

Supporting Information

Pseudo-Code of the Random Search Algorithm:

Input: $F = \{f_1, f_2, \dots, f_n\}$

Output: A subset of F

Step 1: Initial $r_0 = r = Q$, $s = \emptyset$, $G_{best} = F$, $k = 0$, C , K are specified

Step 2: Partition r_0

Step 3: Find the most promising index

$\sigma = \{\eta | \eta \in \text{children}(r)\}$, $m = |\sigma|$, $\sigma_{m+1} = s$, $\text{Index} = 0$;

For $i = 1: m + 1$

Randomly sample N subsets in σ_i , find the best G_i^*

End;

$\text{Index} = \arg \max_{1 \leq i \leq m+1} (I(\sigma_i))$,

If $\text{Index} G_{\text{Index}}^* \geq G_{best}$ then $G_{best} = G_{\text{Index}}^*$

If $|\sigma_{\text{Index}}| = 1$ then go to Step 5

Step 4: If $1 \leq \text{Index} \leq m$ then $r = \sigma_{\text{Index}}$, $s = r_0$ else $r = \text{sup}(r)$; $k = k + 1$;

If $k > K$ then go to Step 5 else go to Step 3

Step 5: Output the G_{best}

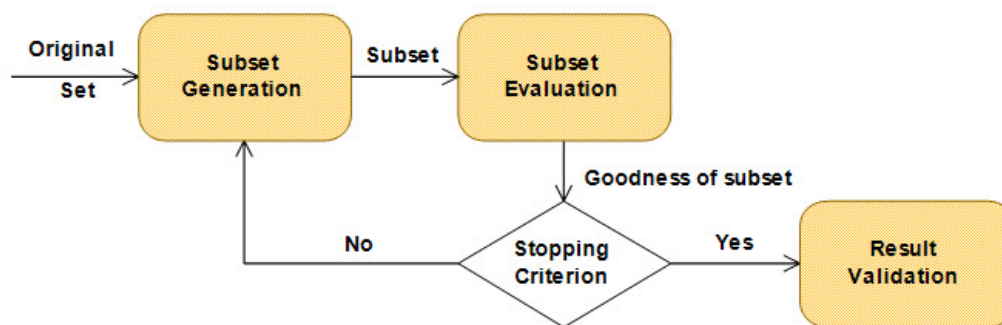


Fig. S1 Process of the feature selection algorithm

Table S1 Characteristics of the heavy metals in soil samples (mg/kg) (average amounts of heavy metals in the soil for each pot in three replicates)

Heavy metal	Contaminated soil		Control sample
	Range (mg/kg)	Average \pm STDEV	Average (mg/kg)
Cd	0.07–0.11	0.09 \pm 0.01	0
Ni	17–23	20 \pm 2.06	1
Pb	12–18	15 \pm 1.87	0.5
Zn	200–230	220 \pm 10	1

Table S2 Selected bands utilizing the random search method

Heavy metal	Selected bands
Pb	<i>b₅₂₀, b₅₇₀, b₆₂₀, b₆₃₀, b₆₄₀, b₆₅₀, b₆₈₀, b₆₉₀, b₇₀₀, b₇₁₀, b₇₄₀, b₇₅₀, b₇₆₀, b₁₀₂₀</i>
Zn	<i>b₅₂₀, b₅₅₀, b₅₈₀, b₉₅₀, b₉₁₀, b₉₄₀, b₅₆₀, b₉₉₀, b₈₇₀, b₇₈₀, b₆₃₀, b₇₇₀, b₇₆₀, b₆₂₀, b₇₅₀, b₆₉₀, b₇₄₀, b₇₃₀, b₇₁₀, b₇₂₀, b₇₀₀, b₉₁₀, b₁₀₅₀</i>
Ni	<i>b₄₀₀, b₆₃₀, b₇₉₀, b₄₁₀, b₇₇₀, b₇₈₀, b₇₆₀, b₇₃₀, b₇₂₀, b₅₀₀, b₅₁₀, b₁₀₃₀</i>
Cd	<i>b₅₈₀, b₅₅₀, b₄₀₀, b₄₈₀, b₄₇₀, b₄₂₀, b₄₉₀, b₄₄₀, b₅₆₀, b₇₈₀, b₆₉₀, b₇₀₀, b₇₉₀, b₇₅₀, b₇₃₀, b₇₁₀, b₇₂₀, b₆₇₀, b₆₅₀, b₆₈₀, b₆₆₀, b₄₅₀, b₉₈₀, b₈₀₀, b₈₇₀, b₈₉₀</i>

Table S3 Summary of THQ Predictive Models for heavy metals contaminated Plants

Heavy metal	Independent Variables	Adjusted R Square	Std. Error of the Estimate
Cd	Constant, <i>b₈₈₀, b₄₀₀</i>	0.848	0.020
Ni	Constant, <i>b₁₀₃₀, b₄₀₀</i>	0.820	0.0003
Pb	Constant, <i>b₇₆₀, b₅₇₀, b₆₅₀</i>	0.830	0.002
Zn	Constant, <i>b₁₀₅₀, b₅₆₀, b₉₁₀</i>	0.831	0.004