24th Annual (Virtual) Summer Research Symposium

Sponsored by
The Bayer School of
Natural and Environmental Sciences

Keynote Address:

Shon Remich, M.D.
VP Global Head of Clinical Development and Operations,
Takeda Pharmaceuticals

“The SARS-CoV2 Pandemic: Perspectives from a Vaccine Developer”

Friday, July 30, 2021
10 a.m. to 2 p.m.
Welcome to the
2021 Virtual Summer Undergraduate Research Symposium!

On behalf of the faculty and staff of the Bayer School of Natural and Environmental Sciences, welcome to the 24th Annual Summer Undergraduate Research Symposium. Each year we are excited to host this event as a culmination of your summer of research experience. Today is an important day for each of you, your research advisor and your parents as you present your work at the symposium. Whether this was your first research experience or you are an experienced student investigator returning for your second or third summer, we know that you have grown as a scientist over the course of this summer. We are looking forward to hearing the presentations today and we hope this experience will only be a starting point for your scientific careers. Good luck today and in your future academic and career endeavors.

Sincerely,

Ellen Gawalt
Interim Dean
Bayer School of Natural and Environmental Sciences

Schedule:

10 a.m. Welcome and Keynote Address Zoom Link
11 a.m. Poster Session I Zoom Links
Noon Break
1 p.m. Poster Session II Zoom Links
2 p.m. Ice Cream Social Mellon Hall

Contents:

About Dr. Shon Remich 3
Index of Authors and Posters 4
Schedule of Presentations 7
Abstracts 16
Representation of Home Institutions 69

Instructions to Authors:

Authors can locate their assigned poster sessions and the time of their presentations, starting at page seven. The abstracts of all the authors’ research begin at page sixteen. Please remember all presentations are up to eight minutes, with two minutes of questions and answers. All Q&A will be conducted on the chat feature in each room.
About Dr. Shon Remich

Dr. Remich received his medical degree from the University of Oklahoma where he conducted his first honors research and was awarded a Health Education Scholarship (HPSP) from the United States Army. After completing his Pediatric internship and residency, he served as Chief of Pediatrics at Reynolds Army Hospital. His formal training in research began with a post-doctorate in Clinical Pharmacology at Georgetown University joining Dr. David Flockhart’s pharmacogenetics lab. In 2001, Dr. Remich joined the Walter Reed Army Institute of Research (WRAIR) and was deployed to Kenya to establish the military’s first dedicated drug development platform at the US Army Medical Directorate-Africa (USAMRD-A) and conducted the first GMP IV Artesunate study on the continent. Leveraging the success of life saving treatments, Dr. Remich developed a passion for playing a role in the prevention as well as the treatment of devastating neglected diseases, culminating in a second post-doctorate in Allergy and Immunology at the joint National Institutes of Health and Walter Reed Medical Center program. In 2008, he returned to Kenya to lead the Department of Defense ‘s Presidential Emergency Plan for Aids Relief (PEPFAR) country program and as the military liaison to the Kenyan Defense Forces HIV prevention program. He was selected by the US ambassador to Kenya to lead select public health initiatives augmenting PEPFAR’s improvement in infant survival and health care infrastructure. Returning to the US in 2012, he became the Senior Director of WRAIR’s Translational Medicine division, conducting clinical trials in Malaria, Dengue, Shigella, Anthrax, Chikungunya, as well as the first study of the VSV-Ebola vaccine with additional duties included overseeing the operations and major expansion of WRAIR’s multiple campaign Pilot Bioproduction Facility.

Following his 23 year military career, he joined Pfizer’s vaccine clinical research and development team executing pivotal phase 3 studies for C difficile, overseeing the expansion and US licensure of Tico-Vax (tick born encephalitis vaccine), and assuming a pivotal role in the development of the Pfizer-BioNTech mRNA COVID vaccine. In 2021, Dr. Remich joined Takeda Pharmaceuticals to lead their clinical development and operational Vaccine branch including vaccine candidates for Dengue, Zika, Norovirus, COVID, and influenza.

Zoom Link to Dr. Remich’s Keynote Address

https://duq.zoom.us/j/3921708843?pwd=cEZqOTZZOWliN3ZHUl0ySm9UaWpmQT09

Meeting ID: 392 170 8843
Passcode: Keynote
<table>
<thead>
<tr>
<th>Name</th>
<th>Poster #</th>
<th>Name</th>
<th>Poster #</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agarwal, Annika</td>
<td>66</td>
<td>Deal, Brooke</td>
<td>86, 88</td>
</tr>
<tr>
<td>Anderson, Carl</td>
<td>91</td>
<td>Dembowski, Jill</td>
<td>97, 100</td>
</tr>
<tr>
<td>Appadoo, Shania</td>
<td>37</td>
<td>Demjanenko, Peter</td>
<td>50</td>
</tr>
<tr>
<td>Armen, Jennifer</td>
<td>50</td>
<td>Deslouches, Jakobi</td>
<td>38</td>
</tr>
<tr>
<td>Aumer, Thomas</td>
<td>24, 49</td>
<td>Dobbins, Duncan</td>
<td>39</td>
</tr>
<tr>
<td>Auron, Philip</td>
<td>57, 74</td>
<td>Doyle, Liam</td>
<td>2</td>
</tr>
<tr>
<td>Bai, Qing</td>
<td>84</td>
<td>Drennen, James K.</td>
<td>91</td>
</tr>
<tr>
<td>Bandosz, Mikolaj</td>
<td>67</td>
<td>Dryzal, Dana</td>
<td>105</td>
</tr>
<tr>
<td>Barner, Grace</td>
<td>1</td>
<td>Durosko, Anna</td>
<td>32</td>
</tr>
<tr>
<td>Baxter, Dylan</td>
<td>61</td>
<td>Eiben, Yael</td>
<td>79</td>
</tr>
<tr>
<td>Bayto, Mikayla</td>
<td>55</td>
<td>Esenwein, Raegen</td>
<td>97</td>
</tr>
<tr>
<td>Bedford, Felicia</td>
<td>56</td>
<td>Evans, Anton</td>
<td>9, 12</td>
</tr>
<tr>
<td>Beidler, Erica</td>
<td>68</td>
<td>Evans, Kelsey</td>
<td>25</td>
</tr>
<tr>
<td>Benmokhtar, Fatiha</td>
<td>6, 93</td>
<td>Evanseck, Jeffrey</td>
<td>27, 29, 30, 34, 36, 40, 78, 95</td>
</tr>
<tr>
<td>Bhatt, Akshita</td>
<td>83</td>
<td>Fadare, Anuoluwapo</td>
<td>98</td>
</tr>
<tr>
<td>Bliss, Shawn</td>
<td>43</td>
<td>Farmen, Christopher</td>
<td>26, 62</td>
</tr>
<tr>
<td>Boesch, Scott</td>
<td>34</td>
<td>Faruk, Asef</td>
<td>42, 83</td>
</tr>
<tr>
<td>Bohrer, Luke</td>
<td>81</td>
<td>Ferrara, Lyndsie</td>
<td>63, 64</td>
</tr>
<tr>
<td>Bojanac, Izayah</td>
<td>95</td>
<td>Fetzer, Nicholas</td>
<td>8</td>
</tr>
<tr>
<td>Brown, Zoey</td>
<td>72</td>
<td>Firek, Julianna</td>
<td>63</td>
</tr>
<tr>
<td>Buckner, Ira S.</td>
<td>90</td>
<td>Flaherty, Patrick</td>
<td>42, 83, 84</td>
</tr>
<tr>
<td>Burns, Austin</td>
<td>28, 36</td>
<td>Fry, Allison</td>
<td>26, 65</td>
</tr>
<tr>
<td>Burton, Edward</td>
<td>84</td>
<td>Frye, C.</td>
<td>32, 106</td>
</tr>
<tr>
<td>Cane, Brandon</td>
<td>31</td>
<td>Fu, Jiahao</td>
<td>9, 12</td>
</tr>
<tr>
<td>Cascio, Michael</td>
<td>15, 24, 49</td>
<td>Gangjee, Aleem</td>
<td>85</td>
</tr>
<tr>
<td>Cavanaugh, Jane</td>
<td>42, 83</td>
<td>Garcia, Emily</td>
<td>40</td>
</tr>
<tr>
<td>Cawley, Hannah</td>
<td>105</td>
<td>Gawalt, Ellen</td>
<td>25, 50, 51, 54</td>
</tr>
<tr>
<td>Celestin, Hervinah</td>
<td>96</td>
<td>Gayluak, Nya</td>
<td>80, 89</td>
</tr>
<tr>
<td>Chandwani, Manisha</td>
<td>76, 98, 99</td>
<td>Gernatt, Grace</td>
<td>96</td>
</tr>
<tr>
<td>Chartier, Eric</td>
<td>78</td>
<td>Gibbs, William</td>
<td>13</td>
</tr>
<tr>
<td>Chase, Daniel</td>
<td>82</td>
<td>Glasser, Sarah</td>
<td>33</td>
</tr>
<tr>
<td>Clark, Russell</td>
<td>94</td>
<td>Goralski, Peter</td>
<td>42</td>
</tr>
<tr>
<td>Clegg, Benjamin</td>
<td>51</td>
<td>Gordon, Andrew</td>
<td>84</td>
</tr>
<tr>
<td>Cocolas, Alex</td>
<td>80, 89</td>
<td>Gray, Carlan</td>
<td>19</td>
</tr>
<tr>
<td>Conklin, Shane</td>
<td>101</td>
<td>Grimaldi, Lydia</td>
<td>14</td>
</tr>
<tr>
<td>Cook, Amy</td>
<td>105</td>
<td>Guan, Y.</td>
<td>31</td>
</tr>
<tr>
<td>Cooke, Lauren</td>
<td>102</td>
<td>Guarinoni, K</td>
<td>32</td>
</tr>
<tr>
<td>Corecvilos, Theodore</td>
<td>24, 49, 58, 92</td>
<td>Gumireddy, Ashwini</td>
<td>90</td>
</tr>
<tr>
<td>Costa, Suzannah</td>
<td>7, 41</td>
<td>Haberstock, Isabella</td>
<td>65</td>
</tr>
<tr>
<td>Cowan, Shane</td>
<td>74</td>
<td>Hajjassani, Arian</td>
<td>15, 24</td>
</tr>
<tr>
<td>Cunningham, Caylee</td>
<td>19, 32, 106</td>
<td>Hallak, Ramez</td>
<td>42, 83, 84</td>
</tr>
<tr>
<td>Daneshwar, Nesa</td>
<td>67</td>
<td>Hammers, Jennifer</td>
<td>71</td>
</tr>
<tr>
<td>Dave, Kandarp</td>
<td>39</td>
<td>Hao, Weier</td>
<td>60</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Harlan, Emery</td>
<td>26</td>
</tr>
<tr>
<td>Name</td>
<td>Poster #</td>
<td>Name</td>
<td>Poster #</td>
</tr>
<tr>
<td>--------------------------------</td>
<td>----------</td>
<td>--------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>Harvey, Lindsay</td>
<td>67</td>
<td>Levine, Stacey</td>
<td>45</td>
</tr>
<tr>
<td>Hatten, Jahmaine</td>
<td>51</td>
<td>Lim, Min</td>
<td>25</td>
</tr>
<tr>
<td>Hawkins, Hailey</td>
<td>70</td>
<td>Loughner, Lindsay</td>
<td>73</td>
</tr>
<tr>
<td>Hemerson, Marlo</td>
<td>99</td>
<td>Lowther, Warren</td>
<td>15, 24</td>
</tr>
<tr>
<td>Henson, Samuel</td>
<td>91</td>
<td>Ludvico, Lisa</td>
<td>61</td>
</tr>
<tr>
<td>Hernandez, Gleymi</td>
<td>52</td>
<td>Lummis, Paul</td>
<td>35, 79</td>
</tr>
<tr>
<td>Higinbotham, Douglas</td>
<td>93</td>
<td>Luong, Ny</td>
<td>82</td>
</tr>
<tr>
<td>Hoenig, Brandon</td>
<td>59, 96</td>
<td>Macar, David</td>
<td>57</td>
</tr>
<tr>
<td>Hoke, Tiffany</td>
<td>60</td>
<td>Mack, Kathryn</td>
<td>4</td>
</tr>
<tr>
<td>Hopkins, Taylor</td>
<td>64</td>
<td>Mackenstein, Nicole</td>
<td>16</td>
</tr>
<tr>
<td>Horton, Camren</td>
<td>85</td>
<td>Makowski, Joseph</td>
<td>30</td>
</tr>
<tr>
<td>Hostetler, John C.</td>
<td>44</td>
<td>Manickam, Devika</td>
<td>39</td>
</tr>
<tr>
<td>Hrach, Victoria</td>
<td>101</td>
<td>Marquis, Sara</td>
<td>28, 36</td>
</tr>
<tr>
<td>Iuliucci, Robbie</td>
<td>34</td>
<td>Marshall, Pamela</td>
<td>71</td>
</tr>
<tr>
<td>Janecka, Jan</td>
<td>57</td>
<td>Massari, Kayla</td>
<td>26, 65</td>
</tr>
<tr>
<td>Janjic, Jelena</td>
<td>86, 88</td>
<td>McCallister, Megan</td>
<td>70</td>
</tr>
<tr>
<td>Jeganathar Kanmanii, Narthana</td>
<td>10</td>
<td>McClure, Taylor</td>
<td>73</td>
</tr>
<tr>
<td>Jemison, Kezia</td>
<td>27</td>
<td>McCormick, Joseph</td>
<td>103, 104</td>
</tr>
<tr>
<td>Jensen-Seaman, Michael I.</td>
<td>13, 17, 73</td>
<td>McIntyre, Clancy</td>
<td>17</td>
</tr>
<tr>
<td>Kaczynski, Katie</td>
<td>80, 89</td>
<td>Metzler, Luke</td>
<td>22, 26, 62, 65</td>
</tr>
<tr>
<td>Kamte, Yashika</td>
<td>76, 98, 99</td>
<td>Mihailescu, Mihaela-Rita</td>
<td>16, 18, 19, 32, 95, 106</td>
</tr>
<tr>
<td>Kane, Ella</td>
<td>3</td>
<td>Milback, Ella</td>
<td>18</td>
</tr>
<tr>
<td>Kazimer, Benjamin</td>
<td>45</td>
<td>Montgomery, Thomas</td>
<td>28, 29, 36, 78, 80, 82, 89</td>
</tr>
<tr>
<td>Kelleher, Bryan</td>
<td>95</td>
<td>Moskal, Lindsay</td>
<td>29</td>
</tr>
<tr>
<td>Kelley, Connor</td>
<td>90</td>
<td>Nayeen, Junayed</td>
<td>85</td>
</tr>
<tr>
<td>Kelly, Jordan</td>
<td>22</td>
<td>Neilian, Rachael</td>
<td>53</td>
</tr>
<tr>
<td>Kelly, Thomas</td>
<td>21</td>
<td>Nelson, Rebecca</td>
<td>58</td>
</tr>
<tr>
<td>Kensinger, Adam</td>
<td>95</td>
<td>Nestler, Matthew</td>
<td>46</td>
</tr>
<tr>
<td>Kessler, Collin</td>
<td>7, 9</td>
<td>Nguyen, Melissa</td>
<td>21</td>
</tr>
<tr>
<td>Kim, Wook</td>
<td>7, 9, 12, 41</td>
<td>O'Donnell, Lauren</td>
<td>76, 98, 99</td>
</tr>
<tr>
<td>King, William</td>
<td>102</td>
<td>Omstead, Madisen</td>
<td>87</td>
</tr>
<tr>
<td>Kingston, Howard “Skip”</td>
<td>60</td>
<td>Orgovan, Jessica</td>
<td>103</td>
</tr>
<tr>
<td>Koch, Andrew</td>
<td>28, 36</td>
<td>Packard, Jessica</td>
<td>100</td>
</tr>
<tr>
<td>Kohler, Olivia</td>
<td>20</td>
<td>Pamuku, Matt</td>
<td>60</td>
</tr>
<tr>
<td>Kolber, Benedict</td>
<td>53</td>
<td>Parshall, Rachel</td>
<td>87</td>
</tr>
<tr>
<td>Kosel, Kelby</td>
<td>68</td>
<td>Parsi, Leeann</td>
<td>106</td>
</tr>
<tr>
<td>Kosowsky, A.</td>
<td>31</td>
<td>Patel, Saloni</td>
<td>42, 83</td>
</tr>
<tr>
<td>Kostek, Matthew</td>
<td>77, 87</td>
<td>Pater, Jordan</td>
<td>96</td>
</tr>
<tr>
<td>Kotsikorou, Evangelia</td>
<td>40</td>
<td>Patterson, Charles</td>
<td>86, 88</td>
</tr>
<tr>
<td>Lackey, Patrick</td>
<td>16, 95</td>
<td>Patton-Vogt, Jana</td>
<td>101, 102</td>
</tr>
<tr>
<td>Lampe, David</td>
<td>21</td>
<td>Pellegrene, Kendy</td>
<td>95</td>
</tr>
<tr>
<td>Lapinsky, David</td>
<td>81</td>
<td>Pereira, Kenzie</td>
<td>38</td>
</tr>
<tr>
<td>Lara, Laura Carolina</td>
<td>57</td>
<td>Perry, Stephanie</td>
<td>74</td>
</tr>
<tr>
<td>Leninkannan, Madhura</td>
<td>69</td>
<td>Pickering, Quinn</td>
<td>34</td>
</tr>
</tbody>
</table>
## Index of Posters and Authors

<table>
<thead>
<tr>
<th>Name</th>
<th>Poster #</th>
<th>Name</th>
<th>Poster #</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pollock, John</td>
<td>86, 88</td>
<td>Tressler, Serina</td>
<td>29, 80, 89</td>
</tr>
<tr>
<td>Porter, Brady</td>
<td>55, 59</td>
<td>Uhrin, Madison</td>
<td>76</td>
</tr>
<tr>
<td>Ports, Brianna</td>
<td>17</td>
<td>Valenty, Hannah</td>
<td>93</td>
</tr>
<tr>
<td>Powell, Meghan</td>
<td>70</td>
<td>Van Stipdonk, Michael</td>
<td>22, 26, 62, 65</td>
</tr>
<tr>
<td>Powers, Elizabeth</td>
<td>70</td>
<td>Wallace, Sarah</td>
<td>67, 70</td>
</tr>
<tr>
<td>Price, Olivia</td>
<td>87</td>
<td>Wells, Meghan</td>
<td>9, 12</td>
</tr>
<tr>
<td>Qoyawayma, Kevin</td>
<td>5</td>
<td>Wetzel, Stephanie</td>
<td>105</td>
</tr>
<tr>
<td>Rague, Andrea</td>
<td>37</td>
<td>Williams, Maya</td>
<td>100</td>
</tr>
<tr>
<td>Rapp, Chloe</td>
<td>71</td>
<td>Wilson, Bethann</td>
<td>8, 11</td>
</tr>
<tr>
<td>Rebel, Lauren</td>
<td>10</td>
<td>Wilson, Kathleen</td>
<td>59</td>
</tr>
<tr>
<td>Recktenwald, Sean</td>
<td>6</td>
<td>Woerpel, Keith</td>
<td>30</td>
</tr>
<tr>
<td>Reeder, Philip</td>
<td>61</td>
<td>Woodley, Sarah</td>
<td>38, 72, 75, 76</td>
</tr>
<tr>
<td>Reith, Carley</td>
<td>53</td>
<td>Woods, Peter</td>
<td>59</td>
</tr>
<tr>
<td>Rodo, Edgar</td>
<td>30</td>
<td>Wood-Vassey, Michael</td>
<td>3</td>
</tr>
<tr>
<td>Rohde, Jeffrey</td>
<td>78</td>
<td>Yerneni, Sai Gopal</td>
<td>57</td>
</tr>
<tr>
<td>Rupprecht, Alexander</td>
<td>54</td>
<td>Young, Zachary</td>
<td>42</td>
</tr>
<tr>
<td>Ryan, Matt</td>
<td>35</td>
<td>Zhang, Yuanshan</td>
<td>94</td>
</tr>
<tr>
<td>Santoro, Ava</td>
<td>41</td>
<td>Zito, Miranda</td>
<td>77</td>
</tr>
<tr>
<td>Schaer, Suzanne</td>
<td>11</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Seibert, Mark</td>
<td>22, 26</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Seybert, David</td>
<td>20, 23</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Shaw, Rosemarie</td>
<td>104</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Shide, Jasper</td>
<td>28, 36</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sipko, Emily</td>
<td>23</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Skomo, Alec</td>
<td>91</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Slater, Tasia</td>
<td>75</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Snidow, Robert</td>
<td>54</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorescu, Monica</td>
<td>22</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spadavecchia, Katelyn</td>
<td>92</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Staton, Chanel</td>
<td>59</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stirrat, Thomas</td>
<td>15, 24</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stolz, John</td>
<td>8, 10, 11, 55</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sugden, Lauren</td>
<td>56</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sullivan, Marie</td>
<td>47</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Summers, Austin</td>
<td>9, 12</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Supinski, Alexandra</td>
<td>48</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Szucs, Kimberly</td>
<td>77</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tamez, Angel</td>
<td>27, 40</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tanyeri, Melikhan</td>
<td>43, 46, 52</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Taylor, Kimberly</td>
<td>84</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Teague, Vaughn</td>
<td>42, 83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Teitelbaum, Taylor</td>
<td>60</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tidgewell, Kevin</td>
<td>37, 52</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Traore, Aboubacar</td>
<td>86, 88</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Poster Session 1: 11 a.m. to 12 p.m.**
Moderator: Ashley Parisi-Goldblatt, Ph.D. Candidate
Zoom Link: [https://duq.zoom.us/j/99477183001](https://duq.zoom.us/j/99477183001)
Meeting ID: 994 7718 3001

1. Grace Barner: “Relativistic Kinematics studies for Kaons and Pions creation in electron proton scattering experiments at Jefferson Lab.” (11 a.m.)

