

NIST/EPA/NIH EI-MS LIBRARY

2023 Release

40K NEW NIST MEASURED/EVALUATED COMPOUNDS

394K Electron Ionization (EI) Spectra

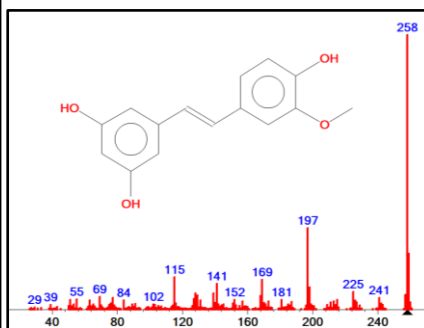
- 347,100 Compounds, 46,954 Replicate Spectra
- 40 K More Compounds than NIST 20

492K Retention Index (RI) Values

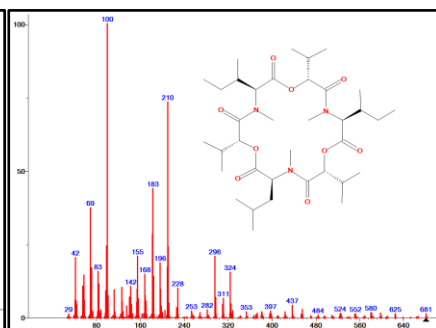
- 153K RI Compounds with EI, >40 K Increase
- AI-RI Estimates for All EI Compounds

COMPOUNDS SELECTED FOR ANALYTICAL RELEVANCE FULLY EVALUATED WITH DERIVATIVES, RETENTION INDICES & CLASS INFORMATION

Citation	New	Total
Wikipedia	1570	6227
EPA Tox	2969	7117
Food DB	582	4273
EU Contaminants	6263	15149
Protein Data Bank	1194	4716
Human Metabolite DB	1992	9393
PFAS	161	749
Adams (Essential Oils)	2136	2136



Plant Stilbenoid



Mycotoxin ENN A

Compound Data

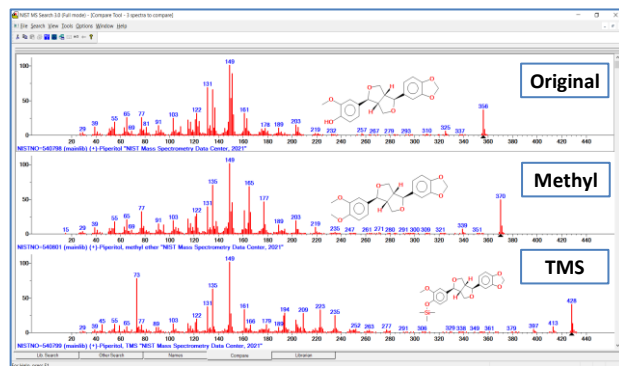
Name: Valeryl fentanyl
Formula: C₂₄H₃₂N₂O
MW: 364 Exact Mass: 364.251463 CAS#: 122882-90-0 NIST#: 463844 IIR: 18711
Contributor: NIST Mass Spectrometry Data Center
InChIKey: VCCPXHWAJYQMR-UHFFFAOYSA-N Non-steroid
Synonyms:
1 Pentanamide, N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]; 2 N-Phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]
Other DBs:
Wikipedia
wikipedia2021 via cheminfo_SMILES
Environmental
SUSDATA22
Experimental RI median+deviation (#data)
Semi-standard non-polar: 2962±18 (2)
Standard non-polar: 2958±N/A (1)
Estimated non-polar retention index (n-alkane scale):
Value: 2938 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu
Retention index:
1. Value: 2980.5 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: HP-5MS
Column Length: 30 m

Collections

RI Averages

AI-RI Estimates

RI Measured



Piperitol with TMS/Me Derivatives (TFA, Acetyl not shown)

ENHANCEMENTS

Hit List

Compound/Spectrum Lookup

New: Retention Index For All Hits (Expt'l or AI-RI*)

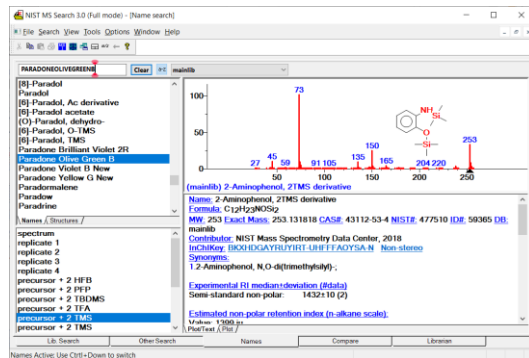
Select Columns
Mass Difference,
Reverse Score,
Probability, ...

