<!DOCTYPE html>

<html lang="zh-TW">

<head>

<meta charset="UTF-8">

<meta name="viewport" content="width=device-width, initial-scale=1.0">

<title>DPPH 抗自由基試紙分析 (修正 CSV 亂碼問題)</title>

<!-- 載入 Tailwind CSS CDN，用於快速美觀的樣式設計 -->

<script src="https://cdn.tailwindcss.com"></script>

<!-- 載入 Inter 字體，提供良好的閱讀體驗 -->

<link href="https://fonts.googleapis.com/css2?family=Inter:wght@400;500;600;700&display=swap" rel="stylesheet">

<!-- 載入 Chart.js CDN，用於繪製圖表 -->

<script src="https://cdn.jsdelivr.net/npm/chart.js"></script>

<style>

/\* 設定全域字體和背景顏色 \*/

body {

font-family: 'Inter', sans-serif;

background-color: #f3f4f6; /\* 淺灰色背景 \*/

}

/\* 確保 canvas 響應式 \*/

canvas {

max-width: 100%;

height: auto;

}

</style>

</head>

<body class="p-4 sm:p-8 md:p-12 lg:p-16">

<!-- 主容器，置中並設定最大寬度、圓角和陰影 -->

<div class="max-w-4xl mx-auto bg-white p-6 sm:p-8 rounded-lg shadow-xl">

<h1 class="text-3xl sm:text-4xl font-bold text-center text-gray-800 mb-6">DPPH 抗自由基試紙分析 App</h1>

<p class="text-gray-600 text-center mb-8">請輸入各組的 CIE LAB (L, a, b\*) 值，App 將自動計算結果。</p>

<div class="grid grid-cols-1 md:grid-cols-2 gap-6 mb-8">

<!-- 輸入數據區塊 -->

<div class="bg-gray-50 p-5 rounded-lg shadow-inner">

<h2 class="text-2xl font-semibold text-gray-700 mb-4">輸入數據</h2>

<!-- 空白試紙組輸入欄位 -->

<div class="mb-4">

<label class="block text-gray-700 text-sm font-bold mb-2">空白試紙組 (白色背景)</label>

<div class="flex space-x-2">

<input type="number" id="blankL" value="49.8" step="0.1" class="shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" id="blankA" value="-1.6" step="0.1" class="shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" id="blankB" value="3.2" step="0.1" class="shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

</div>

</div>

<!-- DPPH 紫色組輸入欄位 -->

<div class="mb-4">

<label class="block text-gray-700 text-sm font-bold mb-2">DPPH 紫色組 (未還原)</label>

<div class="flex space-x-2">

<input type="number" id="dpphL" value="45.8" step="0.1" class="shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" id="dpphA" value="2.3" step="0.1" class="shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" id="dpphB" value="0.8" step="0.1" class="shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

</div>

</div>

<!-- 樣品組輸入欄位 -->

<h3 class="text-xl font-medium text-gray-600 mb-3">樣品組</h3>

<div id="sampleGroups">

<!-- 預設樣品 A 組 -->

<div class="mb-3 flex items-center space-x-1 sample-row">

<input type="text" value="樣品 A" class="sample-name-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="樣品名稱">

<input type="number" data-lab="L" value="41.8" step="0.1" class="sample-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="2.6" step="0.1" class="sample-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="4.1" step="0.1" class="sample-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeSampleRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

</div>

</div>

<!-- 新增/刪除樣品按鈕 -->

<div class="flex justify-end space-x-2 mt-4">

<button onclick="addSampleRow()" class="bg-green-500 hover:bg-green-700 text-white font-bold py-2 px-4 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">

新增樣品

</button>

<button onclick="removeLastSampleRow()" class="bg-red-500 hover:bg-red-700 text-white font-bold py-2 px-4 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">

刪除最後一個樣品

</button>

</div>

<!-- 維生素 C 標準品輸入欄位 -->

<h3 class="text-xl font-medium text-gray-600 mb-3 mt-6">維生素 C 標準品</h3>

<div id="vcStandards">

<!-- VC 0.005 mg/mL -->

<div class="mb-3 flex items-center space-x-1 vc-standard-row">

<input type="number" value="0.005" step="0.001" class="vc-conc-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="濃度 mg/mL">

<input type="number" data-lab="L" value="44.3" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="2.8" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="2.3" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeStandardRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

</div>

<!-- VC 0.01 mg/mL -->

<div class="mb-3 flex items-center space-x-1 vc-standard-row">

<input type="number" value="0.01" step="0.001" class="vc-conc-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="濃度 mg/mL">

<input type="number" data-lab="L" value="41.8" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="2.6" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="4.1" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeStandardRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

</div>

<!-- VC 0.02 mg/mL -->

<div class="mb-3 flex items-center space-x-1 vc-standard-row">

<input type="number" value="0.02" step="0.001" class="vc-conc-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="濃度 mg/mL">

<input type="number" data-lab="L" value="40.0" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="3.7" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="3.9" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeStandardRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

</div>

<!-- VC 0.05 mg/mL -->

<div class="mb-3 flex items-center space-x-1 vc-standard-row">

<input type="number" value="0.05" step="0.001" class="vc-conc-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="濃度 mg/mL">

<input type="number" data-lab="L" value="38.5" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="2.4" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="6.7" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeStandardRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

</div>

<!-- VC 0.1 mg/mL -->

<div class="mb-3 flex items-center space-x-1 vc-standard-row">

<input type="number" value="0.1" step="0.001" class="vc-conc-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="濃度 mg/mL">

<input type="number" data-lab="L" value="37.6" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="2.3" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="5.4" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeStandardRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

</div>

</div>

<!-- 新增/刪除標準品按鈕 -->

<div class="flex justify-end space-x-2 mt-4">

<button onclick="addStandardRow()" class="bg-green-500 hover:bg-green-700 text-white font-bold py-2 px-4 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">

新增標準品

</button>

<button onclick="removeLastStandardRow()" class="bg-red-500 hover:bg-red-700 text-white font-bold py-2 px-4 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">

刪除最後一個標準品

</button>

</div>

<!-- 執行分析按鈕 -->

<button onclick="analyzeDPPH()" class="w-full bg-blue-500 hover:bg-blue-700 text-white font-bold py-3 px-4 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105 mt-6">

執行分析

</button>

<!-- 下載結果按鈕 -->

<button onclick="exportToCsv()" class="w-full bg-purple-600 hover:bg-purple-800 text-white font-bold py-3 px-4 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105 mt-4">

下載結果為 Excel (CSV)

</button>

</div>

<!-- 分析結果區塊 -->

<div class="bg-gray-50 p-5 rounded-lg shadow-inner">

<h2 class="text-2xl font-semibold text-gray-700 mb-4">分析結果</h2>

<div id="results" class="space-y-4">

<!-- Delta E 結果顯示 -->

<div>

<h3 class="text-xl font-medium text-gray-600 mb-2">各組 ΔE 色差值 (與 DPPH 紫色組比較)</h3>

<ul id="deltaEResults" class="list-disc list-inside text-gray-800"></ul>

</div>

<!-- 校正後 Delta E 結果顯示 -->

<div>

<h3 class="text-xl font-medium text-gray-600 mb-2">校正後 ΔE 值 (以空白試紙組 ΔE 校正)</h3>

<ul id="correctedDeltaEResults" class="list-disc list-inside text-gray-800"></ul>

