



Figure S1. Field sites, Yakima River basin catchments sharing similar landscape characteristics and observed water column respiration rates across the Yakima River basin, Washington, USA. (a) Field sites from the 2021 spatial study superimposed on a map of catchment cluster analysis results. U. S. Geological Survey National Hydrography Dataset Plus Version 2.1 (NHDPlusV2.1) catchments were grouped into six classes sharing similar landscape characteristics using key biophysical and hydrologic variables and characterized according to tree height, precipitation, and elevation. Field sites located in cluster 1 are characterized as tree dominated high elevation mesic sites. Field sites located in cluster 3 are characterized as tree dominated, high elevation, hydric sites. Field sites located in cluster 4 are characterized as shrub-steppe, middle elevation, xeric sites. Field sites located in cluster 5 are characterized as tree dominated, middle elevation, mesic sites. Field sites located in cluster 6 are characterized as tree dominated, middle elevation, xeric sites. No sites were in cluster 2, which is characterized as water dominated. (b) Yakima River basin water column respiration rates (ERwc, mg O<sub>2</sub> L<sup>-1</sup> d<sup>-1</sup>) by site overlaid on a shaded hillslope map of the basin and the Yakima River and its tributaries. Map data from the National Hydrography Dataset Plus (NHDPlusV2.1) include catchment boundaries from the Watershed Boundary Dataset (WBD) and hydrography data from the National Hydrography Dataset (NHD) (U.S. Geological Survey, 2019).

15 **Table S1. Key climate, vegetation structure and function, topography, and wildfire potential variables and statistical moments used in the Columbia River basin catchment cluster analysis.**

<b>Variable Name</b>	<b>Description</b>
catchment_ID	Catchment ID number
AreaSqKM	Area of each catchment in sq km
herb_cov_evc_MAX	LANDFIRE - Herbaceous Existing Vegetation Cover (maximum value per catchment)
herb_cov_evc_MEAN	LANDFIRE - Herbaceous Existing Vegetation Cover (mean value per catchment)
herb_cov_evc_MIN	LANDFIRE - Herbaceous Existing Vegetation Cover (minimum value per catchment)
herb_cov_evc_STD	LANDFIRE - Herbaceous Existing Vegetation Cover (standard deviation per catchment)
herb_hgt_evh_MAX	LANDFIRE - Herbaceous Existing Vegetation Height (maximum value per catchment)
herb_hgt_evh_MEAN	LANDFIRE - Herbaceous Existing Vegetation Height (mean value per catchment)
herb_hgt_evh_MIN	LANDFIRE - Herbaceous Existing Vegetation Height (minimum value per catchment)
herb_hgt_evh_STD	LANDFIRE - Herbaceous Existing Vegetation Height (standard deviation per catchment)
MCD15A3H_FPAR_1_MAX	MODIS - January Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_1_MEAN	MODIS - January Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_1_MIN	MODIS - January Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_1_STD	MODIS - January Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_10_MAX	MODIS - October Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_10_MEAN	MODIS - October Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_10_MIN	MODIS - October Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_10_STD	MODIS - October Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_11_MAX	MODIS - November Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_11_MEAN	MODIS - November Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_11_MIN	MODIS - November Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_11_STD	MODIS - November Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_12_MAX	MODIS - December Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_12_MEAN	MODIS - December Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_12_MIN	MODIS - December Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_12_STD	MODIS - December Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_2_MAX	MODIS - February Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_2_MEAN	MODIS - February Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_2_MIN	MODIS - February Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_2_STD	MODIS - February Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_2009_2019_median_MAX	MODIS - Long-Term Median Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_2009_2019_median_MEAN	MODIS - Long-Term Median Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_2009_2019_median_MIN	MODIS - Long-Term Median Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_2009_2019_median_STD	MODIS - Long-Term Median Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_3_MAX	MODIS - March Fraction of Photosynthetically Active Radiation (maximum value per catchment)

<b>Variable Name</b>	<b>Description</b>
MCD15A3H_FPAR_3_MEAN	MODIS - March Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_3_MIN	MODIS - March Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_3_STD	MODIS - March Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_4_MAX	MODIS - April Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_4_MEAN	MODIS - April Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_4_MIN	MODIS - April Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_4_STD	MODIS - April Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_5_MAX	MODIS - May Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_5_MEAN	MODIS - May Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_5_MIN	MODIS - May Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_5_STD	MODIS - May Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_6_MAX	MODIS - June Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_6_MEAN	MODIS - June Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_6_MIN	MODIS - June Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_6_STD	MODIS - June Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_7_MAX	MODIS - July Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_7_MEAN	MODIS - July Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_7_MIN	MODIS - July Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_7_STD	MODIS - July Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_8_MAX	MODIS - August Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_8_MEAN	MODIS - August Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_8_MIN	MODIS - August Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_8_STD	MODIS - August Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_FPAR_9_MAX	MODIS - September Fraction of Photosynthetically Active Radiation (maximum value per catchment)
MCD15A3H_FPAR_9_MEAN	MODIS - September Fraction of Photosynthetically Active Radiation (mean value per catchment)
MCD15A3H_FPAR_9_MIN	MODIS - September Fraction of Photosynthetically Active Radiation (minimum value per catchment)
MCD15A3H_FPAR_9_STD	MODIS - September Fraction of Photosynthetically Active Radiation (standard deviation per catchment)
MCD15A3H_LAI_1_MAX	MODIS - January Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_1_MEAN	MODIS - January Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_1_MIN	MODIS - January Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_1_STD	MODIS - January Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_10_MAX	MODIS - October Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_10_MEAN	MODIS - October Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_10_MIN	MODIS - October Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_10_STD	MODIS - October Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_11_MAX	MODIS - November Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_11_MEAN	MODIS - November Leaf Area Index (mean value per catchment)

<b>Variable Name</b>	<b>Description</b>
MCD15A3H_LAI_11_MIN	MODIS - November Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_11_STD	MODIS - November Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_12_MAX	MODIS - December Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_12_MEAN	MODIS - December Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_12_MIN	MODIS - December Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_12_STD	MODIS - December Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_2_MAX	MODIS - February Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_2_MEAN	MODIS - February Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_2_MIN	MODIS - February Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_2_STD	MODIS - February Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_2009_2019_median_MAX	MODIS - Long-Term Median Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_2009_2019_median_MEAN	MODIS - Long-Term Median Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_2009_2019_median_MIN	MODIS - Long-Term Median Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_2009_2019_median_STD	MODIS - Long-Term Median Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_3_MAX	MODIS - March Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_3_MEAN	MODIS - March Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_3_MIN	MODIS - March Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_3_STD	MODIS - March Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_4_MAX	MODIS - April Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_4_MEAN	MODIS - April Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_4_MIN	MODIS - April Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_4_STD	MODIS - April Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_5_MAX	MODIS - May Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_5_MEAN	MODIS - May Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_5_MIN	MODIS - May Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_5_STD	MODIS - May Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_6_MAX	MODIS - June Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_6_MEAN	MODIS - June Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_6_MIN	MODIS - June Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_6_STD	MODIS - June Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_7_MAX	MODIS - July Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_7_MEAN	MODIS - July Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_7_MIN	MODIS - July Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_7_STD	MODIS - July Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_8_MAX	MODIS - August Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_8_MEAN	MODIS - August Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_8_MIN	MODIS - August Leaf Area Index (minimum value per catchment)

<b>Variable Name</b>	<b>Description</b>
MCD15A3H_LAI_8_STD	MODIS - August Leaf Area Index (standard deviation per catchment)
MCD15A3H_LAI_9_MAX	MODIS - September Leaf Area Index (maximum value per catchment)
MCD15A3H_LAI_9_MEAN	MODIS - September Leaf Area Index (mean value per catchment)
MCD15A3H_LAI_9_MIN	MODIS - September Leaf Area Index (minimum value per catchment)
MCD15A3H_LAI_9_STD	MODIS - September Leaf Area Index (standard deviation per catchment)
MOD16A2_ET_10_MAX	MODIS - October Evapotranspiration (maximum value per catchment)
MOD16A2_ET_10_MEAN	MODIS - October Evapotranspiration (mean value per catchment)
MOD16A2_ET_10_MIN	MODIS - October Evapotranspiration (minimum value per catchment)
MOD16A2_ET_10_STD	MODIS - October Evapotranspiration (standard deviation per catchment)
MOD16A2_ET_11_MAX	MODIS - November Evapotranspiration (maximum value per catchment)
MOD16A2_ET_11_MEAN	MODIS - November Evapotranspiration (mean value per catchment)
MOD16A2_ET_11_MIN	MODIS - November Evapotranspiration (minimum value per catchment)
MOD16A2_ET_11_STD	MODIS - November Evapotranspiration (standard deviation per catchment)
MOD16A2_ET_12_MAX	MODIS - December Evapotranspiration (maximum value per catchment)
MOD16A2_ET_12_MEAN	MODIS - December Evapotranspiration (mean value per catchment)
MOD16A2_ET_12_MIN	MODIS - December Evapotranspiration (minimum value per catchment)
MOD16A2_ET_12_STD	MODIS - December Evapotranspiration (standard deviation per catchment)
MOD16A2_ET_2009_2019_median_MAX	MODIS - Long-Term Median Evapotranspiration (maximum value per catchment)
MOD16A2_ET_2009_2019_median_MEAN	MODIS - Long-Term Median Evapotranspiration (mean value per catchment)
MOD16A2_ET_2009_2019_median_MIN	MODIS - Long-Term Median Evapotranspiration (minimum value per catchment)
MOD16A2_ET_2009_2019_median_STD	MODIS - Long-Term Median Evapotranspiration (standard deviation per catchment)
MOD16A2ET_1_MAX	MODIS - January Evapotranspiration (maximum value per catchment)
MOD16A2ET_1_MEAN	MODIS - January Evapotranspiration (mean value per catchment)
MOD16A2ET_1_MIN	MODIS - January Evapotranspiration (minimum value per catchment)
MOD16A2ET_1_STD	MODIS - January Evapotranspiration (standard deviation per catchment)
MOD16A2ET_2_MAX	MODIS - February Evapotranspiration (maximum value per catchment)
MOD16A2ET_2_MEAN	MODIS - February Evapotranspiration (mean value per catchment)
MOD16A2ET_2_MIN	MODIS - February Evapotranspiration (minimum value per catchment)
MOD16A2ET_2_STD	MODIS - February Evapotranspiration (standard deviation per catchment)
MOD16A2ET_3_MAX	MODIS - March Evapotranspiration (maximum value per catchment)
MOD16A2ET_3_MEAN	MODIS - March Evapotranspiration (mean value per catchment)
MOD16A2ET_3_MIN	MODIS - March Evapotranspiration (minimum value per catchment)
MOD16A2ET_3_STD	MODIS - March Evapotranspiration (standard deviation per catchment)
MOD16A2ET_4_MAX	MODIS - April Evapotranspiration (maximum value per catchment)
MOD16A2ET_4_MEAN	MODIS - April Evapotranspiration (mean value per catchment)
MOD16A2ET_4_MIN	MODIS - April Evapotranspiration (minimum value per catchment)
MOD16A2ET_4_STD	MODIS - April Evapotranspiration (standard deviation per catchment)

