Supporting Information

Evaluating Satellite-Based Water Quality Sensing of Inland Waters on Basis of 100+ German Water Bodies Using 2 Different Processing Chains

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Table S1: Water body characteristics. O = oligotrophic, M = mesotrophic, E = eutrophic, P = polytrophic. Waterbodies with an “x” in the column “S3” are large enough to be evaluated with Sentinel-3 OLCI. See main text for the derivation. In brief, a 5x5 contiguous macro pixel, i.e. 1500*1500 m², can fit into waterbodies with an “x” in this column.

Federal State	Waterbody name	Waterbody type	Longitude	Latitude	Surface (ha)	Max. depth (m)	Tro-phy	S3
Hessia	Aartal Reservoir	Reservoir	50.6998	8.4558	58	9.2	E	
Hessia	Affolderner Reservoir	Reservoir	51.1622	9.0760	159	11.03	E	
Hessia	Borkener See	Mining pit	51.0301	9.2652	139	55.28	M	
Hessia	Diemel Reservoir	Reservoir	51.3770	8.7271	165	34	M	
Hessia	Eder Reservoir	Reservoir	51.1975	9.0596	1050	41.7	E	
Hessia	Kinzig Reservoir	Reservoir	50.3041	9.4051	65	7.3	P	
Hessia	Lampertheimer Altrheinsee	Anabranch	49.6131	8.4404	103	9.9	P	
Hessia	Mainflinger See	Mining pit	50.0188	9.0203	58	5.95	M	
Hessia	Twiste Reservoir	Reservoir	51.3825	9.0627	76	14.5	E	
Hessia	Werratalsee	Mining pit	51.1930	10.0739	117	8.51	E	
Rhineland Palatinate	Krombach Reservoir	Reservoir	50.6194	8.1330	67	9.5	M	
Rhineland Palatinate	Seensystem Neuhofener Altrhein	Lake	49.4327	8.4577	37	10.6	E	
Rhineland Palatinate	Laacher See	Lake	50.4116	7.2706	333	51.7	M	x
Rhineland Palatinate	Dreifelder Weiher	Lake	50.5906	7.8254	95	5.3	E	
Rhineland Palatinate	Wiesensee	Lake	50.5930	7.9940	81	5.5	E	
Rhineland Palatinate	Seehof Erlenbach	Lake	*49.1024*	*7.8714*	*5*	*2.5*	*E*	
Rhineland Palatinate	Badeweiher Neuhofen "Steinerne Brücke"	Lake	*49.4158*	*8.4162*	*6*	*17.1*	*M*	
Rhineland Palatinate	Nachtweideweiher Lambsheim	Lake	*49.5162*	*8.3067*	*19*	*8.8*	*E*	
Rhineland Palatinate	Nachtweideweiher Bobenheim Roxheim	Lake	*49.5866*	*8.3645*	*5*	*8.8*	*E*	
Rhineland Palatinate	Seensystem Binsfeld Speyerlachsee	Lake	*49.3573*	*8.4456*	*9*	*17.2*	*E*	
Schleswig-Holstein	Behlendorfer See	Lake	53.7006	10.6793	63	15.2	M	
Schleswig-Holstein	Bistensee	Lake	54.3897	9.6884	146	14.4	E	
Schleswig-Holstein	Bordesholmer See	Lake	54.1732	10.0205	69	7.8	P	
Schleswig-Holstein	Bothkamper See	Lake	54.2071	10.1343	138	3.2	H	
Schleswig-Holstein	Dieksee	Lake	54.1671	10.5075	375	37.7	M	
Schleswig-Holstein	Dobersdorfer See	Lake	54.3176	10.3179	319	18.4	E	
Schleswig-Holstein	Großer Plöner See	Lake	54.0964	10.4058	2963	56.2	M	
Schleswig-Holstein	Großer Ratzeburger See	Lake	53.7151	10.7594	1326	24.4	E	
Schleswig-Holstein	Großer Segeberger See	Lake	53.9432	10.3201	172	11.8	E	

(Table S1 continued)