2. Liam Doyle: “pPXF and its Applications to Type Ia Supernovae.” (11:10 a.m.)

3. Ella Kane: “Survey of Transiting Extrasolar Planets at the University of Pittsburgh (STEPUP)” (11:20 a.m.)


5. Kevin Qoyawayma: “Simulating the Combined Gravitational Wave Signal from Double White Dwarf Binaries.” (11:40 a.m.)


**Poster Session 2: 11 a.m. to 12 p.m.**
Moderator: Jessica Packard, Ph.D. Student
Zoom Link: [https://duq.zoom.us/j/98714774101](https://duq.zoom.us/j/98714774101)
Meeting ID: 987 1477 4101

7. Suzannah Costa: “Reconstructing naturally acquired mutations that alter the regulation of cyclic di-GMP production in bacteria.” (11 a.m.)

8. Nicholas Fetzer: “Investigation of anaerobic respiration in the selenite respiring Bacillus selenitereducens strain MLS10.” (11:10 a.m.)

9. Jiahao Fu: “Identifying functionally important residues of a bacterial protein through competition assays.” (11:20 a.m.)

10. Lauren Rebel: “Comparing Methods of Extracting RarA, a Membrane Porin from Sulfurospirillum barnesii SES-3” (11:30 a.m.)

11. Suzanne Schaer: “Antibiotic Resistance in Alkalilimnicola ehrlichii strain MLHE-1.” (11:40 a.m.)

12. Austin Summers: “Engineering a library of antibiotic resistant and fluorescent strains of Pseudomonas fluorescens to study the function of RsmE.” (11:50 a.m.)
13. Liam Gibbs: “Dual Affinity Chromatography to Purify Recombinant Seminal Proteins to Analyze Biochemical Differences between Humans and Chimpanzees.” (11 a.m.)

14. Lydia Grimaldi: “Characterization of the (G4C2)45 repeat in the C9ORF72 gene.” (11:10 a.m.)

15. Arian Hajihassani: “Investigation of the human glycine receptor (GlyR) using crosslinking mass spectrometry. (11:20 a.m.)

16. Nicole Mackenstein: “Stability of histone mRNA stem loop degradation intermediates.” (11:30 a.m.)

17. Clancy McIntyre: “Optimization of Purity and Yield of Semenogelin 1 Fragments for Inclusion in Transglutaminase Assays.” (11:40 a.m.)


Poster Session 4: 11 a.m. to 12 p.m.
Moderator: Emily Bierer, Ph.D. Student
Zoom Link: https://duq.zoom.us/j/93508239137
Meeting ID: 935 0823 9137


20. Olivia Kohler: “The effect of polyanions on malate dehydrogenase.” (11:10 a.m.)


22. Mark Seibert: “Gas Phase DNA Cleavage with a Nickel (II) Monoprotic Aminophosphine Complex.” (11:30 a.m.)

23. Emily Sipko: “Macromolecular crowding effects on the kinetic properties of malate dehydrogenase.” (11:40 a.m.)

24. Thomas Stirrat: “Optimization of peptide derivatization for fluorescence normalization and sub-fmol quantitation.” (11:50 a.m.)
Poster Session 5: 11 a.m. to 12 p.m.
Moderator: Benjamin Clegg, Ph.D. Student
Zoom Link: https://duq.zoom.us/j/95620561059
Meeting ID: 956 2056 1059
Passcode: N/A


26. Allison Fry: “A computational investigation of the intrinsic conformation and fragmentation of peptides modified to include N-terminal imine groups.” (11:10 a.m.)

27. Kezia Jemison: “Polarization of three water clusters in quantum mechanical/molecular mechanical calculations reveals novel hydration buckle essential to malonate decarboxylation.” (11:20 a.m.)

28. Sara Marquis: “Comparing DFT and semi-empirical computational methods in the investigation of asymmetric diaryl iodoniums reductive elimination.” (11:30 a.m.)

29. Lindsay Moskal: “Alignment of Computed Gas-Phase Urea Structure with Experiment.” (11:40 a.m.)

30. Edgar Rodo: “DFT-Based Procedure for a Stereocchemical Model for Nucleophilic Substitution with Five-Membered Ring Oxocarbenium Ions.” (11:50 a.m.)

Poster Session 6: 11 a.m. to 12 p.m.
Moderator: Jeff Rohde, Ph.D.
Zoom Link: https://duq.zoom.us/j/98349963158
Meeting ID: 983 4996 3158

31. Brandon Cane: “Using Machine Learning to Produce Better Maps of the CMB.” (11 a.m.)

32. Anna Durosko: “Characterization of secondary structures in C9orf72 hexanucleotide repeat expansions.” (11:10 a.m.)

33. Sarah Glasser: “Mössbauer Spectroscopy of xGd2O3 *(1-x)α-Fe2O3 Nanoparticle System.” (11:20 a.m.)

34. Quinn Pickering: “The use of NMR crystallography to elucidate the structure of an unknown, erlotinib containing compound, a stepwise geometry optimization approach.” (11:30 a.m.)

35. Matt Ryan: “NHC-stabilized SiGe as a soluble materials precursor: a synthetic and computational study.” (11:40 a.m.)

36. Jasper Shide: “Computational mapping of the pathway of reductive eliminations using neutral aromatic nucleophiles with asymmetric diaryl iodanes.” (11:50 a.m.)
Poster Session 7: 11 a.m. to 12 p.m.
Moderator: Warren Lowther, Ph.D. Student
Zoom Link: https://duq.zoom.us/j/98728674712
Meeting ID: 987 2867 4712

37. Shania Appadoo: “Exploring Puerto Rican Cyanobacteria as Neuroscience Leads.” (11 a.m.)

38. Jakobi Deslouches: “Antimicrobial Activity of Salamander Skin Peptides Against ESKAPE Bacterial Pathogens (11:10 a.m.)

39. Duncan Dobbins: “Mitochondrial Transfer from Extracellular Vesicles to the Brain Endothelial Cells—A promising therapy for Ischemic Stroke.” (11:20 a.m.)

40. Emily Garcia: “p',p' -DDE in the BF-3 Site Alters the Allosteric Communications and the Steroid Unbinding Pathways in the Androgen Receptor.” (11:30 a.m.)

41. Ava Santoro: “The impact of zinc pyrithione and coconut oil on the growth and symbiosis of the dominant microbes of the human scalp.” (11:40 a.m.)

42. Zachary Young: “Novel Pharmacological Inhibition of Glioblastoma Cell Proliferation and Migration.” (11:50 a.m.)

Poster Session 8: 11 a.m. to 12 p.m.
Moderator: Brianna Ports, Ph.D. Student
Zoom Link: https://duq.zoom.us/j/97502879941
Meeting ID: 975 0287 9941

43. Shawn Bliss: “Microfluidic-Photoacoustic Flow Cytometry for Diagnosis of Acute Lymphocytic Leukemia.” (11 a.m.)

44. John Hostetler: “Method Development for Fluoride Removal using a Double-Ionic Layer (11:10 a.m.)

45. Ben Kazimer: “Utilizing Geometrically Transformed Data to Train a Convolutional Neural Network for Image Denoising.” (11:20 a.m.)

46. Matthew Nestler: “Rapid Quantification of Bacteria Using Droplet Microfluidics.” (11:30 a.m.)

47. Marie Sullivan: “Comparison of the Accuracy of Satellite Precipitation Measurements to Ground Precipitation Gages in Southern Africa.” (11:40 a.m.)

48. Alexandra Supinski: “Mud in the Water: Using SEM and EDS to Analyze Runoff from Horizontal Directional Drilling.” (11:50 a.m.)
Poster Session 9: 11 a.m. to 12 p.m.  
Moderator: Theodore Corcovilos, Ph.D.  
Zoom Link: [https://duq.zoom.us/j/92308477794?pwd=SHd1ZUtUVjdweGNqSkxXeUpIMINQQT09](https://duq.zoom.us/j/92308477794?pwd=SHd1ZUtUVjdweGNqSkxXeUpIMINQQT09)  
Meeting ID: 923 0847 7794  
Passcode: 265924

49. Thomas Aumer: “Optimization of a Laser Induced Fluorescence Platform.” (11 a.m.)

50. Peter Demjanenko: “Fabrication of an Anti-Inflammatory Surface for Orthopedic Implants.” (11:10 a.m.)

51. Jahmaine Hatten: “Crosslinking of Elaidic Acids on Aluminum-Based Surfaces.” (11:20 a.m.)

52. Gleymi Hernandez: “High Throughput Sensitive Microfluidic Assay for the Measurement of Fluorescently Labeled 5-HTc Binding Kinetics to GPCRs.” (11:30 a.m.)

53. Carley Reith: “3-Dimensional Computational Model of Neural Activity in the Central Nucleus of the Amygdala During Pain.” (11:40 a.m.)

54. Robert Snidow: “Polymerization of Polydicyclopentadiene on Self Assembled Monolayers To Reduce Corrosion In Stainless Steel.” (11:50 a.m.)

Poster Session 10: 1 p.m. to 2 p.m.  
Moderator: Patrick Lackey, Ph.D.  
Zoom Link: [https://duq.zoom.us/j/94129361853](https://duq.zoom.us/j/94129361853)  
Meeting ID: 941 2936 1853

55. Mikayla Bayto: “THE IDENTIFICATION OF GAMMARID AMPHIPOD SPECIES BY SCANNING ELECTRON MICROSCOPY AND DNA BARCODING.” (1 p.m.)

56. Felicia Bedford: “The Effects of Social Structure on Genetic Diversity in Primate Populations, A Modelling Approach.” (1:10 p.m.)

57. Carolina Lara: “Sequence Variation and mRNA Expression of Hypoxia Genes in Felids for Deciphering Molecular Adaptations in Snow Leopards to High Altitude.” (1:20 p.m.)

58. Rebecca Nelson: “Color Based Detection of Fluoride in Drinking Water with Part Per Million Precision.” (1:30 p.m.)

59. Chanel Staton: “eDNA Metabarcoding Assessment of The Powdermill Forestfly (Soyedina merritti) and Other Spring-dwelling Arthropods of The Laurel Highlands of Pennsylvania.” (1:40 p.m.)

60. Taylor Teitlebaum: “Determination of Persistent Organic Pollutants (POPs) in Fruits and Foods.” (1:50 p.m.)
**Poster Session 11: 1 p.m. to 2 p.m.**  
Moderator: Pamela Marshall, Ph.D.  
Zoom Link: [https://duq.zoom.us/j/98411425769](https://duq.zoom.us/j/98411425769)  
Meeting ID: 984 1142 5769

(1 p.m.)


63. Julianna Firek: “Court Proceedings During the COVID-19 Pandemic.” (1:20 p.m.)

64. Taylor Hopkins: “Case Contextual Information and its Variation Among Forensic Laboratories.” (1:30 p.m.)

65. Kayla Massari: “Characterization of Metal-Peroxide Complexes Using Paper Spray Ionization Tandem Mass Spectrometry (PSI-MS).” (1:40 p.m.)

**Poster Session 12: 1 p.m. to 2 p.m.**  
Moderator: Ning Sun, Ph.D. Candidate  
Zoom Link: [https://duq.zoom.us/j/91555708109](https://duq.zoom.us/j/91555708109)  
Meeting ID: 915 5570 8109

66. Annika Agarwal: “Validation and Identity: The Ayurvedic Dichotomy.” (1 p.m.)

67. Nesha Daneshwar: “Posttraumatic Growth and Aphasia: Case Studies of Emotional Growth.” (1:10 p.m.)

68. Kelby Kosel: “Investigating Sex Equity in Concussion Identification, Diagnosis and Recovery in Collegiate Athletes.” (1:20 p.m.)

69. Madhura Leninkannan: “An Evaluation of Health-Related Lifestyle Factors in Spain.” (1:30 p.m.)

70. Elizabeth Powers: “The Impact of Aphasia on Friendship over Time as Seen Through the Lense of Personal Factors.” (1:40 p.m.)

71. Chloe Rapp: “The prevalent miscorrelation between BMI and a standardized healthy individual.” (1:50 p.m.)
Poster Session 13: 1 p.m. to 2 p.m.
Moderator: Kyle Emerson, Ph.D. Candidate
Zoom Link: https://duq.zoom.us/j/7678830592
Meeting ID: 767 883 0592

72. Zoey Brown: “Using pS6-immunoreactivity as a marker of neuronal activity in amphibians.” (1 p.m.)

73. Taylor McClure: “Effect of variation at the RLN2 promoter on expression of human relaxin.” (1:10 p.m.)

74. Stephanie Perry: “Interactions Between Transcription Factors on the Immediate-Early Gene IL1B.” (1:20 p.m.)

75. Tasia Slater: “Mechanisms underlying female courtship behavior in plethodontid salamanders.” (1:30 p.m.)

76. Madison Uhrin: “Comparing brain cell counts in tadpole and metamorph Northern Leopard Frogs (Lithobates pipiens) using isotropic fractionation and flow cytometry.” (1:40 p.m.)

77. Miranda Zito: “The Effects of Mindfulness Meditation Training on Kinesiophobia in Patients with Chronic Low-Back Pain in Patients with Chronic Low-Back Pain.” (1:50 p.m.)

Poster Session 14: 1 p.m. to 2 p.m.
Moderator: Anna Vietmeier, Ph.D. Student
Zoom Link: https://duq.zoom.us/j/99149195397
Meeting ID: 991 4919 5397

78. Eric Chartier: “Formation of a Pyrrolopyridinone Scaffold via the Fischer Indole Synthesis.” (1 p.m.)

79. Yael Eiben: “Metalation of Benzene Rings by Coinage Metals Gold and Silver.” (1:10 p.m.)

80. Ynaluak Gayluak: “Synthesis of Chrysosporazine D&E: Reversing Multidrug Resistance in Cancer Cells.” (1:20 p.m.)

81. Emery Harlan: “One-Step Preparation of Structurally-Diverse Covalent Compounds as Potential Antibacterial Agents via the “Undergraduate Friendly” Ugi and Passerini Multicomponent Reactions.” (1:30 p.m.)

82. Ny Luong: “Synthetic Investigation of Group 13 Metal Chelates Containing the aza–Dipyromethene Core.” (1:40 p.m.)

83. Vaughn Teague: “Dual MEK5 and AKT pathway inhibitors as therapy for treating TNBC.” (1:50 p.m.)
84. Andrew Gordon: “Synthesis of midostaurin analogs for evaluation in a Tau 4R0N zebrafish assay for rescue of a neurodegenerative phenotype.” (1 p.m.)


86. Charles Patterson: “CD68 Positive Macrophages Found Following Injury to the Sciatic Nerve Shows Fluorescently Tagged Nanoemulsion at a Higher Rate at the Site of Injury Compared to Macrophages Filtered to the Liver.” (1:20 p.m.)

87. Olivia Price: “MDX versus D2 Mice: Identifying a Better Model for DMD.” (1:30 p.m.)

88. Aboubacar Traore: “Tracking Nanoemulsion Filled CD68 Positive Macrophages Involved with Inflammation Within Injured Rat Sciatic Nerve and Organs.” (1:40 p.m.)

89. Serina Tressler: “Steps toward the Synthesis of Chrysosporazines.” (1:50 p.m.)

90. Connor Kelley: “Optimization of Spray Dried Amorphous Particles.” (1 p.m.)

91. Alec Skomo: “Effects of Powder Granulation on Theophylline Tablets.” (1:10 p.m.)

92. Katelyn Spadavecchia: “Video Series on applying Geometric Algebra to Introductory Physics.” (1:20 p.m.)

93. Hannah Valenty: “Global fits and extrapolations of the up to down quark ratio contributions to the proton.” (1:30 p.m.)

94. Yuanshan Zhang: “Flight Simulation for a Two-Balloon High-Altitude System.” (1:40 p.m.)
Poster Session 17: 1 p.m. to 2 p.m.  
Moderator: Brandon Hoenig, Ph.D. Candidate  
Zoom Link: https://duq.zoom.us/j/95166562603?pwd=RnNxZXNHem94cW9Oai84NEJIQWNlQT09  
Meeting ID: 951 6656 2603  
Passcode: 245485

95. Izayah Bojanac: “Structural and dynamic differences between SARS-CoV-2 s2m variants.” (1 p.m.)

96. Hervinah Celestin, Grace Gernatt and Jordan Pater: “Reducing COVID-19 Vaccination Hesitancy with Empirically Supported Community Engagement Techniques.” (1:10 p.m.)

