certain byproducts of paracetamol. Then, a method was optimized to detect all three compounds that were tested for at once.
Research Question/Problem/ Need	How can paracetamol and its byproducts in water samples be detected with one overarching method?
	

VOCAB: (w/definition)	Paracetamol-glucuronide: byproduct of paracetamol p-Aminophenol: byproduct of paracetamol
Cited references to follow up on	None currently
Follow up Questions	Could a simple device utilizing these methods be made available for more general use? Could levels be continuously monitored during water treatment with this method? Are there more complex pollution conditions that a similar method could be used to test for (e.g. multiple pollutants and byproducts interacting)?

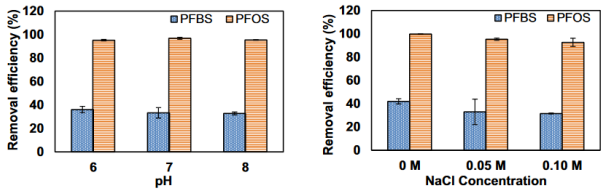
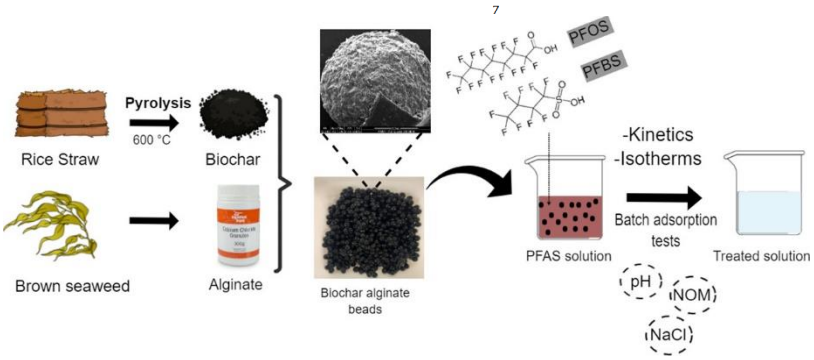
Article #5 Notes: Adsorption mechanism of dichlorvos onto coconut fibre biochar: the significant dependence of H-bonding and the pore-filling mechanism

Source Title	Adsorption mechanism of dichlorvos onto coconut fibre biochar: the significant dependence of H-bonding and the pore-filling mechanism
Source citation (APA Format)	Binh, Q. A., & Kajitvichyanukul, P. (2019). Adsorption mechanism of dichlorvos onto coconut fibre biochar: the significant dependence of H-bonding and the pore-filling mechanism. *Water Science and Technology*, *79*(5), 866-876.
Original URL	https://www.academia.edu/download/99999519/wst079050866.pdf
Source type	Journal article
Keywords	adsorption, biochar, dichlorvos, diffusion, mechanism, pesticide
#Tags	#Introduction
Summary of key points + notes (include methodology)	Coconut fibre biochar was prepared and used to adsorb dichlorovos from water. It was determined that the reaction best fit the psuedo-second order model, and that the rate-limiting step was the modelled liquid film diffusion process. The major factors that contributed to adsorption were pore-filling and hydrogen bonding.
Research Question/Problem/ Need	How does coconut fibre biochar adsorb the chemical contaminant dichlorvos?

Important Figures	 **Figure 6** | Suggested adsorption mechanism of the coconut fibre biochar and dichlorvos.
VOCAB: (w/definition)	**microporous** (having a pore size up to 2 nm) **mesoporous** (having a pore size 2 to 50 nm)
Cited references to follow up on	Tan, X., Liu, Y., Zeng, G., Wang, X., Hu, X., Gu, Y. & Yang, Z. (2015). Application of biochar for the removal of pollutants from aqueous solutions. *Chemosphere 125*, 70–85.
Follow up Questions	What does this tell us about possibilities for adsorbing contaminants with a similar chemical structure? What is the role of acid washing biochars before they are used as adsorbents, in general? Do these findings hold true in a real-world context?

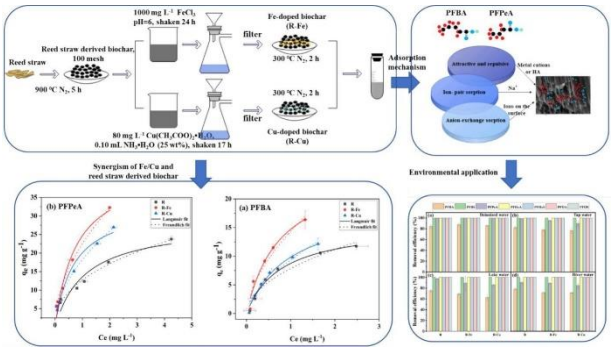
Article #6 Notes: PFAS removal from water by adsorption with alginate-encapsulated plant albumin and rice straw-derived biochar

Source Title	PFAS removal from water by adsorption with alginate-encapsulated plant albumin and rice straw-derived biochar
Source citation (APA Format)	Militao, I. M., Roddick, F., Fan, L., Zepeda, L. C., Parthasarathy, R., & Bergamasco, R. (2023). PFAS removal from water by adsorption with alginate-encapsulated plant albumin and rice straw-derived biochar. *Journal of Water Process Engineering*, *53*, 103616.
Original URL	https://www.sciencedirect.com/science/article/pii/S2214714423001332
Source type	Journal article
Keywords	PFAS Natural material-based adsorbents Remediation Adsorption Biochar
#Tags	#Introduction
Summary of key points + notes (include methodology)	Because there was a gap in the research where the best solution for PFAS removal was slow, inefficient (with short-chain PFAS) activated carbon, the effects of other substances as adsorbents were tested. Sodium alginate beads were combined with biochar treated with different substances, as well as with albumin from seed powder. Then, a model adsorption experiment was conducted. The findings were that the biochar was extremely effective at removing long-chain PFOS and less effective but still promising in removing short-chain PFBS. The adsorption mechanism indicated was hydrophobic interactions.
Research Question/Problem/ Need	How can certain types of PFAS be quickly and efficiently removed from water?

Important Figures	 **Fig. 6.** PFOS removal efficiency by NT biochar-alginate composite and PFBS removal efficiency by DAP biochar-alginate composite containing 3 % biochar, 2 % alginate, 2 % $CaCl_2$ at different a) pH conditions and b) ionic strength ($n = 2$). 
VOCAB: (w/definition)	Langmuir adsorption isotherm: models the kinetics of adsorption on homogeneous monolayer adsorption sites; presumes the adsorbate behaves as an ideal gas
Cited references to follow up on	C. Wu, M.J. Klemes, B. Trang, W.R. Dichtel, D.E. Helbling, Exploring the factors that influence the adsorption of anionic PFAS on conventional and emerging adsorbents in aquatic matrices, Water Res. 182 (2020), 115950, https://doi.org/10.1016/j.watres.2020.115950, 2020/09/01/.
Follow up Questions	How does the presence of coexisting pollutants affect performance? What would improve the success of the biochar at eliminating short-chain PFAS? How could various methods for adsorption be combined for a more effective approach?

