

## Supplementary Information

### Untargeted Mass Spectrometry for Investigating Ocean Acidification in *Cancer borealis* Using Optimized Metabolite Extraction Methods

Yunxiao Yao<sup>1</sup>, Olga Riusech<sup>1</sup>, Shuling Xu<sup>2</sup>, Lingjun Li<sup>\*1,2,3,4</sup>

<sup>1</sup> Department of Chemistry, University of Wisconsin, Madison, WI, USA

<sup>2</sup> School of Pharmacy, University of Wisconsin, Madison, WI, USA

<sup>3</sup>Lachman Institute for Pharmaceutical Development, School of Pharmacy, University of Wisconsin-Madison,  
Madison, WI 53705, USA

<sup>4</sup>Wisconsin Center for NanoBioSystems, School of Pharmacy, University of Wisconsin-Madison, Madison, WI  
53705, USA

**\*Corresponding author:** Lingjun Li

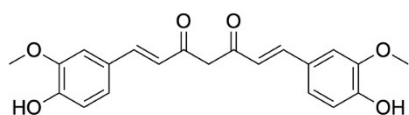
**Post address:** 777 Highland Ave, Madison, Wisconsin, United States

**ZIP Code:** 53705

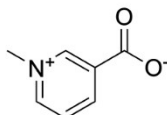
**Email:** lingjun.li@wisc.edu

**Tel:** +1 608-265-8491

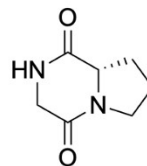
**Fax:** +1 608-262-5345



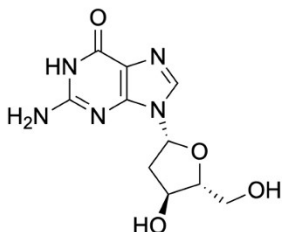
Curcumin (CID: 9690516)



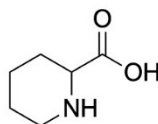
Trigonelline (CID: 5570)



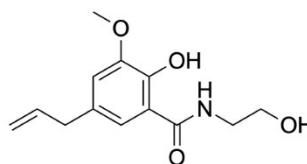
Cyclopropylglycine (CID:126154)



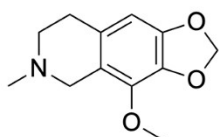
Deoxyguanosine (CID:135398592)



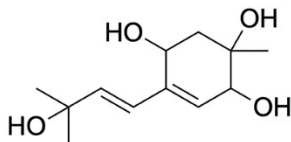
Pilocarpic acid (CID:849)



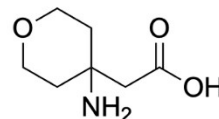
Alibendol (CID:71916)



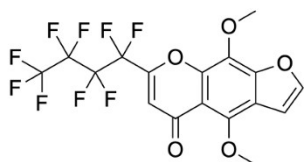
Hydrocotarnine (CID:3646)



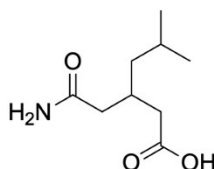
Acremin F (CID:23846553)



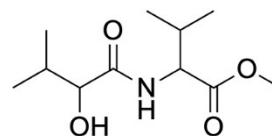
2-(4-aminotetrahydro-2H-pyran-4-yl)acetic acid (CID18379269)



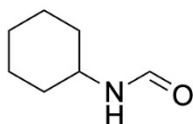
4,9-dimethoxy-7-(perfluorobutyl)-5H-furo[3,2-g]chromen-5-one (CID:1789495)



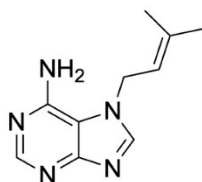
3-(2-amino-2-oxoethyl)-5-methyl-hexanoic acid (CID10867083)



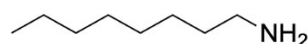
methyl 2-[(2-hydroxy-3-methylbutanoyl)amino]-3-methylbutanoate (CID102571591)



N-Cyclohexylformamide (CID:13017)



Triacanthine (CID:10625)



Octylamine (CID:8143)

19

20 **Supplementary Figure 1.** Molecular structures and PubChem Compound IDs (CIDs) of significantly  
21 altered metabolites identified after 4-hour ocean acidification (OA) exposure.