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Role of Forensic Chemistry and Analytical Intrumentation in the Identification of Designer Drugs

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Role of Forensic Chemistry and Analytical Instrumentation in the Identification of Designer Drugs

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This thesis describes the overall issues that designer drugs are causing in society today. There are three main types of structural differences between designer drugs and the parent drug they are created from. The substances can be direct or indirect regioisomers with the same atomic components as the parent drug or isobaric compounds containing different atomic components than the parent drug. These substances are slowly becoming classified as stimulants, sedatives, dissociative, psychedelics, or synthetic cannabinoids, and scheduled into one of the classes set in place by the Controlled Substances Act of 1970, appropriately once enough information is known about them. Many different instrumentation techniques can be used to help identify these designer drugs and assist with the process of relating them to a specific designer drug family. Some of the most important forensic instruments for this identification process include Gas Chromatography, Mass Spectrometry, and Fourier Transform Infrared Spectroscopy. Overall, these designer drugs need to be analyzed and researched more in order to put proper polices into place to ultimately save the lives of many.

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Over the years within the Forensic Chemistry field there have been major advancement with the technology and instrumentation used to analyze evidence and different compounds. Some of the major compounds that forensic drug chemists analyze in the laboratory include designer drugs, which are normally derivatives, or analogs, of pre-existing drugs where their chemical structure becomes altered by chemical processes. Designer drugs can also have a different structure than any pre-existing drug but produce the same mind-altering effects as a pre-existing drug. The chemical processes make it so that natural drug substances that come from plants and animals are less popular because these synthetic drug substances, that are created within a laboratory, have stronger, more potent, effects on the human body (1). Many synthetically made drugs have a lot of changes made to their structure or structural orientation of substituents in order to create these derivatives which can make it very difficult for the forensic chemists working in the laboratories to identify these newly formed drugs quickly. Without knowing the drug's chemical structure, it can be difficult to know to effects it will cause to the human body. These new designer drugs are being created in order to bypass existing drug laws, like the Controlled Substance Act of 1970 that created a system where drugs were placed into one of five different scheduled levels (2). Schedule I drugs have a very high potential for

abuse and are not acceptable to be prescribed for medical use. Schedule II drugs have a slightly lower potential for abuse and are very rarely prescribed for medical purposes. Schedule III drugs have an intermediate potential for abuse and are more commonly used for medical purposes. Schedule IV drugs have a very low potential for abuse and are prescribed very often for medical uses. Schedule V drugs have the lowest potential for abuse and are most commonly prescribed for medical purposes (2). By creating drugs with no restrictions on them, these drugs become a legal way for people to get high (1). Designer drugs are created in clandestine laboratories, which can be defined by the US Department of Justice (3) as, "An [illegal] operation consisting of a sufficient combination of [equipment] and chemicals that either has been or could be used in the synthesis of [illicit] substances." The illicit substances mentioned are what can be classified as designer dugs.

The types of derivatives that are being created of these drugs include direct regioisomers, indirect regioisomers, and isobaric compounds. Direct regioisomers differ from the original compound by having a different arrangement of the substituents connected to the main structure, but they have the same exact mass as the original compound. Indirect regioisomers differ from the original structure by having a different structural arrangement of the molecules, and they also will have the same exact mass of the original compound. Unlike direct and indirect regioisomers, isobaric compounds have a different atomic composition from the original drug, which results in a differing exact mass from the original compound. Examples of these different derivatives can be seen in **Figure 1**. The top two compounds in this figure can be identified as direct regioisomers because the methyl group moved from being in an ortho-arrangement meta-arrangement

on the aromatic ring. The middle two compounds can be identified as indirect regioisomers because the methyl group in this structure goes from being attached to the Oxygen of one substituent to being connected directly to the aromatic ring. The bottom two compounds shown in this figure can be identified as being isobaric compounds because the atomic composition is different between the two structures. The original drug shown on the right has one methyl group substituent and one methoxy group so overall this compound only contains one Oxygen atom. The isobaric compound differs atomically from the original compound because instead of the two substituents mentioned, this compound contains a methylenedioxy group so overall this compound contains two Oxygen atoms.

Although there is an increasing amount of designer drugs being created by altering other substance's chemical structure, it is also important to realize that not all of the possible derivatives within one drug family are possible drugs of abuse. Some of the derivatives of these substances are inactive derivatives, substances that will not be used for abusive purposes because they lack the structural properties that would cause them to be abusable. Every drug family contains some substances with a specific chemical structure that causes them to be these inactive derivatives. It is very important for forensic chemists to know the differences between abusable derivatives within a drug family and the inactive derivatives that may be used for other chemical purposes. A proper process needs to be put into place to differentiate between the different types of substances so that no chemists run into trouble when using the inactive derivatives of these substances for purposes within the lab just because they could be mistaken for an

active abusable substance. The different types of forensic instrumentation can be used to identify the structure of questioned samples to help with this differentiation process.

