# Supplementary Files

# Application of $^{1}$H HR-MAS NMR-based metabolite fingerprinting of marine microalgae

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†This work is dedicated to the memory of our dear colleague and mentor, Professor Paulo Cesar Abreu, who passed away on July 19, 2022.

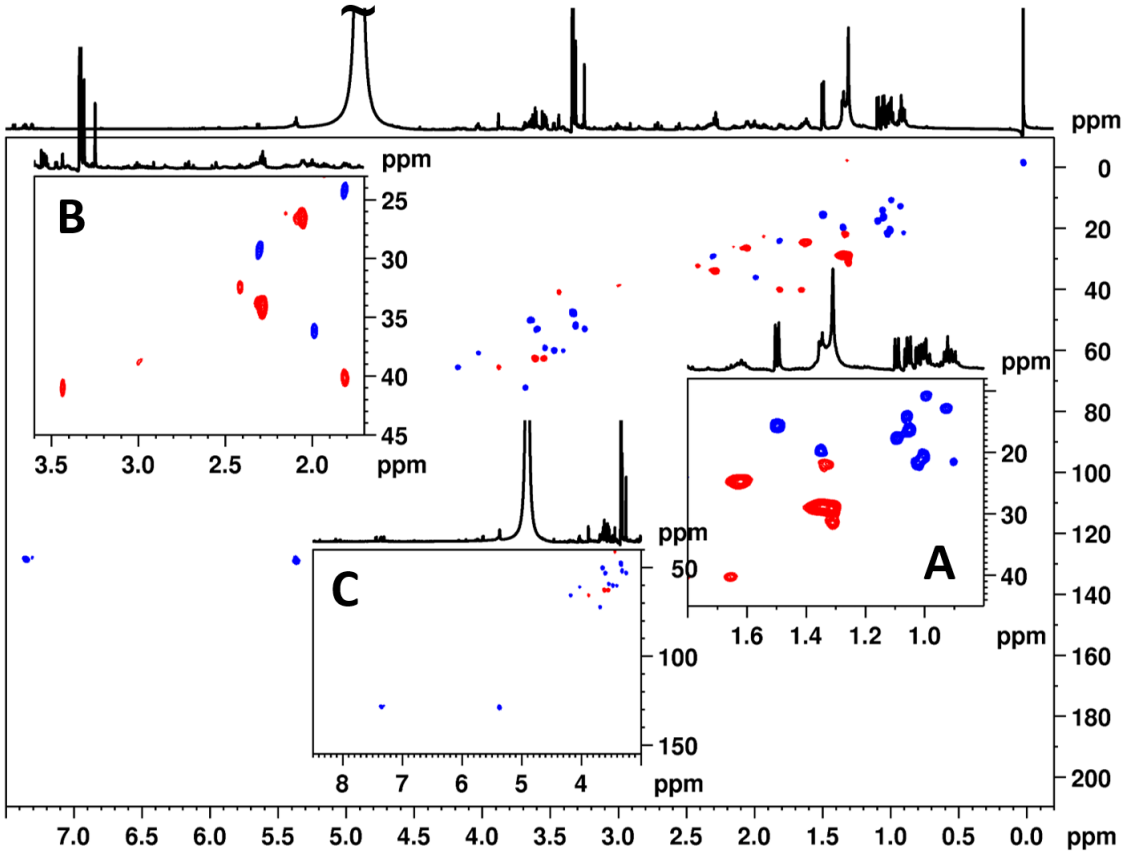


Figure S1. $^{1}$H-$^{13}$C one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Conticribra weissflogii* ($^{1}$H and $^{13}$C, 600 and 150 MHz, $D_2O$) – regions A, B, and C.