97. Raegen Esenwein: “The Role of Topoisomerase 1 in Herpes Simplex Virus Type 1 Infection.” (1:20 p.m.)

98. Anuoloapo (Anu) Fadare: “Pediatric neurotropic infection alters synaptic development in the developing brain.” (1:30 p.m.)


100. Maya Williams: “Elucidating the function of Cellular PCNA in HSV-1 Infection.” (1:50 p.m.)

Poster Session 18: 1 p.m. to 2 p.m.  
Moderator: Victoria Hrach, Ph.D. Student  
Zoom Link: https://duq.zoom.us/j/99339449366  
Meeting ID: 993 3944 9366

101. Shane Conklin: “The impact of saturation status on the regulation of yeast acyltransferase Gpc1.” (1 p.m.)

102. Lauren Cooke: “Glycerophosphocholine as an alternative phosphate source in Candida albicans.” (1:10 p.m.)

103. Jessica Orgovan: “The Use of Streptomyces Spores as a Vaccine Vehicle for Bordetella pertussis via the Adenylate Cyclase Repeat-in-Toxin (RTX) Epitope.” (1:20 p.m.)

104. Rosemarie Shaw: “Characterization of Spore-Associated Protein A Assembly onto the Spore Surface in Streptomyces.” (1:30 p.m.)

105. Amy Cook: “The Effects of Pre-Loading Internal Standards and Storage Time on Recovery of Amphetamines and Barbiturates.” (1:40 p.m.)

106. Leeann Parisi: “Characterization of the dimer initiation site in the SARS-CoV-2 3’-untranslated region and of its interactions with miR-1307-3p.” (1:50 p.m.)
1
Relativistic Kinematics studies for Kaons and Pions creation in electron proton scattering experiments at Jefferson Lab.
Barner, Grace
Department of Physics, Duquesne University

In Hall B at Jefferson Lab, semi-inclusive deep inelastic scattering of electrons off protons is performed. This collision causes hadrons, particles made of two or more quarks held together by the strong force, that are produced through the hadronization of quarks to expel at all different angles and momenta. Jefferson Lab is able to distinguish between types of hadrons, specifically between pions and kaons, that are emitted through use of the Continuous Electron Beam Accelerator Facility (CEBAF) Large Acceptance Spectrometer (CLAS12) detector. This data can then be analyzed through programming using Eclipse, an integrated development environment, Java and CLAS12 software, to measure the momentum and angular distribution of pions and kaons. My work focuses on the study of the kinematical variables for kaons and pions in electron proton scattering.

2
pPXF and its Applications to Type Ia Supernovae
Doyle, Liam
Department of Physics and Astronomy, University of Pittsburgh

pPXF is a data package that fits the spectra of galaxies and measures their spectral lines, which is useful when analyzing the properties of type Ia supernova host galaxies. Specifically, pPXF enables the measuring of the Balmer decrement and its difference from the predicted theoretical value, leading to the understanding of the effect of host galaxy dust on the spectra. This data also provides information on the star formation rates of these galaxies and around type Ia supernovae. My poster discusses the use and application of the pPXF program, calculating star formation rate from its outputs, and its potential use in determining host galaxy dust's effect on type Ia supernovae cosmology.
3
Survey of Transiting Extrasolar Planets at the University of Pittsburgh (STEPUP)
Kane, Ella; Wood-Vasey, Michael
Department of Physics and Astronomy
University of Pittsburgh
STEPUP was founded in 2009 with the purpose of investigating exoplanets and planetary candidates (PCs) with differential photometry using the 16-inch Keeler telescope at the Allegheny Observatory. Since 2018, STEPUP has been collecting follow-up data to confirm exoplanet systems for NASA's Transiting Exoplanet Survey Satellite (TESS). TESS identifies PCs by recording the decrease in apparent brightness of a star as an exoplanet passes in front of it; however, TESS sacrifices angular resolution to maximize data collection, making it prone to false-positive planet identifications. Our ground-based telescope has a higher resolution allowing us to perform follow-up photometry on any PCs that TESS identifies to rule out false positives. In summer 2021 we accomplished the goal of increasing student membership in STEPUP, allowing us to engage in a new project observing and classifying supernovae and to more efficiently process data to contribute to the growing catalogue of exoplanets.

4
Mass-Metallicity Relation of Galaxies in the LEGA-C Survey
Mack, Kathryn
Department of Physics and Astronomy
University of Pittsburgh, Pittsburgh, PA

Galaxies are collections of stars and gas gravitationally bound to each other. Galaxy evolution, the study of how galaxies are formed and change throughout time, can be studied through elemental composition. One primary factor we look at is called metallicity, which is the ratio of heavy elements to hydrogen. With metallicity we can observe how it relates to total stellar mass, this is called the mass-metallicity relation (MZR). The MZR correlates metallicity with mass because it reflects the stellar mass increase as metallicity increases, explained by the formation and death of stars. We then introduce a third parameter, star formation rate (SFR), which is related to the MZR because the rate of star formation depends on the hydrogen levels. Building off of Pitt undergraduate Zach Lewis's previous research on the MZR of the Large Early Galaxy Astrophysics Census (LEGA-C), I am observing how the SFR in this survey affects the relationship between stellar mass and oxygen levels.
Simulating the Combined Gravitational Wave Signal from Double White Dwarf Binaries
Qoyawayma, Kevin
Department of Physics, University of Pittsburgh

Many, if not most, stars are in binary systems, and since the majority of stars end up as white dwarfs, double white dwarf binaries are thought to be common. However, because of their low mass and low luminosity, few of these systems have been detected. Therefore, more can be learned through their combined gravitational wave signal derived from simulations than using their individual electromagnetic profiles found in surveys. The current version of this project uses weighted signal strengths based on the probability density functions from various observational and evolutionary models. This approach makes it easy to swap in different models to create a signature for each set of models. Once LISA, a gravitational wave satellite, launches, these signals can be compared to LISA’s detections. Finally, by finding the best signal fit, this project will allow astronomers to compare the accuracy of double white dwarf binary system evolution and population theories.

Kaon Analysis in High Energy Electron-Proton Scattering at Jefferson Lab.
Recktenwald, Sean and Dr. Benmokhtar, Fathiha
Department of Physics
Duquesne University

The CLAS12 particle spectrometer located in Hall B at Jefferson Lab contains a Ring-Imaging Cherenkov Detector (RICH) that is designed to improve charged particle identification in the momentum range of 3-8 GeV/c. RICH contributes to the studies of the quarks and anti-quarks in the nucleon and Duquesne is leading the Physics and the studies of strangeness by separating kaons. RICH functions by using a system of aerogel tiles, spherical and planar mirrors, and Multi-Anode-Photo-Multiplier tubes (MAPMTs). The particles pass through the aerogel tiles producing Cherenkov radiation cones. The mirrors are used to reduce the area of PMTs needed. The PMTs are used to measure the angle of the Cherenkov photons produced. My work was on improving the java online monitoring system and analysis of the single spin asymmetries for the $ep\rightarrow e'p' K X$ channel. Data analysis is performed using the C++ CERN ROOT data analysis framework.
Reconstructing naturally acquired mutations that alter the regulation of cyclic di-GMP production in bacteria
Costa, Suzannah; Kessler, Collin; Kim, Wook
Department of Biological Sciences
Duquesne University

Bacteria frequently form biofilms on surfaces, comprising densely packed cells that compete for nutrients and space, where cells must adapt to crowded conditions or risk starvation and death. Our lab utilizes a simple experimental system where new multicellular strategies repeatedly evolve in response to space and nutrient limitations. Specifically, two cell types cooperate to move and colonize new surfaces, and this is driven by mutations in diverse genes that converge on cyclic di-GMP (CdG) production. To confirm the causality of naturally acquired mutations on CdG production, we utilized gene splicing by overlap extension, suicide plasmid, and genome sequencing to reconstruct and confirm individual mutations in respective ancestral strains. CdG is a universal signaling molecule in bacteria with a range of applications, but the regulation of its production remains poorly understood. Our results reveal new genes that contribute to CdG production and a broad spectrum of complexities in CdG regulation.

Investigation of anaerobic respiration in the selenite respiring Bacillus selenitereducens strain MLS10.
Fetzer, Nicholas; Wilson, Bethann; Stolz, John F.
Department of Biological Sciences, Duquesne University

Bacillus selenitereducens strain MLS10, a haloalkaliphilic firmicute, is capable of using selenite (Se(IV) as a terminal electron acceptor using the respiratory selenite reductase, Srr. Here we investigated the expression of Srr, nitrate reductase (Nar), and arsenate reductase (Arr) under selenite, nitrate, and arsenate respiratory growth conditions. Cells grown under the different conditions were harvested and cell fractions prepared to determine the cellular location of the different reductases (i.e., Srr, Nar, Arr). Activity assays were performed using the periplasmic fractions, spheroplasts, and whole cells. SDS-PAGE revealed different protein content in each fraction and growth condition. Selenite grown cells showed activity in the spheroplast and whole cells and was specific for selenite. Spheroplasts and the whole cells had the greatest activity for nitrate grown cells and all three substrates were able to be used. Arsenic grown cells could use all three substrates with the greatest activity in the spheroplast.
Identifying functionally important residues of a bacterial protein through competition assays

Fu*, Jiahao; Summers*, Austin; Wells, Meghan; Kessler, Collin; Evans, Anton; Kim, Wook
Department of Biological Sciences
Duquesne University

*Equal contributions

RsmE is a protein in Pseudomonas fluorescens that represses the production of extracellular secretions by inhibitive mRNA binding. In our experimental system, random mutations naturally occur within rsmE that correlate with elevated fitness. We predict that single nucleotide substitutions that alter the amino acid sequence will also alter the protein’s ability to bind to the cognate mRNA; manifest a range of deregulation and differential production of individual secretions. Thus, we expect mutants that produce more secretions to outcompete those that produce less or no secretions. To test this, we conducted a small tournament of select RsmE mutants to assess their competitive advantage. Our results indeed show a spectrum of relative fitness, indicating a range of altered RsmE function. Once we complete the competitions of all mutants in our library, select strains across the competitive scale will be utilized to determine differential mRNA binding and secretion production.

Comparing Methods of Extracting RarA, a Membrane Porin from Sulfurospirillum barnesii SES-3

Rebel, Lauren; Jeganathar Kanmanii, Narthana; Stolz, John
Department of Biological Sciences
Duquesne University

While arsenic contamination of soil and groundwater is toxic to human populations, arsenate can be used as an energy source for certain anaerobic microorganisms. Among these is Sulfurospirillum barnesii SES-3, a bacterium capable of reducing a variety of metals and metalloids. The reductase capabilities of SES-3 are a result of its unique membrane protein, RarA. Based on computational modeling, we hypothesize that RarA is a monomeric, 18-strand antiparallel β-barrel porin. Upon its successful extraction and purification, RarA could be valuable in the bioremediation of contaminated water. This project aimed to compare two methods of extracting the native protein from SES-3 whole cells. Fractions obtained from each method were further purified using anion exchange chromatography and analyzed by western blotting. Activity assays were performed in the presence of various oxyanion substrates to determine specific activity. Furthering our understanding of the kinetics of RarA will assist in the development of bioremediation strategies.
11
Antibiotic Resistance in *Alkalilimnicola ehrlichii* strain MLHE-1
Schaer, Suzanne¹, Wilson, Bethann², Stolz, John²
1. Department of Biology, Shippensburg University of Pennsylvania
2. Department of Biological Sciences, Duquesne University

*Alkalilimnicola ehrlichii* strain MLHE1 is an haloalkaliphilic gammaproteobacterium found in Mono Lake California. MLHE-1 oxidizes arenite to arsenate using the novel arenite oxidase, Arx, to generate energy. Arx is an ancient enzyme in the DMSO reductase family of molybdoenzymes, hence its study can provide a better understanding of the evolution of this family. Here, we determined which antibiotics MLHE-1 is susceptible to in order to develop a genetic system. Agar plates with a synthetic Mono Lake medium, varying salt concentrations, and with and without amino acids and acetate were tested to determine optimal growth conditions. The plates with 15.0g/L NaCl, 20mM acetate, tryptone, peptone, and casamino acids grew best. A disk diffusion test was performed with a variety of antibiotics. MLHE-1 was found to be resistant to ampicillin, bacitracin, oxacillin, polymyxin, tetracycline and vancomycin, and susceptible to chloramphenicol, clarithromycin, erythromycin, streptomycin and sulfamethoxazole/trimethoprim. Funded by NSF-REU-Site Award 1757555.

12
Engineering a library of antibiotic resistant and fluorescent strains of *Pseudomonas fluorescens* to study the function of RsmE
Summers, Austin
Department of Biological Sciences
Duquesne University

*Equal contributions

Within microbial environments bacteria will often position themselves in a fashion that enables them to gain better access to nutrients. Bacteria commonly do so by use of cilia or flagella. In the case *Pseudomonas fluorescens* (Pf0-1), it does so by means of secretions.

Previous research has shown Pf0-1 naturally acquires mutations within the gene RsmE – repeatedly emerge as localized patches and eventually outcompete the parent cells. We have a large collection of independently isolated *rsmE* mutants, and we predict that substitution mutations will exhibit a broad spectrum of altered RsmE function. By utilizing a specialized transposon which integrates as a single copy into the chromosome, we introduced antibiotic resistance or fluorescence protein genes into each missense or nonsense *rsmE* mutant. We confirmed correct insertions by PCR then confirmed expected phenotypes through antibiotic resistance assays or epifluorescence microscopy. This library of labeled mutants will next be utilized in a round-robin tournament to assess their relative fitness and analyzed by microscopy to detect alterations in patch formation against the ancestral strain.
Dual Affinity Chromatography to Purify Recombinant Seminal Proteins to Analyze Biochemical Differences between Humans and Chimpanzees
Gibbs, William\textsuperscript{1}; Jensen-Seaman, Michael I.\textsuperscript{2}
\textsuperscript{1}Forensic Science and Law, \textsuperscript{2}Department of Biological Sciences
Duquesne University

Semenogelin proteins are the most abundant proteins in primate seminal plasma. Differences in the semenogelin proteins help us understand the evolutionary differences among primates caused by varying sexual selection levels. Therefore, recombinant semenogelin 1 (SEMG1) protein fragments in humans and chimpanzees were expressed in an \textit{E.coli} system to produce an optimal yield and purity of the recombinant fragments. This was done by producing human and chimpanzee SEMG1 protein fragments as a fusion with maltose-binding protein on the amino terminus and a hexahistidine tag on the carboxy terminus, followed by tandem affinity chromatography. Once the method was optimized and recombinant fragments were expressed, they were tested using an enzymatic assay for a prostate-specific transglutaminase which crosslinks lysine and glutamine residues and is responsible for the coagulation of seminal fluid. Testing various SEMG1 protein fragments with this assay reveals biochemical differences between fragments and potential differences between humans and chimpanzees.

Characterization of the (G4C2)\textsuperscript{45} repeat in the C9ORF72 gene
Grimaldi, Lydia
Chemistry and biochemistry
Duquesne University

Amyotrophic lateral sclerosis (ALS) is a progressive neurodegenerative disease which leads to degradation of somatic nerves, ultimately causing a loss of neuromuscular function and cell death. A repeat expansion of the G\textsubscript{4}C\textsubscript{2} sequence in the C9ORF72 gene, which codes for the C9ORF72 protein, has been observed in familial ALS and its function is not yet known. This project aims to biophysically characterize this expansion through a (G\textsubscript{4}C\textsubscript{2})\textsuperscript{45} repeat, with particular interest in G quadruplex formation. Binding interactions of targeted proteins and nucleic acids to the G quadruplex formed by the G4C2 expansion will provide insight into the function of the G\textsubscript{4}C\textsubscript{2} expansion and possible effects on gene expression related to pathogenesis. Transcription optimization of a (G\textsubscript{4}C\textsubscript{2})\textsuperscript{45} sequence from bacterial plasmid vectors, followed by native polyacrylamide gel electrophoresis and NMR will biophysically characterize the formation of secondary structures in this expansion and provide insight into the function and stability of the G\textsubscript{4}C\textsubscript{2} repeat.
**Title:** Investigation of the human glycine receptor (GlyR) using crosslinking mass spectrometry.
**Authors:** Arian Hajihassani, Warren Lowther, Thomas Stirrat, and Dr. Michael Cascio

**Abstract:** The glycine receptor (GlyR), a pentameric ligand-gated ion channel (pLGIC) member, is found in the spinal cord and the brain stem of mammals. Dysfunction of GlyR can result in neurological diseases like hyperekplexia and epilepsy. pLGIC structures are known, but there is limited structural information on transitions between their resting, open, and desensitized states. We propose to use site-directed crosslinking studies coupled with mass spectrometry (CX-MS) to examine GlyR conformation in each allosteric state. Homopentameric α1 GlyR containing a single Cys mutant, K6C, was overexpressed in insect cells, purified, and reconstituted into lipid vesicles. The receptor was stabilized in each of its allosteric states before crosslinking with MTS-benzophenone and subsequent analysis by MS/MS to identify intra- and intersubunit crosslinks. The results will be used with analogous CX-MS GlyR studies to refine the current understanding of GlyR structural conformations in a native-like environment.

---

**Stability of histone mRNA stem loop degradation intermediates**
Mackenstein, Nicole M¹; Mihailescu, Mihaela-Rita²; Lackey, Patrick E.¹

¹Department of Biochemistry and Chemistry, Westminster College
²Department of Chemistry and Biochemistry, Duquesne University

In this study we characterize degradation intermediates of the 3' end of histone mRNA. These intermediates were analyzed using biophysical methods to determine the level of association between the RNA and two proteins, SLBP and 3'hExo, in the ternary complex that forms in the cytoplasm. The three RNA intermediates studied were the wildtype stem-loop, a trimmed intermediate with seven nucleotides removed, and uridylated intermediate to allow a representation of the trimming and uridylation that occurs to be shown. To characterize these intermediates both independently and when bound to SLBP, UV-thermal denaturation, circular dichroism, and fluorescence experiments were carried out. In the absence of protein, the wildtype intermediate showed both the most relatively stable structure, as well as the most intense stem loop. Further characterization of the intermediates with protein will allow for further clarity on the ternary complex stability and function.
Optimization of Purity and Yield of Semenogelin 1 Fragments for Inclusion in Transglutaminase Assays
McIntyre, Clancy A.; Ports, Brianna L.; Jensen-Seaman, Michael I.
Department of Biological Sciences, Duquesne University

Differences in mating systems as well as forces of natural and sexual selection have led reproductive proteins found in semen of primate species to diversify and change rapidly. Among these proteins is semenogelin 1 (SEMG1), which is the most abundant protein found in seminal plasma of primates. Differences among species’ SEMG1 proteins could potentially lead to changes in how they interact with enzymes like transglutaminases, which are responsible for coagulation of semen by crosslinking glutamine and lysine residues. In order to quantify these biochemical differences in substrate/enzyme interaction, individual recombinant fragments of the SEMG1 protein of both humans and chimpanzees were produced in an E. coli system and purified by a combination of affinity chromatography methods. With these purified recombinant proteins, we are currently working to understand what SEMG1 sites are responsible for coagulation and how this varies among species.