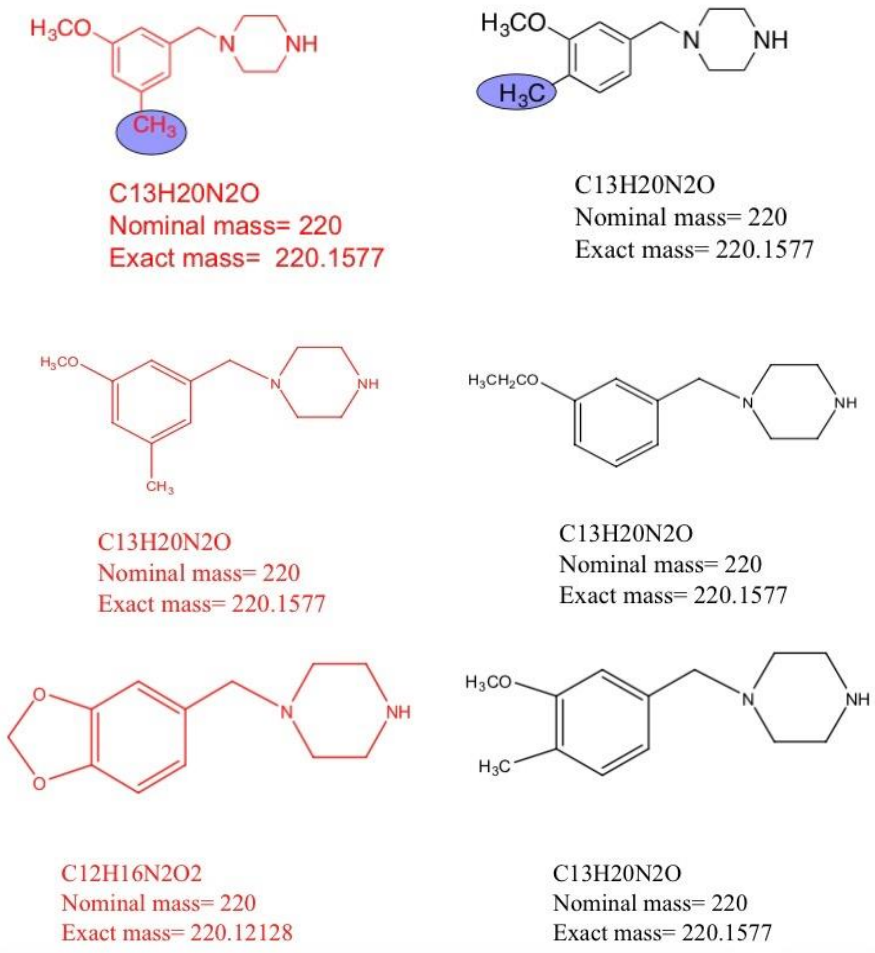


Figure 1: Examples of direct regioisomers, indirect regioisomers, and isobaric compounds (4).

It is very important to recognize that the amount of newly created designer drugs is increasing rapidly at a rate that makes it very difficult for police officers, forensic chemists, medical professional, and the public to keep up with all the new information that is being done to identify and classify these compounds. Many different groups of scientists are working on the identification and classification processes for these drugs so staying up to date on the new research and working well together is very crucial for all

the workers mentioned (5). The different types of designer drugs will produce different types of effects on the human body depending on how they interact with the brain and the body. Many new substances that have similar effects as already existing drugs of abuse will also follow to same biochemical interactions with the human body (6). The constant repeat of abuse of these substances will cause a person to develop a dependance on the euphoric effects.

One classification of these drugs is a stimulant substance, which is normally one of the most widely used type of substance. Stimulants will boost the happiness within a person by interacting with the monoamine transporters in the body and effecting the levels of norepinephrine, dopamine, and serotonin, by increasing them significantly (6). Many normal body functions and a person's mood will be altered if this type of drug is abused. Quite a lot of the different drug families are classified as stimulant substances.

Another classification of designer drug is a sedative substance, medically these are prescribed as pain medication. Sedative substances will relieve people by calming them down, reducing anxiety and creating a euphoric feeling. These substances will bind to the opioid receptors in the brain to cause the effects mentioned (6). There are not as many sedative type substances as there are stimulant substances.

Synthetic cannabinoids have their own classification type when discussing designer drugs. These drugs are very similar to sedative substances because they produce the same effects, however these with interact with the CB_1 and CB_2 receptors in the body (6). This is the largest classification type of designer drugs, containing the most compounds with differing structural components.

One other classification of these substances are ones that create psychedelic effects, and sometimes these were used by religious groups or for people to relax. These substances interact with the 5-HT_{2A} and 5-HT_{2C} receptors to produce their effects in the human body (6). This is a smaller classification type since there is not a large number of psychedelic drugs.

One last classification of designer drugs is the dissociative substances; these substances have very distinctive effects on the human body. An individual will not feel any pain when under the influence of this drug, and these can also be used as a fast-acting anti-depressant substitute. Dissociative substances will interact with the ionotropic glutamatergic NMDA receptors in the body (6). It is very helpful to know which classification each new drug belongs to, but normally the structural components of the sample in question must be identified first, which is completed by using proper analytical instrumentation within the forensic chemistry labs.

There are many different instruments found within a forensic chemistry laboratory that aid in the process of identifying these designer drugs. As the instrumentation used to identify these drugs has improved of the years, the scientists have been able to identify some types of these designer drugs more quickly. It can still be quite difficult to identify the isobaric drug compounds because they do not have a chemical structure that is similar to any pre-existing drugs. Some of the most important forensic instruments that are used to successfully identify designer drugs include Gas Chromatography (GC), Mass Spectrometry (MS), Fourier-Transform Infrared Spectroscopy (FTIR), Liquid Chromatography (LC), Direct Analysis in Real Time (DART), and Nuclear Magnetic Resonance (NMR). These instruments can be used by themselves for an identification

process, or some instruments can be paired together in order to get as much information as possible about the drugs throughout the identification process. Each of the formerly mentioned instruments are used to identify different aspects of compounds, and it is important when forensic chemists do not have any information on a brand-new designer drug that they use all the instrumentation they have at their disposal to gain as much information as quickly as possible. Using these different processes will also help a chemist come to a widely accepted conclusion. If multiple instruments or other analytical tests are used to identify the drug in question. The guidelines that need to be followed to make a clear decision on a drugs identity can be found within the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG). Each of the different instruments and tests are separated into three categories A, B, and C, and only the use of multiple uncorrelated processes will positively confirm the determined identity of the drug in question. If a category A process is used during analysis, then only one other process from any of the categories is required to confirm the results, but if a category A test is not used during the analysis, then three instruments or techniques must be used to confirm the results (7). Ultimately, advancements in forensic instrumentation and technology are improving the speed at which new designer drugs are being identified and scheduled, which will lead to better polices and enforcements, as well as saving lives.

