

Table S1. Statistical values of major and minor ions measured in surface and groundwater from Taxco-Cocula hydrological sub-basin.

Water Source	Season	Statistical values	HCO_3^-	SO_4^{2-}	Cl^-	NO_3^-	Ca^{2+}	Na^+	K^+	Mg^{2+}	SiO_2
mg/L											
Surface water (Rivers or streams)	Dry	Min	129.3	10.0	3.3	1.1	27.9	4.1	0.9	1.6	6.8
		Max	412.4	2600.0	90.0	125.0	183.5	79.1	37.2	102.1	48.9
		Median	197.6	61.5	17.5	7.1	109.5	16.6	4.0	14.7	24.2
		P10	174.5	27.5	10.8	2.6	72.5	11.1	36.3	11.1	21.5
		P90	234.3	163.0	24.2	19.4	147.5	25.8	9.7	18.4	33.1
		IQR	59.8	135.5	13.4	16.8	75.0	14.8	7.4	7.3	11.6
	Rainy	Min	109.8	10.0	2.0	0.5	23.8	2.1	0.3	1.7	7.6
		Max	383.1	460.0	53.0	26.7	170.1	49.4	21.9	19.1	47.4
		Median	201.3	48.0	10.0	9.5	97.7	9.3	2.2	10.2	25.3
		P10	164.7	29.5	4.5	5.2	69.7	6.4	1.5	7.8	18.9
		P90	230.6	74.0	15.0	14.4	128.2	16.9	4.6	12.6	37.3
		IQR	65.9	44.5	10.5	9.2	58.5	10.5	3.1	4.9	18.4
Groundwater (Springs)	Dry	Min	29.3	1.0	1.7	0.3	5.0	1.1	0.2	0.2	9.5
		Max	621.2	1000.0	54.2	57.7	352.2	17.9	3.2	76.4	74.0
		Median	268.4	18.5	5.4	1.4	112.2	5.5	0.9	4.2	18.8
		P10	229.4	5.5	3.3	1.0	59.0	2.8	0.8	2.2	12.6
		P90	408.9	94.0	26.7	7.2	173.3	13.1	2.0	17.7	28.0
		IQR	179.5	88.5	23.4	6.2	114.3	10.3	1.3	15.5	15.4
	Rainy	Min	29.3	1.0	2.0	0.1	4.9	1.0	0.1	0.2	4.0
		Max	407.5	900.0	31.0	39.1	390.5	18.3	4.3	72.9	70.0
		Median	261.1	15.0	5.0	2.6	83.9	4.9	0.9	3.9	17.2
		P10	179.8	3.0	3.0	1.4	48.3	2.3	0.4	1.2	9.5
		P90	292.5	64.0	26.0	10.2	130.4	13.7	2.2	14.1	34.9
		IQR	112.8	61.0	23.0	8.9	82.1	11.4	1.8	12.9	25.4

Min: Minimum; Max: Maximum; P10: 10th percentile; P90: 90th percentile; IQR: Interquartile range

Table S2. Statistical values of heavy metals measured in surface and groundwater from Taxco-Cocula hydrological sub-basin.

