

Supplementary Information

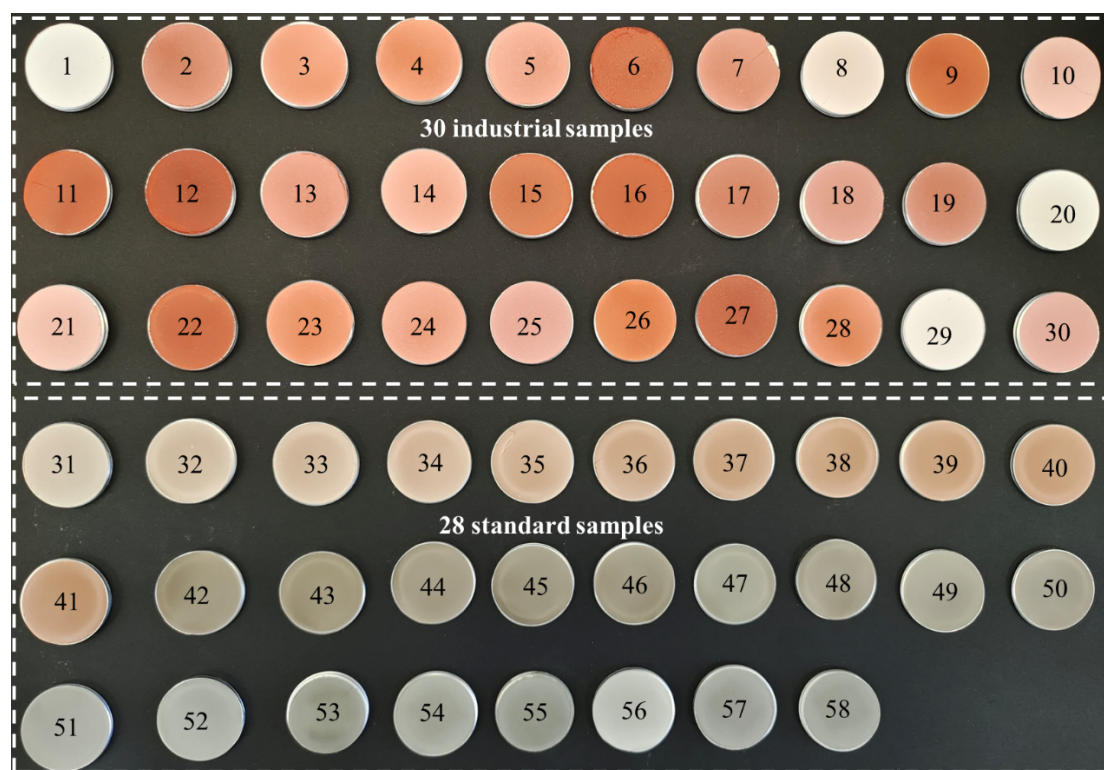


Fig.S1 The 58 samples are arranged in ascending order from left to right and top to bottom according to their respective numbers.

