WHAT'S NEW

MAgenNTA Match 6.1

Everything new since FluoroMatch 5.73, LipidMatch, and PolyMatch

THE TAKE-HOME

MAgenNTA Match enables comprehensive identification, covering metabolite, xenobiotic, PFAS, lipid and polymer annotation. MAgenNTA covers the entire non-targeted analysis workflow including file conversion, peak picking, blank filtering, annotation, and statistics for LC-HRMS/MS based non-targeted analysis. Four benchmarked peak pickers (MZmine 2, MZmine 3, Asari and HRMSKit) are implemented and a modular workflow works with any upstream peak processing and annotation. For annotation MAgenNTA Match 6.1 implements rule-based and spectral matching algorithms for high-confidence screening using fragmentation patterns from real chemicals standards and experimental spectra: Over 2.9 million open MS/MS spectra and over 1 million rule-based diagnostic fragmentation libraries which have been developed with over a decade of contributions are distributed in compressed SQLite databases. Non-targeted analysis for class based screening and completely unknown chemical discovery are also implemented. Schymanski, FluoroMatch, and Charbonnet scores, backed by a retention-time-aware homologous-series model, aid in assigning chemical confidence. Analyze data, review evidence, assign confidence and flag features, reintegrate and export (Excel or Agilent ChemVista) from a browser interface, while an agent-ready evidence database lets AI assistants explore your results right alongside you.

BY THE NUMBERS

2.9 M

open MS/MS spectra in one SQLite library (real LC-HRMS/MS spectra, none are predicted)

12–17×

faster processing (tested on NIST A (AFFF contaminated soil) and SRM 2781 (sewage sludge)

1 M+

MS/MS Rule-based libraries with < 5% false positive rate for lipids, polymers, and PFAS developed over the past decade

4

peak pickers: MZmine 2 & 3, Asari, HRMSKit

3

confidence systems: Schymanski, FluoroMatch, Charbonnet

2000+

Users of FluoroMatch, LipidMatch, and PolyMatch can now benefit from this all-in-one software

01 Spectral Libraries & Matching (Thank you David Schiessel!)

Millions of spectra, one tidy file — with credit to every source.

- **One library to search them all.** Compiled multiple available MS/MS open-source spectral libraries — GNPS[1], LIPID MAPS[2], MassBank[3,4], MoNA[5], MS-DIAL[6,7] and the NIST DIMSpec PFAS database[8,9] — into one compressed SQLite file. These libraries also include the Enveda-180 collection distributed through MoNA[10].

Table 1. Spectral library contents by source and polarity

Source	Polarity	Total spectra	Unique spectra	Total compounds	Unique compounds
GNPS	Positive	637,602	624,485	637,602	103,791
	Negative	196,347	192,041	196,347	41,164
LIPID MAPS	Positive	148	146	148	74
	Negative	1,491	1,485	1,491	483
MassBank	Positive	155,060	78,480	155,060	9,054
	Negative	76,981	38,557	76,981	6,213
MoNA	Positive	406,627	398,987	406,627	76,406
	Negative	94,572	93,433	94,572	42,535
MS-DIAL	Positive	2,475,102	425,426	2,475,102	43,014
	Negative	349,059	105,437	349,059	32,420
NIST	Positive	877	877	877	32
	Negative	6,307	6,307	6,307	101

Table 2. Combined counts by polarity

Polarity	Total spectra	Unique spectra	Total compounds	Unique compounds
Positive	3,675,416	1,525,217	3,675,416	173,603
Negative	724,757	434,900	724,757	90,109

- **Compact by design.** The merged library (SpecDB 6.3, compiled by David Schiessel) takes 1.66 GB instead of the 9.26 GB of its two source files. Duplicate spectra are stored once and every source record links to the retained spectrum, and 63,045 low-intensity spectra that rounding would have erased were rescued and rescaled.
- **Da, not ppm.** Changed ppm MS/MS matching to Da and patched bugs. Annotation coverage: compared to the old version, **+35% more confident IDs** (42 IDs instead of 31) with MZmine 3 on SRM 2781.

- **Smarter fragment counting.** Matched fragments within 2× the MS/MS window now count once on both the experimental and library side, and the reverse cosine uses the most intense peak of each fragment window (forward cosine and spectral entropy[11] are unchanged). A "+" marks each matched fragment on both sides of the library mirror plot.
- **Credit where credit is due.** Ranked candidates now show the library identifier, the library record (linked to its MassBank, GNPS or MoNA page where one exists) and the attribution: the citation or license recorded with each matched spectrum.

