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New Aliphatic Alcohols from Seeds of *Momordica charantia* Linn. and Prediction of their Biological Activity

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ABSTRACT

Momordica charantia is a very well-known traditional medicinal herb. The current research investigation aimed towards the isolation, characterization and prediction of biological activity spectra of the phytoconstituents from the seeds of Momordica charantia Linn. (Cucurbitaceae). The Ethanolic extract of Momordica charantia seeds led to isolate two new aliphatic alcohols: n-nonatriacontan-19α-ol &n-henetetracontan-19α-ol and four known compounds: n-tetracosane, n-pentacosane, n-pentatriacontane, n-heptatriacontan-15α-ol. These isolated phytomolecules can act as the marker compounds in order to establish the identity, quality and purity of the drug. The observations of the in silico profiling of these compounds shall be very useful for the upcoming reaearchers for establishing them as pharmacologically active moieties.

Keywords: *n*-nonatriacontan-19α-ol, *n*-henetetracontan-19α-ol**,** *n*-tetracosane, n-pentacosane, *n*-pentatriacontane, *n*-heptatriacontan-15α-ol.

INTRODUCTION

Momordica charantia Linn. (Family: Cucurbitaceae) is commonly known as karela in hindi; bitter gourd, bitter cucumber, bitter melon or balsam pear in English and karavella in Sanskrit [1]. It is a monoecious annual climber which grows upto 5 m in height cultivated in East Africa, South America, China, Malaya and India upto an altitude of 1500 m and it also grows wildely in tropical and sub-tropical Africa, Asia, America and Caribbean [2]. The plant possesses thin, branched, grooved and twisted stem; glabrous leaves with margin containing sharp protruding points; solitary, unisexual, pale yellow to orange flowers; dark green oblong, 5-25 cm long pepo fruits with compressed brownish 12-16 mm long seeds embedded in red pulp [3].

The Ayurvedic Pharmacopoeia mentions the medicinal uses of *Momordicacharantia* as Laghu (easily digestible), Bhedana (purgative), Javara (fever), Tikta (bitter), Asradosa (dyscarasia), Prameha (obstinate urinary diseases including diabetes), Paandu (anaemia) and Krimi (worm infestation) [4]. Various recent pharmacological studies have displayed the medicinal potential of *M. charantia* as anti-oxidant, anti-viral, anti-bacterial, anti-HIV, anti-cancer, anti-diabetic and anthelmintic. It is also used in hypertension, obesity and modulating immune system [2,5-8]. More than 220 phytoconstituents have been isolated from leaves, fruits, stems, entire plant, pericarp, callus tissues and seeds [9] which include glycosides, alkaloids, terpenoids, fixed oils, steroids, proteins, inorganic compounds, monoterpenes, carbohydrates, benzanoids, sesquiterpenes etc. [8].

Cucurbitacins, momordicins, cucurbitanes, momordenol, cucurbitins, momordicilin, cycloartenols, galactouronic acids, goyaglycosides, multiflorenol, diosgenin, gallic acid etc. have been identified as the major constituents of *Momordica charantia* [9-11]. The major active hypoglycemic constituent is charantin also known as momorcharin which is a 1: 1 mixture of β-sitosterol β-D-glucoside and stigmastandienol β-D-glucoside [12]. Anti-diabetic effects have also been shown due to some other constituents like v-insulin, polypeptide-p, p-insulin (insulin like action) [13-15]; momordin (activates PPAR β/δ) [16]; vicine (hypoglycemic effect) [17] and momordicoside S and T (enhances glucose clearance and basal metabolic rate) [18].

MATERIALS AND METHODS

General chemical procedures

All melting points (mp) were determined in centigrade scale in one–end open capillary on a thermoelectrical melting point apparatus. The IR spectra were measured on IR affinity-1 Fourier transform infrared spectrometer model (Schimadzu). The mass spectra were recorded on a JEOL-Accu TOF (time of flight) JMS-T100LC mass spectrometer having a DART (direct analysis in real time) source. The m/z (mass to charge ratio) values of the more intense peaks are mentioned and the figure in a bracket attached to each m/z values indicated relative intensities with respect to the base peak. The ^{1}H and ^{13}C-NMR spectra were scanned on BrukerAvIII HD-300 and 75 MHz, respectively, an instrument in $CDCl_3$ and MeOD solvents using TMS as an internal standard. The coupling constants (J values) are expressed in Hertz (Hz). Column chromatography was performed on a silica gel (60-120 mesh; Qualigen, Mumbai, India) column. TLC (Thin Layer Chromatography) was run on silica gel G 60 F 254 (Qualigen) coated aluminium sheets. Spots were visualised by exposing to iodine vapors, UV (ultraviolet) radiation and spraying with ceric sulfate solution.

Plant material

The dried seeds of *Momordica charantia* were procured from KhariBaoli market, Delhi. They were authenticated by Dr. SunitaGarg, Chief Scientist, Raw Material Herbarium and Museum, Delhi (RHMD), CSIR-NISCAIR, New Delhi and assigned the voucher specimen/Accession number (Ref No. NISCAIR/RHMD/Consult/ 2015/ 2911/ 104-1). The voucher specimen is preserved in the herbarium section of Department of Pharmacognosy, KIET School of Pharmacy, Ghaziabad, Uttar Pradesh.

Extraction

The dried seeds of *Momordica charantia* (4.0 kg) were crushed to smaller pieces, re-dried, coarsely powdered, defatted with petroleum ether and then extracted in ethanol (95%) using Soxhlet Apparatus for 72 h. The extract was then concentrated under reduced pressureto yield 270.93 g (6.77%) of dark reddish brown orange mass.

Preparation of slurry

The concentrated alcoholic extract of *Momordica charantia* (45 g) was taken in a china dish, placed on water bath and methanol was added in fractions to attain the desired consistency. Silica gel for column chromatography (60-120 mesh) was added gradually with constant mixing with a stainless steel spatula to obtain the slurry required to be packed into the column. Then, it was dried in air and the larger lumps were broken up. Finally, the uniform particle size was obtained by passing it through a sieve (No. 8).