</div>

<!-- DPPH 清除率結果顯示 -->

<div>

<h3 class="text-xl font-medium text-gray-600 mb-2">DPPH 清除率 (%)</h3>

<ul id="scavengingRateResults" class="list-disc list-inside text-gray-800"></ul>

</div>

<!-- 檢量線詳細資訊顯示 -->

<div>

<h3 class="text-xl font-medium text-gray-600 mb-2">檢量線 (DPPH 清除率 vs. 維生素 C 濃度)</h3>

<!-- 線性回歸結果與圖表 -->

<div class="bg-white p-4 rounded-lg shadow mb-4">

<h4 class="text-lg font-semibold text-gray-700 mb-2">線性回歸結果</h4>

<p id="linearRegressionEquation" class="text-gray-800"></p>

<p id="linearRSquared" class="text-gray-800"></p>

<p id="linearRSquaredWarning" class="text-red-600 font-semibold"></p>

<div class="mt-4">

<canvas id="linearChart"></canvas>

</div>

</div>

<!-- 4PL 回歸結果與圖表 -->

<div class="bg-white p-4 rounded-lg shadow">

<h4 class="text-lg font-semibold text-gray-700 mb-2">4PL 回歸結果</h4>

<p id="fourPLRegressionEquation" class="text-gray-800"></p>

<p id="fourPLRSquared" class="text-gray-800"></p>

<p id="fourPLRSquaredWarning" class="text-red-600 font-semibold"></p>

<div class="mt-4">

<canvas id="fourPLChart"></canvas>

</div>

</div>

</div>

<!-- 樣品維生素 C 當量值顯示 -->

<div>

<h3 class="text-xl font-medium text-gray-600 mb-2">樣品維生素 C 當量值</h3>

<ul id="sampleVCEquivalents" class="list-disc list-inside text-gray-800"></ul>

</div>

</div>

</div>

</div>

</div>

<script>

// 全局變量用於存儲 Chart 實例，以便在重新分析時銷毀舊圖表

let linearChartInstance = null;

let fourPLChartInstance = null;

// 全局變量用於存儲分析結果，以便匯出

let analysisResults = {};

/\*\*

\* 計算兩個 CIE LAB 顏色之間的 Delta E (色差)。

\* 使用歐幾里得距離公式。

\* @param {number} L1 - 第一個顏色的 L 值。

\* @param {number} a1 - 第一個顏色的 a 值。

\* @param {number} b1 - 第一個顏色的 b 值。

\* @param {number} L2 - 第二個顏色的 L 值。

\* @param {number} a2 - 第二個顏色的 a 值。

\* @param {number} b2 - 第二個顏色的 b 值。

\* @returns {number} Delta E 值。

\*/

function calculateDeltaE(L1, a1, b1, L2, a2, b2) {

const deltaL = L1 - L2;

const deltaA = a1 - a2;

const deltaB = b1 - b2;

return Math.sqrt(deltaL \* deltaL + deltaA \* deltaA + deltaB \* deltaB);

}

/\*\*

\* 執行簡單線性回歸並計算 R-squared 值。

\* 公式: y = mx + b

\* @param {number[]} x - X 軸數據點 (自變數)。

\* @param {number[]} y - Y 軸數據點 (因變數)。

\* @returns {{m: number, b: number, rSquared: number}} 包含斜率 (m)、截距 (b) 和 R-squared 值的物件。

\*/

function linearRegression(x, y) {

const n = x.length;

let sumX = 0, sumY = 0, sumXY = 0, sumX2 = 0, sumY2 = 0;

for (let i = 0; i < n; i++) {

sumX += x[i];

sumY += y[i];

sumXY += x[i] \* y[i];

sumX2 += x[i] \* x[i];

sumY2 += y[i] \* y[i];

}

const numeratorM = (n \* sumXY - sumX \* sumY);

const denominatorM = (n \* sumX2 - sumX \* sumX);

const m = denominatorM === 0 ? 0 : numeratorM / denominatorM; // 斜率 (Slope)

const b = (sumY - m \* sumX) / n; // Y 軸截距 (Y-intercept)

// 計算 R-squared

let ssTotal = 0;

let ssResidual = 0;

for (let i = 0; i < n; i++) {

const yPred = m \* x[i] + b;

ssTotal += Math.pow(y[i] - (sumY / n), 2);

ssResidual += Math.pow(y[i] - yPred, 2);

}

let rSquared = 0;

if (ssTotal !== 0) {

rSquared = 1 - (ssResidual / ssTotal);

}

if (isNaN(rSquared) || rSquared < 0) rSquared = 0; // 處理無效的 R-squared

return { m, b, rSquared };

}

/\*\*

\* 四參數邏輯 (4PL) 模型函數。

\* y = D + (A - D) / (1 + (x / C)^B)

\* A: 下漸近線 (最低反應值)

\* B: 希爾斜率 (曲線陡峭度)

\* C: 拐點 (EC50/IC50，50% 反應時的 x 值)

\* D: 上漸近線 (最高反應值)

\* @param {number} x - 自變數 (濃度)。

\* @param {number} A - 下漸近線。

\* @param {number} B - 希爾斜率。

\* @param {number} C - 拐點。

\* @param {number} D - 上漸近線。

\* @returns {number} 預測的 y 值。

\*/

function fourParameterLogistic(x, A, B, C, D) {

if (C === 0) return D; // 避免除以零

const term = Math.pow(x / C, B);

return D + (A - D) / (1 + term);

}

/\*\*

\* 計算四參數邏輯模型擬合的平方誤差和 (SSE)。

\* @param {object} params - 包含 A, B, C, D 參數的物件。

\* @param {number[]} xData - X 軸數據。

\* @param {number[]} yData - Y 軸數據。

\* @returns {number} 平方誤差和。

\*/

function calculateSSE\_4PL(params, xData, yData) {

let sse = 0;

for (let i = 0; i < xData.length; i++) {

const yPred = fourParameterLogistic(xData[i], params.A, params.B, params.C, params.D);

sse += Math.pow(yData[i] - yPred, 2);

}

return sse;

}

/\*\*

\* 執行簡化的迭代優化來擬合四參數邏輯 (4PL) 模型。

\* 注意：這是一個基礎的迭代方法，可能不如專業統計軟體中的演算法穩健或精確。

\* @param {number[]} xData - X 軸數據點 (維生素 C 濃度)。

\* @param {number[]} yData - Y 軸數據點 (DPPH 清除率)。

\* @returns {{A: number, B: number, C: number, D: number, rSquared: number, fourPLFunction: function, inverseFourPLFunction: function}} 擬合參數、R-squared 值和 4PL 函數。

\*/

function fit4PL(xData, yData) {

// 初始參數猜測

// A: 下漸近線 (最低清除率，預期接近 0)