A Gas Chromatography instrument is a category B analytical technique. This process will take a liquid sample, usually created from dissolving the solid compound within a solvent and heat it while it goes through the instrument for the analysis. The sample will become separated into all its molecular components which will be displayed on a chromatogram showing a peak for each compound along with the time it took for it to

elute from the instrument. An example chromatogram can be seen in **Figure 2**. In this chromatogram each peak is representative of a designer drug from the Cathinone family each with a different arrangement of one substituent group between the a and b compounds, and a one carbon difference, added to the side chain, between compounds 1, 2, and 3. This figure shows how this instrument can distinguish between regioisomeric compounds as well as isobaric compounds because each compound within the mixture will elute from the sample at a different time, even when the changes are miniscule. This instrument is largely used for samples that have a mixture of compounds within them because it will separate them and give the identity of all of the compounds within the sample. Two forensic instruments that can be used alongside the Gas Chromatographer are a Mass Spectrometer and a Fourier-Transform Infrared Spectrometer.

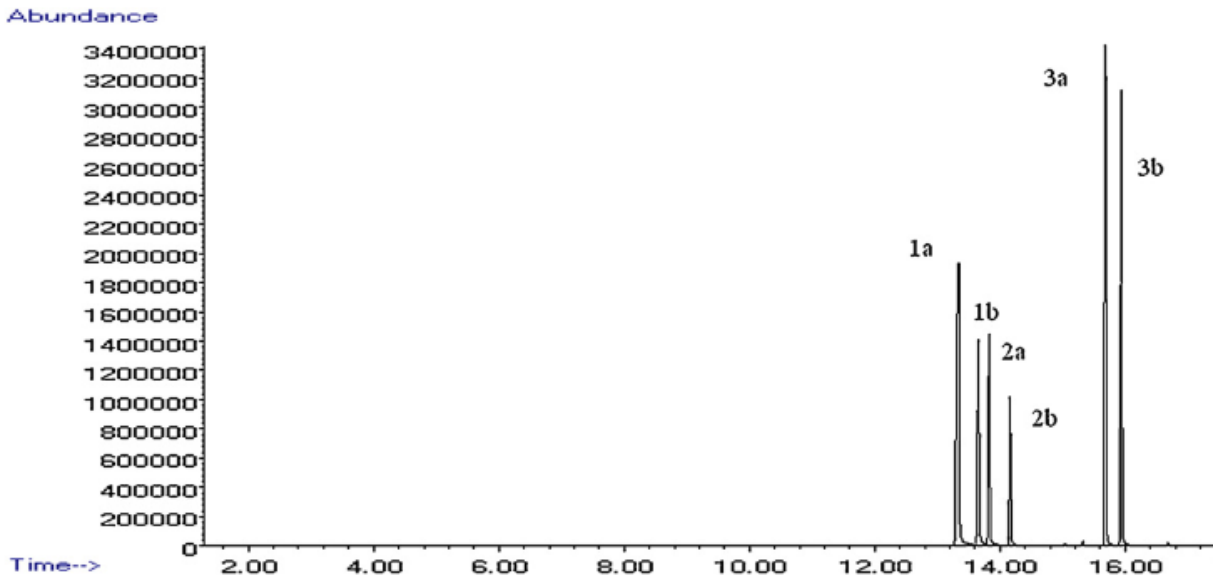


Figure 2: A Gas Chromatogram showing the different elution times between regioisomers, structures a and b, and isobaric compounds, structures 1, 2, and 3 (10).

A Mass Spectrometry instrument is a category A analytical technique. This process will take a sample and break it down into the main structural groups located within the

compound. This process occurs by having the sample travel through a section of the instrument that will electrically charge the compound to create fragmented ions, charged particles. These fragmented ions will then travel through the mass analyzer part of the instrument where they will be separated based on their charge to mass ratio, or their m/z value. The output data for this type of instrument is called a mass spectrum and it will show peaks at specific m/z values for fragmentations of the original compound and the peak height is based on how abundant that fragment is for that compound. An example mass spectrum can be seen in **Figure 3**. This mass spectrum is representative of the compound 2-Ethylenecathinone, also a part of the cathinone family like the compounds discussed on the gas chromatogram. The peaks on this spectrum represent the ways in which this structure can fragment to create ions. The more abundant the peak, the more likely that type of fragmentation will occur much like the peak at the 72 m/z value; the arrows on the structure show where this compound will break apart to create this ion. The process of mass spectrometry is one of the most used during the identification of designer drugs because it will give the fragmentation patterns of the compound based on its structure, as well as the exact mass of the compound in question. Mass spectrometers are very equipped to be used alongside many other forensic instruments and other analysis processes such as mass defect filtering (8). Mass Defect Filtering is a process that is completed after a sample has been ran on the Mass Spectrometer where the structural similarities and differences between the drug in question and other types of known substances are compared using a library system. **Figure 4** shows an example of how Mass Defect Filtering can be used to match compounds in question to the drug family they belong to, in this case completely synthetic cannabinoids. In this figure the diagram

shows a popular abusable designer drug JWH-018 and compounds with identical structures to this drug except the addition or subtraction of on methyl group, CH_3 group, within the alkyl side chain. Because the difference between these derivatives and the original drug is the addition or subtraction of such a small component, then the mass does not change that significantly and ultimately the structures of these two derivatives is almost unnotably different. Using this process has shown to be a very effective method because it compares the sample and the library results by their structural components and their exact atomic mass. This process can be used to identify which of the main drug families the sample would most likely belongs to, or it can at least give a more reasonable starting place to where it may belong if it is an isobaric compound based on the central structural components.

