**Table S1 List of all OS and NOS peaks observed in the mass spectra and their corresponding potential precursors at the four polar sampling sites.** Ion peaks in bold are containing-32S isotope formulas and, and ion peaks in red are their corresponding 34S-containing formulas.

1. **The central Arctic Ocean area**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| NO. | m/z | Theo. Mass (Da) | Delta (ppm) | Formula | Tentatively identified potential precursors |
|  | 279.01038 | 279.01801 | -1.18 | C9H11O8S1 | Diesel/biodiesel A |
|  | 331.08609 | 331.0857 | 1.19 | C14H19O7S1 | Diesel/biodiesel A |
|  | 397.22328 | 397.22655 | 0.25 | C18H37O7S1 |  |
|  | **484.98572** | **484.98539** | **0.68** | **C18H13O12S2** |  |
|  | 486.98255 | 486.98229 | 0.54 | C18H13O12S134S1 |  |
|  | **485.00296** | **485.00315** | **-0.39** | **C18H13O14S1** |  |
|  | 487.00001 | 487.00005 | -0.08 | C18H13O1434S1 |  |
|  | 633.97698 | 633.9774 | -0.67 | C16H16O20N3S2 |  |
|  | 633.99534 | 633.99516 | 0.28 | C16H16O22N3S1 |  |