<b>Variable Name</b>	<b>Description</b>
MOD16A2ET_5_MAX	MODIS - May Evapotranspiration (maximum value per catchment)
MOD16A2ET_5_MEAN	MODIS - May Evapotranspiration (mean value per catchment)
MOD16A2ET_5_MIN	MODIS - May Evapotranspiration (minimum value per catchment)
MOD16A2ET_5_STD	MODIS - May Evapotranspiration (standard deviation per catchment)
MOD16A2ET_6_MAX	MODIS - June Evapotranspiration (maximum value per catchment)
MOD16A2ET_6_MEAN	MODIS - June Evapotranspiration (mean value per catchment)
MOD16A2ET_6_MIN	MODIS - June Evapotranspiration (minimum value per catchment)
MOD16A2ET_6_STD	MODIS - June Evapotranspiration (standard deviation per catchment)
MOD16A2ET_7_MAX	MODIS - July Evapotranspiration (maximum value per catchment)
MOD16A2ET_7_MEAN	MODIS - July Evapotranspiration (mean value per catchment)
MOD16A2ET_7_MIN	MODIS - July Evapotranspiration (minimum value per catchment)
MOD16A2ET_7_STD	MODIS - July Evapotranspiration (standard deviation per catchment)
MOD16A2ET_8_MAX	MODIS - August Evapotranspiration (maximum value per catchment)
MOD16A2ET_8_MEAN	MODIS - August Evapotranspiration (mean value per catchment)
MOD16A2ET_8_MIN	MODIS - August Evapotranspiration (minimum value per catchment)
MOD16A2ET_8_STD	MODIS - August Evapotranspiration (standard deviation per catchment)
MOD16A2ET_9_MAX	MODIS - September Evapotranspiration (maximum value per catchment)
MOD16A2ET_9_MEAN	MODIS - September Evapotranspiration (mean value per catchment)
MOD16A2ET_9_MIN	MODIS - September Evapotranspiration (minimum value per catchment)
MOD16A2ET_9_STD	MODIS - September Evapotranspiration (standard deviation per catchment)
MOD17A3H_NPP_2004_2014_median_MAX	MODIS - Net Primary Productivity Long-Term Median (maximum value per catchment)
MOD17A3H_NPP_2004_2014_median_MEAN	MODIS - Net Primary Productivity Long-Term Median (mean value per catchment)
MOD17A3H_NPP_2004_2014_median_MIN	MODIS - Net Primary Productivity Long-Term Median (minimum value per catchment)
MOD17A3H_NPP_2004_2014_median_STD	MODIS - Net Primary Productivity Long-Term Median (standard deviation per catchment)
ned17_MAX	NHDPlus - National Elevation Dataset (maximum value per catchment)
ned17_MEAN	NHDPlus - National Elevation Dataset (mean value per catchment)
ned17_MIN	NHDPlus - National Elevation Dataset (minimum value per catchment)
ned17_STD	NHDPlus - National Elevation Dataset (standard deviation per catchment)
ned17shadedrelief_MAX	NHDPlus - National Elevation Dataset, Shaded Relief (maximum value per catchment)
ned17shadedrelief_MEAN	NHDPlus - National Elevation Dataset, Shaded Relief (mean value per catchment)
ned17shadedrelief_MIN	NHDPlus - National Elevation Dataset, Shaded Relief (minimum value per catchment)
ned17shadedrelief_STD	NHDPlus - National Elevation Dataset, Shaded Relief (standard deviation per catchment)
pheno_AMP_ltmean_MAX	MODIS Phenology - Amplitude (maximum value per catchment)
pheno_AMP_ltmean_MEAN	MODIS Phenology - Amplitude (mean value per catchment)
pheno_AMP_ltmean_MIN	MODIS Phenology - Amplitude (minimum value per catchment)
pheno_AMP_ltmean_STD	MODIS Phenology - Amplitude (standard deviation per catchment)
pheno_DUR_ltmean_MAX	MODIS Phenology - Duration (maximum value per catchment)

<b>Variable Name</b>	<b>Description</b>
pheno_DUR_Itmean_MEAN	MODIS Phenology - Duration (mean value per catchment)
pheno_DUR_Itmean_MIN	MODIS Phenology - Duration (minimum value per catchment)
pheno_DUR_Itmean_STD	MODIS Phenology - Duration (standard deviation per catchment)
pheno_EOSN_Itmean_MAX	MODIS Phenology - End of Season Normalized Difference Vegetation Index (maximum value per catchment)
pheno_EOSN_Itmean_MEAN	MODIS Phenology - End of Season Normalized Difference Vegetation Index (mean value per catchment)
pheno_EOSN_Itmean_MIN	MODIS Phenology - End of Season Normalized Difference Vegetation Index (minimum value per catchment)
pheno_EOSN_Itmean_STD	MODIS Phenology - End of Season Normalized Difference Vegetation Index (standard deviation per catchment)
pheno_EOST_Itmean_MAX	MODIS Phenology - End of Season Time (maximum value per catchment)
pheno_EOST_Itmean_MEAN	MODIS Phenology - End of Season Time (mean value per catchment)
pheno_EOST_Itmean_MIN	MODIS Phenology - End of Season Time (minimum value per catchment)
pheno_EOST_Itmean_STD	MODIS Phenology - End of Season Time (standard deviation per catchment)
pheno_MAXN_Itmean_MAX	MODIS Phenology - Maximum Normalized Difference Vegetation Index (maximum value per catchment)
pheno_MAXN_Itmean_MEAN	MODIS Phenology - Maximum Normalized Difference Vegetation Index (maximum value per catchment)
pheno_MAXN_Itmean_MIN	MODIS Phenology - Maximum Normalized Difference Vegetation Index (maximum value per catchment)
pheno_MAXN_Itmean_STD	MODIS Phenology - Maximum Normalized Difference Vegetation Index (maximum value per catchment)
pheno_SOSN_Itmean_MAX	MODIS Phenology - Start of Season Normalized Difference Vegetation Index (maximum value per catchment)
pheno_SOSN_Itmean_MEAN	MODIS Phenology - Start of Season Normalized Difference Vegetation Index (mean value per catchment)
pheno_SOSN_Itmean_MIN	MODIS Phenology - Start of Season Normalized Difference Vegetation Index (minimum value per catchment)
pheno_SOSN_Itmean_STD	MODIS Phenology - Start of Season Normalized Difference Vegetation Index (standard deviation per catchment)
pheno_SOST_Itmean_MAX	MODIS Phenology - Start of Season Time (maximum value per catchment)
pheno_SOST_Itmean_MEAN	MODIS Phenology - Start of Season Time (mean value per catchment)
pheno_SOST_Itmean_MIN	MODIS Phenology - Start of Season Time (minimum value per catchment)
pheno_SOST_Itmean_STD	MODIS Phenology - Start of Season Time (standard deviation per catchment)
pheno_TIN_Itmean_MAX	MODIS Phenology - Time Integrated Normalized Difference Vegetation Index (maximum value per catchment)
pheno_TIN_Itmean_MEAN	MODIS Phenology - Time Integrated Normalized Difference Vegetation Index (mean value per catchment)
pheno_TIN_Itmean_MIN	MODIS Phenology - Time Integrated Normalized Difference Vegetation Index (minimum value per catchment)
pheno_TIN_Itmean_STD	MODIS Phenology - Time Integrated Normalized Difference Vegetation Index (standard deviation per catchment)
ppt_30yr_norm_01_MAX	PRISM - Normalized 30-Year Precipitation for January (maximum value per catchment)
ppt_30yr_norm_01_MEAN	PRISM - Normalized 30-Year Precipitation for January (mean value per catchment)
ppt_30yr_norm_01_MIN	PRISM - Normalized 30-Year Precipitation for January (minimum value per catchment)
ppt_30yr_norm_01_STD	PRISM - Normalized 30-Year Precipitation for January (standard deviation per catchment)
ppt_30yr_norm_02_MAX	PRISM - Normalized 30-Year Precipitation for February (maximum value per catchment)
ppt_30yr_norm_02_MEAN	PRISM - Normalized 30-Year Precipitation for February (mean value per catchment)
ppt_30yr_norm_02_MIN	PRISM - Normalized 30-Year Precipitation for February (minimum value per catchment)
ppt_30yr_norm_02_STD	PRISM - Normalized 30-Year Precipitation for February (standard deviation per catchment)
ppt_30yr_norm_03_MAX	PRISM - Normalized 30-Year Precipitation for March (maximum value per catchment)
ppt_30yr_norm_03_MEAN	PRISM - Normalized 30-Year Precipitation for March (mean value per catchment)