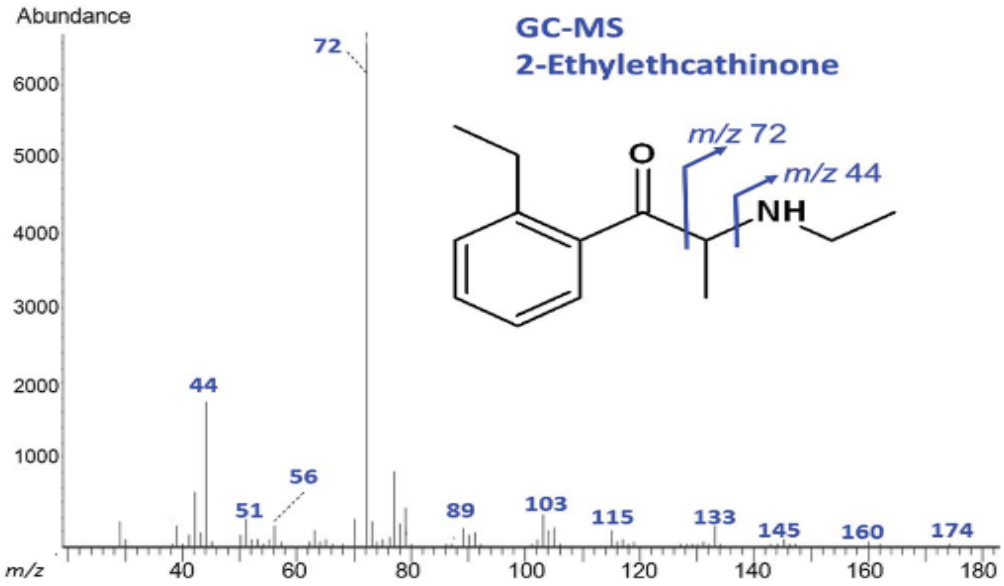


Figure 3: Mass spectrum of a drug within the cathinone family with its most abundant fragments (9).

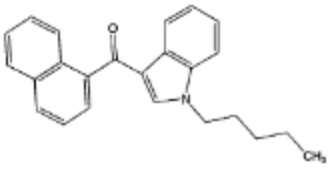
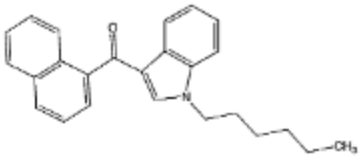
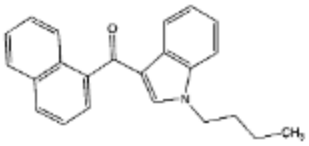
JWH-018		341.17796	0.00000	0.0	N/A
JWH-019		355.19361	14.01565	15.7	+ methyl
JWH-073		327.16231	-14.01565	-15.7	- methyl

Figure 4: Diagram of the Mass Defect Filtering process of cannabinoid compounds (8).

Fourier-Transform Infrared Spectroscopy is a category A analytical technique. This instrument will send infrared light waves towards a sample, some of which will be absorbed by the sample, but the infrared waves that pass through the sample are the ones detected by the instrument. The output data for this process is an Infrared spectrum which will show a unique fingerprint for every sample. An example Infrared spectrum can be seen in **Figure 5**. This spectrum shows another drug compound within the cathinone family. Each peak represented on this spectrum is specific for each molecular group within this compound. The peaks within the 400-1500 cm^{-1} wavelength range can help differentiate between regioisomers because they are very specific for only that compound's arrangement of atoms. This information can give some insight into the possible chemical structure of the compound. The Infrared spectrum of the compound in question can also be compared against library match results of compounds with similar structures and a percentage of how likely the two spectra match will be given as well. Finding out the possible structural matches to the compound in question can be crucial

information when dealing with identifying designer drugs and when looking at multiple drugs within the same family with slight structural changes.

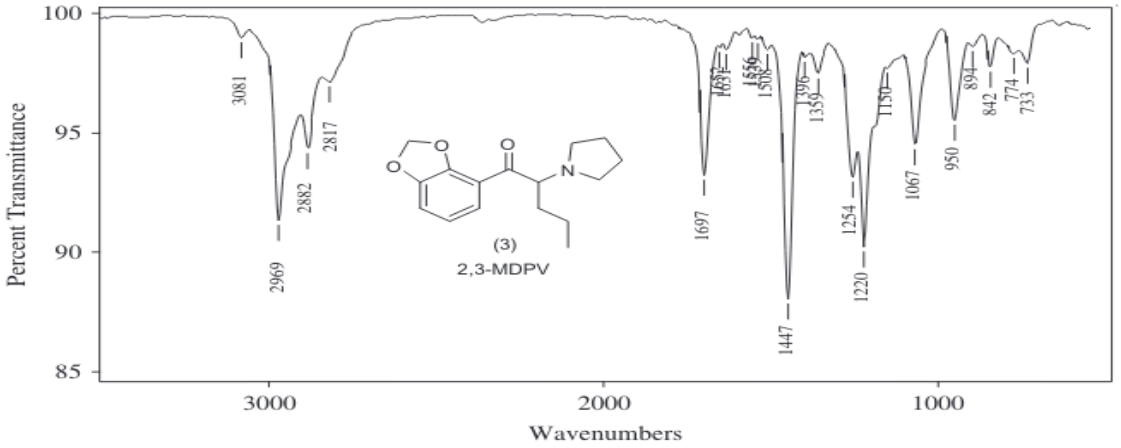


Figure 5: An Infrared spectrum of a cathinone substance (10).

Liquid Chromatography is a category B analytical technique. This instrument is a separation technique much like the Gas Chromatography technique, however Liquid Chromatography is not as sensitive of a technique as Gas Chromatography (11). This process can be beneficial for any compounds that have heat sensitivity. This process uses a liquid sample and by using a large amount of pressure and other solvents, the compound is able to be separated into its molecular components. One type of Liquid Chromatography is High Performance Liquid Chromatography which is a very precise and sensitive process. Liquid Chromatography is also largely used to separate mixtures into their individual molecular components. The output data from this instrument will also be shown on a chromatogram where each peak will represent a compound from within the sample as well as information about its elution time from the instrument. A chromatogram from this instrument would look very similar to a chromatogram from a Gas Chromatographer. The Liquid chromatographer can be connected to a mass

spectrometer to allow for the analysis process to provide data from both instruments and can be used for the same analysis process as a Gas Chromatographer-Mass Spectrometer.

Direct Analysis in Real Time is an ambient instrument that is usually paired with a Time-of-Flight Mass Spectrometer (9). This type of instrument can be used directly in the field when an unknown substance is collected from a scene. This process can be used in place of Gas Chromatography-Mass Spectrometry or Liquid Chromatography-Mass Spectroscopy (12). This instrument pairs well with a Mass Spectrometer because it is also a technique where the atoms of the sample become charged particles, ions, to be analyzed. The output data from this instrument will be shown on a spectrum similarly as well and each peak will represent a fragment of the structure in question. This instrument was used to analyze a mixture of drugs and all the results were accurate when the compounds need to be differentiated form one another. These results were comparable to results from a Gas Chromatogram-Mass Spectrometer but were more easily obtained with absolutely no preparations made to the samples before they were ran through the instrument (9).

