**Description of each abiotic factor (chemical metrics and environmental variables) included in the analysis.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| VARIABLE | DESCRIPTION | DIMENSION | TYPE | REFERENCES\* |
| Chemical metrics | Risk Quotients (RQs) and Toxic Units (TUs) based on measured concentration of pesticides (insecticides, herbicides, and fungicides), Swiss ecotoxicological quality standards and ecotoxicological endpoints, calculated as 'maximum' and 'mixture' values, and represented by (mean, median, max) per time window. | Chemical | Dynamic | (Burdon et al., 2019; Liess et al., 2021) |
| Catchment area (m2) | Estimation of the total area (in m2) of water bodies (including lakes) upstream the sampling point. | Hydrological | Static | (BAFU, 2020; Hutter et al., 2019; Ilg & Alther, 2024) |
| Average discharge (m3/s) | Annual mean modelled discharge (in m3/s) for the watercourse 'Mittlerer modellierter Abfluss'. | Hydrological | Static | (BAFU, 2020; Burdon et al., 2016) |
| Flow velocity (m/s) | Modelled annual flow velocity (based on stream width and slope). | Hydrological | Static | (Khaliq et al., 2024) |
| Stream classification | Waterbody size classification (small 'kleines', medium 'mittel', large 'grosses') based on discharge. | Hydrological | Static | (Ilg & Alther, 2024) |
| Proportion of urban land use | Proportion of the total land upstream categorized as human settlements 'Siedlungsflächen.' | Land Use | Static | (Hutter et al., 2019; Ilg & Alther, 2024; Khaliq et al., 2024; Liess et al., 2021) |
| Proportion of forest land use | Proportion of the total land upstream categorized as forested areas, unproductive areas, artificial meadows, permanent meadows, permanent pastures, and summer grazing area. | Land Use | Static |
| Proportion of agricultural land use | Proportion of the total land upstream categorized as other fruit crops, fruit crops aggregated, perennial berries, stone fruit, pears, apples, open area for production, vines, vineyards with natural biodiversity, and vines (region-specific biodiversity areas). | Land Use | Static |
| Ecomorphology | Classification of the stream based on water body morphology, ranging from 0 (natural or near natural) to 12 (unnatural or artificial). | Morphological | Static | (BAFU, 2022; Hutter et al., 2019; Ilg & Alther, 2024) |
| Altitude (m.a.s.l.) | Measure of the altitude (m.a.s.l.) at the sampling point. | Spatial | Static |  |
| Stream identity | Stream name where macroinvertebrate and chemical sampling occurred. | Spatial | Static | - |
| Maximum summer water temperature (°C) | Modelled maximum morning summer stream temperature predicted from a linear model based on catchment area and mean catchment elevation. | Spatial | Static | (Khaliq et al., 2024) |
| Season | Season (spring or summer) when macroinvertebrate monitoring was performed. | Temporal | Static | (Ilg & Alther, 2024) |
| Year | Year of macroinvertebrate and chemical sampling. | Temporal | Static | (Khaliq et al., 2024) |
| Average of daily precipitation (mm) | Average of daily precipitation (mm) per site from 01-01-2017 to 31-12-2023, separated by chemical sample | Temporal | Dynamic | - |

*\*References that have used the same or equivalent (based on our data availability) abiotic factors to be related to the bioindicators in previous studies*