Isolation of phytoconstituents

The adsorbent cotton was plugged in the lower end of a dry column (5 feet high, 2.5 inches diameter) and then it was filled with petroleum ether upto half of its height. The required length of the packed column was obtained by adding silica gel in small proportions and allowing it to settle down. The blank column was run thrice with solvent to allow the bubbles to escape. Then the column was packed with dried silica gel slurry of the extract and the column was plugged with adsorbent cotton. Different solvents (2.5 l each) with increasing polarity were used to elute the column. The column was developed and eluted with solvents of increasing polarity in various combinations, viz., petroleumether, chloroform in petroleum ether (0.5%, 1%, 2%, 5%, 10%, 15%, 20%, 25%, 30%, 35%, 40%, 45%, 50%, 55%, 60%, 65%, 70%, 75%, 80%, 85%, 90%, 95%) chloroform (100%), and methanol in chloroform. The Thin layer Chromatography was performed for the fractions (250 ml each) thus collected. The fractions exhibiting the similar chromatographic profile were combined and concentrated.

PASS prediction

In this molecular modelling study, structures were generated with the aid of Chem3D Ultra-9.00 and HyperChem-v.6.02, Wolfram Research Mathematics 6.0 software. Lone pairs of electrons and hydrogen atoms were added where appropriated. The equilibrium geometries of compounds were located using MM+(for Hyper Chem) and MM2 (for Chem3D) functional set. In the next step, RHF calculation (semiempirical AM1 method, the self-consistent field of Hartree-Fock) were performed and bond length, angles, torsion angles and partial charges have been calculated. Calculations were performed on a Intel (R) Core2 (TM) CPU 6600 @ 2.4 GHz Pentium IV computer with 2 GB RAM.

RESULTS AND DISCUSSIONS

Isolation and characterization of phytoconstituents

Compound MC-1

Elution of the column with petroleum ether: chloroform (90: 10) yielded colorless powder of MC-1, 85 mg (0.04% yield). R_f: 0.80 (petroleum ether: chloroform: methanol, 2: 4: 0.1). Melting point: 71ºC-72ºC; IR υ_{max} (KBr): 2926, 2854, 1466, 1215, 1077, 929, 757 cm^{-1}; ^{1}H-NMR ($CDCl_3$): δ (ppm)=1.56 (2H, m, CH_2), 1.33 (2H, m, CH_2), 1.31 (2H, m, CH_2), 1.28 (4H, m, 2α CH_2), 1.25 (34 H, brs, 17 × CH_2), 0.88 (3H, t, *J*=6.0 Hz, Me-1), 0.85 (3H, t, *J*=7.5 Hz, Me-24); ^{13}C-NMR ($CDCl_3$): δ (ppm)=32.16 (CH_2), 29.93 (19 × CH_2), 29.59 (CH_2), 22.92 (CH_2), 14.33 (Me-1, Me-24). ESI MS *m/z* (rel. int.): 338 $[M]^+$($C_{24}H_{50}$) (50.3).

The IR spectrum of compound MC-1 exhibited an absorption band for long chain hydrocarbon at 757 cm^{-1}. The absence of any distinctive band in the range 3500-3200 cm^{-1} and 1750-1600 cm^{-1} suggested the saturated nature of the molecule without hydroxyl, amino, carboxylic, carbonyl and other functional groups. The mass spectrum had a molecular ion peak at *m/z* 338 consistent with the molecular formula of a saturated hydrocarbon, $C_{24}H_{50}$. The absence of $[M - Me]^+$ ion peak indicated the straight chain nature of the molecule. The ^{1}H-NMR spectrum of MC-1 showed two three - proton triplets at δ 0.88 (*J*=6.0 Hz) and 0.85 (*J*=7.5 Hz) ascribed to the terminal C-1 and C-24 primary methyl protons, respectively. Three two-proton multiplets at δ 1.56, 1.33 and 1.31, a four-proton multiplet at δ 1.28 and a broad singlet at δ 1.25 (34 H) were associated with the methylene protons. The ^{13}C-NMR spectrum of MC-1 displayed signals at δ 14.33 due to presence of methyl carbons C-1 and C-24, and between δ 32.16-22.50 assigned to the methylene carbons. The absence of any signal beyond δ 1.56 in the ^{1}H-NMR spectrum and δ 32.16 in the ^{13}C-NMR spectrum ruled out the unsaturated nature of the molecule and existence of any functional group in it. On the basis of foregoing spectral data analysis, the structure of MC-1 has been elucidated as *n*-tetracosane (Figure 1).

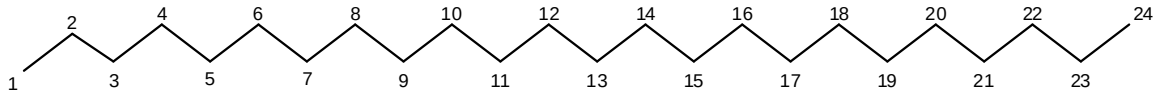

Figure 1: Structure of n-tetracosane (MC-1)

Compound MC-2

Elution of the column with petroleum ether: chloroform (80: 20) afforded colorless powder of MC-2, 97 mg (0.045% yield). R_f: 0.82 (benzene: chloroform: methanol, 2.5: 4.5: 0.6). Melting point: 78ºC-79ºC. IR υ_{max} (KBr): 2927, 2854, 1466, 1378, 1215, 1078, 849, 757 cm^{-1}; ^{1}H-NMR ($CDCl_3$): δ (ppm)=1.64 (2H, m, CH_2), 1.50 (2H, m, CH_2), 1.45 (2H, m, CH_2), 1.41 (2H, m, CH_2), 1.38 (2H, m, CH_2), 1.33 (2H, m, CH_2), 1.29 (6H, s, 3 × CH_2), 1.25 (28H, brs, 14 × CH_2), 0.89 (3H, t, *J*=6.0 Hz, Me-1), 0.85 (3H, t, *J*=7.2 Hz, Me-25); ^{13}C-NMR ($CDCl_3$): δ (ppm)=32.16 (CH_2), 29.93 (20 × CH_2), 29.59 (CH_2), 22.92 (CH_2), 14.33 (Me-1, Me-25). ESI MS *m/z* (rel. int.): 352 $[M]^+$($C_{25}H_{52}O$) (2.1).

The IR spectrum of compound MC-2 displayed an absorption band for long chain hydrocarbon at 757 cm^{-1}. The absence of any prominent band in the range 3500-3200 cm^{-1} and 1750-1600 cm^{-1} indicated the saturated nature of the molecule without any functional group. Its mass spectrum had a molecular ion peak at *m/z* 352 consistent with the molecular formula of a saturated hydrocarbon, $C_{25}H_{52}$. The absence of $[M–Me]^+$ ion peak suggested straight nature of the molecule. The ^{1}H-NMR spectrum of MC-2 showed two three-proton triplets at δ 0.89 (*J* = 6.0 Hz) and 0.85 (*J* = 7.2 Hz) assigned to the terminal C-1 and C-25 primary methyl protons, respectively. Six two - proton multiplets at δ 1.64, 1.50, 1.45, 1.41, 1.38 and 1.33 and two broad singlets at δ 1.29 (6H) and 1.25(28 H) were allied with the methylene protons. The ^{13}C-NMR spectrum of MC-2 showed two signals for methyl carbons at δ 14.33 (C-1 and C-25) and between δ 22.92 to 32.16 for methylene carbons. The absence of any signal beyond δ 1.64 in the ^{1}H-NMR spectrum and δ 32.16 in the ^{13}C-NMR spectrum indicated the unsaturated nature of the molecule and absence of any functional group in it. The above mentioned spectral data interpretation led us to elucidate the structure of MC-2 as *n*-pentacosane (Figure 2).