<b>Variable Name</b>	<b>Description</b>
ppt_30yr_norm_03_MIN	PRISM - Normalized 30-Year Precipitation for March (minimum value per catchment)
ppt_30yr_norm_03_STD	PRISM - Normalized 30-Year Precipitation for March (standard deviation per catchment)
ppt_30yr_norm_04_MAX	PRISM - Normalized 30-Year Precipitation for April (maximum value per catchment)
ppt_30yr_norm_04_MEAN	PRISM - Normalized 30-Year Precipitation for April (mean value per catchment)
ppt_30yr_norm_04_MIN	PRISM - Normalized 30-Year Precipitation for April (minimum value per catchment)
ppt_30yr_norm_04_STD	PRISM - Normalized 30-Year Precipitation for April (standard deviation per catchment)
ppt_30yr_norm_05_MAX	PRISM - Normalized 30-Year Precipitation for May (maximum value per catchment)
ppt_30yr_norm_05_MEAN	PRISM - Normalized 30-Year Precipitation for May (mean value per catchment)
ppt_30yr_norm_05_MIN	PRISM - Normalized 30-Year Precipitation for May (minimum value per catchment)
ppt_30yr_norm_05_STD	PRISM - Normalized 30-Year Precipitation for May (standard deviation per catchment)
ppt_30yr_norm_06_MAX	PRISM - Normalized 30-Year Precipitation for June (maximum value per catchment)
ppt_30yr_norm_06_MEAN	PRISM - Normalized 30-Year Precipitation for June (mean value per catchment)
ppt_30yr_norm_06_MIN	PRISM - Normalized 30-Year Precipitation for June (minimum value per catchment)
ppt_30yr_norm_06_STD	PRISM - Normalized 30-Year Precipitation for June (standard deviation per catchment)
ppt_30yr_norm_07_MAX	PRISM - Normalized 30-Year Precipitation for July (maximum value per catchment)
ppt_30yr_norm_07_MEAN	PRISM - Normalized 30-Year Precipitation for July (mean value per catchment)
ppt_30yr_norm_07_MIN	PRISM - Normalized 30-Year Precipitation for July (minimum value per catchment)
ppt_30yr_norm_07_STD	PRISM - Normalized 30-Year Precipitation for July (standard deviation per catchment)
ppt_30yr_norm_08_MAX	PRISM - Normalized 30-Year Precipitation for August (maximum value per catchment)
ppt_30yr_norm_08_MEAN	PRISM - Normalized 30-Year Precipitation for August (mean value per catchment)
ppt_30yr_norm_08_MIN	PRISM - Normalized 30-Year Precipitation for August (minimum value per catchment)
ppt_30yr_norm_08_STD	PRISM - Normalized 30-Year Precipitation for August (standard deviation per catchment)
ppt_30yr_norm_09_MAX	PRISM - Normalized 30-Year Precipitation for September (maximum value per catchment)
ppt_30yr_norm_09_MEAN	PRISM - Normalized 30-Year Precipitation for September (mean value per catchment)
ppt_30yr_norm_09_MIN	PRISM - Normalized 30-Year Precipitation for September (minimum value per catchment)
ppt_30yr_norm_09_STD	PRISM - Normalized 30-Year Precipitation for September (standard deviation per catchment)
ppt_30yr_norm_10_MAX	PRISM - Normalized 30-Year Precipitation for October (maximum value per catchment)
ppt_30yr_norm_10_MEAN	PRISM - Normalized 30-Year Precipitation for October (mean value per catchment)
ppt_30yr_norm_10_MIN	PRISM - Normalized 30-Year Precipitation for October (minimum value per catchment)
ppt_30yr_norm_10_STD	PRISM - Normalized 30-Year Precipitation for October (standard deviation per catchment)
ppt_30yr_norm_11_MAX	PRISM - Normalized 30-Year Precipitation for November (maximum value per catchment)
ppt_30yr_norm_11_MEAN	PRISM - Normalized 30-Year Precipitation for November (mean value per catchment)
ppt_30yr_norm_11_MIN	PRISM - Normalized 30-Year Precipitation for November (minimum value per catchment)
ppt_30yr_norm_11_STD	PRISM - Normalized 30-Year Precipitation for November (standard deviation per catchment)
ppt_30yr_norm_12_MAX	PRISM - Normalized 30-Year Precipitation for December (maximum value per catchment)
ppt_30yr_norm_12_MEAN	PRISM - Normalized 30-Year Precipitation for December (mean value per catchment)
ppt_30yr_norm_12_MIN	PRISM - Normalized 30-Year Precipitation for December (minimum value per catchment)



Variable Name	Description
ppt_30yr_norm_12_STD	PRISM - Normalized 30-Year Precipitation for December (standard deviation per catchment)
ppt_30yr_norm_annual_MAX	PRISM - Normalized, Annual 30-Year Precipitation (maximum value per catchment)
ppt_30yr_norm_annual_MEAN	PRISM - Normalized, Annual 30-Year Precipitation (mean value per catchment)
ppt_30yr_norm_annual_MIN	PRISM - Normalized, Annual 30-Year Precipitation (minimum value per catchment)
ppt_30yr_norm_annual_STD	PRISM - Normalized, Annual 30-Year Precipitation (standard deviation per catchment)
shrub_cov_evc_MAX	LANDFIRE - Shrub Existing Vegetation Cover (maximum value per catchment)
shrub_cov_evc_MEAN	LANDFIRE - Shrub Existing Vegetation Cover (mean value per catchment)
shrub_cov_evc_MIN	LANDFIRE - Shrub Existing Vegetation Cover (minimum value per catchment)
shrub_cov_evc_STD	LANDFIRE - Shrub Existing Vegetation Cover (standard deviation per catchment)
shrub_hgt_evh_MAX	LANDFIRE - Shrub Existing Vegetation Height (maximum value per catchment)
shrub_hgt_evh_MEAN	LANDFIRE - Shrub Existing Vegetation Height (mean value per catchment)
shrub_hgt_evh_MIN	LANDFIRE - Shrub Existing Vegetation Height (minimum value per catchment)
shrub_hgt_evh_STD	LANDFIRE - Shrub Existing Vegetation Height (standard deviation per catchment)
tree_cov_evc_MAX	LANDFIRE - Tree Existing Vegetation Cover (maximum value per catchment)
tree_cov_evc_MEAN	LANDFIRE - Tree Existing Vegetation Cover (mean value per catchment)
tree_cov_evc_MIN	LANDFIRE - Tree Existing Vegetation Cover (minimum value per catchment)
tree_cov_evc_STD	LANDFIRE - Tree Existing Vegetation Cover (standard deviation per catchment)
tree_hgt_evh_MAX	LANDFIRE - Tree Existing Vegetation Height (maximum value per catchment)
tree_hgt_evh_MEAN	LANDFIRE - Tree Existing Vegetation Height (mean value per catchment)
tree_hgt_evh_MIN	LANDFIRE - Tree Existing Vegetation Height (minimum value per catchment)
tree_hgt_evh_STD	LANDFIRE - Tree Existing Vegetation Height (standard deviation per catchment)
WHP_MAX	USFS - Wildfire Hazard Potential (maximum value per catchment)
WHP_MEAN	USFS - Wildfire Hazard Potential (mean value per catchment)
WHP_MIN	USFS - Wildfire Hazard Potential (minimum value per catchment)
WHP_STD	USFS - Wildfire Hazard Potential (standard deviation per catchment)

A total of 280 variables (i.e., variable-statistical moment combinations) were created as input data to cluster analysis by calculating the four statistical moments (mean, minimum, maximum, and standard deviation values) for each of 16 key biophysical and hydrological attributes. The cluster analysis was performed to group Columbia River basin NHDPlusV2.1 catchments into six classes sharing similar characteristics. The 16 key biophysical and hydrological variables include: 1) MODIS-derived existing vegetation cover, percent (shrub, tree, and herbaceous vegetation; %); 2) MODIS-derived existing vegetation cover (shrub, tree, and herbaceous vegetation), height (m); 3) eMODIS Phenology-derived net primary productivity (NPP), long-term median ( $\text{kg C m}^{-2} \text{y}^{-1}$ ); 4) eMODIS Phenology-derived net ecosystem productivity (NEP), long-term median ( $\text{kg C m}^{-2} \text{y}^{-1}$ ); 5) eMODIS Phenology-derived amplitude (day of the year); 6) eMODIS Phenology-derived length of growing season (number of days); 7) eMODIS Phenology-derived time of growing season, start-of-season and end-of-season (day of year); 8) eMODIS Phenology-derived normalized difference vegetation index (NDVI), start-of-season, end-of-season, maximum, and time-integrated NDVI values; 9) MODIS-derived leaf area index (LAI;  $\text{m}^2$  green leaf area per  $\text{m}^2$  land area); 10) MODIS-derived fraction of photosynthetically active radiation (FPAR), monthly and long-term median (%); 11) MODIS-derived total evapotranspiration (ET), monthly and long-term median ( $\text{kg H}_2\text{O m}^{-2} \text{land area d}^{-1}$ ); 12) PRISM-derived 30-year precipitation (PPT), normalized monthly and normalized annual (mm); 13) National Elevation Dataset (NED)-derived elevation (m); 14) National Elevation Dataset (NED)-derived slope (%); 15) National Elevation Dataset (NED)-derived aspect; and 16) LANDFIRE-derived USFS Wildfire Hazard Potential (WHP). See the Code and Data Availability section for more information on the source of these data and how these data were processed and analyzed for use in this study. and procto the code and data used to perform the catchment cluster analysis.