Article #7 Notes: Efficient adsorption of short-chain perfluoroalkyl substances by pristine and Fe/Cu-loaded reed straw biochars

Source Title	Efficient adsorption of short-chain perfluoroalkyl substances by pristine and Fe/Cu-loaded reed straw biochars
Source citation (APA Format)	Liu, N., Li, Y., Zhang, M., Che, N., Song, X., Liu, Y., & Li, C. (2024). Efficient adsorption of short-chain perfluoroalkyl substances by pristine and Fe/Cu-loaded Reed straw biochars. *Science of The Total Environment*, *946*, 174223. https://doi.org/10.1016/j.scitotenv.2024.174223
Original URL	https://www.sciencedirect.com/science/article/pii/S0048969724043717
Source type	Journal article
Keywords	Perfluorobutyric acid (PFBA) Perfluoropentanoic acid (PFPeA) Biochar Adsorption Mechanisms
#Tags	#Introduction
Summary of key points + notes (include methodology)	Starting from a basis of reed straw biochar, unmodified, Fe-doped, and Cu-doped biochars were prepared. The biochars' adsorption of PFBA and PFPeA was then tested. 0.005 g of each biochar was added to 10 mL of each PFAS solution and shaken for 24 hours. After this, the solutions were filtered through a PES membrane filter and the PFAS remaining in the solution was measured with LC/MS/MS. Then, different factors were tested to measure their impact on the solution to simulate environmental conditions. It was found that both modified biochars were more effective than the initial biochar at adsorbing both types of PFAS. Environmental conditions were able to negatively affect the performance of the biochars, but they still demonstrated >86% efficiency in synthetic wastewater.
Research Question/Problem/ Need	How can biochar be used to efficiently adsorb short-chain PFAS from natural water sources?

Important Figures	
VOCAB: (w/definition)	Doping (chemistry): The introduction of very small amounts of another material into a pure substance to alter its properties.
Cited references to follow up on	Guo, W., Huo, S., Feng, J., & Lu, X. (2017). Adsorption of perfluorooctane sulfonate (PFOS) on corn straw-derived biochar prepared at different pyrolytic temperatures. *Journal of the Taiwan Institute of Chemical Engineers*, *78*, 265-271.
Follow up Questions	Could other metals be introduced into biochar to produce an even more effective adsorbent? What are drawbacks of treatment with this method? Is this method cost-efficient, and if not, how can it be made so? How could we increase the biochar surface area and porosity after doping it with the metals?

Article #8 Notes: Title

Article notes should be on separate sheets

Source Title	The mosquito strategy that could eliminate dengue
Source citation (APA Format)	Callaway, E. (2020, August 27). *The mosquito strategy that could eliminate dengue*. Nature News. https://www.nature.com/articles/d41586-020-02492-1
Original URL	https://www.nature.com/articles/d41586-020-02492-1
Source type	Science news article
Keywords	Wolbachia, insect control, mosquito, A. aegypti, dengue
#Tags	None
Summary of key points + notes (include methodology)	I chose to summarize a science news article on a proposed natural method of mosquito control. A 2020 study shows a positive impact from the release of mosquitoes infected with certain bacteria which prevent mosquitoes from transmitting viruses to curb the spread of dengue (Callaway, 2020). In the study, researchers infected mosquitoes with the *Wolbachia* bacterium, then released them into designated areas of the city of Yogyakarta in Indonesia. Although these bacteria do not naturally infect the dengue-transmitting *Aedes aegypti* mosquito, the bacteria will spread rapidly from the laboratory mosquitoes to the naturally occuring mosquito population. The results of the study showed a dramatic decrease in rates of dengue, which were 77% lower in areas with *Wolbachia*-infected mosquitoes as compared to control areas within the city several years after the mosquitoes' release (Calloway, 2020). A previous study had showed similar improvement, but was conducted in Australia, where dengue outbreaks tend to be smaller and fewer, and did not use controls (Callaway, 2020). This relates to an idea of mine which was researching ways to use natural solutions to help in controlling insect-borne diseases, such as those carried by ticks and mosquitoes. This article was from the summer brainstorming.
Research Question/Problem/ Need	How can natural bacteria be used to curb mosquito-borne disease?
Important Figures	None
VOCAB: (w/definition)	None
Cited references to follow up on	None
Follow up Questions	What other impacts do the bacteria used have on mosquitoes? Can a similar method be used with ticks? Do the modified mosquitoes have any drawbacks related to human health?

Article #9 Notes: Title

Article notes should be on separate sheets

Source Title	Evaluation of the effectiveness of the FOCUS ADHD app in monitoring adults with attention-deficit/hyperactivity disorder.
Source citation (APA Format)	Carvalho, L. R., Haas, L. M., Zeni, G., Victor, M. M., Techele, S. P., Marrone Castanho, J., Meneghetti Coimbra, I., de Freitas de Sousa, A., Ceretta, N., Garrudo, A., Grevet, E. H., & Rohde, L. A. (2023). Evaluation of the effectiveness of the focus ADHD app in monitoring adults with attention-deficit/hyperactivity disorder. *European Psychiatry*, *66*(1). https://doi.org/10.1192/j.eurpsy.2023.2422
Original URL	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC10377453/
Source type	Journal article
Keywords	ADHD, mobile app, digital, discount, adherence, attention-deficit/hyperactivity disorder
#Tags	None
Summary of key points + notes (include methodology)	For this assignment, I chose to read a study of an app for people with ADHD. The purpose of the FOCUS ADHD App was to provide a host of digital tools to assist those with ADHD. The primary functions mentioned in the study included tracking of medication, reminders to take medication, and educational content about ADHD. The results from the study did not seem to produce many useful insights. By the metrics of the study, no significant difference was found between the control group or either of the two app user groups in either adherence to medication regimens or knowledge of ADHD, though the latter may have been due to high baseline levels of knowledge creating a ceiling effect. The authors did note that the group who were offered a discount on their medication for logging their medication intake on the app were more likely to log their medication intake than those only using the app with no financial incentive. In conclusion, this study did not generate many useful insights, but the app was rated as useful by participants and appears to have the possibility to produce better results with an expanded sample. This article was from the summer brainstorming.
Research Question/Problem/ Need	What is the role of mobile applications in the treatment of ADHD?
Important Figures	None
VOCAB: (w/definition)	None
Cited references to follow up on	None
Follow up Questions	What could improve the app so that the users were more likely to use it? What

	features could be added to the app to improve its usefulness for users? Is the data from the app stored securely?

