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Identification of Bioactive compounds of pyrolysis oil obtained from cotton residues (*Gossypium arboreum*) by flash pyrolysis

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Abstract : Pyrolysis oils have attracted a lot of interest, as they are liquid energy carriers and general sources of chemicals. In this work the gas chromatography–mass spectroscopy was developed and applied for the analysis of bioactive and hydrocarbons of pyrolysis bio oil. More than 250bioactive compounds such as normal saturated hydrocarbons, cyclopentane, cyclohexane, esters, alcohols, sulfur- and bromo-containing compounds, simple pyrane, and benzene derivatives, were identified. Most of these compounds have not been reported earlier. The increase in the number of identified products is due to increased separations. This increased understanding of pyrolytic product distribution can be used to enhance our understanding of the formation mechanisms of pyrolytic products. The method described in this article is a suitable research tool for the determination of various chemical compounds from pyrolysis bio oil derives from cotton shell.
Keywords : Cotton shell, Fluidized bed, Pyrolysis, Bio-oil, GC-MS, bioactive compounds.

1. Introduction

The environmental problems related with the extended use of fossil fuels are well known and established, and in addition to their forthcoming shortage, scientific interest has turned towards the development of technologies exploiting renewable energy sources. Such an alternative source is biomass, which as a term is used to define any type of organic residue or certain types of energy crops that may be used as a renewable energy source. Biomass isa complex material, mainly composed of hemicellulose, cellulose and lignin in addition to extractives (tannins, fatty acids, resins) and inorganic salts [1].With an increasing global population, more and more biomass residues are being generated, due to higher demands for food and shelter. Development of advanced state-of-the-art commercial technologies such as fast pyrolysis will help treating the waste generated, thereby decreasing environmental pollution, and permitting conversion of agricultural biomass into useful bioproducts[2]. Fast pyrolysis is a process that produces gas, solid and liquid products. The liquid product of fast pyrolysis is commonly called bio-oil or pyrolysis oil. Bio-oils find applications as sources of chemicals, as fuels, mainly in mixtures or emulsions with fossil fuels [3,4], while their use as fungicides or wood preservatives, has also been proposed [5,6]. They can also be upgraded through hydrodeoxygenation or catalytic cracking, so as to reduce their viscosity or oxygen content in order for them to be incorporated into existing technologies. Bio-oil is a mixture of various chemical compounds including phenols, carboxylic acids, guaiacols, syringols, etc., as a result of the rapid depolymerization and the chemical fragmentation of lignin, cellulose and hemicellulose during the fast pyrolysis. The chemical composition of bio-oils is determined by the

nature of the biomass from which they originate and the pyrolysis conditions employed [7,8]. The bio-oil resulting from such a process usually consists of two phases: a lower mainly organic phase containing oligomeric lignin molecules and other compounds with high molecular weight, and an upper aqueous phase, which is rich in low molecular weight compounds with added value, such as carboxylic acids, phenols, guaiacols, syringols, etc. The chemical composition of this aqueous phase renders it suitable as feed stock in a steam reforming process for the production of hydrogen [9] or after further fractionation for the extraction of specific chemicals for other applications, such as syringols or guaiacols that may be used as flavorings [7]. The bio-oil's complex nature renders essential the use of high resolution chromatographic techniques. Both HPLC [10, 11] and GC [12-14] have been employed, since the bio-oil contains both volatile and non-volatile compounds, The increase in the number of identified products is due to increased number of separations [15].Characterization of structure and confirmation of identity are usually achieved by comparison of the massspectra with library spectra and determination of the chromatographic retention indexes [16, 17].Faull et al [18] have reported that the separation and quantitative determination of a wide variety of organic and inorganic components in microorganisms are carried out by chromatographic methods. At present, analysis by GC–MS is essential for the identification of natural organics. Usually, determination of bioactive compounds, such as aromatic compounds, fatty acids, general hydrocarbons, and hydroxy or amino metabolites is achieved using GC–MS techniques.

Cotton shell: *Gossypium arboreum*, commonly called tree cotton is one of the largest sources of biomass for agricultural residues in India. It is a species of cotton native to India, Pakistan and other tropical and subtropical regions of the world. There is a lot of evidence of its cultivation as longago as the Harappan civilization of the Indus Valley for cotton textile production. The cotton crop occupies more than 9.2 million hectares and its share 27 percent of the world total production. The country has three main cotton growing zones: the northern zone in the States of Punjab, Rajasthan and Haryana, accounting for about 1.9million hectares; the major central zone in the States of Gujarat, Madhya Pradesh and Maharashtra with 5.4 millionhectares; and the southern zone in the states of Andhra Pradesh, Karnataka and Tamil Nadu accounting for about1.8 million hectares. India has the largest area under cotton and its cotton production is about 15.8 million bales. The seeds are removed from cotton and can be used to prepare highly viscous cotton seed oil which can be used directly for burning and further it can be converted into biodiesel. In the previous paper [19] the process optimization of the flash pyrolysis of cotton shell for the maximum bio oil production using an electrically heated fluidized bed reactor has been reported. In the present study further detection of a wide range of bioactive compounds from the cotton shell pyrolysis bio oils has been carried out.

2. Pyrolysis process Method

The pyrolysis product yields are affected by the process temperature, feedstock particle size, feeding rate and sweep gas flow rate. In another study used palm shell as the biomass, the effect of particle size on the slow pyrolysis has been investigated between the range of 0.224–1.8 mm [20], In our study all the experiments are conducted at the particle size of 1 mm for the yield of maximum bio oil. From the brief review, the increase in the particle size enhances the solid yield in the slow, fast and flash pyrolysis process due to the larger temperature gradient inside the particles.[21,22].The sweep gas (nitrogen) flow rate directly affects the residence time of the evolved gases produced from the pyrolysis reactions and minimizes the secondary decomposition of higher molecular weight products. However, it has been observed that the yield of the bio oil decreases when the nitrogen flow rate exceeds. This elevates the heat transfer rate and increased production of volatiles. At the same time, the vapor residence time is shortened leading to lower probability of the secondary tar cracking reaction.T he suitable flow rate is 1.75 m^3/h for higher yield. Pyrolysis temperature greatly affects the type and amount of the reaction products; at a relatively low temperature, say below 350 °C, the main products are char, whereas at higher temperature exceeding 700 °C, most of the reaction products are non-condensable gases. So the suitable temperature for the pyrolysis process is in the range of400–600 °C [23].

3. Experimental set up

3.1 Flash Pyrolyser

The experimental set up used for the present study is same as that used in previous paper [19] and is explained in this section. The devolatilization fraction samples are prepared from the flash pyrolysis of the cotton shell in an electrically heated fluidized-bed reactor. Pyrolysis experiments were carried out under

nitrogen atmosphere at the temperatures of 350, 400, 450, 500 and 550 °C. The pyrolysis experiments conducted in the reactor is made up of stainless steel tube of internal diameter 50 mm. The reactor is filled with sand of particle size of0.71 mm supported with the perforated base for enabling fluidization. The reactor is heated using 2000W electrical heater with ammeter and voltmeter setup to measure the power input and is controlled by an autotransformer and temperature cut off unit. The temperatures of the reactor are measured with the help of thermocouple located at five different points along the reactor, and is well insulated with mineral wool and Chromel-Alumel. The cotton shell particles are kept in the hopper and are fed into the reactor through screw feeder. Fluidization is first done by air till the reactor reaches the uniform temperature and then in inert atmosphere using nitrogen gas. The flow rate of the nitrogen was measured with the help of a rotameter. A distributor valve was utilized to separate the flow of air and nitrogen. The fluidizing gas velocity was approximately maintained two times greater than the minimum fluidization velocity of 0.11 m/s and the flow rate was maintained to 1.75 m^3/h. Figure 1 shows the layout of an electrically heated fluidized bed pyrolyser.

