# SUPPLEMENTARY INFORMATION

Dereplication of Microbial Metabolites Through Database Search of Mass Spectra

Mohimani et al.

# SUPPLEMENTARY FIGURES

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   | Peptides (RiPPs)<br>PP Natural Products work<br>erimental MS/MS spectr<br>them for possible RIPP<br>dy in beta development<br>ove analysis and usability  | <ul> <li>RiPPquest<br/>flow. This analysis will<br/>against full genome<br/>natural products. This<br/>lages so any feedback<br/>b. it is available http://www.</li> </ul>  |                  |  |   |   |      |   |   | | | | | | | | | | | | | | | | | | | | |
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   | SpeckIZ C<br>427.39<br>513.32<br>45 21  
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  | Fraj   | Min<br>gmentation<br>Score C<br>-<br>-<br>18<br>18<br>18  | MetMass 3<br>426.39<br>512.31<br>434.32<br>510.22   
   
   
   
   
   
   
   | SpecMZ C<br>427.39<br>513.32<br>435.33<br>511.23  
   | RT C  | Adduct C<br>M+H<br>M+H<br>M+H   |                  |  |   |   |      |   |   | | | | | | | | | | | | | | | | | | | | |
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| Workflow Submiss   | Max Charge:<br>ion Ema Filename  Filename  Show Show Show Show Show  | Scan 0         Image: Scan 0 </td <td>Sexample.com<br/>Metaboli<br/>(+)-squalene-11<br/>Angunorycin-A<br/>beta-Citzaurinoi; 8-A<br/>antimyc<br/>Pristinamycin IC; Vern</td> <td>Fray</td> <td>Min<br/>gmentation<br/>Score C<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td> <td>MetMass 2<br/>48-24<br/>48-23<br/>434.32<br/>510.22<br/>852.38</td> <td>SpecAX C<br/>427.39<br/>435.33<br/>511.23<br/>427.39</td> <td>NT         H           4076.73         2996.03           2447.53         2447.53</td> <td>1-6 \$ Submit Submit M+H M+H M+H M+H M+2H</td>  | Sexample.com<br>Metaboli<br>(+)-squalene-11<br>Angunorycin-A<br>beta-Citzaurinoi; 8-A<br>antimyc<br>Pristinamycin IC; Vern   
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  | Frag   | Min<br>gmentation   | MetMass -           -         -      -         - <tr <="" tblood<="" td=""><td>spec.MZ =<br/></td><td>Att         -           Idic-Total):         6           Idic-Total):         7           Idic-Total):         7           Idi:         7</td><td>Adduct *</td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:<br/>sion<br/>Email<br/>Filename<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show</td><td>scan -             sil me at user           6867           7143           316           9377           516           9377           575</td><td>Artabolt  Argunomycin-A beta-Citraurinol.g-N-A beta-Citraurinol.g-N</td><td>Frag</td><td>Min<br/>gmentation<br/>Score ()<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18</td><td>Mactilians         Mactilians           426.39         512.31           434.32         510.22           852.38         448.24           410.28         738.28</td><td>SpeckXZ C<br/>SpeckXZ C<br/>427.39<br/>513.32<br/>511.23<br/>427.20<br/>943.53<br/>427.20<br/>943.53<br/>427.20<br/>943.53<br/>427.20<br/>943.53<br/>427.20<br/>943.53<br/>427.20<br/>943.53<br/>427.20<br/>943.53<br/>427.20<br/>943.53<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20<br/>427.20</td><td>RT C Litic-Total J: 6</td><td>1-6 ¢           Submit           M+H           M+H</td></tr> <tr><td>Workflow Submiss<br/>d)<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary<br/>AddtoGNPSLIbrary</td><td>Max Charge:<br/>Ion Ema<br/>Flienane C<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show</td><td>Scan = 1         Image: Scan = 1           sil me at user         Scan = 1           6667         7143           3148         3156           92777         5116           7576         5727           5728         5128</td><td>Antaboli 
(+)-squalene-1  Angulonycin-A  beta-Citraurinol; 8-A  antimyc Pristinamyc)_L/C; Vern 10-acetylircit "Azafrinaldehyde(58, Amych nona</td><td>Fray</td><td>Min<br/>gmentation<br/>Score C<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td><td>MetMass -<br/>426.39<br/>510.22<br/>510.22<br/>52.31<br/>510.22<br/>52.38<br/>942.52<br/>418.24<br/>410.28<br/>718.28<br/>418.24<br/>410.28<br/>718.28<br/>418.24<br/>410.28<br/>718.28<br/>470.34</td><td>Ider a PSM as 5<br/>aks: Linear-Cyc<br/>SpecMZ C<br/>H<br/>427,39<br/>513,32<br/>513,32<br/>513,33<br/>511,23<br/>427,20<br/>943,53<br/>403,54<br/>419,24<br/>411,29<br/>729,29<br/>471,35</td><td>RT:<br/>Idic-Total):<br/>6<br/>8<br/>8<br/>7<br/>9<br/>9<br/>9<br/>102<br/>9<br/>102<br/>9<br/>102<br/>102<br/>102<br/>102<br/>102<br/>102<br/>102<br/>102</td><td>Adduct 2<br/>M+H<br/>M+H<br/>M+H<br/>M+H<br/>M+H<br/>M+H<br/>M+H<br/>M+H</td></tr> <tr><td>Workflow Submiss<br/>d)<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary</td><td>Max Charge:</td><td>Scan ÷         I           sil me at user         -           Scan ÷         I           H         -           6667         7143           5132         3348           3376         90777           91777         5116           7576         5726           9175         5128           4872         -</td><td>Rexample.com Actaboli (+)-squalene-10 Anguinomycin-A beta-Citrauriou, 8-A antimyc Pristinamycin, JC, Vern Soyasap 4,4-Diaponeurosporen 10-acetylircit razafrinaldryder (58,<br/>Amychyder (58,<br/>Amychyder (58, Amychyder (58, Amychyddia))))</td><td>Frag<br/>20<br/>21<br/>21<br/>21<br/>22<br/>23<br/>24<br/>25<br/>24<br/>25<br/>24<br/>25<br/>24<br/>25<br/>24<br/>25<br/>25<br/>25<br/>25<br/>25<br/>25<br/>25<br/>25<br/>25<br/>25</td><td>Min<br/>gmentation<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td><td>Methass 2         A           40.3         3           41.3         3</td><td>Ider a PSM as 5<br/>aks: Linear-Cyc<br/>sec. 12<br/>47, 39<br/>513, 32<br/>47, 20<br/>943, 53<br/>511, 23<br/>403, 34<br/>403, 34<br/>419, 24<br/>411, 29<br/>419, 23<br/>419, 33</td><td>HT         I           III         -         -           III         -         -         -           III         -         -         -         -           IIII         -          -</td><td>Adduct -</td></tr> <tr><td>Workflow Submiss<br/>d)<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary<br/>AddtoGNPSLibrary</td><td>Max Charge:<br/>sion Ema Show Show Show Show Show Show Show Show</td><td>Scan -           -           sil me at user         -           6867         -           7143         -           3346         -           93777         -           516         -           93777         -           512         -           3346         -           93777         -           512         -           3346         -           93777         -           5128         -           4972         -           9372         -</td><td>Pristinamycin_LC; Vern Yraziniaidenyde; SR, Ar-Diaponurospore 10-acetylioriol Yazafrinaidenyde; SR, Armoh beta-Citararinene; JF: Virginiamycin_S1; Stap</td><td>Frag</td><td>Min<br/>gmentation<br/>Score ()<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>17<br/>17<br/>17<br/>17<br/>17<br/>17<br/>17</td><td>Matthens         Anatomic           48.39         512.31           434.32         510.22           852.33         418.24           402.8         702.34           418.24         823.35           823.35         823.35</td><td>SpeckXZ C<br/>SpeckXZ C<br/>427,39<br/>513,32<br/>427,20<br/>940,53<br/>427,20<br/>940,53<br/>427,20<br/>940,53<br/>427,20<br/>940,53<br/>427,20<br/>940,53<br/>427,20<br/>940,53<br/>427,20<br/>940,53<br/>427,20<br/>940,53<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>941,55<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,20<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35</td><td>RT C<br/>H<br/>H<br/>S487, 38<br/>3709, 99<br/>4076, 73<br/>2946, 52<br/>437, 73<br/>3458, 13<br/>3459, 14<br/>319(2), 52<br/>1049, 55<br/>4074, 43<br/>3991, 14<br/>319(2), 52<br/>1049, 55<br/>4074, 43<br/>3091, 38</td><td>Adduct *</td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:<br/>Max Charge:<br/>Fliename :<br/>Fliename
:<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Sh</td><td>Scan +         I           sil me at         user           Scan +         I           B         -           6867         7143           31346         3316           3277         5716           5727         572           6727         5128           4872         3227           2757         2257</td><td>Rexample.com Metaboli (+)-squalene-11 Anguinomycin-A beta-Citraurino(:, 8-A antimyc Pristinamycin_UC, Yern Systapa 4.4'-Diaponeurosporei 10-acetylicrif "Azafrinaldehyde;(SR,<br/>Amych beta-Citraurinet;, 8-Yinghiamycin-51, Stag beta-Citraurinet;, 8-Yinghiamycin-51, Stag Ostreogrycin, A.; Miami</td><td>Frag</td><td>Min<br/>gmentation</td><td>MetMass -<br/>426.39<br/>426.39<br/>424.31<br/>42.31<br/>42.31<br/>42.31<br/>42.32<br/>42.32<br/>42.32<br/>42.23<br/>418.24<br/>410.28<br/>470.24<br/>418.23<br/>418.24<br/>410.28<br/>470.34<br/>418.32<br/>552.25<br/>552.25</td><td>Speckiz C<br/>+ 427,39<br/>513,33<br/>511,23<br/>427,20<br/>943,53<br/>511,23<br/>427,20<br/>943,53<br/>511,23<br/>427,20<br/>943,53<br/>511,23<br/>427,20<br/>943,53<br/>511,23<br/>427,20<br/>943,53<br/>511,23<br/>427,20<br/>943,53<br/>511,23<br/>427,29<br/>427,39<br/>513,23<br/>511,23<br/>512,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,23<br/>513,25<br/>513,25<br/>513,25<br/>513,25<br/>513,25<br/>513,25<br/>513,25<br/>513,25<br/>513,25<br/>5</td><td>KT C           -         -      <tr td=""> <tr td=""> <tr td=""></tr></tr></tr></td><td>Adduct :<br/>MoH<br/>MoH<br/>MoH<br/>MoH<br/>MoH<br/>MoH<br/>MoH<br/>MoH</td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:</td><td>scan ÷         1           sll me at         user           sll me at         user</td><td>Control Control Contr</td><td>Frag</td><td>Min<br/>gmentation<br/>Score ()<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td><td>Methass         Methass         <t< td=""><td>Ider a PSM as 5<br/>aks: Linear-Cyc<br/>aks: Linear-Cyc<br/></td><td>Itic-TotalJ: 6     Itic-TotalJ: 7     Itic-To</td><td>Adduct *</td></t<></td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:<br/>Max
Charge:<br/>Filename<br/>Filename<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Sh</td><td>Regular •<br/>2 •<br/>stil me at usern<br/>stil me at use</td><td>Aretabolt     (+)-squalene-10     (+)-squalene-10     (+)-squalene-10     (-)-squalene-10     (-)-taponourospore     (-)-taponourosp</td><td>Frag</td><td>Min<br/>gmentation<br/>Score ©<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td><td>MetMoss         C           40,000         -         <t< td=""><td>SpocM2 C<br/></td><td>RT C<br/>HT C<br/>H</td><td>Adduct *</td></t<></td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:</td><td>Scan 0         Image: Scan 0<!--</td--><td>Antaboli<br/>(+)-squalene-11<br/>Anguinomycin-A<br/>beta-Citraurinol; 8-A<br/>antimyc<br/>Pristinamycin, JC; Ven<br/>10-acetylicci<br/>*Azafrinadetyde(SR,<br/>Amych<br/>Virginiamycin-51; Stap<br/>Virginiamycin-51; Stap<br/>Virginiamycin-51; Stap<br/>Stareogrycin, A; Mikam<br/>Phrotoce<br/>phakellist<br/>(5)-(-)-squalene<br/>2: 15-(-)-squalene</td><td>Frag</td><td>Min<br/>gmentation<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td><td>MetMass         Construction           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:00000         -         -           9:00000         -         -           9:000000         -         -           9:000000000         -         -           9:000000000000000000000000000000000000</td><td>Spec.M.Z =<br/>Spec.M.Z =<br/>427.39<br/>513.32<br/>435.33<br/>511.23<br/>403.34<br/>419.24<br/>411.29<br/>419.33<br/>427.20<br/>141.29<br/>419.33<br/>427.20<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.