Article #10 Notes: Title

Article notes should be on separate sheets

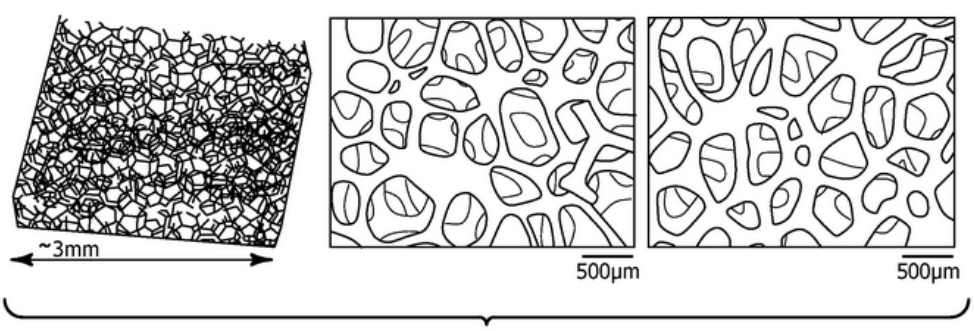
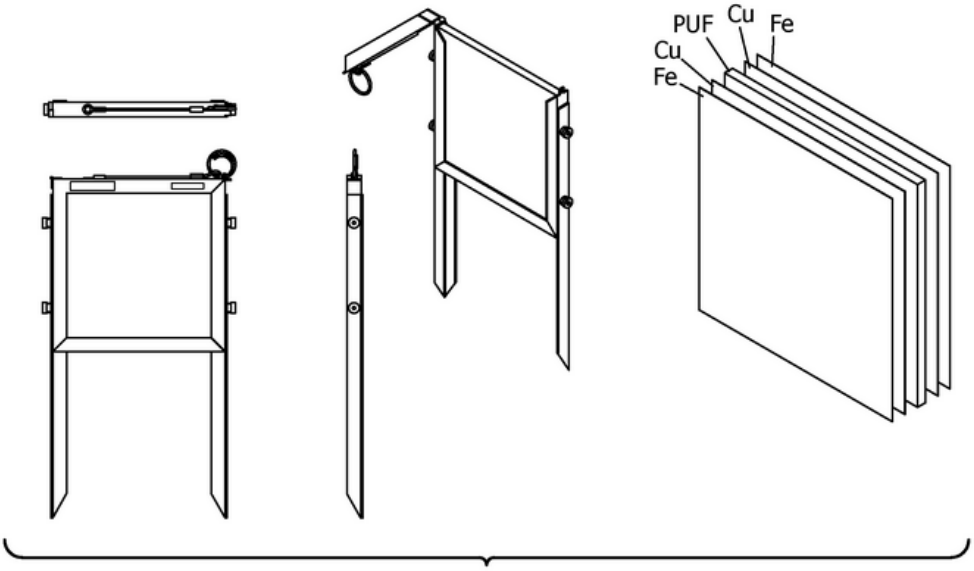
Source Title	Structures of the dopamine transporter point to ways to target addiction and disease.
Source citation (APA Format)	Sitte, H. H. (2024, August 7). *Structures of the dopamine transporter point to ways to target addiction and disease*. Nature News. https://www.nature.com/articles/d41586-024-02435-0
Original URL	https://www.nature.com/articles/d41586-024-02435-0
Source type	Science news article
Keywords	Human dopamine transmitter, ADHD, addiction, binding site, dopamine, zinc, cholesterol, drug development
#Tags	None
Summary of key points + notes (include methodology)	This article summarized new research about the human dopamine transporter (DAT). Recent studies have solved the structure of DAT for the first time. They also have provided new information about how compounds bind to it and sites where this occurs. A fourth cholesterol binding site was discovered for the first time. It was also noted that it had binding ability with zinc. These new discoveries may have implications for a variety of different dopamine-related conditions, including ADHD and addiction. In the case of a dopamine imbalance, the new information about the structure and binding sites may help with the development of drugs in the future.
Research Question/Problem/ Need	What role does the human dopamine transmitter play in addiction and disease?
Important Figures	None
VOCAB: (w/definition)	None
Cited references to follow up on	None
Follow up Questions	How can this new structure help in the development of ADHD medications? Does this play a role in drug tolerance? Which other compounds can bind to the human dopamine transmitter?

Patent #1 Notes: Title

Source Title	Modified polyamines grafted to a particulate, solid support as sorbent materials for removal of target substances from fluids.
Source citation (APA Format)	Modified polyamines grafted to a particulate, solid support as sorbent materials for removal of target substances from fluids (2024). Reeve, B. D., Li, W., Reeh, K., You, A. Y. F., & Hagemann, H. *European Patent No. 4321248A3*. European Patent Office.
Original URL	https://patentimages.storage.googleapis.com/91/94/08/35b59ae693f656/EP3774026B1.pdf
Source type	Patent
Keywords	Adsorption, PFAS, Hydrophobicity, Reuse, Functional Group, Linkage
#Tags	#Introduction
Summary of key points + notes (include methodology)	The purpose of the patent is to provide sorption of various contaminants, such as pharmaceuticals, precious metals, and PFAS from water. To do this, a branched polyamine is linked to a cellulose support material. Then, a hydrophobic functional group is linked to the polyamine. This can be used to adsorb contaminants from water which flows through it in a stream. The material can be reused by back-rinsing the adsorbent.
Research Question/Problem/ Need	It is costly and inefficient to adsorb PFAS and precious metals from water, and the adsorbent cannot be reused.
Important Figures	None
VOCAB: (w/definition)	None
Cited references to follow up on	None
Follow up Questions	How can the hydrophobic functional group be linked to the PFAS molecule instead? How can biochars be applied instead of the cellulose material? What contaminants is this unable to adsorb? What limitations exist in this process?

