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Data Article

Biochemical characterization data from Fourier transform infra-red spectroscopy analyses of *Rhizophora mangle* L. bark-extract

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ABSTRACT

This article presents biochemical characterization data, of organic functional groups and 3-D optimized structures of identified organic chemicals, from the Fourier transform infra-red (FT-IR) spectroscopy analyses of *Rhizophora mangle* L. bark-extract. Spectral plot from FT-IR spectroscopy instrumentation application to the *Rhizophora mangle* L. bark-extract, which includes numerical data of adsorbed frequencies for indicating fingerprints/vibration modes of organic functional groups, is supplied in the paper. The obtained spectrum was also rendered to the computer-based Euclidean Search® of the Fluka Library® reference database, for obtaining hit-list of organic chemical compounds constituted in the bark-extract. Adsorbed functional groups from the FT-IR spectroscopy, including N–H, C–N, –C≡N, O–P(=O)(H–O) and S-containing ligands, are corroborated by the chemical compounds identified by the computer-based hit-list. These data of biochemical constituent characterizations are useful for gaining insights into the prospects of using bark-extract from *Rhizophora mangle* L. natural-plant for corrosion-protection of metallic materials in aggressive service-environments.

Specifications table

Subject area	*Engineering, Materials Science and Engineering, Chemical Engineering, Biochemistry, Organic Chemistry, Spectroscopy, Plant Science*
Compounds	*Bio-organic chemical functional groups, bio-organic chemical compounds*
Data category	*Fourier transform infra-red spectroscopic spectrum, numerical data of adsorbed frequencies of organic functional groups, computer-based Euclidean Search hit list from Fluka Library*
Data acquisition format	*Spectrum from FT-IR spectroscopy instrumentation, analyzed for organic bio-constituent characterization*
Data type	*Spectrum, in-plot numerical data of adsorbed ligand frequency on FT-IR spectrum, computer-based Euclidean Search hit list of organic chemical rendered in 3-D optimized structure*
Procedure	*Methanolic extract of Rhizophora mangle L. bark was mounted in KBr pellet on the Spectrum BX® model of Perkin-Elmer® FT-IR spectrophotometer instrument. The FT-IR spectrum acquired was rendered to the Euclidean Search of the Fluka Library of the Perkin-Elmer® instrument*
Data accessibility	*A comprehensive dataset of physicochemical and mineralogical characterization of oil drill cuttings for comparison with other types of cement and assessing suitability for partial replacement of cements in concrete is provided in this article*

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1. Rationale

Metallic materials for many engineering applications are employed in service-environments that are aggressively corrosive, in detriments to the durability, in-service performance, and structural integrity of the materials and of the installation of their application [1-8]. Averting catastrophic failure from insidious corrosion deterioration of metals and the attendant huge costs necessitates use of methods for mitigating the metallic corrosion in their service-environments [9-13]. A highly effective and low cost approach for metallic corrosion-protection includes use of corrosion inhibitors, for which studies have reported effective corrosion inhibiting substances for specified metals in also specified aggressive environments [14-17]. Problems arise, however, from the toxicity, hazardousness, and the non-environmentally friendliness of corrosion inhibitor compounds, either from their synthesis procedures or applications for corrosion inhibition [2,18-23]. These engender interests in the search for environmentally-friendly ‘green’, i.e. non-toxic and non-hazardous, corrosion inhibiting substances.

It has been identified in reported works that extracts from plants are highly rich bio-resource of naturally synthesized mixtures of organic compounds combining advantages of non-toxicity, eco-friendliness, biodegradability, renewability, cost-effectiveness with positive potentials of metallic corrosion-protection [24-30]. Extracts of natural-plants, especially habitat in West Africa had been used for inhibiting metallic corrosion. Among them are *Anthocleista djalonensis* [31-35], *Cassia fistula* [24,25], *Cymbopogon citratus* [11,19,36-38], *Morinda lucida* [29,39], *Phyllanthus muellerianus* [40,41], *Phyllanthus amarus* [42,43], *Solanum aethiopicum* [45,46], *Spondia mombin* L. [47], *Rhizophora mangle* L. [28,48-50], and *Terminalia catappa* [22,51]. These extracts have been employed for the corrosion inhibition of metals including aluminum [24,35,43,47], carbon steel [37,38,42], mild steel [22,34,44,51], reinforcing steel in concrete [11,19,29,31-33,36,39-41,45,46,48-50] and stainless steel [25]. Also, these had been used for aggressive media such as acidic sulfate/industrial/microbial [22,24,25,29,33,38,40,44-45,47,49,50], hydrochloric acid [44,51], sodium chloride/saline [39,41,46,48], alkaline [44] and produced water [37] environments.