</td><td>Att         12           Lile-Total]s:         6           Lile-Total]s:         6           Statistics         6           Jane Statistics         7           Jane Statistics         7      &lt;</td><td>Adduct -<br/>Submit<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H</td></td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:</td><td>scan :                     sill me at         useri           sill me at         useri</td><td>Actaboli     (+)-squalene-1(         Anguinomycin-A         Anguinomycin-A         Anguinomycin-A         beta-Citraurinol.; 8-A         antimyc     Pristinamycin_JC; Vem         Soyasap         Ar-Diaponeurosporer         10-acetylirci         T-azafrinaldetyde;(58,         Amych         beta-Citraurinene; 8-         Virginiamycin-51; Stag         Ostroopycin.4: "Miam         Prorocei         phakelilis         (5)-(-)-squalene         7.11-cyclobotryococ         Chalcomperies.Mecmonic</td><td>Frag</td><td>Min<br/>gmentation<br/>Score ©<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18<br/>18</td><td>MetMass         MetMass           426.39         512.31          
434.32         510.23           434.32         510.23           434.32         510.23           418.24         418.24           418.28         832.35           523.35         525.23           418.24         418.24           418.28         833.35           510.54.50         448.35           418.44         418.32           414.42         20.33</td><td>Ider a PSM as 5<br/>aks: Linear-Cyc<br/>saks: Linear-Cyc<br/>saks: 2<br/>427,39<br/>427,30<br/>427,20<br/>447,33<br/>427,20<br/>443,31<br/>427,20<br/>443,31<br/>427,20<br/>443,31<br/>411,29<br/>427,39<br/>427,39<br/>427,39<br/>427,35<br/>429,26<br/>427,39<br/>427,35<br/>429,26<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,35<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>427,45<br/>45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45<br/>45,4545,45<br/>45,45<br/>45,45<br/>45,4545,45<br/>45,45<br/>45,45<br/>45,45<br/>45,45</td><td>RT -<br/>ILIC-TotalJ: 6<br/>ILIC-TotalJ: 6</td><td>Adduct =</td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:<br/>Max Charge:<br/>Max Charge:<br/>Email<br/>Email<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show<br/>Show</td><td>Scan +         I           sill me at         user           sill me at         user           Scan +         I           6667         7143           7143         3346           3316         907177           5716         5775           572         5775           572         3900           5007         6554           5485         100731*</td><td>Sexample.com<br/>Metaboli<br/>(+)-squalene-II<br/>Anguinomycin-A<br/>beta-Citraurinot,:::-A-<br/>antimyc<br/>Pristinamycin_JC; Vern<br/>Soyaspa<br/>4,6-Daponeurosporen<br/>10-acetylicti<br/>"Azafrinaldehyde (SR,<br/>Amych<br/>nonan<br/>beta-Citraurinem;<br/>Virginiamycin_S1; Stap<br/>Ostreogrycin, A:, Mikam<br/>Proroce<br/>phakellist<br/>(S)-(-)-squalene<br/>7,11-Cyclostrycoco<br/>Chalcomycin; Wyconom</td><td>Frag<br/>b: 1<br/>c: 1<br/>c: 2<br/>c: 2</td><td>Min<br/>gmentation<br/>Score C<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td><td>MetMass         Construction           HetMass         H           426.39         H           510.22         B52.38           942.53         402.33           418.24         410.28           173.82.8         470.34           418.32         515.25           488.35         1036.50           426.39         416.42           700.37         1268.41</td><td>Speck82 C<br/></td><td>RT C<br/>FT Cotal J: 6<br/>5467, 28<br/>3709, 99<br/>4076, 73<br/>2998, 03<br/>2467, 52<br/>937, 17<br/>3488, 83<br/>3891, 14<br/>3190, 52<br/>1049, 55<br/>4074, 43<br/>3904, 38<br/>2207, 40<br/>3876, 45<br/>3060, 14<br/>4687, 25<br/>5107, 91<br/>3194, 45<br/>3107, 19<br/>3197, 45<br/>3107, 19<br/>3197, 45<br/>3107, 19<br/>3197, 45<br/>3107, 19<br/>3197, 45<br/>3107, 19<br/>3197, 45<br/>3107, 19<br/>3197, 45<br/>3107, 19<br/>3107, 19<br/>3107,</td><td>1-6 ¢ Submit Submit Adduct M+H M+H M+H M+H M+H M+H M+H M+H M+H M+H</td></tr> <tr><td>Workflow Submiss</td><td>Max Charge:</td><td>Scan ÷         I           sil me at         user           sil me at         user</td><td>Rexample.com Actaboli (+)-squalene-11 Angulnomycin-A beta-Citraurinol.g.*A. beta-Citraurinol.g.*G. Pristinamycin_JC, Vern 10-acetylicri 10-acetylicri tasfraidavide(158,<br/>Amychyle(158,<br/>Amychyle(158,<br/>Amychyle(158,<br/>Amychyle(151, Stage)) Ostrogoyrch. Skilland Ostrogoyrch. Skilland Protoce phakellist (5)-(-)-squalene 7,11-Cyclobotryooco Chalcomycin, Wyconon Actinomycin, X2, Actino designal</td><td>Frag<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011<br/>2011</td><td>Min<br/>gmentation<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td><td>MectAlass C           48.30           49.39           49.39           40.39           40.39           40.39           40.39           40.31           40.32           512.31           414.32           852.38           402.33           418.32           823.35           1036.50           1036.50           426.39           410.42           70.37           1268.61           586.31</td><td>spec.4.2 C</td><td>AT         I           Identificant:         12          
Ident</td><td>Adduct<br/>Submit<br/>Submit<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H</td></tr> | spec.MZ =<br>   | Att         -           Idic-Total):         6           Idic-Total):         7           Idic-Total):         7           Idi:         7  | Adduct *  |