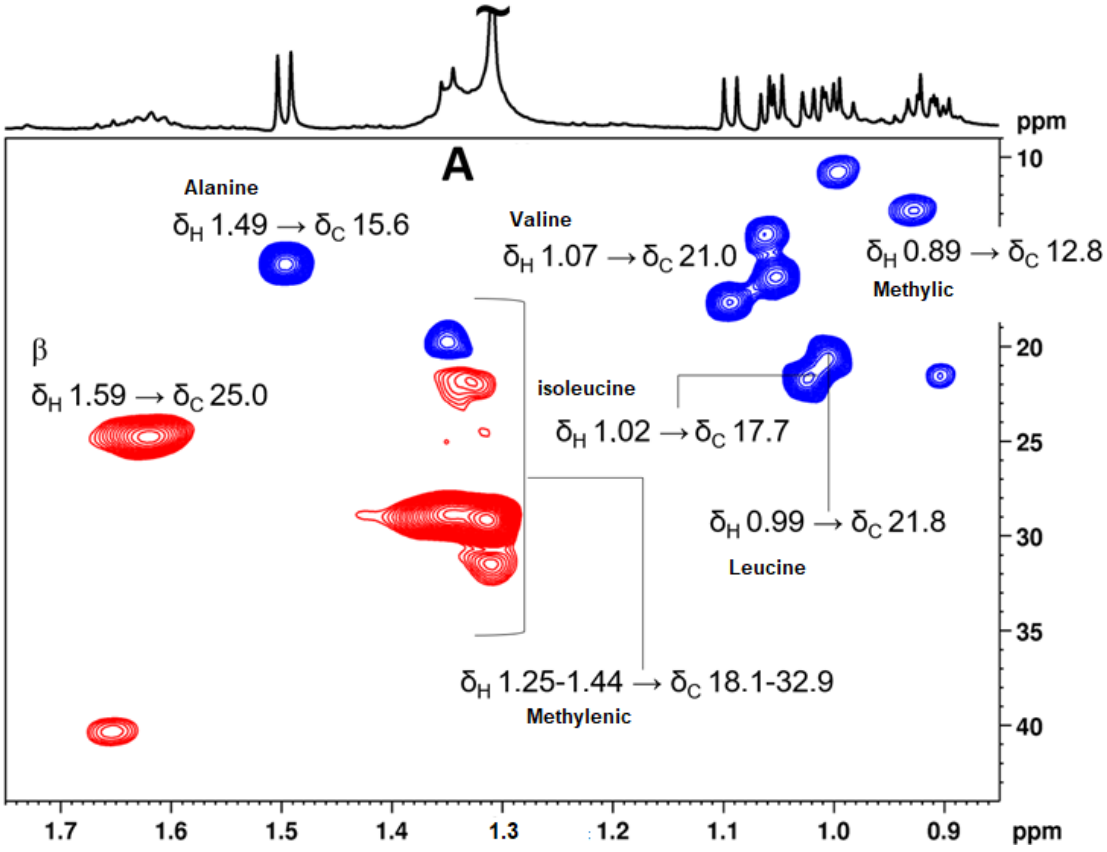


Figure S2. Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Conticribra weissflogii* ($^{1}H$ and $^{13}C$, 600 and 150 MHz, $D_2O$) – region *A*.

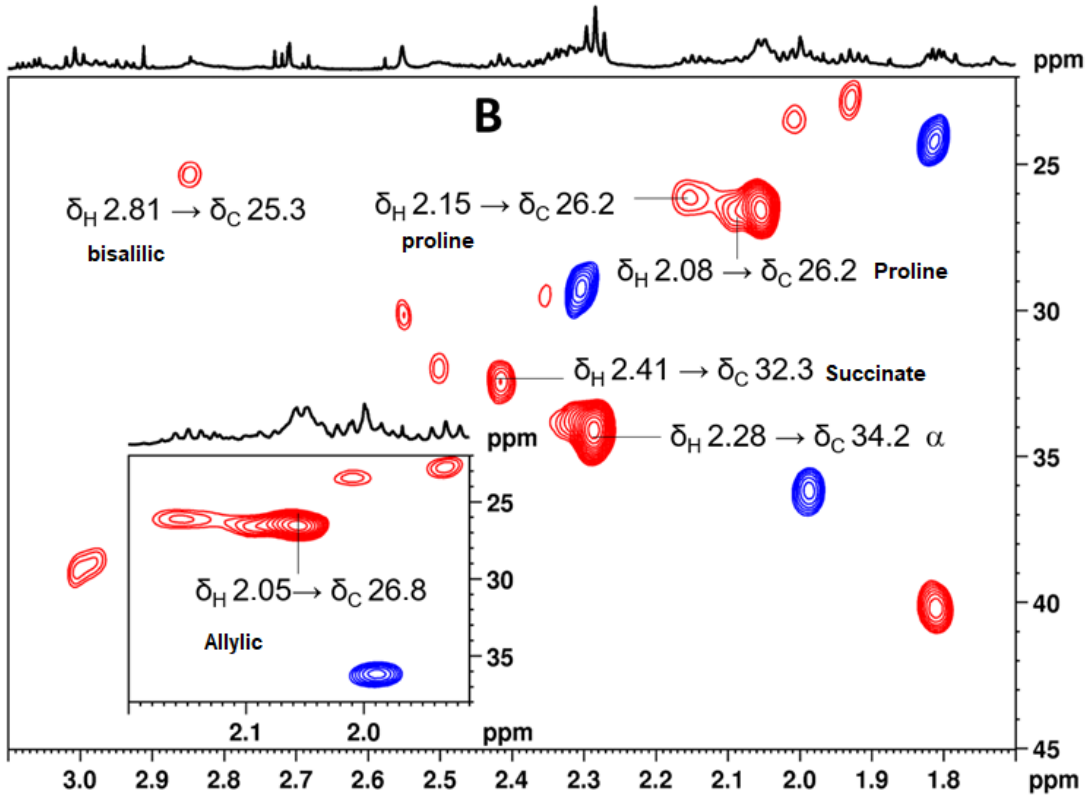


Figure S3. Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Conticribra weissflogii* ($^{1}H$ and $^{13}C$, 600 and 150 MHz, $D_2O$) – region *B*.