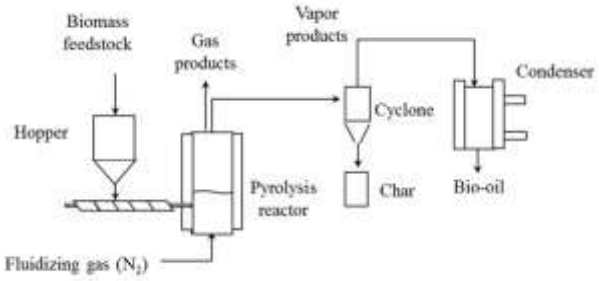

Fig. 1 Layout of the electrically heated fluidized bed pyrolyser

The rising gas from the reaction first passes through the cyclone separator wherethe particulate matters are dropped and thereby preventing char from reaching the condensing unit. The vapours and the gases are passed through a water cooled condenser to a series of ice cooled to entrap the derived bio oil. The char and other particulate matters are collected in a cyclone separator and weighed. The liquid phase condensed in the condenser is weighed. The gaseous phase is then calculated by the remaining material balance.

3.2 Apparatus and chromatography conditions

Gas chromatography Mass spectroscopy is a technique that can be used to characterize the structure and composition of the various components of lignocellulosic and microalgal biomass based on their pyrolysate distributions. For the identification and quantitative measurement of bioactive compounds in the pyrolysis bio oil obtained from the cotton shellwas performed on a GC-MS equipment (South Indian Textile Research Association) THERMO GC-TRACE ULTRA VER: 5.0,THERMO MS DSQ II were used for the analysis under the following experimental conditions: A capillary column coated with a 0.25 µm film of DB-35 with length of 30 m and diameter 0.25 mm. The GC was equipped with Helium gas as carrier gas was set at the flow rate of 10 ml/min. The oven initial temperature was set to 70 °C for 2 min and then increased to 250 °C at a rate of 10 °C/min. Massspectrometer was operated at an interface temperature with ion source temperature of 200 °C. The sample was run fully at a range of 40–650 m/z.

4. Results and discussion

4.1 Characterization of cotton shell

The proximate and ultimate analysis of the dried cotton shell was carried out and presented in Table 1. The result confirmed that cotton shell restrained maximum volatile matters (62.64%), fixed carbon (25.02%) contents and ash (2.82%) with lower percentage of moisture (9.52). More amount of volatile matter produces more liquid and gaseous fuel during pyrolysis. The ultimate analysis determined the presence of carbon (45.09%), oxygen (49.32%), hydrogen (4.9%),nitrogen (0.68%) and sulfur (0.01%) in cotton shell. Lower sulfur content in the raw materials makes them suitable feed for pyrolysis to produce good quality of liquid and gaseous fuels. The presence of volatiles determines the combustibility of biomass. Normally thermal degradation is a function of composition such as celluloses, hemi-celluloses, lignin and extractives [20, 24, 25]. Initially, moisture and more volatile compounds were removed within 150 °C and after that the thermal

degradation of cotton shell started and proceeded followed by two steps such as degradation of hemicelluloses and cellulose. At higher temperature lignin degrades. Hemicelluloses degrade at lower temperature than cellulose. At higher temperature lignin degrades slowly till the end stage of degradation. At the end of pyrolysis, residue of cotton shell remained as char. It was observed that maximum degradation occurred during second and third stage in the temperature range between 150 and 450 °C. This temperature range was considered as active pyrolytic zone for cotton shell where maximum volatilization took place.

Table 1. Cotton shell characteristics

Elements	Value (wt %)
Proximate analysis	
Volatile matter	62.64
Fixed Carbon	25.02
Moisture Content	09.52
Ash Content	02.82
Ultimate analysis	
Carbon	45.09
Hydrogen	04.90
Nitrogen	00.68
Oxygen[a]	49.32
Sulfur	00.01
Calorific Value in MJ/kg	13.72

[a]by difference

4.2 Pyrolysis of cotton shell and the effect of temperature on pyrolysis

Thermal pyrolysis of cotton shell was performed in an electrically heated fluidized bed reactor. The result revealed the influence of temperature with relation to weight % yield of liquid, char and non-condensable gases. It was confirmed that temperature had a positive affinity towards the yield of oil and non-condensable gas. The various pyrolysis product distribution of flash pyrolysis of cotton shell at the temperatures of 350, 400, 450, 500 and 550 °C are listed in Table 2. With increasing the temperature, the product distributions of the biomass material changed. By increasing the pyrolysis temperature from 400 to 450 °C, the bio-oil yield increased and the bio-char yield decreased. The results show that the liquid yield increases up to51wt% at 450 °C. Due to incomplete decomposition, the maximum bio oil yield was only 29 wt% at 350 °C whereas the char yield is 35wt%. When the temperature exceeds 500 °C the gas yield increases but it decreases the char and liquid yield. The secondary reaction of the liquid fraction of the volatile matter causes the decomposition of the char particles at higher temperature. Literature reported that pyrolysis at elevated temperature produce more amount of H2 and CO which results in less liquid yield. The release of gases may be due to the reduction reaction of char at high temperatures. In most cases, incomplete decomposition of the biomass at lower temperatures favor char yields. With increasing the pyrolysis temperature, both liquid and gaseous yields increase. The physical properties of the raw bio oil is listed in the table 3.

Table 2.Product distributions of pyrolysis of biomass

Temperature in °C	Reaction products		
	Bio oil	Bio char	Bio gas
350	29.7	35.1	35.2
400	35.2	34.3	30.5
450	51.2	18.4	30.4
500	45.4	17.2	37.4
550	36.8	15.6	47.6

Table 3. Physical and elemental analysis of pyrolytic oil

Properties	Values
Density in kg/m^3	1005
Viscosity at 40 °C in cSt	7.87
Flash point in °C	160
pH	3.3
Ash content in %	<0.1
Elemental Analysis in %	
Carbon	38.14
Hydrogen	11.24
Nitrogen	00.94
Sulfur	00.11
Oxygen[a]	49.57
Calorific value in MJ/kg	19.32

[a]By difference

4.3Compound analysis of bio oil

The results pertaining to GC-MS analysis of the cotton shell pyrolysis oil lead to the identification of a number of compounds. These compounds were identified through mass spectrometry attached with GC. The increase in the number of identified products is due to increased separations. A number of compounds can be identified and listed in Table 4. They include acids, alcohols, ketones, aldehydes, phenols, esters, sugars, furans, guaiacols and multifunctional compounds. These compounds are also found in other bio-oils produced from different biomass resources [26].The presence of carboxylic acids seems to be the reason for the low pH value of the bio-oil. Cellulose and hemicelluloses are the major components of the biomass feedstock as they are the sources of these aromatic and oxygenated compounds [27].This class of compounds abundantly occursin bio-oil since they are present as the monomeric units and oligomers from the lignin in the biomass feedstock [28]. Some of these compounds have beneficial applications in the medical, industrial, and agricultural fields. This increased understanding of pyrolytic product distribution can be used to enhance our understanding of the formation mechanisms of important pyrolytic products.

