Trans Fats

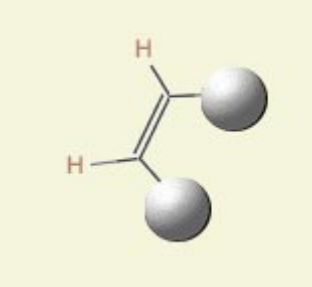
What is a trans fat? Trans fatty acids, or trans fats as they are known, are certain fats found in such foodstuffs as vegetable shortenings, margarines, crackers, candies baked goods and many more processed foods. Trans fats, as detrimental as they are for one's health, are surprisingly prolific in today's food market.

These trans fats have been proven to cause health problems. There has been a direct, proven relationship in diets that have high trans fat contents of high LDL levels (LDLs are Low Density Lipoproteins, or Bad Cholesterol. The good type of lipoproteins is HDL or High Density Lipoproteins.) If LDL levels are too high in a person's body, they will have higher cholesterol and subsequently will be more prone to coronary disease, which is a leading cause of death in the United States.

The reason that these foods have made such a noticeable impact in the United States is due to their purpose. Hydrogenated oils, or oils that have gone through a special process to produce a more solidified oil for texture resembling that of butter and having increased "spreadability", are able to be produced cheaply and effectively. The hydrogenation process is one in which a vegetable oil is reacted under pressure with hydrogen gas at about 250-400 degrees Fahrenheit for several hours in the presence of a catalyst such as nickel or platinum. This allows for many natural foods to be chemically converted into different compounds. One compound that made its away out of all this hydrogenation is the trans fat. Trans fats have double bonds on their molecules that are located in irregular and unnatural positions.

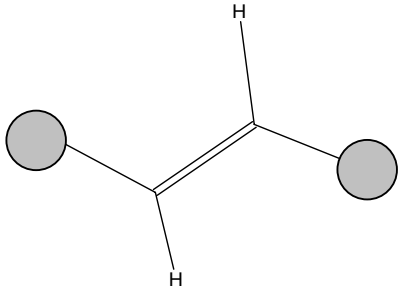
The two types of unsaturated fats that are available are the "cis" and "trans", both denoting the general location of the double bond in the fatty acid molecule. When atoms

are added to the same side of the double bond, the compound is called “cis” and the molecule is bent in an irregular shape due to this crowding of molecules.



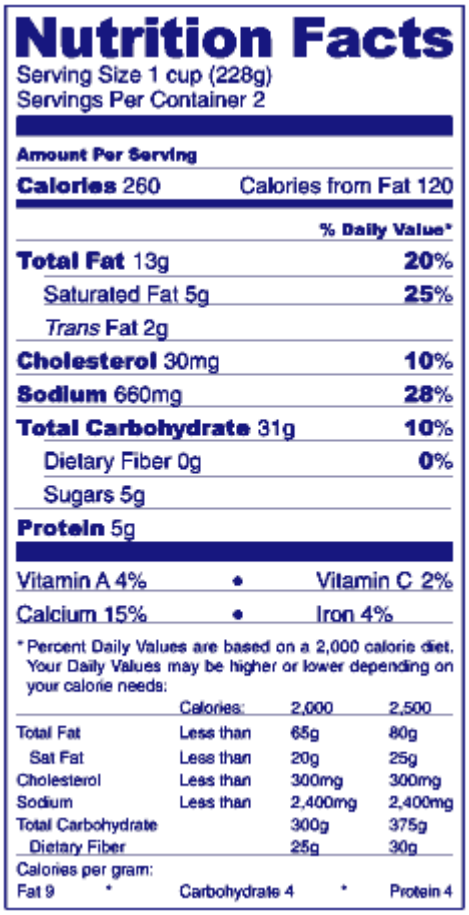
“Cis” molecule

The other type of trans fat is the “trans”. When a molecule is “trans” that means that the atoms are added to the opposite sides of the chain and it is subsequently less balanced than that of a “cis” molecule. Since the atoms are added to opposite sides of the molecule, a kink is made in the molecule offsetting its natural balance. Both setups of the molecules are different than they would be found in nature and for that reason react with peoples’ metabolisms differently while processing these molecules. The trans fats, when introduced in a diet, lower the HDL level in the body and raise the LDL, and for this reason, trans fats are extremely detrimental to one’s health.



“Trans” Molecule

Due to these health concerns, the FDA is requiring a nutrition label that specifies the trans fat content. This means that food companies have had to develop a standardized test for trans fat so they can properly label their products.



Nutrition Facts

Serving Size 1 cup (228g)
Servings Per Container 2

Amount Per Serving

Calories 260 Calories from Fat 120

	% Daily Value*
Total Fat 13g	**20%**
Saturated Fat 5g	**25%**
Trans **Fat** 2g	
Cholesterol 30mg	**10%**
Sodium 660mg	**28%**
Total Carbohydrate 31g	**10%**
Dietary Fiber 0g	**0%**
Sugars 5g	
Protein 5g	

Vitamin A 4% • Vitamin C 2%

Calcium 15% • Iron 4%

* Percent Daily Values are based on a 2,000 calorie diet. Your Daily Values may be higher or lower depending on your calorie needs:

	Calories:	2,000	2,500
Total Fat	Less than	65g	80g
Sat Fat	Less than	20g	25g
Cholesterol	Less than	300mg	300mg
Sodium	Less than	2,400mg	2,400mg
Total Carbohydrate		300g	375g
Dietary Fiber		25g	30g

Calories per gram:
Fat 9 * Carbohydrate 4 * Protein 4

Food Label containing Trans fat content

The test is a gas chromatography test (a temperature controlled oven with a “boiling tube” built into it.) We wanted to determine if NMR could be used to determine trans fat as a fast alternative to gas chromatography (which takes approximately 20-40 minutes to complete and requires calibration standards). NMR takes about one minute and needs no calibration making it faster and easier to test with than gas chromatography.