It is well-known that major factors supporting the suitability, for metallic corrosion-protection application, of a particular extract from natural-plant include the biochemical constituents of the extract [52]. This is because the bio-constituent characterizations of the plant-extracts are also useful for elucidating the corrosion-protection mechanisms of the extracts on the specified metallic material and in the specific environment of their anticorrosion application [42,53,54]. Methods that could be used for detailing organic components constituted in a specific plant-extract include the phytochemical screening procedures and the use of spectroscopy analyses [55-57]. The phytochemical screening method employs systems of set procedures involving chemical reactions, and with the needs to visually observe the reaction product for qualitative determination of the presence or otherwise of a specific constituent, for each system of set procedures. By this, identifications different phytochemical compounds require different system of set procedures for each specified compound. In contrasts, the spectroscopy analyses utilize specialized and robust instrumentation that is capable of identifying wide range of functional groups constituted in given test-sample, via a single application of the spectroscopy instrumentation. Particularly, the FT-IR spectroscopy analyses have the advantage of functional group identifications from characteristic and reproducible vibrations at the frequencies of electromagnetic radiation (infra-red light) adsorptions by the structural features of the chemical compounds constituted in the test-sample. These vibrations at adsorption frequencies also find usefulness for indicating backbones or fingerprints organic ligands within the spectra that could be further subjected to comparisons with references and databases [58-60].

Unlike many other plant-extracts that had been used for metallic corrosion-protection in aggressive environments, there is dearth of study on the biochemical characterization of the bark-extract from *Rhizophora mangle* L., especially via use of FT-IR spectroscopy analyses. While a recent research work published elsewhere [61] has included *R. mangle* L. leaf-extract characterization, there is dearth of study in the literature that has presented data on the FT-IR based characterization of *Rhizophora mangle* L. bark-extract. Therefore, this article presents data of biochemical characterization of organic bio-constituents from the Fourier transform infra-red (FT-IR) spectroscopy analyses of *Rhizophora mangle* L. bark-extract. Thus, the present data article will be both useful for complementing the cited work in [61] and for comparisons of the biochemical compounds that are constituted in the leaf as well as the bark of *R. mangle* L. natural-plant.

2. Procedure

Extract from the dried bark of *Rhizophora mangle* L. (*R. mangle* L.) Rhizophoraceae (identified at Forestry Research Institute with the voucher FHI No. 109501) was obtained using method that has been detailed in [61,62]. The bark of *R. mangle* L. natural-plant itself was sourced from Ehin-moore, at Ilaje Ese-odo environs in Ondo State, Southwest Nigeria [61]. The bark-extract was grinded in pestle into powdery form before mixing with KBr (potassium bromide) for hydraulically pressing into pellet [61,63], using the Specac® Press from Perkin–Elmer®. The obtained pellet held in cell holder for mounting on a Spectrum BX® model of FT-IR spectrophotometer equipment, also from Perkin–Elmer®. This FT-IR instrument has interface with Spectrum V5.3.1 software installed on an Intel® Core 2 Pro computer. It is from this system that the *R. mangle* L. bark-extract FT-IR spectrum for the study was obtained.

From the software system of the Spectrum BX®, and after the FT-IR spectrum for the *R. mangle* L. bark-extract had been obtained, the spectrum was first processed for the numerical indication, directly on the FT-IR spectrum chart, of the

