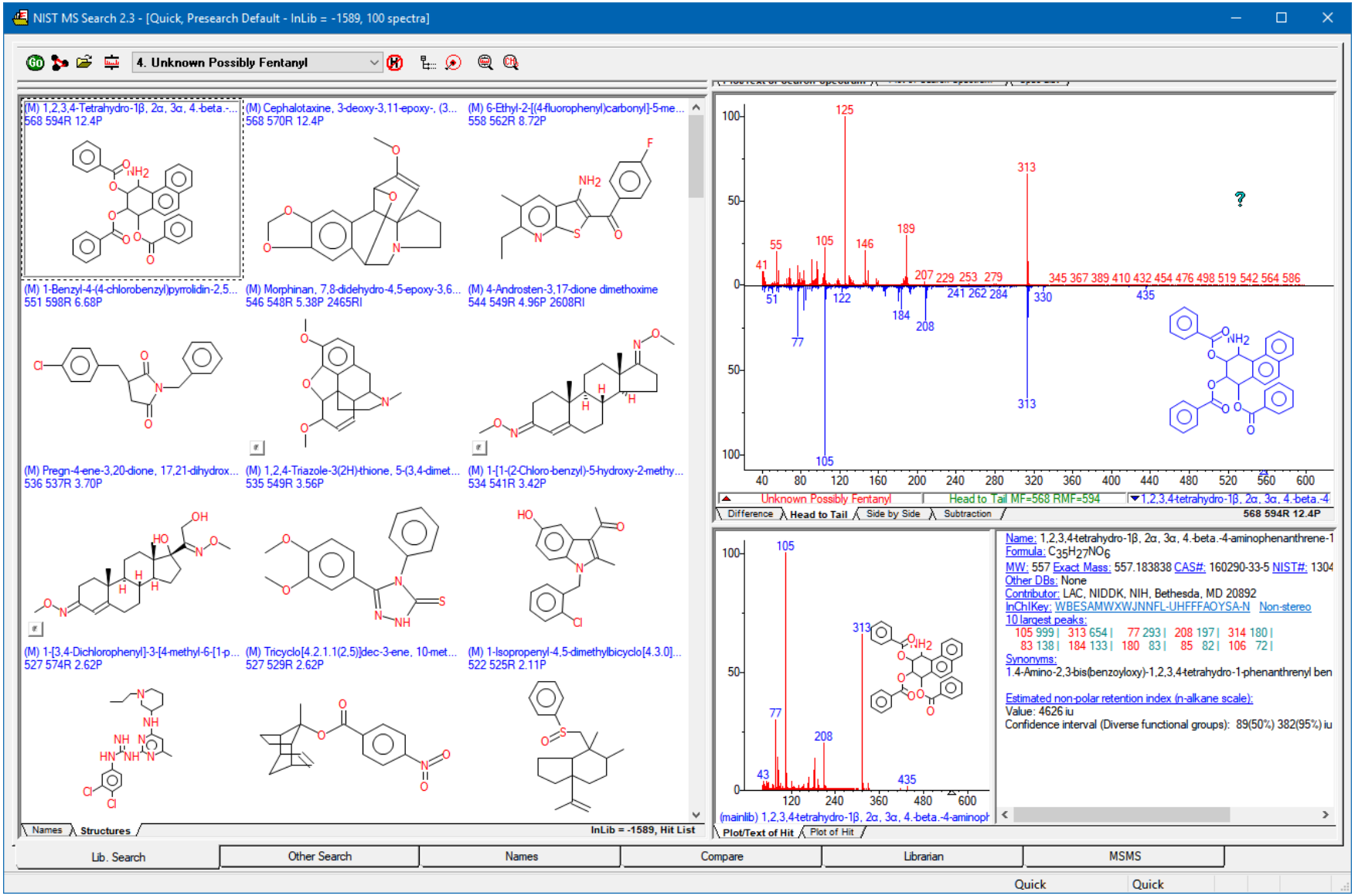
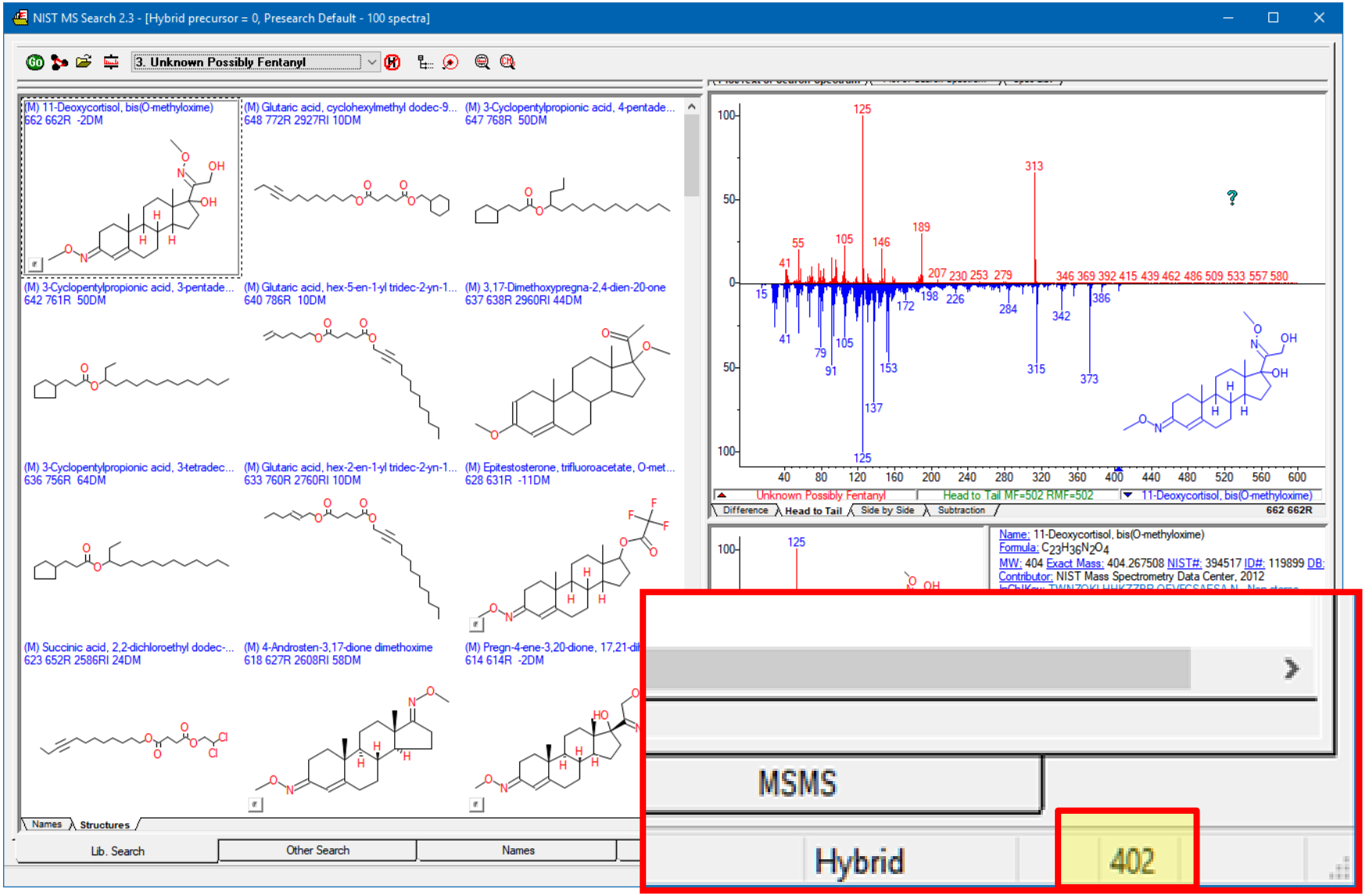
A compound suspected of being a Fentanyl

