

**Supporting Information**  
**Visualization and Identification of Neurotransmitters in**  
**Crustacean Brain via Multifaceted Mass Spectrometric**  
**Approaches**

**Qinjingwen Cao<sup>1</sup>, Yijia Wang<sup>2</sup>, Bingming Chen<sup>3</sup>, Fengfei Ma<sup>3</sup>, Ling Hao<sup>3</sup>, Gongyu Li<sup>3</sup>,**  
**Chuanzi Ouyang<sup>1</sup>, Lingjun Li<sup>1,3\*</sup>**

*<sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, 1101 University Avenue, Madison, Wisconsin, 53706, United States*

*<sup>2</sup>Department of Chemical Physics, School of Chemistry and Materials Science, University of Science and Technology of China, 96 Jinzhai Road, Hefei, Anhui, 230026, China*

*<sup>3</sup>School of Pharmacy, University of Wisconsin-Madison, 777 Highland Avenue, Madison, Wisconsin, 53705, United States*

**\*Corresponding author**

Tel.: (608) 265-8491

Fax: (608) 262-5345

E-mail: lingjun.li@wisc.edu

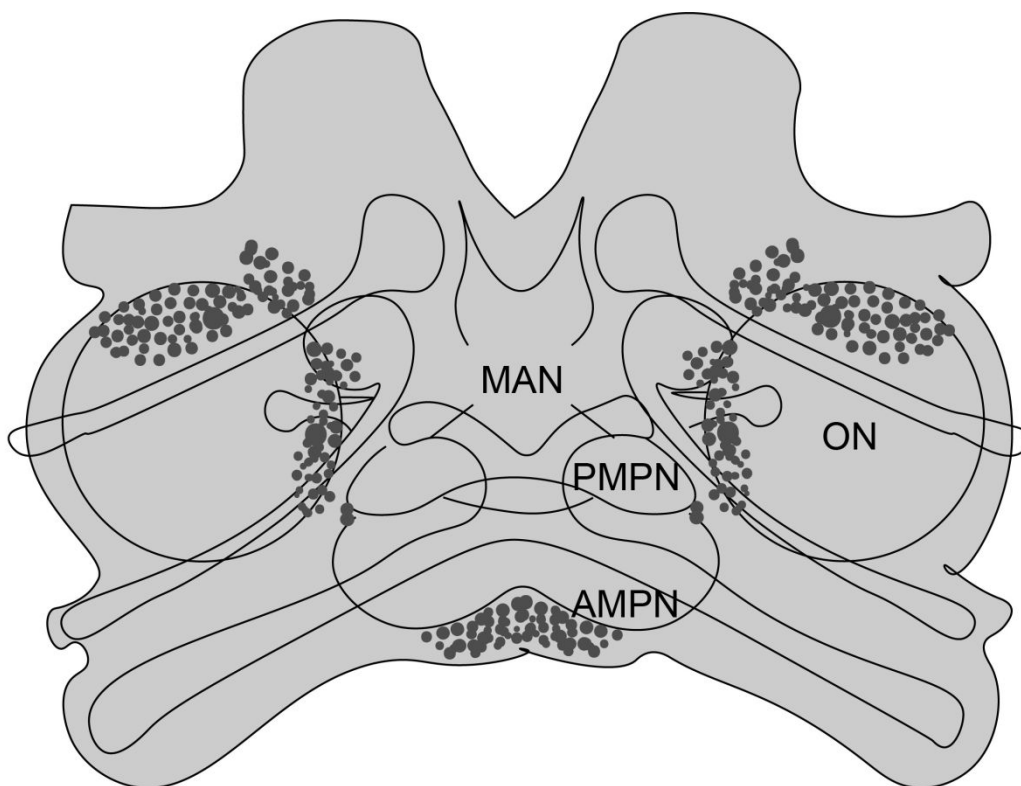
**Table S1.** Neurotransmitters and metabolites identified from crab brain tissue via HRAM MALDI-LTQ-Orbitrap XL platform