30 **Table S2. Key biophysical and hydrological variable-statistical moment combinations evaluated for use in the Columbia River catchment cluster analysis.**

Variable Set	Description	Variables <sup>b</sup>	Moments <sup>c</sup>	Months	<i>n</i>	Notes
0	All zonal and tabulation statistical moments for all variables	All	All	January–December	280	
1	All variables using zonal mean only	All	zonal mean	January–December	70	
2	Set 1 AND only months 3, 7, and 11 for FPAR, LAI, ET, and PPT	FPAR, LAI, ET, PPT	zonal mean	March, July, November	30	
3	Set 1 AND only long-term median for FPAR, LAI, ET, and PPT	FPAR, LAI, ET, PPT	long-term median	March, July, November	22	
4	Set 3 with FPAR and PPT	FPAR, PPT	long-term median	March, July, November	20	Dropped LAI, ET
5	Set 3 with LAI and PPT	LAI, PPT	long-term median	March, July, November	20	Dropped FPAR, ET
6	Set 3 with ET and PPT	ET, PPT	long-term median	March, July, November	20	Dropped FPAR, LAI
7	All variables using zonal SD only	All	zonal SD	January–December	70	
8 <sup>a</sup>	All variables using zonal mean and SD	All	zonal mean, zonal SD	January–December	140	
9	Set 2 with only FPAR and PPT	FPAR, PPT	zonal mean	March, July, November	24	
10	Set 2 with only LAI and PPT	LAI, PPT	zonal mean	March, July, November	24	
11	Set 2 with only ET and PPT	ET, PPT	zonal mean	March, July, November	24	
12	PCA derived from means of all variables	All	mean	January - December	30	Used top 30 PCA components (PC1–PC30)

<sup>a</sup> Variable set 8 was used in the final Columbia River basin catchment cluster analysis. The data set includes two statistical moments (zonal mean and zonal SD) for the key biophysical and hydrological variables shown in Table S1.

<sup>b</sup> The description for the 13 variable sets analyzed using cluster analysis lists the key biophysical and hydrological variables and the statistical moments for each key variable included in a specific variable set. FPAR (%) is the MODIS-derived fraction of photosynthetically active radiation for the month(s) indicated. LAI (m<sup>2</sup> green leaf area per m<sup>-2</sup> land area) is the MODIS-derived Leaf Area Index for the month(s) indicated. ET (kg H<sub>2</sub>O m<sup>-2</sup> d<sup>-1</sup>) is the MODIS-derived total evapotranspiration for the month(s) indicated. PPT (mm) is the PRISM-derived, normalized 30-year precipitation for the month(s) indicated.

<sup>c</sup> Key biophysical and hydrological variables in each variable includes either 1) all the key variables shown in Table S1 or 2) a subset of the key variables shown in Table S1.

<sup>d</sup> “All” includes the following four statistical moments calculated for the key variables in each variable set: 1) mean value, 2) minimum value, 3) maximum value, and 4) standard deviation (SD), and 5) long-term median value calculated for the variables listed.

<sup>e</sup> *n* is the total number of key variable-statistical moment combinations in each variable set.

**Table S3. Expanded cluster analysis results characterizing NHDPlusV2.1 catchments across the Columbia River basin and Yakima River basin with similar biophysical and hydrologic characteristics and the number and percentage of sites in each.**

<b>Cluster</b>	<b>Name</b>	<b>CRB Catchments</b>	<b>CRB Drainage Area</b>	<b>YRB Catchments</b>	<b>YRB Drainage Area</b>	<b>YRB Sites Per Cluster</b>	<b>Percent YRB Sites Per Cluster</b>
<b>1</b>	Tree dominated high elevation mesic	41,153	23%	1,553	27%	9	19%
<b>2</b>	Water dominated	6,188	34%	127	2%	0	0%
<b>3</b>	Tree dominated high elevation hydric	13,223	7%	136	2%	2	4%
<b>4</b>	Shrub-steppe middle elevation xeric	46,028	25%	1,591	28%	10	21%
<b>5</b>	Tree dominated middle elevation mesic	31,549	17%	982	17%	13	28%
<b>6</b>	Tree dominated middle elevation xeric	43,390	24%	1,282	23%	13	28%

“CRB Catchments” is the number of NHDPlusV2.1 catchments within the Columbia River basin classified in each cluster type. “CRB Drainage Area” is the percentage of the total drainage area of the Columbia River basin that was classified in each cluster. “YRB Catchments” is the number of NHDPlusV2.1 catchments within the Yakima River basin classified in each cluster. “YRB Drainage Area” is the percentage of the total drainage area of the Yakima River basin that was classified in each cluster. “YRB Sites Per Cluster” is the total number of field sites in the Yakima River basin located in each cluster. “YRB Sites Per Cluster” is the percentage of field sites located in each cluster.

Table S4. Name or molecular formula and mass for 1,255 commonly observed biochemical transformations.

Name	Mass
CH4_O	0.036380
NH_CH2	0.995250
2ndIP	1.997000
Na_H	21.981940
CH3COO-	59.013305
PO43-	94.953423
SO42-	95.951732
NO3-	61.987819
NH4+	18.034374
H2S	33.987722
S2O32-	111.928889
Alanine	71.037114
Arginine	156.101111
Asparagine	114.042928
Aspartic Acid	115.026943
Cysteine	103.009186
Cystine	222.013286
Glutamic Acid	129.042593
Glutamine	128.058578
Glycine	57.021464
Histidine	137.058912
Isoleucine	113.084064
Lysine	128.094963
Methionine	131.040486
Phenylalanine	147.068414
Proline	97.052764
Serine	87.032028
Threonine	101.047679
Tryptophan	186.079313
Tyrosine	163.063329
Valine	99.068414
acetotacetate (-H2O)	84.021129
acetone (-H)	57.034040
adenylate (-H2O)	329.052522
biotinyl (-H)	243.080339
biotinyl (-H2O)	226.077600
carbamoyl P transfer (-H2PO4)	44.013639
co-enzyme A (-H)	765.099566
co-enzyme A (-H2O)	748.096826
glutathione (-H2O)	289.073243
isoprene addition (-H)	67.054775
malonyl group (-H2O)	86.000394
palmitoylation (-H2O)	238.229666
pyridoxal phosphate (-H2O)	229.014011
urea addition (-H)	59.024538
adenine (-H)	134.046670
adenosine (-H2O)	249.086189
Adenosine 5'-diphosphate (-H2O)	409.018854
cytidine 5' diphosphate (-H2O)	385.007621
cytidine 5' monophosphate (-H2O)	305.041288

Name	Mass
cytosine (-H)	110.035437
Guanosine 5- diphosphate (-H2O)	425.013769
Guanosine 5- monophosphate (-H2O)	345.047436
guanine (-H)	150.041585
guanosine (-H2O)	265.081104
deoxythymidine 5' diphosphate (-H2O)	384.012372
thymidine (-H2O)	224.079707
thymine (-H)	125.035103
thymidine 5' monophosphate (-H2O)	304.046039
uridine 5' diphosphate (-H2O)	385.991636
uridine 5' monophosphate (-H2O)	306.025304
uracil (-H)	111.019452
uridine (-H2O)	226.058972
acetylation (-H)	59.013304
acetylation (-H2O)	42.010565
C2H2	26.015650
Carboxylation	43.989829
CHO2	44.997654
condensation/dehydration	18.010565
diphosphate	160.940490
ethyl addition (-H2O)	28.031300
Formic Acid (-H2O)	27.994915
glyoxylate (-H2O)	55.989829
hydrogenation/dehydrogenation	2.015650
hydroxylation (-H)	15.994915
Inorganic Phosphate	30.973763
methanol (-H2O)	14.015650
phosphate	79.966332
primary amine	16.018724
pyrophosphate	61.947527
secondary amine	15.010899
sulfate (-H2O)	79.956816
tertiary amine	14.003074
C6H10O5	162.052824
C6H10O6	178.047738
D-Ribose (-H2O) (ribosylation)	132.042259
disaccharide (-H2O)	340.100562
glucose-N-Phosphate (-H2O)	242.019156
Glucuronic Acid (-H2O)	176.032088
trisaccharide (-H2O)	486.158471
erythrose (-H2O)	102.031695
transamination (-O)	2.039459
H2N1O_1	0.023809
C_1H_5N_1O2	0.947631
H_1O1N_1	0.984016
C_1H_1N1	0.995249
C12_C13	1.003355
H1	1.007825
H3N1O_3S1	1.013876
H3O_1N1	1.031634
H_2N_2O2	1.968032
H_1O_2C11	1.971200

Name	Mass
C_1H_2O1	1.979265
N_1O1	1.991841
H_1O_1F1	1.995700
H2	2.015650
CH6O_1	2.052035
H_3N_3O3	2.952048
C_1H1N1O_2S1	2.993141
H1O1N_1	2.999666
H3	3.023475
H5O_1N1	3.047284
C_1O1	3.994915
H4	4.031300
H3N_1O1	5.015316
C4H6N1O_2P_1	5.086431
C_2H_2O2	5.974180
H_4N3O_2	5.988092
C2H_2O_1	5.989435
C_1H2O	6.010565
C3H2O_2	6.025820
H6	6.046950
C_1H1N_1S1	6.976823
H5O1N_1	7.030966
CH_4	7.968700
C_2O2	7.989830
C2O_1	8.005085
C_1H4O	8.026215
C3H4O_2	8.041470
H8	8.062600
C_2N_1O1P1	8.965604
C1H_1N1O_1	9.000334
C2H3N1O_2	9.036719
H_6O1	9.947965
C_3H_2O3	9.969095
H_2C1	9.984350
C_2H2O2	10.005480
C2H2O_1	10.020735
H10	10.078250
N1H_3	10.979599
C1H_1	10.992175
C1H1N1O_1	11.015984
H_4O1	11.963615
C1	12.000000
C2H4O_1	12.036385
H_3O1	12.971440
CH_1N_1O	12.984016
H_1N1	12.995249
CH	13.007825
C1H3N1O_1	13.031634
C_1H_6O2	13.942880
H_2O1	13.979265
N1	14.003074
CH2	14.015650