// D: 上漸近線 (最高清除率，預期接近 100)

// C: 拐點 (IC50，50% 反應時的 x 值)

// B: 希爾斜率 (曲線陡峭度，預期為正值)

let A = 0; // 假定最低清除率為 0%

let D = 100; // 假定最高清除率為 100%

let C = xData.length > 0 ? xData[Math.floor(xData.length / 2)] : 0.01; // 以中間濃度作為 IC50 的初始猜測

if (C === 0) C = 0.01; // 避免 C 初始值為 0

let B = 1.0; // 初始希爾斜率

// 迭代優化設置

const learningRate = 0.0005; // 學習率，調整每次迭代的步長

const numIterations = 50000; // 迭代次數

const paramStepFactor = 0.01; // 參數調整步長的因子

let params = { A, B, C, D };

let currentSSE = calculateSSE\_4PL(params, xData, yData);

for (let iter = 0; iter < numIterations; iter++) {

let improved = false;

let bestParams = { ...params };

let bestSSE = currentSSE;

// 嘗試微調每個參數，並朝著減少 SSE 的方向移動

// A

let testA\_plus = params.A + learningRate \* paramStepFactor \* (D - A);

let sse\_A\_plus = calculateSSE\_4PL({ ...params, A: testA\_plus }, xData, yData);

if (sse\_A\_plus < bestSSE) { bestParams.A = testA\_plus; bestSSE = sse\_A\_plus; improved = true; }

let testA\_minus = params.A - learningRate \* paramStepFactor \* (D - A);

let sse\_A\_minus = calculateSSE\_4PL({ ...params, A: testA\_minus }, xData, yData);

if (sse\_A\_minus < bestSSE) { bestParams.A = testA\_minus; bestSSE = sse\_A\_minus; improved = true; }

// D

let testD\_plus = params.D + learningRate \* paramStepFactor \* (D - A);

let sse\_D\_plus = calculateSSE\_4PL({ ...params, D: testD\_plus }, xData, yData);

if (sse\_D\_plus < bestSSE) { bestParams.D = testD\_plus; bestSSE = sse\_D\_plus; improved = true; }

let testD\_minus = params.D - learningRate \* paramStepFactor \* (D - A);

let sse\_D\_minus = calculateSSE\_4PL({ ...params, D: testD\_minus }, xData, yData);

if (sse\_D\_minus < bestSSE) { bestParams.D = testD\_minus; bestSSE = sse\_D\_minus; improved = true; }

// C (IC50 應為正值)

let testC\_plus = params.C + learningRate \* paramStepFactor \* params.C;

if (testC\_plus < 1e-9) testC\_plus = 1e-9; // 避免 C 過小或負值

let sse\_C\_plus = calculateSSE\_4PL({ ...params, C: testC\_plus }, xData, yData);

if (sse\_C\_plus < bestSSE) { bestParams.C = testC\_plus; bestSSE = sse\_C\_plus; improved = true; }

let testC\_minus = params.C - learningRate \* paramStepFactor \* params.C;

if (testC\_minus < 1e-9) testC\_minus = 1e-9; // 避免 C 過小或負值

let sse\_C\_minus = calculateSSE\_4PL({ ...params, C: testC\_minus }, xData, yData);

if (sse\_C\_minus < bestSSE) { bestParams.C = testC\_minus; bestSSE = sse\_C\_minus; improved = true; }

// B (希爾斜率，對於增加的曲線應為正值)

let testB\_plus = params.B + learningRate \* paramStepFactor;

if (testB\_plus < 0.01) testB\_plus = 0.01; // 避免 B 過小或負值，對於增加曲線

let sse\_B\_plus = calculateSSE\_4PL({ ...params, B: testB\_plus }, xData, yData);

if (sse\_B\_plus < bestSSE) { bestParams.B = testB\_plus; bestSSE = sse\_B\_plus; improved = true; }

let testB\_minus = params.B - learningRate \* paramStepFactor;

if (testB\_minus < 0.01) testB\_minus = 0.01; // 避免 B 過小或負值，對於增加曲線

let sse\_B\_minus = calculateSSE\_4PL({ ...params, B: testB\_minus }, xData, yData);

if (sse\_B\_minus < bestSSE) { bestParams.B = testB\_minus; bestSSE = sse\_B\_minus; improved = true; }

if (improved) {

params = { ...bestParams };

currentSSE = bestSSE;

} else {

// 如果沒有改善，可能已收斂或達到局部最小值，可以提前結束

// break;

}

}

// 計算 R-squared

let ssTotal = 0;

let meanY = yData.reduce((sum, val) => sum + val, 0) / yData.length;

for (let i = 0; i < yData.length; i++) {

ssTotal += Math.pow(yData[i] - meanY, 2);

}

let rSquared = 1 - (currentSSE / ssTotal);

if (isNaN(rSquared) || rSquared < 0) rSquared = 0; // 處理無效的 R-squared

/\*\*

\* 四參數邏輯 (4PL) 模型的反函數，用於從 y 值計算 x 值。

\* x = C \* ((A - D) / (y - D) - 1)^(1/B)

\* @param {number} y - 因變數 (清除率)。

\* @param {object} params - 包含 A, B, C, D 參數的物件。

\* @returns {number} 預測的 x 值 (濃度)。

\*/

function inverseFourPL(y, params) {

const { A, B, C, D } = params;

if (y === D) return Infinity; // y 達到上漸近線時 x 趨近無限大

if (y === A) return 0; // y 達到下漸近線時 x 趨近 0

const numerator = A - D;

const denominator = y - D;

if (denominator === 0) return NaN; // 避免除以零

const base = numerator / denominator - 1;

// 確保 base 為正數，因為 B 通常為正且 1/B 可能不是整數

if (base <= 0) {

// 如果 base 非正，且 B 不是奇數整數，則結果為複數或無效

// 對於增加的曲線 (A < D, B > 0)，y 在 A 和 D 之間時 base 應為正

// 如果 base <= 0，表示 y 值超出模型有效範圍，或擬合有問題

console.warn("Inverse 4PL: Base for power is non-positive. Result might be invalid.", {y, A, B, C, D, base});

return NaN;

}

// 避免 Math.pow(x, y) 中 x 為負數且 y 不是整數的情況

const power = 1 / B;

return C \* Math.pow(base, power);

}

return { A: params.A, B: params.B, C: params.C, D: params.D, rSquared, fourPLFunction: fourParameterLogistic, inverseFourPLFunction: inverseFourPL };

}

/\*\*

\* 建立一個新的樣品數據輸入列。

\* @param {string} name - 樣品名稱的預設值。

\* @param {number} L - L 值的預設值。

\* @param {number} a - a 值的預設值。

\* @param {number} b - b\* 值的預設值。

\* @returns {HTMLElement} 新的樣品列 DOM 元素。

\*/

function createSampleRow(name = '', L = '', a = '', b = '') {

const div = document.createElement('div');

div.className = 'mb-3 flex items-center space-x-1 sample-row';

div.innerHTML = `

<input type="text" value="${name}" class="sample-name-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="樣品名稱">