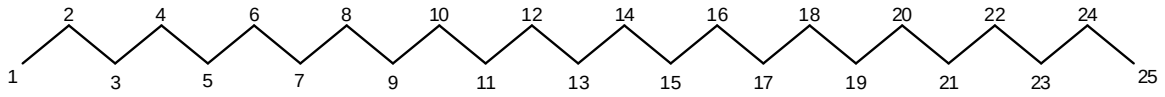

Figure 2: Structure of n-pentacosane (MC-2)

Compound MC-3

Elution of the column with petroleum ether-chloroform (70: 30) furnished colorless crystals of MC-3, 81 mg (0.038% yield). R_f: 0.74 (benzene-chloroform-methanol, 2.5: 4.5: 0.6). Melting point: 81ºC- 82ºC; IR υ_{max} (KBr): 2927, 2854, 1466, 1215, 1075, 929, 757 cm^{-1}; ^{1}H-NMR ($CDCl_3$): δ (ppm)=1.44 (2H, m, CH_2), 1.41 (2H, m, CH_2), 1.33 (2H, m, CH_2), 1.31 (2H, m, CH_2), 1.30 (2H, m, CH_2), 1.28 (8H, brs, 4 × CH_2), 1.25 (48H, brs, 24 × CH_2), 0.89 (3H, t, *J*=6.0 Hz, Me-1), 0.85 (3H, t, *J*=6.9 Hz, Me-35); ^{13}C-NMR ($CDCl_3$): δ (ppm)=32.15 (CH_2), 30.43 (CH_2), 29.92 (CH_2), 29.58 (29 × CH_2), 22.91 (CH_2), 14.33 (Me-1, Me-35). ESI MS *m/z* (rel. int.): 492 $[M]^+$($C_{35}H_{72}$) (1.3).

The IR spectrum of MC-3 demonstrated the presence of an absorption band for long chain hydrocarbon at 757 cm^{-1}. The absence of any distinct band in the range 3500-3200 cm^{-1} and 1750-1600 cm^{-1} indicated the saturated nature of the molecule and ruled out the existence of any functional group. The mass spectrum had a molecular ion peak at *m/z* 492 corresponding to the molecular formula of a saturated hydrocarbon, $C_{35}H_{72}$. The deficiency of $[M – Me]^+$ ion peak indicated the straight chain nature of the molecule. The ^{1}H-NMR spectrum of MC-3 showed two three - proton triplets at δ 0.89 (*J*=6.0 Hz) and 0.85 (*J*=6.9 Hz) accounted to the terminal C-1 and C-35 primary methyl protons, respectively. Five two-proton multiplets from δ 1.44-1.30 and two broad singlets at δ 1.28 (8H) and 1.25 (48 H) were associated with the methylene protons. The ^{13}C-NMR spectrum of MC-3 exhibited two signals at δ 14.33 due to presence of methyl groups at C-1 and C-35 and between δ 22.91 to 32.15 ascribed to the presence of methylene carbons. The absence of any signal beyond δ 1.44 in the ^{1}H-NMR spectrum and δ 32.15 in the ^{13}C-NMR spectrum supported the unsaturated nature of the molecule and absence of any functional group in it. This discussion of the spectral data analysis led us to explicate the structure of MC-3 as *n*-pentatriacontane (Figure 3).

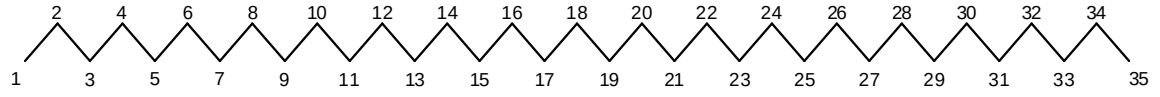

Figure 3: Structure of n-pentatriacontane (MC-3)

Compound MC-4

Elution of the column with chloroform-methanol (99.1: 0.1) produced colorless crystals of MC-4, 94 mg (0.044% yield). R_f: 0.55 (benzene-chloroform-methanol, 2.5: 4: 0.6). Melting point: 83ºC-84ºC; IR υ_{max} (KBr): 3401, 2926, 2854, 1602, 1466, 1378, 1215, 1079, 1020, 929, 849, 757 cm^{-1}; ^{1}H-NMR (MeOD): δ (ppm)=3.31 (1H, m, *w1/2*=6.6 Hz, H-19β), 1.45 (2H, m, CH_2), 1.43 (2H, m, CH_2), 1.41 (2H, m, CH_2), 1.37 (2H, m, CH_2), 1.34 (2H, m, CH_2), 1.32 (2H, m, CH_2), 1.30 (2H, m, CH_2), 1.26 (6H, s, 3 × CH_2), 1.24 (2H, m, CH_2), 0.92 (3H, t, *J*=8.1Hz, Me-1), 0.87 (3H, t, *J*=6.9Hz, Me-39); ^{13}C-NMR (MeOD): δ (ppm)=73.27 (C-19), 45.31 (C-18), 41.16 (C-20), 34.11 (C-20), 30.89 (28 × CH_2), 30.28 (CH_2), 29.51 (CH_2), 27.42 (CH_2), 25.19 (CH_2), 22.68 (CH_2), 14.16 (Me-1), 14.07 (Me-39). ESI MS *m/z* (rel. int.): 564 $[M]^+$($C_{39}H_{80}O$) (68.5), 311 $[CH_3(CH_2)_{19}CHOH]^+$ (19.3), 253 [M-311, $CH_3(CH_2)_{17}]^+$ (12.4).