Name	Mass
H2N2O_1	14.026883
C2H6O_1	14.052035
H_1S1O_1	14.969332
H_1O1	14.987090
CHN_1O	14.999666
H1N1	15.010900
C1H3	15.023475
CH5NO_1	15.047284
C_1H_4O2	15.958530
O_1S1	15.977157
O1	15.994915
H1O1P1S_1	16.004431
H2N1	16.018724
C1H4	16.031300
O_1H4N2	16.042533
C2H8O_1	16.067685
H16	16.125200
H_1O2N_1	16.978931
O1H1	17.002740
C3H_1N1O_2	17.005419
H3N1	17.026549
C1H5	17.039125
H_1C11O_1	17.966100
C_1H_2O2	17.974180
H2O_1S1	17.992807
H2O	18.010565
CH6	18.046950
H6N2O_1	18.058183
C_8H_9N1O1P2S1	18.847162
H1O2N_1	18.994581
H3O1	19.018390
H5N1	19.042199
C_10H_2O5P2	19.906451
C_1O2	19.989830
C3O_1	20.005085
H4O	20.026215
C2H_2	21.984350
C_1H2O2	22.005480
C3H2O_1	22.020735
CH_4O	23.963615
C2	24.000000
C1O_1N2	24.011233
C_1H4O2	24.021130
C3H4O_1	24.036385
C1H_1N1	24.995249
C2H3NO_1	25.031634
H_2C1O1	25.979265
C1H2O_1N2	26.026883
C2H2O2S_1	26.033408
C3H6O_1	26.052035
C2HN_1O	26.999666
C1H1N1	27.010900

Name	Mass
H3C2	27.023475
C2H5O_1N1	27.047284
H_4O2	27.958530
C_4H1N2O1P1	27.982651
Formic Acid_(H2O)_CO	27.994915
N2	28.006148
ethyl addition_(H2O)_C2H4	28.031300
C15H22O_7P_2	28.260219
H_1N1O1	28.990164
CHO	29.002740
CH3N	29.026549
C2H7N1O_1	29.062934
H_2S1	29.956422
H_2O2	29.974180
O1N1	29.997989
C1H2O1	30.010565
H_1S1	30.964247
CHN_1O2	30.994581
H1N1O1	31.005814
C1H5N1	31.042200
H_3Cl1	31.945400
O_2S2	31.954314
S1	31.972072
O2	31.989830
C1H4O_1S1	32.008457
C1H4O1	32.026215
C2H8	32.062600
H3O_1N1S1	33.003706
H_1Cl1	33.961000
H2O2	34.005480
C4H2O_1	34.020735
C1H6O1	34.041865
H2O_1Cl1N1	34.992700
H3O2	35.013305
C3H1N1O_1	35.015984
C4H4N1P_1	35.060611
C_1H1O1P1	35.976500
H1Cl1	35.976600
C_1O3	35.984745
C3	36.000000
H4O2	36.021130
C4H4O_1	36.036385
C3H3N1O_1	37.031618
C5H2N5O_4P_1	37.077600
C2H_2O	37.979265
C3H2	38.015650
O2H6	38.036780
C4H6O_1	38.052035
C3H5N1O_1	39.047284
C4H9N1O_2	39.083669
C_7H_2O4P2	39.911536
CH_4O2	39.958530



Name	Mass
C2O1	39.994915
C3H4	40.031300
C4H8O_1	40.067685
C2HO	41.002740
C2H3N	41.026549
C3H7N1O_1	41.062934
H_2S1C1	41.956422
C1H_2O2	41.974180
acetylation_(H2O)_C2H2O	42.010565
C1H2N2	42.021800
C3H6	42.046950
C1H_1O2	42.982005
C1H1O1N1	43.005814
C2H3O	43.018390
C2H5N	43.042199
C2H5N1	43.042200
C3H7	43.054775
Carboxylation_CO2	43.989830
C2H4O1	44.026215
C3H8	44.062600
C4H12O_1	44.098985
H_1N1O2	44.985079
C2H3N_1O2	45.010231
CH3NO	45.021464
C2H5O1	45.034040
C2H7N1	45.057849
H_2O3	45.969095
C1H2O2	46.005480
C2H6O1	46.041865
H1O2N1	47.000729
C1H5N1O_1S1	47.019356
O1S1	47.966987
O3	47.984745
C4	48.000000
C1H4S1	48.003372
C1H4O2	48.021130
C2H8O	48.057515
H1O3	48.992570
C1H5O2	49.028955
H2O3	50.000379
C4H2	50.015650
C3H2N2O_1	50.026883
CH6O2	50.036757
C4H5N1O_1	51.047284
C3H13N7O_6	51.153753
C_1H1O2P1	51.971418
C3O	51.994927
H4O3	52.016012
C4H4	52.031300
C3H4N2O_1	52.042533
C5H8O_1	52.067685
C2H_1O_1N1S1	52.972406

Name	Mass
C3H3N	53.026581
C5H7N_1	53.051701
C_7H_4O5P2	53.890801
C_2H_2O1S2	53.923409
O_1Cl2	53.942800
C2H_2O2	53.974182
C3H2O1	54.010565
C4H6	54.046947
C3H3O1	55.018390
#N/A-1	55.042199
C7H5N1O_3	55.057454
H_1O_3Cl3	55.914000
CH_4O3	55.953422
glyoxylate_(H2O)_C2O2	55.989830
C2H3Cl_1O2S1	56.016500
C3H4O1	56.026215
C2H4N2	56.037448
C4H8	56.062585
Glycine_C2H3NO	57.021464
acetone_(H)_C3H5O	57.034040
C3H7N1	57.057840
C1H_1o1	57.925300
#N/A-2	57.969083
C2H2O2	58.005480
C1H2N2O1	58.016713
C3H6O1	58.041864
C3H8N1	58.065674
C3H10N2O_1	58.089483
C2H5N1O_1S1	59.019356
C2H5N1O1	59.037114
CO3	59.984729
C2H4O2	60.021129
C1H4N2O1	60.032363
C3H8O1	60.057489
C3H10N1	60.081324
C1H3N1S1	60.998621
C1H3N1O2	61.016379
C2H7O1N1	61.052764
C1H7N3	61.063997
#N/A-3	61.964011
C1H3Cl1	61.992300
C1H2O3	62.000376
C2H6S1	62.019022
C2H6O2	62.036765
C4H3O_1N2	63.034708
O2S1	63.961902
H1O2P1	63.971418
O4	63.979660
H1O4S_1P1	63.989176
C4O	63.994945
C1H1O2F1	63.996000
C1H4O1S1	63.998287

<b>Name</b>	<b>Mass</b>
C1H4O3	64.016034
C5H4	64.031300
C4H3N1	65.026549
#N/A-4	65.031479
H2O2S1	65.977552
H3O2P1	65.987068
H2O4	65.995310
C5H3Cl1O_2	66.002500
C4H2O	66.010585
C4O2	66.031707
C5H6	66.046935
H1C2N3	67.017047
C5H5N_1O1	67.030966
C4H5N1	67.042199
C3O2	67.989843
C4H4O1	68.026215
C5H8	68.062600
C4H6N1O2S_1	68.067782
C3H3N1O1	69.021452
C4H7N1	69.057849
Cl2	69.937700
CH_2O3	69.969101
C3H2O2	70.005480
C4H6O1	70.041867
C4H10N2O_1	70.089483
C6H14O_1	70.114635
C2H1N1O2	71.000729
C3H3O2	71.013305
Alanine_C3H5NO	71.037114
C4H9N1	71.073499
C5H13O_1N1	71.109884
H_1O_2Cl3	71.908900
C2O3	71.984745
C3H4O2	72.021131
C4H8O1	72.057515
C4H12N2O_1	72.105133
C2H3N1O2	73.016379
C3H7O1N1	73.052761
C2H2O3	74.000388
C3H6O2	74.036780
C4H10O	74.073184
C8H10O_2	74.088420
C2H5N1O2	75.032029
C6H5N1O_1	75.047284
C1H_2N_1O5	75.955851
C2H1O1Cl1	75.971600
C2H4O3	76.016045
C6H4	76.031300
C5H3N1	77.026549
C1H7N3O1	77.058912
CH2O4	77.995309
C5H2O	78.010626

Name	Mass
C2H6O3	78.031687
C5H4N1	78.034374
C5H8N3O_2	78.081992
H_1O3S1	78.948992
O3P1	78.958508
C5H5N1	79.042199
O3S1	79.956817
H1O3P1	79.966333
C1H5O2P1	80.002718
#N/A-5	80.018600
C5H4O1	80.026215
C6H8	80.062600
H1O3S1	80.964642
H3N1O2S1	80.988451
C5H7N1	81.057849
C6H11O_1N1	81.094234
H2O3S1	81.972467
C4H2O2	82.005480
C5H6O1	82.041872
C6H9O2P_1	82.086492
H2N_1O4P1	82.965999
C5H9N1	83.073499
C3O3	83.984740
acetotacetate_(H2O)_C4H4O2	84.021137
C4H4O4S_1	84.038888
C5H8O1	84.057515
C3H3N1O2	85.016379
C4H7N1O1	85.052738
malonyl_group_(H2O)_C3H2O3	86.000421
C4H6O2	86.036780
C5H10O1	86.073165
C5H12N1	86.096974
C6H14	86.109550
C7H1N_1O1	86.999666
C4H9O1N1	87.068414
C3H4O3	88.016045
C7H4	88.031300
C3H6N1O2	88.039854
C4H8O2	88.052422
C3H3N_1O4	89.000061
C6H3N1	89.026549
C3H7N1O2	89.047679
C7H7O_1N1	89.062934
C2H2O4	89.995294
C3H6O3	90.031695
C2O2H6N2	90.042928
C7H6	90.046950
C6H5N1	91.042199
C2H4O4	92.010938
C6H4O1	92.026215
C3H8O3	92.047367
C7H8	92.062600