Biophysical Characterization of G-quadruplex and i-motif Secondary Structures in the MBNL1 Promoter
Milback, Ella; Mihailescu, Mihaela Rita,
Department of Chemistry and Biochemistry Duquesne University

Myotonic dystrophy (DM) is an autosomal dominant neuromuscular disease characterized by myotonia, progressive muscle atrophy, and other multisystemic impairments, with no curative options for treatment. The more prevalent type, DM1, results from CTG trinucleotide repeat expansions in the 3’ untranslated region (UTR) of the dystrophia myotonica protein kinase (DMPK) gene. The translated repeats cause sequestration of key RNA-binding proteins (RBPs), including muscleblind like protein 1 (MBNL1). As MBNL1 regulates muscle splicing interactions involved in DM1 pathogenesis, current research suggests overexpression as a viable therapy. In this study, we characterized a selected portion of the MBNL1 promoter region for the presence of regulatory secondary structures. This study hypothesized that an equilibrium exists between canonical Watson-Crick base pairing and noncanonical G-quadruplex (GQ) and i-motif (IM) structures, providing a potential therapeutic target for the treatment of DM1. This hypothesis was supported through biophysical analyses conducted on respective strands of the selected sequences.
Biophysical Characterization of G-quadruplex Structures in NEAT1 lncRNA and their Contribution to Paraspeckle Formation in ALS
Carlan Gray, Caylee Cunningham, and Rita Mihailescu
Chemistry and Biochemistry Department at Duquesne University
600 Forbes Ave, Pittsburgh, PA 15282

Amyotrophic lateral sclerosis (ALS) is one of the most prominent neurological diseases and no cure currently exists. An expanding area of research involves paraspeckles, which regulate gene expression through nuclear retention of RNA transcripts. This discovery has promoted interest in their role in ALS pathogenesis. An integral component of paraspeckles’ composition is the long noncoding RNA (lncRNA) nuclear enriched abundant transcript 1 (NEAT1). Without this lncRNA, no scaffold for paraspeckle formation exists. To better understand how these nuclear bodies assemble, this study investigated the potential for NEAT1 to form G-quadruplexes (GQ), a structure known to facilitate protein binding. This study has revealed the presence of five GQs in NEAT1 and showed they are recognized by Fused in Sarcoma (FUS), a protein prominent in paraspeckles. Characterizing these interactions will elucidate the role of NEAT1 in paraspeckle formation, providing insight into ALS pathogenesis.

The effect of polyanions on malate dehydrogenase
Kohler, Olivia; Seybert, David W. Department of Chemistry and Biochemistry
Duquesne University

A recent study reported that polyanions exert a protein destabilizing effect through preferential binding to unfolded intermediates. Since RNA exists in cells as a polyanion, we wished to determine whether polyanions, including RNA, exert broader effects upon enzyme stability as probed by steady-state kinetics. Malate dehydrogenase (MDH) was selected as the model enzyme for this study. Km and Vmax values were determined for MDH as a function of concentration of the variable substrate oxaloacetate (OAA). Others in our group have shown that MDH displays substrate inhibition with OAA. Inclusion of the mono-anions chloride and acetate at 100 mM concentrations did not significantly alter this inhibition. Polyacetate at 100 mM, however, significantly diminished substrate inhibition. Work in the immediate future will examine the polyanion concentration dependence of this phenomenon. In anticipation of future studies, a pilot extraction of total RNA from bovine liver with an A260/A280 of 1.75 was successfully implemented.
Optimization of a homologous recombination protocol for future insertion of an antiplasmodial effector into *Asaia bogorensis* genome

Nguyen, Melissa; Kelly, Thomas; Lampe, David
Department of Biological Sciences
Duquesne University

Current malaria control strategies such as insecticide use lack long-term effects due to rising resistance within mosquito populations. Another approach, paratransgenesis, attempts to combat malaria by modifying the genome of an existing symbiotic bacteria, *Asaia bogorensis*, within the midgut of mosquitoes. It has been shown that expression of an antiplasmodial effector inside *Asaia* makes the mosquito resistant to *Plasmodium berghei*, which causes malaria in rodents. However, the antiplasmodial effectors within these strains are maintained on plasmids with antibiotic resistance markers, making them unstable and unfit for long term use. To prepare for stable insertion into *Asaia*, we used homologous recombination to delete a neutral phage site within the *Asaia* genome using one kilobase homologous regions. However, the protocol for homologous recombination within *Asaia* is still unoptimized. To optimize the protocol, we have modified the length of the homologous regions used for the deletion and analyzed relative recombination efficiency.

Gas Phase DNA Cleavage with a Nickel (II) Monoprotic Aminophosphine Complex

Seibert, Mark; Kelly, Jordan; Metzler, Luke; van Stipdonk, Michael
Department of Chemistry and Biochemistry
Duquesne University
seibma02@gettysburg.edu

Testing inorganic compounds for their ability to cleave DNA can be performed to identify potential biological activity. This study investigates DNA cleavage in the gas phase with a nickel (II) monoprotic aminophosphine complex, which has not previously been reported. Samples were prepared with 1.4 mg of the metal complex dissolved in 10 mL of acetonitrile and final solutions were made with 100 µL of the metal solution mixed with 200 µL of acetonitrile. A 1:20 v/v solution of DNA was made and combined with the metal solution and analyzed with an electrospray ionization mass spectrometer (ESI-MS). ESI-MS analysis aides in determining fragmentation patterns, which were collected for the metal complex and DNA solutions individually. Differences between the spectra were hypothesized to show successful DNA cleavage in the gas phase. DFT calculations were performed to support experimental results and identify binding sites and cleaving interactions.
23

Macromolecular crowding effects on the kinetic properties of malate dehydrogenase
Sipko, Emily; Seybert, David W.
Department of Chemistry and Biochemistry
Duquesne University

The *in vivo* cell environment is crowded with macromolecules, affecting a variety of cellular processes, particularly the kinetic properties of enzymes. Most *in vitro* studies, however, are conducted in dilute buffer solution. The use of model macromolecular (MM) crowding agents, such as bovine serum albumin (BSA), enables the crowded *in vivo* cell environment to be mimicked *in vitro*. The effects of MM crowding on the kinetics of malate dehydrogenase (MDH) were investigated. MDH is a tricarboxylic acid cycle enzyme and catalyzes the NAD$^+$/NADH-dependent reversible interconversion of malate and oxaloacetate (OAA). MDH is subject to substrate inhibition by OAA, and MM crowding was hypothesized to enhance substrate binding affinity of MDH for OAA and decrease substrate inhibition by OAA. Initial experiments with increasing BSA concentration show decreases in both $K_m$ and $V_{max}$ for OAA, but substrate inhibition was unexpectedly enhanced, as reflected by a decrease in $K_i$ for OAA.

24

Title: Optimization of peptide derivatization for fluorescence normalization and sub-fmol quantitation
Authors: Thomas Stirrat, Warren Lowther, Arian Hajihassani, Tom Aumer, Dr. Theodore Corcovillos and Dr. Michael Cascio

Mass spectrometry (MS) is limited in its quantification capabilities as spectral mass ion peaks represent ionization frequencies rather than abundance, making it impossible to distinguish the abundance of crosslinking events and hindering MS interpretation. This project has focused on optimizing chemical derivatization of trypsin proteolyzed peptides from purified glycine receptors and bovine serum albumin (a control protein) using Naphthalene-2,3-Dicarboxaldehyde (NDA), an amine-reactive fluorescent tag, for eventual conjunction with a microfluidic-laser induced fluorescence (LIF) platform to reach sub-fmol levels of detection. However, before we can utilize this method for on-chip reactions, the NDA-modified peptides containing single Arg or Lys residues are currently being assessed to determine their relative fluorescence, as fluorescence emission intensities are composition-dependent. Nonetheless, the use of this LIF detection platform offers unparalleled sensitivity with detection limits lower than current MS platforms and thus may be easily adapted for complementary quantification studies.
Frictional Properties of Single and Mixed Monolayers of 16-Hydroxydecanoic Acid and Hexadecanoic Acid

Evans, Kelsey; Lim, Min; Gawalt, Ellen
Department of Chemistry and Biochemistry
Duquesne University and Slippery Rock University

The continuing desire to reduce the size of devices such as microelectromechanical systems (MEMS) and hard disc drives (HDD) and improve their lifespans requires for those systems to contain molecularly thin protective lubricant layers. The lubricant layers must be resistant to interfacial friction and wear. Self-assembled monolayers (SAMs) can be utilized to form a protective film between the moving parts of a device and resist against mechanical damage by reducing interfacial friction. Single and mixed monolayers with hydroxyl- and methyl- terminations were formed on single crystalline sapphire substrates by solution deposition. Atomic force microscopy (AFM) was employed to explore the frictional properties of single and mixed monolayers of 16-hydroxyhexadecanoic acid and hexadecanoic acid. Diffuse reflectance infrared Fourier transformation spectroscopy (DRIFT) was adopted to determine the alkyl chain ordering and binding nature of the monolayers. Water wettability of the monolayers were investigated with contact angle goniometry.

A computational investigation of the intrinsic conformation and fragmentation of peptides modified to include N-terminal imine groups

Fry, Allison; Metzler, Luke; Massari, Kayla; Farmen, Christopher; Seibert, Mark; Van Stipdonk, Michael
1 Department of Chemistry and Biochemistry
Duquesne University

Tandem mass spectrometry-based approaches are effective for the identification of peptides in peptidome studies. For characterization of new peptide sequences, de-novo methods and direct interpretation of fragmentation patterns is often necessary. This study investigates the use of an N-terminal derivatization technique to improve accuracy of sequence determination. Derivatization to create an N-terminal imine reduces sequence scrambling, decreases the complexity of fragmentation spectra, and increases the yield of N-terminal, sequence-specific ions.

The working hypothesis is that the basicity of the imine may enhance the tendency for the N-terminal dissociation products (b_n- and a_n-type ions) to retain the ionizing proton. The experimental data confirms that dissociation occurs through the b_n/a_n series to reveal the complete peptide sequence.

Density functional theory (DFT) was used to determine protonation sites, and structures of key intermediates and transition states to provide a better understanding of the mechanism(s) and energetics for the dissociation reactions of derivatized peptides.
Polarization of three water clusters in quantum mechanical/molecular mechanical calculations reveals novel hydration buckle essential to malonate decarboxylation

Jemison, Kezia M.; Tamez, Angel; Evanseck, Jeffrey D.
Center for Computational Sciences and Department of Chemistry and Biochemistry
Duquesne University

Decarboxylation of β-keto acids is essential to biochemical processes, yet the origins of non-catalytic effects remain undefined. Quantum mechanical/molecular mechanical (QM/MM) calculations were employed on three models of malonate decarboxylation using the ONIOM/PCM-X method to reproduce experimental enthalpy of activation (∆H‡) of 30.0 kcal/mol. Monoanionic malonate was treated in QM using M06-2X, with the jul-cc-pVDZ basis set, while water clusters of 3, 10, and 15 were treated in MM with the AMBER forcefield. Different charge schemes were used to polarize water molecules within the AMBER forcefield. A discrete continuum model was used with bulk solvation effects was approximated by Tomasi’s polarizable continuum model (PCM) for all cluster systems investigated. We found that polarization of the novel hydration buckle, an interfacial network of hydrogen bonds that modifies malonates conformational energetics, with CHelpG reproduces experiment. This work has further implications to similar solvent-substrate interactions, other β-keto acids, and enzymatic processes.

Comparing DFT and semi-empirical computational methods in the investigation of asymmetric diaryl iodoniums reductive elimination

Authors: Marquis, Sara; Shide, Jasper; Burns, Austin; Koch, Andrew; Montgomery, Thomas; Evanseck, Jeffrey
Department of Chemistry and Biochemistry
Duquesne University and St. Mary’s College of Maryland

Diaryl iodoniums are arylation agents that have a high efficiency toward introducing nucleophiles to a wide variety of aromatic rings. Asymmetric diaryl iodoniums with small anionic nucleophiles favor the electron deficient ring, while neutral azoaryl ring prefers adding to the electron rich ring. This work investigates the position of a cyano group around the electron deficient ring compared to an asymmetrical iodane with a 4-methoxyphenyl group. The large aryl nucleophiles differ from small anionic nucleophiles in their ability to form different conformations when coordinated to the iodine. We have calculated different conformations of the iodine ready to accept the electron rich ring and the electron poor ring with a common nucleophile and compared DFT computational results to semi-empirical results. This will allow us to determine which semi-empirical method can be used as either a good starting point for DFT calculations or possibly a faster method of explaining experimental results.
Alignment of Computed Gas-Phase Urea Structure with Experiment

Moskal, Lindsay1-3; Tressler, Serina1,2; Montgomery, Thomas D.1,2; Evanseck, Jeffrey D.1,2
1Department of Chemistry and Biochemistry; 2Center for Computational Sciences; 3Department of Mathematics and Computer Science, Duquesne University

While urea is critical in agriculture, biochemistry, and catalysis, its structure in the gas-phase remains unresolved. Early microwave studies indicate that in the gas-phase, unsubstituted monomeric urea adopts an intuitive nonplanar conformation known as anti (nitrogens pyramidalized on opposite sides). Yet, certain quantum chemical computations locate an additional and unexpected syn-conformation (nitrogens pyramidalized on the same sides). Other computational theories, like density functional theory, however, do not locate syn. Hence, a consistent potential energy surface (PES) is missing. We utilized the M06-2X functional and second-order Møller-Plesset theory (MP2) with Dunning basis sets to investigate the PES of urea—particularly the anti to syn interconversion. We find that thermodynamic energy corrections and complete basis set limit calculations eliminate the interconversion barrier through nitrogen pyramidalization. We conclude that the syn-conformation is not a distinct conformation. Rather, only the anti-conformation exists with a large-amplitude motion originating from torsional rotation, aligning computation with experiment.

DFT-Based Procedure for a Stereochemical Model for Nucleophilic Substitution with Five-Membered Ring Oxocarbenium Ions

Rodo, Edgar; Makowski, Joseph; Woerpel, Keith1; Evanseck, Jeffrey D.

New York University, New York City, NY 100031
Center for Computational Chemistry and Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA 15282

Striking reversal of stereoselective reactions of five-membered-ring oxocarbenium-ions have been previously reported by experiment to proceed with high stereoselectivity dictated by C-3 substitution. To date, no stereochemical model has been able to predict accurately this dramatic change in stereoselectivity. The use of CCSD(T), or “golden standard,” for the precise characterization of the noncovalent interactions thought to yield the observed stereochemistry would be ideal. Nevertheless, the method is both unfeasible and impractical due to the size of computations. In response, we chose the smallest experimentally reported system, 3-benzyl ether five-membered-ring oxocarbenium ion, and systematically compared DFT, MP2, and CCSD(T) energy profiles of two torsional angles and the activation energies to assess whether DFT can be a trustworthy and practical substitute for CCSD(T) when studying larger five-, six-, and seven-membered systems. We find that DFT is within the range of 2 kcal/mol and 0.3 Å from CCSD(T)’s results, thus a practical method.
Using Machine Learning to Produce Better Maps of the CMB
Cane, B., Guan, Y., Kosowsky, A.
Department of Physics and Astronomy
University of Pittsburgh

The Cosmic Microwave Background (CMB) is light from the early universe and holds secrets to how the universe was formed. In particular, astrophysicists focus on the microwave photon radiation of the CMB -- electromagnetic radiation, with wavelengths 1000 times longer than visible light. The light from the CMB encounters many different galaxies in its journey to our detectors, and this allows us to see how galaxies formed at the beginning of the universe. Naturally, for astrophysicists to come to these inferences about the evolution of the universe and the early formation of galaxies, the CMB map must be as accurate as possible. Maps of the CMB are made from very careful measurements of temperature fluctuations. The temperature of the CMB averages at 2.726 Kelvin. This is because the universe is not uniformly dense. These fluctuations in temperature are minute, and thus require extremely precise telescope measurements.

Characterization of secondary structures in C9orf72 hexanucleotide repeat expansions
Durosko, A; Guarinoni, K; Cunningham, C; Frye, C; Mihailescu, MR
Department of Chemistry and Biochemistry
Duquesne University

GGGGCC (G_4C_2)_x hexanucleotide repeat expansions in the first intron of the C9orf72 gene are the leading cause of familial amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD) and have been proven to form stable G-quadruplexes. These secondary structures provide specificity as targets for PNA oligomers. However, very little research has been done on how increasing number of repeats affects these structures. This study sought to explore the structural and dynamic changes of secondary structures as the number of repeats is increased using molecular dynamics simulations in VMD and the calculation of RMSD and RMSF values. In addition, it attempted to bind PNA oligomers to G-quadruplexes formed by (G_4C_2)_4.
Altogether, the study was a preliminary analysis of the structural diversity and potential function of secondary structures in C9orf72 hexanucleotide repeat expansions.
Mössbauer Spectroscopy of $\text{xGd}_2\text{O}_3 \ast (1-x)\alpha\text{-Fe}_2\text{O}_3$ Nanoparticle System
Glasser, Sarah and Sorescu, Monica
Department of Physics
Duquesne University

The Mössbauer spectra of Gadolinium oxide were recorded for molar concentrations of $x=0.1$, 0.3, 0.5, and 0.7. These concentrations were ball milled and data were taken at 0, 2, 4, 8, and 12 hours. This data were loaded into IGOR Pro and were fitted. Only hematite was present in the 0 hour and all concentrations were fitted with a single sextet and doublet. The $x=0.1$ concentration was fitted using two sextets at BMT=2 h and 8 h, three sextets at BMT=4 h, and two sextets and one doublet at BMT=12 h. The rest of the concentrations at BMT=2, 4, 8, and 12 h were fitted using two sextets and one doublet. Using SigmaPlot, these fits were graphed. The Hyperfine Field of the sextets and the Percent Abundance of the doublets were both graphed against the Ball Milling Time. Gadolinium perovskite nanoparticles were identified as an end product.

The use of NMR crystallography to elucidate the structure of an unknown, erlotinib containing compound, a stepwise geometry optimization approach
Pickering, Quinn; Iuliucci, Robbie; Evanseck, Jeffrey; Boesch, Scott
Department of Chemistry and Biochemistry
Duquesne University
Department of Chemistry
Washington and Jefferson College

Many anticancer drugs are hindered by their bioavailability. To improve a drug’s bioavailability, it can be synthesized within a novel metal complex. This study used NMR crystallography to analyze a zinc and erlotinib containing crystal. Isolated complexes were constructed and optimized on Gaussian using a 6-31G (d) basis set and PBEPBE functional. Geometry optimizations using lattice including planewave DFT with the RPBE functional and dispersion corrections with the D2* method on CASTEP provided crystalline models for NMR calculations. The DFT NMR data was compared to experimental data using root mean square deviation (RMSD) to quantify structural similarities. RMSD findings reveal the impact of each successive optimization on the constructed complexes’ structures. This study and its stepwise approach to NMR crystallography show an effective and reliable method for the computational technique. Moreover, these findings support the conclusion that a metal erlotinib complex has been synthesized – the first of its kind.
NHC-stabilized SiGe as a soluble materials precursor: a synthetic and computational study
Matt Ryan, Dr. Paul Lummis
Department of Chemistry and Biochemistry
Duquesne University

Silicon Germanium is an industry established, widely-used semiconducting material, however the manufacturing process uses toxic and pyrophoric SiH₄ and GeH₄ gases as precursors. Two potential alternative SiGe precursors, both N-heterocyclic carbene (NHC) stabilized, SiGe-containing molecules, NHC:→SiGe←NHC (NHC=MeIPr, IPr) and NHC:→SiGe→BCF [BCF = B(C₆F₅)₃], were targeted for synthesis and computational analysis to determine their molecular structure, thermal behavior, and reactivity. Synthetic pathways and computational techniques have been identified, with execution still underway. DFT optimization and frequency calculations on NHC:→SiGe←NHC using ωb97xd/6-311+G* and ωb97xd/cc-PVTZ show multiple bond character between Si and Ge with a nearly 90° trans-bent geometry between each NHC and the SiGe core. A relatively high energy separation (~6 ev) in the HOMO/LUMO gap suggests this will be a stable molecule.