The compound MC-4 displayed IR absorption bands for a hydroxyl group (3401 cm^{-1}) and long aliphatic chain (757 cm^{-1}). Its mass spectrum exhibited a molecular ion peak at *m/z* 564 consequent to the molecular formula of a saturated aliphatic alcohol, $C_{39}H_{80}O$. The prominent ion peaks generating at *m/z* 311 $[CH_3\ (CH_2)_{10}CHOH]^+$ and 253 $[CH_3(CH_2)_{17}]$ due to fission of linkage between C-18 and C-19 suggested the occurrence of the hydroxyl group at C-19. The ^{1}H NMR spectrum of MC-4 displayed a one-proton multiplet at δ 3.31 with half width of 6.6 Hz associated with β-oriented carbinol H-19 proton. Two three - proton triplets at δ 0.92 (*J*=8.1 Hz) and 0.87 (*J*=6.9 Hz) were accounted to terminal C-1 and C-39 primary methyl protons respectively. Seven two-proton multiplets from δ 1.45-1.30 and two broad singlets at δ 1.26 (6H) and 1.24 (52 H) were ascribed to the remaining methylene protons. The ^{13}C-NMR spectrum of MC-4 displayed the signals for carbinol carbon at δ 73.27 (C-19), methyl carbons at δ 14.16 (C-1) and 14.07 (C-39) and methylene carbons in the range of δ 45.31 to 22.68. The deficiency of any signal further δ 3.54 in ^{1}H NMR and 66.11 in ^{13}C-NMR suggested the saturated nature of the molecule. On the basis of the foregoing discussion the

structure of the MC-4 has been formulated as *n*-nonatriacontan-19α-ol (Figure 4), an unknown aliphatic alcohol.

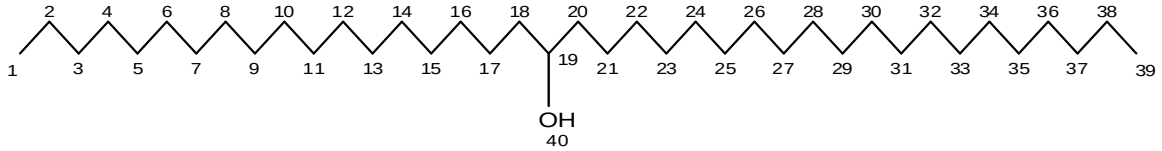

Figure 4: Structure of n-nonatriacontan-19α-ol (MC-4)

Compound MC-5

Elution of the column with chloroform-methanol (99.1: 0.1) gave a semisolid mass of MC-5, 79 mg (0.037% yield). R_f: 0.58 (Benzene-chloroform-methanol, 2.5: 4: 0.6). Melting point: 75ºC-76ºC. IR υ_{max} (KBr): 3400, 2926, 2854, 1467, 1422, 1215, 1072, 929, 756 cm^{-1}; ^{1}H-NMR (MeOD): δ (ppm)=3.31 (1H, m, *w1/2*=6.6 Hz, H-19β), 1.37 (2H, m, CH_2), 1.35 (2H, m, CH_2), 1.34 (2H, m, CH_2), 1.32 (2H, m, CH_2), 1.30 (2H, m, CH_2), 1.29 (4H, s, 2 × CH_2), 1.26 (H, brs, CH_2), 1.23 (2H, m, CH_2), 0.90 (3H, t, *J*=6.3 Hz, Me-1), 0.87 (3H, t, *J*=6.9Hz, Me-41); ^{13}C-NMR (MeOD): δ (ppm)=68.26 (C-19), 37.11 (CH_2), 34.52 (CH_2), 31.18 (CH_2), 30.89 (CH_2), 29.84 (CH_2), 27.60 (CH_2), 24.71 (CH_2), 22.69 (CH_2), 16.16 (C-1), 14.18 (C-41). ESI MS *m/z* (rel. int.): 592 $[M]^+$($C_{41}H_{84}O$) (18.7), 339 $[CH_3(CH_2)_{21}CHOH]^+$ (100), 253 [M-339, $CH_3(CH_2)_{17}]^+$(1.1)
The compound MC-5 exhibited characteristic IR absorption bands for a hydroxyl group (3400 cm^{-1}) and long aliphatic chain (756 cm^{-1}). Its mass spectrum displayed a molecular ion peak at *m/z* 592 corresponding to the molecular formula of a saturated aliphatic alcohol, $C_{41}H_{84}O$. The distinct ion peaks were produced at *m/z* 339 $[CH_3(CH_2)_{21}CHOH]^+$ and 253 $[CH_3(CH_2)_{17}]$ due to fission of the linkage between C-18 and C-19 suggesting the occurrence of hydroxyl group at C-19. The ^{1}H-NMR spectrum of MC-5 showed a one-proton multiplet at δ 3.31 with half width of 6.6 Hz associated with β-oriented carbinol H-19 proton. Two three- proton triplets at δ 0.90 (*J*=6.3 Hz) and 0.87 (*J*=6.9 Hz) were ascribed to terminal C-1 and C-41 primary methyl protons, respectively. Six two-proton multiplets between δ 1.37-1.30 and at δ 1.23 and as broad singlets at δ 1.29 (4H) and 1.26 (30 H) were associated to the methylene protons. The ^{13}C-NMR spectrum of MC-5 displayed the signals for carbinol carbon at δ 68.26 (C-19), methyl carbons at δ 16.16 (C-1) and 14.18 (C-41) and methylene carbons between δ 22.69 to 37.11. The deficiency of any signal ahead of δ 3.31 in ^{1}H-NMR and δ 68.26 in ^{13}C-NMR supported the saturated nature of the compound. On the basis of the spectral data analysis the structure of the compound MC-5 has been elucidated as *n*-henetetracontan-19α-ol (Figure 5), a new aliphatic alcohol.

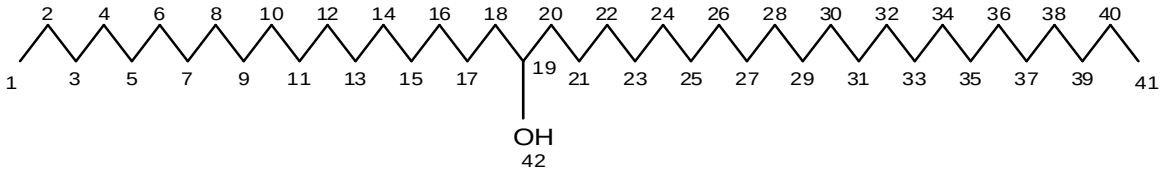

Figure 5: Structure of n-henetetracontan-19α-ol (MC-5)