Gaschromatography–mass spectrometry was developed and applied for the analysis of bioactive compounds derived from the cotton shell pyrolysis oil. Most of these compounds have not been reported earlier. Bio-oil consists mostly of phenolic and oxygenated compounds with aliphatic compounds in significant amounts. The elements and its derivatives found in the GC–MS analysis are used medicinally and also feed for the chemical industries. Boron trichloride is a starting material for the production of elemental boron. It is also used in the refining of aluminium, magnesium, zinc, and copper alloys to remove nitrides, carbides, and oxides from molten metal. It has been used as a soldering flux for alloys of aluminium, iron, zinc, tungsten, and monel. Aluminum castings can be improved by treating the melt with boron trichloride vapors. In the manufacture of electrical resistors, a uniform and lasting adhesive carbon film can be put over a ceramic base using BCl_3. It has been used in the field of high energy fuels and rocket propellants as a source of boron to raise BTU value. BCl_3 is also used in plasma etching in semiconductor manufacturing. 4 - propyl – syringol is the class of Flavor and Fragrance Chemical Compounds, colorless clear liquid with specific gravity 1.071 to 1.076 at 25.00 °C having Flash Point 276.00 °F. Linalool is used as a scent in 60–80% of perfumed hygiene products and cleaning agents including soaps, detergents, shampoos, and lotions. Linalool is used in some mosquito-repellent products. Linalool gradually breaks down when in contact with oxygen, forming an oxidized by-product that may cause allergic reactions such as eczema in susceptible individuals.Phenol,2-methoxy, which is used as a precursor to various flavorants such as eugenol and vanillin. Its derivatives are used medicinally as an expectorant, antiseptic. It also can be used as an indicator in chemical reactions that produce oxygen. 2,6-Dimethoxyphenolis a dimethyl ether of pyrogallol. It is slightly soluble in water and it is combustible with flash point 140 °C.

Table 4. GC–MS analysis of the cotton shell pyrolysis oil

S. N	RT	Compound name	Probability	Molecular formula	Molecular weight	Area %
1	3.07	2-Butanone, 3,3-dimethyl-1 (methylsulfinyl), [(methylamino) carbonyl]oxime	33.67	$C_9H_{18}N_2O_3S$	234	17.21
2		cis- and trans-N-Formyl-N,2,3-trimethylacrylamide	25.79	$C_7H_{11}NO_2$	141	
3		11á-methoxy-1á,4,4 trimethylbicyclo [5.4.0]undeca-5,9-dien-2-one	6.18	$C_{15}H_{22}O_2$	234	
4		2-Hexene	5.22	C_6H_{12}	84	
5		3-Hexene	3.59	C_6H_{12}	84	
6	4.42	Linalyl 2-methylpropanoate	13.30	$C_{14}H_{24}O_2$	224	3.32
7		9-methyl-6,7-dihydroxy-di(1,4-dioxo-naphtho)[3,4a,c] carbazole-9H	11.23	$C_{29}H_{15}NO_6$	473	
8		Linalyl butyrate	7.03	$C_{14}H_{24}O_2$	224	
9		Cyclopent-2-enethione	5.94	C_5H_6S	98	
10		Linalyl propionate	4.78	$C_{13}H_{22}O_2$	210	
11		Linalool	4.04	$C_{10}H_{18}O$	154	
12		Pyridine, 2-propyl-	3.73	$C_8H_{11}N$	121	
13		2,6,10-trimethyl-2,5:7,10-dioxido-dodeca-1,11-dien- 3-ol-5-one	2.85	$C_{15}H_{24}O_3$	252	
14		Pyridine, 2-tridecyl	2.74	$C_{18}H_{31}N$	261	
15	4.74	1-(1',3'-Dioxolane)-4a,8-epoxy-9a-methyl-7-oxabicyclo[5.4.094a,9a)]undec-5-ene	31.15	$C_{13}H_{18}O_4$	238	4.45
16		2,6-dimethyl-6-(8-methyl-4-methylene-7-nonenyl)-2-cyclohexene-1á-methanol	14.18	$C_{20}H_{34}O$	290	
17		7,7-Dimethyl-1-(1-methylethyl)tricyclo[2.2.1.0(2,6)]heptan-3-ol	3.86	$C_{12}H_{20}O$	180	
18		[4,4,10á-Trimethyl-7-methylidene-(trans)-decal-3á-ol]-7-spiro[1'-cyclopropane]	2.96	$C_{15}H_{26}O$	222	
19		2-[5-(2-Hydroxy-propyl)-furan-2-yl]-propan-1-ol	2.15	$C_{10}H_{16}O_3$	184	
20		Butane-1,1-D2, 1-iodo	2.15	$C_{10}H_{16}O_3$	184	
21		2-[5-(2-Hydroxy-propyl)-furan-2-yl]-propan-1-ol	2.15	$C_{10}H_{16}O_3$	184	
22		(5à,7à)-3,4,7-Trimethylcholest-3-en-7-ol	2.06	$C_{30}H_{52}O$	428	
23		Bromoethylmethanesulfonate	1.98	$C_3H_7BrO_3S$	202	
24		Triamcinolone	1.98	$C_{21}H_{27}FO_6$	394	
25	4.93	3,4-Dimethylthiophene	19.12	C_6H_8S	112	2.22
26		Thiophene, 2,3-dimethyl-	9.28	C_6H_8S	112	
27		2H-Pyran, 2-(2 heptadecynyloxy) tetrahydro-	6.92	$C_{22}H_{40}O_2$	336	
28		2H-Pyran, 2-(2-heptadecynyloxy) tetrahydro	6.92	$C_{22}H_{40}O_2$	336	
29		Thiophene, 2,5-dimethyl	5.44	C_6H_8S	112	
30		3,4 and 2,4-dimethylthiophene	5.23	C_6H_8S	112	
31		6-Methyl-5-(1'-phenylhydroxy methyl)4,5-dihydro-(2H)-3-pyridaz	5.03	$C_{12}H_{14}N_2O_2$	218	