Water Source	Season	Statistical values	Al	As	Ba	Cd	Cu	Fe	Mn	Pb	Sr	Zn
mg/L												
Surface water (Rivers/streams)	Dry	Min	0.030	0.010	0.020	0.010	0.080	0.030	0.030	0.010	0.060	0.050
		Max	28.630	0.600	0.180	1.780	1.050	68.270	21.470	0.020	0.740	208.800
		Median	0.060	0.015	0.050	0.085	0.135	0.085	0.670	0.015	0.280	0.200
		P10	0.035	0.010	0.035	0.015	0.100	0.050	0.060	0.010	0.200	0.080
		P90	1.105	0.025	0.065	0.105	0.600	0.285	1.580	0.020	0.370	1.200
		IQR	1.070	0.015	0.030	0.090	0.500	0.235	1.520	0.010	0.170	1.120
	Rainy	Min	0.050	0.010	0.030	0.010	ND	0.040	0.030	0.030	0.030	0.020
		Max	2.150	0.090	0.230	0.020	ND	3.730	0.590	0.050	0.980	1.410
		Median	0.265	0.020	0.045	0.015	ND	0.330	0.050	0.040	0.230	0.050
		P10	0.120	0.010	0.040	0.010	ND	0.160	0.030	0.030	0.185	0.030
		P90	0.520	0.030	0.050	0.020	ND	0.645	0.230	0.050	0.305	0.110
		IQR	0.400	0.020	0.010	0.010	ND	0.485	0.200	0.020	0.120	0.080
Groundwater (Springs)	Dry	Min	0.030	0.010	0.030	ND	ND	0.030	0.030	ND	0.030	0.030
		Max	0.370	0.080	0.100	ND	ND	0.130	0.030	ND	2.520	0.230
		Median	0.120	0.045	0.040	ND	ND	0.060	0.030	ND	0.130	0.110
		P10	0.030	0.010	0.030	ND	ND	0.050	0.030	ND	0.070	0.070
		P90	0.150	0.080	0.050	ND	ND	0.100	0.030	ND	0.530	0.130
		IQR	0.120	0.070	0.020	ND	ND	0.050	0.000	ND	0.460	0.060
	Rainy	Min	0.030	0.150	0.030	ND	ND	0.020	0.030	ND	0.030	0.030
		Max	0.250	0.150	0.070	ND	ND	0.250	0.030	ND	2.800	0.060
		Median	0.100	0.150	0.050	ND	ND	0.060	0.030	ND	0.060	0.045
		P10	0.060	0.150	0.040	ND	ND	0.045	0.030	ND	0.040	0.030
		P90	0.190	0.150	0.055	ND	ND	0.135	0.030	ND	0.255	0.060
		IQR	0.130	0.000	0.015	ND	ND	0.090	0.000	ND	0.215	0.030

Min: Minimum; Max: Maximum; P10: 10th percentile; P90: 90th percentile; IQR: Interquartile range; ND: No detected

Table S3. Multivariate analysis by using Principal Component Analysis.

Component	Factor 1	Factor 2	Factor 3	Factor 4
HCO_3^-	-0.57	0.6	-0.15	0.05
SO_4^{2-}	0.99	-0.03	0	0.03
Cl^-	-0.12	0.97	-0.05	0.12
NO_3^-	0.6	0.77	-0.15	-0.02
Ca^{2+}	0.24	-0.05	0.1	0.92
Na^+	0.07	0.96	0.08	-0.05
K^+	-0.07	0.85	0.33	0.14
Mg^{2+}	0.95	0.02	0.14	0.22
SiO_2	-0.12	0.47	-0.25	0.73
Al	1	-0.03	0.01	0
As	0.99	-0.04	-0.02	-0.01
Ba	-0.15	0.07	0.97	-0.14
Cd	1	-0.04	-0.01	0
Cu	0.95	0.06	0.05	0.13
Fe	1	-0.03	0	0.02
Mn	1	0	-0.01	0.04
Pb	0.99	-0.03	0.01	0.03
Sr	0.2	0.04	0.96	0.09
Zn	1	-0.03	-0.01	0.01
Variance (%)	55	20.5	11.2	7.1

Table S4. Diversity of chemical reactive phases in the surface water of Taxco-Cocula sub-basin in dry season.