Compound MC-6

Elution of the column with chloroform-methanol (99.8: 0.2) gave colorless amorphous powder of MC-6, 73 mg (0.034% yield). R_f: 0.73 (chloroform-methanol, 10: 1). Melting point: 81ºC-82ºC; IR υ_{max} (KBr): 3401, 2927, 2854, 1618, 1475, 1215, 1072, 929, 757 cm^{-1}; ^{1}H-NMR (MeOD): δ (ppm)=3.65 (1H, m, *w1/2*=6.6Hz, H-15β), 2.31 (2H, m, CH_2), 1.89 (2H, m, CH_2), 1.60 (2H, m, CH_2), 1.58 (2H, m, CH_2), 1.40 (2H, m, CH_2), 1.38 (2H, m, CH_2), 1.33 (2H, m, CH_2), 1.32 (2H, m, CH_2), 1.30 (2H, m, CH_2), 1.28 (48 H, brs, 2H α CH_2), 1.23 (2H, m, CH_2), 0.92 (3H, t, *J*=6.0 Hz, Me-1), 0.85 (3H, t, *J*=7.2 Hz, Me-37); ^{13}C-NMR (MeOD): δ (ppm)=68.21 (C-15), 45.65 (CH_2), 37.23 (CH_2), 34.48 (CH_2), 30.89 (26 α CH_2), 29.15 (CH_2), 28.67 (CH_2), 25.33 (CH_2), 24.74 (CH_2), 22.68 (CH_2), 16.18 (C-1), 14.05 (C-37). ESI MS *m/z* (rel. int.): 536 $[M]^+$ ($C_{37}H_{76}O$) (5.8), 339 $[CH_3(CH_2)_{21}CHOH]^+$(14.8).

The compound MC-6 showed IR absorption bands for hydroxyl group (3401 cm^{-1}) and long aliphatic chain (757 cm^{-1}). Its mass spectrum exhibited a molecular ion peak at *m/z* 536 corresponding to the molecular formula of a saturated aliphatic alcohol, $C_{37}H_{76}O$. The mass spectrum showed C_nH_{2n} and C_nH_{2n-1} fragmentation peaks most of which were separated by 14 mass units indicating the straight chain characteristic of the compound. The prominent ion peak arising at *m/z* 339 $[CH_3 (CH_2)_{21}CHOH]^+$ due to fission between C-14 and C-15 indicated the presence of the hydroxyl group at C-15. The ^{1}H-NMR spectrum of MC-6 showed a one-proton multiplet at δ 3.65 with half width of 6.6 Hz ascribed to β-oriented carbinol H-15 proton. Two three proton triplets at δ 0.92 (*J*=6.0 Hz) and 0.85 (*J*=7.2 Hz) were accounted to terminal C-1 and C-37 primary methyl protons, respectively. Nine two - proton multiplets at from δ 2.31 to 1.23 and a broad singlet at δ 1.28 (48 H) were associated with the methylene protons. The ^{13}C-NMR spectrum of MC-6 exhibited signals for carbinol carbon at δ 68.21 (C-15), methyl carbons at δ 16.18 (C-1) and 14.05 (C-37) and methylene carbons between δ 45.65- 22.68. The absence of any signal ahead of δ 3.54 in ^{1}H-NMR and 66.11 in ^{13}C-NMR further supported that the molecule possessed the saturated nature. On the basis of these evidences the structure of MC-6 was elucidated as: *n*-heptatriacontan-15α-ol (Figure 6).

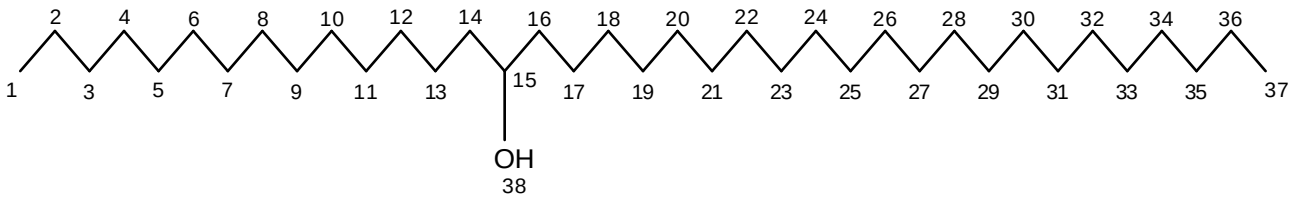

Figure 6: Structure of n-heptatriacontan-15α-ol (MC-6)

PASS prediction

The PASS computer program, which is able to simultaneously predict more than one thousand biological and toxicological activities from only the structural formulas of the chemicals, was used to predict the biological activity profile of the compounds isolated from *Momordica charantia*. Various novel pharmaceuticals have been discovered using PASS prediction. This application is a wonderful gift of technology to the mankind because it helps to discover new, potent and safe medicinal agents. It also provides an excellent opportunity for the multidisciplinary professionals (e.g. Pharma and Computational experts) to work together on a single platform and serve the society. Currently, PASS web-service is being utilised by more than 8700 registered users from more than 70 countries. Predictions for more than 250000 organic compounds have been obtained from this computer program. More than 4000 pharmacological effects, specific toxicities, mode of action, effect on gene expression, the interaction of metabolic enzymes, etc. have been predicted so far.

The predicted biological activities of the isolated phytoconstituents have been mentioned in Tables 1-6.

Table 1: Biological activity for *n*-Tetracosane

Percentage activity	Percentage inactivity	Name of activity
95.4	0.2	Sugar-phosphatase inhibitor
95	0.2	Acrocylindropepsin inhibitor
94	0.2	Carboxypeptidase Taq inhibitor
93.5	0.2	Cutinase inhibitor
93	0.2	Pullulanase inhibitor
92.6	0.3	CYP2J substrate
92.5	0.3	Taurine dehydrogenase inhibitor
92.4	0.4	Phobic disorders treatment
91.8	0.3	CYP2J2 substrate
91.5	0.2	Poly(alpha-L-guluronate) lyase inhibitor
91	0.2	Xylan endo-1,3-beta-xylosidase inhibitor
90.7	0.3	Dextranase inhibitor

Table 2: Biological activity for *n*-Pentacosane

Percentage activity	Percentage inactivity	Name of activity
95.4	0.2	Sugar-phosphatase inhibitor
95	0.2	Acrocylindropepsin inhibitor
95	0.2	Chymosin inhibitor
95	0.2	Saccharopepsin inhibitor
94	0.2	Carboxypeptidase Taq inhibitor
93	0.2	Pullulanase inhibitor
92.9	0.6	CYP2C12 substrate
91	0.2	Xylan endo-1,3-beta-xylosidase inhibitor
90.4	0.2	Poly(beta-D-mannuronate) lyase inhibitor
89	0.3	Cl--transporting ATPase inhibitor
89	0.3	Lysine 2,3-aminomutase inhibitor