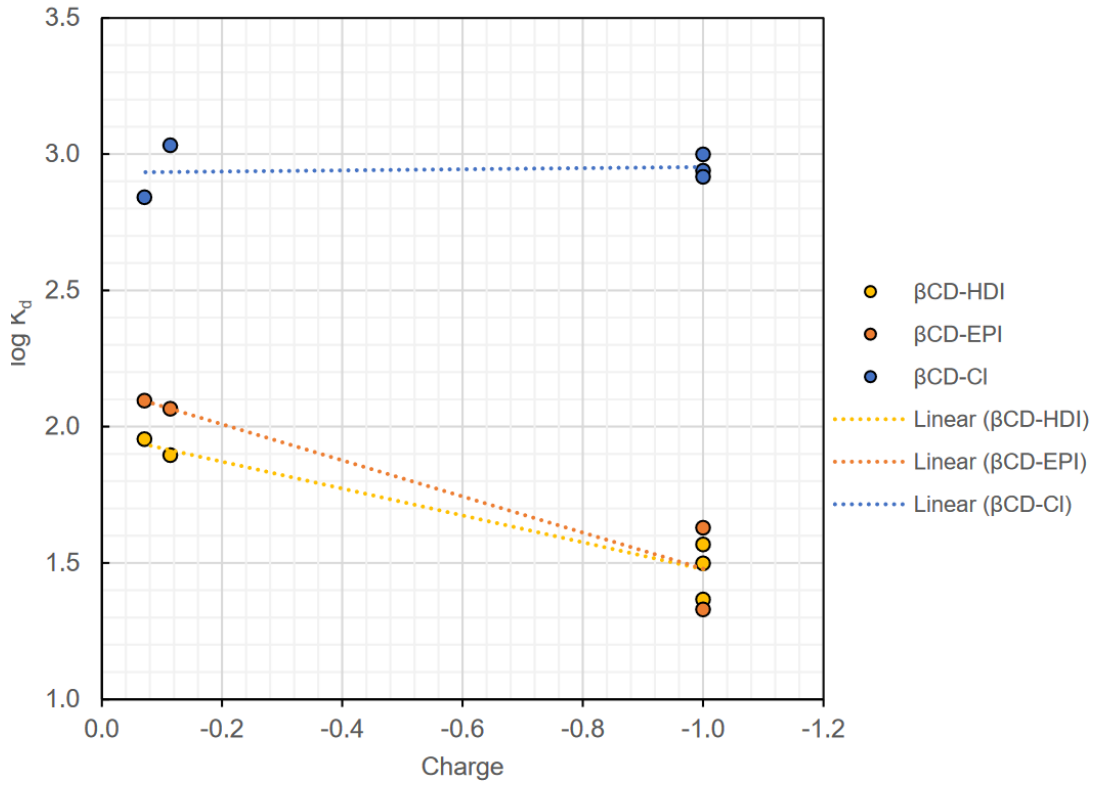
Patent #2 Notes: Title

Source Title	**Sampling for monitoring Per- and Polyfluoroalkyl Substances (PFAS) in surface water, groundwater and pore water**
Source citation (APA Format)	Sampling for monitoring Per- and Polyfluoroalkyl Substances (PFAS) in surface water, groundwater and pore water (2023). Kaltenberg, E.M., Pala, F., Dasu, K., Griesemer, F., Westlake, B., & Nanes, G. *U.S Patent No. 20230238849A1.* U.S. Patent Office.
Original URL	https://patentimages.storage.googleapis.com/a8/e8/44/5dc43bdcf3f908/US20230238849A1.pdf
Source type	Patent
Keywords	PFAS, Detection, Adsorbent, Kinetic, Equilibrium
#Tags	#Introduction
Summary of key points + notes (include methodology)	The invention is a PFAS absorbent that works in different scenarios and has a log K_d of greater than two for multiple types of PFAS. Additionally, the invention had a housing for the adsorbent and a way to detect in groundwater specifically. The adsorbent used was a polyurethane foam with both hydrophobic and hydrophilic parts, which was thought to be the best at adsorbing PFAS with various chain lengths. The temperature, pH, DOC, and ionic strength of the water were measured and used to find its K_d, which then provided a method to determine the concentration of PFAS.
Research Question/Problem/ Need	How can PFAS be effectively detected in water?

Important Figures	 FIG. 1  FIG. 2
VOCAB: (w/definition)	None
Cited references to follow up on	None
Follow up Questions	What coexisting pollutants would affect the results? How can other variables be used to indirectly track concentration? What other adsorbents with both hydrophilic and hydrophobic presentations are broadly used?

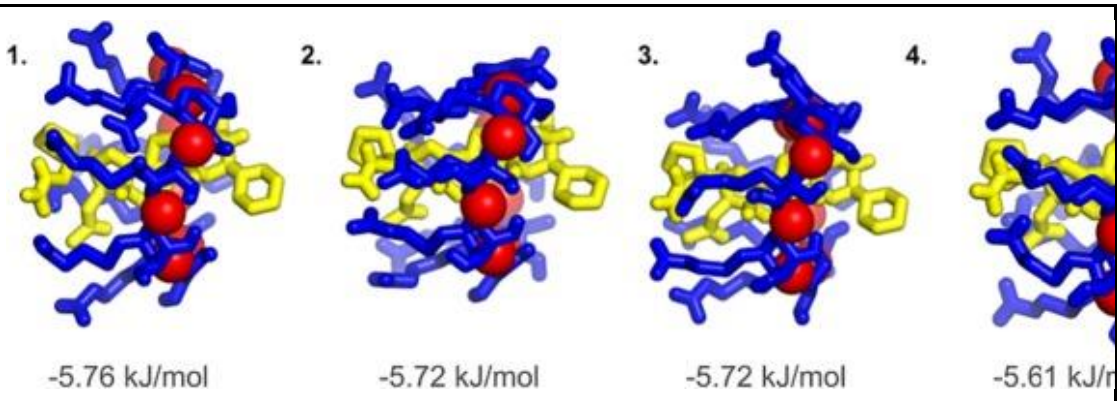
Article #11 Notes: Application of β-Cyclodextrin Adsorbents in the Removal of Mixed Per- and Polyfluoroalkyl Substances

Source Title	Application of β-Cyclodextrin Adsorbents in the Removal of Mixed Per- and Polyfluoroalkyl Substances
Source citation (APA Format)	Abaie, E., Kumar, M., Kumar, N., Sun, Y., Guelfo, J., Shen, Y., & Reible, D. (2024). Application of β-Cyclodextrin Adsorbents in the Removal of Mixed Per- and Polyfluoroalkyl Substances. *Toxics (Basel)*, *12*(4), 264. https://doi.org/10.3390/toxics12040264
Original URL	https://go-gale-com.ezpv7-web-p-u01.wpi.edu/ps/i.do?p=AONE&u=mlin_c_worpoly&id=GALE%7CA793552668&v=2.1&it=r&u group=outside&aty=ip
Source type	Journal article
Keywords	PFAS; groundwater contamination; β-cyclodextrin; adsorption; fluorine-free adsorbents
#Tags	#Introduction
Summary of key points + notes (include methodology)	This paper wanted to see the effects of beta-cyclodextrin polymers on adsorbing PFAS. They took 15 mL vials, added one of three different modified beta-cyclodextrins to each one, then filled them with 10 mL of nano-pure water and PFAS at known concentration. They let it adsorb and then centrifuged to separate the mixture. They used Liquid chromatography–quantitative time-of-flight mass spectrometry to analyze the adsorption capabilities. They found that β-CD-Cl adsorbed anionic and nonionic PFAS but not zwitterionic PFAS, but β-CD-HDI and β-CD-EPI adsorbed zwitterionic PFAS. The PFAS charge played a role in how well the latter two adsorbed it but not the first one.
Research Question/Problem/ Need	How can beta-cyclodextrins of different types be used to remove PFAS from natural water sources?