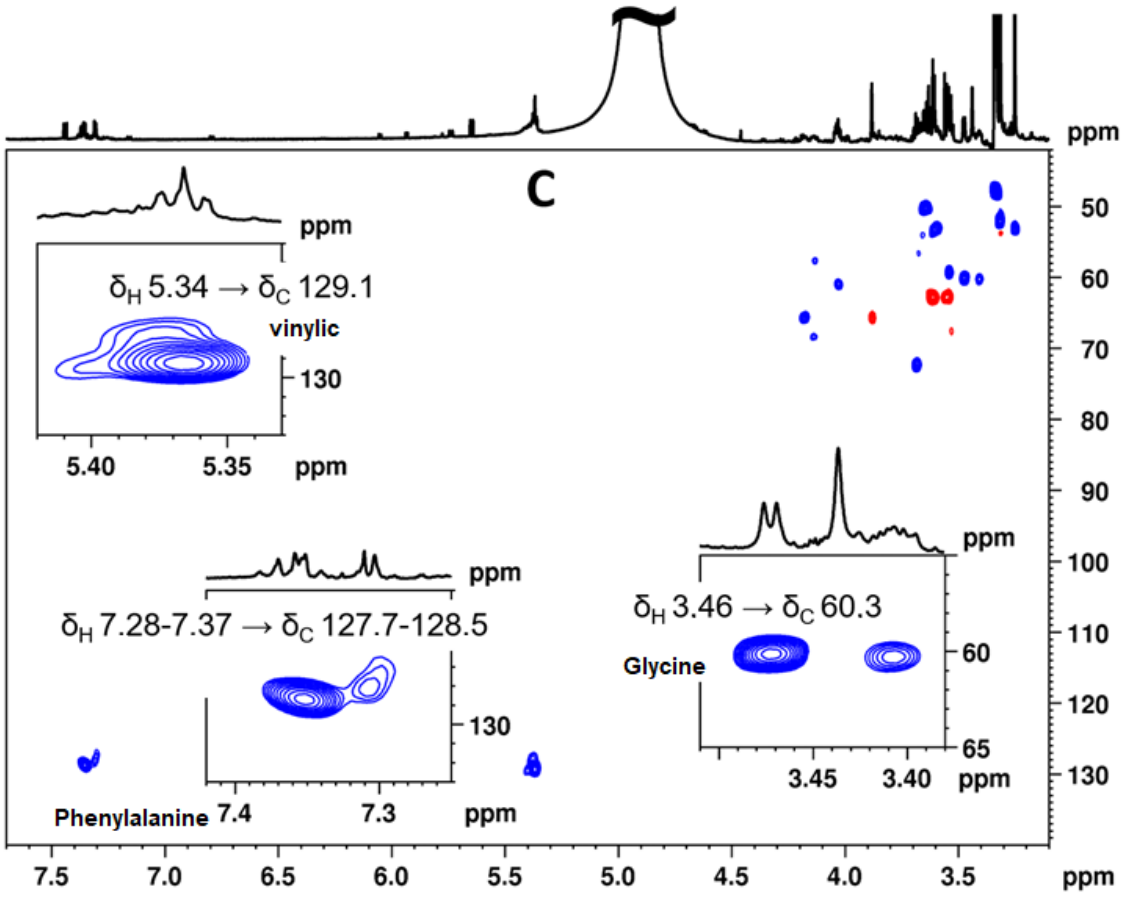


Figure S4. Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Conticribra weissflogii* ($^{1}H$ and $^{13}C$, 600 and 150 MHz, $D_2O$) – region *C*.

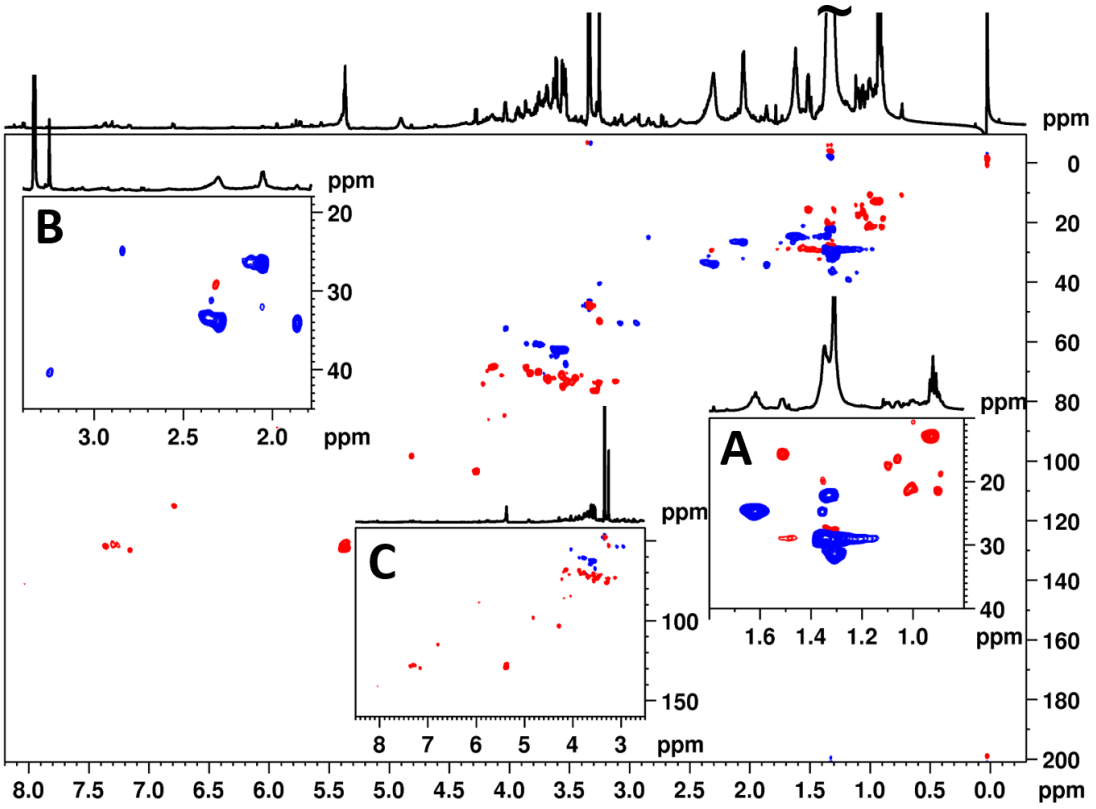


Figure S5. $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Chaetoceros muelleri* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – regions A, B, and C.