**Data Dictionary: Abiotic\_factors\_41\_streams\_ds\_prepared**

|  |  |
| --- | --- |
| Column Name | Description |
| Gewasser | Stream name (character). The river or stream where the abiotic measurements were taken. |
| Messstelle\_ID | Unique identifier for the sampling station (factor). |
| Catch\_area\_m2 | Catchment area in square meters for the stream section (numeric). |
| Avg\_mod\_discharge\_m3\_s | Average modelled discharge (flow) in cubic meters per second (numeric). |
| Proportion\_of\_wastewater\_l\_s | Proportion of wastewater in liters per second in the stream at the sampling point (numeric). |
| FLOZ | Stream order or hydrological classification (integer). |
| Flow\_velocity | Mean flow velocity at the sampling site (meters per second, numeric). |
| Ecomorphology\_class | Ecomorphological class of the stream section (integer, usually 1-5). |
| Ecomorphology\_categories23 | Categorical variable describing the ecomorphological status (factor, e.g., "Eingedolt", "Stark beeinträchtigt"). |
| Ecomorphology\_values23 | Numeric or categorical code for the ecomorphological category (factor, 1-4). |
| Urban\_area\_frac | Proportion (%) of urban area in the catchment (numeric). |
| Forest\_area\_frac | Proportion (%) of forest area in the catchment (numeric). |
| Agricultural\_area\_frac | Proportion (%) of agricultural area in the catchment (numeric). |
| Mod\_max\_temp\_summer | Modelled maximum summer water temperature (°C, numeric). |
| Ecomorphology\_cont23\_Langhans | Continuous ecomorphology index (numeric, typically 0-1). |
| Ecomorphology\_0\_12 | Ecomorphological score or classification on a 0-12 scale (numeric). |
| Stream\_bed\_construction | Categorical description of stream bed construction (factor, e.g., "0%, natural", "100%, artificial"). |

**Data Dictionary: metrics\_3.5d\_0\_R12\_pp\_ds**

|  |  |
| --- | --- |
| Column Name | Description |
| Gewasser | Stream name (character). Refers to the river or stream where the sample was collected. |
| OBSERVATIONDATE | Date and time of the biological/chemical observation (POSIXct). |
| ARQmix\_max | Maximum mixture Acute Risk Quotient (RQ) for all detected substances in the composite sample. |
| ARQmix\_max\_Probe | Unique identifier for the probe/sample with the maximum ARQmix value (factor). |
| ARQmix\_max\_DIF\_DATE | Time difference category between sampling and observation (e.g., "Less than 1 week", "1-2 weeks"). |
| ARQmix\_max\_num\_Substances | Number of substances contributing to the maximum ARQmix value. |
| ARQmix\_mean | Mean mixture Risk Quotient (RQ) across all substances in the sample. |
| ARQmix\_median | Median mixture Risk Quotient (RQ) across all substances in the sample. |
| ARQmix\_n | Number of samples or measurements included in the ARQmix calculation. |
| ARQmix\_mean\_num\_substances | Mean number of substances per sample for ARQmix calculation. |
| ARQmax\_max | Maximum individual Risk Quotient (RQ) found in the sample (i.e., for a single substance). |
| ARQmax\_max\_Probe | Unique identifier for the probe/sample with the maximum ARQmax value (factor). |
| ARQmax\_max\_DIF\_DATE | Time difference category for the maximum ARQmax value. |