New: Expanded
Compound Classes

#	Match	R.M.	RI	Del...	S	DBs	Name
1	R	999	999	1442	0	1	2-Aminophenol, 2TMS deriva
2	M	965	965	1930	-50	0	3-Amino-2-naphthol, N,O-bis
3	M	965	965	1489*	-14	1	2-Amino-m-cresol, N,O-bis
4	R	956	956	1309	-1	9	38 W...
5	M	955	957	1582	-17	1	5 E
6	M	953	953	2023*	-49	1	2,3-Naphthalenediamine, 2T
7	M	949	949	1449	-29	3	7 EFGM
8	M	947	947	1600	-34	4	2-amino-5-chlorophenol, N, C
9	M	941	942	1388	-15	2	21 W...
10	M	939	951	1778	-33	0	1 M
11	M	938	946	1469	-17	1	7 EM
12	M	936	945	1755	-33	1	2 E
13	M	933	937	1470	-43	9	8 EGM
14	M	931	931	1550	-28	1	2-Amino-4-ethylphenol, 2TMS
15	M	929	929	1930	-50	0	2-Amino-1-naphthol, N,O-bis

Names

Spectra
Replicates
Derivatives
Stereo



NIST EI LIBRARY SOFTWARE

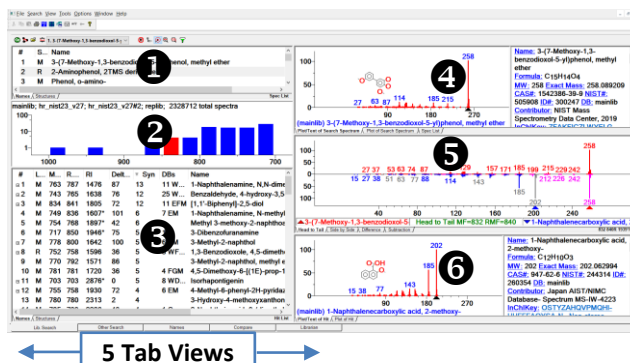
2023 EI Release EI MS ANALYSIS TOOLS

NISTMS

FULL FEATURED MS LIBRARY
SEARCH/DISPLAY PROGRAM

MULTIPLE SEARCH TYPES & DISPLAY
MODES

5 VIEWS: SPECTRUM SEARCH, FEATURE
SEARCH, COMPARE, NAME/SPECTRUM,
USER LIBRARY



- 1 Query spectrum list
- 2 Score Histogram
- 3 Hit List—multiple values
- 4 Query spectrum
- 5 Query/Library Compare
- 6 Library Spectrum

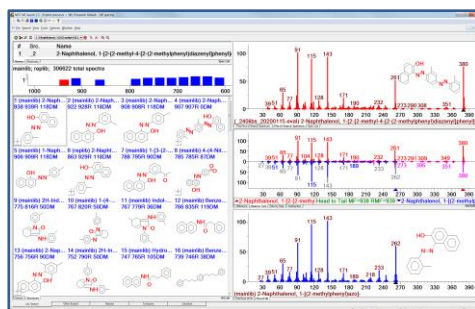
Hybrid Search

FOR COMPOUNDS NOT FOUND IN
LIBRARY & ID CONFIRMATION

FINDS 'MODIFIED' LIBRARY IDS
AND MASSES OF MODIFICATIONS
WITH THEIR SHIFTED PEAKS

USES MW ESTIMATE

DELTA MASS => CHEMICAL FORMULA

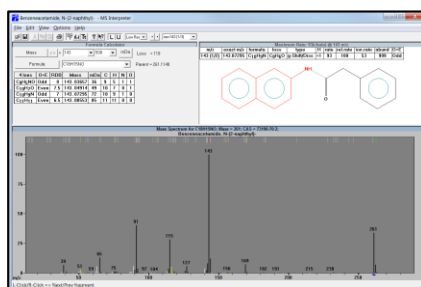


DMass	Replace or Insert
1	H->D, C->C13, NH->O, CH->N
2	CH2->O, C=C->C-C
12	CH2->C=CH2
14	X-Y->X-CH2-Y
16	X-Y->X-O-Y
17	NH->S
18	H->F
28	X-Y->X-CO-Y
30	H->CH3O-H
32	X-Y->X-S-Y
34	H->Cl
50	Phenyl->Naphthyl
76	H->Phenyl
162	H->Glucose