Computational mapping of the pathway of reductive eliminations using neutral aromatic nucleophiles with asymmetric diaryl iodanes
Shide, Jasper; Marquis, Sara; Burns, Austin; Koch, Andrew; Montgomery, Thomas; Evanseck, Jeffrey
Department of Chemistry and Biochemistry, St. Mary’s College of Maryland and Duquesne University

N-arylation of nitrogen-bearing heterocyclic rings can be used to produce useful compounds in a number of industries. In the investigation of asymmetric iodanes as arylating agents a difference in the resultant product distribution based on the nature of the nucleophile exists. In reactions featuring point-like anionic nucleophiles with asymmetric diaryliodonium salts, arylation proceeds through reductive elimination, leaving the less electron-rich ring attached to the incoming nucleophile. We have observed that in some systems featuring neutral heterocyclic nucleophiles, the observed distribution of products favors arylation with the more electron-rich ring. Current mechanistic descriptions do not adequately explain these observations, suggesting that further investigations of the electronic interactions between various aryls and the incoming neutral heterocyclic nucleophile are necessary to obtain a more complete mechanistic picture. We present the investigation of noncovalent interactions between the aromatic rings of the diaryliodonium and of the nucleophile, and the best theoretical approach to such investigations.
Exploring Puerto Rican Cyanobacteria as Neuroscience Leads
Appadoo, Shania, Rague, Andrea, and Tidgewell, Kevin
Graduate School of Pharmaceutical Sciences
Duquesne University

Even though over 60% of drugs are inspired by nature, the ocean remains underexplored. Bioactive compounds synthesized by marine cyanobacteria as defense mechanisms are isolated by members of the Tidgewell lab using chromatographic techniques to develop neuroscience leads. Once isolated, these chemicals are tested for central nervous system (CNS) activity against receptors implicated in the treatment of depression and chronic pain. My project investigated a green paintbrush *Symphloca* collected from Punta Arenas, Puerto Rico. Nine fractions were created using silica column chromatography to enhance the likelihood of discovering minor secondary metabolites. Nuclear magnetic resonance (NMR) and mass spectroscopy were then utilized to evaluate the chemical profile of the fractions. The results suggest that one fraction contained a compound with structural features similar to endogenous human neurotransmitters. Chemical characterization and structure elucidation efforts of the fraction will be presented. The fraction will be tested for CNS receptor affinity following elucidation efforts.

Antimicrobial Activity of Salamander Skin Peptides Against ESKAPE Bacterial Pathogens
Jakobi Deslouches 2, Kenzie Pereira 1, Sarah K. Woodley 1
1. Department of Biological Sciences, Duquesne University, Pittsburgh, PA 2. College of Computer, Mathematical, and Natural Sciences, University of Maryland, College Park, College Park, MD

Multidrug resistant bacteria known as ESKAPE pathogens threaten vulnerable hospital patients, increasing the need for novel therapeutics. Amphibians are a promising source of such therapeutics because many secrete skin peptides with broad-spectrum antimicrobial activity. To explore clinical applications of amphibian skin peptides, additional studies are needed. The objective of this study was to explore antimicrobial activity of skin peptides from twelve amphibian species against six ESKAPE pathogens and Serratia marcescens. Bacteria were grown to a standard concentration and combined with skin peptides in a 96-well plate. Optical density of each plate was read at 600 nm to determine antimicrobial activity. For the two ESKAPE pathogens tested so far, skin peptides from only one amphibian species (Amphiuma tridactylum) have demonstrated potent antimicrobial activity. Additional analyses including RP-HPLC and peptide sequencing are needed to characterize skin peptides from A. tridactylum. This research was supported by the Charles Henry Leach II fund.
Mitochondrial Transfer from Extracellular Vesicles to the Brain Endothelial Cells—A promising therapy for Ischemic Stroke
Duncan Dobbins, Kandarp Dave, and Devika Manickam.
Neurodegenerative Undergraduate Research Experience (NURE)
School of Pharmacy & Graduate School of Pharmaceutical Sciences
Duquesne University, Pittsburgh PA.

Extracellular Vesicles (EVs) are known to transfer healthy and functional mitochondria to recipient cells and have tremendous potential to treat hypoxic conditions like ischemic stroke. Our goal in this study was to determine the subcellular localization of the EV-transferred mitochondria in the recipient brain endothelial cells—a critical protection target in stroke. We isolated EVs from brain endothelial cells and characterized EVs using dynamic light scattering (DLS) and western blotting. We found that the EVs retained consistent particle characteristics upon freeze-thaw cycles using DLS and verified characteristic EV protein markers using western blotting. We successfully demonstrated mitochondrial transfer from donor EVs to recipient brain endothelial cell models by staining the mitochondria in the EVs and the recipient cell mitochondria using different mitochondria-specific dyes that label functional mitochondria. Our microscopy data demonstrated co-localization of the mitochondria signals confirming the transfer of functional mitochondria from donor EVs to recipient cells.

p’,p’-DDE in the BF-3 Site Alters the Allosteric Communications and the Steroid Unbinding Pathways in the Androgen Receptor
Emily Garcia, Angel Tamez, Jeffrey Evanseck, and Evangelia Kotsikorou
Duquesne University

The androgen receptor (AR), a steroid binding receptor, can get dysregulated by endocrine disrupting chemicals (EDCs). It was thought that EDCs act by binding in the steroid binding pocket disrupting its function; however, recent data suggests they may also act allosterically via binding to the surface site BF-3. This study investigated the effect p’,p’-DDE, an EDC, bound to BF-3 site has on the stability of the bound steroid dihydrotestosterone (DHT). A network-based method, Ohm, was used to identify allosteric communication networks within AR. It revealed different allosteric communication paths between the steroid pocket and the BF-3 site for AR in the presence and absence of p’,p’-DDE. Random accelerated molecular dynamics (RAMD) showed that DHT follows only a subset of the exit paths when p’,p’-DDE was present in the BF-3 site compared to the AR-DHT complex. Further studies will measure binding and dissociation energies of DHT via steered MD simulations.
The impact of zinc pyrithione and coconut oil on the growth and symbiosis of the dominant microbes of the human scalp
Santoro*, Ava; Costa*, Suzannah; Kim, Wook
Department of Biological Sciences
Duquesne University

*Equal contributions

The human body is colonized by diverse microbes, but the human scalp is uniquely dominated by Malassezia restricta (Mr), Cutibacterium acnes (Ca), and Staphylococcus epidermidis (Se). These three organisms likely form a symbiotic relationship, and recent reports indicate that a specific shift in their relative abundance is strongly correlated with dandruff – Ca decreases while Mr and Se increase – Ca’s fitness appears to be the key driver of a healthy scalp. Anti-dandruff shampoos provide only transient relief and thus require continuous application. Here, we test the impact of two major anti-dandruff compounds, zinc pyrithione and coconut oil, on the growth of the three dominant scalp microbes. Although zinc pyrithione is described to suppress fungal growth, we find that it is highly toxic to all microbes. In contrast, coconut oil appears to selectively promote Ca’s growth, exhibiting a promising potential for restoring the symbiotic balance of a healthy scalp.

Novel Pharmacological Inhibition of Glioblastoma Cell Proliferation and Migration
Young, Zach1, Faruk, Asef2, Goralski, Peter3, Teague, Vaughn4, Hallak, Ramez5, Patel, Saloni6, Cavanaugh, Jane7, and Flaherty, Patrick8
Department of Pharmacology
Neurodegenerative Undergraduate Research Experience (NURE)
Duquesne University, Pittsburgh, PA

Glioblastomas are the most common form of malignant brain tumors, however, most existing treatments are detrimental to both healthy and cancerous cells. Given the relatively high incidence of disease and the poor prognoses that affected individuals often face, it is crucial to investigate cellular mechanisms for preventing tumor growth and metastasis. We hypothesized that newly synthesized kinase inhibitors would reduce proliferation and migration of U87MG glioblastoma cells by targeting two kinase signaling pathways known for their roles in proliferation, motility, and apoptosis. Specifically, novel compounds were hypothesized to inhibit phosphorylation of extracellular signal-related kinase 1/2 (ERK1/2) and ERK5 in the mitogen-activated protein kinase pathway as well as protein kinase B in the phosphatidylinositol-3 kinase-protein kinase B pathway. Immunoblotting was used to analyze relative abundances of phosphorylated kinases to their respective unphosphorylated counterparts. Further tests will be conducted to determine how the synthesized inhibitors affect cell proliferation and migration.
Leukemia is one of the most prevalent forms of cancer, ranking as the 10th most diagnosed cancer in the US in 2020 and the most common cancer in children and adolescents. More specifically, acute lymphocytic leukemia (ALL) is the most frequently diagnosed cancer in children and progresses very rapidly; ALL can be fatal within a few months if left untreated. Current methods of diagnosis include biopsy, marrow aspirations, and blood smear analysis, but these techniques are invasive, expensive, and time-costly. We propose the use of a microfluidic-photoacoustic system to detect ALL through the analysis of small volumes of white blood cells, which does not require invasive procedures. The use of PA flow cytometry enables near-instant identification of cells of interest and allows for a quicker diagnosis. We have fabricated a three-part prototype as a model for the microfluidic-photoacoustic device that we will use to detect and analyze ALL cells.

The utilization of a double-ionic layer has proven to be an effective measure of fluoride removal in drinking water. This concept was originally based on aluminum cations that were attached to bentonite clay. However, a concern arose with the potential leaching of aluminum into the water, making the harmful water even more dangerous. Therefore, other cations have been introduced as a replacement to the aluminum. The cations (calcium, zinc, and sodium) have been tested using experimental procedures like isotherm analysis and EDX scanning to verify their effectiveness in fluoride removal. Throughout this project, a social aspect has been noted, especially in the aspect of future use of this research in remote areas. The newly introduced cations are cost effective and aid in internal homeostatic processes. The future of this research includes the creation of an effective point of use water treatment using a double-ionic layer.
Utilizing Geometrically Transformed Data to Train a Convolutional Neural Network for Image Denoising
Kazimer, Benjamin, Dr. Levine, Stacey
Department of Mathematics and Computer Science
Duquesne University

Removing Gaussian noise from images is a widely researched topic in the field of image processing. Deep learning models have been the most successful algorithms to perform such a task, with their power coming from learning a large number of parameters based on massive training data sets. Their drawbacks include that many of these models are not based on solid mathematical foundations, and these models must undergo a computationally intensive training process to "learn" these parameters. This work is focused on adapting the feed-forward denoising convolutional neural networks (DnCNN) of Zhang et.al. to operate on the components of images in a geometrically motivated moving frame of the image. This new approach incorporates the geometry of the image in a mathematically sound way, with the intent of better preserving fine details in the denoised data as well as improving quantitative image quality metrics. Numerical results and future work will be presented.

Rapid Quantification of Bacteria Using Droplet Microfluidics
Nestler, Matthew, Tanyeri, Melikhan,
Rangos School of Health Sciences
Duquesne University

Bacteria enumeration is a technique used in many applications including clinical, environmental, and food testing. However, the current standard for bacteria quantification, agar plating, is labor intensive and can take up to several weeks to complete. For many applications, this long timespan produces a bottleneck for increasing throughput and reducing cost. Therefore, alternative techniques are required for rapid detection and quantification of bacteria. Here, we describe a new method based on droplet microfluidics and machine learning to rapidly quantify bacteria in liquid samples. Our method relies on encapsulating and culturing single bacterial cells in droplets, and imaging them subsequent to an incubation period. Finally, we analyze these images using machine learning algorithms for fast and accurate quantification of bacteria in the sample. Our method holds potential for reducing cost and time for applications requiring accurate quantification of bacteria using small sample volumes.
Comparison of the Accuracy of Satellite Precipitation Measurements to Ground Precipitation Gages in Southern Africa
Sullivan, Marie Center for Environmental Research and Education Duquesne University

Precipitation data are needed for water resources management in agriculture and for drought and flood models. The Limpopo River Basin of southern Africa has a sparsely distributed precipitation gage network. Global Precipitation Measurement (GPM) mission uses satellites to take temporally (daily) and spatially distributed measurements. To validate the GPM data, they were compared to standard precipitation gage data in R. The data were compared at a range of temporal and spatially averaged resolutions. The results showed that precipitation measurements from satellites are reliable when the area covered is fairly large. This accuracy wanes as the areas become more precise. The GPM daily measurements were less accurate compared to the GPM monthly measurements.

Mud in the Water: Using SEM and EDS to Analyze Runoff from Horizontal Directional Drilling
Alexandra Supinski
Department of Biological Sciences
Duquesne University

Horizontal Directional Drilling (HDD) is regarded as a more environmentally-sound way for the construction of underground pipelines and cables. The Mariner East is a pipeline that spans from East Ohio and the entirety of Pennsylvania, including West Chester County, Pennsylvania. Bentonite is typically used in the drilling fluid and has reportedly been found in private water wells and a lake near pipeline construction in West Chester County. Samples of putative bentonite were obtained from private water wells, road run off, and Marsh Creek Lake. The samples were analyzed by Scanning Electron Microscope (SEM) and Energy Dispersive Spectroscopy (EDS). The particles ranged in size from 5 to 700 um, and composed mainly of Al, Si, O, and other minor constituents (i.e., Fe, Ca, K, Ti). The analysis confirmed the presence of aluminosilicate with a signature similar to the pure bentonite standard. Confirmation awaits further analysis with X-Ray Diffraction (XRD).
Optimization of a Laser Induced Fluorescence Platform
Thomas Aumer¹ Michael Cascio² and Theodore Corcovilos¹
Duquesne Department of Physics¹; Duquesne Department of Chemistry & Biochemistry²
Neurodegenerative Undergraduate Research Experience (NURE)
Duquesne University, Pittsburgh, PA

Laser Induced Fluorescence (LIF) complements mass spectrometry (MS). Fluorescence allows for quantification as the amount of light absorbed by the sample and subsequently re-emitted is proportional to fluorophore concentration, whereas MS can sensitively and accurately identify peptide sequences, but cannot quantify them. In our platform, derivatization reactions will be run on a polydimethylsiloxane microfluidic chip, requiring nanoliter droplets of reactants and quick reaction times due to advective mixing before LIF measurements via confocal imaging of the microdroplets. Peptides are tagged with the amine-reactive naphthalene-2,3-dicarboxaldehyde, which only fluoresces at 470 nm upon excitation from a 405-nm laser after conjugation. Significantly, this LIF platform is more sensitive than modern MS platforms, allowing contemporaneous quantification with parallel MS-based identification. Objectives completed this summer include optimization of the hardware by aligning the microscope, optimizing the output signal of the laser beam, and the production of new microfluidic chips.

Fabrication of an Anti-Inflammatory Surface for Orthopedic Implants
Demjanenko, Peter; Armen, Jennifer; Gawalt, Ellen
Department of Chemistry and Biochemistry
Duquesne University

Total hip and total knee arthroplasties are some of the most commonly performed surgical procedures, yet there is still a significant rate of revision surgeries. No biomaterial, alone, addresses the two largest causes of orthopedic implant failure: aseptic loosening and bacterial infection. In this work, a novel surface for orthopedic implants is being designed to address these issues. It consists of a TiO₂ coupon coated with an artificial extracellular matrix of collagen I and high-sulfated hyaluronic acid, a synthetic glycosaminoglycan with immunomodulatory and anti-inflammatory properties. The matrix will be further modified with vancomycin. Collagen I was covalently immobilized using a self-assembled monolayer of 16-phosphonohexadecanoic acid using an acyl chloride reaction. After confirmation of matrix attachment by FTIR, hyaluronic acid will be sulfated and integrated into the matrix, and the surface will be evaluated by ELISA for immune cell cytokines after exposure of monocytes to treated surfaces.
Crosslinking of Elaidic Acids on Aluminum-Based Surfaces
Hatten, Jahmaine; Clegg, Benjamin; Gawalt, Ellen
Department of Chemistry and Biochemistry
Duquesne University

Aluminum is among the most commonly used metals in the industrial setting and is a constituent of numerous alloys due to its lightweight, high strength-to-weight ratio, and low-density properties. Despite its moderate corrosion resistance, the dominant cause of aluminum infrastructural and equipment failure is corrosion. To address this problem, self-assembling monolayers (SAMs) were used to create a protective film on the surface of aluminum metal to protect the surface from oxidizing species. A SAM composed of elaidic acid, a long chain unsaturated carboxylic acid, was formed and then crosslinked through thermal initiation by a free radical process. DRIFT spectroscopy was used to monitor the crosslinking of the SAM with additional characterization by contact angle goniometry to characterize changes in surface wettability. Corrosion resistance of aluminum oxide and the SAM-protected surfaces will be measured by cyclic voltammetry to determine the increase in corrosion resistance afforded by a crosslinked SAM.

High Throughput Sensitive Microfluidic Assay for the Measurement of Fluorescently Labeled 5-HTc Binding Kinetics to GPCRs
Authors: Hernandez, Gleymi; Tanyeri, Melikhan; Tidgewell, Kevin
Department: Biomedical Engineering, Pharmacy
Pain Undergraduate Research Experience (PURE)
Duquesne University, Pittsburgh, PA

Opioids, often prescribed to patients with chronic pain disorders, are addictive in nature, and reported as the leading cause of death due to drug overdose; therefore, development of alternative, non-opioid pain medication is imperative. Drug discovery for pain medication is hampered by lack of low-cost, high throughput and sensitive assays. In this work, using simple microfluidic devices and fluorescence microscopy, we developed a highly sensitive, competitive fluorescence assay for measuring affinity and binding kinetics of 5-Hydroxy Tryptamine (5-HT) or serotonin to the 5-HT\textsubscript{2c} receptor, a subtype of the 5-HT receptors which may be a promising target for pain medication. We implemented this method on human 5-HT\textsubscript{2c} GPCR membrane preparation as well as HEK293 cells. Our results show that our assay can measure affinity and binding kinetics of 5-HT to the 5-HT\textsubscript{2c} receptor with high sensitivity using nanomolar concentrations of ligand.
3-Dimensional Computational Model of Neural Activity in the Central Nucleus of the Amygdala During Pain
Reith, Carley¹,²; Neilan, Rachael¹; Kolber, Benedict²

¹ Department of Mathematics and Computer Science, Duquesne University
² Department of Neuroscience and Center for Advanced Pain Studies, University of Texas at Dallas

The central nucleus of the amygdala (CeA) is a region of the brain important in pain processing. Neurons within the CeA expressing protein kinase c-delta (PKC-δ) or somatostatin (SOM) have opposing roles in pain modulation. A computational space was created in an in silico manner to study the role of these cell populations in whole animal “wet lab” experiments. We developed a 3-dimensional computational model of these neuron populations and their connectivity to predict system-level measures of pain. The model consists of 5000 neurons with cell-type specific properties and behaviors estimated from laboratory data. During each model time step, neuron firing rates update based on an external stimulus, and a network of directed links sends inhibitory signals between neurons. A measure of pain is calculated as the difference in the cumulative firing rates of PKC-δ and SOM neurons. Results demonstrate the model’s ability to produce both spontaneous and evoked pain in response to noxious stimuli.