02 Speed & Scalability

From an overnight run to a coffee break: SRM 2781 now finishes in about 20 minutes instead of 4.5 hours.

- **A rapid test bench.** Made a synthetic NIST A mzML test set for rapid testing.
- **A whole-code speed audit.** Did an entire audit of slow portions of the code using the synthetic NIST A set, SRM 2781 (40,000 features) and NIST A, and sped up and parallelized the code:

Table 3. Processing time before and after the speed-up

Dataset	Release	Full processing time (with MZmine)	R processing time
NIST A	5.73	1h 13m 12s 4,392.5 s	1h 10m 56s 4,256.4 s
	5.75*	6m 10s 370.4 s	4m 10s 250.2 s
	Speed-up (old/current)	**12×**	**17×**
SRM 2781	5.73	4h 29m 01s 16,140.7 s	4h 26m 08s 15,967.8 s
	5.75*	20m 46s 1,245.6 s	18m 03s 1,083.5 s
	Speed-up (old/current)	**13×**	**15×**

**Release 5.75 is the development build that became MAgenNTA Match 6.1.*

- **…and then faster still.** A further round of R parallelization in 6.1 cut the R stage for a 76,452-feature SRM 2781 HRMSKit table from 5,150 s to 1,702 s (3×) and for NIST A from 511 s to 272 s, with results identical to the previous code.
- **Sized to your computer.** Parallel stages size themselves automatically: one worker per physical core (leaving headroom for Windows), limited by free memory, with a simple override (`FLUOROMATCH_WORKERS`).
- **A snappier dashboard.** SRM 2781 (76,452 features) opens in 7.2 s instead of 19.5 s, GPU-drawn (WebGL) scatter plots cut hover steps from 243 ms to 52 ms, and a selected feature's evidence loads in under half a second.

03 Peak Picking: Four Engines, One Fair Race

Benchmarked against manually annotated reference samples.

- **Four engines under one hood.** Integrated Asari[12] and HRMSKit[13] alongside MZmine 2[14] and MZmine 3[15]. Vendor files are converted automatically with ProteoWizard MSConvert[16].
- **Benchmarked, not guessed.** Benchmarked Asari, HRMSKit and MZmine 3 against manually annotated NIST A and NIST C samples. Also benchmarked against sewage sludge (SRM 2781[17]).

NIST A

- All software covered every single spiked chemical standard and in-source fragment.
- MZmine 3 and HRMSKit got all peaks across all dilutions; Asari missed some in NIST A.
- MZmine 3 and HRMSKit had the fastest run times and Asari was much slower, with all having highly permissive parameters for NIST A, NIST C and sewage sludge.

NIST C

- HRMSKit had the fewest false peaks detected and integrated.
- HRMSKit had the smallest peak list.
- MZmine 3 had the most coverage. HRMSKit did the worst for isomer detection; without considering isomers, it had similar coverage to MZmine 3.

SRM 2781 (sewage sludge)

Table 4. High-scoring annotations (score A and B+) and peak-table size per peak picker

Peak picker	Score A	Score B+	A + B+	Features in peak table
MZmine 3	10	21	31	64,799
HRMSKit (permissive)	7	25	32	86,591
Asari (permissive)	8	29	37	105,755

- Asari actually covered the most high-scoring peaks when ignoring isomers, but had massive peak table sizes. MZmine 3 and HRMSKit performed similarly.

04 Annotation, Scoring & Confidence

More evidence behind every ID, and clearer language for how sure we are.

- **Three ways to say "how sure."** Updated the scoring algorithm: updated Schymanski scoring[18], FluoroMatch scoring[19,20], and added Charbonnet scoring[21].
- **Homologous series, generalized.** Made a generalized homologous series detection script, which is implemented. It searches every enabled repeating unit (CF_2, CH_2, CH_2CH_2O) and also discovers new repeat intervals directly from the data, with Kendrick mass defect[22] views of each.
- **Retention-time trend model.** A new RT series model decides, for every PFAS, lipid and polymer series, whether each feature is a member, unsure or an outlier, formalizing a reviewer's visual check of RT vs. m/z. It reached 0.955 precision and 0.843 recall against reviewer-checked tables, now gates Charbonnet Level 2C/3D

homologue promotions, and fills blank names, formulas and SMILES of members from the nearest confident anchor.