MS Interpreter

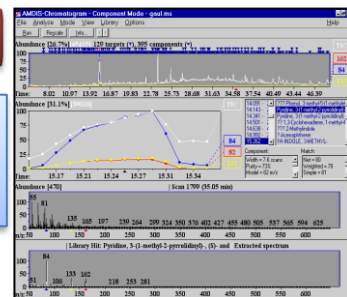
CONNECT PEAKS TO PLAUSIBLE
FRAGMENTS (IN RED)

CONFIRM ID
COMPUTE FRAGMENT MASSES
CONNECT PEAKS TO STRUCTURES



AMDIS

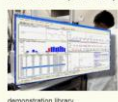
'PURIFIES'
SPECTRA AND
CONNECTS
TO NISTMS



FREELY AVAILABLE DATA AND SOFTWARE

NIST Website
chemdata.nist.gov

Libraries, Tools, Service



This site provides information and access to NIST mass spectral data products. A variety of data products are available, including EI and tandem MS libraries (small molecule and peptide), a GC retention index collection as well as certain freely available, specialized spectral libraries. Freely available data analysis tools include AMDIS (Automated Mass Spectral Deconvolution and Identification System for GC/MS), the Mass Spectrum Interpreter (connects chemical structures with mass spectra), and the Mass Spectral Digitizer Program. Also available is a fully functional, version of NIST MS Search Program v2.9.0 with a small

Tools

- Mass Spectrum Interpreter - Major New Release - February 2019 (v. 3.4). Information and downloads for version 3.4 of this program which connects mass spectral peaks to their probable chemical structure origin (EI and MS/MS, both nominal and accurate mass).
- NIST MS Software and Data - updates, demo, documentation, MSPepSearch, Lib2NIST, RUS libraries and support programs.
- AMDIS - computer program that extracts spectra for individual components in a GC/MS data file (Instructions for using AMDIS with MS Search - 11-25-2019)
- Mass Spectrum Digitizer Program - a tutorial on how to use the program (includes program download) that allows the digitization of graphical spectra
- The NIST Glyco Mass Calculator - a tool to aid in the analysis of glycoforms
- DIMEDR - A Novel Algorithm for Agglomerating Incongruent LC-MS Metabolomics Datasets.
- MS_Piano (New, 2021) - A new software tool for annotating peaks in collision induced dissociation (CID) tandem mass spectra of peptides and N-glycopeptides.

Recurrent Unidentified Spectral Libraries

There are three NIST user libraries of recurrent unidentified spectra (RUS):

- Food:** A set of 650+ spectra extracted from a set of dried food material, some of these spectra have tentative identifications. These experiments were done with methoximation and TMS derivatization. Data
- PedUrine:** A set of 200+ spectra from a large set of pediatric urine samples. All of these samples were derivatized with TMS after forming the ethoxime for the non-acid carbonyl groups; the majority of this
- EssOil:** A set of 1000+ spectra derived from a large set of essential oils (both commercial and laboratory distilled), solvent extract of various plant materials (leaves, flowers, roots, etc). Most of these data were



<http://chemdata.nist.gov>

NIST Tandem Mass Spectral Library

2023 Release

51,501 Compounds, 60% More than 2020
400 K Precursor Ions – 2.4 M Spectra

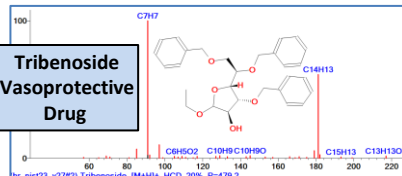
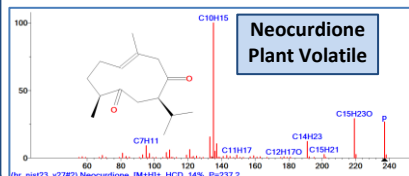
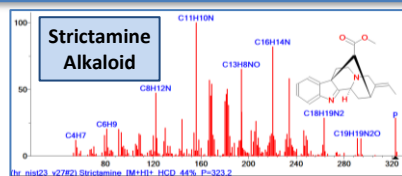
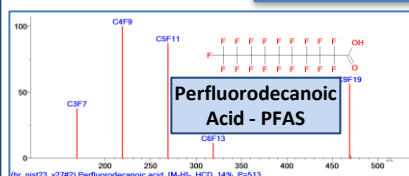
Fragmentation Methods