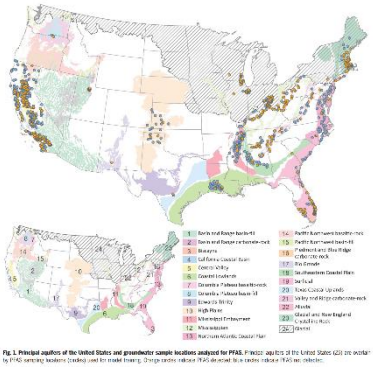
Important Figures	 **Figure 5.** Effect of PFAS charge on log K_d values. The data points correspond to PFOS, PFNA, N-MeFOSAA, and N-EtFOSAA, all of which share the same chain length of 8 fluorinated carb exhibit different charges. Surface charges were extracted from literature [39].
VOCAB: (w/definition)	N/A
Cited references to follow up on	Xiao, L.; Ling, Y.; Alsbaiee, A.; Li, C.; Helbling, D.E.; Dichtel, W.R. β-Cyclodextrin Polymer Network Sequesters Perfluorooctanoic Acid at Environmentally Relevant Concentrations. J. Am. Chem. Soc. 2017, 139, 7689–7692. https://pubmed.ncbi.nlm.nih.gov/28558203/
Follow up Questions	How can this be improved to adsorb zwitterionic compounds? What are some drawbacks to this particular cyclodextrin? What is its performance for short-chain PFAS?

Article #12 Notes: Unraveling the molecular dynamics of sugammadex-rocuronium complexation: A blueprint for cyclodextrin drug design.

Source Title	Unraveling the molecular dynamics of sugammadex-rocuronium complexation: A blueprint for cyclodextrin drug design.
Source citation (APA Format)	Anderson, A., García-Fandiño, R., Piñeiro, Á., & O'Connor, M. S. (2024). Unraveling the molecular dynamics of sugammadex-rocuronium complexation: A blueprint for cyclodextrin drug design. *Carbohydrate Polymers*, *334*, 122018. https://doi.org/https://doi.org/10.1016/j.carbpol.2024.122018
Original URL	https://www.sciencedirect.com/science/article/pii/S0144861724002443#f0010
Source type	Journal article
Keywords	Cyclodextrin Inclusion complex Affinity constant Sugammadex Rocuronium Molecular dynamics Potential of mean force Metadynamics
#Tags	#Methodology
Summary of key points + notes (include methodology)	The researchers first performed simulations to determine 8 different structures that Sugammadex could exist in in solution. Next, they used AutoDock Vina to determine the optimal poses that rocuronium could dock into each of those initial structures with. They selected the pose with the minimum docking score for each. Then they used molecular dynamics simulations, varying the distance between the center of mass of rocuronium and the center of mass of the O4 atoms in Sugammadex and seeing how the interactions changed to determine the properties at different locations. This can be used for further cyclodextrin drug design as an experimental model.
Research Question/Problem/ Need	How does sugammadex work to adsorb rocuronium in the body?

Important Figures	
VOCAB: (w/definition)	N/A
Cited references to follow up on	N/A
Follow up Questions	How can we use this outside of the drug design field? If we replaced the terminal anionic groups with cationic groups, would it bind anionic PFAS? What CV (here distances between centers of mass) would be most appropriate for PFAS?

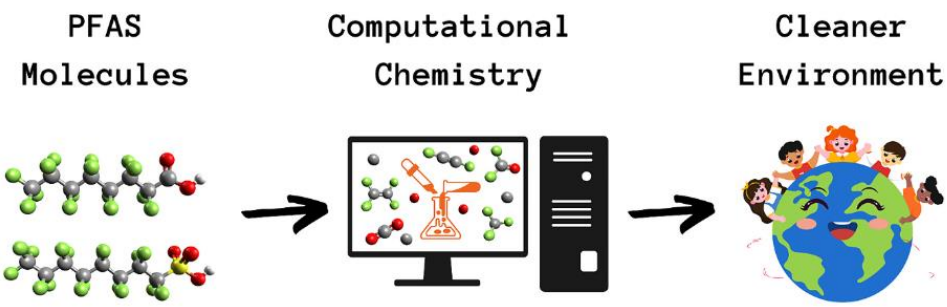
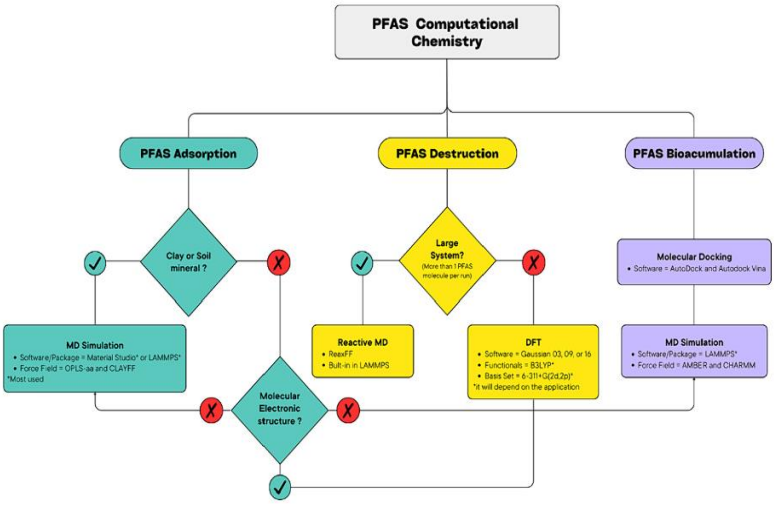
Article #13 Notes: Predictions of groundwater PFAS occurrence at drinking water supply depths in the United States.

Source Title	Predictions of groundwater PFAS occurrence at drinking water supply depths in the United States.
Source citation (APA Format)	Tokranov, A. K., Ransom, K. M., Bexfield, L. M., Lindsey, B. D., Watson, E., Dupuy, D. I., Stackelberg, P. E., Fram, M. S., Voss, S. A., Kingsbury, J. A., Jurgens, B. C., Smalling, K. L., & Bradley, P. M. (2024). Predictions of groundwater PFAS occurrence at drinking water supply depths in the United States. *Science*, *386*(6723), 748-755. https://doi.org/doi:10.1126/science.ado6638
Original URL	https://www.science.org/doi/epdf/10.1126/science.ado6638
Source type	Journal article
Keywords	PFAS, contamination, groundwater, dataset, mathematical model, prediction
#Tags	#Introduction
Summary of key points + notes (include methodology)	This study used a variety of data. They collected samples from 2019 to 2022 of well water for public, private, and agricultural use. Then they modeled potential PFAS sources and combined these into a single parameter. They took this data to create a mathematical model to predict the occurrence of PFAS at different places in the U.S. Significant data included that about 80% of those who rely on groundwater have PFAS contamination in it.
Research Question/Problem/ Need	Finding information about the occurrence of PFAS in U.S. groundwater
Important Figures	

VOCAB: (w/definition)	N/A
Cited references to follow up on	N/A
Follow up Questions	How can we add potential remediation strategies to the model? What analysis methods would help to better detect PFAS? How can PFAS be removed effectively so this problem is reduced?

Article #14 Notes: Insights into PFAS environmental fate through computational chemistry: A review.