| ARQmax\_max\_Param | Name of the substance/parameter with the maximum ARQmax value. |
| ARQmax\_max\_Substance | Unique identifier for the substance with the maximum ARQmax value (factor). |
| ARQmax\_mean | Mean of the maximum individual RQ values across all samples. |
| ARQmax\_median | Median of the maximum individual RQ values across all samples. |
| ARQmax\_n | Number of samples or measurements included in the ARQmax calculation. |
| TU\_ECmix\_max | Maximum mixture Toxic Unit (TU) based on EC50 values for all detected substances in the sample. |
| TU\_ECmix\_max\_Probe | Unique identifier for the probe/sample with the maximum TU\_ECmix value (factor). |
| TU\_ECmix\_max\_DIF\_DATE | Time difference category for the maximum TU\_ECmix value. |
| TU\_ECmix\_max\_num\_Substances | Number of substances contributing to the maximum TU\_ECmix value. |
| TU\_ECmix\_mean | Mean mixture Toxic Unit (TU) across all substances in the sample. |
| TU\_ECmix\_median | Median mixture Toxic Unit (TU) across all substances in the sample. |
| TU\_ECmix\_n | Number of samples or measurements included in the TU\_ECmix calculation. |
| TU\_ECmix\_mean\_num\_substances | Mean number of substances per sample for TU\_ECmix calculation. |
| TU\_ECmax\_max | Maximum individual Toxic Unit (TU) found in the sample (i.e., for a single substance). |
| TU\_ECmax\_max\_Probe | Unique identifier for the probe/sample with the maximum TU\_ECmax value (factor). |
| TU\_ECmax\_max\_DIF\_DATE | Time difference category for the maximum TU\_ECmax value. |
| TU\_ECmax\_max\_Param | Name of the substance/parameter with the maximum TU\_ECmax value. |
| TU\_ECmax\_max\_Substance | Unique identifier for the substance with the maximum TU\_ECmax value (factor). |
| TU\_ECmax\_mean | Mean of the maximum individual TU values across all samples. |
| TU\_ECmax\_median | Median of the maximum individual TU values across all samples. |
| TU\_ECmax\_n | Number of samples or measurements included in the TU\_ECmax calculation. |
| SPEAR | Value of the SPEARpesticides bioindicator index for the sample. |
| IBCH\_2019 | Value of the IBCH (Swiss biological index) for the sample. |
| GI\_VALUE | Value of another macroinvertebrate-based bioindicator. |
| VT\_VALUE | Value of another macroinvertebrate-based bioindicator. |
| EPT | Proportion of EPT taxa (Ephemeroptera, Plecoptera, Trichoptera) in the sample. |
| Kanton | Swiss canton where the stream is located (factor). |
| Kategorie\_FG\_Grosse | Stream size category (e.g., "Kleine", “Mittel”, "Gross "; factor). |
| YEAR | Year of sampling or observation. |
| OID | Unique identifier for the observation or site (factor). |
| X.y | X-coordinate (e.g., Swiss coordinate system) of the sampling location. |
| Y.y | Y-coordinate of the sampling location. |
| Z | Elevation (meters above sea level) of the sampling location. |
| Season\_MZB | Season of macroinvertebrate sampling (e.g., "Spring", "Summer"; factor). |
| scenario | Scenario or time window used for the aggregation of the composite samples (e.g., "3.5\_days\_1\_month", "3.5\_days\_2\_weeks"). |
| Gewasser\_clean | Cleaned/lowercase version of the stream name for easier merging. |
| PP\_mean\_mean | Mean value of daily precipitation. |