		Inone				
32		1-Oxaspiro[2.5]octan-4-one, 2,2-dimethyl	4.44	$C_9H_{14}O_2$	154	
33		Benzenethiol, 4-chloro-	3.58	C_6H_5ClS	144	
34		Thiophene, 2,3-dimethyl-	9.28	C_6H_8S	112	
35		5-(Benzyloxymethyl)uracil	24.0	$C_{12}H_{12}N_2O_3$	232	
36		1,5-dimethyl-2-aminomethylpyrrole	15.5	$C_7H_{12}N_2$	124	
37		Benzeneethanamine, 3-fluoro-4-hydroxy-	6.13	$C_8H_{10}FNO$	155	
38		M-Hydroxy-à,à-dideuterobenzyl alcohol	5.17	$C_7H_6D_2O_2$	124	
39		[Ethyl(methyl)seleno]-sulfenate	3.86	C_3H_8SSe	156	
40	5.52	Silane, phenyl-	2.72	C_6H_8Si	108	0.98
41		cis-4-[(Benzyloxycarbonyl) amino]cyclooctanol	1.98	$C_{16}H_{23}NO_3$	277	
42		Benzenemethanol, 4-hydroxy	1.98	$C_7H_8O_2$	124	
43		M-hydroxy-à-deuterobenzyl alcohol	1.98	$C_7H_7DO_2$	124	
44		(S)-2-Benzyloxycarbonylamino butane-1-sulfonyl chloride	1.82	$C_{12}H_{16}ClNO_4S$	305	
45		(Cyanomethyl)cyclopentane	26.88	$C_7H_{11}N$	109	
46		2,4-methanoproline	6.64	$C_6H_9NO_2$	127	
47		Phenol, 2-methoxy-	6.38	$C_7H_8O_2$	124	
48		5-[4-(2-fluoro-benzyloxy)-benzylidene]-3-furan-2-ylmethyl-2-thioxo-thiazolidin-4-one	4.63	$C_{22}H_{16}FNO_3S_2$	425	
49	6.07	p-Mesyloxyphenol	4.27	$C_7H_8O_4S$	188	12.93
50		4,6-dihydrofuro[3,4-b]furan	4.11	$C_6H_6O_2$	110	
51		endo-d2-2-exo-Acetoxynorbornan-7-one	3.79	$C_9H_{10}D_2O_3$	168	
52		Methyl hept-2-ynoate	2.82	$C_8H_{12}O_2$	140	
53		Phenol, 3-amino	2.82	C_6H_7NO	109	
54		Pyridinium, 1-amino-2,6-dimethyl-, chloride	8.22	$C_7H_{11}ClN_2$	158	
55		1-(1',2'-Dimethylprop-1'-yl)-3-(4'-methylphenylsulfonyl)-3-azabi cyclo[3.1.0]hexane	4.98	$C_{17}H_{23}NO_2S$	305	
56		2-Phenyl-1-p-tolylethanol	3.51	$C_{14}H_{16}O$	200	
57		Benzenamine, 4-methyl-	3.10	C_7H_9N	107	
58	6.94	Benzenamine, 4-methyl-, hydrochloride	2.98	C_7H_9N	107	1.88
59		N-[1-(Benzylamino)-2,2,2-trifluoro-1-(trifluoromethyl)ethyl]benz Amide	2.98	$C_{17}H_{14}F_6N_2O$	376	
60		Phenol, 2,5-dimethyl-	2.87	$C_8H_{10}O$	122	
61		Hydrazine, (3-methylphenyl)-	2.53	$C_7H_{10}N_2$	122	
62		Hydrazine, (4-methylphenyl)-, monohydrochloride	2.43	$C_7H_{10}N_2$	122	
63		10-Chlorodanuphylline	49.36	$C_{24}H_{25}ClN_2O_8$	504	
64		9-(2-Deoxy-3,5-O-(tetraisopropyldisiloxanediyl)-2-methylene-áD -erythro-pentofuranosyl)adenine	22.48	$C_{24}H_{40}N_4O_4Si_2$	504	
65	7.23	2,4-di(-butoxy)-2,4-dimesityl-1,3,2,4-diphosphadisiletane	11.59	$C_{26}H_{42}O_2P_2Si_2$	504	1.35
66		1,10-Dihydro-3,8-bis(2-methoxycarbonylethyl)-2,7-bis-(methoxycarbonylmethyl)-1-	2.64	$C_{24}H_{28}N_2O_{10}$	504	

		oxodipyrrin-9-carbaldehyde				
67		1-(2'-Deoxy-1',2'-seco-D-ribosyl)thymine	1.97	$C_{24}H_{28}N_2O_{10}$	244	
68		(2S,3S)-4-Methyl-5-(3-thienyl)-4-pentene-2,3-diol	1.43	$C_{10}H_{14}O_2S$	198	
69		Methyl 2-allyl-3-hydroxy-4,5,5-trimethylhexanedithioate	1.43	$C_{13}H_{24}OS_2$	260	
70		3á-hydroxy-5à,6á-bis(trimethylsiloxy)-5,6-dihyd roandrenolactone	0.48	$C_{28}H_{50}O_5Si_2$	522	
71		3,7-Anhydro-7-deoxy-7-[(diphenyloxyphosphoryl)amino]-1,2:4,5-di-O-isopropylidene-D-allo-hept-3-ulofuranose	0.48	$C_{25}H_{30}NO_8P$	503	
72	7.59	2-Methoxy-4-methylphenol	19.12	$C_8H_{10}O_2$	138	1.93
73		3-Methoxy-2-methylphenol	13.88	$C_8H_{10}O_2$	138	
74		Phenol, 3-methoxy-2-methyl-	13.88	$C_8H_{10}O_2$	138	
75		2-Methoxy-4-methylphenol	19.12	$C_8H_{10}O_2$	138	
76		Phenol, 2-methoxy-4-methyl-	19.12	$C_8H_{10}O_2$	138	
77		1,4-Dihydrothujopsene-(I1)	6.23	$C_{15}H_{26}$	206	
78	8.19	1,3-Benzenediol,4-(3,4-dihydro-7-hydroxy-2H-1 -benzopyran-3-yl)-	18.49	$C_{15}H_{14}O_4$	258	0.71
79		1,3-Benzenediol, 4-(3,4-dihydro-7-hydroxy- 2H-1-benzopyran-3-yl)-	18.49	$C_{15}H_{14}O_4$	258	
80		4-(3'-isopropoxy-2',6',6'-trimethyl-1'-cyclohexen-1'-yl)-2-butanone	4.29	$C_{16}H_{28}O_2$	252	
81		Nemorensic acid	4.12	$C_{10}H_{16}O_5$	216	
82		Palustrol	3.15	$C_{15}H_{26}O$	222	
83		8-á-Methoxy-5à-hydroxycaryophylla-3(4)-ene	3.03	$C_{16}H_{28}O_2$	252	
84		(1RS,2RS,3RS)-1,2,6,6-tetramethy[-10-oxatricyclo[5.2.1.0(2,7)]] dec-3-yl acetate	2.80	$C_{15}H_{24}O_3$	252	
85		Cyclohexane, 1,1'-(2-propyl-1,3-propanediyl)bis-	2.80	$C_{18}H_{34}$	250	
86		Cyclohexane, 1,1'-(2-propyl-1,3-propanediyl)bis-	2.80	$C_{18}H_{34}$	250	
87		3-Hydroxy-6-(N,N-dimethylamino)methylpyridazine 1-oxide	2.69	$C_7H_{11}N_3O_2$	169	
88	8.84	2,5-Dimethoxytoluene	14.96	$C_9H_{12}O_2$	152	3.07
89		4-ethyl-2-methoxy-6-methylpyrimidine	9.37	$C_8H_{12}N_2O$	152	
90		Benzene, 1,4-dimethoxy-2-methyl-	14.96	$C_9H_{12}O_2$	152	
91		Phenol, 4-ethyl-2-methoxy-	7.36	$C_9H_{12}O_2$	152	
92		Ethanone, 1-(2,5-dihydroxyphenyl)-	7.07	$C_8H_8O_3$	152	
93		Ethanone, 1-(2,5-dihydroxyphenyl)-	7.07	$C_8H_8O_3$	152	
94		Benzaldehyde, 4-hydroxy-3-methoxy-	6.80	$C_8H_8O_3$	152	
95		(5E)-5-Ethylidene-2-hydroxy-3,4-dimethylcyclopent-2-enone	6.27	$C_9H_{12}O_2$	152	
96		1-(Thien-2-yl)but-1-en-3-one	4.30	C_8H_8OS	152	
97	9.43	3-(4'-Bromophenyl)-5,6-diphenylimidazo[2,1-b]thiazole	26.18	$C_{23}H_{15}BrN_2S$	430	1.25
98		1,3-Bis(4-chlorobenzyl)-5,6-dihydrobenzo[f]quinazoline	20.05	$C_{26}H_{20}C_{l2}N_2$	430	