<input type="number" data-lab="L" value="${L}" step="0.1" class="sample-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="${a}" step="0.1" class="sample-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="${b}" step="0.1" class="sample-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeSampleRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

`;

return div;

}

/\*\*

\* 新增一個樣品數據輸入列。

\*/

function addSampleRow() {

const sampleGroupsDiv = document.getElementById('sampleGroups');

sampleGroupsDiv.appendChild(createSampleRow());

}

/\*\*

\* 刪除指定的樣品數據輸入列。

\* @param {HTMLElement} buttonElement - 觸發刪除的按鈕元素。

\*/

function removeSampleRow(buttonElement) {

const sampleGroupsDiv = document.getElementById('sampleGroups');

// 確保至少保留一個樣品

if (sampleGroupsDiv.children.length > 0) {

const rowToRemove = buttonElement.closest('.sample-row');

if (rowToRemove) {

sampleGroupsDiv.removeChild(rowToRemove);

}

} else {

showMessageBox('至少需要保留一個樣品數據。');

}

}

/\*\*

\* 刪除最後一個樣品數據輸入列。

\*/

function removeLastSampleRow() {

const sampleGroupsDiv = document.getElementById('sampleGroups');

// 確保至少保留一個樣品

if (sampleGroupsDiv.children.length > 0) {

sampleGroupsDiv.removeChild(sampleGroupsDiv.lastElementChild);

} else {

showMessageBox('至少需要保留一個樣品數據。');

}

}

/\*\*

\* 建立一個新的維生素 C 標準品數據輸入列。

\* @returns {HTMLElement} 新的標準品列 DOM 元素。

\*/

function createStandardRow() {

const div = document.createElement('div');

div.className = 'mb-3 flex items-center space-x-1 vc-standard-row';

div.innerHTML = `

<input type="number" value="" step="0.001" class="vc-conc-input shadow appearance-none border rounded w-16 py-2 px-2 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="濃度 mg/mL">

<input type="number" data-lab="L" value="" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="L">

<input type="number" data-lab="A" value="" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="a">

<input type="number" data-lab="B" value="" step="0.1" class="vc-lab-input shadow appearance-none border rounded w-full py-2 px-3 text-gray-700 text-sm leading-tight focus:outline-none focus:shadow-outline" placeholder="b\*">

<button onclick="removeStandardRow(this)" class="ml-1 bg-red-500 hover:bg-red-700 text-white font-bold py-1.5 px-1 rounded-lg focus:outline-none focus:shadow-outline transition duration-300 ease-in-out transform hover:scale-105">刪除</button>

`;

return div;

}

/\*\*

\* 新增一個維生素 C 標準品數據輸入列。

\*/

function addStandardRow() {

const vcStandardsDiv = document.getElementById('vcStandards');

vcStandardsDiv.appendChild(createStandardRow());

}

/\*\*

\* 刪除指定的維生素 C 標準品數據輸入列。

\* @param {HTMLElement} buttonElement - 觸發刪除的按鈕元素。

\*/

function removeStandardRow(buttonElement) {

const vcStandardsDiv = document.getElementById('vcStandards');

// 確保至少保留兩個標準品，以便回歸

if (vcStandardsDiv.children.length > 2) {

const rowToRemove = buttonElement.closest('.vc-standard-row');

if (rowToRemove) {

vcStandardsDiv.removeChild(rowToRemove);

}

} else {

showMessageBox('至少需要保留兩個標準品數據才能進行回歸分析。');

}

}

/\*\*

\* 刪除最後一個維生素 C 標準品數據輸入列。

\*/

function removeLastStandardRow() {

const vcStandardsDiv = document.getElementById('vcStandards');

// 確保至少保留兩個標準品，以便回歸

if (vcStandardsDiv.children.length > 2) {

vcStandardsDiv.removeChild(vcStandardsDiv.lastElementChild);

} else {

showMessageBox('至少需要保留兩個標準品數據才能進行回歸分析。');

}

}

/\*\*

\* 顯示自定義訊息框。

\* @param {string} message - 要顯示的訊息。

\*/

function showMessageBox(message) {

let messageBox = document.getElementById('customMessageBox');

if (!messageBox) {

messageBox = document.createElement('div');

messageBox.id = 'customMessageBox';

messageBox.className = 'fixed inset-0 bg-gray-600 bg-opacity-75 flex items-center justify-center z-50 hidden';

messageBox.innerHTML = `

<div class="bg-white p-6 rounded-lg shadow-xl max-w-sm w-full text-center">

<p class="text-gray-800 text-lg mb-4">${message}</p>

<button onclick="closeMessageBox()" class="bg-blue-500 hover:bg-blue-700 text-white font-bold py-2 px-4 rounded-lg focus:outline-none focus:shadow-outline">

確定

</button>

</div>

`;

document.body.appendChild(messageBox);

} else {

messageBox.querySelector('p').innerText = message;

}

messageBox.classList.remove('hidden');

}

/\*\*

\* 關閉自定義訊息框。

\*/

function closeMessageBox() {

const messageBox = document.getElementById('customMessageBox');

if (messageBox) {

messageBox.classList.add('hidden');

}

}

/\*\*

\* 繪製線性回歸圖表。

\* @param {HTMLElement} canvasElement - Canvas DOM 元素。

\* @param {Array<Object>} dataPoints - 原始數據點 {x, y}。

\* @param {Object} linearRegParams - 線性回歸參數 {m, b}。

\* @param {number} maxConc - 標準品最高濃度。

\*/

function drawLinearChart(canvasElement, dataPoints, linearRegParams, maxConc) {

if (linearChartInstance) {

linearChartInstance.destroy(); // 銷毀舊圖表實例

}

const ctx = canvasElement.getContext('2d');

// 獲取數據點的 x 範圍

const minX = Math.min(...dataPoints.map(p => p.x));

const maxX = maxConc \* 1.1; // X軸最高值為最高濃度\*1.1

// 生成回歸線上的點

const linePoints = [];

// 在數據範圍內生成更多點以平滑曲線

for (let i = 0; i < 100; i++) {

const x = minX + ((maxX - minX) / 99) \* i;

const y = linearRegParams.m \* x + linearRegParams.b;

linePoints.push({ x, y });

}

linearChartInstance = new Chart(ctx, {

type: 'scatter', // 使用散點圖類型

data: {

datasets: [

{

label: '標準品數據',

data: dataPoints,

backgroundColor: 'rgba(75, 192, 192, 0.8)',

borderColor: 'rgba(75, 192, 192, 1)',

pointRadius: 5,

},

{

label: '線性回歸線',

data: linePoints,

type: 'line', // 設置為線圖類型

borderColor: 'rgba(255, 99, 132, 1)',

backgroundColor: 'rgba(255, 99, 132, 0.2)',

fill: false,

pointRadius: 0, // 不顯示線上的點

borderWidth: 2,

}

]

},

options: {

responsive: true,

maintainAspectRatio: true,

aspectRatio: 1, // 將長寬比設為 1:1，使圖表更高

plugins: {

title: {

display: true,

text: '線性回歸檢量線',

font: { size: 16 }

},

legend: {

display: true,

position: 'top',

}

},

scales: {

x: {

type: 'linear',

position: 'bottom',

title: {

display: true,

text: '維生素 C 濃度 (mg/mL)'