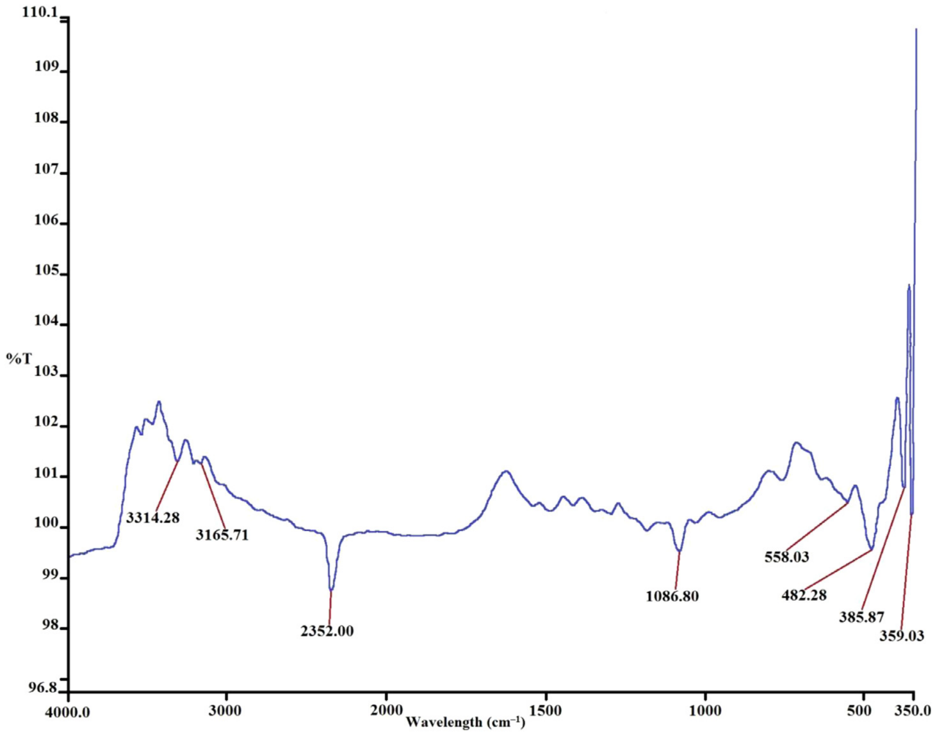


Fig. 1. FT-IR spectrum of *R. mangle* L. bark extract obtained from the Spectrum BX®, FT-IR spectrophotometer of the Perkin–Elmer® system.

adsorption band frequencies for the functional groups present in the *R. mangle* L. bark-extract being studied. After this, the FT-IR spectrum of the *R. mangle* L. bark-extract was also rendered to the computer-based search utilizing the Euclidean Search® of the Fluka® Library reference database, also supplied by Perkin–Elmer® for obtaining hit-list of organic chemical compounds.

The 3-D optimized structure of the organic compounds from the Euclidean Search® hit list was obtained through use of the Jmol® software development version 14.20.3, from Oracle Corporation® as the Java® vendor, and which therefore runs through platform of the Java® software, version 1.8.0_171.

3. Data, value and validation

The spectrum obtained from the FT-IR spectroscopy analyses of *R. mangle* L. bark-extract is presented in Fig. 1. The horizontal axis indicates the absorbance frequencies, while the vertical axis in the spectrum is for indicating the percentage transmitted intensity relative to the input intensity, hence its representation as %T (i.e. %transmittance). On the spectra chart in the figure, the numerical data adsorbed band frequencies, in cm^{-1} unit, of organic functional group, representing backbones and fingerprints of organic chemical compounds that were naturally synthesized in the bark by the *R. mangle* L. natural-plant, are indicated.

3.1. Values of the R. mangle L. FT-IR spectrum

The value of the *R. mangle* L. bark-extract FT-IR spectrum first followed from the adsorbed band frequencies. These include the fact that the numerical data of adsorbed frequencies can be subjected to interpretations from the literature for assignments that suggest the functional group(s) of organic chemical(s) that adsorbed or overlapped at each of the bands of frequencies. This value is explored in Table 1 for assigning the numerical data of absorbed bands of frequency to fingerprints and overlaps of organic functional groups. For these assignments in the table, validation obtained from standard assignments that had been detailed in the literature [60,64-67], especially for indicating presence or absence of specific functional groups known with vibrations exhibiting particular frequency of adsorption band.

Another value of the *R. mangle* L. bark-extract FT-IR analyses follows from the rendering of the bark-extract spectrum to the computer-based Euclidean Search® hit list of the Fluka® Library reference database of the Perkin-Elmer® facility [36,53,55-57]. These further gave the dataset of organic chemical compounds presented in Table 2. The content of Table 2 includes:

Table 1
Assignments of adsorbed band frequency data from FT-IR spectrum of *R. mangle* L. bark-extract.