(a) Comparison of theoretical and detected  $m/z$  values in derivatized crab brain tissue

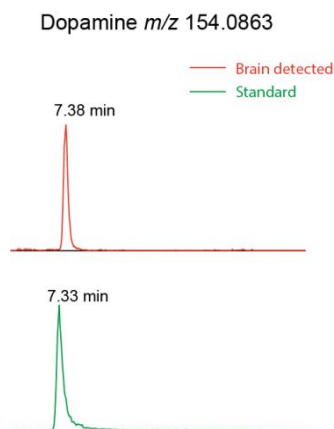
Compound	Theoretical $m/z$	Detected $m/z$	Error (ppm)
Glycine+DPP <sup>+</sup>	290.1176	290.1175	-0.2
Alanine+DPP <sup>+</sup>	304.1332	304.1332	-0.1
GABA+DPP <sup>+</sup>	318.1489	318.1488	-0.2
Histamine+DPP <sup>+</sup>	326.1652	326.1650	-0.6
Proline+DPP <sup>+</sup>	330.1489	330.1489	0.2
Threonine+DPP <sup>+</sup>	334.1438	334.1435	-0.9
Phenethylamine+DPP <sup>+</sup>	336.1747	336.1745	-0.6
Taurine+DPP <sup>+</sup>	340.1002	340.0999	-0.9
3-Methylhistamine+DPP <sup>+</sup>	340.1808	340.1806	-0.7
Agmatine+DPP <sup>+</sup>	345.2074	345.2073	-0.3
Adenine+DPP <sup>+</sup>	350.1400	350.1400	-0.1
Tyramine+DPP <sup>+</sup>	352.1696	352.1695	-0.3
Lysine+DPP <sup>+</sup>	361.1911	361.1908	-0.8
Dopamine+DPP <sup>+</sup>	368.1645	368.1642	-0.9
Tryptamine+DPP <sup>+</sup>	375.1856	375.1851	-1.3
Phenylalanine+DPP <sup>+</sup>	380.1645	380.1641	-1.1
Serotonin+DPP <sup>+</sup>	391.1805	391.1811	1.6
Dopa+DPP <sup>+</sup>	412.1543	412.1538	-1.3
Biopterin+DPP <sup>+</sup>	452.1717	452.1719	0.5
Adenosine+DPP <sup>+</sup>	482.1823	482.1820	-0.6

(b) Comparison of theoretical and detected  $m/z$  values in non-derivatized crab brain tissue

Compound	Theoretical $m/z$	Detected $m/z$	Error (ppm)
Choline	104.1070	104.1068	-1.8
Acetylcholine	146.1176	146.1175	-0.4
Carnitine+H <sup>+</sup>	162.1125	162.1124	-0.5
Arginine+H <sup>+</sup>	175.1190	175.1191	0.9
Phosphocholine	184.0733	184.0734	0.6
N6,N6,N6-Trimethyl-lysine+H <sup>+</sup>	189.1598	189.1596	-0.9
Arginine+Na <sup>+</sup>	197.1009	197.1010	0.6
Acetyl-carnitine+H <sup>+</sup>	204.1230	204.1230	-0.2



**Figure S1.** Illustration of a crab brain from the dorsal view. Main structures are revealed, including olfactory lobes (ON), median antenna I neuropil (MAN), anterior medial protocerebral neuropil (AMPN) and posterior medial protocerebral neuropil (PMPN).



**Figure S2.** Identification of dopamine by matching ion  $m/z$  154.0863 retention time with dopamine standard. Top panel: extracted ion chromatogram (EIC) of dopamine ( $m/z$  154.0863) from crab brain extract; bottom panel: EIC of dopamine ( $m/z$  154.0863) from purchased standard compound.

## **References:**

Sandeman, David, et al. "Morphology of the brain of crayfish, crabs, and spiny lobsters: a common nomenclature for homologous structures." *The Biological Bulletin* 183.2 (1992): 304-326.