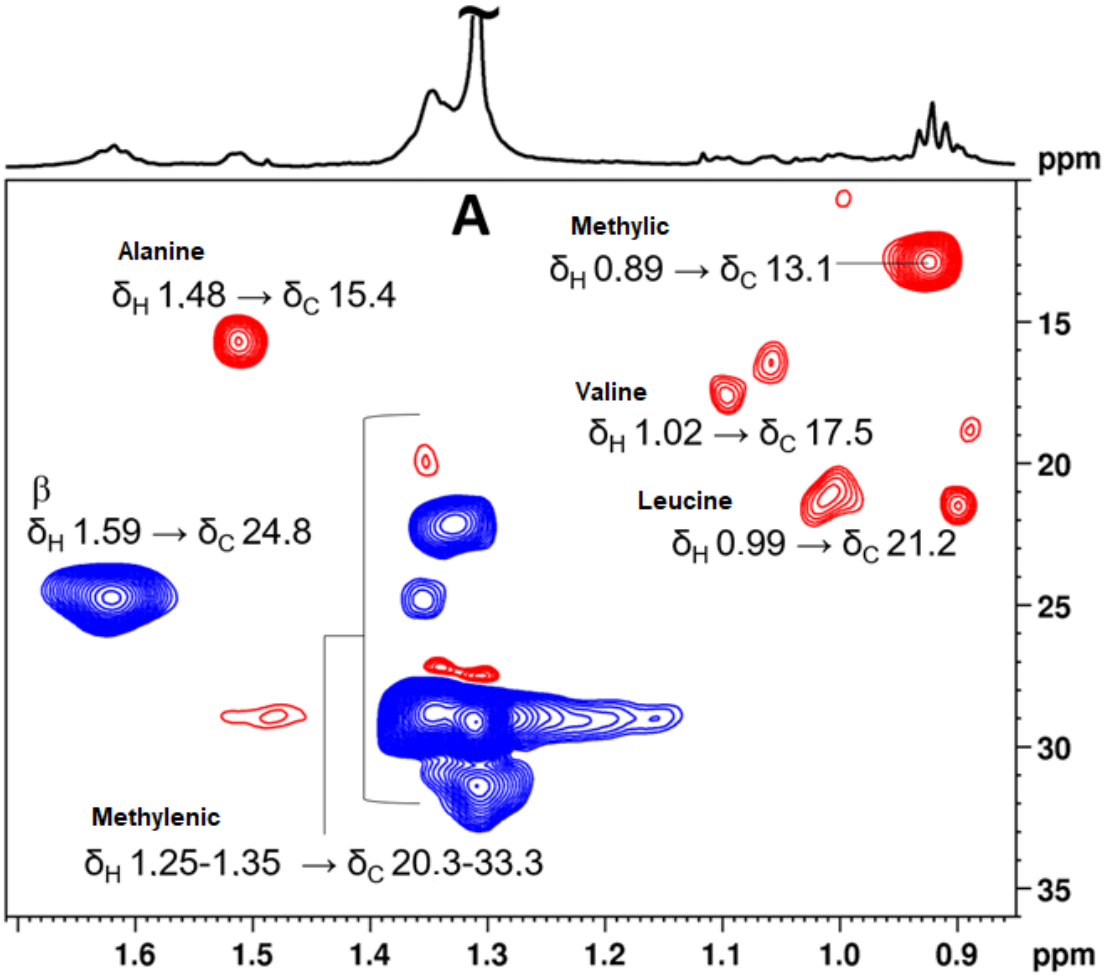


Figure S6. Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Chaetoceros muelleri* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – region *A*.