Workflow Submiss | Max Charge:<br>sion<br>Email<br>Filename<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show | scan -             sil me at user           6867           7143           316           9377           516           9377           575 | Artabolt  Argunomycin-A beta-Citraurinol.g-N-A beta-Citraurinol.g-N | Frag | Min<br>gmentation<br>Score ()<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18 | Mactilians         Mactilians           426.39         512.31           434.32         510.22           852.38         448.24           410.28         738.28 | SpeckXZ C<br>SpeckXZ C<br>427.39<br>513.32<br>511.23<br>427.20<br>943.53<br>427.20<br>943.53<br>427.20<br>943.53<br>427.20<br>943.53<br>427.20<br>943.53<br>427.20<br>943.53<br>427.20<br>943.53<br>427.20<br>943.53<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20<br>427.20 | RT C Litic-Total J: 6 | 1-6 ¢           Submit           M+H           M+H | Workflow Submiss<br>d)<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary<br>AddtoGNPSLIbrary | Max Charge:<br>Ion Ema<br>Flienane C<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show | Scan = 1         Image: Scan = 1           sil me at user         Scan = 1           6667         7143           3148         3156           92777         5116           7576         5727           5728         5128 | Antaboli  (+)-squalene-1  Angulonycin-A  beta-Citraurinol; 8-A  antimyc Pristinamyc)_L/C; Vern 10-acetylircit "Azafrinaldehyde(58, Amych nona | Fray | Min<br>gmentation<br>Score C<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>- | MetMass -<br>426.39<br>510.22<br>510.22<br>52.31<br>510.22<br>52.38<br>942.52<br>418.24<br>410.28<br>718.28<br>418.24<br>410.28<br>718.28<br>418.24<br>410.28<br>718.28<br>470.34 | Ider a PSM as 5<br>aks: Linear-Cyc<br>SpecMZ C<br>H<br>427,39<br>513,32<br>513,32<br>513,33<br>511,23<br>427,20<br>943,53<br>403,54<br>419,24<br>411,29<br>729,29<br>471,35 | RT:<br>Idic-Total):<br>6<br>8<br>8<br>7<br>9<br>9<br>9<br>102<br>9<br>102<br>9<br>102<br>102<br>102<br>102<br>102<br>102<br>102<br>102 | Adduct 2<br>M+H<br>M+H<br>M+H<br>M+H<br>M+H<br>M+H<br>M+H<br>M+H | Workflow Submiss<br>d)<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary | Max Charge: | Scan ÷         I           sil me at user         -           Scan ÷         I           H         -           6667         7143           5132         3348           3376         90777           91777         5116           7576         5726           9175         5128           4872         - | Rexample.com Actaboli (+)-squalene-10 Anguinomycin-A beta-Citrauriou, 8-A antimyc Pristinamycin, JC, Vern Soyasap 4,4-Diaponeurosporen 10-acetylircit razafrinaldryder (58,<br>Amychyder (58,<br>Amychyder (58, Amychyder (58, Amychyddia)))) | Frag<br>20<br>21<br>21<br>21<br>22<br>23<br>24<br>25<br>24<br>25<br>24<br>25<br>24<br>25<br>24<br>25<br>25<br>25<br>25<br>25<br>25<br>25<br>25<br>25<br>25 | Min<br>gmentation<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>- | Methass 2         A           40.3         3           41.3         3 | Ider a PSM as 5<br>aks: Linear-Cyc<br>sec. 12<br>47, 39<br>513, 32<br>47, 20<br>943, 53<br>511, 23<br>403, 34<br>403, 34<br>419, 24<br>411, 29<br>419, 23<br>419, 33 | HT         I           III         -         -           III         -         -         -           III         -         -         -         -           IIII         -          - | Adduct - | Workflow Submiss<br>d)<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary<br>AddtoGNPSLibrary | Max Charge:<br>sion Ema Show Show Show Show Show Show Show Show | Scan -           -           sil me at user         -           6867         -           7143         -           3346         -           93777         -           516         -           93777         -           512         -           3346         -           93777         -           512         -           3346         -           93777         -           5128         -           4972         -           9372         - | Pristinamycin_LC; Vern Yraziniaidenyde; SR, Ar-Diaponurospore 10-acetylioriol Yazafrinaidenyde; SR, Armoh beta-Citararinene; JF: Virginiamycin_S1; Stap | Frag | Min<br>gmentation<br>Score ()<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>17<br>17<br>17<br>17<br>17<br>17<br>17 | Matthens         Anatomic           48.39         512.31           434.32         510.22           852.33         418.24           402.8         702.34           418.24         823.35           823.35         823.35 | SpeckXZ C<br>SpeckXZ
C<br>427,39<br>513,32<br>427,20<br>940,53<br>427,20<br>940,53<br>427,20<br>940,53<br>427,20<br>940,53<br>427,20<br>940,53<br>427,20<br>940,53<br>427,20<br>940,53<br>427,20<br>940,53<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>941,55<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,20<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35 | RT C<br>H<br>H<br>S487, 38<br>3709, 99<br>4076, 73<br>2946, 52<br>437, 73<br>3458, 13<br>3459, 14<br>319(2), 52<br>1049, 55<br>4074, 43<br>3991, 14<br>319(2), 52<br>1049, 55<br>4074, 43<br>3091, 38 | Adduct * | Workflow Submiss | Max Charge:<br>Max Charge:<br>Fliename :<br>Fliename 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| Scan +         I           sil me at         user           Scan +         I           B         -           6867         7143           31346         3316           3277         5716           5727         572           6727         5128           4872         3227           2757         2257 | Rexample.com Metaboli (+)-squalene-11 Anguinomycin-A beta-Citraurino(:, 8-A antimyc Pristinamycin_UC, Yern Systapa 4.4'-Diaponeurosporei 10-acetylicrif "Azafrinaldehyde;(SR,<br>Amych beta-Citraurinet;, 8-Yinghiamycin-51, Stag beta-Citraurinet;, 8-Yinghiamycin-51, Stag Ostreogrycin, A.; Miami | Frag | Min<br>gmentation | MetMass -<br>426.39<br>426.39<br>424.31<br>42.31<br>42.31<br>42.31<br>42.32<br>42.32<br>42.32<br>42.23<br>418.24<br>410.28<br>470.24<br>418.23<br>418.24<br>410.28<br>470.34<br>418.32<br>552.25<br>552.25 | Speckiz C<br>+ 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| KT C           -         - <tr td=""> <tr td=""> <tr td=""></tr></tr></tr> | Adduct :<br>MoH<br>MoH<br>MoH<br>MoH<br>MoH<br>MoH<br>MoH<br>MoH | Workflow Submiss | Max Charge: | scan ÷         1           sll me at         user           sll me at         user | Control Contr | Frag | Min<br>gmentation<br>Score ()<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>- |