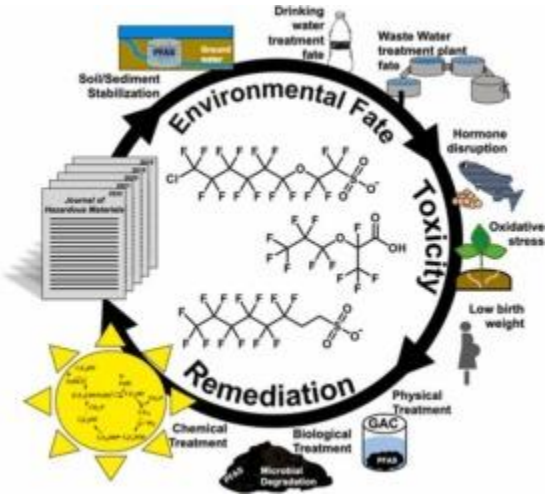
Source Title	Insights into PFAS environmental fate through computational chemistry: A review
Source citation (APA Format)	de Souza, B. B., & Meegoda, J. (2024). Insights into PFAS environmental fate through computational chemistry: A review. *The Science of the total environment*, *926*, 171738-171738. https://doi.org/10.1016/j.scitotenv.2024.171738
Original URL	https://www.sciencedirect.com/science/article/pii/S0048969724018813
Source type	Journal article
Keywords	PFAS computational modeling Molecular dynamics DFT PFAS adsorption PFAS destruction PFAS bioaccumulation
#Tags	#Introduction
Summary of key points + notes (include methodology)	-PFAS causes cancer, childhood obesity -Computational chemistry can help design adsorbents for PFAS -Molecular dynamics – drug discovery and protein characterization -Density functional theory – quantum chemistry (optimize geometries of molecules, calculating properties, determining thermodynamics) which helps study PFAS – can be used intermolecularly as well – reaction mechanisms -DFT computationally expensive -Reactive MD force field combines elements of both -Types of force field – AMBER and CHARMM (AMBER is the primary choice, CHARMM is used for proteins and larger biomolecules as well as small organic molecules), both are public domain -Previous papers have modeled the adsorption of PFAS onto different types of clay and found that PFAS behaves heterogeneously on a homogeneous surface. -Nutrient-amended montmorillonite clays suggested as poss. solution to PFAS -Grand Canonical Monte Carlo (GCMC) simulations study how many individual molecules are in a pore of the adsorbent. This can show the adsorption mechanism works in real-life. These simulations were used to study metal-organic frameworks and polymers for PFAS removal. -Revealed that some MOFs (MIL-101(Cr)s) can adsorb PFAS via Lewis acid/base complex -For destruction of PFAS, quantum chemistry mainly used -Regular molecular docking software used to model bioaccumulation with

	Molecular dynamics being used for further analysis -This last provides some of the evidence that short-chain/alternative PFAS are just as harmful as long-chain/legacy PFAS -In conclusion, MD is broadly useful and DFT is useful in providing specific details but is computationally very expensive. Computational chemistry is a useful tool to get information about PFAS environmental behavior and removal.
Research Question/Problem/ Need	To use computational chemistry to determine how PFAS behaves in the environment
Important Figures	GRAPHICAL ABSTRACT   Fig. 5. Flowchart of PFAS computational chemistry.
VOCAB: (w/definition)	N/A
Cited references to follow up on	N/A
Follow up Questions	How can these techniques be used with cyclodextrins? What are the disadvantages of MD compared to a physical experiment (wet bench)? What

	programs could be used to suggest modifications to be made?

Article #15 Notes: A review of recent studies on toxicity, sequestration, and degradation of per- and polyfluoroalkyl substances (PFAS).

Source Title	A review of recent studies on toxicity, sequestration, and degradation of per- and polyfluoroalkyl substances (PFAS).
Source citation (APA Format)	Dickman, R. A., & Aga, D. S. (2022). A review of recent studies on toxicity, sequestration, and degradation of per- and polyfluoroalkyl substances (PFAS). *Journal of Hazardous Materials*, *436*, 129120. https://doi.org/https://doi.org/10.1016/j.jhazmat.2022.129120
Original URL	https://www.sciencedirect.com/science/article/pii/S0304389422009104
Source type	Review Article
Keywords	Per- and polyfluoroalkyl substances (PFAS) Toxicity Remediation Decarboxyation, defluorination
#Tags	#Introduction
Summary of key points + notes (include methodology)	This review article summarizes the health hazards, frequency, and current treatment methods for PFAS. Treatment methods such as adsorption by AC, ion-exchange resins, and membrane filtration are ineffectual for short-chain PFAS and can be more expensive than they are worth. However, they work pretty well for long-chain PFAS. Long-chain PFAS have been shown to impede plant growth. Additionally, they have reproductive toxicity and can cause liver damage. Notably, short-chain PFAS share some of these effects due to their potential for bioaccumulation. *In silico* studies with regards to humans showed that the PFAS are able to penetrate lipid bilayers and cause hormone/endocrine disruption. Epidemiological studies revealed a positive correlation between body fat levels and PFOS/ 6:2 Cl-PFESA. The previously mentioned physical methods also leave behind PFAS that must be stored and can leach back into the environment. Chemical techniques need further research but redox reactions seem promising. Biodegradation is rare. PFAS do not break down much in the environment
Research Question/Problem/ Need	To find out more about the current state of PFAS

Important Figures	 Graphical abstract
VOCAB: (w/definition)	n/a
Cited references to follow up on	n/a
Follow up Questions	Which physical adsorbents would make chemical methods of breakdown easier to implement later? How do short-chain PFAS impact plants? What are safer methods of storing PFAS-contaminated adsorbents?

Article #16 Notes: Short-chain per- and polyfluoroalkyl substances in aquatic systems: Occurrence, impacts and treatment

Article notes should be on separate sheets

Source Title	**Short-chain per- and polyfluoroalkyl substances in aquatic systems: Occurrence, impacts and treatment**
Source citation (APA Format)	Li, F., Duan, J., Tian, S., Ji, H., Zhu, Y., Wei, Z., & Zhao, D. (2020). Short-chain per- and polyfluoroalkyl substances in aquatic systems: Occurrence, impacts and treatment. *Chemical Engineering Journal*, *380*, 122506. https://doi.org/https://doi.org/10.1016/j.cej.2019.122506
Original URL	https://www.sciencedirect.com/science/article/pii/S1385894719319096
Source type	Review article
Keywords	PFAS PFOA PFOS Persistent organic pollutant Emerging contaminant Water treatment
#Tags	#Introduction
Summary of key points + notes (include methodology)	-Short chain PFAS becoming more prevalent due to increase in regulation of PFOA and PFOS (common long-chain PFAS) and breakdown of longer PFAS -Less regulatory influence for short-chain PFAS -More hydrophilic and water soluble; less bioaccumulation and immediate toxic effects -More persistent (cleanup will be long-term) -East China, India, coastal US and Canada most impacted -PFBA and PFBS most prevalent -Thyroid/hormone changes, body weight changes -Missing health data but can spread fast so more data needed -Adsorption usually dependent on hydrophobicity -Anion exchange resins have functional groups and can do electrostatic interactions -Redox? -Need more cost info -Further research needed

Research Question/Problem/ Need	To find out a list of the ways short-chain PFAS are affecting things and how they can be removed
Important Figures	n/a
VOCAB: (w/definition)	n/a
Cited references to follow up on	n/a
Follow up Questions	How can we get more information on the effects of short-chain PFAS? Are short-chain PFAS carcinogenic? Can redox reactions be used to detect PFAS?