<b>Name</b>	<b>Mass</b>
C5H3N1O1	93.021464
C4H3N3	93.032697
C6H7N1	93.057849
C5H7N3O_1	93.069082
C5H2O2	94.005480
C4H2O1N2	94.016713
C2H6O4	94.026603
C1H5O_1N1S1e1	94.963800
C5H5N1O1	95.037114
H1O4P1	95.961248
C4O3	95.984745
C5H4O2	96.021130
C4H4N2O1	96.032363
C6H8O	96.057515
H_1N_1O3S2	96.917990
H3O3N1S1	96.983366
H4N1O3P1	96.992882
C4H3O2N1	97.016379
Proline_C5H7NO	97.052764
H3O4P1	97.976898
C4H2O3	98.000395
C5H6O2	98.036780
C6H10O1	98.073165
C4H5N1O2	99.032029
C8H5N1O_1	99.047284
Valine_C5H9NO	99.068414
C4H4O3	100.016045
C5H8O2	100.052430
C4H8O1N2	100.063663
C3H3O3N1	101.011294
Threonine_C4H7NO2	101.047679
C5H11N1O1	101.084064
C4H6O1S1	102.013937
C5H2O_1N4	102.033031
C5H10O2	102.068080
C6H14O1	102.104465
C6H1N1O1	103.005814
C8H9N1O_1	103.078584
C6O2	103.989830
C3H4O4	104.010960
C7H4O1	104.026215
C6H4N2	104.037448
C4H8O3	104.047345
C8H8	104.062600
C6H3N1O1	105.021464
C3H7N1O1S1	105.024836
C6H5N2	105.045273
C4H11N1O2	105.078979
C3H6O4	106.026640
C6H4O1N1	106.029289
C2H5O2N1S1	107.004101
C2H6N1O2P1	107.013617

<b>Name</b>	<b>Mass</b>
C6H5N1O1	107.037114
C7H9N1	107.073499
C1H1O4P1	107.961248
C6H4O2	108.021130
C3H8O4	108.042293
C7H8O1	108.057515
C8H12	108.093900
C5H3O2N1	109.016379
C2H7O2N1S1	109.019751
C6H7O1N1	109.052764
C5H2O3	110.000454
cytosine_(H)_C4H4N3O	110.035437
C6H6O2	110.036780
C5H6O1N2	110.048013
C7H10O1	110.073165
C13H16O2P_2S_1	110.195432
C1H1N_1O3S2	110.933640
C3H1N3O2	111.006877
uracil_(H)_C4H3N2O2	111.019453
C6H5Cl1	112.008000
C5H4O3	112.016045
C4H4N2O2	112.027278
C6H8O2	112.052473
C5H12N4O_1	112.111281
C8H16	112.125200
H1S2O3	112.936714
C1H4N_1O5P1	112.976564
C5H7N1O2	113.047679
Isoleucine_C6H11NO	113.084064
C4H2O4	113.995310
C4H3F1N2O1	114.022941
C5H6O3	114.031695
Asparagine_C4H6N2O2	114.042928
C6H10O2	114.068080
C5H10N2O1	114.079313
Aspartic_Acid_C4H5NO3	115.026944
C5H7O3	115.039520
C8H5N1	115.042199
C5H9N1O2	115.063329
C4H4O4	116.010960
C3H4N2O3	116.022193
C5H8O1S1	116.029587
C5H8O3	116.047345
C8H8O_1N2	116.073833
C5H12O1N2	116.094963
C4H7N1O1S1	117.024836
C4H7O3N1	117.042594
C5H3N5O_1	117.043930
C8H7N1	117.057849
C3H2O5	117.990225
C4H6O4	118.026610
C5H2N4	118.027946

<b>Name</b>	<b>Mass</b>
<b>C8H6O1</b>	118.041865
<b>C9H10</b>	118.078250
<b>C3H5N1O2S1</b>	119.004101
<b>C7H5N1O1</b>	119.037114
<b>C6H5N3</b>	119.048347
<b>C5H5N5O_1</b>	119.059580
<b>C7H4O2</b>	120.021130
<b>C6H4N2O1</b>	120.032363
<b>C3H8O1N2S1</b>	120.035735
<b>C4H8O4</b>	120.042334
<b>C8H8O1</b>	120.057515
<b>C6H3N1O2</b>	121.016379
<b>C3H7N1O2S1</b>	121.019751
<b>C8H11N1</b>	121.089149
<b>C2H2O4S1</b>	121.967382
<b>C7H6O2</b>	122.036780
<b>C6H8N3</b>	122.071822
<b>C8H10O1</b>	122.073165
<b>C5H1N1O3</b>	122.995644
<b>C2H6N1O3P1</b>	123.008532
<b>C6H7N2O1</b>	123.055838
<b>C8H13N1</b>	123.104799
<b>H1C1O5P1</b>	123.956163
<b>C2H4O2S2</b>	123.965274
<b>C2H5O4P1</b>	123.992548
<b>C6H4O3</b>	124.016172
<b>C6H6N1O2</b>	124.039854
<b>C2H3N_1O3S2</b>	124.949290
<b>C4H3N3O2</b>	125.022527
<b>thymine_(H)_C5H5N2O2</b>	125.035103
<b>C7H7Cl1</b>	126.023700
<b>C6H6O3</b>	126.031695
<b>C6H8N1S1</b>	126.037746
<b>C5H6N2O2</b>	126.042928
<b>C6H10N2O1</b>	126.079313
<b>C5H10N4</b>	126.090546
<b>C8H14O1</b>	126.104465
<b>C5H5O3N1</b>	127.026944
<b>C6H9O2N1</b>	127.063329
<b>C7H17N3O_1</b>	127.147332
<b>C5H4O4</b>	128.010960
<b>C6H8O3</b>	128.047345
<b>Glutamine_C5H8N2O2</b>	128.058578
<b>Lysine_C6H12N2O</b>	128.094963
<b>Glutamic_Acid_C5H7NO3</b>	129.042594
<b>C6H11N1O2</b>	129.078979
<b>C7H19N3O_1</b>	129.162982
<b>C2H_6O7</b>	129.917455
<b>C5H3Cl1O2</b>	129.982200
<b>C5H6O4</b>	130.026610
<b>C9H6O1</b>	130.041865
<b>C6H10O3</b>	130.062995

<b>Name</b>	<b>Mass</b>
<b>C10H10</b>	130.078250
<b>C6H14O1N2</b>	130.110613
<b>C7H16N1O1</b>	130.123189
<b>C8H5O1N1</b>	131.037114
<b>Methionine_C5H9NOS</b>	131.040486
<b>C5H9N1O3</b>	131.058244
<b>C6H5O_1N5</b>	131.059580
<b>C4H4O5</b>	132.005875
<b>C8H4O2</b>	132.021130
<b>pentose_C5H8O4</b>	132.042260
<b>C9H8O1</b>	132.057515
<b>C8H8N2</b>	132.068748
<b>C10H12</b>	132.093900
<b>C7H3N1O2</b>	133.016379
<b>C4H7N1O2S1</b>	133.019751
<b>C5H3N5</b>	133.038845
<b>C5H9O4</b>	133.050085
<b>C8H7N1O1</b>	133.052764
<b>H7O6P1</b>	133.998028
<b>C5H2O1N4</b>	134.022861
<b>C8H6O2</b>	134.036780
<b>adenine_(H)_C5H4N5</b>	134.046670
<b>C4H10O1N2S1</b>	134.051385
<b>C5H10O4</b>	134.057910
<b>C8H8N1O1</b>	134.060589
<b>C7H5N1O2</b>	135.032029
<b>C4H9N1O2S1</b>	135.035401
<b>C8H9N1O1</b>	135.068414
<b>C2O7</b>	135.964405
<b>C4H9O3P1</b>	136.028933
<b>C4H8O5</b>	136.037175
<b>C5H4O1N4</b>	136.038511
<b>C8H8O2</b>	136.052430
<b>C9H12O1</b>	136.088815
<b>C10H16</b>	136.125200
<b>C3H8N1O3P1</b>	137.024182
<b>C7H7N1O2</b>	137.047679
<b>Histidine_C6H7N3O</b>	137.058912
<b>C7H6O3</b>	138.031695
<b>C6H6N2O2</b>	138.042928
<b>C9H14O1</b>	138.104465
<b>C2H4O3S2</b>	139.960189
<b>C6H4O4</b>	140.010960
<b>C7H8O3</b>	140.047488
<b>C8H14N1O1</b>	140.107539
<b>C2H8O4N1P1</b>	141.019097
<b>C8H15N1O1</b>	141.115364
<b>C8H19N3O_1</b>	141.162982
<b>O5P2</b>	141.922101
<b>C1H3O6P1</b>	141.966728
<b>C2H6O3S2</b>	141.975839
<b>C10H6O1</b>	142.041865



<b>Name</b>	<b>Mass</b>
C7H10O3	142.062995
C6H10N2O2	142.074228
C11H10	142.078250
C10H10N2O_1	142.089483
C6H9N1O3	143.058244
C10H9N1	143.073499
C7H13N1O2	143.094629
C3H1N2O3P1	143.972481
C6H8O4	144.042260
C5H8N2O3	144.053493
C10H8O1	144.057515
C7H12O1S1	144.060887
C7H12O3	144.078645
C5H7N1O4	145.037509
C6H4Cl2	145.969000
C9H6O2	146.036780
C6H10O4	146.057910
C10H10O1	146.073165
C7H1N1O3	146.995644
C8H5N1O2	147.032029
C8H4O3	148.016045
C5O5H8	148.037175
C9H8O2	148.052430
C6H12O4	148.073560
C10H12O1	148.088815
C6H5O1N4	149.046336
C8H7N1O2	149.047679
C9H11N1O1	149.084064
C5H2N4S1	150.000018
C8H6O3	150.031695
guanine_(H)_C5H4N5O	150.041585
C5H10O5	150.052825
C6H6O1N4	150.054161
C9H10O2	150.068080
C5H13N1O2P1	150.068392
C10H14O1	150.104465
C3H6N1O4P1	151.003447
C7H5N1O3	151.026944
C7H9N3O1	151.074562
C3H5O5P1	151.987463
C4H9O2P1S1	152.006090
C3H8O1N2S2	152.007807
C7H4O4	152.010960
C8H8O3	152.047345
C6H8N4O1	152.069811
C10H16O1	152.120115
C3H6O5S1	153.993597
C3H7O5P1	154.003113
C11H6O1	154.041865
C10H18O1	154.135765
C8H13O2N1	155.094629
C7H8O4	156.042260