Sample	Minerals								Others
	Aragonite	Calcite	Gypsum	Jarosite-K	Goethite	Quartz	Barite	ZnO	
Taxco-Cocula River									
S1	0.99	1.14	-1.59	-4.25	8.13	0.72	0.05	-1.48	Ba ₃ (AsO ₄) ₂ (8.84), AlOOH (1.94)
S2	ND	ND	-0.49	-20.38	-3.15	0.59	0.55	-8.83	CuFeO ₂ (1.21), PbSO ₄ (-2.10), CuO (-7.42), As ₂ O ₃ (-8.67), CdSO ₄ (-7.75)
S3	ND	0.15	-1.37	1.81	9.17	0.73	0.16	-1.65	Ba ₃ (AsO ₄) ₂ (7.09), AlOOH (2.48), CdCO ₃ (0.44), FeCO ₃ (0.50)
S8	0.85	1.00	-1.81	1.24	9.74	0.97	0.46	0.44	Ba ₃ (AsO ₄) ₂ (9.70), AlOOH (3.71), CdCO ₃ (0.87), CuO (0.03)
S10	0.79	0.94	-1.10	0.86	9.83	0.91	0.44	0.73	Ba ₃ (AsO ₄) ₂ (10.27), AlOOH (1.88), CuFeO ₂ (16.16), ZnCO ₃ (0.57), MnCO ₃ (0.60)
S11	1.18	1.34	-1.12	-2.98	8.95	0.79	0.39	0.49	Ba ₃ (AsO ₄) ₂ (10.29), AlOOH (0.62), CdCO ₃ (1.16), MnCO ₃ (1.45)
S12	1.41	1.56	-1.12	-6.80	7.89	0.56	0.23	0.23	AlOOH (1.28), CdCO ₃ (0.86), MnCO ₃ (0.57), MgCO ₃ (0.54)
S14	1.77	1.92	-1.39	-11.31	7.14	0.42	0.08	0.26	Ba ₃ (AsO ₄) ₂ (11.57), CdCO ₃ (0.98), MnCO ₃ (1.01), MgCO ₃ (0.84)
S16	1.38	1.52	-1.95	-10.01	7.28	0.49	-0.50	-1.05	Zn ₂ SiO ₄ (1.75), MgCO ₃ (0.44), SrSO ₄ (-2.90)
S22	1.53	1.67	-1.86	-9.66	7.39	0.52	ND	-1.29	Zn ₂ SiO ₄ (0.89), MgCO ₃ (-0.12), FeCO ₃ (-4.45)
S23	1.56	1.70	-1.84	-10.61	7.11	0.51	-0.41	-1.23	Zn ₂ SiO ₄ (1.40), MgCO ₃ (0.58), kaolinite (1.43)
Cacalotenango stream									
S4	0.66	0.81	-2.83	-9.32	7.82	0.64	-0.79	-1.53	Al(OH) ₃ (0.71), Zn ₂ SiO ₄ (1.40), MgCO ₃ (0.58), kaolinite (1.43)
S5	0.78	0.93	-2.41	-9.22	7.63	0.55	-0.59	-1.32	Zn ₂ SiO ₄ (0.83), MgCO ₃ (-0.56), FeCO ₃ (-3.80)
S6	1.04	1.19	-1.76	-6.70	8.05	0.88	0.03	-1.00	Zn ₂ SiO ₄ (1.95), MgCO ₃ (-0.10), FeCO ₃ (-3.17)
S7	1.01	1.16	-1.29	-4.82	8.12	0.91	0.30	-1.44	AlOOH (0.35), Al(OH) ₃ (0.95), MgCO ₃ (-0.19)
Buenavista stream									
S19	0.69	0.84	-1.17	-2.14	8.17	0.93	0.60	-1.17	Ba ₃ (AsO ₄) ₂ (8.80), AlOOH (0.06), MnCO ₃ (0.94), Zn ₂ SiO ₄ (0.38)
S17	1.38	1.52	-1.30	-7.37	7.39	0.75	ND	-1.98	FeCO ₃ (-2.30), MgCO ₃ (0.27), SrSO ₄ (-2.23)
S18	0.61	0.76	-1.41	-5.28	7.31	0.77	0.09	ND	FeCO ₃ (-1.90), MnCO ₃ (-0.34), MgCO ₃ (-0.45)
S20	0.57	0.72	-1.90	-4.22	8.24	0.16	0.42	-1.09	Zn ₂ SiO ₄ (0.94), MgCO ₃ (-0.06), Al(OH) ₃ (1.57)
S21	1.35	1.49	-1.93	-10.35	7.11	-0.11	0.37	ND	FeCO ₃ (-5.34), MgCO ₃ (0.57), AlOOH (-0.17)

ND: No detected.

Table S5. Diversity of chemical reactive phases in the surface water of Taxco-Cocula sub-basin in rainy season.