Table 3: Biological activity for *n*-Pentatriacontane

Percentage activity	Percentage inactivity	Name of activity
95.4	0.2	Sugar-phosphatase inhibitor
95	0.2	Acrocylindropepsin inhibitor
95	0.2	Chymosin inhibitor
95	0.2	Saccharopepsin inhibitor
94	0.2	Carboxypeptidase Taq inhibitor
93.5	0.3	Alkenylglycerophosphocholine hydrolase inhibitor
93	0.2	Pullulanase inhibitor
91.8	0.3	CYP2J2 substrate

91.5	0.4	Sphinganine kinase inhibitor
90.7	0.3	Dextranase inhibitor

Table 4: Biological Activity for *n*-Nonatriacontan-19*α*-ol

Percentage activity	Percentage inactivity	Name of activity
95.5	0.2	Alkylacetylglycerophosphatase inhibitor
95.3	0.2	Acrocylindropepsin inhibitor
95.3	0.2	Chymosin inhibitor
95.3	0.2	Saccharopepsin inhibitor
94.8	0.3	Sphinganine kinase inhibitor
94.4	0.2	Sugar-phosphatase inhibitor
94.3	0.2	Acylcarnitine hydrolase inhibitor
93.7	0.3	Polyporopepsin inhibitor
93	0.1	Beta-mannosidase inhibitor
92.9	0.6	CYP2C12 substrate
92.1	0.3	Fucosterol-epoxide lyase inhibitor
91.9	0.4	Alkenylglycerophosphocholine hydrolase inhibitor

Table 5: Biological activity for *n*-Henetetracontan-19*α*-ol

Percentage activity	Percentage inactivity	Name of activity
95.5	0.2	Alkylacetylglycerophosphatase inhibitor
95.3	0.2	Acrocylindropepsin inhibitor
95.3	0.2	Chymosin inhibitor
95.3	0.2	Saccharopepsin inhibitor
94.8	0.3	Sphinganine kinase inhibitor
94.4	0.2	Sugar-phosphatase inhibitor
94.3	0.2	Acylcarnitine hydrolase inhibitor
93.7	0.3	Polyporopepsin inhibitor
93.6	0.4	5 Hydroxytryptamine release stimulant
93.4	0.1	Xylan endo-1,3-beta-xylosidase inhibitor
93	0.1	Beta-mannosidase inhibitor

Table 6: Biological activity for *n*-Heptatriacontan-15*α*-ol

Percentage activity	Percentage inactivity	Name of activity
95.5	0.2	Alkylacetylglycerophosphatase inhibitor
95.3	0.2	Acrocylindropepsin inhibitor
95.3	0.2	Chymosin inhibitor
95.3	0.2	Saccharopepsin inhibitor
94.8	0.3	Sphinganine kinase inhibitor
94.4	0.2	Sugar-phosphatase inhibitor
94.3	0.2	Acylcarnitine hydrolase inhibitor
93.7	0.3	Polyporopepsin inhibitor
93.6	0.4	5 Hydroxytryptamine release stimulant
93.4	0.1	Xylan endo-1,3-beta-xylosidase inhibitor

CONCLUSION

Two unknown aliphatic alcohols *n*-nonatriacontan-19α-ol and *n*-henetetracontan-19α-ol along with four known phytomolecules: *n*-tetracosane, *n*-pentacosane, *n*-pentatriacontane and *n*-heptatriacontan-15α-ol were isolated from the ethanolic extract of the seeds of *Momordica charantia*

Linn. The various chromatographic techniques might use these compounds as fingerprinting markers. Thus these shall be beneficial for establishing the identity, quality and purity of the drug. These phytoconstituents shall be explored for their pharmacological activity, especially the new compounds. For this the PASS prediction for the biological activity spectra shall be of great help. The Biological Activity Spectrum of *n*-tetracosane, *n*-pentacosane and *n*-pentatriacontane exhibited their maximun probability to be active as Sugar-phosphatase inhibitor, Acrocylindropepsin inhibitor, Chymosin inhibitor and Saccharopepsin inhibitor while that of *n*- nonatriacontan-19α-ol, henetetracontan-19α-ol and *n*-heptatriacontan-15α-ol showed their highest probability to be potent as Alkylacetylglycerophosphatase inhibitor, Acrocylindropepsin inhibitor, Chymosin inhibitor, Saccharopepsin inhibitor, Sphinganine kinase inhibitor. Thus, the PASS prediction of the various isolated compounds also supported the fact that the compounds having similar chemical structures possess similar Biological activity spectrum.

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SUPPLEMENTARY MATERIAL

Spectrums of isolated phytoconstituents (Figures S1-S21)