},

min: 0, // 確保 x 軸從 0 開始

max: maxX, // 設定 X 軸最高值

ticks: {

callback: function(value, index, values) {

// 隱藏最高值標籤

if (index === values.length - 1 && value !== 0) {

return '';

}

return value;

}

}

},

y: {

title: {

display: true,

text: 'DPPH 清除率 (%)'

},

min: 0, // 確保 y 軸從 0 開始

max: 120, // 設定 Y 軸最高值為 120%

ticks: {

callback: function(value, index, values) {

// 隱藏最高值標籤

if (index === values.length - 1 && value !== 0) {

return '';

}

return value;

}

}

}

}

}

});

}

/\*\*

\* 繪製 4PL 回歸圖表。

\* @param {HTMLElement} canvasElement - Canvas DOM 元素。

\* @param {Array<Object>} dataPoints - 原始數據點 {x, y}。

\* @param {Object} fourPLRegParams - 4PL 回歸參數 {A, B, C, D}。

\* @param {number} maxConc - 標準品最高濃度。

\*/

function drawFourPLChart(canvasElement, dataPoints, fourPLRegParams, maxConc) {

if (fourPLChartInstance) {

fourPLChartInstance.destroy(); // 銷毀舊圖表實例

}

const ctx = canvasElement.getContext('2d');

// 獲取數據點的 x 範圍

const minX = Math.min(...dataPoints.map(p => p.x));

const maxX = maxConc \* 1.1; // X軸最高值為最高濃度\*1.1

// 生成 4PL 曲線上的點

const curvePoints = [];

// 在數據範圍內生成更多點以平滑曲線

for (let i = 0; i < 100; i++) {

const x = minX + ((maxX - minX) / 99) \* i;

const y = fourParameterLogistic(x, fourPLRegParams.A, fourPLRegParams.B, fourPLRegParams.C, fourPLRegParams.D);

curvePoints.push({ x, y });

}

fourPLChartInstance = new Chart(ctx, {

type: 'scatter', // 使用散點圖類型

data: {

datasets: [

{

label: '標準品數據',

data: dataPoints,

backgroundColor: 'rgba(75, 192, 192, 0.8)',

borderColor: 'rgba(75, 192, 192, 1)',

pointRadius: 5,

},

{

label: '4PL 回歸曲線',

data: curvePoints,

type: 'line', // 設置為線圖類型

borderColor: 'rgba(153, 102, 255, 1)',

backgroundColor: 'rgba(153, 102, 255, 0.2)',

fill: false,

pointRadius: 0, // 不顯示線上的點

borderWidth: 2,

}

]

},

options: {

responsive: true,

maintainAspectRatio: true,

aspectRatio: 1, // 將長寬比設為 1:1，使圖表更高

plugins: {

title: {

display: true,

text: '4PL 回歸檢量線',

font: { size: 16 }

},

legend: {

display: true,

position: 'top',

}

},

scales: {

x: {

type: 'linear',

position: 'bottom',

title: {

display: true,

text: '維生素 C 濃度 (mg/mL)'

},

min: 0, // 確保 x 軸從 0 開始

max: maxX, // 設定 X 軸最高值

ticks: {

callback: function(value, index, values) {

// 隱藏最高值標籤

if (index === values.length - 1 && value !== 0) {

return '';

}

return value;

}

}

},

y: {

title: {

display: true,

text: 'DPPH 清除率 (%)'

},

min: 0, // 確保 y 軸從 0 開始

max: 120, // 設定 Y 軸最高值為 120%

ticks: {

callback: function(value, index, values) {

// 隱藏最高值標籤

if (index === values.length - 1 && value !== 0) {

return '';

}

return value;

}

}

}

}

}

});

}

/\*\*

\* 執行 DPPH 抗自由基試紙分析的主要函數。

\* 獲取輸入值，執行所有計算，並更新 UI。

\*/

function analyzeDPPH() {

// 重置 analysisResults

analysisResults = {};

// 獲取各組的 CIE LAB 輸入值

const blankL = parseFloat(document.getElementById('blankL').value);

const blankA = parseFloat(document.getElementById('blankA').value);

const blankB = parseFloat(document.getElementById('blankB').value);

const dpphL = parseFloat(document.getElementById('dpphL').value);

const dpphA = parseFloat(document.getElementById('dpphA').value);

const dpphB = parseFloat(document.getElementById('dpphB').value);

// 儲存原始輸入數據

analysisResults.rawInputs = {

blank: { L: blankL, a: blankA, b: blankB },

dpph: { L: dpphL, a: dpphA, b: dpphB }

};

// 獲取樣品組的輸入值

const samples = [];

document.querySelectorAll('#sampleGroups .sample-row').forEach(row => {

const nameInput = row.querySelector('.sample-name-input');

const LInput = row.querySelector('.sample-lab-input[data-lab="L"]');

const AInput = row.querySelector('.sample-lab-input[data-lab="A"]');

const BInput = row.querySelector('.sample-lab-input[data-lab="B"]');

const name = nameInput.value.trim();

const L = parseFloat(LInput.value);

const a = parseFloat(AInput.value);

const b = parseFloat(BInput.value);

// 檢查輸入是否有效

if (!name || isNaN(L) || isNaN(a) || isNaN(b)) {

showMessageBox('請檢查所有樣品的名稱和 CIE LAB 值是否為有效輸入。');

// 清空結果並終止分析

document.getElementById('deltaEResults').innerHTML = '';

document.getElementById('correctedDeltaEResults').innerHTML = '';

document.getElementById('scavengingRateResults').innerHTML = '';

document.getElementById('linearRegressionEquation').innerText = '';

document.getElementById('linearRSquared').innerText = '';

document.getElementById('linearRSquaredWarning').innerText = '';

document.getElementById('fourPLRegressionEquation').innerText = '';

document.getElementById('fourPLRSquared').innerText = '';

document.getElementById('fourPLRSquaredWarning').innerText = '';

document.getElementById('sampleVCEquivalents').innerHTML = '';

if (linearChartInstance) linearChartInstance.destroy();

if (fourPLChartInstance) fourPLChartInstance.destroy();

return;

}

samples.push({ name, L, a, b });

});

analysisResults.samples = samples; // 儲存樣品原始數據

// 如果沒有樣品數據，顯示警告並清空結果

if (samples.length === 0) {

showMessageBox('請至少輸入一個樣品數據進行分析。');

document.getElementById('deltaEResults').innerHTML = '';

document.getElementById('correctedDeltaEResults').innerHTML = '';

document.getElementById('scavengingRateResults').innerHTML = '';

document.getElementById('linearRegressionEquation').innerText = '';

document.getElementById('linearRSquared').innerText = '';

document.getElementById('linearRSquaredWarning').innerText = '';

document.getElementById('fourPLRegressionEquation').innerText = '';

document.getElementById('fourPLRSquared').innerText = '';

document.getElementById('fourPLRSquaredWarning').innerText = '';

document.getElementById('sampleVCEquivalents').innerHTML = '';