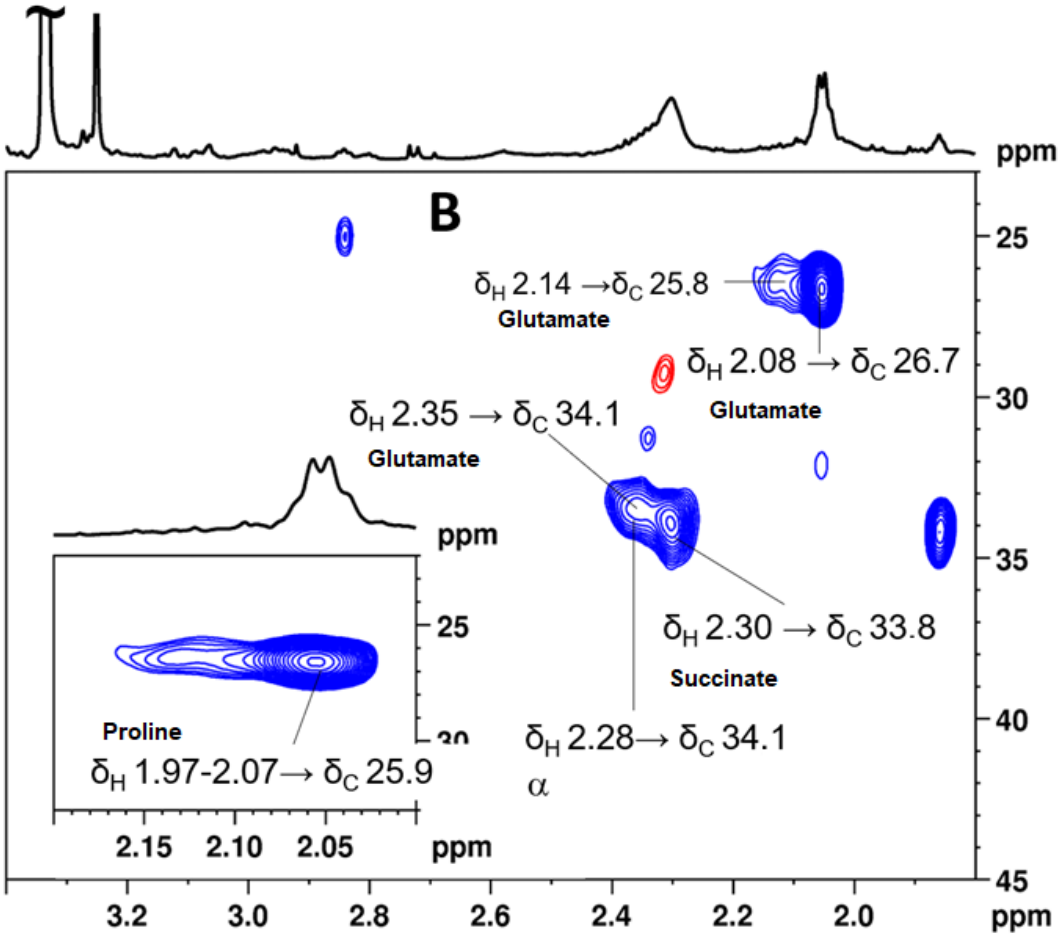


Figure S7. Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Chaetoceros muelleri* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – region *B*.

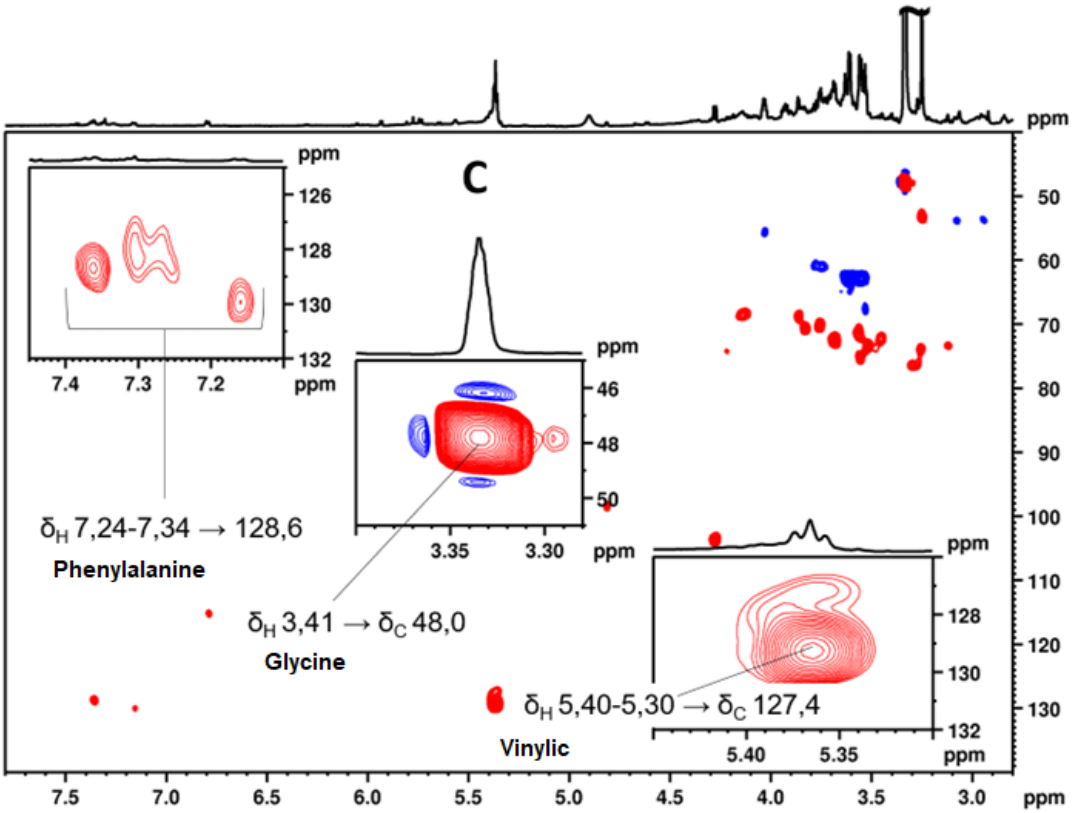


Figure S8. Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Chaetoceros muelleri* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – region *C*.