1. **The Arctic pack ice zone**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | m/z | Theo. Mass (Da) | Delta (ppm) | Formula | Tentatively identified potential precursors |
|  | 167.03853 | 167.03835 | 1.05 | C5H11O4S1 | isoprene B |
|  | 175.00673 | 175.00705 | -1.85 | C6H7O4S1 |  |
|  | 181.05365 | 181.05400 | -1.95 | C6H13O4S1 |  |
|  | 191.00229 | 191.00197 | 1.68 | C6H7O5S1 |  |
|  | 193.01778 | 193.01762 | 0.82 | C6H9O5S1 |  |
|  | 195.03304 | 195.03327 | -1.19 | C6H11O5S1 | Diesel/biodiesel A, pinonaldehyde C |
|  | 198.98862 | 198.99100 | 0.96 | C4H7O7S1 | Diesel/biodiesel A, isoprene D, E |
|  | 199.02786 | 199.02818 | -1.62 | C5H11O6S1 | 2-methyl-3-buten-2-ol F |
|  | 212.98669 | 212.98632 | 1.76 | C8H5O5S1 | Diesel/biodiesel A |
|  | 213.02304 | 213.02270 | 1.59 | C9H9O4S1 | Diesel/biodiesel A |
|  | 215.00180 | 215.00197 | -0.78 | C8H7O5S1 | Diesel/biodiesel A, 2-MeNAP G |
|  | 225.04414 | 225.04383 | 1.38 | C7H13O6S1 | Diesel/biodiesel A |
|  | 226.96561 | 226.96558 | 0.11 | C8H3O6S1 |  |
|  | 231.06989 | 231.06965 | 1.01 | C10H15O4S1 |  |
|  | 235.00752 | 235.00705 | 2 | C11H7O4S1 |  |
|  | 235.06467 | 235.06457 | 0.42 | C9H15O5S1 | Diesel/biodiesel A, isoprene H, β-caryophyllene I |
|  | 246.95557 | 246.95541 | 0.63 | C7H3O8S1 |  |
|  | 249.08059 | 249.08022 | 1.48 | C10H17O5S1 | diesel/biodiesel A, cyclodecane J, pinonaldehydeC, isoprene D, H |
|  | **267.01755** | **267.01801** | **-1.74** | **C8H11O8S1** | diesel/biodiesel A |
|  | 269.01456 | 269.01491 | -1.30 | C8H11O834S1 |  |
|  | **269.03360** | **269.03366** | **-0.23** | **C8H13O8S1** | diesel/biodiesel A |
|  | 271.03044 | 271.03056 | -0.44 | C8H13O834S1 |  |
|  | 274.94986 | 274.95033 | -1.69 | C8H3O9S1 |  |
|  | 275.02280 | 275.02310 | -1.09 | C10H11O7S1 | diesel/biodiesel A |
|  | 275.03879 | 275.03835 | 1.58 | C14H11O4S1 |  |
|  | 280.99150 | 280.99140 | 0.35 | C15H5O4S1 |  |
|  | 281.01230 | 281.01253 | -0.83 | C11H21O6S1 |  |
|  | 283.08585 | 283.08570 | 0.53 | C10H19O7S1 | diesel/biodiesel A, isoprene D |
|  | 287.04459 | 287.04423 | 1.25 | C8H15O9S1 |  |
|  | 292.99734 | 292.99728 | 0.24 | C9H9O9S1 |  |
|  | 293.04849 | 293.04892 | -1.45 | C14H13O5S1 |  |
|  | 296.00760 | 296.00817 | -1.95 | C8H10O9N1S1 |  |
|  | **297.02286** | **297.02270** | **0.52** | **C16H9O4S1** |  |
|  | 299.01979 | 299.01960 | 0.66 | C16H9O434S1 |  |
|  | 305.01239 | 305.01253 | -0.47 | C14H9O6S1 |  |
|  | 305.17877 | 305.17920 | -1.41 | C15H29O4S1 |  |
|  | 309.15588 | 309.15549 | 1.27 | C13H25O6S1 |  |
|  | 321.04941 | 321.04971 | -0.93 | C8H17O11S1 |  |
|  | 321.06540 | 321.06496 | 1.36 | C12H17O8S1 | diesel/biodiesel A |
|  | 324.07523 | 324.07586 | -1.95 | C11H18O8N1S1 |  |
|  | **325.02395** | **325.02349** | **1.4** | **C10H13O10S1** | diesel/biodiesel A |
|  | 327.02064 | 327.02039 | 0.78 | C10H13O1034S1 |  |
|  | 325.98193 | 325.98235 | -1.29 | C8H8O11N1S1 |  |
|  | 327.07539 | 327.07553 | -0.42 | C11H19O9S1 | diesel/biodiesel A |
|  | 329.05504 | 329.05479 | 0.75 | C10H17O10S1 | diesel/biodiesel A |
|  | 329.06949 | 329.07005 | -1.7 | C14H17O7S1 | diesel/biodiesel A |
|  | 329.17902 | 329.17920 | -0.57 | C17H29O4S1 |  |
|  | 330.94016 | 330.94015 | 0 | C10H3O11S1 |  |
|  | 330.95193 | 330.95139 | 1.65 | C9H3O10N2S1 |  |
|  | 330.99215 | 330.99180 | 1.08 | C15H7O7S1 |  |
|  | 337.00232 | 337.00236 | -0.12 | C14H9O8S1 |  |
|  | 339.03882 | 339.03914 | -0.95 | C11H15O10S1 | diesel/biodiesel A |
|  | 339.18494 | 339.18468 | 0.75 | C15H31O6S1 | diesel/biodiesel A |
|  | 340.05014 | 340.04965 | 1.45 | C14H14O7N1S1 |  |
|  | 340.99377 | 340.99325 | 1.53 | C8H9O11N2S1 |  |
|  | 341.08511 | 341.0853 | -0.56 | C19H17O4S1 |  |
|  | 347.08365 | 347.08398 | -0.96 | C11H23O8S2 |  |
|  | 348.93242 | 348.93296 | -1.55 | C10H5O10S2 |  |
|  | 349.09283 | 349.09224 | 1.71 | C9H21O10N2S1 |  |
|  | 352.94615 | 352.94563 | 1.46 | C9H5O13S1 |  |
|  | 353.12811 | 353.12756 | 1.54 | C14H25O8S1 | diesel/biodiesel A, β-caryophyllene I |
|  | 353.14287 | 353.14282 | 0.16 | C18H25O5S1 |  |
|  | 354.99114 | 354.9918 | -1.85 | C17H7O7S1 | diesel/biodiesel A |
|  | 355.10065 | 355.10095 | -0.87 | C20H19O4S1 |  |
|  | 362.94067 | 362.94122 | -1.51 | C9H3O12N2S1 |  |
|  | 362.94865 | 362.94861 | 0.1 | C11H7O10S2 |  |
|  | 363.02140 | 363.02138 | 0.05 | C13H15O8S2 |  |
|  | 363.07181 | 363.0715 | 0.84 | C9H19O11N2S1 |  |
|  | 363.09711 | 363.09666 | 1.24 | C11H23O11S1 |  |
|  | 365.10589 | 365.10643 | -1.49 | C18H21O6S1 |  |
|  | 365.17886 | 365.1792 | -0.93 | C20H29O4S1 |  |
|  | 365.95660 | 365.95614 | 1.27 | C13H4O10N1S1 |  |
|  | 367.01248 | 367.01293 | -1.21 | C15H11O9S1 |  |
|  | 367.07032 | 367.07044 | -0.32 | C13H19O10S1 | diesel/biodiesel A |
|  | 369.03128 | 369.03195 | -1.81 | C12H17O9S2 |  |
|  | 380.93863 | 380.93805 | 1.53 | C14H5O9S2 |  |
|  | 383.03851 | 383.03835 | 0.42 | C23H11O4S1 |  |
|  | 384.96591 | 384.96598 | -0.17 | C17H5O9S1 | diesel/biodiesel A |
|  | 385.00224 | 385.00236 | -0.32 | C18H9O8S1 |  |
|  | 385.01999 | 385.01947 | 1.35 | C10H13O12N2S1 |  |
|  | 387.03403 | 387.03327 | 1.96 | C22H11O5S1 |  |
|  | 388.96152 | 388.96089 | 1.61 | C16H5O10S1 |  |
|  | 388.99670 | 388.99728 | -1.47 | C17H9O9S1 |  |
|  | 389.03430 | 389.03366 | 1.65 | C18H13O8S1 |  |
|  | 393.01270 | 393.01332 | -1.59 | C13H13O12S1 | diesel/biodiesel A |
|  | 393.06903 | 393.06833 | 1.78 | C15H21O8S2 |  |
|  | 393.10727 | 393.10722 | 0.13 | C12H25O12S1 |  |
|  | 393.17334 | 393.17412 | -1.98 | C21H29O5S1 |  |
|  | 397.07568 | 397.07513 | 1.39 | C21H17O6S1 |  |
|  | 399.01866 | 399.01801 | 1.61 | C19H11O8S1 |  |
|  | 410.97781 | 410.9776 | 0.51 | C14H7O11N2S1 |  |
|  | 411.12778 | 411.12717 | 1.48 | C23H23O5S1 | diesel/biodiesel A |
|  | 442.97556 | 442.97483 | 1.65 | C16H11O11S2 |  |
|  | 443.04376 | 443.04423 | -1.05 | C21H15O9S1 |  |
|  | 443.08563 | 443.08648 | -1.92 | C15H23O13S1 |  |
|  | 445.12137 | 445.12076 | 1.36 | C16H29O10S2 |  |
|  | 447.12664 | 447.12717 | -1.17 | C26H23O5S1 | diesel/biodiesel A |
|  | 449.00137 | 449.00065 | 1.62 | C19H13O9S2 |  |
|  | 449.03342 | 449.03366 | -0.54 | C23H13O8S1 |  |
|  | 449.13409 | 449.13343 | 1.47 | C15H29O13S1 | isoprene L |
|  | 468.96732 | 468.96783 | -1.09 | C12H9O16N2S1 |  |
|  | 469.05511 | 469.05585 | -1.59 | C18H17O11N2S1 |  |
|  | 469.12109 | 469.12076 | 0.71 | C18H29O10S2 |  |
|  | 470.20703 | 470.20654 | 1.04 | C19H36O10N1S1 |  |
|  | 471.04840 | 471.04838 | 0.03 | C12H23O15S2 |  |
|  | 471.17020 | 471.16943 | 1.63 | C22H31O9S1 | diesel/biodiesel A |
|  | 484.98848 | 484.98789 | 1.21 | C14H13O17S1 |  |
|  | 485.10675 | 485.10643 | 0.66 | C28H21O6S1 |  |
|  | 485.27807 | 485.27898 | -1.86 | C22H45O9S1 |  |
|  | 500.28955 | 500.28988 | -0.65 | C22H46O9N1S1 |  |
|  | 503.01382 | 503.01371 | 0.22 | C18H15O15S1 |  |
|  | 503.10285 | 503.10359 | -1.47 | C12H27O17N2S1 |  |
|  | 504.19187 | 504.19089 | 1.95 | C22H34O10N1S1 |  |
|  | 504.93137 | 504.93144 | -0.15 | C14H5O17N2S1 |  |
|  | 504.97278 | 504.97185 | 1.85 | C20H9O14S1 |  |
|  | 505.01190 | 505.01161 | 0.58 | C18H17O13S2 |  |
|  | 505.03015 | 505.02936 | 1.56 | C18H17O15S1 |  |
|  | 505.06842 | 505.06912 | -1.39 | C16H25O14S2 |  |
|  | 560.10193 | 560.10208 | -0.26 | C29H22O9N1S1 |  |
|  | 560.13178 | 560.13245 | -1.2 | C16H34O16N1S2 |  |
|  | 560.25299 | 560.25349 | -0.89 | C26H42O10N1S1 |  |
|  | 560.90936 | 560.91004 | -1.2 | C17H5O20S1 |  |
|  | 560.92877 | 560.92866 | 0.19 | C18H9O17S2 |  |
|  | 561.06866 | 561.06833 | 0.59 | C29H21O8S2 |  |
|  | 562.08606 | 562.08656 | -0.89 | C13H28O17N3S2 |  |
|  | 562.10193 | 562.10247 | -0.96 | C25H24O12N1S1 |  |
|  | 633.96907 | 633.96816 | 1.43 | C26H8O15N3S1 |  |
|  | 633.98613 | 633.98527 | 1.36 | C18H12O19N5S1 |  |
|  | 634.00154 | 634.00256 | -1.6 | C18H20O20N1S2 |  |
|  | 634.26862 | 634.26914 | -0.83 | C32H44O10N1S1 |  |
|  | 634.34845 | 634.34778 | 1.05 | C27H56O13N1S1 |  |
|  | 634.93481 | 634.93442 | 0.61 | C26H7O14N2S2 |  |
|  | 634.96231 | 634.96142 | 1.41 | C16H15O21N2S2 |  |
|  | 634.96231 | 634.96207 | 0.38 | C24H11O19S1 |  |
|  | 634.98272 | 634.9832 | -0.75 | C21H15O21S1 |  |
|  | 635.00401 | 635.00433 | -0.5 | C18H19O23S1 |  |
|  | 635.00401 | 635.00382 | 0.31 | C31H11O12N2S1 |  |
|  | 635.02824 | 635.02832 | -0.12 | C25H19O14N2S2 |  |
|  | 635.02824 | 635.02897 | -1.15 | C33H15O12S1 |  |
|  | 635.07793 | 635.0771 | 1.3 | C20H27O21S1 |  |
|  | 635.07793 | 635.07844 | -0.81 | C21H23O17N4S1 |  |
|  | 635.10300 | 635.10359 | -0.93 | C23H27O17N2S1 |  |
|  | 635.15355 | 635.15324 | 0.49 | C19H39O19S2 |  |
|  | 635.15355 | 635.15338 | 0.27 | C40H27O6S1 |  |
|  | 635.17377 | 635.17451 | -1.17 | C37H31O8S1 |  |
|  | 635.19343 | 635.19347 | -0.06 | C17H39O19N4S1 |  |
|  | 635.21934 | 635.22014 | -1.27 | C28H43O12S2 |  |
|  | 635.24010 | 635.24127 | -1.84 | C25H47O14S2 |  |
|  | 635.27013 | 635.27026 | -0.2 | C24H47O15N2S1 |  |
|  | 635.29389 | 635.29291 | 1.54 | C30H51O10S2 |  |
|  | 635.31293 | 635.31404 | -1.75 | C27H55O12S2 |  |
|  | 635.33294 | 635.3318 | 1.79 | C27H55O14S1 |  |
|  | 635.96008 | 635.96069 | -0.96 | C20H14O19N1S2 |  |
|  | 636.03691 | 636.03596 | 1.49 | C18H22O22N1S1 |  |
|  | 636.10807 | 636.10874 | -1.05 | C20H30O20N1S1 |  |
|  | 636.13363 | 636.13338 | 0.4 | C35H26O9N1S1 |  |
|  | 636.19997 | 636.20013 | -0.25 | C23H42O15N1S2 |  |
|  | 636.26257 | 636.26366 | -1.72 | C35H42O8N1S1 |  |
|  | 792.07440 | 792.0742 | 0.25 | C20H30O28N3S1 |  |