Nuclear Magnetic Resonance Spectroscopy is a category A analytical technique. This is used to determine the exact chemical structure of an unknown sample (13). This type of spectroscopy will normally be used after the sample has already been ran on other forensic instruments in the lab like Gas Chromatography-Mass Spectrometry. Similar to the Mass Spectrometer, Nuclear Magnetic Resonance Spectroscopy will break the sample down into fragmented sections, but this instrument will be able to determine the exact chemical structure of the sample in question. A spectrum from this type of instrument can be seen in **Figure 6**. This spectrum is representative of a synthetic cannabinoid

compound. On this spectrum every peak is labeled and corresponds to a specific part of the structure showing just how accurate the process is in identifying the exact chemical structure for samples. This process has been proven to work significantly well when identifying the aromatic substituents as well as other aliphatic compounds (13).

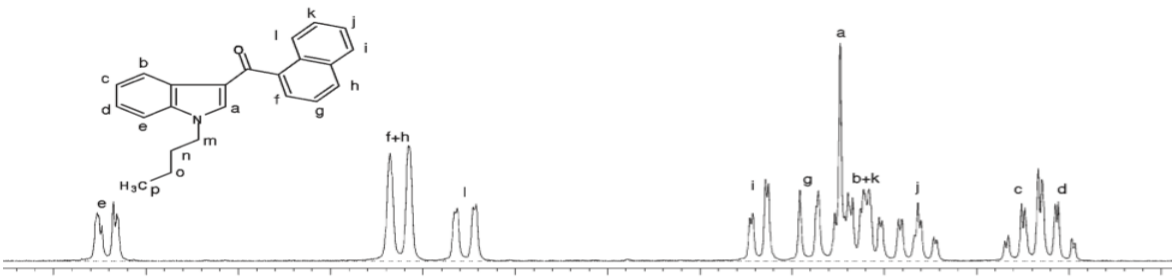


Figure 6: A Nuclear Magnetic resonance spectrum of a fully synthetic cannabinoid compound (13).

Out of all the forensic instruments mentioned so far, the Gas Chromatography-Mass Spectrometry combination of instruments is used the most often when determining the structure of the unknown substances when they are tested by the labs to see if they are designer drugs. The process of using these instruments will allow the chemists to have a better understanding of the number of compounds within the sample and the structure of each compound found. Another way of looking at it, is that this process will tell the chemists the DNA structure of the drug in question. The chromatogram obtained would have a peak on it for every compound within the structure. Each peak would then have a specific mass spectrum that correlates to it to give the overall structure of that particular compound within the sample.

Because there is such a large demand for these types of substances, there is an abundance of designer drugs that are on the streets today and the market for them keeps growing and so many more are made every day. While these designer drugs are not just normal drugs of abuse, they do normally originate from one type of drug of abuse and

become synthetically altered to have a different structure or become a derivative of the original structure. Because of this, designer drugs can be classified as being related to many of the abusable drug families. Some of the main abusable drug families include Cathinones, Cannabinoids, Amphetamines, Opioids, and of course there are many more. Once chemists identify the chemical structure of the samples they are testing in the labs, they can more easily classify which drug family they might belong to which can help know what type of effects they will have on the human body.

The cathinone family contains some drugs that were widely used for medical purposes until the addictive properties of these drugs were discovered then they were classified as Schedule I stimulant compounds (2)(6). The abusable substances within the Cathinone family are more widely known as bath salts. Cathinone drugs are normally created from naturally occurring substances, but the bath salt derivatives have synthetically altered chemical structures turning them into designer drugs. Another popular designer drug within the cathinone family is MDPV, methylenedioxypyrovalerone, MDPV is a very popular designer drug because it is easily purchased on the internet and will produce similar effects to another widely abused drug ecstasy (14). There are three distinct regions within the cathinone chemical structure where structural changes can be made to make the possible derivatives. These three regions are on the aromatic ring, differing lengths of the alkyl side chain, and within the amino group (10). The inactive derivatives within this family have no alkyl side chain group within their structure (15). **Figure 7** highlights the parts of this drugs structure where changes are made for each derivative. The aromatic ring can be seen circled in blue, the alkyl side chain can be seen circled in red and the amino group can be seen circled in black. The instruments that have been able

to accurately identify these types of drug compounds include Gas Chromatography-Mass Spectrometry, Liquid Chromatography-Mass Spectrometry, Fourier Transform Infrared Spectroscopy, and Nuclear Magnetic Resonance Spectroscopy (10)(13)(14)(16).

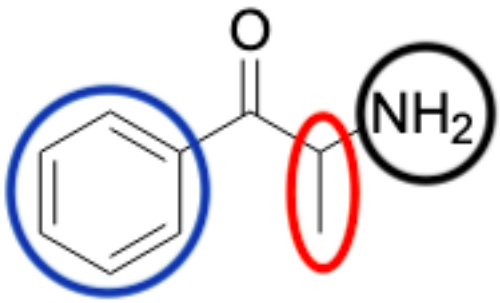


Figure 7: A cathinone structure labeled at the places where changes are made within the structure for derivative compounds.

