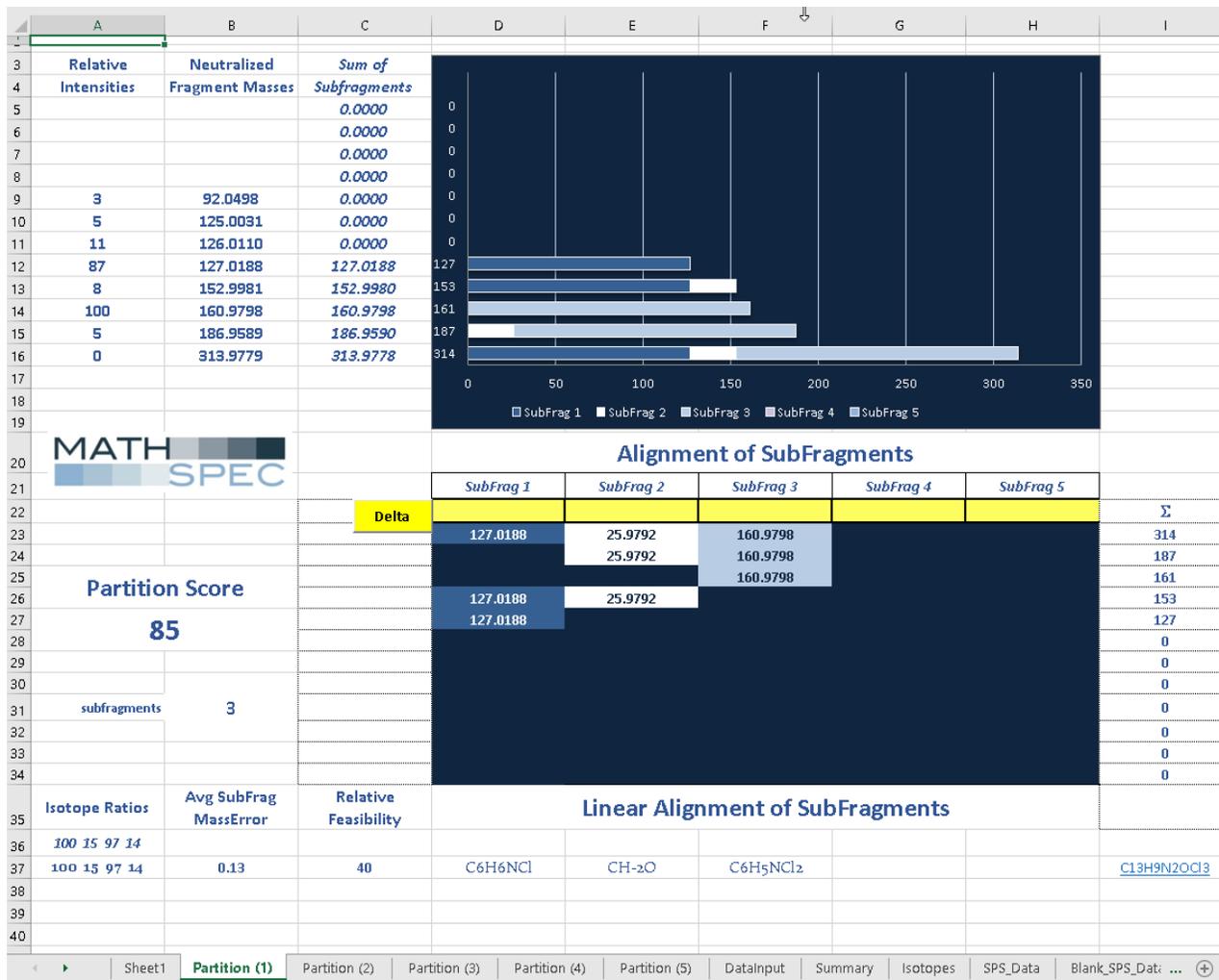An ms2 (MS/MS) spectrum of triclocarban (Massbank-EA298803) was analyzed with the Excel Add-In, using the default parameters except putting no limit on the number of fluorine atoms. The result for the first partition and highest scoring partition is shown below. (The complete set of partitions can be viewed here: **triclocarban example**).

The CH-2O subfragment looks strange at first glance. Keep in mind that subfragment formulas like CH-2O are not meant to denote real molecular entities, but rather represent a form of atomic bookkeeping. Subfragments with negative hydrogens represents a bridge between two other heteroatoms. The CH-2O is a carbonyl attached to two heteroatoms.
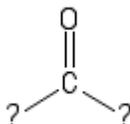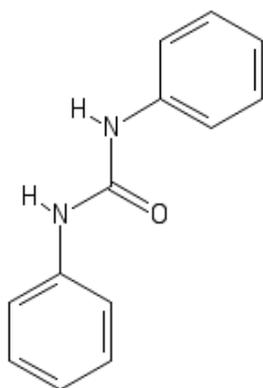
The formula for the whole molecule is found in cell I37, C13H9N2OCl3. Besides this carbonyl oxygen, the other heteroatoms are the three chlorines and the two nitrogens. Because chlorine atoms have only one connection possible, chlorines are always found in "outside" positions. This implies that the CH-2O must be connected on each side to a nitrogen atom. Now the substructure below can be drawn:
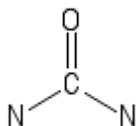
Since the CH-2O subfragment must have lost two hydrogen atoms relative to the corresponding substructure of the actual molecule and because the total number of hydrogens must balance, each of the other two subfragment formulas must have one more hydrogen than their corresponding substructures. For example, the C6H6NCl subfragment must correspond to a C6H5NCl substructure in the molecule.

The two remaining subfragments both have six carbons and 4 ring and double bond equivalents, using the RDBE() function. Most likely, these two are benzene rings with chlorine substituents. Neither one could be a pyridine ring because we know that these subfragments are attached at the nitrogen atom to the carbonyl.

Because we do not know where the chlorines are attached, for substructure searching we can just add them "in space". The substructure combination below was searched in Pubchem Compound:

The search of Pubchem Compound gave 1471 hits with this substructure. These 1471 compounds were then "pushed to Entrez". Next the formula for the whole molecule in cell I37, $C_{13}H_9N_2OCl_3$, was searched yielding a group of 424 compounds each having that molecular formula. Again, these results were pushed to Entrez.

Going to the advanced search builder in Entrez, we know that the compound must be the intersection of the two sets of compounds; basically we want to know which compounds were found in both searches. The intersection ("AND") had 25 compounds.

Lastly, we need to find, visually, all compounds where 2 chlorines are on one benzene ring and only one chlorine is on the other benzene ring, to be consistent with the benzene ring substructures from the Excel Add-In. Four of the compounds have three chlorines on one ring and no chlorine on the other and so these four compounds can be eliminated from consideration. There were also two isotopically labeled compounds which will have the same formula but the wrong accurate-mass. Nineteen compounds remained.

There are six possible arrangements of two chlorines on the one ring and three possible arrangements of the single chlorine on the other. Thus the maximum possible number of geometric isomers is 6 x 3 = 18. All 18 isomers are found in Pubchem. The extra compound was a duplicate structure of triclocarban. The remaining eighteen Pubchem CID numbers of compounds that were consistent with the data are shown below - along with the structure of triclocarban (CID: 7547) :

7547	898729
25784	2057290
294986	3367854
302779	4050201
352823	4335030
726151	4487707
742727	5087463
765417	5174981
853651	5174982