Sample	Minerals								Others
	Aragonite	Calcite	Gypsum	Jarosite-K	Goethite	Quartz	Barite	ZnO	
Taxco-Cocula River									
S1	0.99	1.14	-1.59	-4.25	8.13	0.72	0.05	-1.48	Zn ₂ SiO ₄ (1.50), MnCO ₃ (0.20), Al(OH) ₃ (1.59), AlOOH (2.81)
S2	1.23	1.37	-0.83	-2.79	8.69	0.36	ND	-0.30	AlOOH (0.52), MgCO ₃ (0.22), CdCO ₃ (0.67)
S3	0.72	0.86	-1.51	-2.73	9.03	0.89	-0.40	-0.60	PbSO ₄ (-3.84), Pb(OH) ₂ (0.32), AlOOH (1.40), MnCO ₃ (0.49)
S8	0.77	0.92	-1.60	-1.45	9.39	0.87	0.01	-0.67	AlOOH (1.67), MgCO ₃ (-0.32), Pb(OH) ₂ (-0.65)
S10	1.82	1.96	-1.51	-8.59	7.92	0.64	-0.17	-0.92	CdCO ₃ (0.93), ZnCO ₃ (-2.05), MnCO ₃ (0.22)
S11	1.72	1.86	-1.79	-10.13	7.59	0.55	-0.37	-1.49	Zn ₂ SiO ₄ (0.55), MgCO ₃ (0.51), AlOOH (1.13)
S12	1.76	1.90	-1.80	-11.29	7.44	0.33	-1.32	-1.26	AlOOH (0.91), MgCO ₃ (0.65), Zn ₂ SiO ₄ (0.80)
S14	1.72	1.86	-1.86	-10.76	7.53	0.41	-0.43	ND	Al(OH) ₃ (-0.23), MgCO ₃ (0.60), AlOOH (-0.71)
S16	1.52	1.66	-1.90	-7.82	8.21	0.54	-0.60	-1.19	Zn ₂ SiO ₄ (1.11), MgCO ₃ (0.43), Al(OH) ₃ (0.65)
S22	1.41	1.63	-2.01	-7.84	8.25	0.43	-0.51	-1.09	Ba ₃ (AsO ₄) ₂ (10.66), AlOOH (1.65), MgCO ₃ (0.42), Zn ₂ SiO ₄ (1.18)
S23	1.50	1.64	-1.93	-7.83	8.18	0.38	-0.38	-1.49	AlOOH (0.20), MgCO ₃ (0.40), MnCO ₃ (-0.11)
Cacalotenango stream									
S4	1.27	1.41	-2.64	-11.15	7.71	0.64	-0.80	ND	Al(OH) ₃ (0.15), AlOOH (-0.41), MgCO ₃ (-0.05)
S5	1.25	1.39	-2.51	-13.57	7.05	0.18	ND	ND	AlOOH (-1.06)
S6	1.71	1.86	-1.84	-11.03	7.59	0.71	-0.14	-0.61	MnCO ₃ (0.13), MgCO ₃ (0.57), Al(OH) ₃ (-0.16)
S7	1.76	1.91	-1.66	-9.75	7.68	0.71	-0.14	-1.01	Ba ₃ (AsO ₄) ₂ (11.59), MgCO ₃ (0.64), AlOOH (0.97)
Buenavista stream									
S19	0.83	0.98	-2.14	-4.28	8.57	0.81	-0.19	ND	Ba ₃ (AsO ₄) ₂ (11.12), MnCO ₃ (0.70), AlOOH (2.45), MgCO ₃ (0.01)
S17	1.67	1.78	-1.57	-9.68	7.22	0.77	-0.04	ND	MgCO ₃ (0.54), FeCO ₃ (-4.49)
S18	1.69	1.73	-1.69	-10.42	7.10	0.69	-0.03	-1.54	Ba ₃ (AsO ₄) ₂ (11.71), MgCO ₃ (0.56), FeCO ₃ (-5.09), Zn ₂ SiO ₄ (0.58)
S20	1.53	1.66	-2.07	-12.57	7.22	-0.42	0.50	-0.39	Al(OH) ₃ (-0.30), MgCO ₃ (1.05), MnCO ₃ (-0.04), Zn ₂ SiO ₄ (1.70)
S21	1.49	1.63	-2.07	-11.67	7.31	-0.38	0.52	-0.54	Al(OH) ₃ (-0.32), MgCO ₃ (1.04), Zn ₂ SiO ₄ (1.44)

ND: No detected.