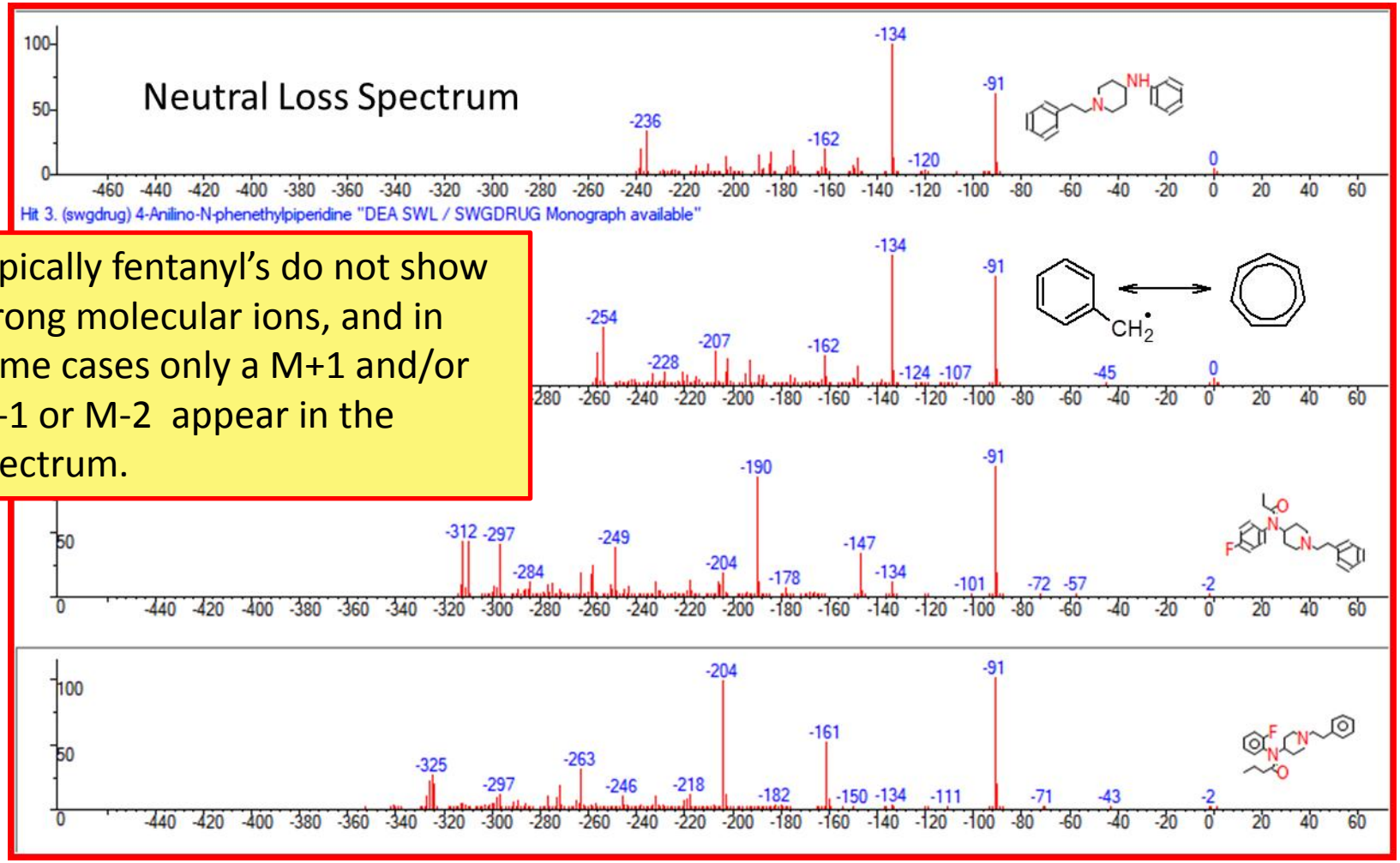
The search gives no hint – best MF 568 – no interesting substructures