1. **The Antarctic Kunlun Station**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | m/z | Theo. Mass (Da) | Delta (ppm) | Formula | Tentatively identified potential precursors |
|  | **241.07467** | **241.07513** | **-0.46** | **C8H17O6S1** | diesel/biodiesel A |
|  | 243.07198 | 243.07203 | -0.2 | C8H17O634S1 |  |
|  | 250.96540 | 250.96558 | -0.18 | C10H3O6S1 |  |
|  | 300.98102 | 300.98123 | -0.21 | C14H5O6S1 |  |
|  | 301.05991 | 301.05988 | 0.03 | C9H17O9S1 |  |
|  | **326.99724** | **326.99688** | **0.35** | **C16H7O6S1** |  |
|  | 328.99403 | 328.99378 | 0.76 | C16H7O634S1 |  |
|  | 334.93533 | 334.93507 | 0.26 | C9H3O12S1 |  |
|  | 335.02277 | 335.02310 | -0.33 | C15H11O7S1 |  |
|  | 362.94876 | 362.94861 | 0.15 | C11H7O10S2 |  |
|  | 372.06007 | 372.06060 | -0.53 | C11H18O11N1S1 |  |
|  | 372.07639 | 372.07586 | 0.53 | C15H18O8N1S1 |  |
|  | 375.02385 | 375.02388 | -0.03 | C10H15O13S1 |  |
|  | 375.07571 | 375.07553 | 0.19 | C15H19O9S1 | diesel/biodiesel A |
|  | 376.92734 | 376.92788 | -0.54 | C11H5O11S2 |  |
|  | **377.09439** | **377.09455** | **-0.16** | **C12H25O9S2** |  |
|  | 379.09127 | 379.09145 | -0.47 | C12H25O9S134S1 |  |
|  | **377.12811** | **377.12756** | **0.55** | **C16H25O8S1** | diesel/biodiesel A |
|  | 379.12454 | 379.12446 | 0.21 | C16H25O834S1 |  |
|  | 410.06038 | 410.06100 | -0.62 | C10H20O14N1S1 |  |
|  | 410.07553 | 410.07625 | -0.72 | C14H20O11N1S1 |  |
|  | 411.98233 | 411.98275 | -0.42 | C11H10O14N1S1 |  |
|  | 412.00159 | 412.00137 | 0.21 | C12H14O11N1S2 |  |
|  | 427.21579 | 427.21598 | -0.19 | C22H35O6S1 |  |
|  | 484.93353 | 484.93375 | -0.22 | C13H9O16S2 |  |
|  | 484.96289 | 484.96274 | 0.14 | C12H9O17N2S1 |  |
|  | 485.01260 | 485.01253 | 0.07 | C29H9O6S1 |  |
|  | 485.05847 | 485.05816 | 0.31 | C20H21O10S2 |  |
|  | 485.11533 | 485.11568 | -0.35 | C18H29O11S2 |  |
|  | **485.12775** | **485.12756** | **0.18** | **C25H25O8S1** | diesel/biodiesel A |
|  | 487.12466 | 487.12446 | 0.42 | C25H25O834S1 |  |
|  | **485.29504** | **485.29423** | **0.81** | **C26H45O6S1** |  |
|  | 487.29180 | 487.29113 | 1.39 | C26H45O634S1 |  |
|  | 626.02433 | 626.02396 | 0.37 | C19H20O17N3S2 |  |
|  | 626.02433 | 626.02461 | -0.28 | C27H16O15N1S1 |  |
|  | 626.03979 | 626.03987 | -0.07 | C31H16O12N1S1 |  |
|  | 626.07111 | 626.07024 | 0.87 | C18H28O19N1S2 |  |
|  | **634.02020** | **634.02031** | **-0.12** | **C18H20O22N1S1** |  |
|  | 636.01697 | 636.01721 | -0.37 | C18H20O22N1S1 |  |
|  | 634.09265 | 634.09309 | -0.43 | C20H28O20N1S1 |  |
|  | 634.10931 | 634.10834 | 0.97 | C24H28O17N1S1 |  |
|  | 636.11508 | 636.11410 | 0.98 | C26H26O14N3S1 |  |
|  | 636.21593 | 636.21539 | 0.54 | C27H42O12N1S2 |  |
|  | 636.23742 | 636.23652 | 0.9 | C24H46O14N1S2 |  |