Federal State	Waterbody name	Waterbody type	Longitude	Latitude	Sur-face (ha)	Max. depth (m)	Tro-phy	S3
Schleswig-Holstein	Hemmelsdorfer See	Lake	53.9506	10.7773	462	39.0	P	
Schleswig-Holstein	Lanker See	Lake	54.2146	10.3019	359	19.8	P	
Schleswig-Holstein	Schaalsee	Lake	53.6307	10.8895	2199	49.4	M	
Schleswig-Holstein	Selenter See	Lake	54.3017	10.4409	2125	36.8	M	x
Schleswig-Holstein	Trammer See	Lake	54.1698	10.4095	160	33.4	E	
Schleswig-Holstein	Westensee	Lake	54.2871	9.9310	724	17.5	E	
Schleswig-Holstein	Wittensee	Lake	54.3817	9.7557	993	21.4	E	x
Mecklenburg Pomerania	Ivenacker See	Lake	53.7099	12.9548	73	2.13	E	
Mecklenburg Pomerania	Schmachter See	Lake	54.3953	13.5954	119	2.50	H	
Mecklenburg Pomerania	Haussee	Lake	53.3473	13.4402	132	12.50	M	
Mecklenburg Pomerania	Borgwallsee	Lake	54.2653	13.0214	369	4.80	P	x
Mecklenburg Pomerania	Röggeliner See	Lake	53.7324	10.9350	184	7.01	E	x
Mecklenburg Pomerania	Schweriner See	Lake	53.6125	11.4552	6155	44.63	E	x
Mecklenburg Pomerania	Goldensee	Lake	53.6911	10.9328	101	9.05	E	
Mecklenburg Pomerania	Lankower See	Lake	53.7137	10.8664	89	11.30	E	
Mecklenburg Pomerania	Woezer See	Lake	53.5814	11.0832	57	3.85	P	
Mecklenburg Pomerania	Plauer See	Lake	53.4930	12.3410	3814	25.20	M	x
Mecklenburg Pomerania	Müritz	Lake	53.5113	12.6727	10867	30.50	M	x
Mecklenburg Pomerania	Tiefwaren	Lake	53.5262	12.6918	138	23.60	M	
Mecklenburg Pomerania	Breiter Luzin	Lake	53.3582	13.4660	337	58.25	M	x
Mecklenburg Pomerania	Zierker See	Lake	53.3603	13.0408	351	3.46	P	x
Mecklenburg Pomerania	Schmaler Luzin	Lake	53.3197	13.4368	146	33.50	O	
Mecklenburg Pomerania	Kummerower See	Lake	53.8058	12.8497	3236	23.31	E	x
Mecklenburg Pomerania	Tollensesee	Lake	53.5141	13.2182	1775	31.25	M	x
Mecklenburg Pomerania	Teterower See	Lake	53.7928	12.6151	312	10.70	E	
Mecklenburg Pomerania	Lieps	Lake	53.4526	13.1699	426	3.77	P	x

(Table S1 continued)

Federal State	Waterbody name	Waterbody type	Longitude	Latitude	Sur-face (ha)	Max. depth (m)	Tro-phy	S3
Saxony-Anhalt	Arendsee	Lake	52.8866	11.4590	510	50.1	P	x
Saxony-Anhalt	Barleber See 1	Lake	52.2230	11.6451	102	10.4	E	
Saxony-Anhalt	Muldestausee	Dammed river	51.6321	12.4125	600	28.4	E	x
Saxony-Anhalt	Neustädter See	Lake	52.1808	11.6400	82	8.4	M	
Saxony-Anhalt	Schollener See	Lake	52.6701	12.2009	92	2.2	P	x
Saxony-Anhalt	Süßer See	Lake	51.4950	11.6775	265	7.4	P	x
Saxony-Anhalt	Reservoir Kelbra	Reservoir	51.4418	10.9962	600	15.8	E	x
Saxony-Anhalt	Reservoir Rappbode	Reservoir	51.7385	10.8911	359	82.4	M	
Brandenburg	Parsteiner See	Lake	52.9256	13.9912	995	30	M	x
Brandenburg	Grimnitzsee	Lake	52.9772	13.7870	777	10	E	x
Brandenburg	Werbellinsee	Lake	52.9206	13.7109	796	55	M	
Brandenburg	Unteruckersee	Lake	53.2765	13.8668	1028	19	M	x
Brandenburg	Schwielochsee	Lake	52.0492	14.2070	1040	7	E	x
Brandenburg	Senftenberger See	Lake	51.4992	14.0152	1081	26	M	x
Brandenburg	Reservoir Spremberg	Reservoir	51.6455	14.3948	683	9	E	x
Brandenburg	Wolziger See	Lake	52.2554	13.8273	528	13	E	x
Brandenburg	Gülper See	Lake	52.7398	12.2547	481	4	P	x
Brandenburg	Blankensee	Lake	52.2255	13.1186	283	4	E	x
Bavaria	Ammersee	Lake	47.9821	11.1224	4630	81.1	O	x
Bavaria	Starnberger See	Lake	47.9284	11.3241	5620	127.8	O	x
Bavaria	Gr. Alpsee bei Immenstadt	Lake	47.5737	10.1792	236	22.7	M	
Bavaria	Grüntensee	Lake	47.6196	10.4578	125	11.2	E	
Bavaria	Simssee	Lake	47.8782	12.2469	640	22.5	M	
Lower Saxony	Steinhuder Meer	Lake	52.4759	9.3369	2910	2.9	P	x
Lower Saxony	Dümmer	Lake	52.5140	8.3402	1240	1.4	P	x
Baden-Württemberg	Bodensee	Lake	47.6101	9.4226	53148	253	O	x
Baden-Württemberg	Illmensee	Lake	47.8544	9.3802	66	17	M	
Baden-Württemberg	Ruschweiler See	Lake	*47.8695*	*9.3681*	*22*	*17*	*M*	
Baden-Württemberg	Mindelsee	Lake	47.7543	9.0217	102	14	M	
Baden-Württemberg	Titisee	Lake	47.8928	8.1442	107	39	O	
Baden-Württemberg	Federsee	Lake	48.0842	9.6293	145	3	E	
Baden-Württemberg	Schluchsee	Lake	47.8240	8.1651	472	63	O	x