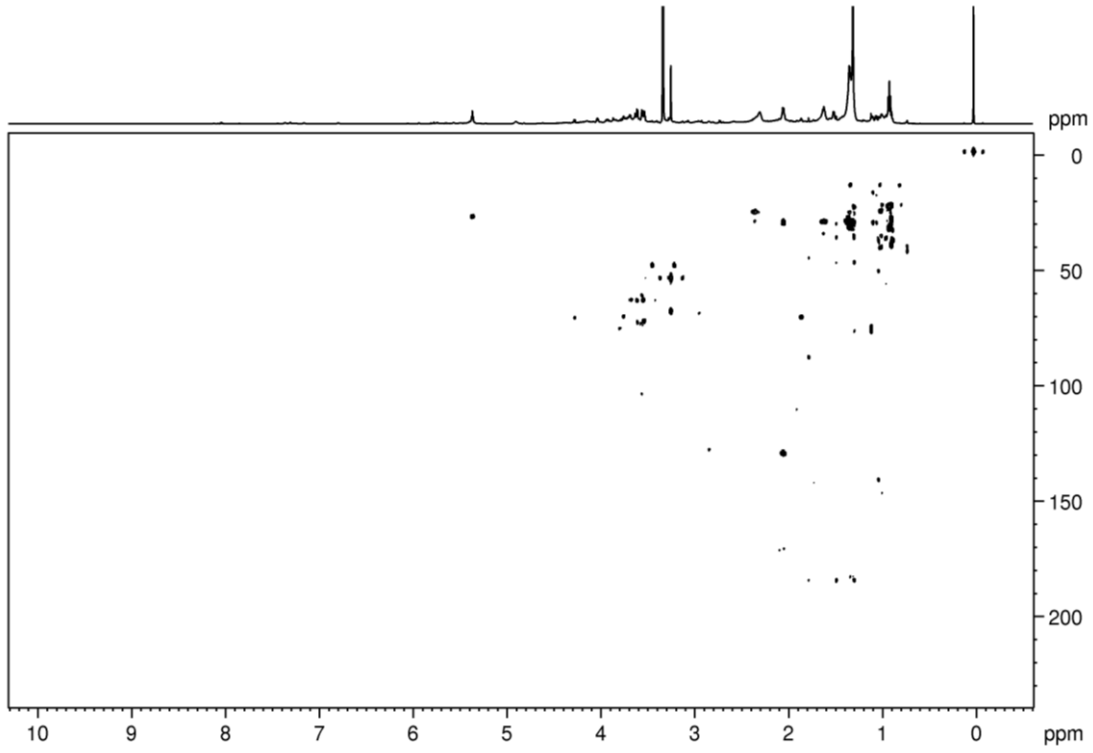


Figure S9. $^{1}H$-$^{13}C$ long-distance correlation map HMBC NMR experiment acquired from *Chaetoceros muelleri* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$).