99		Cyclohexasiloxane, dodecamethyl-	15.36	$C_{12}H_{36}O_6Si_6$	444	
100		2,2-Dimesityl-2 silatetracyclo [7.6.0.0(3,8).0(10,15)]hexadecadoDecae ne	9.92	$C_{32}H_{32}Si$	444	
101		Diethyl N-Methyl-10H-1]Benzoselinopheno [3,2-b]indole-2,7-dicarboxyLate	8.77	$C_{21}H_{19}NO_4Se$	429	
102		bis(trimethylsilyl)-lorazepam	7.40	$C_{21}H_{26}Cl_2N_2O_2Si_2$	464	
103		(5à,6à)-4,5-Epoxy-6-Methoxy-17-propyl-3á-phthalimidomorphin An	4.63	$C_{28}H_{30}N_2O_4$	458	
104		12-Phenyl-2,3,7,8-tetramethoxy-5H-(1)-benzopyrano[4,3-c]isoquInoline	3.73	$C_{26}H_{23}NO_5$	429	
105		cyclohexasiloxane, dodecamethyl-	15.36	$C_{12}H_{36}O_6Si_6$	444	
106		Phenol, 2,6-dimethoxy-	50.77	$C_8H_{10}O_3$	154	
107		Phenol, 2,6-dimethoxy-	50.77	$C_8H_{10}O_3$	154	
108		2-Methoxy-3-methylhydroquinone	20.06	$C_8H_{10}O_3$	154	
109	9.80	2,4-Dimethoxyphenol	14.97	$C_8H_{10}O_3$	154	10.42
110		Phenol, 2,6-dimethoxy-	50.77	$C_8H_{10}O_3$	154	
111		Phenol, 3,4-dimethoxy-	5.01	$C_8H_{10}O_3$	154	
112		2-Acetylcycloheptaneone	4.62	$C_9H_{14}O_2$	154	
113	10.54	Tetradecane	35.33	$C_{14}H_{30}$	198	0.35
115		Kaempferol	26.75	$C_8H_8O_4$	168	
116		3-Hydroxy-4-methoxybenzoic acid	26.75	$C_8H_8O_4$	168	
117		2-Hydroxy-3-methyl-5-methoxy-p-benzoquinone	20.49	$C_8H_8O_4$	168	
118		1,4-Dideuterio-2,5-dimethoxy-3,6-dimethylbenzene	5.47	$C_{10}H_{12}D_2O_2$	166	
119	11.40	4,5-Dimethoxy-2-methylphenol	3.75	$C_9H_{12}O_3$	168	1.61
120		5-Acetyl-2-methylthiopyrimidine	3.61	$C_7H_8N_2OS$	168	
121		4-(1-Hydroxyethyl)-2-methoxyphenol	3.05	$C_9H_{12}O_3$	168	
122		1,2,4-Trimethoxybenzene	1.11	$C_9H_{12}O_3$	168	
123		2,5-Dimethoxybenzyl alcohol	1.07	$C_9H_{12}O_3$	164	
124		2-Hydroxy-2-methoxy-6-pentadecyl-1,4-benzoquinone	1.02	$C_{22}H_{36}O_4$	364	
125		3-(5'-Chloro-1',3'-diphenylpyrazol-4'-yl)-1-oxo(1H)-pyrido[2,1-b] benzothiazole-2,4-carbonitrile	55.90	$C_{28}H_{14}ClN_5OS$	503	
126		N(1)-{4'-[3''-Oxo-4''-(p-fluorophenyl)-3'',3''a,4'',5''-tetrahydro-2''-methyl-(2H)-6''- indazolyl)]phenyl}-5-chloro-2-methoxybenzami De	22.10	$C_{28}H_{23}ClFN_3O_3$	503	
127	12.43	1-Phenyl-3-(2''-chlorophenyl)-6-(p-chlorophenyl)-3a,4,4a,7a,8,8a-hexahydro-4,8-epoxypyrrolo [3,4-f]indazole-5,7-(1H,6H)-dione-	16.04	$C_{27}H_{19}Cl_2N_3O_3$	503	0.96
128		6-(4-Chlorophenyl)-2,5,5-triphenyl-5,8-dihydro-6H-azeto[1,2-a][1,3]thiazolo[4,5-d]pyrimidine	5.85	$C_{31}H_{22}ClN_3S$	503	
129		tetradecamethylcycloheptasiloxane	0.05	$C_{14}H_{42}O_7Si_7$	518	
130		Cycloheptasiloxane, tetradecamethyl-	0.05	$C_{14}H_{42}O_7Si_7$	518	
131		tetradecamethyl - cyclo - hepta - siloxane	0.05	$C_{14}H_{42}O_7Si_7$	518	
132		2,9-Bis(5-tert-butyl-2-methoxyphenyl)-1,10-phenanthroline	0.01	$C_{34}H_{36}N_2O_2$	504	