- **Where was the MS/MS taken?** Added points of trigger for MS/MS (RT) and MS1 at the point of MS/MS trigger to determine if a spectrum is chimeric and where the MS/MS was taken for that peak.
- **PFAS fingerprints in every spectrum.** Each feature's representative MS/MS is screened for a curated set of diagnostic PFAS fragments (e.g., CF_3^-, $C_2F_5^-$, SF_5^-, $CF_3SO_3^-$), its spectral purity (the precursor vs. co-isolated ions at the trigger) and signal thresholds. These new columns support the "PFAS Class Candidate" level of the final report, even without a library match.
- **One chemical, one compound ID.** Adducts, isotopes, dimers and in-source fragments of the same chemical are grouped under one `Compound_ID_MAgenNTA` when their EIC profiles correlate ($r > 0.6$), even across polarities.
- **Formula prediction, refreshed.** Both workflows share a common formula policy (CHNOSFBrCl first, then CHNOSFP; top 10 candidates) built on Rdisop[23], enviPat[24] and MetaboCoreUtils[25], and any feature can be sent for on-demand formula prediction from the dashboard's Formula Hypotheses panel.

05 Libraries & Data Architecture

Leaner, cleaner, and all in SQLite.

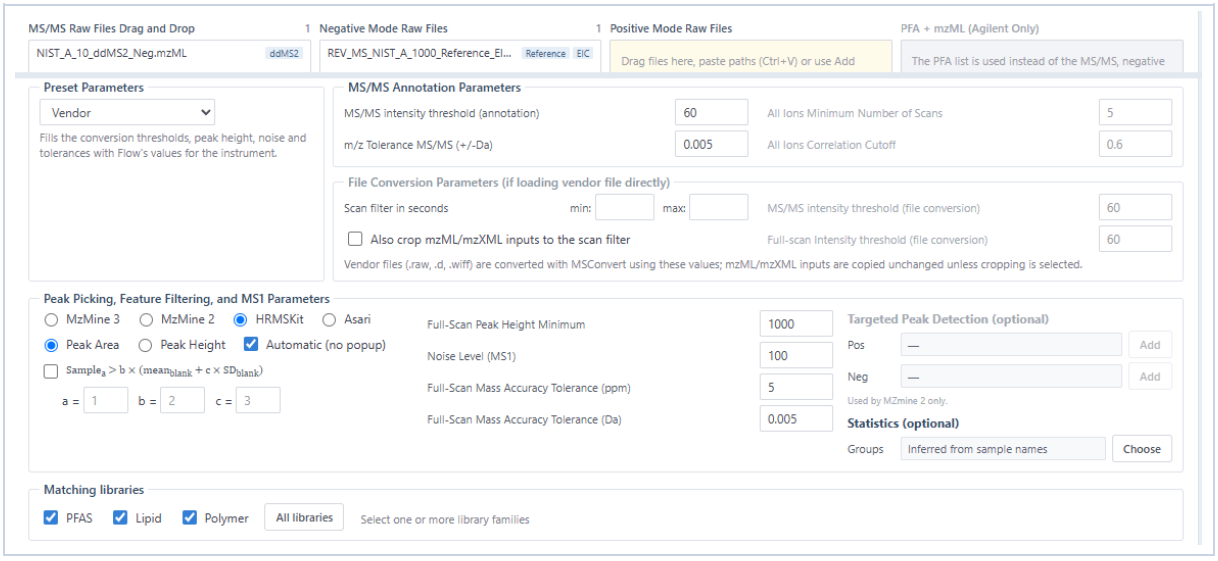
- **From CSV sprawl to SQLite.** Compressed and combined all CSV library files into 3 RDS files (R's native serialized data format), covering in-silico libraries from EPA[26], Biotransformation and rule-based libraries (and removed separate fragment-screening CSVs), and then into SQLite.
- **Lipids and polymers, PFAS-style.** Added SMILES and Formula to the Lipid Libraries and formatted the Lipid and Polymer Libraries to be the same as PFAS. 160,399 previously missing lipid SMILES and 28,838 formulas were added, and all three families now carry structure identifiers (SMILES, InChIKeys and formulas): nearly 1.6 million identifier records.
- **One software, every library.** Compressed and combined all libraries into a single software, with toggles to turn specific libraries (PFAS, Lipid and Polymer) on and off.
- **A lighter download.** Further cleaned up files within the project for a 3× reduction in the file size of the distribution, including 58 unused R packages removed from the bundled R.
- **One result database per run.** Every analysis produces `MAgenNTA_Agent.sqlite`, an indexed result store with completion and provenance recorded inside, alongside the familiar `NegIDed_FIN.csv` / `PosIDed_FIN.csv`. Exact duplicate feature rows are detected and canonicalized, and original inputs are never overwritten.
- **Move it anywhere.** The release finds its bundled R, Python, peak pickers and libraries from wherever it lives, so the folder can be moved or renamed.