Article #17 Notes: AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings.

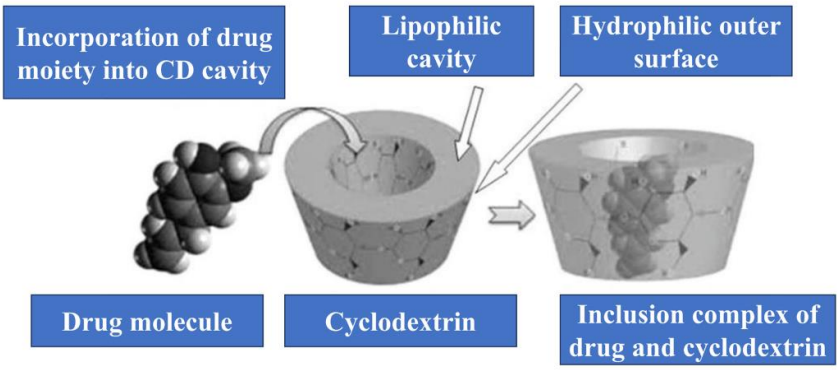
Article notes should be on separate sheets

Source Title	AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings.
Source citation (APA Format)	Eberhardt, J., Santos-Martins, D., Tillack, A. F., & Forli, S. (2021). AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings. *Journal of Chemical Information and Modeling*, *61*(8), 3891-3898. https://doi.org/10.1021/acs.jcim.1c00203
Original URL	https://pubs.acs.org/doi/10.1021/acs.jcim.1c00203
Source type	Article
Keywords	Algorithms, ligands, macrocycles, receptors, molecules
#Tags	#Methodology
Summary of key points + notes (include methodology)	-AutoDock Vina uses a more efficient search function than AutoDock 4 but is missing some of the special features like explicit water molecules, coarse-grained ligand molecules, and other things -This is due to the simplified interface -AutoDock 4 uses a physics-based scoring function which models electrostatic interactions, van der Waals, hydrogen bonds -AutoDock Vina is 3x faster and uses a function with an “electrostatic-like” term, a hydrogen bond term, a hydrophobic term, and entropy penalties -They added a way to model multiple ligands to Vina -And a way to model hydration. How this works is that water molecules are represented by a water “atom” which is attached to the ligand explicitly. They are ignored in the electrostatic calculations. If they overlap with the protein, a reward is added to the function to represent the entropy increase from that water molecule being released back into solution -Also they added Python bindings
Research Question/Problem/ Need	Vina is missing some important functions which were included in AutoDock 4, so the authors had to include them
Important Figures	n/a
VOCAB: (w/definition)	n/a
Cited references to follow up on	n/a
Follow up Questions	What are alternatives to Vina? How can Vina results be validated? How useful is the hydration feature?

Article #18 Notes: Cyclodextrins: Advances in Chemistry, Toxicology, and Multifaceted Applications.

Article notes should be on separate sheets

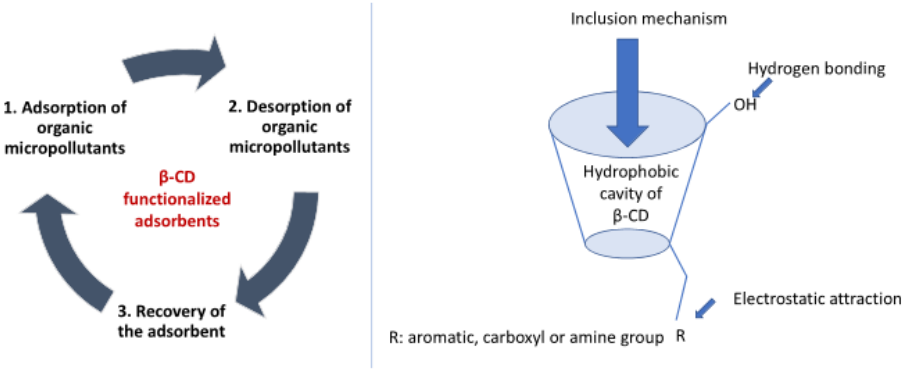
Source Title	**Cyclodextrins: Advances in Chemistry, Toxicology, and Multifaceted Applications**
Source citation (APA Format)	Musuc, A. M. (2024). Cyclodextrins: Advances in Chemistry, Toxicology, and Multifaceted Applications. *Molecules (Basel, Switzerland)*, *29*(22), 5319. https://doi.org/10.3390/molecules29225319
Original URL	https://www.mdpi.com/1420-3049/29/22/5319
Source type	Review article
Keywords	cyclodextrins; inclusion complexes; drug delivery; pharmacokinetics; nanomaterials; environmental remediation; supramolecular chemistry; smart materials
#Tags	#Introduction
Summary of key points + notes (include methodology)	-Cyclodextrins: hollow truncated cone -alpha have 6 D-glucose groups, beta 7, gamma 8 -There are bigger ones (like delta and epsilon) -Derived from starch -Hydrophobic cavity and hydrophilic exterior -Drug delivery -Food, cosmetics, textile uses -Methylation modification: hydroxyl groups replaced with methyl groups (this enhances hydrophobicity) -Other modifications involve the improvement of solubility, selectivity and effectiveness for guest molecules -Potential toxicity of beta-cyclodextrins (reduced when given orally instead of IV and mostly applicable in high doses, likely safe for water remediation) -Modify hydroxyl groups on the smaller rim of the cone (larger rim more difficult) -Enthalpy-entropy conversion -Determining molar ratios can be difficult -Influenced by pH, temp, solvent, concentration -Stabilizing volatile compounds in food industry, cosmetics -Trap organic pollutants and and heavy metals, environmentally friendly -In drug delivery, cyclodextrins improve solubility and bioavailability -Grafting onto cellulose for improved binding properties – used as an adsorbent for pesticides (!) -Orally: low toxicity (poorly adsorbed) -Must consider how modifications affect toxicity -Incorporate molecular dynamics

Research Question/Problem/ Need	To find out how cyclodextrins are being used and study their properties
Important Figures	 **Figure 2.** Schematic representation of the inclusion mechanism of a drug into the cyclodextrin cavity (adapted from [5]).
VOCAB: (w/definition)	n/a
Cited references to follow up on	n/a
Follow up Questions	Can cyclodextrins be used to detect PFAS? Can random modification work to create a PFAS adsorbent? How can cyclodextrins be disposed of once having adsorbed the PFAS?