If we do a hybrid search we do not get much more information



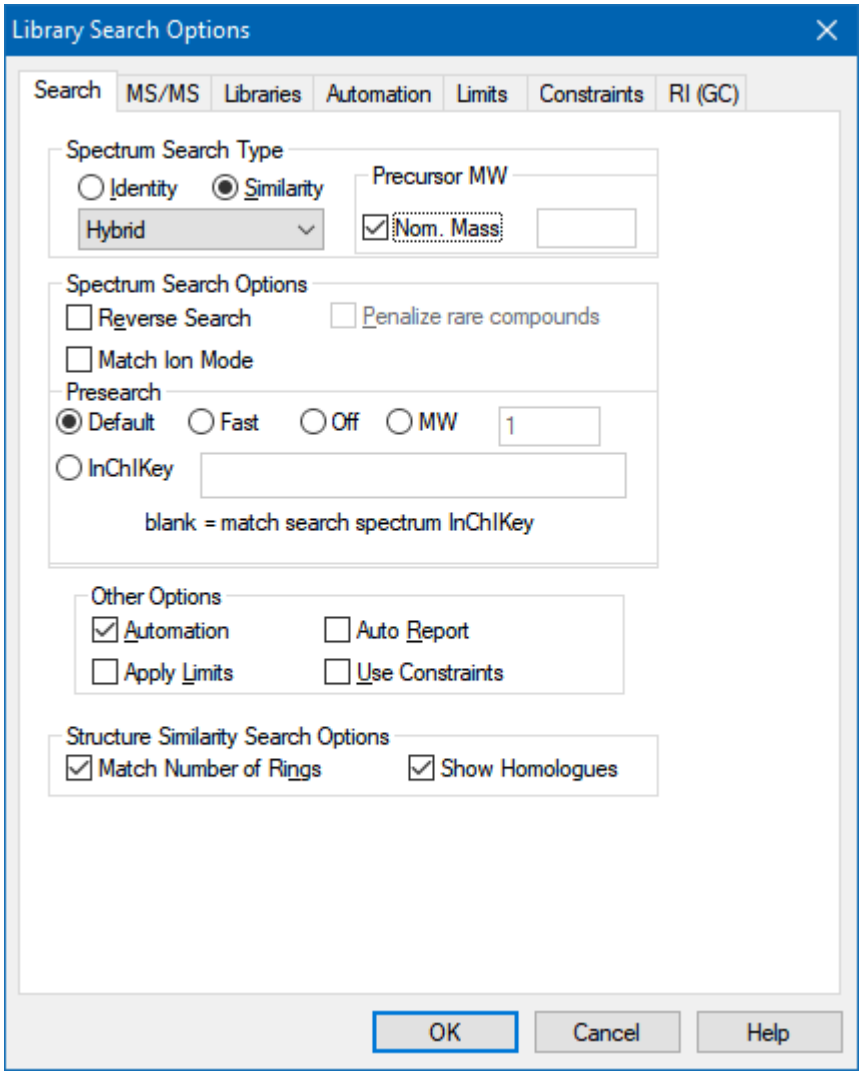
A very common (almost universal) neutral loss for fentanyl is the 91, so a good guess for a molecular ion is the highest mass major ion + 91



