

# MALDI-TOF Search

1. Search website :

<http://169.230.19.26:8080/cgi-bin/msform.cgi?form=msfitstandard>

2. Parameter setting

The screenshot shows a web form for MALDI-TOF search with various input fields and buttons. Red circles highlight specific areas, and callout boxes provide Chinese instructions for each.

**Annotations:**

- 選擇蛋白質資料庫 (Select protein database) - points to the Database field (NCBI nr.2005.01.06).
- 選擇物種 (Select species) - points to the Species dropdown (All).
- 選擇分子量及PI值範圍 (Select molecular weight and pI range) - points to the MW of Protein and Protein pI input fields.
- 開始搜尋 (Start search) - points to the Start Search button.
- 選擇輸出資料之筆數 (Select the number of output records) - points to the Maximum Reported Hits input field (5).
- 調整誤差範圍 (可先設定 200-300 ppm, 再依結果調整) (Adjust error range (can first set 200-300 ppm, then adjust according to results)) - points to the Mass Tolerance input field (+/- 50 ppm).
- 選擇水解酵素及相關選項 (Select protease and related options) - points to the Digest dropdown (Trypsin) and other enzyme-related options.
- 選擇可能產生之修飾反應 (Select possible modifications) - points to the Possible Modifications dropdown.
- 輸入 mass list (Input mass list) - points to the Data Paste Area.

**Form Fields and Values:**

- Database: NCBI nr.2005.01.06
- DNA Frame translation: 3
- Search Hits:  From: msfit
- Filename: lastres1
- Output Type: HTML
- Save Hits to file:  Filename: lastres1
- Accession Numbers: [empty]
- Species: All
- Species Codes: [empty]
- Names: [empty]
- MW of Protein: (from 1000 Da to 100000 Da) All
- Protein pI: (from 3.0 to 10.0) All
- Start Search
- Maximum Reported Hits: 5
- Sample ID (comment): Magic Bullet digest
- Sort By: Score Sort
- Min. # peptides required to match: 4
- Report MOWSE Scores:  Pfactor: 0.4
- Chem Score:  Met Ox Factor: 1.0
- Possible Modifications Mode (default):
  - Peptide N-terminal Gln to pyroGlu
  - Oxidation of M
  - Protein N-terminus Acetylated
  - Acrylamide Modified Cys
  - User Defined Modification 1:
    - Phosphorylation of S, T and Y
- OR
- Homology Mode (select any mode but identity)
- Search mode: identity
- Min. # matches with NO AA substitutions: 1
- Instrument: MALDI-TOF
- Peptide masses are: monoisotopic
- Mass Tolerance: +/- 50 ppm
- Systematic Error: 0
- Data Format: PP M/Z Charge
- Data Paste Area:
  - 676.3718
  - 825.4571
  - 1017.5370
  - 1026.5964
  - 1040.6121
  - 1105.4550
  - 1196.7132
  - 1218.5796