1. **The Antarctic Zhongshan Station**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | m/z | Theo. Mass (Da) | Delta (ppm) | Formula | Tentatively identified potential precursors |
|  | 176.98642 | 176.98632 | 0.58 | C5H5O5S1 |  |
|  | **187.00728** | **187.00705** | **1.23** | **C7H7O4S1** | diesel/biodiesel A, 2-MeNAP G |
|  | 189.00428 | 189.00395 | 1.78 | C7H7O434S1 |  |
|  | 192.98116 | 192.98123 | -0.4 | C5H5O6S1 |  |
|  | 193.01758 | 193.01762 | -0.2 | C6H9O5S1 | diesel/biodiesel A |
|  | 207.03332 | 207.03327 | 0.27 | C7H11O5S1 | diesel/biodiesel A |
|  | 213.04353 | 213.04383 | -1.4 | C6H13O6S1 |  |
|  | **215.03871** | **215.03835** | **1.67** | **C9H11O4S1** |  |
|  | 217.03558 | 217.03525 | 1.53 | C9H11O434S1 |  |
|  | 217.01743 | 217.01762 | -0.88 | C8H9O5S1 |  |
|  | 225.04355 | 225.04383 | -1.26 | C7H13O6S1 | diesel/biodiesel A |
|  | 228.01845 | 228.01835 | 0.45 | C5H10O7N1S1 |  |
|  | 232.97648 | 232.97615 | 1.44 | C7H5O7S1 |  |
|  | 239.00220 | 239.00197 | 0.96 | C10H7O5S1 |  |
|  | 241.07529 | 241.07513 | 0.65 | C8H17O6S1 | diesel/biodiesel A |
|  | 243.01797 | 243.01801 | -0.16 | C6H11O8S1 | diesel/biodiesel A |
|  | 243.03299 | 243.03327 | -1.16 | C10H11O5S1 | diesel/biodiesel A |
|  | 247.98680 | 247.98705 | -0.99 | C7H6O7N1S1 |  |
|  | 249.02244 | 249.02270 | -1.07 | C12H9O4S1 |  |
|  | 249.08068 | 249.08022 | 1.86 | C10H17O5S1 | diesel/biodiesel A, cyclodecane J, isoprene K, β-pinene L |
|  | 254.97603 | 254.97575 | 1.07 | C13H3O4S1 |  |
|  | 256.01324 | 256.01326 | -0.06 | C6H10O8N1S1 |  |
|  | 265.00283 | 265.00236 | 1.78 | C8H9O8S1 | diesel/biodiesel A |
|  | 265.11191 | 265.11152 | 1.49 | C11H21O5S1 | diesel/biodiesel A |
|  | 277.00226 | 277.00236 | -0.37 | C9H9O8S1 |  |
|  | 282.95501 | 282.95541 | -1.42 | C10H3O8S1 |  |
|  | 292.99197 | 292.99140 | 1.95 | C16H5O4S1 |  |
|  | 295.08597 | 295.08570 | 0.93 | C11H19O7S1 | diesel/biodiesel A |
|  | **297.06525** | **297.06496** | **0.96** | **C10H17O8S1** | diesel/biodiesel A, decalin J, isoprene D, K |
|  | 299.06214 | 299.06186 | 0.94 | C10H17O834S1 |  |
|  | 299.09583 | 299.09587 | -0.14 | C14H19O5S1 | diesel/biodiesel A |
|  | 299.13251 | 299.13225 | 0.85 | C15H23O4S1 |  |
|  | **311.08088** | **311.08061** | **0.86** | **C11H19O8S1** | diesel/biodiesel A |
|  | 313.07783 | 313.07751 | 1.04 | C11H19O834S1 |  |
|  | 313.01775 | 313.01762 | 0.43 | C16H9O5S1 |  |
|  | **339.03897** | **339.03914** | **-0.5** | **C11H15O10S1** | diesel/biodiesel A |
|  | 341.03586 | 341.03604 | -0.53 | C11H15O1034S1 |  |
|  | 340.96106 | 340.96089 | 0.5 | C12H5O10S1 |  |
|  | 341.09085 | 341.09118 | -0.97 | C12H21O9S1 | diesel/biodiesel A |
|  | 365.14294 | 365.14282 | 0.35 | C19H25O5S1 | diesel/biodiesel A |
|  | 375.02315 | 375.02388 | -1.95 | C10H15O13S1 |  |
|  | 375.09674 | 375.09666 | 0.23 | C12H23O11S1 | isoprene K |
|  | 375.18408 | 375.18468 | -1.6 | C18H31O6S1 | diesel/biodiesel A |
|  | 375.25714 | 375.25745 | -0.83 | C20H39O4S1 |  |
|  | 484.94955 | 484.94900 | 1.13 | C17H9O13S2 |  |
|  | 485.00659 | 485.00652 | 0.15 | C15H17O14S2 |  |
|  | 485.22165 | 485.22146 | 0.39 | C24H37O8S1 |  |
|  | 634.34238 | 634.34191 | 0.73 | C34H52O8N1S1 |  |
|  | 634.92511 | 634.92503 | 0.12 | C15H11O22N2S2 |  |
|  | 634.92511 | 634.92569 | -0.91 | C23H7O20S1 |  |
|  | 634.94583 | 634.94682 | -1.55 | C20H11O22S1 |  |
|  | 635.00426 | 635.00433 | -0.12 | C18H19O23S1 |  |
|  | 635.00426 | 635.00382 | 0.69 | C31H11O12N2S1 |  |
|  | 635.02970 | 635.03082 | -1.77 | C21H19O19N2S1 |  |
|  | 635.02970 | 635.02897 | 1.14 | C33H15O12S1 |  |
|  | 635.04708 | 635.04760 | -0.82 | C34H19O9S2 |  |
|  | 635.06602 | 635.06655 | -0.84 | C14H27O20N4S2 |  |
|  | 635.06602 | 635.06536 | 1.04 | C34H19O11S1 |  |
|  | 635.08628 | 635.08583 | 0.71 | C23H27O15N2S2 |  |
|  | 635.08628 | 635.08648 | -0.32 | C31H23O13S1 |  |
|  | 635.10578 | 635.10696 | -1.86 | C20H31O17N2S2 |  |
|  | 635.10578 | 635.10511 | 1.05 | C32H27O10S2 |  |
|  | 635.13217 | 635.13211 | 0.09 | C22H35O17S2 |  |
|  | 635.13217 | 635.13225 | -0.13 | C43H23O4S1 |  |
|  | 635.15757 | 635.15708 | 0.77 | C16H35O20N4S1 |  |
|  | 635.17713 | 635.17636 | 1.21 | C25H35O15N2S1 |  |
|  | 635.17713 | 635.17788 | -1.19 | C34H35O8S2 |  |
|  | 635.22214 | 635.22264 | -0.8 | C24H43O17S1 |  |
|  | 635.27133 | 635.27026 | 1.68 | C24H47O15N2S1 |  |
|  | 635.27133 | 635.27178 | -0.71 | C33H47O8S2 |  |
|  | 635.31374 | 635.31404 | -0.48 | C27H55O12S2 |  |
|  | 635.34311 | 635.34303 | 0.12 | C26H55O13N2S1 |  |
|  | 635.38403 | 635.38344 | 0.93 | C32H59O10S1 |  |
|  | 635.49284 | 635.49260 | 0.38 | C35H71O7S1 |  |