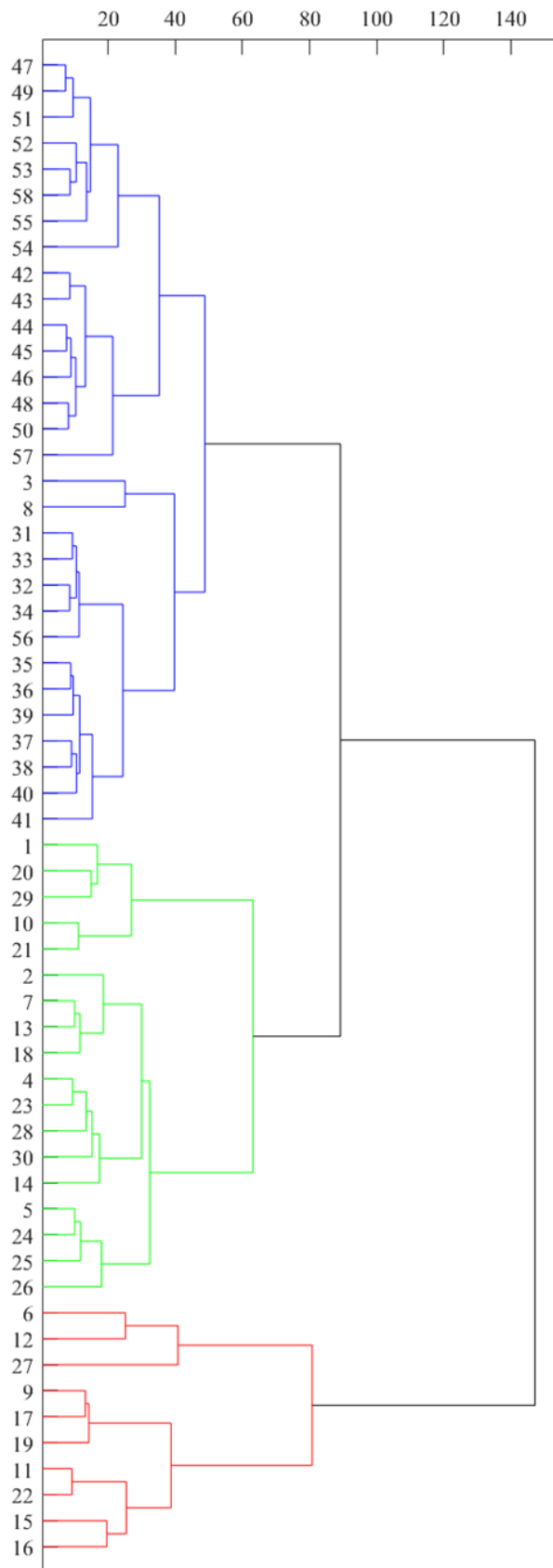


Fig.S2 Dendrogram of 58 cement samples generated by hierarchical clustering.

Table S1 The concentration information of target elements in 58 cement samples.

| Samples number | Ca (%) | Si (%) | Fe (%) | Al (%) | Mg (%) | K (%) |
|----------------|--------|--------|--------|--------|--------|-------|
| #1 | 53.78 | 1.14 | 0.05 | 0.09 | 1.33 | 0.04 |
| #2 | 41.79 | 13.00 | 2.96 | 3.33 | 2.23 | 0.33 |
| #3 | 34.42 | 14.18 | 1.42 | 0.78 | 5.18 | 0.94 |
| #4 | 45.09 | 11.77 | 2.42 | 2.24 | 1.26 | 0.11 |
| #5 | 38.80 | 16.59 | 1.51 | 4.74 | 1.78 | 0.61 |
| #6 | 20.45 | 38.65 | 6.74 | 7.69 | 1.07 | 1.85 |
| #7 | 39.22 | 13.41 | 2.15 | 3.83 | 2.85 | 1.30 |
| #8 | 28.65 | 28.51 | 0.08 | 6.55 | 5.73 | 0.05 |
| #9 | 32.40 | 20.28 | 6.15 | 7.11 | 2.08 | 0.30 |
| #10 | 38.84 | 21.15 | 0.49 | 3.22 | 1.03 | 1.30 |
| #11 | 40.63 | 11.94 | 7.22 | 2.85 | 1.03 | 1.04 |
| #12 | 30.05 | 13.47 | 14.50 | 2.38 | 3.53 | 1.49 |
| #13 | 27.60 | 28.84 | 1.69 | 6.76 | 2.11 | 1.83 |
| #14 | 36.08 | 26.30 | 1.03 | 2.09 | 1.58 | 0.32 |
| #15 | 28.12 | 32.16 | 3.79 | 4.77 | 2.32 | 0.39 |
| #16 | 19.44 | 42.09 | 5.87 | 5.91 | 2.74 | 0.50 |
| #17 | 35.42 | 12.20 | 3.04 | 3.04 | 3.05 | 2.57 |
| #18 | 44.99 | 10.01 | 2.00 | 0.13 | 2.00 | 0.04 |
| #19 | 42.78 | 4.13 | 2.55 | 4.08 | 4.10 | 1.56 |
| #20 | 53.68 | 1.14 | 0.05 | 0.09 | 1.33 | 0.04 |
| #21 | 38.74 | 21.25 | 0.48 | 3.32 | 1.08 | 1.32 |
| #22 | 40.23 | 11.54 | 7.28 | 2.75 | 1.13 | 1.05 |
| #23 | 45.29 | 11.72 | 2.33 | 2.28 | 1.22 | 0.14 |
| #24 | 38.77 | 16.61 | 1.49 | 4.64 | 1.74 | 0.54 |
| #25 | 38.26 | 14.33 | 1.45 | 4.16 | 2.20 | 0.95 |
| #26 | 40.77 | 13.32 | 2.91 | 3.60 | 1.03 | 1.93 |
| #27 | 25.56 | 18.70 | 9.13 | 7.51 | 2.90 | 2.19 |
| #28 | 41.92 | 14.17 | 1.94 | 3.28 | 1.94 | 0.17 |