Name	Mass
C6H7N1O4	157.037509
C10H7N1O1	157.052764
C7H11O3N1	157.073894
C6H11N3O2	157.085127
C8H15N1O2	157.110279
O6P2	157.917016
C6H6O5	158.021525
C10H6O2	158.036780
C7H10O4	158.057910
C10H10N2	158.084398
C6H14O1N4	158.116761
H3N1O5P2	158.948650
C6H9N1O4	159.053159
H2O6P2	159.932666
C5H8N2O2S1	160.030650
C6H8O5	160.037175
C7H12O4	160.073560
N3O2C6H14	160.108602
C13H20O_1	160.161585
H1O7P2N_1	160.916682
diphosphate_H3O6P2	160.940491
C6H11N1O4	161.068809
H4O6P2	161.948316
C9H6O3	162.031695
C6H10O3S1	162.035067
C10H10O2	162.068080
C5H10O3N1P1	163.039832
C6H11O5	163.060650
Tyrosine_C9H9NO2	163.063329
C10H13N1O1	163.099714
C5H12N2S2	164.044192
C6H12O5	164.068475
C7H8O1N4	164.069811
C10H12O2	164.083730
C12H20	164.156500
C3H8N3O3P1	165.030330
C5H12N1O3P1	165.055482
C9H11N1O2	165.078979
C8H10N2S1	166.056470
C9H10O3	166.062995
C5H13N1O3P1	166.063307
C10H14O2	166.099380
C9H13N1O2	167.094629
C6H3N1O3S1	168.983366
C4H10O5P1	169.026588
C1O6P2	169.917016
C3H7O6P1	169.998028
C6H10O_1C11N5	171.067600
C10H8N2O1	172.063663
C7H12N2O3	172.084793
C9H16O3	172.109945
C8H15N1O3	173.105194

<b>Name</b>	<b>Mass</b>
C6H6O6	174.016440
C7H10O5	174.052825
C8H14O4	174.089210
C6H14O2N4	174.111676
C9H5N1O3	175.026944
C7H13N1O4	175.084459
H2O7P2	175.927581
C4O8	175.959320
C6H8O6	176.032090
C10H8O3	176.047345
C7H12O5	176.068475
C9H7N1O3	177.042594
C7H7N5O1	177.065060
H4O7P2	177.943231
C9H9N1O3	179.058244
C6H3Cl3	179.930000
glucose_C6H12O6	180.063390
C10H12O3	180.078645
C10H15O2N1	181.110279
C5H12Cl1O1N2P1	182.037600
C8H10O1N2S1	182.051385
C13H10O1	182.073165
C10H14O3	182.094295
C12H22O1	182.167065
C7H9O3N3	183.064392
C8H13N3O2	183.100777
C7H4O4S1	183.983032
C7H4O6	184.000790
C4H9O6P1	184.013678
C8H12N2O3	184.084793
C10H24N4O_1	184.205181
C10H11O_1N5	185.106530
C11H6O3	186.031695
C8H14N2O3	186.100443
C8H13N1O4	187.084459
C7H13N3O3	187.095692
C8H12O1S2	188.032959
C11H8O3	188.047345
C12H12O2	188.083730
C10H7N1O3	189.042594
C10H10O2N2	190.074228
C14H22	190.172150
C10H8O4	192.042260
C7H12O6	192.063390
C11H12O3	192.078645
C12H16O2	192.115030
C7H3N3O4	193.012357
C9H7N1O4	193.037509
C9H11O2N3	193.085127
C5H7O4P1S1	193.980270
C9H6O5	194.021525
C9H8N1O4	194.045334

<b>Name</b>	<b>Mass</b>
C11H18N2O1	194.141913
C15H30O_1	194.239835
C9H9N1O4	195.053159
C7H9O2N5	195.075625
C9H13O2N3	195.100777
C6H12O7	196.058305
C8H10N2O2S1	198.046300
C8H13N3O3	199.095692
C3H6O6P2	199.963966
C4H9O7P1	200.008593
C12H8O3	200.047345
C12H24O2	200.177630
C9H15N1O4	201.100109
C10H11N5	201.101445
C8H14N2O2S1	202.077600
C8H14N2O4	202.095358
C10H18O4	202.120510
C11H9N1O3	203.058244
glcnac_C8H13N1O5	203.079374
C10H13N5	203.117095
C10H4O5	204.005875
C11H8O4	204.042260
C15H24	204.187800
C10H11N3S1	205.067369
C9H11O1N5	205.096360
C1H4O8P2	205.938146
C6H6O8	206.006270
C11H10O4	206.057910
C10H10O3N2	206.069143
C8H14O6	206.079040
C14H8O2	208.052430
C6H11O6P1	210.029328
C14H26O1	210.198365
C5H10N1O6P1	211.024577
C5H9O7P1	212.008593
C12H20O3	212.141245
C5H10O7P1	213.016418
C13H10O3	214.062995
C12H10N2O2	214.074228
C12H8S2	216.006744
C11H4Cl1N1O2	216.993000
C8H11N1O6	217.058639
C6H3I1O1	217.922800
C6H7N2O5P1	218.009261
C12H10O4	218.057910
C15H22O1	218.167065
C12H11O4	219.065735
C4H11O2Cl2N2P1	219.993500
C8H12O7	220.058305
C13H16O3	220.109945
C14H20O2	220.146330
C16H28	220.219100

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C8H15O6N1	221.089939
C15H26O1	222.198365
C17H34O_1	222.271135
C12H17O3N1	223.120844
C3H2N2O6P2	223.938814
C12H8N4O1	224.069811
C12H16O4	224.104860
C15H28O1	224.214015
C6H10O7S1	226.014727
C14H26O2	226.193280
C18H26O_1	226.208535
C10H16N2O4	228.111008
C19H32O_2	228.260570
C5H11O8P1	230.019158
C8H10N2O6	230.053888
C9H14N2O5	230.090273
C8H12N2O4S1	232.051780
C19H36O_2	232.291870
C15H22O2	234.161980
C19H38O_2	234.307520
C6H10O5P1N3	235.035810
C8H12O8	236.053220
C19H26O_1	238.208535
C6H10N1O7P1	239.019492
H3O9P3	239.898999
C11H12O6	240.063390
C18H24	240.187800
C16H32O1	240.245315
C6H12O7N1P1	241.035142
C6H11O8P1	242.019158
C11H18N2O4	242.126658
C18H26	242.203450
C12H20O5	244.131075
C10H15O6N1	245.089939
C9H14N2O4S1	246.067430
C15H18O3	246.125595
C8H12N2O5S1	248.046695
C16H24O2	248.177630
C7H8N1O5P1S1	248.986084
C7H12O5N3P1	249.051460
C9H15N1O5S1	249.067096
C10H12N5O3	250.094015
C15H8O4	252.042260
C17H16O2	252.115030
C15H24O3	252.172545
C20H28O_1	252.224185
C13H6N2O4	254.032758
C10H10O4N2S1	254.036130
C18H22O1	254.167065
C16H17O2N1	255.125929
C18H24O1	256.182715
C7H8N5O4P1	257.031393

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H5O10P3	257.909564
C10H14N2O6	258.085188
C13H14O2N4	258.111676
C7H4Cl4O2	259.896500
C13H16N4O2	260.127326
C16H20O3	260.141245
C18H28O1	260.214015
C9H15N2O5P1	262.071861
C18H30O1	262.229665
C11H8N2O4S1	264.020480
C10H16O8	264.084520
C18H32O1	264.245315
C_8H_6N7O9P3S1	264.822164
C18H34O1	266.260965
C_10H_12N7O11P3S1	266.765044
C16H13N1O3	267.089544
C17H17O2N1	267.125929
C10H8O3N2S2	267.997637
C7H13O7N2P1	268.046041
C20H12O1	268.088815
C20H28	268.219100
C17H19O2N1	269.141579
C19H10O2	270.068080
C19H26O1	270.198365
C10H10F1N3O5	271.060450
C10H16Cl_1O6N3S1	271.107100
C19H28O1	272.214015
C20H32	272.250400
C14H10O2S2	274.012224
C11H17N1O7	275.100504
C14H15O5N1	277.095024
C5H12O9P2	277.995661
C14H14O6	278.079040
C20H38	278.297350
C11H13N5O2S1	279.078997
C18H14N1F1O1	279.105942
C_9H_10N7O11P3S1	280.780694
C9H16N1O7P1	281.066442
C18H19O2N1	281.141579
C_8H_4N7O10P3S1	282.832729
C8H14N1O8P1	283.045707
C17H17N1O3	283.120844
C2H7O10P3	283.925214
C15H8O6	284.032090
C16H12O5	284.068475
C20H28O1	284.214015
C_10H_10N7O12P3S1	284.775609
C11H14N2O7	286.080103
C20H30O1	286.229665
C21H34	286.266050
C17H21O3N1	287.152144
C18H8O4	288.042260