49,590 HRAM (High Res Accurate Mass) Compounds
50,071 QTOF, HCD, IT-HRAM, QqQ Compounds
49,561 Ion Trap Compounds (Low Res., up to MS⁴)
561 APCI HRAM Compounds

Precursor Ion Types

44,191 Protonated
19,620 Deprotonated
14,318 Water/Ammonia Loss
44,547 Other In-Source Generated

ALL COMPOUNDS SELECTED FOR RELEVANCE MEASURED AT NIST, THOROUGHLY EVALUATED

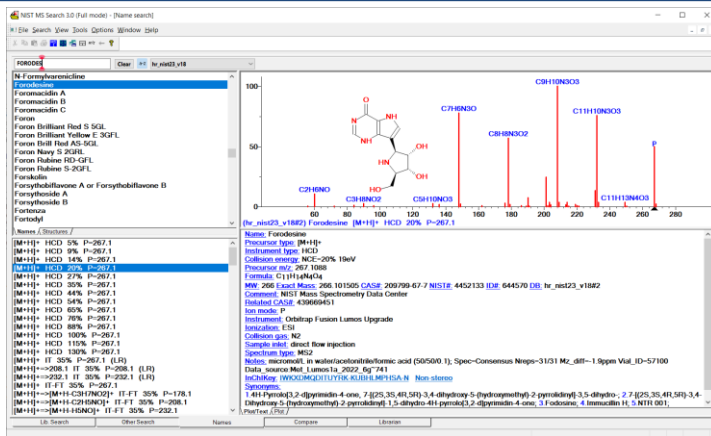


Citation	New	Total
Wikipedia	1618	6424
EPA Tox	3181	8146
Food DB	602	4491
EU Contaminants	6553	15818
Protein Data Bank	1246	4945
Human Metabolite DB	2071	9686
PFAS	90	116

All Spectra Shown for Each Compound

1. Compound Name Many Synonyms

2. All Related Spectra All Energies Fragmentation Types In-Source Ions, ...



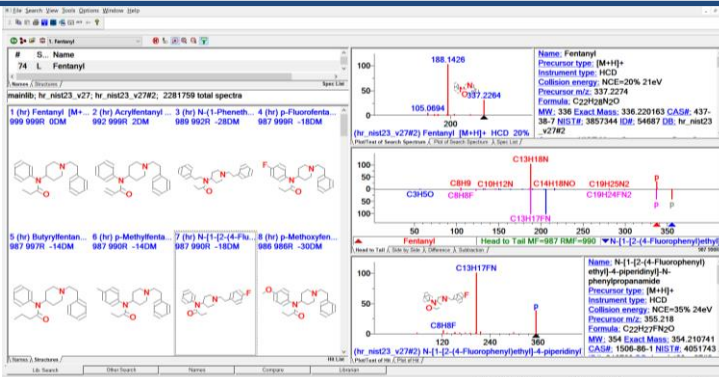
Full Spectrum
Selected from List
at Lower Left

All Spectrum Text
Information

Hybrid Search Recommended for All Tandem MS Searches

Find Related
Compounds Even if
Query is not in Library

Differences in masses
are 'Modifications'



Query Spectrum

Shifted Library Peaks
(gray->red)
Contain Modification

Library Spectrum

NIST TANDEM LIBRARY SOFTWARE

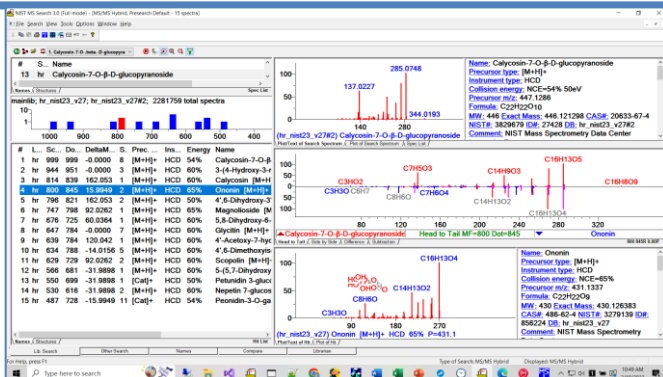
2023 Tandem Release

TANDEM (MS/MS) ANALYSIS TOOLS

NISTMS

ALL SPECTRA FOR EACH
COMPOUND IN ONE LIST

MULTIPLE ENERGIES
ION MODES
FRAGMENTATION TYPE
IN SOURCE IONS



FILTER IDS BY SPECTRUM TYPE

MS/MS Hit List Filter

☐ Enable Filtering (Tandem Only)