A Blair et al. (2017); B Surratt et al. (2010); C Liggio et al. (2006); D Nozière et al. (2010); E Lin et al. (2013);

F Zhang et al. (2012); G Rive et al. (2015); H Surratt et al. (2008); I Chan et al. (2011); J Riva et al. (2016b);

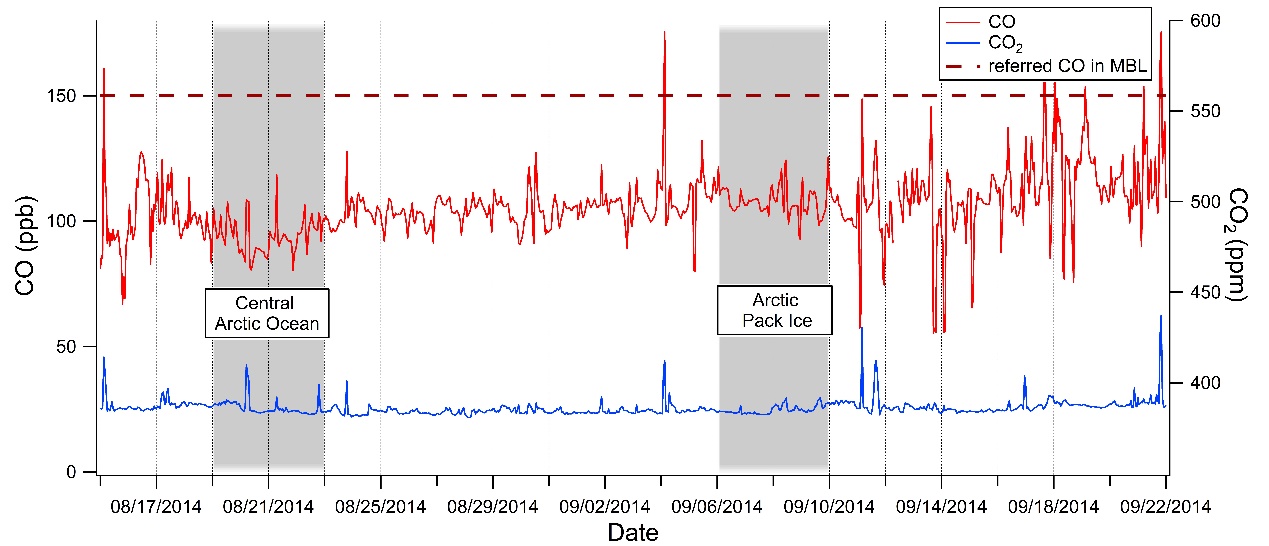
K Riva et al. (2016a); L Iinuma et al. (2007).

**Table S2 The input for ISORROPIA II to calculate pH.**

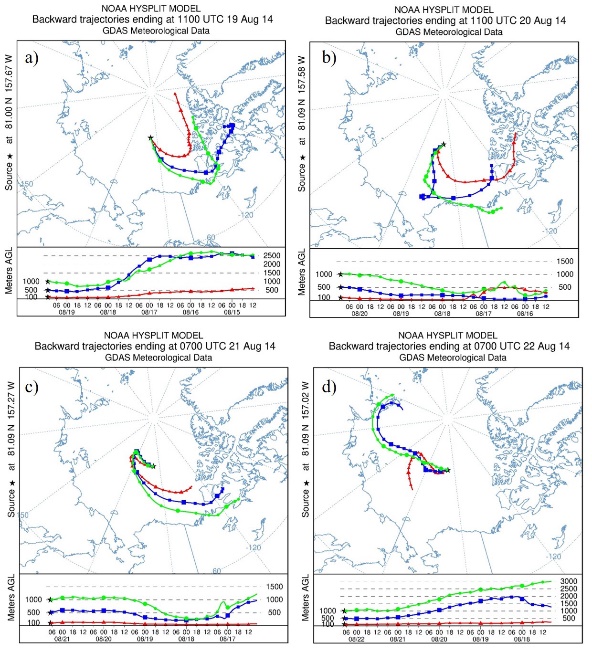
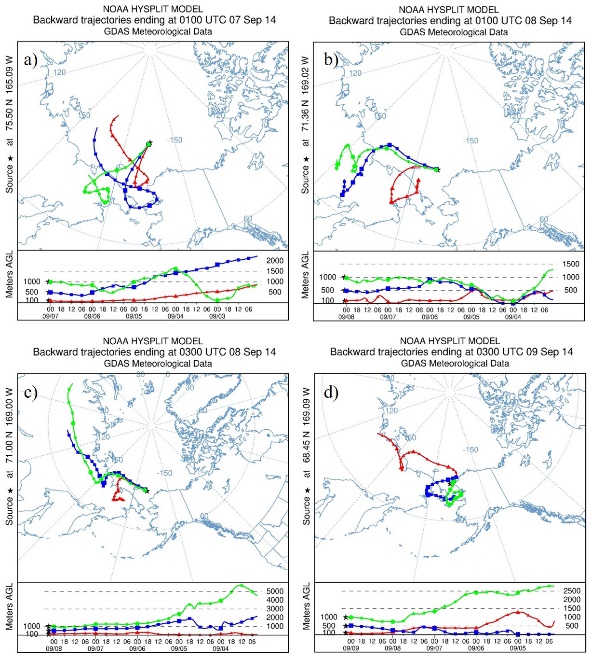
|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sampling Sites** | | **Na+**  **(μg m-3)** | **K+**  **(μg m-3)** | **Mg2+**  **(μg m-3)** | **Ca2+**  **(μg m-3)** | **NH4+**  **(μg m-3)** | **SO42-**  **(μg m-3)** | **NO3-**  **(μg m-3)** | **Cl-**  **(μg m-3)** | **RH (%)** | **T (K)** |
| Arctic | central ocean | 0.34 | - | 0.05 | 0.03 | 0.15 | 0.24 | 0.02 | 0.03 | 90 | 275.15 |
| pack ice | 0.68 | 0.12 | 0.07 | 0.02 | 0.17 | 2.04 | 0.14 | 0.26 | 90 | 260.05 |
| Antarctic | Kunlun Station | 0.48 | 0.11 | 0.02 | 0.05 | - | 0.40 | 0.06 | 0.18 | 65 | 246.98 |
| Zhongshan Station | 0.11 | 0.12 | 0.05 | 0.07 | - | 0.31 | 0.06 | 0.16 | 50 | 266.10 |