S/no.	Adsorption frequency (cm^{-1})	Chemical bond	Compound type(s)
1.	3314.28	N–H stretch	Amines or amino compounds
2.	1086.80	C–N stretch (overlapping with)	Amines or amino compounds (and, due to the overlaps)
		H–P–H in-plane scissors and/or P–O–C stretch	Phosphonic or phosphinic derivatives
3.	3165.71	=C–H stretching vibration	Unsaturated alkenes and/or arenes[a]
4.	385.87	C–H bending overlap(s)	Mono/multiatomic ring substitution of the aromatic H–bond by X–group ligand
5.	359.03		
6.	2352.00	Multiple bond overlaps of bonds such as: triple bonds C≡C, –C≡N, or Accumulated double bonds of the form –C=C=C–, –N=C=O; more specifically, –C≡N → O group overlap	Nitrile oxide
		Or	Or
		P–H stretching vibration characteristics of O–P(=O)(H–O) of phosphonic or of O–P(=O)(H–O) or of phosphinic derivatives	Suspects of hetero-oxy compounds[b]
7.	558.03	C–S stretching vibration	Aliphatic halogenated compound or overlap of S-containing or other ligand substitutions
8.	482.28	or C–Cl stretching vibration	

[a] It is worth noting that the non observation of absorption band characteristics of C=C (alkenes/arenes) at 1600 cm^{-1} in the *R. mangle* L. bark-extract FT-IR spectrum further hinted on a para system of arenes having center of symmetry that eliminates change in dipole moment during vibration via rule of mutual exclusion [66].

[b] These suspects follows from the combining the adsorption at 2352.00 cm^{-1} with the multiple (identified and unidentified) bands observable from the lesser than 1500 cm^{-1} region of the *R. mangle* L. bark-extract FT-IR spectrum [60,67].

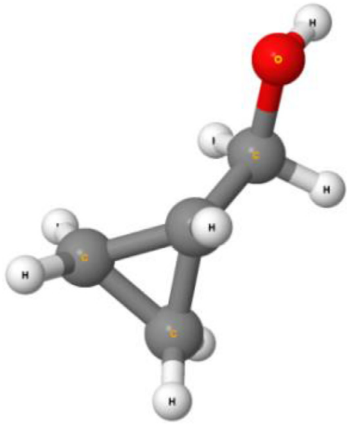
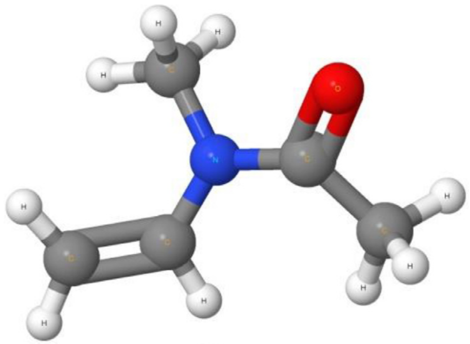
- The Fluka number, by the Spectrum BX® system and which is useful for validating the link of the identified compound to the Fluka® Library from which they were obtained;
- The chemical formula; and
- The nomenclature of chemical compound;
- The 3-D optimized structure of each chemical compound, via the Jmol® software usage.

In furtherance of data value detailing, the FT-IR spectroscopy analyses of *R. mangle* L. bark-extract from the present study foster comparisons with what obtained from the similar spectroscopy applications to the leaf-extract from this same natural-plant in the recently published research detailed in [61]. By these comparisons, therefore, it could be noted from Fig. 1 that the FT-IR spectra of the bark-extract exhibited the contrasts of being more predominated with weak to medium adsorbed frequencies. This is much unlike the FT-IR spectra obtained from the leaf-extract of *R. mangle* L. in [61], which exhibited more of strong and sharp frequency vibration modes. However, both the bark-extract, from the present work, and the leaf-extract from the recent study, exhibited the similarities of constituting N-, S-, Cl- and O-containing ligands, as detailed in Table 1, from their FT-IR spectroscopy analyses. Despite these, it is worth noting from Table 2 that all the ten biochemical compounds identified via computer-based reference database searching for the bark-extract in the present data article are entirely different from those identified for the leaf-extract of *R. mangle* L. in [61]. This is unlike the biochemical compounds identified from other studies on FT-IR spectroscopy applications to extract from leaves of other plants [36,53,55-57,61], and from which some similarities of biochemical compounds among the leaf-extracts were observed. Yet, the findings from those studies on the positive performance of heteoratomic/lone-pair rich organic compounds constituted plant-extracts on metallic corrosion-protection strongly spark interests on utilizing the also lone-pair rich *R mangle* L. bark-extract, from this work, for anticorrosion applications.

Overall, these detailed data of *R. mangle* L. bark-extract biochemical characterization from the FT-IR analyses of the natural plant find useful values that include the following.