06 A Brand-New Interface

Run it, review it, report it, all in your browser.

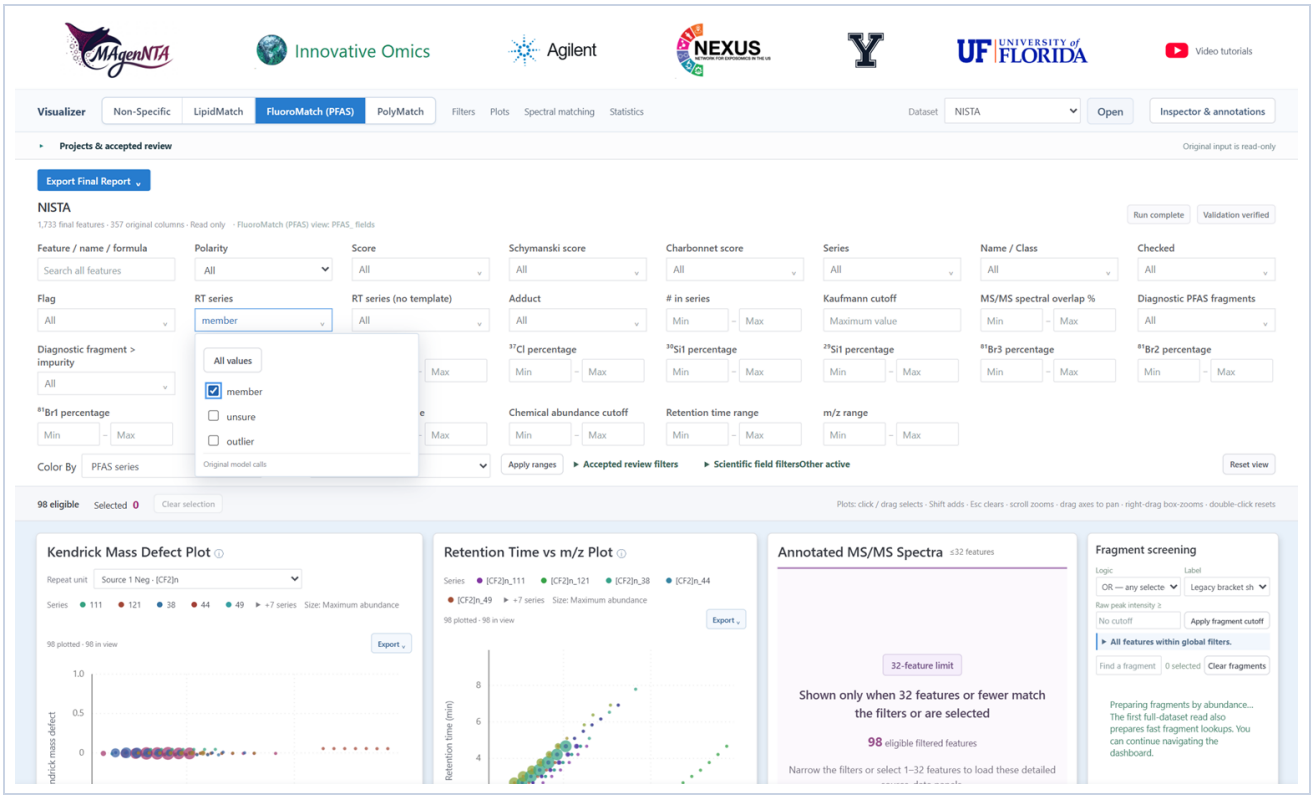
- **Built from the ground up.** Made an entirely new interface (both for running Flow and for the dashboard) from the bottom up, using React/TypeScript with a small Rust service and SQLite[27] underneath.
- **Run analysis.** `Flow.bat` now opens Run analysis in your browser with Flow's familiar layout. Each analysis runs in its own background process, so closing or refreshing the browser doesn't stop it. Analyses queue one after another, can be cancelled without touching any other program, and open automatically in Review results with their provenance.

- **Clear file roles.** Added new naming conventions: EIC and Reference are now different key words.



Run analysis: Flow's layout in the browser, with EIC/Reference file tags, four peak pickers and library toggles.