(Table S1 continued)

Federal State	Waterbody name	Waterbody type	Longitude	Latitude	Surface (ha)	Max. depth (m)	Trophy	S3
Saxony	Speicher Witznitz	Reservoir	51.1462	12.4813	225	18.2	E	x
Saxony	Reservoir Bautzen	Reservoir	51.2267	14.4614	500	13.5	E	x
Saxony	Reservoir Quitzdorf	Reservoir	51.2843	14.7568	661	6.5	E	x
Saxony	Reservoir Saidenbach	Reservoir	50.7358	13.2342	146	46	O	
North Rhine Westphalia	Wupper Reservoir	Reservoir	51.1822	7.3143	227	32	M	
North Rhine Westphalia	Große Dhünn-Reservoir	Reservoir	51.0721	7.2121	440	53	O	
Hamburg	Außenalster	Lake	53.5652	10.0068	164	4.5		x
Hamburg	Eichbaumsee	Lake	53.4856	10.1022	24	16	P	
Hamburg	Dove-Elbe	Lake	53.4828	10.1003	77			
Hamburg	Hohendeicher See	Lake	53.4414	10.1047	62	19	M	
Hamburg	*Öjendorfer See*	Lake	53.5589	10.1392	*43*	*3.4*	*E*	
Hamburg	Neuländer See	Lake	53.4580	10.0203	41	17	E	
Hamburg	*See Hinterm Horn*	Lake	53.4731	10.1556	*10*	*16*	*M*	
Hamburg	*Allermöher See*	Lake	53.4806	10.1625	*9*	*16*	*M*	
Hamburg	Alte Süderelbe	Lake	53.5164	9.8464	60	3.5	E	
Thuringia	Reservoir Ohra	Reservoir	50.7655	10.7214	82	54	O	
Thuringia	Reservoir Leibis/Lichte	Reservoir (Raw water)	50.5983	11.1732	110	85	M	
Thuringia	Reservoir Zeulenroda	Reservoir	50.6633	11.9695	245	25	E	
Thuringia	Reservoir Großbrembach	Reservoir	51.1097	11.3164	55	9	P	
Thuringia	Reservoir Dachwig	Reservoir (Raw water)	51.0666	10.8308	70	8	P	
Lower Saxony	Zwischenahner Meer	Lake	53.1942	8.0136	540	6		x
Thuringia	Vorsperre Dees zu Reservoir Leibis Lichte	Reservoir	50.5735	11.1691	21			

Supplementary Information SI 1 – Projects for developing workflows on incorporating remote sensing in waterbody monitoring