| | | | | | | |
|-----|-------|-------|------|------|------|------|
| #29 | 38.15 | 15.09 | 0.09 | 1.01 | 5.02 | 2.05 |
| #30 | 47.55 | 6.96 | 1.19 | 2.28 | 1.19 | 0.48 |
| #31 | 46.00 | 10.50 | 1.58 | 2.06 | 1.13 | 0.30 |
| #32 | 45.39 | 10.66 | 1.63 | 2.20 | 1.36 | 0.33 |
| #33 | 44.63 | 11.31 | 1.76 | 2.44 | 1.51 | 0.38 |
| #34 | 43.85 | 11.92 | 1.98 | 2.64 | 1.63 | 0.41 |
| #35 | 43.17 | 12.47 | 2.09 | 2.84 | 1.77 | 0.47 |
| #36 | 41.91 | 13.56 | 2.46 | 3.14 | 1.83 | 0.52 |
| #37 | 41.16 | 14.00 | 2.51 | 3.33 | 2.06 | 0.57 |
| #38 | 40.44 | 14.52 | 2.64 | 3.48 | 2.25 | 0.62 |
| #39 | 39.37 | 15.33 | 2.84 | 3.73 | 2.41 | 0.67 |
| #40 | 38.30 | 16.23 | 3.17 | 3.96 | 2.56 | 0.72 |
| #41 | 37.61 | 16.71 | 3.16 | 4.16 | 2.74 | 0.75 |
| #42 | 51.18 | 25.49 | 3.31 | 6.96 | 3.94 | 1.07 |
| #43 | 53.59 | 24.10 | 3.20 | 6.93 | 3.70 | 1.06 |
| #44 | 54.14 | 23.78 | 3.19 | 6.56 | 3.47 | 1.00 |
| #45 | 55.50 | 23.30 | 3.05 | 6.33 | 3.28 | 0.94 |
| #46 | 57.08 | 23.13 | 3.00 | 6.10 | 3.13 | 0.89 |
| #47 | 58.14 | 22.80 | 2.91 | 5.82 | 2.93 | 0.85 |
| #48 | 59.44 | 22.56 | 2.83 | 5.55 | 2.66 | 0.79 |
| #49 | 60.63 | 22.27 | 2.74 | 5.32 | 2.47 | 0.75 |
| #50 | 61.50 | 22.02 | 2.69 | 5.09 | 2.26 | 0.68 |
| #51 | 62.65 | 21.81 | 2.58 | 4.78 | 2.07 | 0.62 |
| #52 | 64.01 | 21.45 | 2.49 | 4.46 | 1.85 | 0.57 |
| #53 | 65.78 | 22.07 | 3.22 | 4.56 | 2.11 | 0.69 |
| #54 | 57.22 | 21.36 | 2.78 | 6.50 | 4.12 | 0.86 |
| #55 | 62.23 | 20.41 | 3.20 | 4.68 | 2.66 | 0.71 |
| #56 | 42.40 | 13.76 | 2.13 | 3.12 | 2.11 | 0.50 |
| #57 | 47.57 | 32.67 | 3.54 | 6.52 | 1.86 | 1.43 |

| | | | | | | |
|----------|--------|-------|-------|------|------|------|
| #58 | 55.21 | 24.78 | 3.00 | 7.24 | 2.64 | 0.71 |
| Average | 44.10 | 17.92 | 2.93 | 4.09 | 2.35 | 0.82 |
| Max. | 65.78 | 42.09 | 14.50 | 7.69 | 5.73 | 2.57 |
| Min. | 19.44 | 1.14 | 0.05 | 0.09 | 1.03 | 0.04 |
| Variance | 119.85 | 64.75 | 5.57 | 3.91 | 1.16 | 0.33 |

Table S2 Number of latent variables (LVs) in the optimized PLSR model.

| Model | Elements | LVs |
|-------------------|----------|-----------|
| HC-PLSR Cluster 1 | Ca | 7 |
| | Si | 8 |
| | Fe | 6 |
| | Al | 6 |
| | Mg | 8 |
| | K | 7 |
| HC-PLSR Cluster 2 | Ca | 10 |
| | Si | 10 |
| | Fe | 10 |
| | Al | 10 |
| | Mg | 6 |
| | K | 10 |
| HC-PLSR Cluster 3 | Ca | 10 |
| | Si | 10 |
| | Fe | 7 |
| | Al | 9 |
| | Mg | 10 |
| | K | 10 |
| PLSR | Ca | 10 |
| | Si | 13 |
| | Fe | 14 |
| | Al | 12 |
| | Mg | 10 |
| | K | 11 |