The Cannabinoid family is very similar to the Cathinone family because it is also normally a naturally occurring substance, cannabis, but can be modified structurally into a designer drug. Cannabinoids will produce more potent effects on the human body than normal cannabis would produce and, a large number of recently identified cannabinoid derivatives have been classified as Schedule I drugs (8)(17). The derivatives within this family can be broken down into three categories: psychoactive, active but not psychoactive, and inactive, and interestingly there are more inactive derivatives than active derivatives within this family (18). Psychoactive drugs will cause psychological and behavioral effects and can be abusive. Substances that are active but not psychoactive will cause some effects to the human body but are not abusive. Like mentioned previously, inactive substances will have no abusable effect on the human body. The most psychoactive derivative in the cannabinoid family is the delta 9-tetrahydrocannabinol and structurally this compound only differs from an inactive

derivative by one oxygen atom (18). Another very popular designer drug within this family, that has recently been classified as a synthetic cannabinoid, scheduled, and made illegal, is JWH-018, more widely known as spice (6)(17). This drug is a fully synthetic compound and although this original compound is now scheduled and considered an illegal substance, there have been a large number of compounds created by changing small aspects to this drugs structure (8). These cannabinoid compounds will be mislabeled and discretely sold as incense or a type of smokable herbs to not get recognized by anyone in law enforcement (19). The main instruments that have been used in the forensic chemistry labs to identify the structures of cannabinoid derivates include Gas-Chromatography-Mass Spectrometry, Liquid Chromatography-Mass Spectrometry with Mass Defect Filtering, Nuclear Magnetic Resonance, and Gas Chromatography-Infrared Analysis (8)(17)(14).

The amphetamine family of drugs are used as stimulants on the Central Nervous System in the human body. The most popular designer drug derivative within this family is methamphetamine. The only structural difference between amphetamine and methamphetamine is the addition of one methyl group to the drugs structure, however the processes to create each substance is slightly different from one another. Another designer drug that is a part of the amphetamine family is *p*-fluoroamphetamine. The designer drugs in this family have a decently high abuse potential, so they are labeled as a Schedule II stimulant drug (2)(6). The instruments used to analyze these drugs structures include Gas Chromatography-Mass Spectrometry and Nuclear Magnetic Resonance Spectroscopy (13).

The Opioid family has a large number of designer drugs within it all having a decently high abuse potential and are considered Schedule II sedative drugs, however, these drugs are regularly used for medical purposes, usually in hospitals (2)(6). A couple of the designer drug derivatives within the Opioid family include acetylfentanyl, a derivative of fentanyl, and Krokodil, a derivative of Codeine. The use of acetylfentanyl as an abuse able drug became very popular in 2013, and since has grown in popularity amongst people creating designer drugs. Acetylfentanyl is much more potent than normal fentanyl so it is used in combination with other drugs like heroine to make it more cost efficient to produce the designer drugs and they can still be sold at the same high price (2). The chemical structure of the acetylfentanyl is very different than the more common opioids like heroine or morphine so it can be hard to determine that it is a substance that is part of the Opioid family. Acetylfentanyl can sometimes be detected by a process that is screening for fentanyl, but these times of processes are not always used in the forensic chemistry lab (2). Some of the previously mentioned instruments that can detect these opioid derivatives within samples are Gas Chromatography-Mass Spectrometry and Liquid Chromatography-Mass Spectrometry. Krokodil has become increasingly popular across North America and European countries after it originated in Russia (20). This drug was created for the sole purpose of being an inexpensive replacement for heroine. The process, which can be seen in **Figure 8**, of making this drug consists of starting with tablets of codeine that undergo synthetic changes within a clandestine lab with items that can be easily bought, like gasoline and other chemicals, to create a deosmorphine salt (21). The image of this process highlights the areas that change within the structure between the normal opioid drug and its more potent derivative. Many presumptive tests

can be done in the forensic labs to narrow down the possibility of if the substance in question Krokodil, but the main two types of instruments used to analyze the compound will be Gas Chromatography-Mass Spectrometry and Liquid Chromatography-Mass Spectrometry (21). The deosmorphine salt has been detected and quantified by many chemists using either one of these processes.

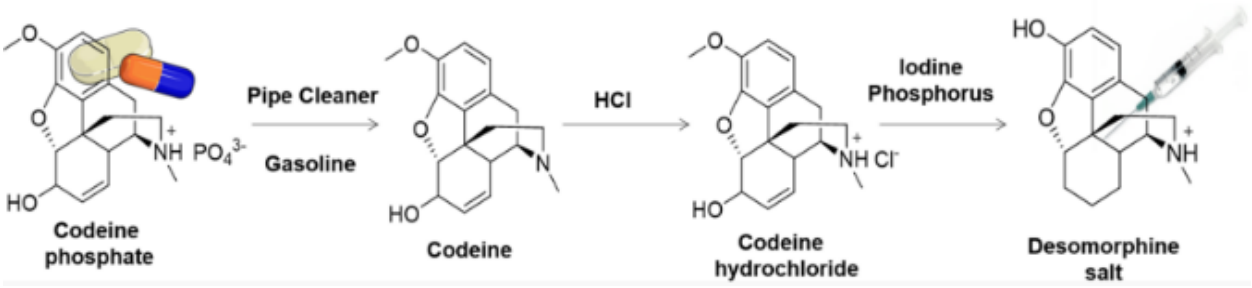


Figure 8: Chemical process of creating Krokodil, deosmorphine salt (21).

Like mentioned earlier, it is very important that forensic chemists are able to identify the characteristics that will differentiate between active designer drugs, normally derivatives of drugs of abuse, and substances that are inactive compounds which produce zero abusive side effects. The most important information to determine about samples like these types of derivatives is their analytical information. Out of all the techniques discussed previously there are only really one instrumentation process that can properly differentiate between active abusive compounds and inactive derivatives. This technique is Gas Chromatography paired with an Infrared Detector; this detector follows the same process as a Fourier Transform Infrared Spectrometer (11). This process can be considered a confirmatory test when determining the identity of a designer drug since it uses a category A and a category B technique. Even though Fourier Transform Infrared Spectroscopy is within a category under SWGDRUG guidelines, this process goes more in depth because it can separate all the compound within the sample before they are

examined by the Fourier Transform Infrared instrument (5). This technique can differentiate between compounds like indirect and direct regioisomers better than a Gas Chromatographer-Mass spectrometer instrument because of the uniqueness in the fingerprint range on the spectra.