// 清空圖表

if (linearChartInstance) linearChartInstance.destroy();

if (fourPLChartInstance) fourPLChartInstance.destroy();

return;

}

// 獲取維生素 C 標準品的輸入值

const vcStandards = [];

document.querySelectorAll('#vcStandards .vc-standard-row').forEach(row => {

const concInput = row.querySelector('.vc-conc-input');

const LInput = row.querySelector('.vc-lab-input[data-lab="L"]');

const AInput = row.querySelector('.vc-lab-input[data-lab="A"]');

const BInput = row.querySelector('.vc-lab-input[data-lab="B"]');

const conc = parseFloat(concInput.value);

const L = parseFloat(LInput.value);

const a = parseFloat(AInput.value);

const b = parseFloat(BInput.value);

// 檢查輸入是否有效

if (isNaN(conc) || isNaN(L) || isNaN(a) || isNaN(b) || conc < 0) {

showMessageBox('請檢查所有維生素 C 標準品的濃度和 CIE LAB 值是否為有效數字，且濃度不能為負數。');

// 清空結果並終止分析

document.getElementById('deltaEResults').innerHTML = '';

document.getElementById('correctedDeltaEResults').innerHTML = '';

document.getElementById('scavengingRateResults').innerHTML = '';

document.getElementById('linearRegressionEquation').innerText = '';

document.getElementById('linearRSquared').innerText = '';

document.getElementById('linearRSquaredWarning').innerText = '';

document.getElementById('fourPLRegressionEquation').innerText = '';

document.getElementById('fourPLRSquared').innerText = '';

document.getElementById('fourPLRSquaredWarning').innerText = '';

document.getElementById('sampleVCEquivalents').innerHTML = '';

if (linearChartInstance) linearChartInstance.destroy();

if (fourPLChartInstance) fourPLChartInstance.destroy();

return;

}

vcStandards.push({ conc, L, a, b });

});

analysisResults.vcStandards = vcStandards; // 儲存標準品原始數據

// 確保有足夠的標準品進行回歸

if (vcStandards.length < 2) {

showMessageBox('至少需要兩個維生素 C 標準品數據才能進行回歸分析。');

// 清空圖表

if (linearChartInstance) linearChartInstance.destroy();

if (fourPLChartInstance) fourPLChartInstance.destroy();

return;

}

// 將 DPPH 紫色組設為 Delta E 計算的參考點

const dpphRef = { L: dpphL, a: dpphA, b: dpphB };

// --- 1. 計算各組的 ΔE 色差值 (與 DPPH 紫色組比較) ---

const deltaEResultsDisplay = []; // 用於顯示在 UI 上

const deltaE\_Blank = calculateDeltaE(blankL, blankA, blankB, dpphRef.L, dpphRef.a, dpphRef.b);

deltaEResultsDisplay.push({ name: '空白試紙組', value: deltaE\_Blank });

const deltaE\_DPPH = calculateDeltaE(dpphL, dpphA, dpphB, dpphRef.L, dpphRef.a, dpphRef.b);

deltaEResultsDisplay.push({ name: 'DPPH 紫色組', value: deltaE\_DPPH }); // 理論上應為 0

samples.forEach(sample => {

const deltaE = calculateDeltaE(sample.L, sample.a, sample.b, dpphRef.L, dpphRef.a, dpphRef.b);

deltaEResultsDisplay.push({ name: `${sample.name} 組`, value: deltaE });

sample.deltaE = deltaE; // 儲存以供後續使用

});

const vcDeltaEs = {}; // 儲存維生素 C 標準品的 Delta E

vcStandards.forEach(vc => {

const deltaE = calculateDeltaE(vc.L, vc.a, vc.b, dpphRef.L, dpphRef.a, dpphRef.b);

vcDeltaEs[vc.conc] = deltaE;

deltaEResultsDisplay.push({ name: `維生素 C ${vc.conc} mg/mL`, value: deltaE });

vc.deltaE = deltaE; // 儲存以供後續使用

});

analysisResults.deltaEValues = deltaEResultsDisplay; // 儲存 Delta E 結果

// 顯示 Delta E 結果到 UI

const deltaEResultsUl = document.getElementById('deltaEResults');

deltaEResultsUl.innerHTML = '';

deltaEResultsDisplay.forEach(res => {

deltaEResultsUl.innerHTML += `<li>${res.name}: ${res.value.toFixed(3)}</li>`;

});

// --- 2. 計算校正後 ΔE 值 (以空白試紙組 ΔE 校正) ---

const correctedDeltaEResultsDisplay = []; // 用於顯示在 UI 上

// 檢查空白試紙組的 Delta E 是否為零，避免除以零錯誤

if (deltaE\_Blank === 0) {

showMessageBox('錯誤：空白試紙組的 ΔE 為零，無法進行校正。請檢查輸入數據。');

document.getElementById('correctedDeltaEResults').innerHTML = '';

document.getElementById('scavengingRateResults').innerHTML = '';

document.getElementById('linearRegressionEquation').innerText = '';

document.getElementById('linearRSquared').innerText = '';

document.getElementById('linearRSquaredWarning').innerText = '';

document.getElementById('fourPLRegressionEquation').innerText = '';

document.getElementById('fourPLRSquared').innerText = '';

document.getElementById('fourPLRSquaredWarning').innerText = '';

document.getElementById('sampleVCEquivalents').innerHTML = '';

// 清空圖表

if (linearChartInstance) linearChartInstance.destroy();

if (fourPLChartInstance) fourPLChartInstance.destroy();

return;

}

const correctedDeltaE\_Blank = deltaE\_Blank / deltaE\_Blank; // 理論上應為 1

correctedDeltaEResultsDisplay.push({ name: '空白試紙組', value: correctedDeltaE\_Blank });

const correctedDeltaE\_DPPH = deltaE\_DPPH / deltaE\_Blank; // 理論上應為 0

correctedDeltaEResultsDisplay.push({ name: 'DPPH 紫色組', value: correctedDeltaE\_DPPH });

samples.forEach(sample => {

const correctedDeltaE = sample.deltaE / deltaE\_Blank;

correctedDeltaEResultsDisplay.push({ name: `${sample.name} 組`, value: correctedDeltaE });

sample.correctedDeltaE = correctedDeltaE; // 儲存以供後續使用

});

const vcCorrectedDeltaEs = {}; // 儲存維生素 C 標準品的校正後 Delta E

vcStandards.forEach(vc => {

const correctedDeltaE = vcDeltaEs[vc.conc] / deltaE\_Blank;

vcCorrectedDeltaEs[vc.conc] = correctedDeltaE;

correctedDeltaEResultsDisplay.push({ name: `維生素 C ${vc.conc} mg/mL`, value: correctedDeltaE });

vc.correctedDeltaE = correctedDeltaE; // 儲存以供後續使用

});

analysisResults.correctedDeltaEValues = correctedDeltaEResultsDisplay; // 儲存校正後 Delta E 結果