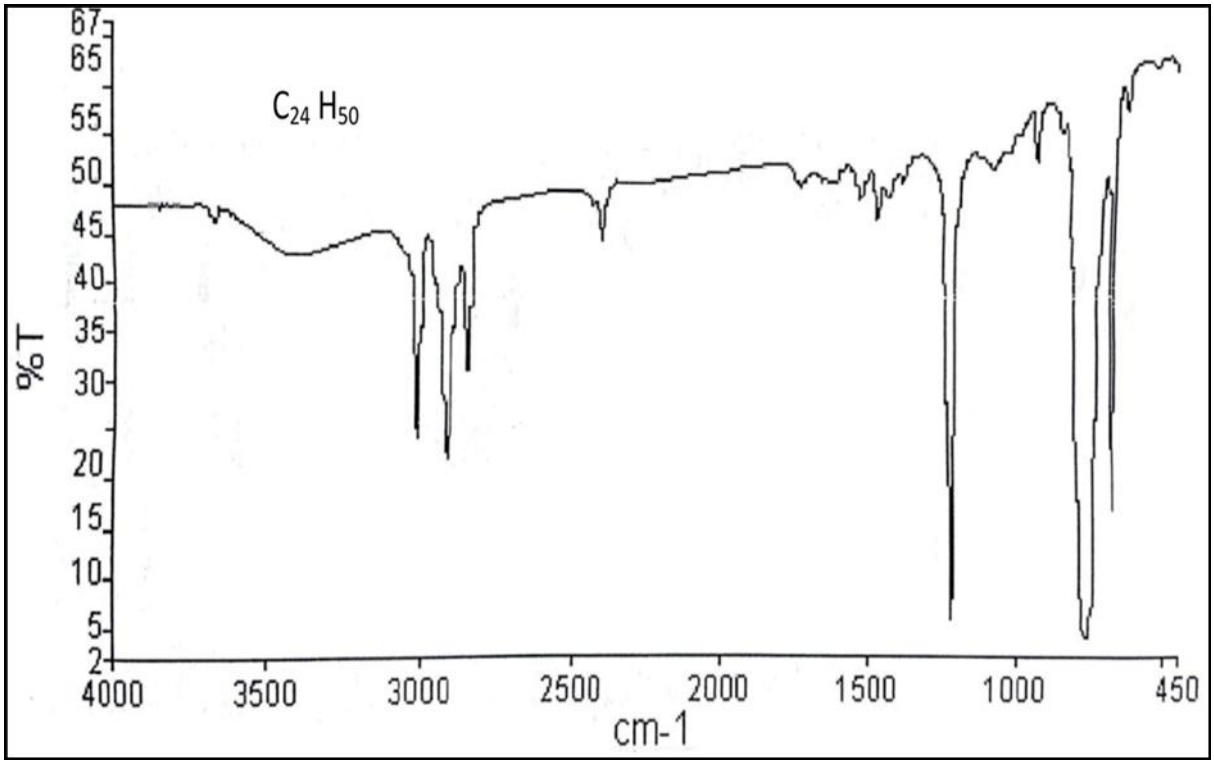

Figure S1: IR spectrum of *n*-Tetracosane (MC-1)

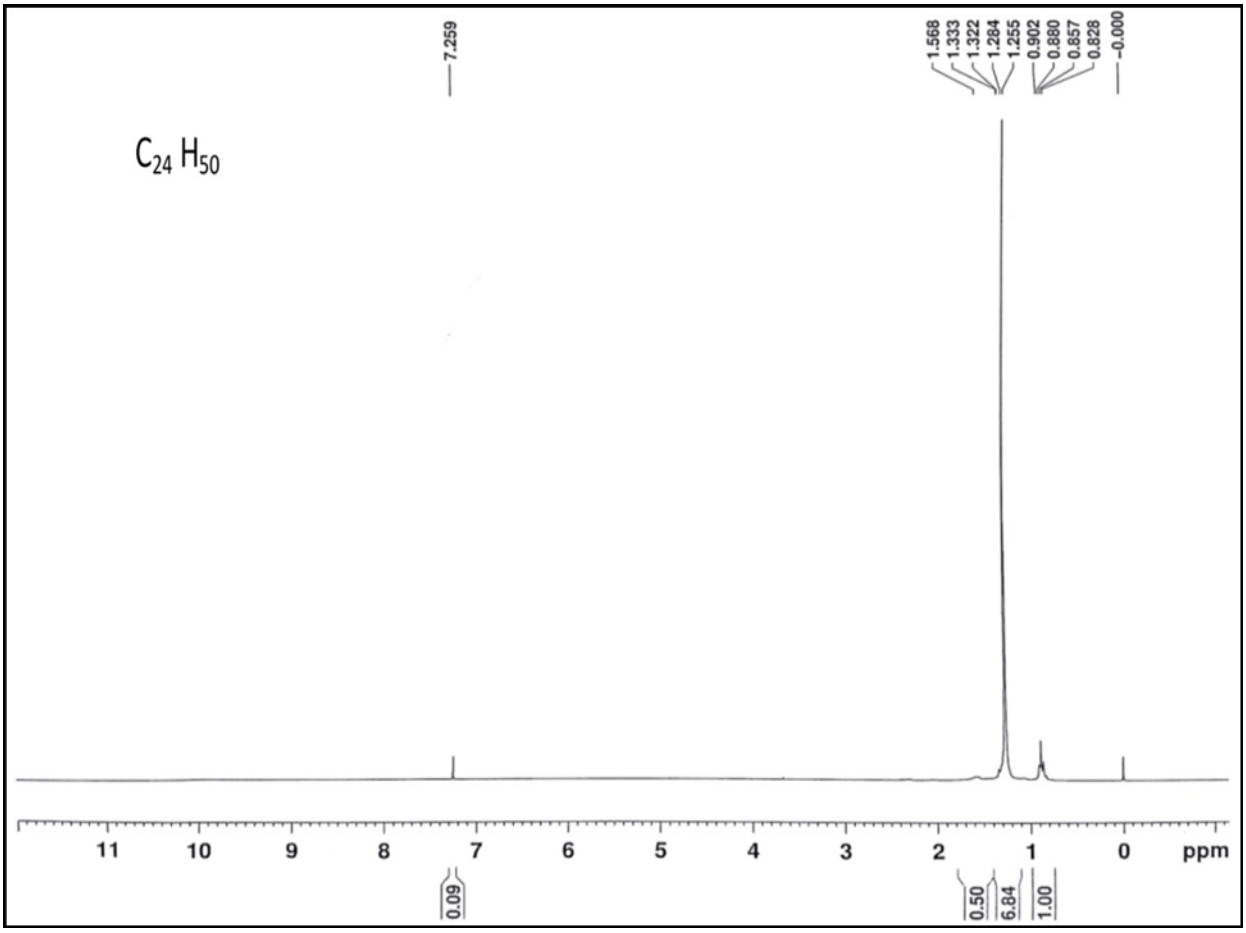

Figure S2: ^{1}H-NMR spectrum *of n*-Tetracosane (MC-1)