The reason why this process works better than using Fourier Transform Infrared Spectroscopy by itself, is because normally the singular instrument cannot identify the compounds well if there are multiple components within it because there is no separation before the identification process, so more likely than not the only the compound that will be identified is the most abundant one within the sample. The reason that the Gas Chromatography-Fourier Transform Infrared Spectroscopy would work more efficiently than Gas Chromatography-Mass Spectrometry is because the fingerprint range on the Fourier Transform Infrared Spectra will be unique for each different arrangement of the components in the sample (10). It will explain how the location of the substituents create different peak patterns on the chromatogram. This is very different than the output data from a mass spectrometer because the mass spectra will look the same for any drugs within the same family that has the same atomic components in a similar chemical structure, like regioisomers (11). Because they have this very similar composition, on the spectra they will usually fragment within the same ways when they have the same substituents, even in different locations. Mass Spectra showing two types of cathinone substances can be seen in **Figure 9**, these two structures are direct regioisomers because they have a differing arrangement of their methoxy group, the OCH_3 group. Even though these two structures have this different arrangement of their components, the fragment peaks are located at the same m/z values with almost identical abundances for

compounds. It would be very difficult to distinguish between these two compounds if only a Mass Spectrometer was used to identify them. Infrared spectra showing the differentiations between these same two samples with the Infrared Detector can be seen in **Figure 10**. These are the same two structures as show in the previous photo, but on this set of spectra there is differences spotted between the two compounds. The different colored circles highlight an example of how two different clusters of three peaks will look different between derivative structures. In the top spectrum the blue circled peaks are not as defined from one another like they are in the bottom spectrum, but in the top spectrum the red circled peaks are very separated from one another unlike the peaks highlighted in the bottom spectrum. This process overall will give more accurate data that can differentiate between these closely related derivatives like the direct and indirect regioisomers between compounds within the same drug family then the Gas Chromatography-Mass Spectrometry process because the Gas Chromatography Infrared Detection process has the unique fingerprint marker for every small difference (10).

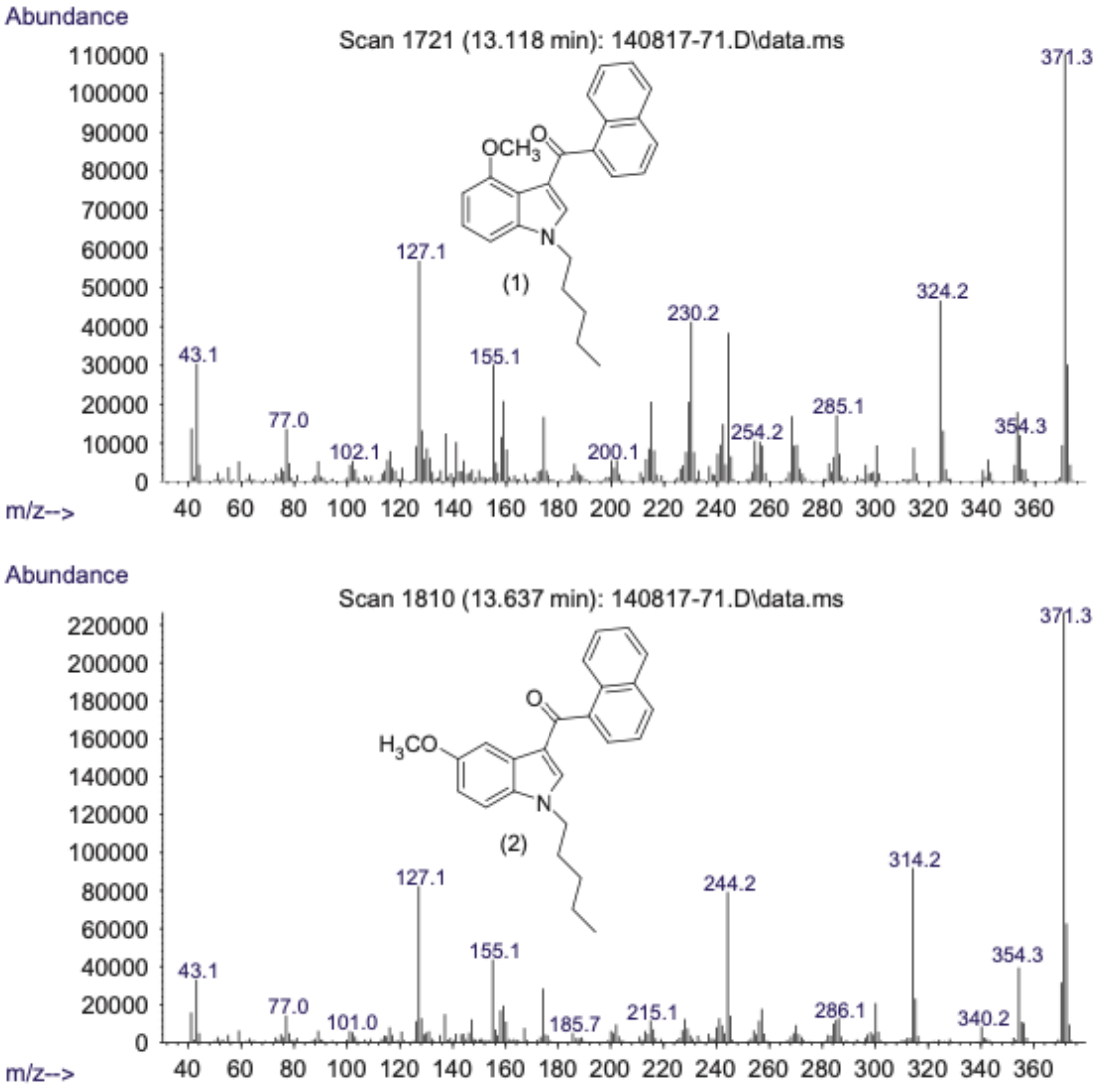


Figure 9: Mass Spectra of two direct regioisomeric compounds (17).