Nuclear Magnetic Resonance

Nuclear Magnetic Resonance, or NMR as it is commonly known, is the process through which the magnetized nucleus of a molecule, such as hydrogen-1 or carbon-13, is studied by aligning the magnetized nucleus using a strong electromagnetic field. The ways that these molecules respond to this magnetic disturbance or "perturbing" is the result in NMR and Magnetic Resonance Imaging (MRI). NMR spectroscopy allows people to get physical, chemical and electric information about any given molecule in solution. It is also the only technique that provides a three-dimensional model of the molecules that are being observed.

NMR was first discovered by Felix Bloch and Edward Mills Purcell, both of which worked separately and shared the Nobel Prize in physics in 1952 for this groundbreaking discovery. Bloch and Purcell both noticed through their studies that magnetized nuclei, such as H-1 and P-31, could absorb Radiofrequency energy (RF energy) when placed in a magnetic field of a certain strength. When perturbed by this magnetic field, the atoms are said to "resonate" and different molecules resonate at different frequencies. This allows scientists to classify and recognize the structure of a molecule based solely on its magnetic resonance.

NMR in the real world is used widely for medical diagnostics, but is also used for chemical studies. In observing the ways that the molecules interact with each other, one is able to discern what kind of molecule it is. A hydrogen bonded to an oxygen, for example will react differently than a hydrogen bonded to a carbon. These interactions all produce different peaks on a graph, which tell chemists what the structure really is. NMR is also

extremely useful for observing a compound without destroying it. Radio waves and static magnetic fields can penetrate many types of matter and many things that are not ferromagnetic (high magnetic permeability) with relative ease. DNA, RNA and other nucleic acids can be easily studied through NMR before any destructive observational experiments. Apart from saving the sample, NMR also helps scientists to analyze dangerous samples without putting themselves into harm's way. NMR, as it can be seen, is a very effective technique for studying chemical samples.

Experimental

The NMR instrument was a Varian 300 MHz superconducting NMR spectrometer operating at 299.96 MHz for 1H and 75.63 MHz for 13C. The samples were dissolved in CDCl3 for the 1H experiments and CDCl3-CrAcAc in the 13C experiments. CrAcAc is a paramagnetic relaxation agent that reduces 13C relaxation times and facilitates quantitative 13C data. 1H NMR was acquired with a 3.6 s acquisition time and a 2 second relaxation delay. The 13C NMR was acquired with a 45 degree tip angle, a 1.3 second acquisition, a 1 second relaxation delay and 1H high power decoupling was applied during the acquisition to remove 1H-13C coupling. The data was Fourier Transformed, phased, referenced, and integral binned with the following parameters: 1H spectra binned at 0.1 ppm intervals from 12 to -2 ppm, 13C spectra binned at 1 ppm intervals from 220 to -20 ppm excluding the CDCl3 region of the spectrum (79-75 ppm). All binned data was normalized to 100 for 1H and 1000 for 13C. The data was associated with the fat chemical data (MONO, PolyUn, Trans, SAFA) and regressed in Galactic Grams PLS/IQ chemometric software utilizing internal prediction and PLS-1 algorithms.

Results

^{1}H		
Parameter	R^2	Error wt%
Trans Fat	0.996	0.95
Monounsaturated Fat	0.985	2.52
Saturated Fat	0.997	1.5
Polyunsaturated Fat	0.999	0.32

^{13}C		
Parameter	R^2	Error wt%
Trans Fat	0.994	1.68
Monounsaturated Fat	0.996	1.88
Saturated Fat	0.996	2.2
Polyunsaturated Fat	0.997	0.77

Discussion

For the experiment, we took 14 samples of trans fats and put them through the NMR machine. Using the data that we got, we were able to figure out how much total fat, polyunsaturated fat and monounsaturated fat there was in the sample. By observing the changes in peak intensity on each of the spectra, we were able to get this information. We then took the information that we collected and compared it to the information that was provided to us (by the American Oil Chemists Society or AOCS, who sent us the samples) and calculated the correlation (R^2 value) and our percent error. All the samples in the dataset were readily modeled. This process also allows outliers (samples that were so off in value by a large enough margin that it can be determined that the lab value is wrong or something wrong with the spectrum and the data can be ignored) to be identified if present. We were quite close in our tests. Most of our results were 96% to almost 100% correct, so it can be inferred that we did quite well and were quite accurate in our tests.

Conclusion

The calibrations developed by both ^{1}H and ^{13}C NMR showed an accuracy that was equal to the accuracy of the GC lab data that was used to correlate with the NMR data – in fact, the ^{1}H results were a factor of 2 better for trans, SAFA and PUFA tests than the ^{13}C NMR. As both techniques worked well, it would be advantageous to utilize the ^{1}H NMR as a quick screening method as ^{1}H NMR takes 1 minute to get a spectrum while ^{13}C takes 20 to 30 minutes.

All of our results were consistent and the inconsistencies can be blamed on minor natural problems (such as minor perturbances and issues while acquiring the signal) or preparation issues on our part. Despite this, our data was quite accurate and came out better than I would ever have expected it to.