Polymerization of Polydicyclopentadiene on Self Assembled Monolayers To Reduce Corrosion In Stainless Steel
Snidow, Robert; Gawalt, Ellen, Rupprecht, Alexander
Department of Chemistry and Biochemistry
Duquesne University

Corrosion of metals such as Stainless Steel 316L leads to a loss of integrity of the structure the metal composes. In this project, surface-initiated ring opening metathesis polymerization of polydicyclopentadiene (pDCPD) was performed. The surface of 11-hydroxyundecylphosphonic acid (11-HUPA) self-assembled monolayers (SAMs) was modified by attaching a terminal norbornene functional group to the hydroxyl terminus via esterification. This was used as an initiator for polymerization of dicyclopentadiene (DCPD) in vapor phase. Diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy, and contact angle analysis were used to characterize the SAM surface after deposition, norbornene attachment, and polymerization. The DRIFT spectra indicated successful formation of 11-HUPA SAMs and terminal norbornene attachment with C=O stretching present at 1730 cm⁻¹ and C-O ester stretching at 1250 cm⁻¹. Future work includes the polymerization of DCPD, characterization with DRIFT spectroscopy, contact angle analysis, and corrosion resistance of the film will be tested with cyclic voltammetry.
THE IDENTIFICATION OF GAMMARID AMPHIPOD SPECIES BY SCANNING ELECTRON MICROSCOPY AND DNA BARCODING
Bayto, Mikayla¹; Brady Porter, Ph.D.²; John F. Stolz, Ph.D.¹&²
Center for Environmental Research and Education¹ & Department of Biological Sciences²
Duquesne University

Amphipods – also known as scuds or freshwater shrimp – are bottom-dwelling members of subphylum Crustacea. Scuds exhibit collector-gather feeding behavior and are moderately-tolerant to pollution. The identification of amphipod species is difficult due to small specimen size, little morphological variance, and lack of study at the species level. We were interested in examining the morphological diversity of Gammarid amphipod specimens from the Mingo Creek watershed of Washington County, PA. Specimens from the Gammaridae family – *Gammarus* and *Crangonyx* genera, specifically – were analyzed by scanning electron microscope (SEM), dissection microscope, and DNA barcoding. The SEM allowed for enhanced viewing of setae and comb spines not as easily viewed with a dissecting microscope. Dissection microscopy and DNA barcoding were utilized to support the scud species identifications determined from SEM imaging as well as existing Gammarid literature. SEM analysis of Gammarid specimens proved helpful in determining Gammaridae specimen genera and species.

The Effects of Social Structure on Genetic Diversity in Primate Populations, A Modelling Approach
Bedford, Felicia, Sugden, Lauren Department of Math and Computer Science
Duquesne University

In an investigation into the nature of socialization in bonobo and chimpanzee populations, there were patterns of genetic diversity that have been found to differ among primate species (Ishizuka). To better understand the effect of social structures on genetic diversity, we are simulating primate-like genomes using demographic simulator SLiM (Haller). Specifically, 50 separate subpopulations with varying numbers of individuals were created, originating from an ancestral population. We created a code that would allow for all of the populations to interbreed and move around amongst each other, with options for female-specific dispersal (male philopatry). These specifics, which were designed to represent a typical chimpanzee population, required us to deviate from typical Wright-Fisher simulations. We believe that this model is the model that could help us to understand genetic patterns in chimpanzee society, and helps to explain the effects of socialization on genetic diversity.
57
Sequence Variation and mRNA Expression of Hypoxia Genes in Felids for Deciphering Molecular Adaptations in Snow Leopards to High Altitude
Lara, Laura Carolina1,2; Macar, David1; Sai, Gopal Yerneni3; Phil Auron1; Janecka, Jan1
1. Duquesne University, Department of Biological Sciences
2. Furman University, Department of Biology
3. Carnegie Mellon University, Department of Biomedical engineering

Snow leopards (Panthera uncia) live across wide ranges of altitudes with higher elevations having lower O₂ availability. In mammals, the transcriptional response to hypoxia (low O₂) is primarily regulated by oxygen-sensing EGLN1, and Hypoxia-Inducible Factors, HIF1α and EPAS1 (HIF2α). While HIFα subunits are constitutively degraded in normoxic conditions, hydroxylation by EGLN1 during hypoxia allows for protein stabilization which turns on hypoxia response genes such as EPO, VEGF, and GLUT1. These downstream genes are crucial for immunological responses, vascularization, and homeostasis. Interestingly, there are snow leopard-specific mutations in EPAS1 and EGLN1, suggesting a molecular basis for hypoxia adaptations. In this study, cell lines and immune cells isolated from peripheral blood are used to compare hypoxic gene response to pseudohypoxia (Cobalt Chloride treatments) and hypoxia (low oxygen chamber). This, in addition to accurate genome/transcript sequence reconstruction and phylogenetic analysis, allows for insight into adaptive hypoxic-response mechanisms in snow leopards. Funded by NSF-REU site award 1757555.

58
Color Based Detection of Fluoride in Drinking Water with Part Per Million Precision
Nelson, Rebecca; Corcovilos, Theodore
Physics Department
Duquesne University

The ability to easily and inexpensively measure contaminants in drinking water is an important step to improving water quality. Color-based chemical sensors can quantitatively determine contaminant levels when measured with a colorimeter. In our study, we measured fluoride concentrations using an eriochrome sensor molecule that bleaches from red to yellow when fluoride is present. We improved an existing sample preparation protocol in order to create more precise samples. Data was then taken with various known concentrations of the fluoride mixture in order to calibrate the colorimeter, demonstrating a resolution of 0.06 parts per million for fluoride solutions in the range of 0-3 ppm. An LCD touch screen was installed in order to make the device more user friendly, and it has the capability to display results with more comprehensibility in the form of graphs and raw data by only pressing a button.
59

**eDNA Metabarcoding Assessment of The Powdermill Forestfly (Soyedina merritti) and Other Spring-dwelling Arthropods of The Laurel Highlands of Pennsylvania**

Staton, Chanel¹, Hoenig, Brandon¹, Wilson, Kathleen¹, Woods, Peter³. Porter, Brady¹

¹Department of Biological Sciences, Duquesne University.
²Department of Biology, Norfolk State University.
³Pennsylvania Natural Heritage Program, Western Pennsylvania Conservancy.

Department of Biological Sciences
Duquesne University

The Powdermill Forestfly (Soyedina merritti) is one of Pennsylvania’s few endemic species. However, surveying for it is difficult due to their brief and varied flight window. Our objective is to investigate efficacy of eDNA barcoding in detecting the presence of the Powdermill Forestfly and other aquatic macroinvertebrates. Advancements in DNA-based taxa detection, DNA barcoding, allow for rapid identification of taxa based on the presence of species-specific DNA segments shed in the environment (eDNA). To detect and report mitochondrial DNA (mtDNA) we used 1 L water samples from several springs, filtered through 0.7 um glass fiber filters stacked on Whatman No 1 filters. We were able to extract DNA with modified DNeasy kits and amplify mtDNA COI-gene with barcode primers (ANML and ZBJ). We used the Illumina MiSeq NGS instrument followed by bioinformatics pipeline to generate a list of arthropod species from each sample site. Funded by NSF-REU Site Award 1757555.

60

**Determination of Persistent Organic Pollutants (POPs) in Fruits and Foods**

Taylor Teitelbaum¹, Weier Hao¹, Tiffany Hoke¹, Matt Pamuku², and H. M. “Skip” Kingston¹

¹Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA
²Applied Isotope Technologies Company, Pittsburgh, PA

Persistent organic pollutants (POPs) are toxic organic molecules found at significant concentrations in the food chain with negative health effects on the people and environment. POPs’ semi-volatility and resistance to natural degradation enable them to disperse throughout the environment and bioaccumulate. Some food may be unfit for human consumption and open for debate with regard to toxicity and health due to contamination. Food safety necessitates a method that enables accurate quantification of simultaneous POPs in fruits. Stir-bar sorptive extraction (SBSE) in combination with gas chromatography mass spectrometry and isotope dilution mass spectrometry (IDMS-GC/MS) quantification is being utilized to determine the concentration of POPs in a variety of fruits. This method is very sensitive and has a low limit of detection. Tested fruits provide assessment of labeling of foods as organic and demonstrates inaccurate labeling.
Determining the Location of Human Remains Using Various Detection Methods
Baxter, Dylan; Reeder, Philip PhD; Ludvico, Lisa PhD
Forensic Science and Law Program
Duquesne University

Locating human remains that have been buried poses a unique problem for the forensic science and archaeological community. If and when remains are buried in unmarked graves it is difficult to locate them by normal methods. The focus of this research is to improve upon this by looking for human remains at the Battlefield of Braddock's Defeat in North Braddock, PA using ground penetrating radar, cadaver dogs, and phosphorus soil testing. By combining these techniques, it is the hope of the researchers that remains of soldiers from the battles will be found to allow for the preservation of history and improve these techniques to allow for law enforcement and archaeologists to locate human remains that have been obscured. These techniques have been used separately in the past but combining them it will allow for confirmation that human remains are present at a location.

Christopher T. Farmen, Luke Metzler, Michael J. Van Stipdonk
Department of Chemistry and Biochemistry
Duquesne University

Breath excretion analysis is emerging as a non-invasive, inexpensive, and time-efficient technique for drug testing. A Simulated Breathing Apparatus (SBA) was built with a venturi to atomize liquid solutions containing a drug analyte of interest. Caffeine, theobromine, and taurine solutions were aerosolized onto a surgical mask with various concentrations according to a serial dilution. The mask was subjected to Paper Spray Ionization- Mass Spectrometry (PSI-MS) with an LTQ XL® Linear Ion Trap Mass Spectrometer. The analytes were detected, and fragmentation pathways were collected via Collision-Induced Dissociation (CID) and compared to reference spectra in order to confirm the analyte identity. All analytes were detected and confirmed in micromolar concentrations of solution (picogram mass range) to emulate detection quantities under physiological conditions. This method allows both volatile and non-volatile drugs to be detected, and future directions of the research will be discussed.
Court Proceedings During the COVID-19 Pandemic
Firek, Julianna Firek and Ferrara, Lyndsie, Ph.D.
Forensic Science and Law
Duquesne University

As of March 2020, the courts shut down, along with the rest of the world. During this unprecedented time, figuring out a way to continue with legal proceedings was a difficult feat that each court did independently, without universal guidelines. Prior to the pandemic, the court was extremely slow to make changes, but the pandemic forced many quick changes along with significant investment into new courtroom technology. These significant changes are important to document and analyze. The goal of this research was to collect firsthand accounts of court adaptations and operation throughout the pandemic. Interviews were conducted of various professionals within the court system in order to gather information on their experiences during the pandemic. Documenting how the courts adapted is important for future events that may also require virtual court as well as for analyzing if what was changed was effective and fair.

Case Contextual Information and its Variation Among Forensic Laboratories
Hopkins, Taylor and Ferrara, Lyndsie
Forensic Science and Law Program
Duquesne University

Contextual bias is a common bias discussed in the forensic science community as it can unintentionally cause scientists to let case contextual information guide their decisions as opposed to the actual evidence. This project investigated the amount of information requested by forensic laboratories, via their lab submission forms, and how they vary between forensic disciplines. Data was collected using a survey that asked participants about their laboratory, laboratory submission form, and laboratory procedures as it relates to case contextual information and how it is transmitted. The responses showed that while many laboratories implement bias training, there are still many laboratories that do not have a protocol in place to guard an analyst from potential biasing effects of case contextual information. Overall, the data provided a comprehensive outlook on what different laboratories and disciplines are doing, or not doing, to mitigate the effects of contextual bias.
Characterization of Metal-Peroxide Complexes Using Paper Spray Ionization Tandem Mass Spectrometry (PSI-MS)

Massari, Kayla; Metzler, Luke; Haberstock, Isabella; Fry, Allison; Van Stipdonk, Michael
Department of Chemistry and Biochemistry
Duquesne University

The instability of the peroxide bond makes it susceptible to extremely exothermic reactions, making them a common agent in improvised explosive devices (IEDs). Thus, a reliable and rapid detection method for organic peroxides is of interest. The goal of this project was to utilize paper spray ionization tandem mass spectrometry (PSI-MS) with collision induced dissociation (CID) for detection and identification of peroxide-based explosives using the ThermoScientific LTQ-XL. Benzoyl peroxide and dicumyl peroxide were used as model compounds that formed complexes with Li⁺, Na⁺, K⁺ and Ag⁺ metals. PSI produced 1:1 complexes between the peroxides and Li⁺, Na⁺ and K⁺, and 2:1 complexes between the peroxides and Ag⁺. Metal-peroxide complex fragmentation patterns suggested that common losses were formaldehyde through the heterolytic cleavage of the peroxide bond and carbon dioxide. Density functional theory (DFT) was used to probe ion structures and their relative energies at the B3LYP/3-21G* and B3LYP/MWB28/6-311+G(d) level of theory.

Validation and Identity: The Ayurvedic Dichotomy
Annika Agarwal Anthropology Department University of Pittsburgh

Ayurveda, an ancient medical system, has been getting plenty of traction in recent news and culture, yet this rising popularity presents an interesting dichotomy with the system’s identity in the modern world. This literature review includes a brief introduction, challenges currently facing the medicine, movements to ensure its validity and to preserve its identity. Ultimately, it is important to recognize that change is inevitable, but from an anthropological perspective, authenticity may be lost entirely. Hence, being aware of this loss may be the key to minimizing it and perhaps even preserving this age-old medicine.
Posttraumatic Growth and Aphasia: Case Studies of Emotional Growth
Daneshwar, Nesha; Harvey, Lindsay; Bandosz, Mikolaj; Wallace, Sarah
Department of Speech-Language Pathology
Neurodegenerative Undergraduate Research Experience (NURE)
Duquesne University, Pittsburgh, PA

Posttraumatic growth (PTG) is a phenomenon where a person experiences emotional growth after a traumatic event, like a stroke. Aphasia is often caused by stroke but individuals with aphasia are excluded from studies measuring PTG because of their communication impairments. This study aims to explore the efficacy of the posttraumatic growth inventory for people with aphasia (PTGIA) at assessing an individual’s experience with aphasia. Participants completed the PTGIA and psychological well-being assessments to understand the degree they experience PTG. Two cases from the larger study were examined, a 48-year-old woman who is 16 months post-stroke, and a 59-year-old man who is 108 months post-stroke. Factors such as time post-stroke and history of anxiety and/or depression can affect how a person experiences PTG after acquiring aphasia. An understanding of PTG can help clinicians better understand how a patient experiences emotional growth and thus individualize therapeutic treatments.

Investigating Sex Equity in Concussion Identification, Diagnosis and Recovery in Collegiate Athletes
Kosel, Kelby and Beidler, Erica
Department of Athletic Training
Neurodegenerative Undergraduate Research Experience (NURE)
Duquesne University, Pittsburgh, PA

Background: Previous literature indicates differences in concussion recovery between male and female athletes, which may suggest health inequities at the collegiate level.
Purpose: This study investigated concussion management and recovery trajectories based on sex.
Participants: This study included 96 collegiate athletes who sustained at least one concussion from one NCAA Division I institution (males 48%, females 52%).
Methods: Extracted data from 2015-2020 athlete medical records include demographics and information related to concussion identification, diagnosis, and recovery. T-tests and odds ratios were used to assess concussion outcomes between sexes.
Results: Although male athletes had a higher odds of accessing an athletic trainer at the time of injury, no significant differences were found regarding removal from play mechanism or acute symptom severity, and identical recovery patterns were observed in both sexes.
Conclusion: Sex inequities exist regarding on-site sports medicine care, but ultimately injury timelines were consistent between sexes at the institutional level.
An Evaluation of Health-Related Lifestyle Factors in Spain
Leninkannan, Madhura
Interdisciplinary Studies
University of Pittsburgh

In 2019, Spain was ranked first as the healthiest country in the world in the most recent Bloomberg Healthiest Country Index. However, there is limited research analyzing the lifestyle factors that contribute to Spain’s positive health outcomes. This study aimed to identify such lifestyle factors through comparing available datasets in the Eurostat database about health-related lifestyle factors amongst other European Union countries. We found that Spain had high fruit and vegetable consumption, low fat and oil intake, increased daily time spent walking, strong social support, and frequent engagement with friends and family in comparison to other European Union countries. Furthermore, Spain consistently ranked the highest on factors related to social relationships, indicating that those factors could potentially have strong influences on Spain’s health. Further research on the association of these lifestyle factors and health outcomes is needed to test these predictions from retrospective data.

The Impact of Aphasia on Friendship over Time as Seen Through the Lense of Personal Factors
Powers, Elizabeth; Hawkins, Hailey; Powell, Meghan; McCallister, Megan; Faculty Advisor: Wallace, Sarah
Department of Speech-Language Pathology
Neurodegenerative Undergraduate Research Experience (NURE)
Duquesne University, Pittsburgh, PA

Aphasia is a language disorder that usually occurs after stroke, and the impact of it can vary across personal and environmental factors. As friends are an important part of having a healthy life and good mental state, it is important to look further into these differences and seek ways to increase the ways in which people with aphasia can make and maintain friendships. A series of interviews with people with aphasia provided insight into how aphasia has impacted friendships over time, both in the time spent with friends and in how satisfied people are with their friends. The participants were given the Comprehensive Aphasia Test to assess the impairments from aphasia. This study looks at one male and one female participant comparing their experiences with aphasia and focuses on some of the possible causes behind the difference, such as how some lose more friends after aphasia onset than others.
The prevalent miscorrelation between BMI and a standardized healthy individual
Rapp, Chloe; Marshall, Pamela; Hammers, Jennifer, DO
Forensic Science and Law Program
Duquesne University

With increasing media attention towards creating a definition of “healthy” to categorize people into a traditional beauty standard, it is important to bring attention to the fact that an external appearance of “skinny” is not equivalent to being in good health. Hidden fat deposits around the major organs like heart, liver, and lungs are sneakily growing to cause fatal health problems in so many Americans, with cardiovascular disease at hand for 25% of deaths in 2019. This study used varying methods of measurement like bioelectrical impedance, a hand-held caliper, and a standard tape measure on different locations of the body to collect and compare the accuracy of these society-accepted systems. Focused on the organ condition, body fat percentage, and BMI on decedents of all sex and ages, it was found that the accepted quantifications of BMI, based solely on height and weight, failed to consider key factors, further establishing its inaccuracy.