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8-A<br/>antimyc<br/>Pristinamycin, JC; Ven<br/>10-acetylicci<br/>*Azafrinadetyde(SR,<br/>Amych<br/>Virginiamycin-51; Stap<br/>Virginiamycin-51; Stap<br/>Virginiamycin-51; Stap<br/>Stareogrycin, A; Mikam<br/>Phrotoce<br/>phakellist<br/>(5)-(-)-squalene<br/>2: 15-(-)-squalene</td> <td>Frag</td> <td>Min<br/>gmentation<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td> <td>MetMass         Construction           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:00000         -         -           9:00000         -         -           9:000000         -         -           9:000000000         -         -           9:000000000000000000000000000000000000</td> <td>Spec.M.Z =<br/>Spec.M.Z =<br/>427.39<br/>513.32<br/>435.33<br/>511.23<br/>403.34<br/>419.24<br/>411.29<br/>419.33<br/>427.20<br/>141.29<br/>419.33<br/>427.20<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.</td> <td>Att         12           Lile-Total]s:         6           Lile-Total]s:         6           Statistics         6           Jane Statistics         7           Jane Statistics         7      &lt;</td> <td>Adduct -<br/>Submit<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H</td> | Antaboli<br>(+)-squalene-11<br>Anguinomycin-A<br>beta-Citraurinol; 8-A<br>antimyc<br>Pristinamycin, JC; Ven<br>10-acetylicci<br>*Azafrinadetyde(SR,<br>Amych<br>Virginiamycin-51; Stap<br>Virginiamycin-51; Stap<br>Virginiamycin-51; Stap<br>Stareogrycin, A; Mikam<br>Phrotoce<br>phakellist<br>(5)-(-)-squalene<br>2: 15-(-)-squalene | Frag | Min<br>gmentation<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>- | MetMass         Construction           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000   
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8-A         antimyc     Pristinamycin_JC; Vem         Soyasap         Ar-Diaponeurosporer         10-acetylirci         T-azafrinaldetyde;(58,         Amych         beta-Citraurinene; 8-         Virginiamycin-51; Stag         Ostroopycin.4: "Miam         Prorocei         phakelilis         (5)-(-)-squalene         7.11-cyclobotryococ         Chalcomperies.Mecmonic | Frag | Min<br>gmentation<br>Score ©<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18<br>18 | MetMass         MetMass           426.39         512.31           434.32         510.23           434.32         510.23           434.32         510.23           418.24         418.24           418.28         832.35           523.35         525.23           418.24         418.24           418.28         833.35           510.54.50         448.35           418.44         418.32           414.42         20.33 | Ider a PSM as 5<br>aks: Linear-Cyc<br>saks: Linear-Cyc<br>saks: 2<br>427,39<br>427,30<br>427,20<br>447,33<br>427,20<br>443,31<br>427,20<br>443,31<br>427,20<br>443,31<br>411,29<br>427,39<br>427,39<br>427,39<br>427,35<br>429,26<br>427,39<br>427,35<br>429,26<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,35<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>427,45<br>45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,45<br>45,4545,45<br>45,45<br>45,45<br>45,4545,45<br>45,45<br>45,45<br>45,45<br>45,45 | RT -<br>ILIC-TotalJ: 6<br>ILIC-TotalJ: 6 | Adduct = | Workflow Submiss | Max Charge:<br>Max Charge:<br>Max Charge:<br>Email<br>Email<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show<br>Show | Scan +         I           sill me at         user           sill me at         user           Scan +         I           6667         7143           7143         3346           3316         907177           5716         5775           572         5775           572         3900           5007         6554           5485         100731* | Sexample.com<br>Metaboli<br>(+)-squalene-II<br>Anguinomycin-A<br>beta-Citraurinot,:::-A-<br>antimyc<br>Pristinamycin_JC; Vern<br>Soyaspa<br>4,6-Daponeurosporen<br>10-acetylicti<br>"Azafrinaldehyde (SR,<br>Amych<br>nonan<br>beta-Citraurinem;<br>Virginiamycin_S1; Stap<br>Ostreogrycin, A:, Mikam<br>Proroce<br>phakellist<br>(S)-(-)-squalene<br>7,11-Cyclostrycoco<br>Chalcomycin; Wyconom | Frag<br>b: 1<br>c: 1<br>c: 2<br>c: 2 | Min<br>gmentation<br>Score C<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>- | MetMass         Construction           HetMass         H           426.39         H           510.22         B52.38           942.53         402.33           418.24         410.28           173.82.8         470.34           418.32         515.25           488.35         1036.50           426.39         416.42           700.37         1268.41 | Speck82 C<br> | RT C<br>FT Cotal J: 6<br>5467, 28<br>3709, 99<br>4076, 73<br>2998, 03<br>2467, 52<br>937, 17<br>3488, 83<br>3891, 14<br>3190, 52<br>1049, 55<br>4074, 43<br>3904, 38<br>2207, 40<br>3876, 45<br>3060, 14<br>4687, 25<br>5107, 91<br>3194, 45<br>3107, 19<br>3197, 45<br>3107, 19<br>3197, 45<br>3107, 19<br>3197, 45<br>3107, 19<br>3197, 45<br>3107, 19<br>3197, 45<br>3107, 19<br>3197, 45<br>3107, 19<br>3107, | 1-6 ¢ Submit Submit Adduct M+H | Workflow Submiss | Max Charge: | Scan ÷         I           sil me at         user           sil me at         user | Rexample.com Actaboli (+)-squalene-11 Angulnomycin-A beta-Citraurinol.g.*A. beta-Citraurinol.g.*G. Pristinamycin_JC, Vern 10-acetylicri 10-acetylicri tasfraidavide(158,<br>Amychyle(158,<br>Amychyle(158,<br>Amychyle(158,<br>Amychyle(151, Stage)) Ostrogoyrch. Skilland Ostrogoyrch. Skilland Protoce phakellist (5)-(-)-squalene 7,11-Cyclobotryooco Chalcomycin, Wyconon Actinomycin, X2, Actino designal |
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Amychyddia))))  | Frag<br>20<br>21<br>21<br>21<br>22<br>23<br>24<br>25<br>24<br>25<br>24<br>25<br>24<br>25<br>24<br>25<br>25<br>25<br>25<br>25<br>25<br>25<br>25<br>25<br>25   | Min<br>gmentation<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-                                | Methass 2         A           40.3         3           41.3         3   
   