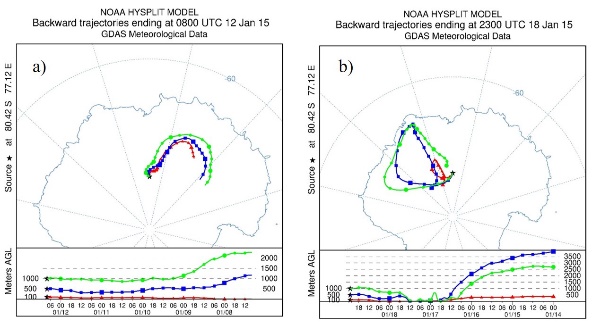
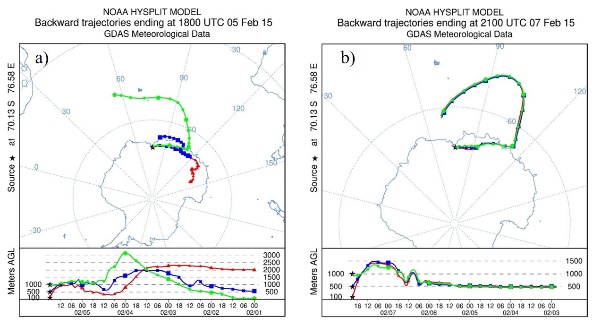
**Table S3 Lists of OSs which had a potential source of phytoplankton at the Arctic pack ice site and Antarctic Zhongshan Station.** OSs in red are those unknown precursor-derived (UP-D) OSs. OSs in blue are those found in Zhu et al. (2019). OSs in purple are those UP-D OSs found in Zhu et al. (2019).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Arctic Pack Ice | | | Antarctic Zhongshan Station | | |
| Formula | Neutral Mass (Da) | DBE | Formula | Neutral Mass (Da) | DBE |
| C4H8O7S1 | 199.99882 | 1 | C6H10O5S1 | 193.01762 | 2 |
| C5H12O4S1 | 168.04617 | 0 | C6H14O6S1 | 213.04383 | 0 |
| C5H12O6S1 | 200.03600 | 0 | C6H12O8S1 | 243.01801 | 1 |
| C6H14O4S1 | 182.06182 | 0 | C7H12O5S1 | 207.03327 | 2 |
| C6H12O5S1 | 196.04109 | 1 | C7H14O6S1 | 225.04383 | 1 |
| C6H10O5S1 | 194.02544 | 2 | C8H18O6S1 | 241.07513 | 0 |
| C7H14O6S1 | 226.05165 | 1 | C10H18O5S1 | 249.08022 | 2 |
| C8H18O11S1 | 322.05753 | 0 | C10H18O8S1 | 297.06496 | 2 |
| C8H16O9S1 | 288.05205 | 1 | **C11H22O5S1** | 265.11152 | 1 |
| C8H14O8S1 | 270.04148 | 2 | C11H20O7S1 | 295.08570 | 2 |
| C9H16O5S1 | 236.07239 | 2 | C11H20O8S1 | 311.08061 | 2 |
| C10H20O7S1 | 284.09352 | 1 | C12H22O9S1 | 341.09118 | 2 |
| C10H18O5S1 | 250.08804 | 2 | C12H24O11S1 | 375.09666 | 1 |
| C10H18O10S1 | 330.06261 | 2 | **C18H32O6S1** | 376.19250 | 3 |
| C11H24O8S2 | 348.09180 | 0 | C20H40O4S1 | 375.25745 | 1 |
| C11H24O11S1 | 364.10448 | 0 |
| C11H20O9S1 | 328.08335 | 2 |
| C12H26O12S1 | 394.11504 | 0 |
| C12H24O15S2 | 472.05620 | 1 |
| C14H26O8S1 | 354.13538 | 2 |
| C15H30O4S1 | 306.18702 | 1 |
| C15H30O13S1 | 450.14125 | 1 |
| C16H30O10S2 | 446.12858 | 2 |
| C25H48O14S2 | 636.24909 | 2 |



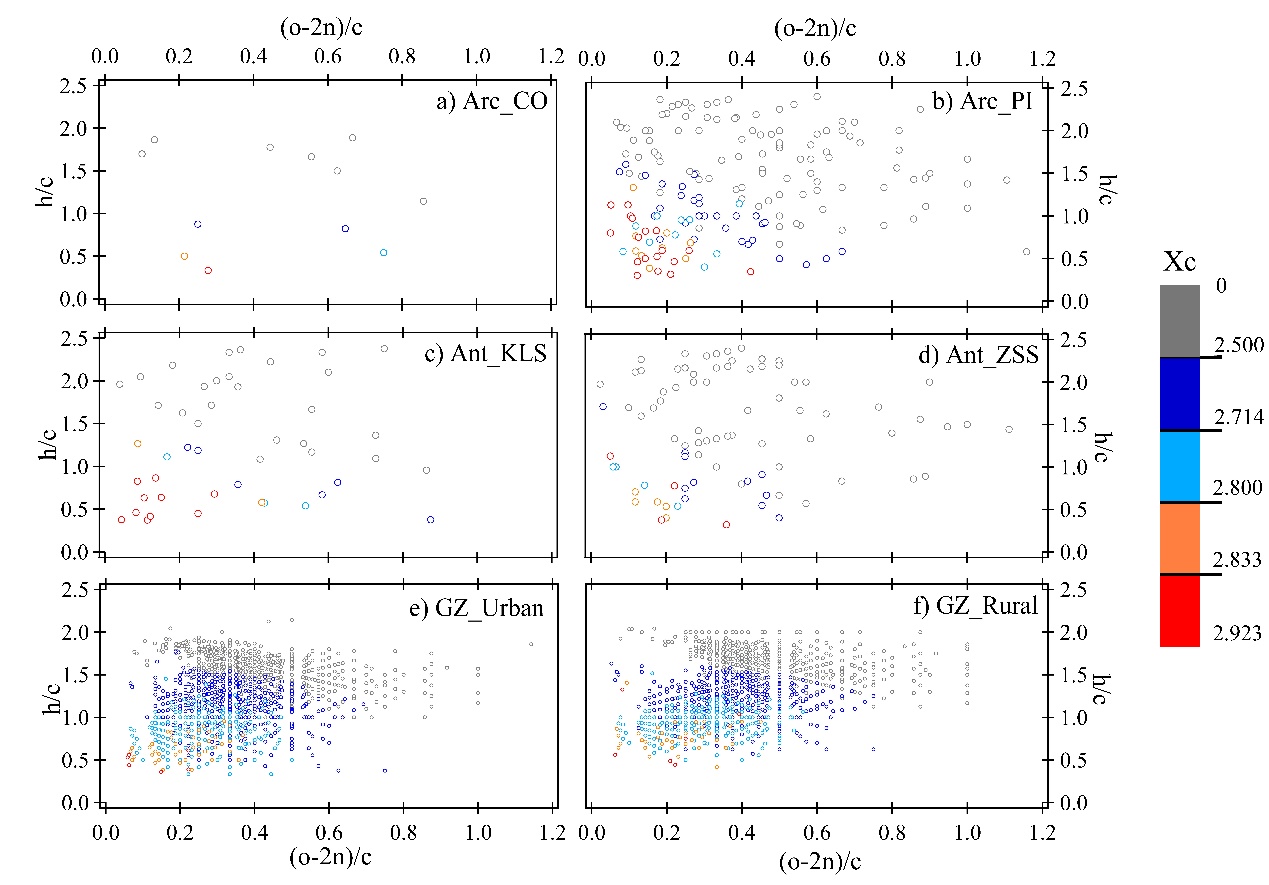
**Figure S1 Concentrations of atmospheric CO and CO2 during the Arctic cruise of 6th CHINARE in 2014.** The two grey area corresponds to the sampling periods selected for this study.