133		deuteratedetioporphyrine	0.00	$C_{32}H_{15}D_{23}N_4$	478	
134		1-Methyl-5-t-butyluracil	26.34	$C_9H_{14}N_2O_2$	182	
135		1-(5-Pentyl-2-furyl)ethan-1-ol	19.65	$C_{11}H_{18}O_2$	182	
136		Benzene, 1,1'-ethylidenebis-	16.60	$C_{14}H_{14}$	182	
137		2,3,5-Trimethoxytoluene	10.06	$C_{10}H_{14}O_3$	182	
138		1,2,4,5-Tetravinylbenzene	7.70	$C_{14}H_{14}$	182	
139		1-(3,4-Dimethoxyphenyl)-1-ethanol	6.81	$C_{10}H_{14}O_3$	182	
140	12.99	2-Carboxy-4-methylbicyclo[2.2.2]oct-2-en-1-ol	4.94	$C_{10}H_{14}O_3$	182	2.27
141		methyl 4-T-butyl-2-furoate	0.95	$C_{10}H_{14}O_3$	182	
142		N-(Diphenylmethyl)-6-(hydroxymethyl)-2-aza-spiro[4,5]decan-1- One	0.92	$C_{23}H_{27}NO_2$	349	
143		2,4-Dihydroxy-6-methoxy-acetophenone	0.61	$C_9H_{10}O_4$	182	
144		1-Ethynyl-1,2,3,4-tetrahydro-á-carboline	59.91	$C_{13}H_{12}N_2$	196	
145		4-(2'-Methyl-3'-butenyl)azulene	15.36	$C_{15}H_{16}$	196	
146		3-phenyl-cis-3,3a,4,5,6,6a-hexahydro-4,5,6-methenocyclopentap Yrazole	15.36	$C_{13}H_{12}N_2$	196	
147		2,2-Diphenylpropane-1,3-dial	2.77	$C_{15}H_{12}O_2$	224	
148	14.72	2,6-Dimethyl-4-propylphenol	2.12	$C_{11}H_{16}O_3$	196	0.36
149		4 - propyl – syringol	1.96	$C_{11}H_{16}O_3$	196	
150		homosyringaldehyde	0.49	$C_{10}H_{12}O_4$	196	
151		4-ethyl-	0.45	$C_{15}H_{16}$	196	
152		1-cyano-2-methyl-3,4 benzotricyclo[3.3.0.0(2,8)]octene	0.36	$C_{14}H_{13}N$	196	
153		2-Chloro-1-phenyl-1-penten-3-ol	0.21	$C_{11}H_{13}ClO$	196	
154		4-Amino-6-methyl-1,5,6,8-tetrahydropyrido[2,3-d]pyrimidin-2,7-Dione	23.31	$C_8H_{10}N_4O_2$	194	
155		4,5-Dimethoxy-2-(2-propenyl)phenol	13.42	$C_{11}H_{14}O_3$	194	
156		Phenol, 2,6-dimethoxy-4-(2-propenyl)-	10.55	$C_{11}H_{14}O_3$	194	
157		5-Methyl-7-(trimethylsilyl)-4-hepten-6-in-2-one	8.50	$C_{11}H_{18}OSi$	194	
158	16.63	2-Methyl-5-methoxy-6-hydroxybenzofuran	7.18	$C_{11}H_{14}O_3$	194	0.48
159		Phenol, 2,6-dimethoxy-4-(2-propenyl)-	10.55	$C_{11}H_{14}O_3$	194	
160		2-Amino-6-methyl-3,5,6,8-tetrahydropyrido[2,3-d]pyrimidin-4,7-Dione	5.79	$C_8H_{10}N_4O_2$	194	
161		(E)-1-(4-methylphenyl)-2-phenylethene	4.32	$C_{15}H_{14}$	194	
162		2',6'-Difluorophenyl 10-Methylacridan-9-carboxylate	3.64	$C_{21}H_{15}F_2NO_2$	351	
163		1-{2'[(Trimethylsilyoxy) carbonyl]piperidin-1'-yl}-3,7-bis[(trimethylsilyloxy)carbonyl]-7-(trimethylsilyl)amino-4-azaheptane	16.35	$C_{26}H_{57}N_3O_6Si_4$	619	
164	29.23	4-sphingenine methaneboronate	16.35	$C_{19}H_{38}BNO_2$	323	0.70
165		1,4-Bis[(Trifluoromethanosulfonyl) oxy]benzene	4.98	$C_8H_4F_6O_6S_2$	374	
166		Morpholine, 4-(2-methyl-1-propenyl)-	3.52	$C_8H_{15}NO$	141	
167		Borane, trichloro-	2.97	BCl_3	116	
168		strongyloster (tursch) #158-4	2.62	$C_{30}H_{50}O$	426	

169		(E/Z)-1-Tosyl-1-(tetrahydro-2-furanyl)-1-butene	2.32	$C_{15}H_{20}O_3S$	280	
170		Boron trichloride	2.97	BCl_3	116	
171		8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, endo-	1.82	$C_8H_{15}NO$	141	
172		(3S,3aS,4S,5S,7S,7aS)-7-Iodo-4,5-di(4-methoxybenzyl)oxy-3-methyl-3a, 4,6,6,7,7a-hexahydrobenzo[b]furan-2(3H)-one	56.38	$C_{25}H_{29}IO_6$	552	
173		Digitoxigenin 3-tert-Bytyldimethylsilyl Ether	17.19	$C_{29}H_{48}O_4Si$	488	
174		1-Benzenesulfonyl-3-(6-butyl-2-thiophen-2-ylpyrimidin-4-yl)-1H-indole	10.42	$C_{26}H_{23}N_3O_2S_2$	473	
175		Methyl 8-hydroxy-10-(tributylstannyl)-4Z,9E-decadienoate	7.77	$C_{23}H_{44}O_3Sn$	488	
176		1,4-Dimethyl-3-(((tert-butyldimethylsilyl)oxy)methyl)-3-methoxy-6-(3'-((ter-butyldimethylsilyl)oxy)propyl)-2,5-piperazinedione	6.56	$C_{23}H_{48}N_2O_5Si_2$	488	
177	30.35	3-tert-Butyldimethylsiloxycyclohex-1-enyl(dimethylamino)methylene pentacarbonylchromium	1.28	$C_{20}H_{29}CrNO_6Si$	459	3.50
178		[.eta(5).Pentamethylcyclopentadienyl]cobalt-. eta(6).-tricyclo[6.4.0.0(3,6)]-2,4,4,5,5,7-hexamethyl-2,7-diboradodeca- 1,3,9,11-tetraene	0.26	$C_{26}H_{37}B_2Co$	430	
179		[3-Deuterium)-ç-tocopheryl methyl ether	0.03	$C_{29}H_{49}DO_2$	430	
180		bis[.eta(5).-Pentamethylcyclopentadienylcobalt]-.eta(6).-tricyclo[6.4.0.0(3,6)]-2,4,4,5,5,7-hexamethyl-2,7-diboradodeca-1,3,9,11-t Etraene	0.01	$C_{36}H_{52}B_2Co_2$	624	
181		(5-(Hexylsulfanyl)-3-(trimethylsilyl)biphenyl-2-yl)phenylmethan One	0.01	$C_{28}H_{34}OSSi$	446	
182		6-(4-Chlorophenyl)-2,5,5-triphenyl-5,8-dihydro-6H-azeto[1,2-a][1,3]thiazolo[4,5-d]pyrimidine	65.44	$C_{31}H_{22}ClN_3S$	503	
183		N(1)-{4'-[3''-Oxo-4''-(p-fluorophenyl)-3'',3''a,4'',5''-tetrahydro-2''-methyl-(2H)-6''-indazolyl)]phenyl}-5-chloro-2-methoxybenzamiDe	14.93	$C_{28}H_{23}ClFN_3O_3$	503	
184	31.43	3-(5'-Chloro-1',3'-diphenylpyrazol-4'-yl)-1-oxo(1H)-pyrido[2,1-b]benzothiazole-2,4-carbonitrile	12.03	$C_{28}H_{14}ClN_5OS$	503	0.37
185		eicosamethylcyclodecasiloxane	2.40	$C_{20}H_{60}O_{10}Si_{10}$	740	
186		Cyclodecasiloxane, eicosamethyl-	2.40	$C_{20}H_{60}O_{10}Si_{10}$	740	
187		1-Phenyl-3-(2''-chlorophenyl)-6-(p-chlorophenyl)-3a,4,4a,7a,8,8a-hexahydro-4,8-epoxypyrrolo [3,4-f]indazole-5,7-(1H,6H)-dione-	1.69	$C_{27}H_{19}Cl_2N_3O_3$	503	
188		1H-Purin-6-amine, [(2-fluorophenyl)methyl]-	1.04	$C_{12}H_{10}FN_5$	243	