Using pS6-immunoreactivity as a marker of neuronal activity in amphibians
Brown¹, Zoey, Woodley², Sarah
Department of Biological Sciences
Clarion University of Pennsylvania¹, Duquesne University²

Chemical signaling via pheromones is an important mode of communication used by many animals. In Allegheny Mountain Dusky salamanders (Desmognathus ochrophaeus), pheromones are transported across the skin, a very unusual mode of pheromone transfer. To understand how these signals are interpreted by the central nervous system, I tested the method of immunohistochemistry for phosphorylated ribosomal protein S6 (pS6), which is a potential indicator of neural activity. I predicted that pS6 immunoreactivity (ir) in the brain would be higher in salamanders exposed to stress from capture and handling compared to unstressed controls. Levels of pS6-ir were higher throughout the brain in stressed animals compared to controls. This suggests that pS6 proteins could be used to track brain activity in response to a variety of stimuli. Future studies will use the pS6 method to investigate how and where pheromonal cues are processed in the brain. Funded by NSF-REU Site Award 1757555.
Effect of variation at the \textit{RLN2} promoter on expression of human relaxin

McClure, Taylor M.; Loughner, Lindsay G.; Jensen-Seaman, Michael I.

\textsuperscript{1}Forensic Science & Law Program; \textsuperscript{2}Department of Biological Sciences

Duquesne University

Preterm birth is the largest factor associated with neonatal death in the United States. Among the various risk factors contributing to preterm delivery is genetics. Studies have shown a link between genetic variation of the relaxin 2 (\textit{RLN2}) gene of the mother and preterm birth. This gene codes for the hormone relaxin, which moderates various pregnancy-related changes to the body, primarily in fetal membranes and tissues at the cervix at the onset of labor. In order to examine variation at the \textit{RLN2} promoter region, two alleles that differ in the length of a microsatellite found within this promoter were ligated into the pNL1.1 reporter vector. These constructs were transfected into human placental JAR cells in vitro. A luciferase reporter assay was used to measure the level of expression of these alleles. The differences in expression observed, along with potential implications for susceptibility to preterm birth, will be discussed.

Interactions Between Transcription Factors on the Immediate-Early Gene IL1B

Stephanie C. Perry, Shane P. Cowan, Philip E. Auron

Department of Biological Sciences, University of Pittsburgh Greensburg

Department of Biological Sciences, Duquesne University

Transcription of the immediate-early IL1B gene is initiated by activation of the cell surface Toll-Like Receptor 4 on myeloid cells. This results in activation and translocation of NF-\kappa B and C/EBP\textbeta to the nucleus and subsequent binding to the IL1B promoter and enhancer, respectively. These transcription factors can then interact with constitutively promoter-bound Spi-1, forming a long-range chromatin loop that organizes the transcriptional machinery and recruits RNA Polymerase II. Molecular interaction studies show that Spi-1 interacts with the NF-\kappa B heterodimer p65 subunit. Molecular modeling was used to predict a theoretical binding mode of this complex using their crystal structures and suggests that Spi-1 interacts with p65, but not p50. SDS-Polyacrylamide Gel Electrophoresis and Western Immunoblot was used to analyze a GST-pulldown in order to test Spi-1 interaction with the p50 subunit. These results suggest a novel mechanism for the induction of immediate early gene transcription. Funded by NSFREU-Site Award 1757555.
Mechanisms underlying female courtship behavior in plethodontid salamanders
Slater, Tasia E & Woodley, Sarah K.
1Department of Biological Sciences, Duquesne University, Pittsburgh, PA

Plethodontid salamander courtship is a well-studied, prime example of behavioral evolution. However, studies have focused on how males “persuade” females to engage in courtship, largely ignoring the role of females. Salamander mate multiple times over the breeding season, but females are refractory to further mating for several days after mating, even though they are attractive to males. I hypothesized that females are refractory because they 1) lack energy reserves to support mating or 2) are sexually unmotivated after insemination. If females are energetically drained, it is predicted they will be less active and forage more. If sexually unmotivated, they should be uninterested in male cues. To test the predictions, females were paired once a week with a male. Controls were unpaired. Locomotory behavior, hunger, and interest in male cues were measured the following day. Results should provide novel information on the role of females in salamander courtship behavior.

Comparing brain cell counts in tadpole and metamorph Northern Leopard Frogs (Lithobates pipiens) using isotropic fractionation and flow cytometry
Uhrin, Madison1, Kamte, Yashika2, Chandwani, Manisha2, O’Donnell, Lauren2 and Woodley, Sarah1
1Department of Biological Sciences
2Graduate School of Pharmaceutical Sciences
Duquesne University

Brain development is shaped by internal and external factors which affect cell differentiation and function. Amphibians are a useful model of vertebrate brain development; unlike mammals, post-embryonic development occurs outside the maternal environment which allows easy manipulation of the developmental environment. I am adapting the methods of isotropic fractionation (IF) and flow cytometry (FC) to count neurons and glial cells in frog brains. With IF, fixed tissue is homogenized, and cells are visualized using immunohistochemistry and counted under a microscope. To validate these methods, I am comparing the numbers of different cell types in tadpole and metamorph brains. I predict that tadpoles will have more immature cells compared to metamorphs. IF is proving difficult to validate, but initial results with FC indicate that tadpole brains have more cells with nestin, a marker of neural stem cells. Thus, FC may allow assessment of environmental impacts on amphibian brain development.
The Effects of Mindfulness Meditation Training on Kinesiophobia in Patients with Chronic Low-Back Pain
Zito, Miranda, Szucs, Kimberly, Ph.D., OTR/L, Kostek, Matthew, Ph.D.
Rangos School of Health Sciences
Duquesne University

Chronic low-back pain, which affects over 100 million adults in the U.S., often discourages individuals’ participation in physical activity in an attempt to avoid pain. This fear-avoidance, known as kinesiophobia, counterproductively leads to an exacerbation of one’s pain. The hypothesized idea is that, by creating a sense of mindfulness and acceptance towards a participant’s pain through 2 weeks of mindfulness meditation training, sedentary time will decrease and break this vicious cycle. This will be measured and quantified through utilization of wrist-worn ActiGraph accelerometers and daily surveys related to pain and pain acceptance. A pilot study of similar nature conducted by the team suggests that these methods are effective in increasing mindfulness and decreasing disability, however, pain acceptance was not considered. If this study also proves effective in reducing kinesiophobia and pain, it has the potential to be marketed as an alternate chronic low-back pain treatment through hospitals and therapy centers.

Formation of a Pyrrolopyridinone Scaffold via the Fischer Indole Synthesis
Chartier, Eric; Montgomery, Thomas; Rohde, Jeffrey; Evanseck, Jeffrey
Department of Chemistry and Biochemistry
Duquesne University and Franciscan University of Steubenville

To treat diseases, large libraries of organic compounds are screened to discover promising molecular scaffolds (starting points) for drug development. We are examining the aza-indole scaffold formed from reacting 4-hydrazinylpyridinone and cyclohexanone by studying the regioselectivity during the key aza-Cope rearrangement. We hypothesized that one of the two products would be major due to favorable positioning of the pi cloud in the Woodward-Hoffman electrocyclization. Using semi-empirical and density functional models, the relative electronic energies of the ground and transition states were computed and compared to determine which regioisomer, and thus, which product is favored. The density functional model displayed a 20 kcal/mol difference between the transition states at the rate limiting step, indicating a single product formation under standard conditions. We conclude that only one rotamer would follow a thermally-allowed pericyclic reaction yielding this product, with the other requiring significant perturbation of the pi cloud as a forbidden reaction pathway.
Metalation of Benzene Rings by Coinage Metals Gold and Silver
Eiben, Yael and Lummis, Paul
Department of Chemistry and Biochemistry
Bryn Mawr College

Aromatic compounds are particularly useful in industry, as these stabilized molecules have important applications for the development of electronic devices. We aim to fully substitute the positions around a benzene ring with metal atoms to form compounds of general formula C₆M₆, which will feature traditional π-aromaticity within the ring, and a second σ-aromatic ring external to the benzene ring. As coinage metals have the ability to access different oxidation states, we believe that our work will open up a class of target molecules with a rich chemistry and interesting electronic properties. Two types of N-Heterocyclic carbene (NHC), imidazolium and benzimidazolium, are being investigated as stabilizing ligands. The target C₆M₆ compounds will be formed via the [2+2+2] cyclotrimerization of an NHC-stabilized alkyne, (NHC)M-C≡C-M(NHC), where M = Ag or Au. Additionally, theoretical investigations of the target compounds at the PBE0PBE/LANL2DZ level of theory are underway and will be discussed.

Synthesis of Chrysosporazine D&E: Reversing Multidrug Resistance in Cancer Cells
Nya Gayluak, Alex Cocolas, Katie Kaczynski, Serina Tressler, and Thomas D. Montgomery*
Department of Chemistry and Biochemistry
Pain Undergraduate Research Experience (PURE)
Duquesne University, Pittsburgh, PA

Cancer is the second leading cause of death in America with roughly 1.8 million cancer cases being diagnosed during 2020. Standard cancer treatment options, like chemotherapy, are effective at suppressing tumor growth and improving patient outcomes. However, all chemotherapeutics, specifically Doxorubicin, are susceptible to multidrug resistance (MDR). MDR serves to decrease the efficacy of life-saving drugs over time, eventually rendering them ineffective. One common mechanism of MDR is the upregulation of P-glycoproteins (P-gp), which decreases intracellular drug concentrations. Our study aims to reverse drug resistance in human cancer cell lines by investigating a natural product family, the chrysosporazines, that were identified in fish gut. Chrysosporazine’s chemical structure has shown inhibitory effects on the P-gp transmembrane protein and this knowledge allows chrysosporazine and Doxorubin to be co-administered efficiently at low dosages. In this project, we have made inroads into the first total synthesis of a member of the chrysosporazine family.
One-Step Preparation of Structurally-Diverse Covalent Compounds as Potential Antibacterial Agents via the “Undergraduate Friendly” Ugi and Passerini Multicomponent Reactions

Harlan, Emery; Bohrer, Luke; Lapinsky, David J.
Graduate School of Pharmaceutical Sciences
Duquesne University School of Pharmacy

Antibiotic resistance is a tremendous threat to global health. As a result, the development of novel antibacterial drugs with the ability to overcome drug resistance is urgently needed. Towards addressing this need, a small library of covalent bactericidal drug candidates was prepared in one step by easily incorporating several different electrophilic warheads into an Ugi four-component reaction (U-4CR) or a Passerini three-component reaction (P-3CR) chemical scaffold. In particular, the U-4CR and P-3CR served as “undergraduate friendly” multicomponent reactions (i.e., typically high-yielding, easy to carry out, no special equipment or experimental conditions such as an inert atmosphere, dry solvents, or catalysts were needed), which allowed the rapid preparation of twenty-two structurally diverse covalent compounds over nine weeks by one undergraduate student and one second-year graduate student. These covalent compounds are currently being screened for antibacterial activity by the Trun lab within the Department of Biological Sciences at Duquesne University.

Synthetic Investigation of Group 13 Metal Chelates Containing the aza–Dipyrromethene Core

Department of Chemistry and Biochemistry
Duquesne University and St. Mary’s College of Maryland

Since its synthetic revival in the early 2000’s, the aza–dipyrromethene (aza–DIPY) core has received significant attention with respect to its boron difluoride chelates, also known as aza–BODIPYs, which have utility as near–infrared (NIR) dyes in both the physical and biological sciences. However, no other chelates outside of boron are currently known with this core. This presentation details the synthetic investigation of chelating heavier Group 13 elements (Al, Ga, In) to the aza–DIPY core, which can be done in a reliable and high yielding process. Also outlined are the absorption and emission profiles of these complexes which have been found to be highly sensitive to axially coordinated solvents such as methanol and pyridine. Further investigations of these compounds will include crystallographic identification and computational modeling of their frontier molecular orbitals.
83

Dual MEK5 and AKT pathway inhibitors as therapy for treating TNBC
Teague, Vaughn; Flaherty, Patrick T; Cavanaugh, Jane E.; Patel, Saloni; Hallak, Ramez; Bhatt, Akshita; Faruk, Asef
Division of Pharmaceutical, Administrative, and Social Sciences
Duquesne University

The presence of triple negative breast cancer presents a serious prognosis for those afflicted with the disease. This disease state is characterized by the lack of target enzymes traditionally used by the current standards of care. With over 280,000 cases of breast cancer diagnoses estimated to occur in 2021, this leaves approximately 28,000-42,000 patients without targeted cancer therapy. Through our research, we are aiming to create a dual inhibitor of both the MEK5 and AKT pathways, enzymes that foster cell growth and division. The chemical starting point is a quinazoline core containing 3-fluorophenyl substitution at the C-6 position. We are exploring saturated amine ring variations at the C-4 position of the quinazoline ring, aiming to identify novel quinazoline derivatives with dual MEK5 and PI3K inhibitory potential.

84

Title: Synthesis of midostaurin analogs for evaluation in a Tau 4R0N zebrafish assay for rescue of a neurodegenerative phenotype
Authors: Gordon, Andrew W., Hallak, Ramez, Taylor, Kimberly S., Bai, Qing, Burton, Edward A., Flaherty, Patrick T.
Division of Medicinal Chemistry, Duquesne University School of Pharmacy
Duquesne University

Neurodegenerative diseases such as Alzheimer's and Progressive Supranuclear Palsy affect people worldwide, but there are no well-established disease modifying therapies for these complex disease states. Protein kinases are relevant biological targets which may contribute to the accumulation of insoluble Tau and amyloid beta protein deposits in the central nervous system (CNS). Many neurodegenerative diseases are characterized by these deposits. The ATP-binding sites of protein kinases can be inhibited by small molecules, and the molecule midostaurin has been identified as an early lead compound. The lower portion amide of midostaurin provides kinase isoform selectivity and is subject to functional modifications. Active synthetic analogs of midostaurin will be synthesized and tested in a Tau 4R0N zebrafish assay to determine their ability to rescue CNS neurotoxicity. The most active compounds will be utilized to determine relevant kinase targets and possible lead compounds for additional optimization of CNS permeability and drug delivery.
Synthesis of 5-Substituted Pyrrolo[3,2-d]pyrimidine Folate Analogues as Potential Anticancer Agents
Horton, Camren; Gangjee, Aleem; Nayeen, Junayed
Graduate School of Pharmacy, Department of Medicinal Chemistry
Duquesne University

In a variety of cancers, folate-mediated one carbon (1C) metabolism is reprogrammed to facilitate growth and survival of tumor cells. Selective targeting of 1C metabolism in the mitochondrial and cytosolic compartments with multitargeting antifolates is a viable aspect of chemotherapy. Pyrrolo[3,2-d]pyrimidine based antifolates, designed and synthesized by the Gangjee group exhibit efficacy in vitro and in vivo patient derived xenograft (PDX) mouse model studies. Their underlying mechanism involves specific targeting 1C metabolism of tumors at multiple sites to impede de novo purine biosynthesis and inhibit the 1C metabolic pathway. Traditional bulk synthesis of select antifolates was unsuccessful due to chemical instability of specific scaffolds. A modified procedure outlined in the literature posed an alternative synthetic route. This study aims to modify this literature method to bulk synthesize the protected pyrrolo[3,2-d]pyrimidine scaffold intermediate to facilitate the synthesis of a variety of novel antifolates for in vivo and in vitro evaluation.

CD68 Positive Macrophages Found Following Injury to the Sciatic Nerve Shows Fluorescently Tagged Nanoemulsion at a Higher Rate at the Site of Injury Compared to Macrophages Filtered to the Liver
Patterson, Charles2, Traore, Aboubacar1, Deal, Brooke2,3, Janjic, Jelena M.3,4, Pollock, John A.2,3
1Biology Department, Colby College, Waterville, ME 04901
2Department of Biological Sciences, Duquesne University, Pittsburgh PA 15219
3Chronic Pain Research Consortium, Duquesne University, Pittsburgh PA 15219
4Graduate School of Pharmaceutical Sciences, Duquesne University, Pittsburgh, PA,15219

During a neuroinflammatory response, macrophages naturally infiltrate into the site of injury. To study neuroinflammation, these cells can act as a delivery method for nanotherapeutics. Once phagocytosed the fluorescently tagged nanoemulsion can be visualized inside CD68 positive macrophages using fluorescent microscopy. Macrophages can be found both at the site of injury as well as in other organs. Here we assess the aggregation of CD68 positive cells with nanoemulsion in off target organs, which could contribute to unwanted side effects. In this study, macrophage number was explored in the injured nerve as well as the liver. The percentage of CD68 positive macrophages with nanoemulsion were compared between the two tissues and reveal that while in the injured nerve ~50% of the macrophages have nanoemulsion, only ~10% of the cells do in the liver. Also, the macrophages appear to dramatically change morphology depending on which tissue they are found in.
MDX versus D2 Mice: Identifying a Better Model for DMD
Price, Olivia; Omstead, Madisen; Parshall, Rachel; Kostek, Matt Rangos School of Health Sciences Department of Physical Therapy Duquesne University

Duchenne Muscular Dystrophy (DMD) is an X-linked, lethal genetic disorder caused by a mutation in the gene dystrophin that causes the degradation of skeletal muscle. There are two mouse models used to study DMD: MDX and D2. Previous studies have suggested the D2 model is a better replication of DMD in humans due to the disease severity in these mice. The current study will further clarify specific functional and pathological differences. 8 male D2 mice, 8 male MDX mice, and 4 male wild-type control mice 8-10 weeks of age were used in the study. A preliminary analysis of the data supports that the D2 mice had greater inflammation (quantified by immunohistochemistry) and lower muscle function than MDX mice. The D2 mice suffer from more severe muscle dysfunction, pathology, and inflammation than do the MDX mice. Our study confirms that the D2 model is more similar to the human condition.

Tracking Nanoemulsion Filled CD68 Positive Macrophages Involved with Inflammation Within Injured Rat Sciatic Nerve and Organs
Traore, Aboubacar1, Patterson, Charles2, Deal, Brooke2,3, Janjic, Jelena M.3,4, Pollock, John A.3,4

1Biology Department, Colby College, Waterville, ME 04901
2Department of Biological Sciences, Duquesne University, Pittsburgh PA 15219
3Chronic Pain Research Consortium, Duquesne University, Pittsburgh PA 15219
4Graduate School of Pharmaceutical Sciences, Duquesne University, Pittsburgh, PA,15219

Chronic pain is a neurobiological disease that plagues 20% of adults worldwide. Non-steroidal anti-inflammatory drugs (NSAIDs) provide relief but cause off target effects due to the high systemic dosage needed. Using the innate inflammatory response, nanoemulsion therapy can utilize macrophages to naturally deliver drug to the site of injury. Using the rat sciatic nerve chronic constriction injury (CCI) model to induce a neuroinflammatory response we explored the presence of CD68 positive macrophages carrying the nanotherapy within the site of injury and the spleen. We were able to visualize this using fluorescent staining and microscopy. This study showed that at the site of injury, there were significantly more macrophages containing nanoemulsion than in the spleen. These findings give insight into the efficacy and longevity of macrophages to transport the nanotherapy throughout the body. Funded by NSF-REU-Site Award 1757555.
Steps toward the Synthesis of Chrysosporazines
Tressler, Serina; Kaczynski, Katie; Cocolas, Alex; Gayluak, Nya; Montgomery, Thomas*
Department of Chemistry and Biochemistry
Duquesne University

The chrysosporazines are a family of alkaloid natural products found to be effective at reversing multidrug resistance in cancer cells lines. Given their promising bioactivities and natural scarcity, we have designed a novel synthetic pathway towards these compounds. Portions of the synthetic route towards several members of the chrysosporazine family were considered and performed using standard organic lab techniques. While our overall isolated yields were low, the desired compounds were synthesized and fully characterized, indicating the feasibility of this synthetic route for future development. These findings have provided insights into the direction of our future work on the chrysosporazines.