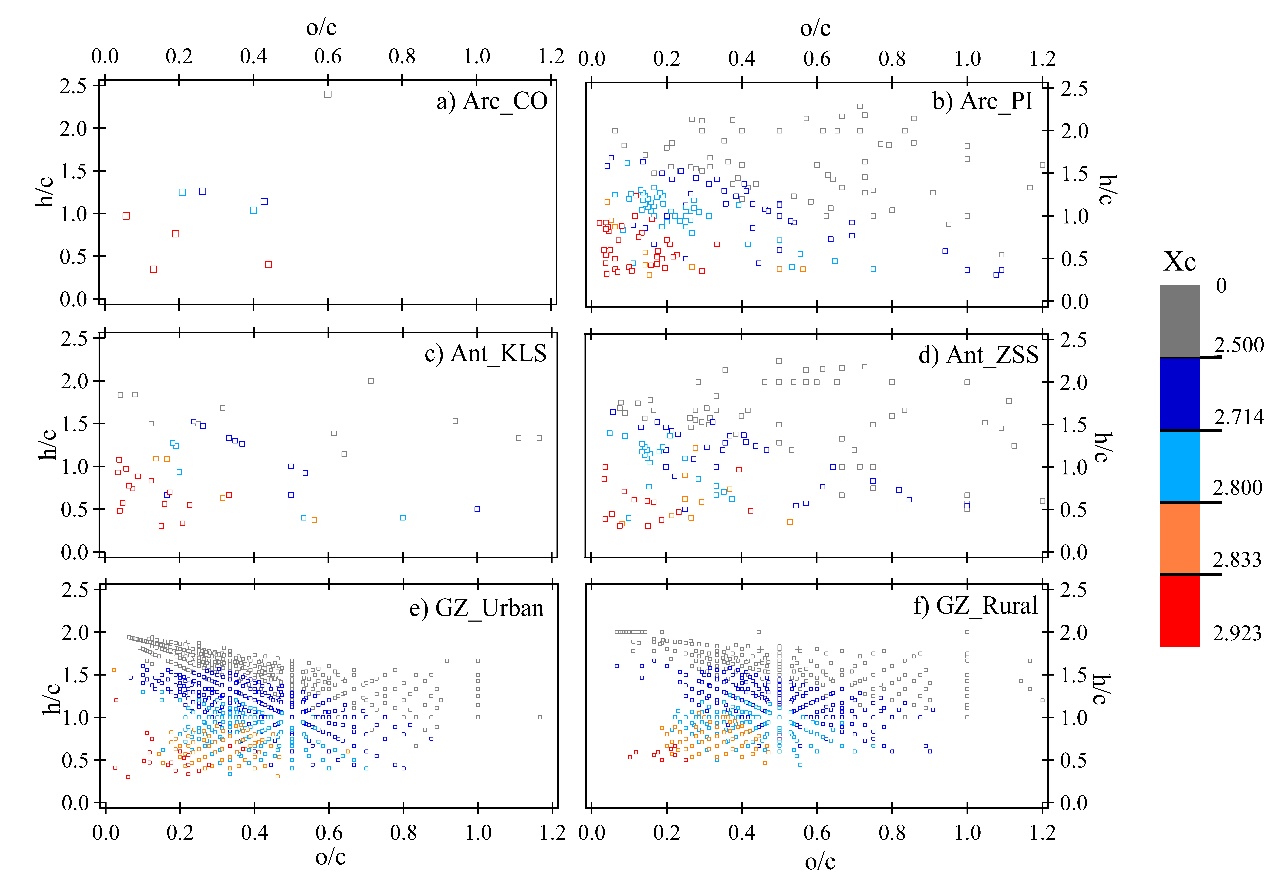
**A)** **Central Arctic Ocean B) Arctic Pack Ice**