189		2-Chloro-3-(2-chlorophenyl)-6-phenyl-3,6-dihydro-2H-1,3,2-oxazaphosphinine 2-oxide #	7.47	$C_{15}H_{12}C_{l2}NO_2P$	339	
191		2-chloro-3-(ortho-chlorophenyl)-6-phenyl-3,4-dihydro-1,3,2-oxazaphosphorin-2-oxide	6.60	$C_{15}H_{12}Cl_2NO_2P$	339	
192		2',4'-Dibutyl-6'-hydroxymethyl-4-nitrobiphenyl	4.53	$C_{21}H_{27}NO_3$	341	
193		3-(2-Hydroxy-2,2-diphenylethyl)-1H-quinoxaline-2-thione	4.35	$C_{22}H_{18}N_2OS$	358	
194		Ethyl 2-[3'-(p-chlorophenyl)-4',5'-dihydrofuran-2(3H)-ylidene]-propion Ate	3.85	$C_{15}H_{17}ClO_3$	280	
195	31.76	N-[3,3-bis(dimethylamino)-1-ethylthio)-2-propenylidene]benzolsUlfonamide	3.85	$C_{15}H_{23}N_3O_2S_2$	341	0.68
196		Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, acetate (ester),(5à,6à)-	3.85	$C_{20}H_{23}NO_4$	341	
197		4-acetyloxyimino-6,6-dimethyl-3-methylsulfan YL-4,5,6,7- tetrahydro-benzo [C]thiophene-1-carboxylic acid methyl ester	3.70	$C_{15}H_{19}NO_4S_2$	341	
198		4-Acetyloxyimino-6,6-dimethyl-3-methylsulfanyl-4,5,6,7-tetrahydro-benzo[c]thiophene-1-carboxylic acid methylester	3.70	$C_{15}H_{19}NO_4S_2$	341	
199		3-hydroxy-2-(3,4-dimethoxyphenyl)-6,7-dimethoxytetralone	2.90	$C_{20}H_{22}O_6$	358	
200		Methyl 5-(p-bromophenyl)amino-2-(tri-n-butylphosphoranylideneamino)-1,4-benzoquinone -3-carboxylate	37.28	$C_{26}H_{36}BrN_2O_4P$	550	
201		Rhodium Bromo[(1,2,3,4,5-.elita.) -1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl] (3-thienyl) (trimethylphosphine)	7.58	$C_{17}H_{27}BrPRhS$	476	
202		Rhodiumbromo[(1,2,3,4,5-.elita.) -1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl](2-thienyl)(trimethylphosphine)-	5.35	$C_{17}H_{27}BrPRhS$	476	
203	33.57	2,2'-dioxospirilloxanthin	4.52	$C_{42}H_{56}O_4$	624	1.72
204		Carotene, 3,3',4,4'-tetradehydro-1,1',2,2'-tetrahydro-1,1'-dimethoxy-2,2'-dio xo	4.52	$C_{42}H_{56}O4$	624	
205		1,5-Dichloro-9,10-bis(p-diphenyl)anthracene	4.17	$C_{38}H_{24}Cl_2$	550	
206		Methyl (E)-3-(2,3-dichlorophenyl)-2-(thiomethyl)-2-propenoate dimer	3.28	$C_{22}H_{18}Cl_4O_4S_2$	550	
207		(22S,24R)-3á-Acetoxy-22-bromo-24-methyl-5à-cholestan-6,23-d Ione	2.18	$C_{30}H_{47}BrO_4$	550	
208		(Trimethylsilyl)adamantanole	1.76	$C_{13}H_{24}OSi$	224	
209		Nabilone, tert-butyldimethylsilyl ether	1.69	$C_{30}H_{50}O_3Si$	486	
210	35.10	trans-3,4,5-Trimethoxy-7-phenyl-8-trimethylsilyl-7-(trimethylsilyloxy)bicyclo[4.2.0] octa-	5.35	$C_{23}H_{34}O_4Si_2$	430	6.0

		1,3,5-triene				
211		Cholan-24-oic acid, 3,12-bis(acetyloxy)-,methylester, (3á,5à,12à)-	3.99	$C_{29}H_{46}O_6$	490	
212		Cholan-24-oic acid, 3,12-bis(acetyloxy)-, methylester, (3á,5à,12à)-	3.99	$C_{29}H_{46}O_6$	490	
213		(22S,23S,25R)-3-ü-Methoxy-16á,23:22,26-diepoxy-5à-cholestane	3.84	$C_{28}H_{46}O_3$	430	
214		(N-(methylthiomethyl) trimethylsilylamino) (trimethylsilylamino) (trimethylsilylimino) (trimethylsiloxy) phosphorane	3.39	$C_{14}H_{42}N_3OPSSi_4$	443	
215		5-(3,6-Di-t-butyl-1-azulenyl)-5H-dibenzo[a,d]cycloheptene	3.26	$C_{33}H_{34}$	430	
216		epoxygedunin	3.26	$C_{28}H_{34}O_8$	498	
217		D-Homo-24-nor-17-oxachola-20,22-diene-3,16-dione,7-(acetyloxy)-1,2:14,15:21,23-triepoxy-4,4,8-trimethyl-	3.26	$C_{28}H_{34}O_8$	498	
218		3,3,7,8-tetramethyl-11-(4-trifluoromethoxy-phenyl)-2,3,4,5,10,11-hexahydro-dibenzo[B,E][1,4]diazepin-1-one	2.56	$C_{24}H_{25}F_3N_2O_2$	430	
219		Pregn-4-ene-3,20-dione, 11,21-dihydroxy-,(11á)-	2.56	$C_{21}H_{30}O_4$	346	
220		Cyclodecasiloxane, eicosamethyl-	5.46	$C_{20}H_{60}O_{10}Si_{10}$	740	
221		eicosamethylcyclodecasiloxane	5.46	$C_{20}H_{60}O_{10}Si_{10}$	740	
222		Cyclotetrasiloxane, (iodomethyl)heptamethyl	4.61	$C_8H_{23}IO_4Si_4$	422	
223	35.96	Cyclotetrasiloxane, (iodomethyl)heptamethyl-	4.61	$C_8H_{23}IO_4Si_4$	422	0.35
224		Fumarylacetoacetic acid, tetrakis(O-trimethylsilyl)-	4.07	$C_{20}H_{40}O_6Si_4$	488	
225		1H-Purin-6-amine, [(2-fluorophenyl)methyl]-	3.91	$C_{12}H_{10}FN_5$	243	
226		fumarylacetoacetic acid	3.76	$C_{20}H_{40}O_6Si_4$	488	
227		6-(4-Chlorophenyl)-2,5,5-triphenyl-5,8-dihydro-6H-azeto[1,2-a][1,3]thiazolo[4,5-d]pyrimidine	62.09	$C_{31}H_{22}ClN_3S$	503	
228		2,9-Bis(5-tert-butyl-2-methoxyphenyl)-1,10-phenanthroline	12.99	$C_{34}H_{36}N_2O_2$	504	
229	37.18	N(1)-{4'-[3"-Oxo-4"-(p-fluorophenyl)-3",3"a,4",5"-tetrahydro-2"-methyl-(2H)-6"-indazolyl)] phenyl}-5-chloro-2-methoxybenzamide	7.87	$C_{28}H_{23}ClFN_3O_3$	503	0.81
230		3-(5'-Chloro-1',3'-diphenylpyrazol-4'-yl)-1-oxo(1H)-pyrido[2,1-b]benzothiazole-2,4-carbonitrile	7.87	$C_{28}H_{14}ClN_5OS$	503	
231		1-Phenyl-3-(2"-chlorophenyl)-6-(p-chlorophenyl)-3a,4,4a,7a,8,8a-hexahydro-4,8-epoxypyrrolo [3,4-f]indazole-5,7-(1H,6H)-dione-	1.88	$C_{27}H_{19}Cl_2N_3O_3$	503	
232		deuteratedetioporphyrine	0.85	$C_{32}H_{15}D_{23}N_4$	478	