// 顯示校正後 Delta E 結果到 UI

const correctedDeltaEResultsUl = document.getElementById('correctedDeltaEResults');

correctedDeltaEResultsUl.innerHTML = '';

correctedDeltaEResultsDisplay.forEach(res => {

correctedDeltaEResultsUl.innerHTML += `<li>${res.name}: ${res.value.toFixed(3)}</li>`;

});

// --- 3. 計算 DPPH 清除率 (%) ---

const scavengingRateResultsDisplay = []; // 用於顯示在 UI 上

// 以 0.1 mg/mL 維生素 C 組的校正 ΔE 為 100% 清除率的基準

// 需要找到 0.1 mg/mL 的數據，如果不存在則使用最高濃度作為參考

let referenceConc = 0.1;

let correctedDeltaE\_VC\_Reference = vcCorrectedDeltaEs[referenceConc];

// 如果沒有 0.1 mg/mL 的數據，則找最大的濃度作為參考

if (correctedDeltaE\_VC\_Reference === undefined || correctedDeltaE\_VC\_Reference === 0) {

const maxConcVC = vcStandards.reduce((max, vc) => Math.max(max, vc.conc), 0);

if (maxConcVC > 0) {

referenceConc = maxConcVC;

correctedDeltaE\_VC\_Reference = vcCorrectedDeltaEs[referenceConc];

}

}

// 檢查參考組的校正 ΔE 是否為零，避免除以零錯誤

if (correctedDeltaE\_VC\_Reference === undefined || correctedDeltaE\_VC\_Reference === 0) {

showMessageBox(`錯誤：用於計算清除率的參考維生素 C 組（${referenceConc} mg/mL）的校正 ΔE 為零或不存在。請檢查輸入數據。`);

document.getElementById('scavengingRateResults').innerHTML = '';

document.getElementById('linearRegressionEquation').innerText = '';

document.getElementById('linearRSquared').innerText = '';

document.getElementById('linearRSquaredWarning').innerText = '';

document.getElementById('fourPLRegressionEquation').innerText = '';

document.getElementById('fourPLRSquared').innerText = '';

document.getElementById('fourPLRSquaredWarning').innerText = '';

document.getElementById('sampleVCEquivalents').innerHTML = '';

// 清空圖表

if (linearChartInstance) linearChartInstance.destroy();

if (fourPLChartInstance) fourPLChartInstance.destroy();

return;

}

const scavengingRate\_Blank = (correctedDeltaE\_Blank / correctedDeltaE\_VC\_Reference) \* 100;

scavengingRateResultsDisplay.push({ name: '空白試紙組', value: scavengingRate\_Blank });

const scavengingRate\_DPPH = (correctedDeltaE\_DPPH / correctedDeltaE\_VC\_Reference) \* 100;

scavengingRateResultsDisplay.push({ name: 'DPPH 紫色組', value: scavengingRate\_DPPH });

samples.forEach(sample => {

const scavengingRate = (sample.correctedDeltaE / correctedDeltaE\_VC\_Reference) \* 100;

scavengingRateResultsDisplay.push({ name: `${sample.name} 組`, value: scavengingRate });

sample.scavengingRate = scavengingRate; // 儲存以供後續使用

});

const vcScavengingRates = {}; // 儲存維生素 C 標準品的清除率

vcStandards.forEach(vc => {

const scavengingRate = (vcCorrectedDeltaEs[vc.conc] / correctedDeltaE\_VC\_Reference) \* 100;

vcScavengingRates[vc.conc] = scavengingRate;

scavengingRateResultsDisplay.push({ name: `維生素 C ${vc.conc} mg/mL`, value: scavengingRate });

vc.scavengingRate = scavengingRate; // 儲存以供後續使用

});

analysisResults.scavengingRates = scavengingRateResultsDisplay; // 儲存清除率結果

// 顯示清除率結果到 UI

const scavengingRateResultsUl = document.getElementById('scavengingRateResults');

scavengingRateResultsUl.innerHTML = '';

scavengingRateResultsDisplay.forEach(res => {

scavengingRateResultsUl.innerHTML += `<li>${res.name}: ${res.value.toFixed(3)} %</li>`;

});

// --- 4. 建立檢量線並計算回歸方程式與相關係數 (R²) ---

// X 值為維生素 C 濃度，Y 值為對應的清除率

const xValues = vcStandards.map(vc => vc.conc);

const yValues = vcStandards.map(vc => vc.scavengingRate);

// 準備 Chart.js 的數據點格式

const chartDataPoints = xValues.map((x, i) => ({ x: x, y: yValues[i] }));

// 獲取標準品最高濃度，用於 X 軸最大值設定

const maxConc = xValues.length > 0 ? Math.max(...xValues) : 0.1;

// 執行線性回歸

const linearReg = linearRegression(xValues, yValues);

document.getElementById('linearRegressionEquation').innerText = `回歸方程式: y = ${linearReg.m.toFixed(4)}x + ${linearReg.b.toFixed(4)}`;

document.getElementById('linearRSquared').innerText = `相關係數 (R²): ${linearReg.rSquared.toFixed(4)}`;

const linearRSquaredWarning = document.getElementById('linearRSquaredWarning');

if (linearReg.rSquared < 0.95) {

linearRSquaredWarning.innerText = '警告：相關係數 R² 低於 0.95，線性檢量線可能不適用。';

} else {

linearRSquaredWarning.innerText = '';

}

analysisResults.linearRegression = {

equation: `y = ${linearReg.m.toFixed(4)}x + ${linearReg.b.toFixed(4)}`,

rSquared: linearReg.rSquared.toFixed(4),

m: linearReg.m,

b: linearReg.b

};

// 繪製線性回歸圖表

drawLinearChart(document.getElementById('linearChart'), chartDataPoints, linearReg, maxConc);

// 執行 4PL 擬合

const fourPLReg = fit4PL(xValues, yValues);

document.getElementById('fourPLRegressionEquation').innerText = `回歸方程式: y = ${fourPLReg.D.toFixed(4)} + (${fourPLReg.A.toFixed(4)} - ${fourPLReg.D.toFixed(4)}) / (1 + (x / ${fourPLReg.C.toFixed(4)})^${fourPLReg.B.toFixed(4)})`;

document.getElementById('fourPLRSquared').innerText = `相關係數 (R²): ${fourPLReg.rSquared.toFixed(4)}`;

const fourPLRSquaredWarning = document.getElementById('fourPLRSquaredWarning');

if (fourPLReg.rSquared < 0.95) {

fourPLRSquaredWarning.innerText = '警告：相關係數 R² 低於 0.95，4PL 檢量線擬合可能不佳。';

} else {

fourPLRSquaredWarning.innerText = '';

}

analysisResults.fourPLRegression = {

equation: `y = ${fourPLReg.D.toFixed(4)} + (${fourPLReg.A.toFixed(4)} - ${fourPLReg.D.toFixed(4)}) / (1 + (x / ${fourPLReg.C.toFixed(4)})^${fourPLReg.B.toFixed(4)})`,

rSquared: fourPLReg.rSquared.toFixed(4),

A: fourPLReg.A, B: fourPLReg.B, C: fourPLReg.C, D: fourPLReg.D,

inverseFourPLFunction: fourPLReg.inverseFourPLFunction // 儲存函數以便後續使用

};