Typically fentanyl's do not show strong molecular ions, and in some cases only a M+1 and/or M-1 or M-2 appear in the spectrum.

With the highest mass of our unknown (313) the 91 neutral loss gives 404 (not 402) as M+

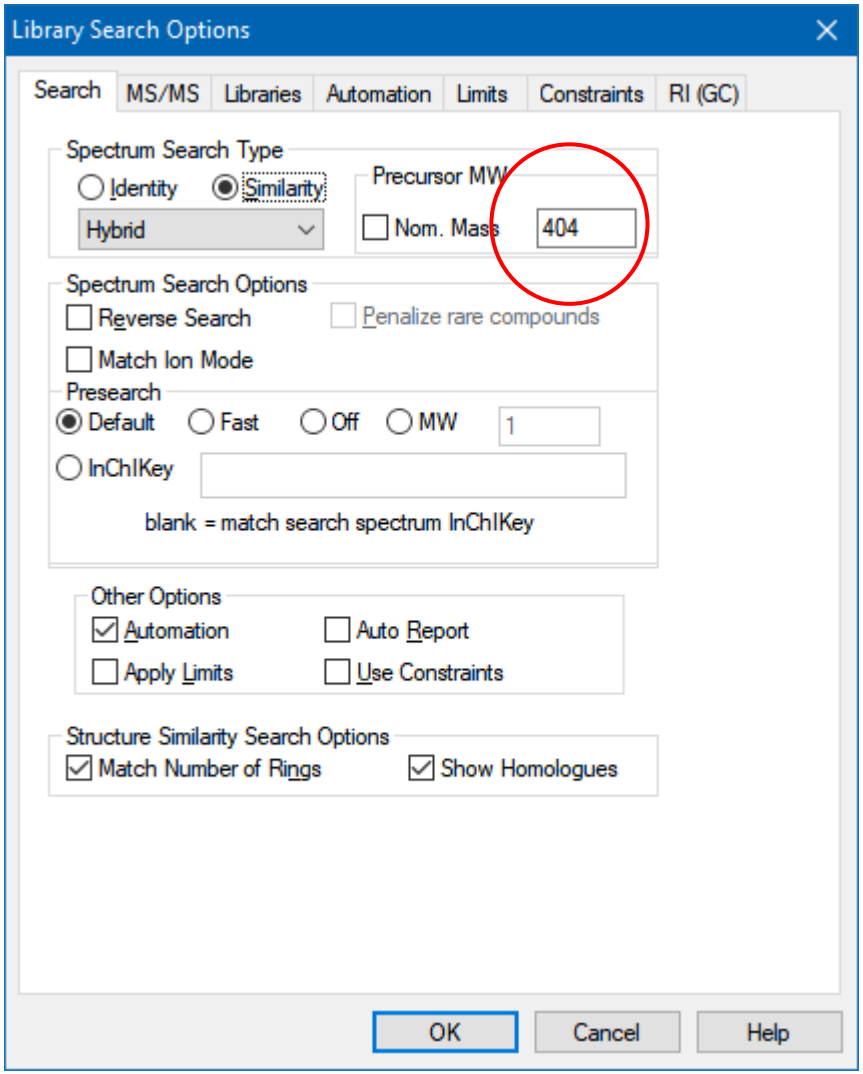
The default condition is to allow the program to estimate a molecular mass if it is not in the spectrum



This works for most unknown spectra, but it is not foolproof.

When it does not work the results do not show the common structural elements that are expected if the search is working.

The program's nominal mass calculation can be overridden.



Here we specify the molecular ion m/z value, here derived from the assumed loss of 91 from M+ to yield the large 313 peak..

With the M+ specified, the hybrid search yields a large number of fentanyls (all of the first 12 hits)