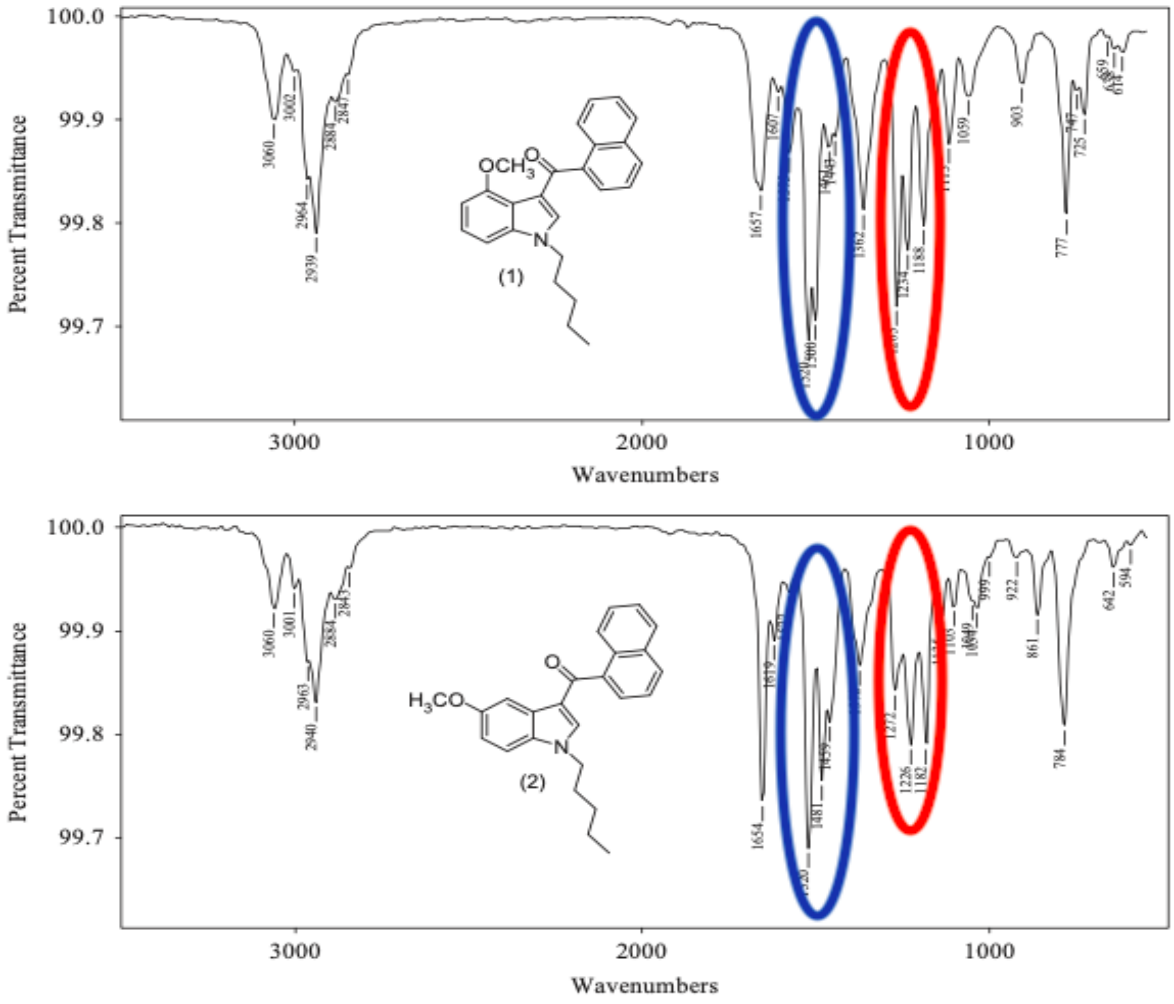


Figure 10: Infrared spectra of two regioisomeric compounds (17).

Many of these new designer drugs are responsible for dozens of fatalities before they can even be recognized as a problem and even more before they can be identified and made illegal. And as always, as soon as one drug can be classified, another new synthetically created drug pops up in its place flooding the streets for the process to begin all over again (22). These designer drugs are being created either by altering the structure of an already existing drug or by trying to recreate the effects of an already existing drug. The main types of structures that can be created to make these different illicit substances include direct regioisomers, indirect regioisomers, and isobaric compounds. Both types of

regioisomers contain the same atomic components as the parent drug, but they are just arranged in a different way. On the other hand, isobaric compounds do not contain the same atomic components as the drug they are trying to mimic.

To speed up the process of identifying these new substances and their effects many scientists are completing various types of research studies and forensic analysis tests (8)(9)(10)(12)(13)(14)(16)(17)(19)(23)(24)(25)(26)(27)(28). These different studies are focused on analyzing and identifying one drug substance or one drug family by preforming many analytical tests with forensic instrumentation. Another type of study that is very relevant to scientists, medical professionals, and police officers is one that takes all known data for one specific drug or drug family and complies a very informative review for those substances (15)(18)(29)(30). Because they the different structural changes and the number of new substances is increasing rapidly, these types of articles help keep everyone up to date as best as possible on the designer drug substances.

The different forensic instruments discussed earlier all have key components during the analysis process that assist in the identification and classification of these illicit substances. The Gas Chromatography and Liquid Chromatography instruments can separate the multiple components of a sample from each other for better analysis. The Mass Spectrometry instrument can determine the possible chemical structure of the questioned sample to help determine which drug family it may belong in. The Direct analysis in Real Time and Nuclear Magnetic Resonance instruments have very similar output data to the Mass Spectrometry instrument. The Fourier Transform Infrared Spectroscopy instrument and the Infrared detector are both able to produce the structural information for a compound in question, however this instrument differs from Mass

Spectrometry because it can tell the difference between active compounds and inactive derivatives within the same drug family based on the unique fingerprint region on the spectrum.

The two most important aspects to the identification process of these designer drugs are: 1) making it possible for these drugs to become scheduled appropriately under the Controlled Substance Act so that these substances can no longer be considered a legal way to get high and 2) making sure the differences are known between the active abusable compounds and their inactive derivatives so that no scientists receive punishment for analyzing a non-abuseable compound in the laboratory. The most effective forensic instrument to be used for this process is the Gas Chromatographer with an Infrared detector.

Due to the major advancements in with the technology and instrumentation used in the Forensic Chemistry laboratories the analysis process for evidence and different questioned compounds are conducted much easier and more time efficient. Because these designer drugs are being identified more quickly and more efficiently, then they can be classified and scheduled within a faster time frame as well. All of this will lead to even faster identification processes in the future as well as the placement of better policies against these substances, which will ultimately save many lives globally.

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