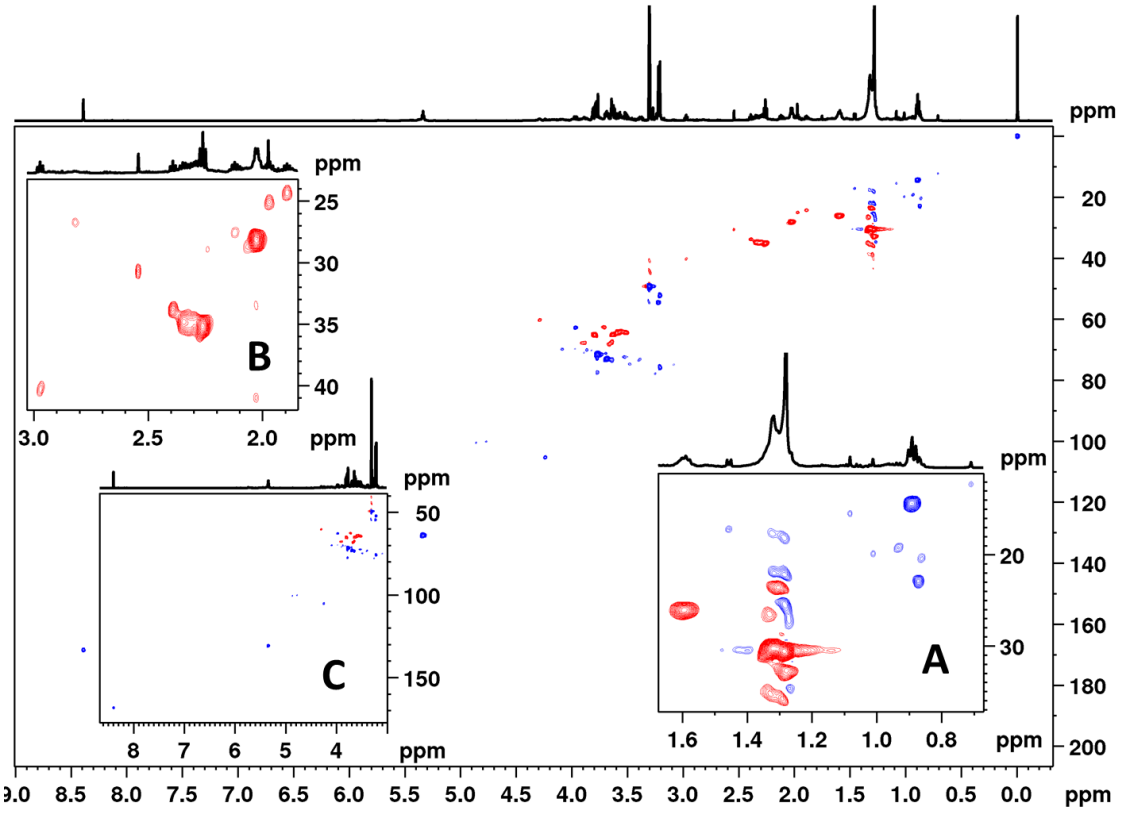


Figure S10. $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Nannochloropsis oceanica* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – regions A, B, and C.

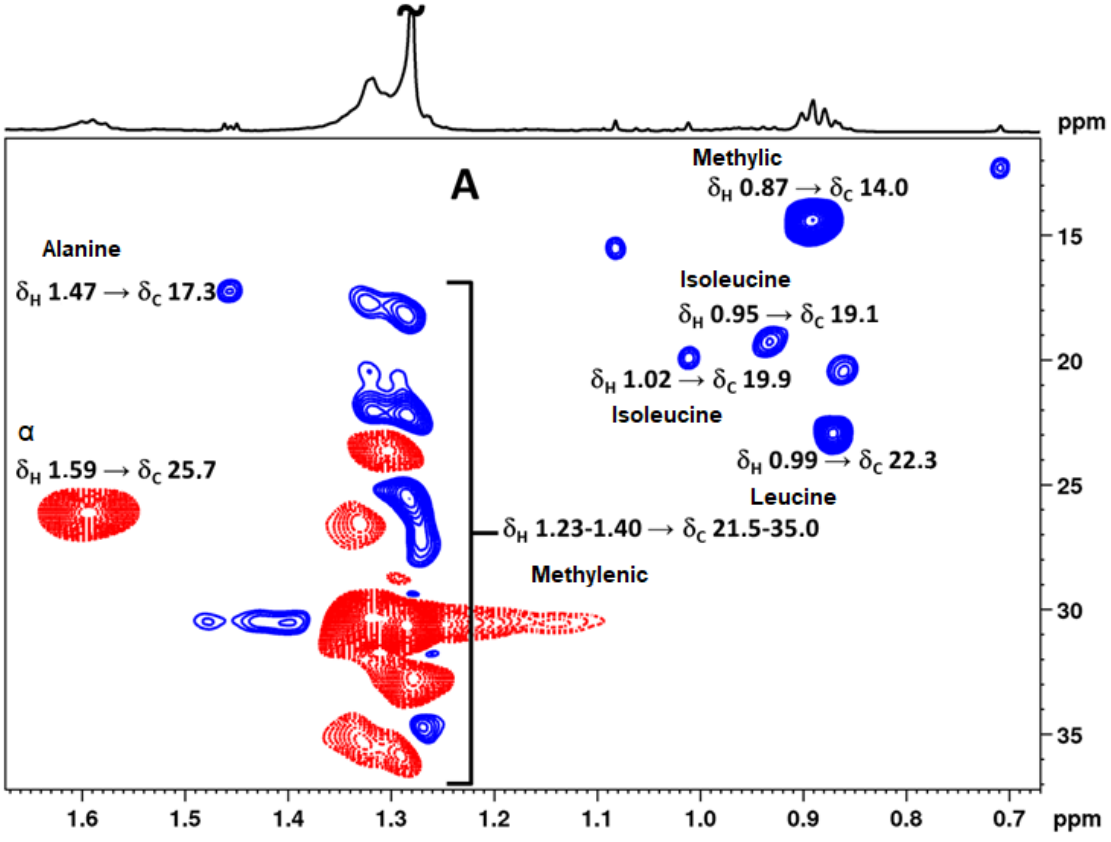


Figure S11.Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Nannochloropsis oceanica* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – region *A*.