Instrument Type: ☐ Ion Trap ☐ Ion Trap + FT ☐ Other

Allow Precursors: ☐ C16-18 ☐ C18-20 ☐ C20-22 ☐ C22-24 ☐ C24-26 ☐ C26-28 ☐ C28-30 ☐ C30-32 ☐ C32-34 ☐ C34-36 ☐ C36-38 ☐ C38-40 ☐ C40-42 ☐ C42-44 ☐ C44-46 ☐ C46-48 ☐ C48-50 ☐ C50-52 ☐ C52-54 ☐ C54-56 ☐ C56-58 ☐ C58-60 ☐ C60-62 ☐ C62-64 ☐ C64-66 ☐ C66-68 ☐ C68-70 ☐ C70-72 ☐ C72-74 ☐ C74-76 ☐ C76-78 ☐ C78-80 ☐ C80-82 ☐ C82-84 ☐ C84-86 ☐ C86-88 ☐ C88-90 ☐ C90-92 ☐ C92-94 ☐ C94-96 ☐ C96-98 ☐ C98-100 ☐ C100-102 ☐ C102-104 ☐ C104-106 ☐ C106-108 ☐ C108-110 ☐ C110-112 ☐ C112-114 ☐ C114-116 ☐ C116-118 ☐ C118-120 ☐ C120-122 ☐ C122-124 ☐ C124-126 ☐ C126-128 ☐ C128-130 ☐ C130-132 ☐ C132-134 ☐ C134-136 ☐ C136-138 ☐ C138-140 ☐ C140-142 ☐ C142-144 ☐ C144-146 ☐ C146-148 ☐ C148-150 ☐ C150-152 ☐ C152-154 ☐ C154-156 ☐ C156-158 ☐ C158-160 ☐ C160-162 ☐ C162-164 ☐ C164-166 ☐ C166-168 ☐ C168-170 ☐ C170-172 ☐ C172-174 ☐ C174-176 ☐ C176-178 ☐ C178-180 ☐ C180-182 ☐ C182-184 ☐ C184-186 ☐ C186-188 ☐ C188-190 ☐ C190-192 ☐ C192-194 ☐ C194-196 ☐ C196-198 ☐ C198-200 ☐ C200-202 ☐ C202-204 ☐ C204-206 ☐ C206-208 ☐ C208-210 ☐ C210-212 ☐ C212-214 ☐ C214-216 ☐ C216-218 ☐ C218-220 ☐ C220-222 ☐ C222-224 ☐ C224-226 ☐ C226-228 ☐ C228-230 ☐ C230-232 ☐ C232-234 ☐ C234-236 ☐ C236-238 ☐ C238-240 ☐ C240-242 ☐ C242-244 ☐ C244-246 ☐ C246-248 ☐ C248-250 ☐ C250-252 ☐ C252-254 ☐ C254-256 ☐ C256-258 ☐ C258-260 ☐ C260-262 ☐ C262-264 ☐ C264-266 ☐ C266-268 ☐ C268-270 ☐ C270-272 ☐ C272-274 ☐ C274-276 ☐ C276-278 ☐ C278-280 ☐ C280-282 ☐ C282-284 ☐ C284-286 ☐ C286-288 ☐ C288-290 ☐ C290-292 ☐ C292-294 ☐ C294-296 ☐ C296-298 ☐ C298-300 ☐ C300-302 ☐ C302-304 ☐ C304-306 ☐ C306-308 ☐ C308-310 ☐ C310-312 ☐ C312-314 ☐ C314-316 ☐ C316-318 ☐ C318-320 ☐ C320-322 ☐ C322-324 ☐ C324-326 ☐ C326-328 ☐ C328-330 ☐ C330-332 ☐ C332-334 ☐ C334-336 ☐ C336-338 ☐ C338-340 ☐ C340-342 ☐ C342-344 ☐ C344-346 ☐ C346-348 ☐ C348-350 ☐ C350-352 ☐ C352-354 ☐ C354-356 ☐ C356-358 ☐ C358-360 ☐ C360-362 ☐ C362-364 ☐ C364-366 ☐ C366-368 ☐ C368-370 ☐ C370-372 ☐ C372-374 ☐ C374-376 ☐ C376-378 ☐ C378-380 ☐ C380-382 ☐ C382-384 ☐ C384-386 ☐ C386-388 ☐ C388-390 ☐ C390-392 ☐ C392-394 ☐ C394-396 ☐ C396-398 ☐ C398-400 ☐ C400-402 ☐ C402-404 ☐ C404-406 ☐ C406-408 ☐ C408-410 ☐ C410-412 ☐ C412-414 ☐ C414-416 ☐ C416-418 ☐ C418-420 ☐ C420-422 ☐ C422-424 ☐ C424-426 ☐ C426-428 ☐ C428-430 ☐ C430-432 ☐ C432-434 ☐ C434-436 ☐ C436-438 ☐ C438-440 ☐ C440-442 ☐ C442-444 ☐ C444-446 ☐ C446-448 ☐ C448-450 ☐ C450-452 ☐ C452-454 ☐ C454-456 ☐ C456-458 ☐ C458-460 ☐ C460-462 ☐ C462-464 ☐ C464-466 ☐ C466-468 ☐ C468-470 ☐ C470-472 ☐ C472-474 ☐ C474-476 ☐ C476-478 ☐ C478-480 ☐ C480-482 ☐ C482-484 ☐ C484-486 ☐ C486-488 ☐ C488-490 ☐ C490-492 ☐ C492-494 ☐ C494-496 ☐ C496-498 ☐ C498-500 ☐ C500-502 ☐ C502-504 ☐ C504-506 ☐ C506-508 ☐ C508-510 ☐ C510-512 ☐ C512-514 ☐ C514-516 ☐ C516-518 ☐ C518-520 ☐ C520-522 ☐ C522-524 ☐ C524-526 ☐ C526-528 ☐ C528-530 ☐ C530-532 ☐ C532-534 ☐ C534-536 ☐ C536-538 ☐ C538-540 ☐ C540-542 ☐ C542-544 ☐ C544-546 ☐ C546-548 ☐ C548-550 ☐ C550-552 ☐ C552-554 ☐ C554-556 ☐ C556-558 ☐ C558-560 ☐ C560-562 ☐ C562-564 ☐ C564-566 ☐ C566-568 ☐ C568-570 ☐ C570-572 ☐ 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C754-756 ☐ C756-758 ☐ C758-760 ☐ C760-762 ☐ C762-764 ☐ C764-766 ☐ C766-768 ☐ C768-770 ☐ C770-772 ☐ C772-774 ☐ C774-776 ☐ C776-778 ☐ C778-780 ☐ C780-782 ☐ C782-784 ☐ C784-786 ☐ C786-788 ☐ C788-790 ☐ C790-792 ☐ C792-794 ☐ C794-796 ☐ C796-798 ☐ C798-800 ☐ C800-802 ☐ C802-804 ☐ C804-806 ☐ C806-808 ☐ C808-810 ☐ C810-812 ☐ C812-814 ☐ C814-816 ☐ C816-818 ☐ C818-820 ☐ C820-822 ☐ C822-824 ☐ C824-826 ☐ C826-828 ☐ C828-830 ☐ C830-832 ☐ C832-834 ☐ C834-836 ☐ C836-838 ☐ C838-840 ☐ C840-842 ☐ C842-844 ☐ C844-846 ☐ C846-848 ☐ C848-850 ☐ C850-852 ☐ C852-854 ☐ C854-856 ☐ C856-858 ☐ C858-860 ☐ C860-862 ☐ C862-864 ☐ C864-866 ☐ C866-868 ☐ C868-870 ☐ C870-872 ☐ C872-874 ☐ C874-876 ☐ C876-878 ☐ C878-880 ☐ C880-882 ☐ C882-884 ☐ C884-886 ☐ C886-888 ☐ C888-890 ☐ C890-892 ☐ C892-894 ☐ C894-896 ☐ C896-898 ☐ C898-900 ☐ C900-902 ☐ C902-904 ☐ C904-906 ☐ C906-908 ☐ C908-910 ☐ C910-912 ☐ C912-914 ☐ C914-916 ☐ C916-918 ☐ C918-920 ☐ C920-922 ☐ C922-924 ☐ C924-926 ☐ C926-928 ☐ C928-930 ☐ C930-932 ☐ C932-934 ☐ C934-936 ☐ C936-938 ☐ C938-940 ☐ C940-942 ☐ C942-944 ☐ C944-946 ☐ C946-948 ☐ C948-950 ☐ C950-952 ☐ C952-954 ☐ C954-956 ☐ C956-958 ☐ C958-960 ☐ C960-962 ☐ C962-964 ☐ C964-966 ☐ C966-968 ☐ C968-970 ☐ C970-972 ☐ C972-974 ☐ C974-976 ☐ C976-978 ☐ C978-980 ☐ C980-982 ☐ C982-984 ☐ C984-986 ☐ C986-988 ☐ C988-990 ☐ C990-992 ☐ C992-994 ☐ C994-996 ☐ C996-998 ☐ C998-1000 ☐ C1000-1002 ☐ C1002-1004 ☐ C1004-1006 ☐ C1006-1008 ☐ C1008-1010 ☐ C1010-1012 ☐ C1012-1014 ☐ C1014-1016 ☐ C1016-1018 ☐ C1018-1020 ☐ C1020-1022 ☐ C1022-1024 ☐ C1024-1026 ☐ C1026-1028 ☐ C1028-1030 ☐ C1030-1032 ☐ C1032-1034 ☐ C1034-1036 ☐ C1036-1038 ☐ C1038-1040 ☐ C1040-1042 ☐ C1042-1044 ☐ C1044-1046 ☐ C1046-1048 ☐ C1048-1050 ☐ C1050-1052 ☐ C1052-1054 ☐ C1054-1056 ☐ C1056-1058 ☐ C1058-1060 ☐ C1060-1062 ☐ C1062-1064 ☐ C1064-1066 ☐ C1066-1068 ☐ C1068-1070 ☐ C1070-1072 ☐ C1072-1074 ☐ C1074-1076 ☐ C1076-1078 ☐ C1078-1080 ☐ C1080-1082 ☐ C1082-1084 ☐ C1084-1086 ☐ C1086-1088 ☐ C1088-1090 ☐ C1090-1092 ☐ C1092-1094 ☐ C1094-1096 ☐ C1096-1098 ☐ C1098-1100 ☐ C1100-1102 ☐ C1102-1104 ☐ C1104-1106 ☐ C1106-1108 ☐ C1108-1110 ☐ C1110-1112 ☐ C1112-1114 ☐ C1114-1116 ☐ C1116-1118 ☐ C1118-1120 ☐ C1120-1122 ☐ C1122-1124 ☐ C1124-1126 ☐ C1126-1128 ☐ C1128-1130 ☐ C1130-1132 ☐ C1132-1134 ☐ C1134-1136 ☐ C1136-1138 ☐ C1138-1140 ☐ C1140-1142 ☐ C1142-1144 ☐ C1144-1146 ☐ C1146-1148 ☐ C1148-1150 ☐ C1150-1152 ☐ C1152-1154 ☐ C1154-1156 ☐ C1156-1158 ☐ C1158-1160 ☐ C1160-1162 ☐ C1162-1164 ☐ C1164-1166 ☐ C1166-1168 ☐ C1168-1170 ☐ C1170-1172 ☐ C1172-1174 ☐ C1174-1176 ☐ C1176-1178 ☐ C1178-1180 ☐ C1180-1182 ☐ C1182-1184 ☐ C1184-1186 ☐ C1186-1188 ☐ C1188-1190 ☐ C1190-1192 ☐ C1192-1194 ☐ C1194-1196 ☐ C1196-1198 ☐ C1198-1200 ☐ C1200-1202 ☐ C1202-1204 ☐ C1204-1206 ☐ C1206-1208 ☐ C1208-1210 ☐ C1210-1212 ☐ C1212-1214 ☐ C1214-1216 ☐ C1216-1218 ☐ C1218-1220 ☐ C1220-1222 ☐ C1222-1224 ☐ C1224-1226 ☐ C1226-1228 ☐ C1228-1230 ☐ C1230-1232 ☐ C1232-1234 ☐ C1234-1236 ☐ C1236-1238 ☐ C1238-1240 ☐ C1240-1242 ☐ C1242-1244 ☐ C1244-1246 ☐ C1246-1248 ☐ C1248-1250 ☐ C1250-1252 ☐ C1252-1254 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