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C20H32O1	288.245315
C20H34O1	290.260965
C11H17N1O8	291.095419
C5H10O10P2	291.974926
C6H12O9S2	291.992279
C12H20O8	292.115820
C20H36O1	292.276615
C5H_6O15	293.876775
C11H18O9	294.095085
C19H22O1N2	294.173213
C20H38O1	294.292265
C_8H_8N7O11P3S1	294.796344
C14H12N6O2	296.102174
C11H15N5O3S1	297.089562
C18H19N1O3	297.136494
C_9H_8N7O12P3S1	298.791259
C19H25N1O2	299.188529
C17H18O5	302.115425
C9H11N3O7P1	304.033465
C15H12O7	304.058305
C10H16N4O5S1	304.084143
C9H12N3O7P1	305.041290
C10H15N3O6S1	305.068159
C11H20O5N3P1	305.114060
C12H23O6N3	305.158687
C18H10O5	306.052825
C10H17N3O6S1	307.083809
neugc_C11H17N1O9	307.090318
C18H12O5	308.068475
C10H17N2O7P1	308.077341
C15H16O7	308.089605
C12H20O9	308.110735
C20H24O1N2	308.188863
C19H20N1O3	310.144319
C22H30O1	310.229665
C19H21O3N1	311.152144
C8H13N2O9P1	312.035871
C22H32O1	312.245315
C_8H_6N7O12P3S1	312.806909
C16H10O7	314.042655
C22H34O1	314.260965
C12H12O10	316.043050
C11H14N2O7P1	317.053866
C11H13N1O8P1	318.037882
C20H18O2N2	318.136828
C20H30O3	318.219495
C21H34O2	318.255880
C22H38O1	318.292265
C9H13O7N4P1	320.052189
C22H40O1	320.307915
C6H11O10N1S2	320.982443
C9H12N3O8P1	321.036205

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C22H42O1	322.323565
C9H14N3O8P1	323.051855
C12H21N1O9	323.121634
C20H21N1O3	323.152144
C18H12O6	324.063390
C15H16O8	324.084520
C12H22O6P2	324.089166
C12H20O10	324.105650
C17H12O7	328.058305
C10H13N6O5P1	328.068507
C10H12N5O6P1	329.052523
C10H11N4O7P1	330.036539
C10H13N5O6P1	330.060348
C21H20O2N2	332.152478
C11H14N2O6S2	334.029332
C9H14O7N5P1	335.063088
C21H24N2O2	336.183778
C9H15N4O4P2S1	337.028929
C9H15O8N4P1	338.062754
C9H14N3O9P1	339.046770
C15H17N1O8	339.095419
C18H12O7	340.058305
C11H21N2O6P1S1	340.085798
C25H40	340.313000
C11H20O7S1N1P1	341.069814
C18H14O7	342.073955
C6H2I2O1	343.819500
C27H36O_1	344.286785
C6H4I2O1	345.835200
C12H10O12	346.017230
C10H11N4O8P1	346.031454
C10H14N5O7P1	347.063088
C12H17N3O7S1	347.078724
C16H28O8	348.178420
C24H44O1	348.339215
C3H13O11P3S1	349.939151
C21H22O3N2	350.163043
C25H34O1	350.260965
C24H46O1	350.354865
C12H16O12	352.064180
C21H23O4N1	353.162709
C18H14N2O6	354.085188
C14H17O6N3S1	355.083809
C18H30O7	358.199155
C14H20N2O9	360.116883
C24H40O2	360.302830
C14H23O10N1	365.132199
C27H44	368.344300
C17H22O9	370.126385
C5H11O13P3	371.941259
C11H12N5O8P1	373.042353
C22H18N2O4	374.126658



<b>Name</b>	<b>Mass</b>
C24H38O3	374.282095
C20H7O1Cl2N3	374.996600
C11H19O5N4P2S1	381.055144
C27H44O1	384.339215
C10H15N3O6S2e1	384.984700
C9H12N2O11P2	385.991639
C24H38O4	390.277010
C27H40O2	396.302830
C30H40	400.313000
C10H16O11N2P2	402.022939
C30H48	408.375600
C10H14N5O9P3S_1	409.028372
C18H24O11	416.131865
C24H32O6	416.219890
C17H32N6O4S1	416.220576
C27H44O3	416.329045
C11H22N2O9P2S1	420.052131
C23H35N1O4S1	421.228681
C12H19O7N4P2S1	425.044974
C19H19O5N7	425.144768
C19H21N7O5	427.160418
C18H34N6O4S1	430.236226
C27H44O4	432.323960
C3H2N7O11P3S1	436.874594
C17H19N4O8P1	438.094054
C27H18O6	438.110340
C46H77N_2O_8P_1	442.663294
C35H46O_1	450.365035
C7H12O12N5P3	450.969539
C30H44O3	452.329045
C22H27O4N7	453.212453
C18H30O13	454.168645
C20H21N7O6	455.155333
C25H32N2O6	456.226038
C1N7O14P3S1	458.843689
C9H13N2O14P3	465.957972
C18H30O14	470.163560
C2H2N7O14P3S1	472.859339
C20H39N7O4S1	473.278425
C35H56	476.438200
C32H60O2	476.459330
C9H14N5O12P3	476.985189
C25H38N2O5S1	478.250145
C4H2N7O13P3S1	480.864424
C17H28N2O12S1	484.136300
C17H30O12N2S1	486.151950
C18H30O15	486.158475
C28H30O4N4	486.226706
C10H14N5O12P3	488.985189
C5H4N7O13P3S1	494.880074
C9H16O13N5P3	494.995754
C19H20N3O11P1	497.083550

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C4H6N7O14P3S1	500.890639
C10H14N5O13P3	504.980104
C10H13N4O14P3	505.964120
C5H8N7O14P3S1	514.906289
C23H21O11N3	515.117612
C21H25N1O14	515.127509
C15H17N5O10P2S1	521.017143
C46H78N_2O_5	522.629627
C27H27O10N1	525.163499
C18H28O18	532.127570
C29H31O9N1	537.199884
C15H21N5O13P2	541.061116
C15H22N5O13P2	542.068941
C40H64	544.500800
C28H51N1O9	545.356384
C29H31O10N1	553.194799
C21H41N5O12	555.275175
C7H10N7O15P3S1	556.916854
C34H32O4N4	560.242356
C27H20N2O12	564.101628
S2O9C20H32N6	564.167223
C44H72O_2	568.573570
C10H15N5O15P4	568.951522
C8H12N7O15P3S1	570.932504
C14H24N7O10P3S1	575.051829
C14H26N7O11P3S1	593.062394
C35H32O4M1g1N4	596.227400
C23H43O13N5	597.285740
C16H28N7O10P3S1	603.083129
C14H21N6O13P3S1	606.010025
C35H30O5M1g1N4	610.206700
C45H72	612.563400
C34H63N1O8	613.455369
C12H26N7O14P3S1	617.047139
C17H30N7O10P3S1	617.098779
C16H27N6O12P3S1	620.062060
C27H24O17	620.101355
C16H26N5O13P3S1	621.046076
C15H23N5O16P3	622.035274
C13H21N6O15P3S1	625.999855
C24H27N4O14P1	626.126144
C30H32N2O13	628.190443
C16H26N7O12P3S1	633.057309
C28H39O13S_2N6P1	634.287133
C15H30N7O13P3S1	641.083524
C21H26N7O13P2	646.106389
C13H28N7O15P3S1	647.057704
C17H28N7O12P3S1	647.072959
C24H40O20	648.211300
C10H16N5O18P5	648.917855
C14H22N7O15P3S1	653.010754
C15H30N7O14P3S1	657.078439

<b>Name</b>	<b>Mass</b>
C15H32N7O14P3S1	659.094089
C20H29N3O18P2	661.092143
C15H24N7O15P3S1	667.026404
C21H33N7O12P2S1	669.138321
C19H32N7O12P3S1	675.104259
C50H80	680.626000
C14H20N7O17P3S1	682.984934
C28H38N5O13P1	683.220378
C16H30N7O15P3S1	685.073354
C39H60O10	688.418650
C19H31N6O14P3S1	692.083190
C34H64N1O11P1	693.421702
C43H71O5P1	698.503913
C39H60O11	704.413565
C19H29N6O15P3S1	706.062455
C19H32N7O14P3S1	707.094089
C43H87O5P1	714.629113
C20H34O14N7P3S1	721.109739
C19H29N6O16P3S1	722.057370
C34H42O14N4	730.269756
C23H34N4O19P2	732.129257
C21H36N7O14P3S1	735.125389
C39H42O11N4	742.285011
C21H34N7O15S1P3	749.104654
C21H35N7O15P3S1	750.112479
C29H34N5O17P1	755.168738
C30H43N6O15P1	758.252407
C21H32N7O16P3S1	763.083919
C21H36N7O16P3S1	767.115219
C29H49O17N3P2	773.253728
C22H38N7O16P3S1	781.130869
C22H35N8O16P3S1	792.110468
C23H37N7O16P3S1	792.123044
H39C24O16N7P3S1	806.138694
C23H38O17N7P3S1	809.125784
C30H50O25	810.264125
C24H40O17N7P3S1	823.141434
C31H52N7O17P1	825.315736
H41C26O16N7P3S1	832.154344
C25H41O16N8P3S1	834.157418
C27H40O17N7P3S1	859.141434
C28H41N5O22P2	861.171851
C43H50O15N4	862.327271
C45H72O16	868.482040
C32H52N7O19P1	869.305566
C41H60N12O10	880.455538
H49C31O16N7P3S1	900.216944
C46H63N10O7o1	914.421300
C30H48O18N7P3S1	919.198949
C44H48O15o1N4	919.244800
C44H49O15o1N4	920.252700
C60H98O6N1P1	959.713177

<b>Name</b>	<b>Mass</b>
<b>C36H60O30</b>	972.316950
<b>C34H53N7O23P2</b>	989.266814
<b>C35H53N7O25P2</b>	1033.256644
<b>C51H80O22</b>	1044.514130
<b>C37H58N8O24P2</b>	1060.303928
<b>C38H58N8O26P2</b>	1104.293758
<b>C56H75N15O10o1</b>	1164.515400
<b>C60H64O28</b>	1232.358420
<b>C59H83N16O13P1o1</b>	1301.539500

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## **References for Supplementary Material**

U.S. Geological Survey: National Hydrography Dataset Plus Version 2 [dataset], 2019.