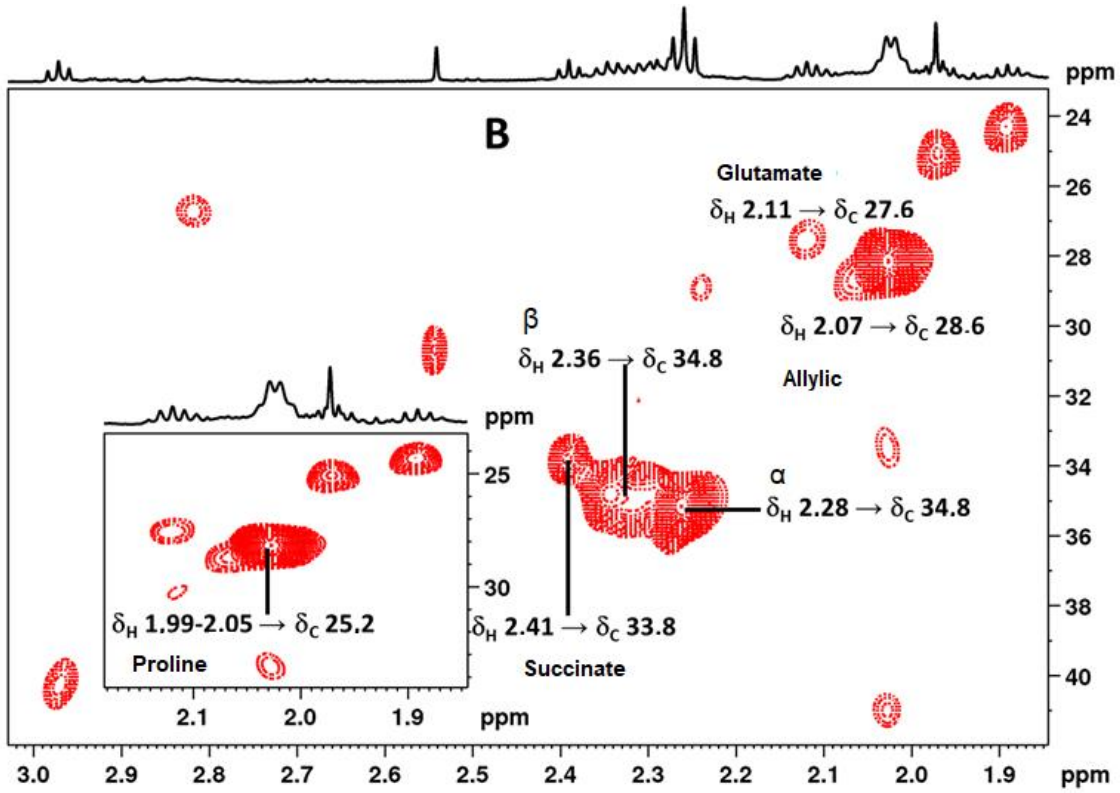


Figure S12. Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Nannochloropsis oceanica* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – region *B*.

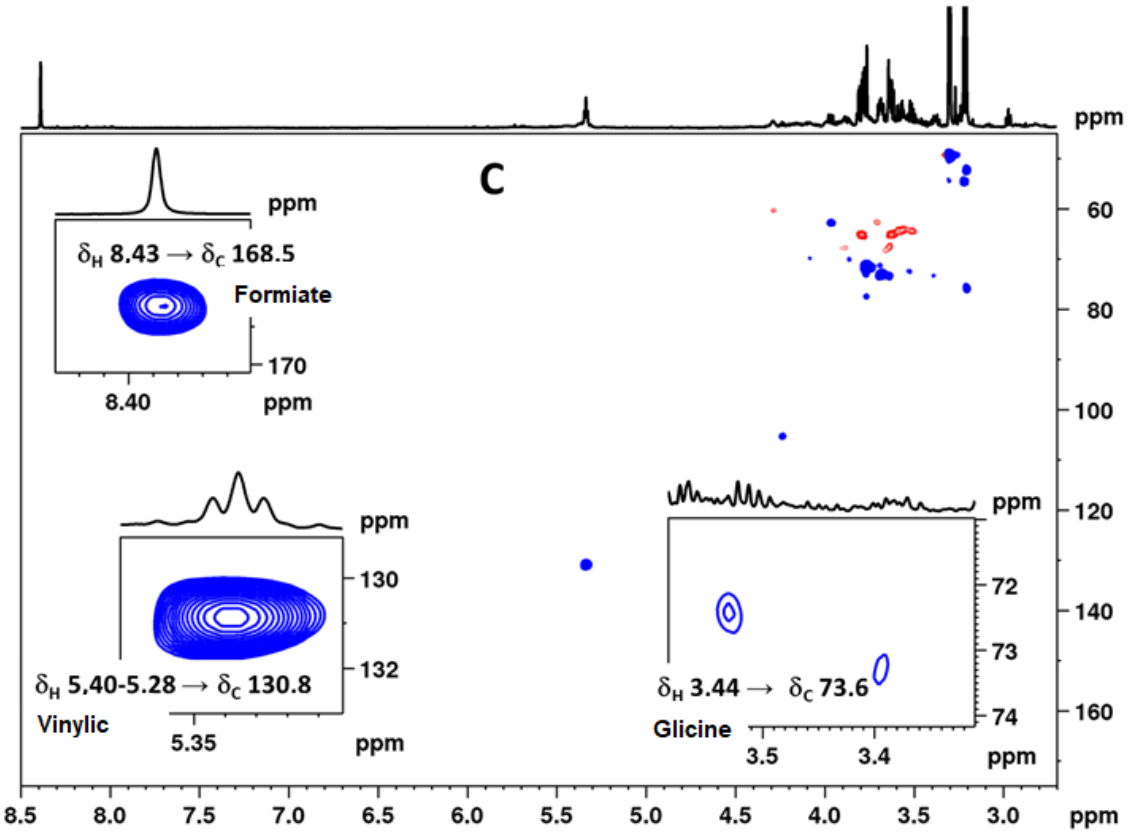


Figure S13.Ampliation from $^{1}H$-$^{13}C$ one-bond correlation map from multiplicity edited HSQC NMR experiment acquired from *Nannochloropsis oceanica* ($^{1}H$ and $^{13}C$, 600.13 and 150.92 MHz, $CD_3OD$) – region *C*.