   
   
   
   
   
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   | HT         I           III         -         -           III         -         -         -           III         -         -         -         -           IIII         -          -  | Adduct -  |                  |  |   |   |      |   |   | | | | | | | | | | | | | | | | | | | | |
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  | Ider a PSM as 5<br>aks: Linear-Cyc<br>aks: Linear-Cyc<br>   | Itic-TotalJ: 6     Itic-TotalJ: 7     Itic-To  | Adduct *  |                  |  |   | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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  | Min<br>gmentation<br>Score ©<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-                     | MetMoss         C           40,000         - <t< td=""><td>SpocM2 C<br/></td><td>RT C<br/>HT C<br/>H</td><td>Adduct *</td></t<>  
   
   
   
   
   
   
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| Workflow Submiss   | Max Charge:  | Scan 0         Image: Scan 0 </td <td>Antaboli<br/>(+)-squalene-11<br/>Anguinomycin-A<br/>beta-Citraurinol; 8-A<br/>antimyc<br/>Pristinamycin, JC; Ven<br/>10-acetylicci<br/>*Azafrinadetyde(SR,<br/>Amych<br/>Virginiamycin-51; Stap<br/>Virginiamycin-51; Stap<br/>Virginiamycin-51; Stap<br/>Stareogrycin, A; Mikam<br/>Phrotoce<br/>phakellist<br/>(5)-(-)-squalene<br/>2: 15-(-)-squalene</td> <td>Frag</td> <td>Min<br/>gmentation<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-<br/>-</td> <td>MetMass         Construction           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           40:000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:0000         -         -           9:00000         -         -           9:00000         -         -           9:000000         -         -           9:000000000         -         -           9:000000000000000000000000000000000000</td> <td>Spec.M.Z =<br/>Spec.M.Z =<br/>427.39<br/>513.32<br/>435.33<br/>511.23<br/>403.34<br/>419.24<br/>411.29<br/>419.33<br/>427.20<br/>141.29<br/>419.33<br/>427.20<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.42<br/>435.</td> <td>Att         12           Lile-Total]s:         6           Lile-Total]s:         6           Statistics         6           Jane Statistics         7           Jane Statistics         7      &lt;</td> <td>Adduct -<br/>Submit<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H<br/>M-H</td> | Antaboli<br>(+)-squalene-11<br>Anguinomycin-A<br>beta-Citraurinol; 8-A<br>antimyc<br>Pristinamycin, JC; Ven<br>10-acetylicci<br>*Azafrinadetyde(SR,<br>Amych<br>Virginiamycin-51; Stap<br>Virginiamycin-51; Stap<br>Virginiamycin-51; Stap<br>Stareogrycin, A; Mikam<br>Phrotoce<br>phakellist<br>(5)-(-)-squalene<br>2: 15-(-)-squalene  | Frag   
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| Workflow Submiss   | Max Charge:  | scan :                     sill me at         useri   | Actaboli     (+)-squalene-1(         Anguinomycin-A         Anguinomycin-A         Anguinomycin-A         beta-Citraurinol.; 8-A         antimyc     Pristinamycin_JC; Vem         Soyasap         Ar-Diaponeurosporer         10-acetylirci         T-azafrinaldetyde;(58,         Amych         beta-Citraurinene; 8-         Virginiamycin-51; Stag         Ostroopycin.4: "Miam         Prorocei         phakelilis         (5)-(-)-squalene         7.11-cyclobotryococ         Chalcomperies.Mecmonic  
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**Supplementary Figure 1:** Running DEREPLICATOR+ on the GNPS web server. (a) Image of the GNPS web page at www.gnps.edu. DEREPLICATOR+ users click on "Browse" in the section "GNPS Theoretical/Insilico" (b) At "DEREPLICATOR+, Identification of Metabolites Through Database Search of Mass Spectra" section, users click on "here". (c) To select input files, users click on "Select Input Files". Users can either import one of the existing GNPS public datasets from the "Share Files" section, or use their own data from "Upload Files" section. Users select a title/email for the job and specify the DEREPLI-CATOR+ accuracy mode (precursor and fragment ion mass tolerances). Users receive a notification email after the job is completed. (d) When the job is completed, users click on "View Significant Matches" to see all the identifications. Further guidelines and information on using DEREPLICATOR+ are available at: "https://bix-lab.ucsd.edu/display/Public/Insilico+Natural+Products+Dereplicator+Documentation"

. The search results for Spectra<sub>ActiSeq</sub>, Spectra<sub>Cyan</sub>, and Spectra<sub>Lichen</sub> are available at "https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=5ea18d0c3b1d4018b7e0e79445ca8c18", "https://gnps.ucsd.edu/ProteoSAFe/result.jsp?task=95ebc1c169654d838c41df41cc24f88a", and "https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=00c03bdbdae644e4935a8e094f249c2a" respectively.



**Supplementary Figure 2:** DEREPLICATOR p-values versus DEREPLICATOR+ p-values. Peptides are shown in black, lipids in blue and polyketides in red.



**Supplementary Figure 3:** Dereplicator+ annotation of arylomycin and antrimycin spectra. (a) Arylomycin mass spectra, (b) annotation of arylomycin mass spectra, (c) antrimycin mass spectra, and (d) annotation of antrimycin mass spectra. DEREPLICATOR annotations (amide bonds at depth 1) are shown in red, DEREPLICATOR-G annotations (general bonds at depth 1) are shown in green, DEREPLICATOR-PEP-FG annotations (amide bonds, depth 2 or more) are shown in light blue, DEREPLICATOR+ annotations (general bonds, depth 2 or more) are shown in light blue, DEREPLICATOR+ annotations (general bonds, depth 2 or more) are shown in dark blue. In case of Arylomycin we have 5 DEREPLI-CATOR annotations, and 6 more DEREPLICATOR-G annotations (total score 11). In case of antrimycin we have 5 DEREPLICATOR annotations, 3 DEREPLICATOR-PEP-FG annotations, 3 DEREPLICATOR-G annotations, 3 DEREPLICATOR-G annotations, 3 DEREPLICATOR-G annotations, 4 an



**Supplementary Figure 4:** Dereplicator+ identification of salinamide matches GNPS spectral library. (a) Spectra of salinamide identified by DEREPLICATOR+ in Spectra<sub>ActiSeq</sub>. (b) Spectra of Salinamide from GNPS spectral library.