- **WasMon-CT** with the federal state of Baden-Württemberg (https://www.d-copernicus.de/fileadmin/Content/pdf/Beispiele-aus-Deutschland/umwelt-naturschutz/WasMon-CT_15.7.16.pdf, and https://geoportal.bafg.de/arcportal/apps/webappviewer/index.html?id=72fdfede0a034e3b9f61b2f9aa75a609, accessed 20th of October 2023)
- **SAMOSEE-BW**, also with the federal state of Baden-Württemberg (https://um.baden-wuerttemberg.de/de/umwelt-natur/nachhaltigkeit/nachhaltige-digitalisierung/projekte/samosee-bw/, and https://pudi.lubw.de/detailseite/-/publication/10383, accessed 20th of October 2023)
- **CIWAWA** with the state of Hamburg (https://www.d-copernicus.de/fileadmin/Content/pdf/Beispiele-aus-Deutschland/Methoden-und-Anwendungsentwicklung/CIWAWA_graphical_abstract.pdf, and https://www.bafg.de/DE/05_Wissen/02_Veranst/2021/2021_09_07_05.pdf?__blob=publicationFile, accessed 20th of October 2023)
- **WaCoDis** with the North Rhine Westphalia association for protecting the drinking water use along the River Wupper (https://wacodis.fbg-hsbo.de/, accessed 20th of October 2023; [1]

Supporting Information SI 2 – Authorities concerned with water quality who contributed *in situ* data

HNLUG (Hessian State Agency for Nature Protection, Environment and Geology)

LfU (State agency for Environment Rhineland-Palatinate)

LLUR (State Agency Agriculture, Environment and Rural Areas, Schleswig Holstein)

Ministry for Climate protection, Agriculture, Rural Areas and the Environment Mecklenburg Pomerania

LHW (State agency for Flood protection and Water Resources Management Saxony Anhalt)

State agency for the Environment Brandenburg

NLWKN (Lower Saxony State Agency for Water Resources Management, Coast and Nature protection)

LUBW (State agency for the Environment Baden Württemberg)

LTV (State agency for Reservoirs Saxony)

Agency for the management of the catchment of the River Wupper, North Rhine Westphalia

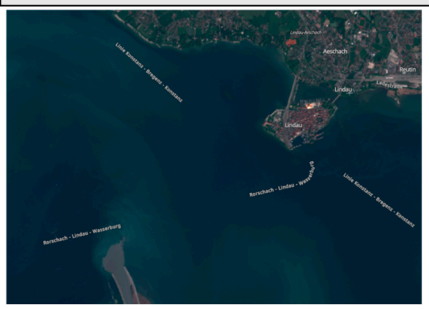
HHU (State Agency for Environment, Climate, Energy and Agricultural Management Institute for Hygiene and the Environment Hamburg

Thuringian Water Resources Provider

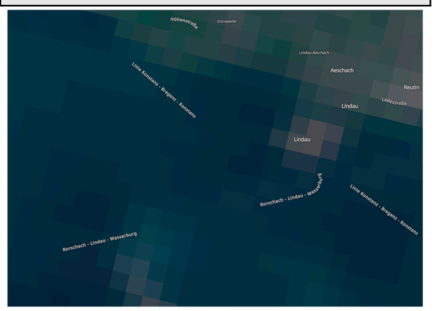
LfU (Bavarian state agency for the Environment)

Supporting Information SI 3 – Satellite specifications

Satellite	Sentinel-2	Sentinel-3
Active since	2015 (A), 2017 (B)	2016 (A), 2018 (B)
Spatial Resolution	10 x 10 m; 30 x 30 m; 60 x 60 m	300x300 m
Temporal Resolution	Overflights every ca. 5 days	Overflights ca. every day
Instruments	Multispectral imager (MSI)	Ocean and Land Colour Instrument (OLCI)
Spectral resolution	13 bands	21 bands for OLCI



Sentinel-2 (11th of May 2022)



Sentinel-3 (11th of May 2022)

Figure S1. Overview over the two satellites used and their specifications, along with two example images from Lindau, Lake Constance, Germany. MSI = Multispectral Instrument; OLCI = Ocean and Land Color Imager.