233		3,3-(Ethylidenedioxy)-20-(tert-butyldimethylsilyloxy)-5-pregnen-7-one	0.64	$C_{30}H_{50}O_4Si$	502	
234		deuteratedetioporphyrine	0.85	$C_{32}H_{14}D_{24}N_4$	478	
235		Androstane,17-(2(5H)-oxofuran-4-yl)-3-(t-butyldimethylsilyloxy)-14-(trimethylsilyloxy)-	0.27	$C_{32}H_{56}O_4Si_2$	560	
236		Androstane,17-(2(5H)-oxofuran-4-yl)-3-(t-butyldimethylsilyloxy)-14-(trimethylsilyloxy)-	0.27	$C_{32}H_{56}O_4Si_2$	560	
237		4,4-dimesityl-11,12-bis(methoxycarbonyl)-3,5,9-trioxa-4-silabicyclo[5.3.2]dodeca-1(10),7,11-triene	26.48	$C_{30}H_{34}O_7Si$	534	
238		17-Methyl[2.2.2](1,3,5)benzeno(3,3',3")triphenylmethanophane	13.65	$C_{32}H_{30}$	414	
239	38.08	1,5-Dimethyl-6-(1,5-dimethylhexyl)-15,16-epoxy-18-oxatetracyclo[9.6.1.0(2,10).0(5,9)]octdecane-13-one	7.04	$C_{28}H_{46}O_2$	414	13.80
240		24(Z)-methyl-25-homocholesterol	7.04	$C_{29}H_{50}O$	414	
241		Spirostan-3-one, (5à,25R)-	6.76	$C_{27}H_{42}O_3$	414	
242		ç-Sitosterol	4.10	$C_{29}H_{50}O$	414	
243		stigmast-5-en-3-OL, (3á,24S)-	4.10	$C_{29}H_{50}O$	414	
244		3-Methoxyergost-8(14)-ene	2.48	$C_{29}H_{50}O$	414	
245		Dimethyl-bis[(trimethylsilyl)-2-thienyl]germane	1.95	$C_{16}H_{28}GeS_2Si_2$	414	
246		1,2-Bis(2'-quinolylmethyl)ethylene	30.05	$C_{20}H_{14}N_2$	282	
247		3',4'-Dihydroxy-(mono-14C)-sudan	13.69	$C_{16}H_{12}N_2O_3$	280	
248		(+-)-(2-Hydroxy-1 naphthyl)methylphenylphosphine Oxide	9.93	$C_{17}H_{15}O_2P$	282	
249		15(13-12)-abeo-Isopimara-8,11,13,15-tetraen-7-one	5.12	$C_{20}H_{26}O$	282	
250		(1-cycloxexen-1-YL)-diphenylphosphanoxide	3.61	$C_{18}H_{19}OP$	282	
251	39.10	2-(3,4-Dimethoxyphenyl)-5-(4-methyl-1-piperazonyl)-1H-benzimidazole	3.05	$C_{20}H_{24}N_4O_2$	352	2.22
252		3-(4-Fluorophenyl)-5-cyano-11-iminopyrano[4,3-b]quinolizine	2.40	$C_{19}H_{10}FN_3O_2$	331	
253		tetramethyl 1,2-diazine-3,4,5,6-tetracarboxylate	1.84	$C_{12}H_{12}N_2O_8$	312	
254		4,4'-(1,4-butanediyl)bis[1,4-dihydro-2,4-diphenylquinazoline	1.55	$C_{44}H_{38}N_4$	622	
255		[(2'-Naphthyl)-phenyl-(methyl)]-phosphinate	1.37	$C_{17}H_{15}O_2P$	282	
256		cis-trans-cis-2,4,6,8-Tetramethyltetraphenylcyclotetrasiloxane	34.67	$C_{28}H_32O_4Si_4$	544	
257		ç-chloro-aetio-à-oxophlorin	8.89	$C_{32}H_{37}ClN_4O$	528	
258	40.12	2-(2,4,6-Trimethylphenyl)butylamine	6.98	$C_{13}H_{21}N$	191	2.09
259		Tetramethyl ester of 4-(2-Cyano-1-methylethenyl)-7b,11a-dihydrobenzo[a]pyrrolo[1',2':3,4]pyrimido[6,1,2cd]pyrrolizin-8,9,10,11-tetracarboxylic acid	5.63	$C_{28}H_{23}N_3O_8$	529	

260		2-[4-(2-Cyanoethylthio)-5-methylthio-1,3-thiole-2-ylidene]-N-tosyl-[1,3]-dithiolo[4,5-c]pyrrole	4.31	$C_{19}H_{16}N_2O_2S_7$	528	
261		Ethyl 5-Acetyl-3-(3-chloro-1,1,2,2,3,3-hexafluoropropyl)-4-methylene pyrrolo[1,2-a]quinoxaline-2-carbaxylate	3.64	$C_{25}H_{19}ClF_6N_2O_2$	528	
262		9-(4',5'-Diethylsulfanyl-1',3'-dithiol-2'-ylidene)-10-(4",5"-dimethyl-1",3"-dithiol-2"-ylidene)-9,10-dihydroanthracene	3.36	$C_{26}H_{24}S_6$	528	
263		8-(Methoxymethyl)-6-methyl-2-(2"-thienyl)-4H-[1]-benzopyran-4-one	2.50	$C_{16}H_{14}O_3S$	286	
264		2,5-[Bis((4,5-di(methoxycarbonyl)-1,3-dithiaol-2-ylidene)methyl]furan	2.41	$C_{20}H_{16}O_9S_4$	528	
265		(6,7-Methylenedioxy)coumarin	2.31	$C_{10}H_6O_4$	190	

5. Conclusion

In this study, flash pyrolysis of the cotton shell was carried out in an electrically heated fluidized bed reactor with nitrogen gas atmosphere. In this study, pyrolysis temperature was shown to be a significant process parameter as it determines the product yields. The maximum yield of 51 % was obtained at an optimum pyrolysis condition of pyrolysis temperature 450 °C, The pyrolysis oil was identified as a biofuel candidate. The liquid may be used as a source of low-grade fuel directly or it may be upgraded to high quality liquid fuel. Analytical methods for the identification of bioactive compounds are the key to studying their formation and functions in biological interactions. The present study successfully identified their hydrocarbons and other bioactive compounds present in the cotton shell pyrolysis oil and the GC–MS measurement is achieved in a fully programmed way, the presented approach offers an interesting and powerful tool for the study of the dynamic range of bioactive compounds. The application of the method resulted in the identification of more than 250 different bioactive compounds, which have not been ascribed to pyrolysis oils so far.

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