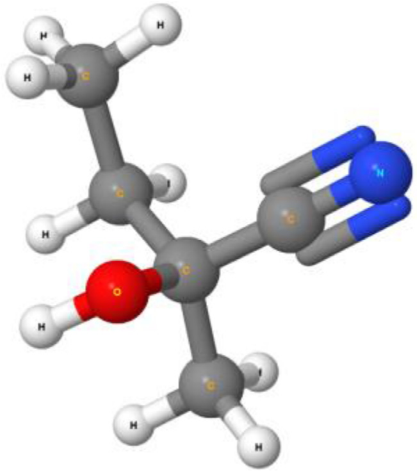
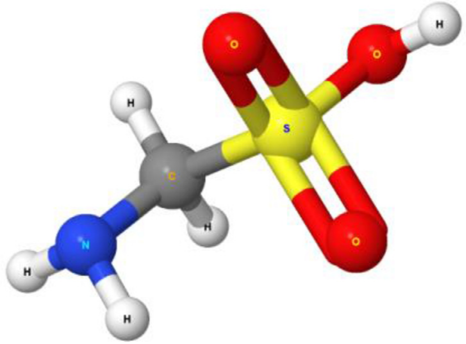
- Since reports from studies showed that N-, S-, P- and O-containing, and lone-pair/π-electrons rich, organic compounds are effective corrosion inhibitors [10,26,68,69], these ligands-containing compounds also identified in this study can be further investigated for metallic corrosion-protection [70];
- The identified ligands of organic functional groups can lend understanding to the corrosion-protection effects and mechanisms observed from using *R. mangle* L. bark-extract on metallic materials in aggressive environments [53,59];
- Knowledge of the organic compound bio-resources identified in the *R. mangle* L. bark-extract can engender further research on usage of the bark-extract on metallic materials and/or corrosive environments for which the natural-plant has not yet been studied for anticorrosion application;
- The characterized bark-extract and the identified naturally-synthesized biochemical compounds can promote usage of environmentally-friendly corrosion inhibitors that combine lower costs, non-toxicity, and non-hazardousness to the environment with positive effectiveness on corrosion-protection for metallic materials in aggressive environments.

Table 2
Euclidean search hit list of the compounds from R. mangle L. bark-extract FT-IR analyses.

S/no.	Fluka® no.	Molecular formula	Chemical nomenclature	3-D optimized structure
1.	F55660	$\mathbf{C_4H_8O}$	(Hydroxymethyl) cyclopropane	
2.	F69670	$\mathbf{C_5H_9NO}$	N-Methyl-N-vinylacetamide	

(*continued on next page*)

Table 2 (*continued*)

S/no.	Fluka® no.	Molecular formula	Chemical nomenclature	3-D optimized structure
3.	F55622	**C_5H_9NO**	2-Hydroxy-2-methylbutanenitrile	
4.	F08398	**CH_5NO_3S**	Aminomethanesulfonic acid	

(*continued on next page*)

Table 2 (*continued*)

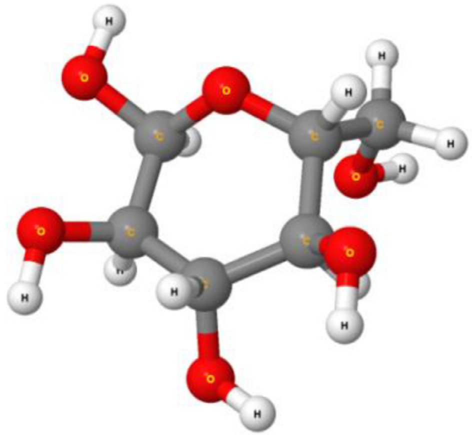
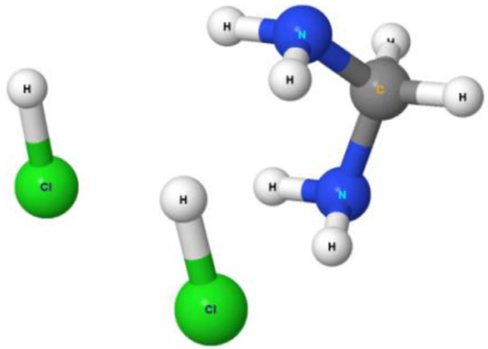
S/no.	Fluka® no.	Molecular formula	Chemical nomenclature	3-D optimized structure
5.	F49140	$\mathbf{C_6H_{12}O_6}$	D(+)-Glucose anhydrous	
6.	F66770	$\mathbf{CH_2(NH_2)_2{\cdot}2HCl}$	Methylenediamine dihydrochloride	