Supporting Information SI 4 – Secchi depth *in situ* measurements

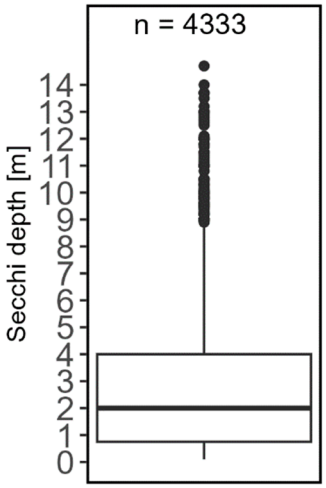
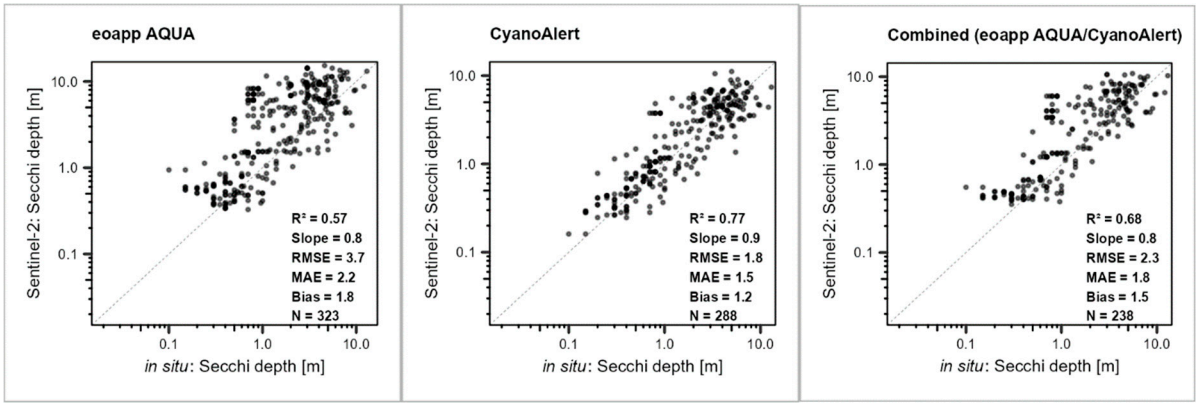


Figure S2. Boxplot of the Secchi depths in the in situ *data. The upper whisker extends here from the upper line of the box to the largest value, with the whisker not being further than 1.5 times the inter-quartile range from the upper line of the box. The inter-quartile range is the distance between the first and third quartiles. The lower whisker extends to the smallest value*

which is maximum 1.5 times the inter-quartile range. Outliers are points outside of the inter-quartile range. They are plotted as separate points.

Supporting Information SI 5 – Results

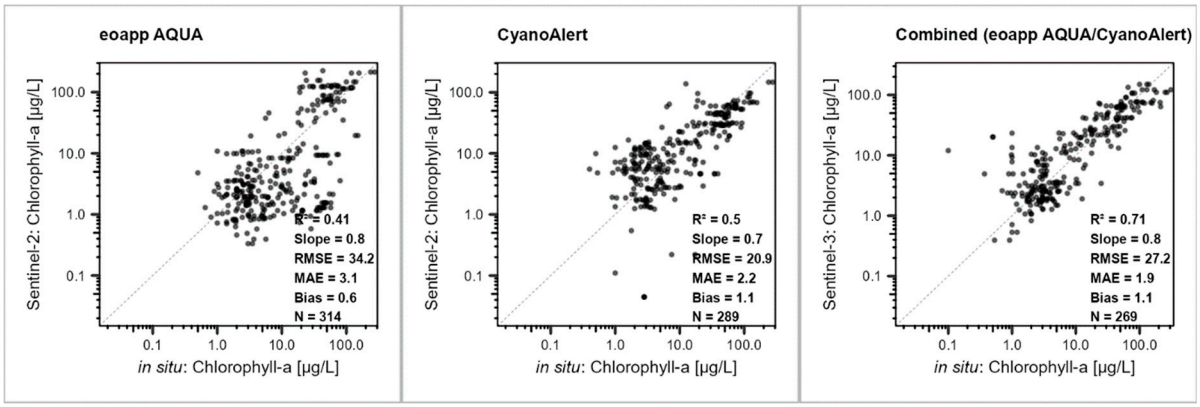
Secchi depth



(a) (b) (c)

Figure S3. Regression between in situ *(x axis) and Sentinel-2 MSI remote sensing Secchi depth values (y axis) from the whole water body, values from the same day, on a logarithmic scale. a), eoapp AQUA processing chain, b) CyanoAlert processing chain, c) combined approach. R^2 = Determination measure, Slope = regression line slope, MAE = Mean average error, all three based on log transformed data, RMSE = root mean square error, Bias =mean bias from the untransformed data, N = number of measurements. For the results for Sentinel-3, refer to Figure 3 of the main paper.*