**Supplementary Figure 5:** Annotation of almiramide biosynthetic gene cluster. (a) Putative almiramide biosynthetic gene cluster starts with a PKS domain and consists adenylation domains encoding a (methylated) phenylalaline, an alaline, a (methylated) alanine, and a (methylated) phenylalaline. (b) The structure of almiramide B.



Supplementary Figure 6: Distribution of the masses for 5336 identifications from whole GNPS.



Supplementary Figure 7: The histograms of experimental and theoretical spectra of Pricestantering Pricestant



**Supplementary Figure 8:** Generating decoy fragmentation graph. For each target fragmentation graph, DEREPLICATOR+ generate a decoy fragmentation graph with the same structure and assigns masses to its nodes in a breadth-first manner as follows. The mass of the root is equal to the total mass of the metabolite, and for each node v, DEREPLISCATOR+ samples mass(v) from the range [0, mass(Parent(v))] of the distribution of all theoretical peaks, where Parent(v) is the parent of node v.



Supplementary Figure 9: Computing the statistical signicance of MSMs. Figure shows a depth-1 fragmentation graph with three peaks at masses 400.0, 500.0 and 800.0. For each peak with mass m, the probability p(m) that a random experimental peak sampled from range [0, M] of the experimental distribution annotates peak m within tolerance  $\delta$  can be computed as  $p(m) = F(m - \delta, m + \delta)$ .



**Supplementary Figure 10:** The molecular networks of the chalcolmycin family. (a) Chalcomycin (shown in yellow) is identied by DEREPLICATOR+. Novel chalcomycin variants are shown in green. Mass spectra of (b) chalcomycin, (c) chalcomycin variant with mass 687, (d) chalcomycin variant with mass 731, (e) chalcomycin variant with mass 699. *CH*2 stands for methylation/demethylation mass difference.

## SUPPLEMENTARY TABLES

Supplementary Table 1. Information about spectral datasets.

dataset	number of spectra	GNPS IDs
$Spectra_{GNPS}$	$\approx 248,000,000$	548 datasets
$Spectra_{Fungi}$	2475907	MSV000079098
$Spectra_{Acti}$	5598651	MSV000078787, MSV000078936, MSV000078937, MSV000078836, MSV000078839
$Spectra_{Pseu}$	3529556	MSV000078803, MSV000078817, MSV000078635, MSV000078606
$Spectra_{Cvan}$	11921457	MSV000078568
$Spectra_{Acti-seq}$	178635	MSV000078604, MSV000078839
$Spectra_{Lichen}$	926864	MSV000078584
$\operatorname{Spectra}_{\operatorname{library}}$	5473	-

most similar gene	coverage	identity	length
lipid-A-disaccharide synthase	64%	77%	645
cobaltochelatase CobN subunit	100%	86%	1330
serine/threonine protein kinase	92%	73%	284
jamJ	95%	77%	1336
jamJ	98%	72%	383
tubC protein	99%	46%	1545
PuwG	94%	55%	1135
tubC protein	99%	45%	1546
$\operatorname{CrpC}$	64%	57%	2303
2-hydroxy-6-oxohepta-2,4-dienoate hydrolase	100%	100%	293
methyltransferase	100%	100%	243
LmbE-like protein	96%	63%	279
glycosyltransferase	100%	99%	694

**Supplementary Table 3.** The most frequent atoms in all metabolites from the AntiMarin database.  $freq_{marin}$  and  $freq_{terres}$  stand for frequencies of different atoms within marine and terrestrial compounds.

atom	frequency	$freq_{marin}$	$fereq_{terres}$
Η	2272193(51.7%)	217513(51.7%)	2054680(51.7%)
С	1597940(36.3%)	153866(36.6%)	1444074(36.3%)
0	400204(9.1%)	37804(8.8%)	362400(9.1%)
Ν	97945(2.2%)	8403(1.9%)	89542(2.2%)
$\mathbf{S}$	8151(0.2%)	842(0.2%)	7309(0.2%)
$\operatorname{Br}$	8002(0.2%)	1403(0.3%)	6599(0.2%)
Cl	6195(0.2%)	824(0.2%)	5371(0.2%)

Supplementary Table 4. The most frequent bonds in all metabolite structures from the AntiMarin database.  $freq_{marin}$  and  $freq_{terres}$  stand for frequencies of different bonds within marine and terrestial compounds.

bond	frequency	$freq_{marin}$	$freq_{terres}$
C-H	2050594(45.4%)	196820(45.6%)	1853774(45.4%)
C-C	1283757(28.4%)	121283(28.1%)	1162474(28.4%)
C-O	356218(7.8%)	34168(7.9%)	322050(7.8%)
C=C	222100(4.9%)	23698(5.4%)	198402(4.9%)
C-N	183013(4.0%)	16505(3.8%)	166508(4.0%)
C=O	140625(3.1%)	11868(2.7%)	128757(3.1%)
O-H	138568(3.0%)	14552(3.3%)	124016(3.0%)
N-H	82728(1.8%)	6130(1.4%)	76598(1.8%)
C=N	11747(0.2%)	1109(0.2%)	10638(0.2%)
C-S	9179(0.2%)	998(0.2%)	8181(0.2%)
C-Br	7998(0.1%)	1403(0.3%)	6595(0.1%)
C-Cl	6191(0.1%)	824(0.1%)	5367(0.1%)
S=O	5007(0.1%)	447(0.1%)	4560(0.1%)

#### SUPPLEMENTARY NOTES

## Supplementary Note 1. Datasets.

MSV000078839 dataset. 36 strains of Streptomyces were grown on A1, MS and R5 agar, extracted sequentially with ethyl acetate, butanol and methanol, and analyzed on Agilent 6530 Accurate-Mass Q-TOF spectrometer coupled to a C18 RP Agilent 1260 LC system (ESI ionization, CID fragmentation).

MSV000078604 dataset. 16 strains of Streptomyces were grown on ISP2 agar plates, extracted by butanol, and analyzed on LTQ Orbitrap Velos coupled to a C18 RP Agilent 1200 LC system (ESI ionization, HCD fragmentation).

MSV000078568 dataset. A total of 317 cyanobacterial collections were extracted repetitively with CH2Cl2:MeOH 2:1, dried in vacuo, and fractionated into nine fractions (A-I) by silica gel vacuum liquid chromatography (VLC) using a stepwise gradient of hexanes/EtOAc and EtOAc/MeOH, and analyzed on a Maxis Impact mass spectrometer coupled to C18 RP-UHPLC (ESI ionization, CID fragmentation).