**Data Dictionary: metrics\_14d\_0\_R12\_pp\_ds**

|  |  |
| --- | --- |
| Column Name | Description |
| Gewasser | Stream name (character). The river or stream where the sample was collected. |
| OBSERVATIONDATE | Date and time of the biological/chemical observation (POSIXct). |
| CRQmix\_max | Maximum mixture Chronic Risk Quotient (RQ) for all detected substances in the composite sample (numeric). |
| CRQmix\_max\_Probe | Unique identifier for the probe/sample with the maximum CRQmix value (factor). |
| CRQmix\_max\_DIF\_DATE | Time difference category between sampling and observation (e.g., "Less than 1 week", "1-2 weeks"). |
| CRQmix\_max\_num\_Substances | Number of substances contributing to the maximum CRQmix value (integer). |
| CRQmix\_mean | Mean mixture Risk Quotient (RQ) across all substances in the sample (numeric). |
| CRQmix\_median | Median mixture Risk Quotient (RQ) across all substances in the sample (numeric). |
| CRQmix\_n | Number of samples or measurements included in the CRQmix calculation (integer). |
| CRQmix\_mean\_num\_substances | Mean number of substances per sample for CRQmix calculation (numeric). |
| CRQmax\_max | Maximum individual Risk Quotient (RQ) found in the sample (i.e., for a single substance, numeric). |
| CRQmax\_max\_Probe | Unique identifier for the probe/sample with the maximum CRQmax value (factor). |
| CRQmax\_max\_DIF\_DATE | Time difference category for the maximum CRQmax value (character). |
| CRQmax\_max\_Param | Name of the substance/parameter with the maximum CRQmax value (character). |
| CRQmax\_max\_Substance | Unique identifier for the substance with the maximum CRQmax value (factor). |
| CRQmax\_mean | Mean of the maximum individual RQ values across all samples (numeric). |
| CRQmax\_median | Median of the maximum individual RQ values across all samples (numeric). |
| CRQmax\_n | Number of samples or measurements included in the CRQmax calculation (integer). |
| TU\_NOECmix\_max | Maximum mixture Toxic Unit (TU) based on NOEC values for all detected substances in the sample (numeric). |
| TU\_NOECmix\_max\_Probe | Unique identifier for the probe/sample with the maximum TU\_NOECmix value (factor). |
| TU\_NOECmix\_max\_DIF\_DATE | Time difference category for the maximum TU\_NOECmix value (character). |
| TU\_NOECmix\_max\_num\_Substances | Number of substances contributing to the maximum TU\_NOECmix value (integer). |
| TU\_NOECmix\_mean | Mean mixture Toxic Unit (TU) across all substances in the sample (numeric). |
| TU\_NOECmix\_median | Median mixture Toxic Unit (TU) across all substances in the sample (numeric). |
| TU\_NOECmix\_n | Number of samples or measurements included in the TU\_NOECmix calculation (integer). |
| TU\_NOECmix\_mean\_num\_substances | Mean number of substances per sample for TU\_NOECmix calculation (numeric). |
| TU\_NOECmax\_max | Maximum individual Toxic Unit (TU) found in the sample (i.e., for a single substance, numeric). |
| TU\_NOECmax\_max\_Probe | Unique identifier for the probe/sample with the maximum TU\_NOECmax value (factor). |
| TU\_NOECmax\_max\_DIF\_DATE | Time difference category for the maximum TU\_NOECmax value (character). |
| TU\_NOECmax\_max\_Param | Name of the substance/parameter with the maximum TU\_NOECmax value (character). |
| TU\_NOECmax\_max\_Substance | Unique identifier for the substance with the maximum TU\_NOECmax value (factor). |
| TU\_NOECmax\_mean | Mean of the maximum individual TU values across all samples (numeric). |
| TU\_NOECmax\_median | Median of the maximum individual TU values across all samples (numeric). |
| TU\_NOECmax\_n | Number of samples or measurements included in the TU\_NOECmax calculation (integer). |
| SPEAR | Value of the SPEARpesticides bioindicator index for the sample (numeric). |
| IBCH\_2019 | Value of the IBCH (Swiss biological index) for the sample (numeric). |
| GI\_VALUE | Value of another macroinvertebrate-based bioindicator. |
| VT\_VALUE | Value of another macroinvertebrate-based bioindicator. |
| EPT | Proportion of EPT taxa (Ephemeroptera, Plecoptera, Trichoptera) in the sample (numeric). |
| Kanton | Swiss canton where the stream is located (factor). |
| Kategorie\_FG\_Grosse | Stream size category (e.g., "Kleine", “Mittel”, "Gross "; factor). |
| YEAR | Year of sampling or observation (integer). |
| OID | Unique identifier for the observation or site (factor). |
| X.y | X-coordinate (e.g., Swiss coordinate system) of the sampling location (numeric). |
| Y.y | Y-coordinate of the sampling location (numeric). |
| Z | Elevation (meters above sea level) of the sampling location (numeric). |
| Season\_MZB | Season of macroinvertebrate sampling (e.g., "Spring", "Summer"; factor). |
| scenario | Scenario or time window used for the aggregation of the composite samples (e.g., "14\_days\_1\_month", "14\_days\_2\_weeks"; factor). |
| Gewasser\_clean | Cleaned/lowercase version of the stream name for easier merging (character). |
| PP\_mean\_mean | Mean value of daily precipitation. |

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