Article #19 Notes: **β-Cyclodextrin functionalized adsorbents for removal of organic micropollutants from water**

Article notes should be on separate sheets

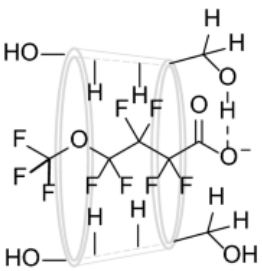
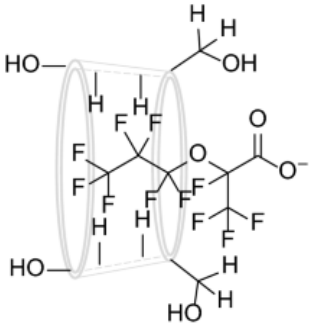
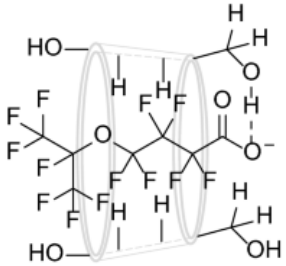
Source Title	**β-Cyclodextrin functionalized adsorbents for removal of organic micropollutants from water**
Source citation (APA Format)	Ozelcaglayan, E. D., & Parker, W. J. (2023). β-Cyclodextrin functionalized adsorbents for removal of organic micropollutants from water. *Chemosphere (Oxford)*, *320*, 137964-137964. https://doi.org/10.1016/j.chemosphere.2023.137964
Original URL	https://www.sciencedirect.com/science/article/pii/S004565352300231X?via%3Dihub
Source type	Article
Keywords	β-Cyclodextrin Organic micropollutants Water Adsorption Reuse Computational chemistry
#Tags	#Introduction
Summary of key points + notes (include methodology)	-Organic micropollutants becoming a problem -Effects may not be well studied -Regulation doesn't typically address them -Existing technologies often transform them into other forms -Beta-cyclodextrin usually modified and then grafted onto a nanocomposite -Or crosslinked polymers (groups of B-CDs), forming micro and mesoporous structures that can have high PFAS affinity -Psuedo-second-order adsorption kinetics as opposed to psuedo-first-order -Adsorption is rapid at first and slows down as the pores are filled -Fast (this is a major advantage over activated carbon) -Need to assess competitive adsorption (other molecules blocking the adsorption of the desired substance) at levels that would exist in the natural environment -Large NOMs like humic acid cannot fit into the B-CD cavity -Sodium and other ions, pH can affect the system -Desorption is feasible (one study with PFOA found over 90% desorption efficiency and no significant change in removal efficiency when reused)
Research Question/Problem/	To investigate how modified beta-cyclodextrins can form host-guest complexes

Need	with organic pollutants
Important Figures	GRAPHICAL ABSTRACT 
VOCAB: (w/definition)	n/a
Cited references to follow up on	Xiao, L., Ling, Y., Alsbaiee, A., Li, C., Helbling, D. E., & Dichtel, W. R. (2017). β-Cyclodextrin polymer network sequesters perfluorooctanoic acid at environmentally relevant concentrations. *Journal of the American Chemical Society*, *139*(23), 7689-7692.
Follow up Questions	Can B-CDs be reused when dealing with short-chain PFAS? How do natural materials compete with short-chain PFAS specifically? Do these findings apply to gamma-cyclodextrins?

Article #20 Notes: **Enhanced host–guest complexation of short chain perfluoroalkyl substances with positively charged β-cyclodextrin derivatives**

Article notes should be on separate sheets

Source Title	**Enhanced host–guest complexation of short chain perfluoroalkyl substances with positively charged β-cyclodextrin derivatives**
Source citation (APA Format)	Weiss-Errico, M. J., & O'Shea, K. E. (2019). Enhanced host–guest complexation of short chain perfluoroalkyl substances with positively charged β-cyclodextrin derivatives. *Journal of inclusion phenomena and macrocyclic chemistry*, *95*(1-2), 111-117. https://doi.org/10.1007/s10847-019-00930-w
Original URL	https://link.springer.com/article/10.1007/s10847-019-00930-w
Source type	Article
Keywords	**β-cyclodextrin** Per- and polyfluoroalkyl substances Short-chain PFAS Emerging contaminants Water remediation Organic pollutants Host-guest chemistry
#Tags	#Introduction
Summary of key points + notes (include methodology)	-Lifetime advisory limit of 70 ppt for PFOA and PFOS established, all PFAS emerging contaminants. -Long-chain being phased out for short-chain like GenX and ether-type which were thought to be less harmful and less persistent. However they can actually be more persistent and just as toxic, so this was a bad decision. -Current methods ineffective for short chain PFAS especially ether-type like PFECAs -Beta-cyclodextrin is a cyclic sugar with seven glucose subunits. It has a smaller rim and a larger rim comprised of hydroxyl groups. It has a hydrophobic interior and hydrophilic exterior. -Negative PFAS head orients toward the smaller rim -Host-guest complexation driven by positive entropy change from displacing water molecules, and the hydrophobic interactions between the cavity and PFAS backbone. Including an ether in the backbone weakens the hydrophobic interactions. Hydrogen bonding can also occur. -Long chain PFAS have very strong association constants, but short chain are weaker in this regard. This is a problem because the cyclodextrins would then be less selective for short-chain PFAS (so NOMs or other pollutants could outcompete

	them.) -Replacing hydroxyl groups (primary groups on the smaller rim) with positively charged groups like amino groups can increase the electrostatic interactions. This study tested amino B-CD (positively charged) molecules for short-chain PFAS with F NMR titration. -Solutions with pH 7 were prepared with a 2.42 × 10 −3 M concentration of PFAS (using PFBA, PFPA, PFMOBA, PFDMMOBA, PFPrOPrA). Then B-CDs were added at various molar ratios. -F NMR spectroscopy – chemical shift of each peak recorded and association constants determined with Matlab. -The shift of peaks corresponding to each fluorine changed with cyclodextrin concentration. The negatively charged cyclodextrin had decreased complexation compared to neutral charge (due to repulsive forces from the negatively charged head). -The positively charged cyclodextrins varied from no change to 20x increase in association constant. -If PFAS is branched at the head, hydrogen bonding is prevented, significantly lowering constant. If PFAS is branched at the tail, hydrogen bonding is forced and encapsulation strengthens. -One positive charge has roughly the same effect as the hydrogen bonds; multiple positive charges significantly strengthen the complex. -If the head is branched the PFAS must go through tail-first which is an unfavorable interaction -In conclusion, positively charged groups modifying the cyclodextrins are effective for the short-chain, ether, PFAS tested and had little to no or a slightly negative effect on association constant for the long-chain and non-ether PFAS.
Research Question/Problem/ Need	How can short-chain PFAS be adsorbed by beta-cyclodextrins?
Important Figures	 **PFMOBA**  **PFPrOPrA**  **PFDMMOBA**
VOCAB: (w/definition)	n/a
Cited references to follow up on	n/a
Follow up Questions	How can computational chemistry be used to confirm these results? How can we make a cyclodextrin that would be applicable for both long- and short-chain PFAS?

	What other positive groups would be cheapest to manufacture (the best solution to do cost-effective remediation?)