MSV000078584 dataset. Metabolites from 110 spots of lichen were extracted with 4:1 ethyl acetate-methanol and 0.1% trifluoroacetic acid (TFA), and analyzed on Maxis Q-TOF mass spectrometer (Bruker Daltonics) coupled to a C18 RP UltiMate 3000 UHPLC (ESI ionization, CID fragmentation).

## Supplementary Note 2. Further analysis of $\operatorname{Spectra}_{\operatorname{ActiSeq}}$ dataset.

We divided Spectra<sub>ActiSeq</sub> into two parts, Spectra<sub>ActiSeq-CID</sub> consisting of 473135 spectra from MSV000078839 dataset and Spectra<sub>ActiSeq-HCD</sub> consisting of 178635 spectra from MSV000078604 dataset. DEREPLICATOR+ identified 2979 spectra (129 compounds) in Spectra<sub>ActiSeq-CID</sub> and 5215 spectra (404 compounds) in Spectra<sub>ActiSeq-HCD</sub>. 45 compounds are found in both CID and HCD datasets. Supplementary Data 1 shows compounds discovered in CID and HCD spectra at 1% FDR.

To evaluate whether DEREPLICATOR+ incorrectly identifies common mass spectrometry contaminants as natural products, we performed an evaluation of the masses of 760 contaminants from Keller et al.

Among these 760 masses, 319 are present at 0.02Da threshold in Spectra<sub>ActiSeq</sub>. However, only m/z 1020.50 (bovine trypsin) identified by DEREPLICATOR+ and reported as Salinamide A at 1% FDR (Supplementary Data 3). We manually confirmed that spectra at m/z 1020.50 is indeed Salinamide A and not a contaminant (Supplementary Figure 4).

DEREPLICATOR+ search of Spectra<sub>ActiSeq</sub> against AntiMarin, HMDB, LipidMaps, DNP, DrugBank, GNPS spectral library, KEGG, MiBIG, StreptomeDB, and UNPD identified 539 compounds at 1% FDR (Supplementary Data 4).

#### Supplementary Note 3. Further analysis of Spectra<sub>library</sub> dataset.

Compounds in Spectra<sub>Library</sub> have on average 8 isomers with identical chemical formula in DNP. Among 4360 compounds (80%) of Spectra<sub>Library</sub>, which have at least one other isomer in the DNP database, DEREPLICATOR+ correctly identified 1746 (40%) of compounds (Supplementary Data 6).

To assess the capability of DEREPLICATOR+ in identifying adducts, we searched 1207 annotated spectra with sodium/potassium adducts from the GNPS spectral library using DEREPLI-CATOR+, and 280 (23%) of them were correctly identified at 1% FDR, while 23 (2%) were falsely identifies as a non-adduct compounds (Supplementary Data 8).

To assess the capability of DEREPLICATOR+ in identifying compounds in the negative ionization modes, we analyzed 341 additional spectra in the GNPS spectral library collected in the ESI (-) mode. DEREPLICATOR+ search correctly identified 88 (26%) of these compounds as top predictions (Supplementary Data 9).

Supplementary Note 4. Fragmentation model selection. To evaluate the rationality of the rules and thresholds in the fragmentation model, we compared 14 fragmentation models with various parameters used in conditions (i)-(iv). The comparison is based on the log-likelihood of these models in explaining the experimental spectrum (in comparison to the null model) over a set of 5473 Metabolite-Spectrum Matches (MSMs) from the Spectra<sub>library</sub> dataset. The models differ from each other in the chemical bonds they fragment, the maximum number of bridges and 2-cuts they allow, and whether or not they allow for the breakage of C-C 2-cuts and multiple C-C bridges.  $\#Max_L$  stands for the maximum number of bridge fragmentations allowed.  $\#Max_C$  stands for the maximum number of the 2-cut fragmentations allowed.  $#Max_{2L+C}$  is an upper-bound on twice the number of 2-cuts plus the number of bridges (i.e. total number of cuts in the fragmentation).  $theo_{ef}$  stands for the size of the effective theoretical spectrum of a MSM, defined as peaks in the theoretical spectrum with annotated parents (the root is always annotated). e stands for the number of explained peaks in the experimental spectrum. For a specific model  $\theta$ ,  $p_{\theta}$  stand for the probability of a peak in the effective theoretical spectrum being explained by the model. The null hypothesis assumes peaks are explained independent of the theoretical spectrum, with a constant probability  $p_{null}$ . LL stands for log-likelihood, defined as the log-ratio of the probability of the match under the model, to that of the match under the null hypothesis.

Given a set L MSMs  $(M_1, S_1), \dots, (M_L, S_L)$ , the log-likelihood score LL for a model  $\theta$  is defined as :

$$LL_{\theta} = \sum_{t=1}^{L} LL_{\theta}(M_t, S_t) \tag{1}$$

where

$$LL_{\theta}(M,S) = \log \frac{p_{\theta}(M,S)}{p_{null}(M,S)} = e * \log \frac{p_{\theta}}{p_{null}} + (theo_{ef} - e) * \log \frac{1 - p_{\theta}}{1 - p_{null}}$$
(2)

Parameters  $p_{\theta}$  is approximated as the probability that a peak in the effective theoretical spectra is explained by a peak in the corresponding theoretical spectra, while  $p_{null}$  is approximated as the probability that a peak in the effective theoretical spectra is explained by a peak in a random spectra.

Supplementary Data 14 shows that addition of the OC and CC bonds increased the log-likelihood score from 7051 to 16054. From depth one to two, the log-likelihood score increased from 16054 to 27121. From depth two to depth three, the log-likelihood score increased from 27121 to 29888. At depth three, allowing for breakage of CC 2-cuts bonds or multiple CC bridges decreased the log-likelihood by 8% (from 29888 to 27565). Increasing the depth from 3 to 6 increased the log-likelihood from 29888 to 32394. Allowing for more than a single 2-cut breakage at depth 6 decreased the log-likelihood by a factor of 3% (from 32394 to 31404). Further increasing the depth from 6 to 9 hardly improved the log-likelihood (from 32394 to 32401). Our results show that, for condition (i), the optimal value of k is 6, and conditions (ii), (iii) and (iv) are crucial to maintain a fragmentation graph consistent with mass spectrometry fragmentation.