// 繪製 4PL 回歸圖表

drawFourPLChart(document.getElementById('fourPLChart'), chartDataPoints, fourPLReg, maxConc);

// --- 5. 計算樣品的維生素 C 當量值 ---

const sampleVCEquivalentsUl = document.getElementById('sampleVCEquivalents');

sampleVCEquivalentsUl.innerHTML = '';

samples.forEach(sample => {

// 線性回歸計算

let linearVCEquivalent = '無法計算 (線性回歸無效)';

let linearVCEquivalentValue = NaN;

if (analysisResults.linearRegression.m !== 0) {

const calculatedX = (sample.scavengingRate - analysisResults.linearRegression.b) / analysisResults.linearRegression.m;

if (!isNaN(calculatedX) && isFinite(calculatedX) && calculatedX >= 0) {

linearVCEquivalent = calculatedX.toFixed(4) + ' mg/mL';

linearVCEquivalentValue = calculatedX;

} else {

linearVCEquivalent = `清除率 (${sample.scavengingRate.toFixed(3)}%) 超出線性模型範圍`;

}

}

sample.linearVCEquivalent = linearVCEquivalent; // 儲存以供匯出

sample.linearVCEquivalentValue = linearVCEquivalentValue; // 儲存數值以供匯出

sampleVCEquivalentsUl.innerHTML += `<li>${sample.name} (線性回歸): ${linearVCEquivalent}</li>`;

// 4PL 回歸計算

let fourPLVCEquivalent = '無法計算 (4PL 回歸無效)';

let fourPLVCEquivalentValue = NaN;

const sampleScavengingRate = sample.scavengingRate;

if (sampleScavengingRate >= Math.min(analysisResults.fourPLRegression.A, analysisResults.fourPLRegression.D) && sampleScavengingRate <= Math.max(analysisResults.fourPLRegression.A, analysisResults.fourPLRegression.D)) {

const calculatedX\_4PL = analysisResults.fourPLRegression.inverseFourPLFunction(sampleScavengingRate, analysisResults.fourPLRegression);

if (!isNaN(calculatedX\_4PL) && isFinite(calculatedX\_4PL) && calculatedX\_4PL >= 0) {

fourPLVCEquivalent = calculatedX\_4PL.toFixed(4) + ' mg/mL';

fourPLVCEquivalentValue = calculatedX\_4PL;

} else {

fourPLVCEquivalent = `清除率 (${sampleScavengingRate.toFixed(3)}%) 超出 4PL 模型範圍`;

}

} else {

fourPLVCEquivalent = `清除率 (${sampleScavengingRate.toFixed(3)}%) 超出 4PL 模型擬合範圍 (${analysisResults.fourPLRegression.A.toFixed(2)}% - ${analysisResults.fourPLRegression.D.toFixed(2)}%)`;

}

sample.fourPLVCEquivalent = fourPLVCEquivalent; // 儲存以供匯出

sample.fourPLVCEquivalentValue = fourPLVCEquivalentValue; // 儲存數值以供匯出

sampleVCEquivalentsUl.innerHTML += `<li>${sample.name} (4PL 回歸): ${fourPLVCEquivalent}</li>`;

});

}

/\*\*

\* 將分析結果匯出為 CSV 檔案。

\*/

function exportToCsv() {

if (!analysisResults || !analysisResults.samples || analysisResults.samples.length === 0) {

showMessageBox('沒有可匯出的分析結果。請先執行分析。');

return;

}

let csvContent = "";

// 添加 UTF-8 BOM

const BOM = "\uFEFF";

csvContent += BOM;

// --- 基礎數據 ---

csvContent += "基礎數據\n";

csvContent += "組別,L,a,b\*\n";

csvContent += `空白試紙組,${analysisResults.rawInputs.blank.L},${analysisResults.rawInputs.blank.a},${analysisResults.rawInputs.blank.b}\n`;

csvContent += `DPPH 紫色組,${analysisResults.rawInputs.dpph.L},${analysisResults.rawInputs.dpph.a},${analysisResults.rawInputs.dpph.b}\n\n`;

// --- 樣品組分析結果 ---

csvContent += "樣品組分析結果\n";

csvContent += "樣品名稱,L,a,b\*,ΔE (與DPPH比較),校正後ΔE (與空白試紙比較),DPPH清除率 (%),線性回歸維生素C當量 (mg/mL),4PL回歸維生素C當量 (mg/mL)\n";

analysisResults.samples.forEach(sample => {

const linearVC = isNaN(sample.linearVCEquivalentValue) ? sample.linearVCEquivalent : sample.linearVCEquivalentValue.toFixed(4);

const fourPLVC = isNaN(sample.fourPLVCEquivalentValue) ? sample.fourPLVCEquivalent : sample.fourPLVCEquivalentValue.toFixed(4);

csvContent += `${sample.name},${sample.L},${sample.a},${sample.b},${sample.deltaE.toFixed(3)},${sample.correctedDeltaE.toFixed(3)},${sample.scavengingRate.toFixed(3)},${linearVC},${fourPLVC}\n`;

});

csvContent += "\n";

// --- 維生素 C 標準品數據與結果 ---

csvContent += "維生素 C 標準品數據與結果\n";

csvContent += "濃度 (mg/mL),L,a,b\*,ΔE (與DPPH比較),校正後ΔE (與空白試紙比較),DPPH清除率 (%)\n";

analysisResults.vcStandards.forEach(vc => {

csvContent += `${vc.conc},${vc.L},${vc.a},${vc.b},${vc.deltaE.toFixed(3)},${vc.correctedDeltaE.toFixed(3)},${vc.scavengingRate.toFixed(3)}\n`;

});

csvContent += "\n";

// --- 檢量線回歸結果 ---

csvContent += "檢量線回歸結果\n";

csvContent += "回歸類型,方程式,R²\n";

csvContent += `線性回歸,"${analysisResults.linearRegression.equation}",${analysisResults.linearRegression.rSquared}\n`;

csvContent += `4PL回歸,"${analysisResults.fourPLRegression.equation}",${analysisResults.fourPLRegression.rSquared}\n`;

csvContent += "\n";

// 創建 Blob 並下載

const blob = new Blob([csvContent], { type: 'text/csv;charset=utf-8;' });

const link = document.createElement('a');

if (link.download !== undefined) { // 檢查瀏覽器是否支援 download 屬性

const url = URL.createObjectURL(blob);

link.setAttribute('href', url);

link.setAttribute('download', 'DPPH\_Analysis\_Results.csv');

link.style.visibility = 'hidden';

document.body.appendChild(link);

link.click();

document.body.removeChild(link);

URL.revokeObjectURL(url); // 釋放 URL 物件

} else {

showMessageBox('您的瀏覽器不支援檔案下載。請嘗試使用其他瀏覽器。');

}

}

// 頁面載入完成後自動執行分析，顯示預設數據的結果

window.onload = analyzeDPPH;

</script>

</body>

</html>