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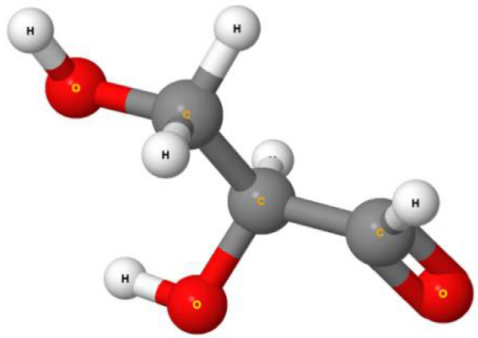
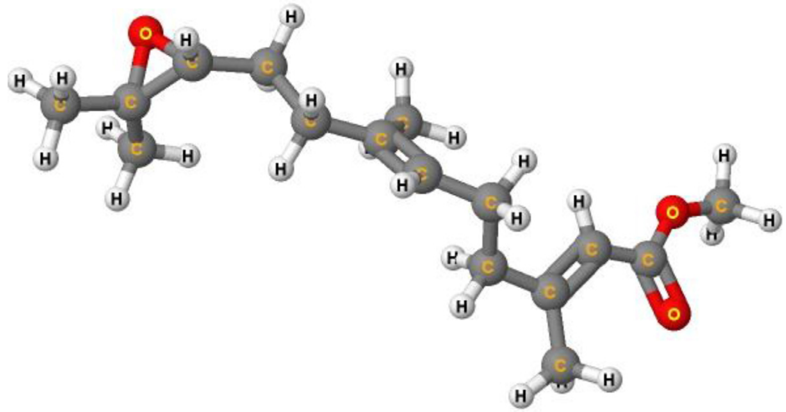
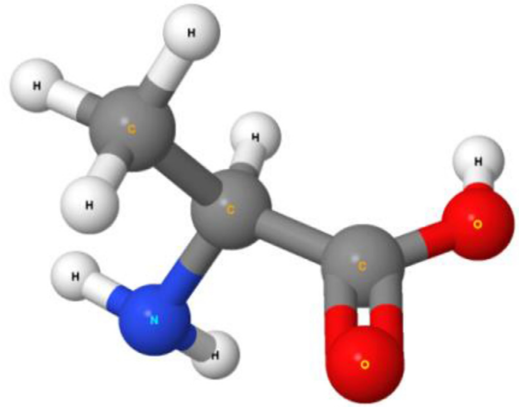
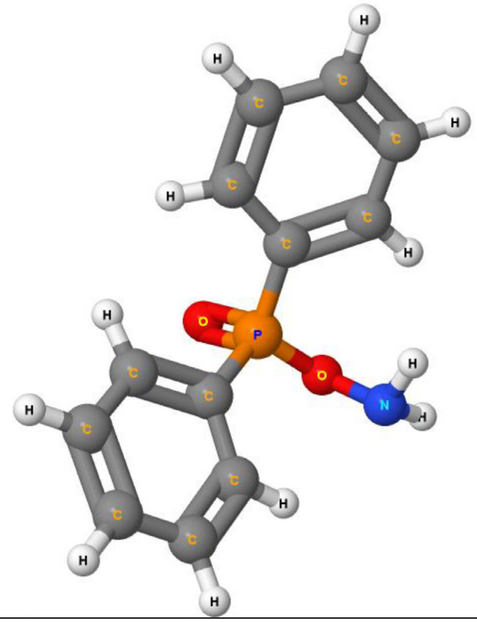
Table 2 (*continued*)

S/no.	Fluka® no.	Molecular formula	Chemical nomenclature	3-D optimized structure
7.	F49790	$\mathbf{C_3H_6O_3}$	L(−)-Glyceraldehyde unnatural form	
8.	F59992	$\mathbf{C_{16}H_{26}O_3}$	C16-Juvenile hormone	

(*continued on next page*)

Table 2 (*continued*)

S/no.	Fluka® no.	Molecular formula	Chemical nomenclature	3-D optimized structure
9.	F05150	$\mathbf{C_3H_7NO_2}$	DL-Alanine	
10.	F43154	$\mathbf{C_{12}H_{12}NO_2P}$	O-(Diphenylphosphinyl) hydroxylamine	

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cdc.2019.100177.

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