- **Statistics that find your groups.** Added more statistical views and automatic detection of groups: PCA scores and loadings, volcano plots, Welch ANOVA[28] with Games–Howell post hoc tests[29] and Benjamini–Hochberg FDR[30], group violins and an abundance heatmap.
- **Review at the speed of thought.** Added an in-app annotation/review workflow, including hotkeys that let you drag to confirm or deny annotations (as well as apply many other user-supplied categories). Reviews autosave to your own project copy; the scientific result stays read-only.
- **One-click family views.** A master toggle switches the whole dashboard between Non-Specific, LipidMatch[31], FluoroMatch (PFAS) and PolyMatch views, with family-specific Kendrick plots ($[CF_2]_n$, $[CH_2]_n$, $[CH_2CH_2O]_n$), Kaufmann plots[32], slicers and tooltips.
- **Reintegration.** Added a reintegration workflow, so peak integration can be adjusted directly on the extracted ion chromatograms (EICs).
- **Export what matters.** Added an Export workflow for a final XLSX report with just the confident annotations (or whichever levels of confidence, criteria, etc. you want to export), as Simple, Verbose and Unique-Chemicals workbooks, with a rule editor for each confidence level.
- **Agilent ChemVista export.** Added Agilent ChemVista[33] export: the features chosen for the Excel report are also written as MassBank records, MoNA-style SDF spectra and EPA CompTox-style compound files, complete with SPLASH identifiers[34] and RDKit[35] structures and InChIKeys.
- **Slide-ready figures.** Every plot exports to an editable PowerPoint slide, as well as PNG, SVG and CSV.
- **Evidence at a glance.** MS/MS trigger EIC overlays, labelled isotope peaks (M, M+1, M+2…), library mirror plots, locally rendered structures (SmilesDrawer[36]) and one mouse scheme on every plot.



Review results: the FluoroMatch (PFAS) view of NIST A, filtered to RT-series members, with coordinated Kendrick mass defect and retention time vs. m/z plots.

07 AI-Ready Tools

Built for humans and their AI agents.

- ☐ **An environment for agents.** Made an Agent environment: a rapidly accessible database with FluoroMatch results, an MD file with instructions to navigate the environment, and Agent tools specific to the environment. Agents can summarize a run, search by m/z, pull every piece of evidence for a feature, and extract and plot raw scans using the bundled Python and R, with no internet required. Results and raw data stay read-only; annotation edits go only to a review copy, after your confirmation.
- ☐ **MAgenNTA Library Explorer.** Made a standalone software, MAgenNTA Library Explorer, distributed within, to read and write libraries and visualize spectral data and metadata. Search offline by name, formula, InChIKey, precursor or fragment mass, instrument, collision energy and even chain length; “Develop libraries” builds new entries from CSV or mzML spectra, fragment rules and Boolean criteria.

READY, SET, MATCH

Keep the release folder together, double-click `Flow.bat`, and Run analysis opens in your browser. HRMSKit (automatic mode), Asari and MZmine 3 need no installation; MZmine 2 needs 64-bit Java 8 and the interactive HRMSKit window needs the Microsoft Edge WebView2 Runtime.

08 Acknowledgments & Attribution

MAgenNTA Match stands on the shoulders of a generous open-science community. Thank you!

- **David Schiessel**, for the spectral matching algorithms and the compiled spectral libraries (SpecDB) at the heart of MAgenNTA's spectral matching.
- **Hyung Won Choi and team** (National University of Singapore; hyung_won_choi@nus.edu.sg), for HRMSKit and its integration into MAgenNTA Match[13].
- **Spectral data providers:** the MassBank consortium and its contributors[3,4]; MassBank of North America (MoNA), Fiehn Laboratory, UC Davis[5]; the GNPS/GNPS2 community libraries[1]; the MS-DIAL libraries[6,7]; LIPID MAPS[2]; the NIST DIMSpec PFAS database (Jared M. Ragland and Benjamin J. Place, NIST)[8,9]; and Enveda for the Enveda-180 collection[10]. Every library spectrum keeps its original source record, citation and license.
- **Open-source software:** Asari (Shuzhao Li laboratory)[12], MZmine 3[15] and MZmine 2[14], ProteoWizard MSConvert[16], R with mzR, Rdisop[23], enviPat[24], MetaboCoreUtils[25] and MassTools, RDKit[35], SmilesDrawer[36], SPLASH[34], SQLite[27], Python, React, TypeScript, Rust, chroma.js and python-pptx. Each is used under its own license, shipped with the release.
- **Scientific frameworks:** confidence levels by Schymanski et al.[18] and Charbonnet et al.[21], spectral entropy by Li et al.[11], Kendrick[22] and Kaufmann[32] mass-defect plots, EPA CompTox chemical lists[26], and NIST SRM 2781[17].

Product names are trademarks of their respective owners.

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