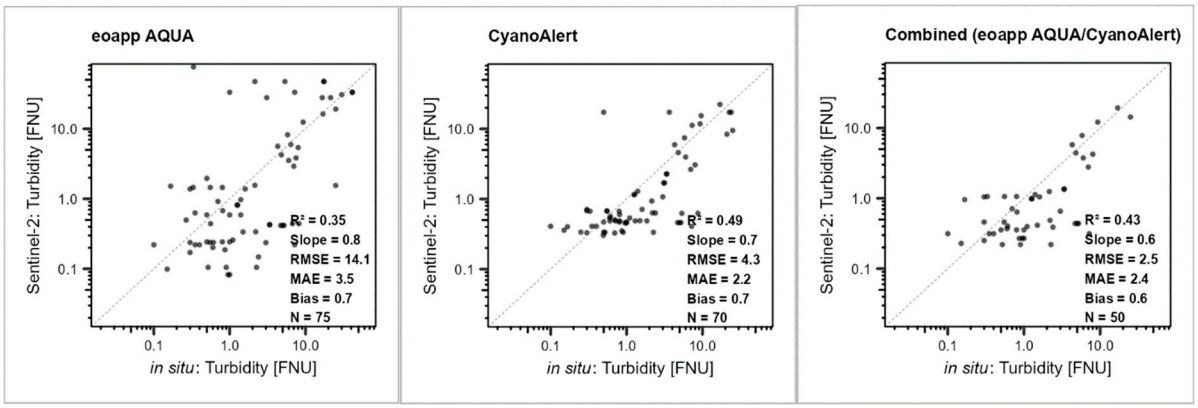
Chlorophyll-a



(a) (b) (c)

Figure S4. Regression between in situ *(x axis) and Sentinel-2 remote sensing chlorophyll-a values (y axis) from the whole water body, values from the same day, on a logarithmic scale. a) eoapp AQUA processing chain, b) CyanoAlert processing chain, c) combined approach. R^2 = Determination measure, Slope = regression line slope, MAE = Mean average error, all three based on log transformed data, RMSE = root mean square error, Bias =mean bias from the untransformed data, N = number of measurements. For the results for Sentinel-3, refer to Figure 4 of the main paper.*

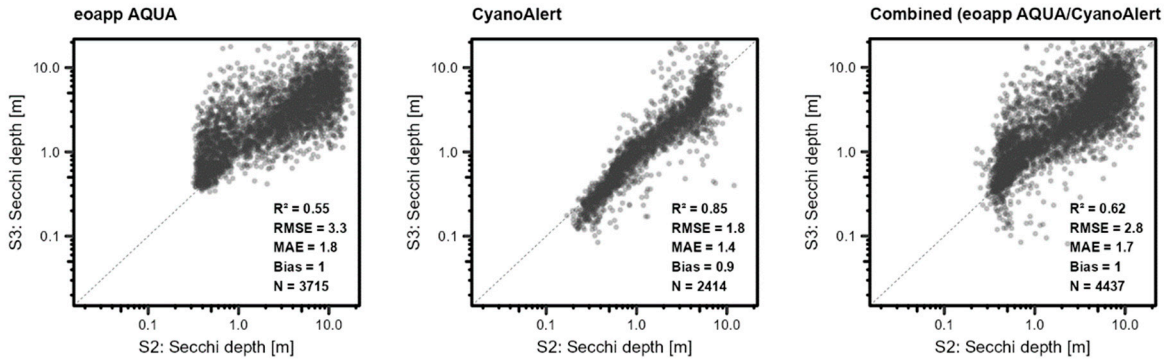
Turbidity



(a) (b) (c)