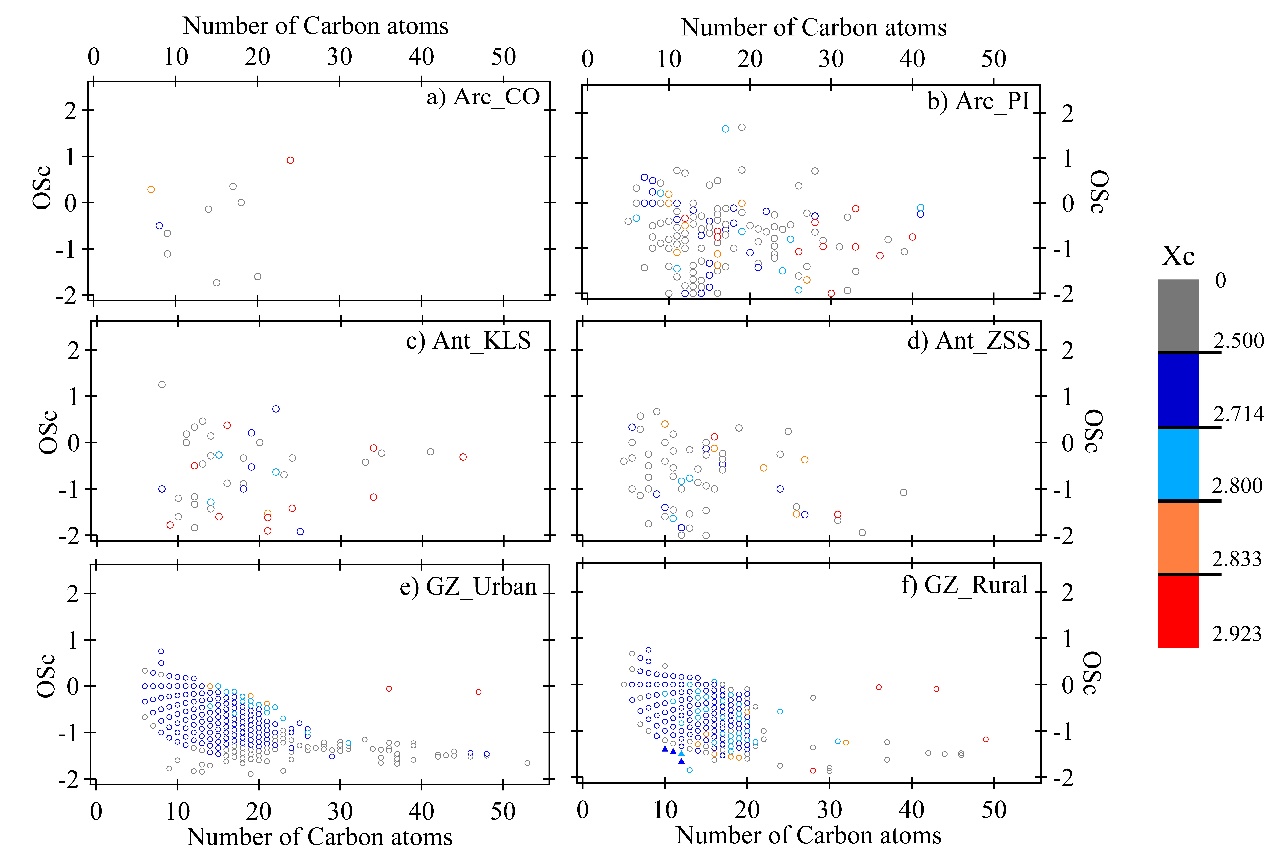
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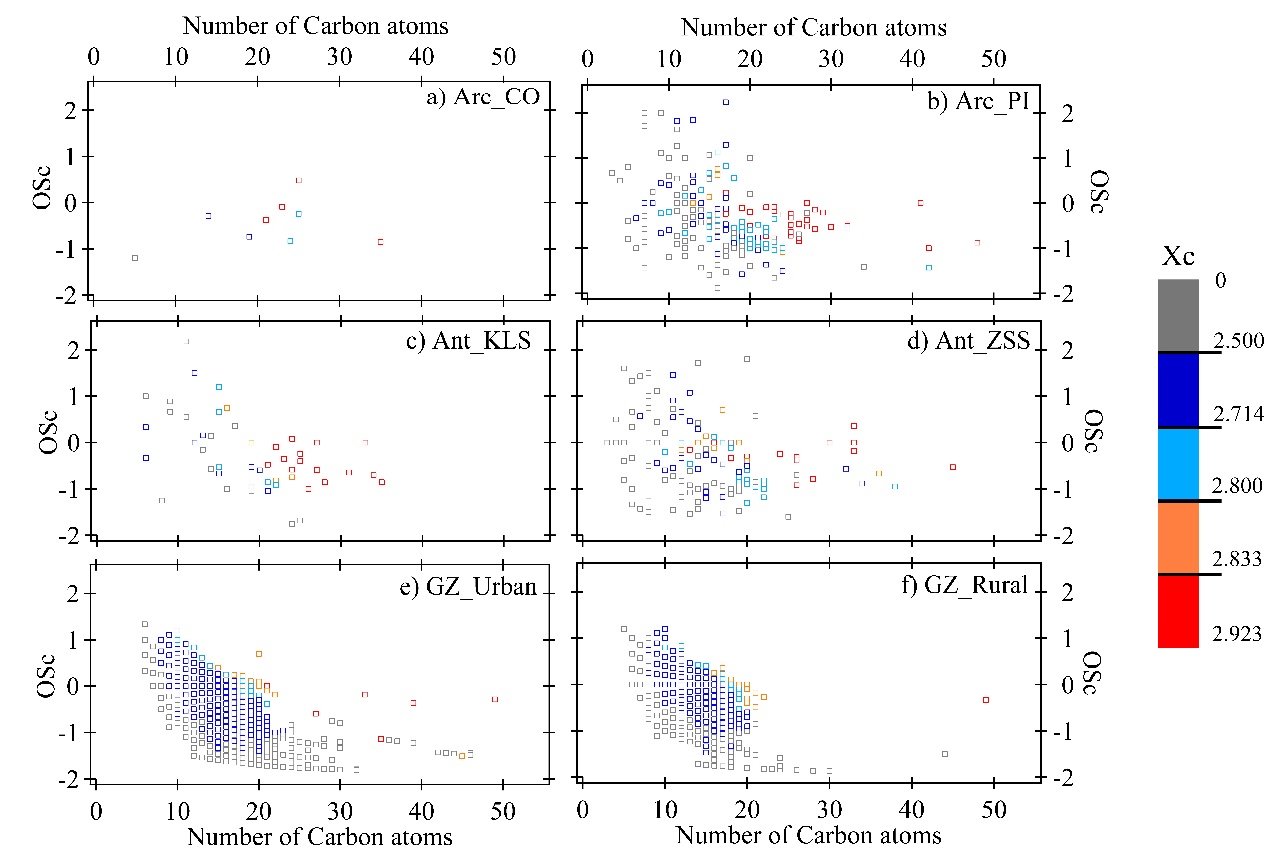
**C) Antarctic Kunlun Station D) Antarctic Zhongshan Station**

**Figure S2 HYSPLIT model results for 120 h back trajectories over the central Arctic Ocean area (A), the Arctic pack ice zone (B), the Antarctic Kunlun Station (C) and the Antarctic Zhongshan Station at start sampling time (D).**

**Figure S3 Van Krevelen Diagrams for ONs molecules in the six sampling sites.** The color-coding represents the Xc values calculated from Eq. (2). The gray marks represent aliphatic compounds (Xc < 2.500), the dark blue marks represent aromatics with a benzene core structure (2.500 ≤ Xc < 2.714), the light blue marks represent aromatics with a naphthalene core structure (2.714 ≤ Xc < 2.800), the orange marks represent aromatics with a anthracene core structure (2.800 ≤ Xc < 2.833), the red marks represent aromatics with a pyrene core structure (2.833 ≤ Xc < 2.923).

**Figure S4 Van Krevelen Diagrams for OxyCs molecules in the six sampling sites.** The color-coding represents the Xc values calculated from Eq. (2). The gray marks represent aliphatic compounds (Xc < 2.500), the dark blue marks represent aromatics with a benzene core structure (2.500 ≤ Xc < 2.714), the light blue marks represent aromatics with a naphthalene core structure (2.714 ≤ Xc < 2.800), the orange marks represent aromatics with a anthracene core structure (2.800 ≤ Xc < 2.833), the red marks represent aromatics with a pyrene core structure (2.833 ≤ Xc < 2.923).

**Figure S5 Oxidation State of Carbon (OSc) for ONs in the six sampling sites.** The color-coding represents the Xc values calculated from Eq. (2). The gray marks represent aliphatic compounds (Xc < 2.500), the dark blue marks represent aromatics with a benzene core structure (2.500 ≤ Xc < 2.714), the light blue marks represent aromatics with a naphthalene core structure (2.714 ≤ Xc < 2.800), the orange marks represent aromatics with a anthracene core structure (2.800 ≤ Xc < 2.833), the red marks represent aromatics with a pyrene core structure (2.833 ≤ Xc < 2.923).

**Figure S6 Oxidation State of Carbon (OSc) for OxyCs in the six sampling sites.** The color-coding represents the Xc values calculated from Eq. (2). The gray marks represent aliphatic compounds (Xc < 2.500), the dark blue marks represent aromatics with a benzene core structure (2.500 ≤ Xc < 2.714), the light blue marks represent aromatics with a naphthalene core structure (2.714 ≤ Xc < 2.800), the orange marks represent aromatics with a anthracene core structure (2.800 ≤ Xc < 2.833), the red marks represent aromatics with a pyrene core structure (2.833 ≤ Xc < 2.923).

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