Title: Optimization of Spray Dried Amorphous Particles
Authors: Connor Kelley, Ashwini Gumireddy, and Ira S. Buckner
Academic Department: Pharmaceutical Sciences, Pharmaceutics
University: Duquesne University

Particle characteristics directly impact the performance of many drug products. The goal of this project is to investigate how three spray drying parameters affect the resulting particles. A two-level full factorial design was used to investigate the effects of atomizing air pressure, pump rate, and concentration of the feed solution. Solutions of poly(vinylpyrrolidone-co-vinyl acetate) dissolved in methanol were sprayed to prepare 10 different batches including replication of the center point. At low atomizing air pressure, high pump rate, and high feed concentration, the largest particle sizes, smallest particle agglomerates, and lowest percent yield were obtained. At high AAP, low pump rate, and low feed concentration, smaller particle size, lower residual solvent concentration, and largest particle agglomerates. These findings suggest spray dried particle properties can be rationally manipulated to improve drug product performance.
Effects of Powder Granulation on Theophylline Tablets
Skomo, Alec; Henson, Samuel; Anderson, Carl A. Ph.D; Drennen, James K. Ph.D
Pharmaceutical Sciences
Duquesne University

Continuous manufacturing of pharmaceutical products is difficult with various raw materials due to their poor flowability. Granulating the powder blend increases the flowability but requires development to be implemented as a continuous process. This study aims to find a consistent set of granulation critical process parameters, making granules with certain critical quality attributes. These properties can then be correlated with tablet properties. Thus, the properties of the tablets can be controlled continuously via the granulation process, an important part of continuous manufacturing. This research investigated the hardness and dissolution properties of tablets made from granules to determine the most appropriate granule size range and seek out connections between tablet properties and dissolution behavior. It was found that addition of disintegrant and lubricant was necessary for proper production and dissolution of tablets made from granules, and tablets that had oversized granules removed yielded the quickest dissolution times.

Video Series on applying Geometric Algebra to Introductory Physics
Spadavecchia, Katelyn and Corcovilos, Theodore A.
Dept. of Physics
Duquesne University

Physics education research investigates effective ways of teaching and learning about physics, however there exist complications in its foundation. For example, there are many different mathematical systems used in physics today. The creation of a unified mathematical language could make physics easier to learn and use, as was recognized by William Clifford when creating his Geometric Algebra (GA) in 1873. Although Clifford Algebras are typically reserved for advanced physics topics like quantum field theory, GA and its extension, Projective Geometric Algebra (PGA), offer an intuitive model for classical mechanics based on the geometry of reflections and rotations unifying many different areas of math including synthetic and coordinate geometry, vector and complex analysis, and differential forms among others. We are creating a video series for entry-level physics students highlighting the benefits of using PGA specifically in unifying rectilinear and rotational motions for solving Newtonian mechanics problems.
Global fits and extrapolations of the up to down quark ratio contributions to the proton
Valenty, Hannah¹; Benmokhtar, Fatiha¹; Higinbotham, Douglas²
¹Department of Physics, Duquesne University, Pittsburgh, PA
²Thomas Jefferson National Accelerator Facility, Newport News, VA

The MARATHON experiment ran in spring 2018 in Hall A at the Thomas Jefferson National Accelerator Facility by a large international Nuclear Physics collaboration. The experiment used two high resolution spectrometers for electron detection, and a cryogenic target system which included a low-activity tritium cell. MARATHON uses a novel method to extract the ratio of neutron to proton structure functions that allows the access to the ratio of the up to down quark contributions to nucleon structure. MARATHON performed deep inelastic electron scattering off Tritium and Helium-3 mirror nuclei over the range x=0.195 to x=0.825. Where x is the fraction of momentum carried by the struck quark.

The results of F2n/F2p from the MARATHON experiment have been released and my work performs a fit of the data to extrapolate to the xB=1 limit. An overview of the MARATHON experiment, the fits and extrapolation work I performed will be presented.

Flight Simulation for a Two-Balloon High-Altitude System
Yuanshan Zhang, Russell Clark, Ph.D.
Department of Physics and Astronomy
The University of Pittsburgh

A typical high-altitude balloon system consists of a single balloon for lift and a parachute to return the payload. Since a parachute has a fixed area and the drag force depends on the air density, the initial descent speed can be extremely large, resulting in chaotic motion. This project explores using two balloons to lift the payload and a single balloon to return it. The advantage of using a balloon for the return instead of a parachute is that the area of the balloon scales with the density producing a more controlled descent. A simple, one-dimensional flight simulator was previously developed for the proposed two-balloon system. The simulator uses Euler’s method to calculate position and velocity and a realistic model for drag. This work has expanded on this by making the simulator three-dimensional, adding crosswinds, translating the simulation coordinate system to latitude and longitude, and adding real-time weather information.
95
Structural and dynamic differences between SARS-CoV-2 s2m variants
Bojanac, Izayah
Pellegrene, Kendy, Kelleher, Bryan, Kensing, Adam.
Dr. Patrick Lackey, Dr. Jeffery Evanseck, Dr. Mihael-Rita Mihaescu
Department of Biochemistry and Chemistry, Westminster College, New Wilmington, Pennsylvania,
Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, Pennsylvania,
Duquesne University

This work has assessed and characterized a mutation in the highly conserved s2m region of the SARS-CoV-2 virus. Our computations studied the change in structure and dynamics due to a G→U mutation in this region. Atomistic models of both the SARS-CoV-2 s2m and G→U mutant were produced using AMBERTOOLS20. Molecular dynamics simulations were performed with TIP3P explicit solvents and 0.05 M Mg²⁺. Sodium ions were added to achieve system neutrality. Two microsecond simulations were performed and analyzed after minimization and equilibration. Structural analysis included RMSD, RMSF, hydrogen bond analysis, and secondary structure analysis using VMD and MINT. These analyses demonstrated differences in the RNA secondary structure caused by the mutation of interest. Visual representations were created from various conformations and used as the basis for final assessment of the impact of the G→U mutation on the motif's structure.

96
Reducing COVID-19 Vaccination Hesitancy with Empirically Supported Community Engagement Techniques
Celestin, Hervinah, Gernatt, Grace, Pater, Jordan; Hoenig, Brandon D.
*These authors contributed equally to this work

Bayer School of Natural and Environmental Sciences, Department of Forensic Science and Law, Department of Biological Sciences
Duquesne University

While experts agree that vaccinations will serve a critical role in eradicating the SARS-CoV-2 virus (hereafter, COVID-19), there has been a high degree of confusion surrounding the efficacy and safety of COVID-19 vaccines. This confusion, which may stem from a disconnect between experts and the population at large as well as the politicization of healthcare decisions, is, at least in part, to blame for the decline in vaccination rates and recent increases in COVID-19 cases. As it is becoming increasingly clear that vaccination hesitancy is a result of societal influences, as opposed to vaccine efficacy or safety, this work aims at identifying potential avenues for reducing vaccine hesitancy using empirically supported community engagement techniques and strategies. Here, we present examples of common concerns surrounding COVID-19 vaccinations as well as strategies to not only reduce vaccination hesitancy, but also develop the relationships necessary for meaningful conversations around other potentially contentious issues.
**The Role of Topoisomerase 1 in Herpes Simplex Virus Type 1 Infection**

Esenwein, Raegen; Dembowski, Jill  
Department of Biological Sciences  
Duquesne University

Human topoisomerase 1 (Top1) is an enzyme required for normal growth and development. Cellular Top1 ensures proper transcription and DNA replication by creating single stranded nicks in DNA to relieve topological stress and allow relaxation of supercoiled DNA. Previous research found Top1 interacts with HSV-1 DNA. Based on its role in cellular processes, we believe that Top1 helps regulate viral transcription and/or replication. We therefore hypothesize that altering Top1 expression in HSV-1 infected cells will decrease viral yield. To alter Top1 expression, the commercial inhibitor, camptothecin (CPT) was used. Our studies revealed that Top1 inhibition via CPT reduces viral yield. Currently, an inducible Top1 shRNA knockdown cell line is being created as another method of alteration. In the future, we will determine if viral transcription or DNA replication are altered after Top1 inhibition or knockdown. These studies will further pinpoint the role of Top1 in HSV-1 infection. Funded by NSF-REU Site Award 1757555

---

**Pediatric neurotropic infection alters synaptic development in the developing brain**

Fadare, Anuoluwapo; O'Donnell, Lauren A.; Chandwani, Manisha; Kamte, Yashika S.  
Natural and Environmental Science  
Duquesne University

Many neurotropic viruses cause more significant pathology in younger hosts as their brains are still developing. This experiment asked how central nervous system (CNS) viral-infections affect the development of synapses in the pediatric brain during infection as well as long-term. We used a transgenic mice model where measles virus (MV) infect only mature neurons, leading us to question whether synaptic proteins were impacted. Synaptogenesis is at its peak in pediatric mice (10 days old) and we hypothesized that a neurotropic infection could disrupt synaptic proteins. We examined synaptic markers in the cerebellum and hippocampus in MV-infected and uninfected mice 9 days and 90 days post-infection through western blot analysis. We found differential downregulation of synapsin isoforms during infection, which was dependent on the brain region and the time point examined. This highlights the short and long-term consequences of a pediatric infection on neurodevelopment and how that impacts brain circuitry.
99
Protecting Future Generations: How do Adult and Newborn Brains Fight Differently Against Neurotropic Viral Infections?
Hemerson, Marlo E.
Chandwani, Manisha N.
Kamte, Yashika S.
O'Donnell, Lauren A.
Graduate School of Pharmaceutical Sciences
Neurogenerative Undergraduate Research Experience (NURE)
Duquesne University

Newborns are vulnerable to brain damage from viral infections. We have observed adult mice successfully fight measles virus in the brain, while neonates (2 days old) die. We hypothesized the development of neonatal brain cells would be disrupted by infection, whereas adult brain cells would be resilient against inflammation. Western blot revealed reduced expression of mature neuronal (BIII-Tubulin) and astrocytic (GFAP) markers in infected adult hippocampus, whereas neonates did not show changes in these markers. These findings suggest adult neural cells experience changes in marker expression during infection, despite 100% survival. In contrast, neonates do not show global changes in expression of neural markers, despite succumbing to the infection with neurological changes. Thus, expression of neural markers does not correlate with survival, suggesting cellular dysfunction, as opposed to cell death, may contribute to mortality. Understanding these differences may identify pathological hallmarks and potential therapeutic targets in the newborn brain.

100
Elucidating the function of Cellular PCNA in HSV-1 Infection
Williams, Maya; Packard, Jessica; Dembowski, Jill
Department of Biological Sciences Duquesne University

Proliferating cell nuclear antigen (PCNA) is a cellular protein that adds processivity to cellular DNA polymerases during DNA replication. PCNA associates with herpes simplex virus type 1 (HSV-1) replication forks. The function PCNA plays during HSV-1 infection and its necessity for a successful infection is unknown. If PCNA is required for viral infection, it is hypothesized that viral yield will decrease when PCNA is knocked down or inhibited. Two inhibitors and two short hairpin RNAs (shRNA) will be used to target and reduce PCNA along with plaque assays to quantify viral yield. Data from the inhibitor plaque assays indicate that viral yield does decrease in the presence of inhibitors. shRNAs have been shown to successfully reduce PCNA levels in the cell. We are currently using plaque assays to determine viral yield after treatment with short hairpin RNAs compared to a control with PCNA present.
101
The impact of saturation status on the regulation of yeast acyltransferase Gpc1
Conklin, Shane; Hrach, Victoria; Patton-Vogt, Jana
Biology
Duquesne University

A vital component of cell viability is membrane homeostasis, which includes lipid synthesis, lipid turnover, and alterations in lipid saturation status. Phosphatidylcholine (PC) is a major membrane phospholipid in eukaryotic cells. The novel PC Deacylation-Reacylation Pathway (PC-DRP) remodels phosphatidylcholine through cleavage of its acyl chains, followed by two reacylations. The first acylation is catalyzed by Gpc1, and results in an increase in PC saturation status. To further explore the relationship between Gpc1 and membrane saturation, we provided Saccharomyces cerevisiae with saturated and unsaturated fatty acids. Expression was assessed for GPC1 and OLE1, the sole desaturase in S. cerevisiae. Additionally, we probed for GPC1 expression upon downregulation of OLE1 transcription. Induction of the UPR was also monitored. Our results indicate that GPC1 expression is responsive to fatty acid saturation.

102
Glycerophosphocholine as an alternative phosphate source in Candida albicans
Cooke, Lauren1; King, William2; and Patton-Vogt, Jana2
1Gettysburg College
2Department of Biological Sciences, Duquesne University

Phosphate is an essential nutrient for cell function and growth. In the fungal pathogen, Candida albicans, perturbations in phosphate acquisition influence virulence phenotypes. For example, phosphate starvation causes increased sensitivity to cell wall stress and oxidative stress. In addition to inorganic phosphate, C. albicans can utilize the renal metabolite, glycerophosphocholine (GPC) as a phosphate source. The goal of this study is to examine virulence phenotypes as a function of the provision of either GPC or inorganic phosphate as a phosphate source. To simulate inorganic phosphate starvation conditions, we utilized a deletion strain of the high affinity inorganic phosphate transporter, Pho84. Our studies show that GPC is able to rescue a variety of phenotypes displayed by pho84ΔΔ, including sensitivity to cell wall stress and oxidative stress. Funded by NSF-REU-Site Award 1757555.
The Use of *Streptomyces* Spores as a Vaccine Vehicle for *Bordetella pertussis* via the Adenylate Cyclase Repeat-in-Toxin (RTX) Epitope
Orgovan, Jessica & McCormick, Joseph
Department of Biological Sciences
Duquesne University

Whooping cough is an upper respiratory infection caused by the bacterial pathogen *Bordetella pertussis*. This study aims to develop an alternative method of vaccine delivery using spores of *Streptomyces coelicolor* as the current acellular vaccine does not provide lifelong immunity. Spores will act as a vehicle to carry an epitope of a *B. pertussis* virulence factor as a passenger protein. The specific goal of this project was to create a protein fusion between the C-terminus of spore associated protein A (SapA) and repeats II-III of the repeat-in-toxin (RTX) domain of *B. pertussis* adenylate cyclase. First, a gene encoding RTXII-III and the apramycin-resistance gene were cloned adjacently into an *E. coli* plasmid. Then, the fragment was isolated via restriction enzyme digestion and will be used as template for synthesis of a mutagenic PCR product. The PCR product will ultimately be fused to sapA by recombineering (an *in vivo* recombination technique).

Characterization of Spore-Associated Protein A Assembly onto the Spore Surface in *Streptomyces*
Shaw, Rosemarie & McCormick, Joseph
Department of Biological Sciences
Duquesne University

*Streptomyces* are Gram positive, filamentous, soil bacteria that produce many medicines and antibiotics. A unique characteristic of these bacteria is the production of sporulating aerial hyphae. During sporulation *Streptomyces* secrete spore-associated proteins to create a spore coat. However, there is little known about how the spore coat proteins assemble. The aim of this study was to further characterize SapA, a 13 kilodalton secreted spore-associated protein of *Streptomyces*. SapA will be used as a model for how *Streptomyces* build a spore coat. SapA will be studied by constructing mutant strains of *Streptomyces* that express variants of a SapA. Spore-associated proteins will be extracted and analyzed by a Western Blot, which will show whether these mutant strains secrete and assemble the SapA variants on the spore surface. Characterizing which portions of SapA are required for secretion and assembly could advance the understanding of the developmental biology of *Streptomyces*.
The Effects of Pre-Loading Internal Standards and Storage Time on Recovery of Amphetamines and Barbiturates
Cook, Amy E; Dryzal, Dana E; Cawley, Hannah M; Wetzel, Stephanie J
Department of Chemistry and Biochemistry
Duquesne University

Toxicological analysis requires high precision and high accuracy sample preparation. Streamlining sample preparation increases laboratory efficiency and cost-effectiveness. Pre-loading deuterated standards to integrate into Solid-Phase Extraction (SPE) could eliminate time-consuming steps in sample preparation and minimize quantitative errors. Using Liquid Chromatography-Mass Spectrometry, recoveries of amphetamines (Cook) and barbiturates (Dryzal, Cawley) were found for several loading conditions, storage times, application materials and types of SPE cartridges pre-loaded with deuterated standards. Fresh samples using no pre-loading technique were prepared as a control. The fresh samples were hypothesized to have the best recovery, with the pre-loaded SPE cartridges second best and decreasing over time. Of the internal standard application materials, nylon was hypothesized to produce the best recovery. The interpretation of these data sets will be used to determine future experiments and expanded application to analyze amphetamines and barbiturates, as well as opioids and benzodiazepines, in one sample.

Characterization of the dimer initiation site in the SARS-CoV-2 3'-untranslated region and of its interactions with miR-1307-3p
Leeann Parsi\(^1\), Caylee Cunningham\(^2\), Caleb Frye\(^2\) and Mihaela Rita Mihăilescu\(^2\)
\(^1\)Saint Joseph High School
\(^2\)Department of Chemistry & Biochemistry, Duquesne University, Pittsburgh PA 15282

The current COVID-19 pandemic, caused by the severe acute respiratory coronavirus 2 (SARS-CoV-2) outbreak, has severely affected millions of people worldwide. Despite the success of the current vaccines developed against SARS-CoV-2, the emergence of variants which are more transmissible and resistant to the vaccines highlight the importance of understanding the coronaviruses’ life cycle. While most of the 3’-untranslated region (UTR) of SARS-CoV-2 is not conserved it harbors a 41 nucleotide s2m element, which is conserved not only in coronaviruses, but also in three other viral families. In this study we have studied an extended stem-loop (50 nucleotides), which we named the dimer initiation site which we proposed to form a kissing complex, initiating the SARS-CoV-2 genome dimerization. Additionally, we characterized the interactions of this stem-loop with the host cellular microRNA miR-1307-3p.
Colleges and High Schools Represented at the 24th Annual Summer Undergraduate Research Symposium:

Arizona State University     University of Texas-Rio Grande Valley
Bryn Mawr College           University of Wisconsin at Parkside
California University of PA Washington & Jefferson College
Carlow University             Waynesburg University
Centre College               Westminster College
Christopher Newport University
Clarion University
Colby College
Concord College
Duquesne University
Franciscan University of Steubenville
Furman University
Georgia Institute of Technology
Gettysburg College
High Point University
Lycoming College
Norfolk State University
Rowan University
Shippensburg University
Slippery Rock University
Saint Joseph High School
St. Mary’s College of Maryland
Stockton University
Texas A&M University
The College of St. Scholastica
University of Maryland
University of Pittsburgh