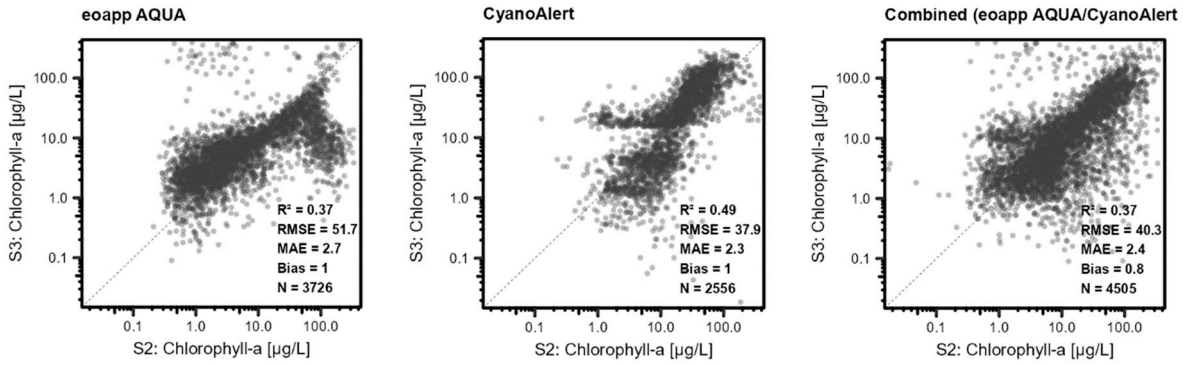
Figure S5. Regression between in situ *(x axis) and Sentinel-2 remote sensing turbidity values (y axis) from the whole water body, values from the same day, on a logarithmic scale. a) eoapp AQUA processing chain, b) CyanoAlert processing chain, c) combined approach. R^2 = Determination measure, Slope = regression line slope, MAE = Mean average error, all three based on log transformed data, RMSE = root mean square error, Bias =mean bias from the untransformed data, N = number of measurements. For the results for Sentinel-3, refer to Figure 5 of the main paper.*

Sentinel-2 versus Sentinel-3



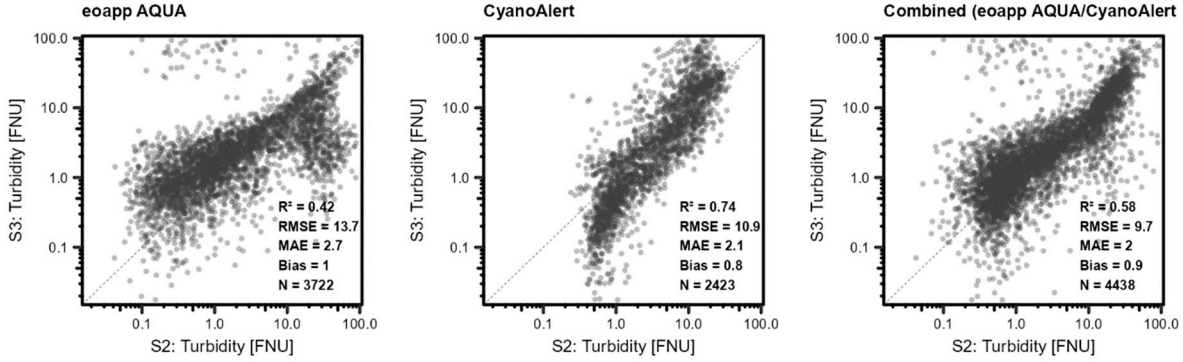
(a) (b) (c)

Figure S6: Regression between remote sensing Secchi depth values from the waterbody-scale Sentinel-2 (x axis) and Sentinel-3 (y axis), values from the same day, on a logarithmic scale. a) eoapp AQUA processing chain, b) CyanoAlert processing chain, c) combined approach. R^2 = Determination measure, Slope = regression line slope, MAE = Mean average error, Bias = mean bias; all four based on log transformed data, RMSE = root mean square error, N = number of measurements.



(a) (b) (c)

Figure S7. Regression between remote sensing chlorophyll-a values from the waterbody-scale Sentinel-2 (x axis) and Sentinel-3 (y axis), values from the same day, on a logarithmic scale. a) eoapp AQUA processing chain, b) CyanoAlert processing chain, c) combined approach. R^2 = Determination measure, Slope = regression line slope, MAE = Mean average error, Bias = mean bias; all four based on log transformed data, RMSE = root mean square error, N = number of measurements.



(a) (b) (c)

Figure S8. Regression between remote sensing turbidity values from the waterbody-scale Sentinel-2 (x axis) and Sentinel-3 (y axis), values from the same day, on a logarithmic scale. a) eoapp AQUA processing chain, b) CyanoAlert processing chain, c) combined approach. R^2 = Determination measure, Slope = regression line slope, MAE = Mean average error, Bias = mean bias; all four based on log transformed data, RMSE = root mean square error, N = number of measurements.

References

1. Kirstein, V.; Bitterich, L.; Drost, S.; Vogt, A.; Pakzad, K. Copernicus Dienste Für Die Wasserwirtschaft – Ergebnisse Aus Dem Projekt WaCoDiS. *kw Korrespondenz Wasserwirtschaft* **2021**, *14*, 486–486.