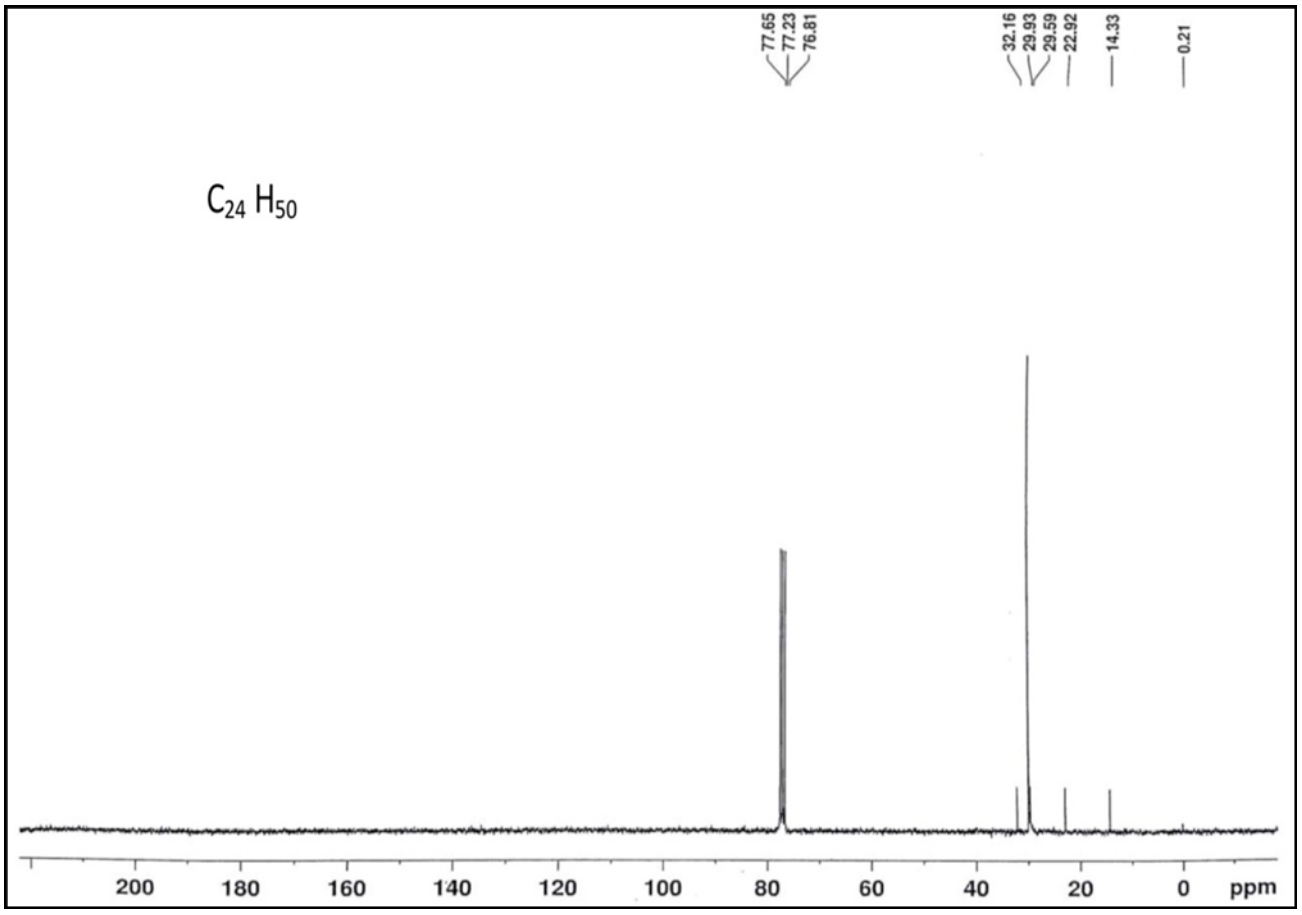

Figure S3: ^{13}C-NMR spectrum of *n*-Tetracosane (MC-1)

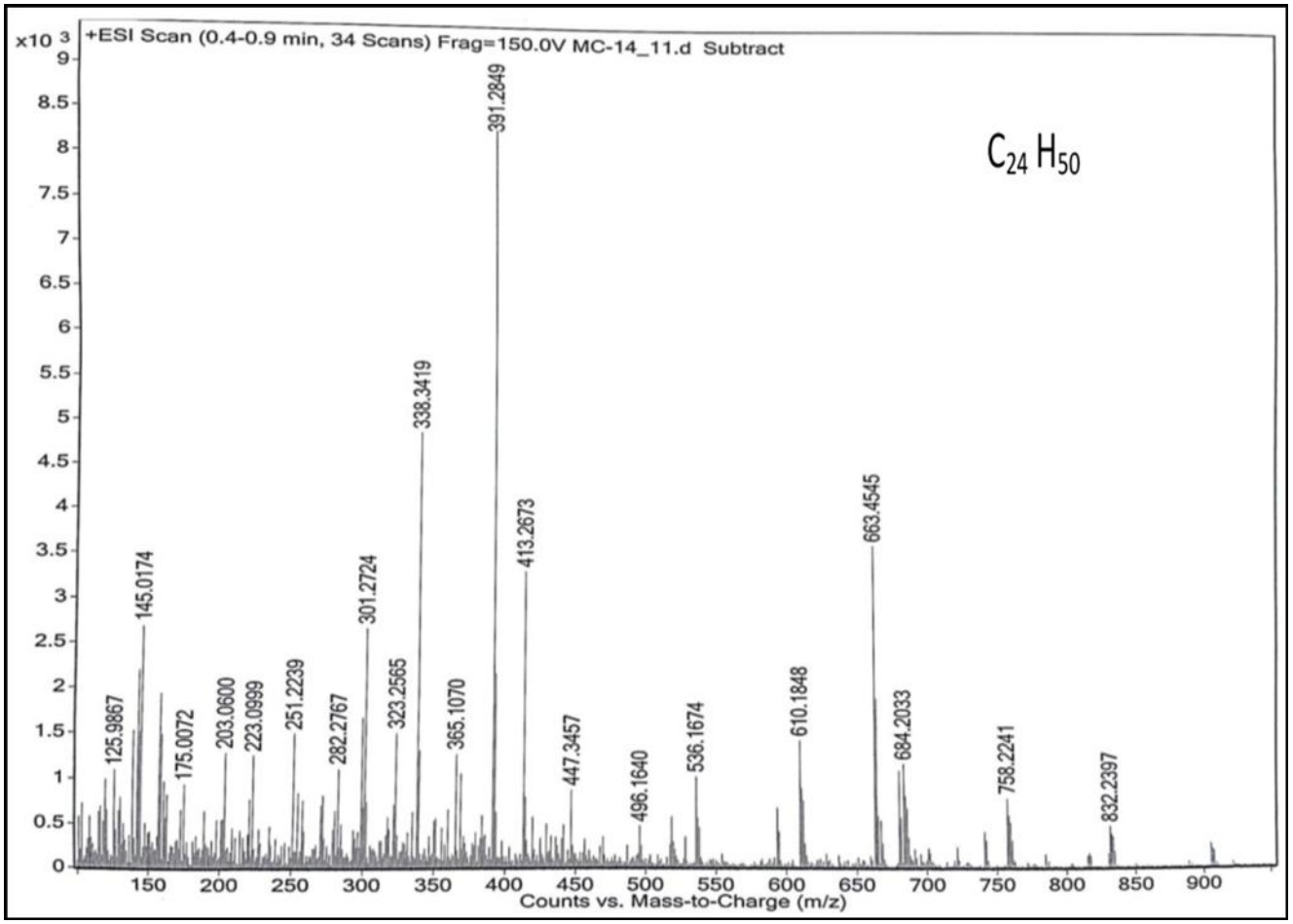

Figure S4: Mass spectrum of *n*-Tetracosane (MC-1)

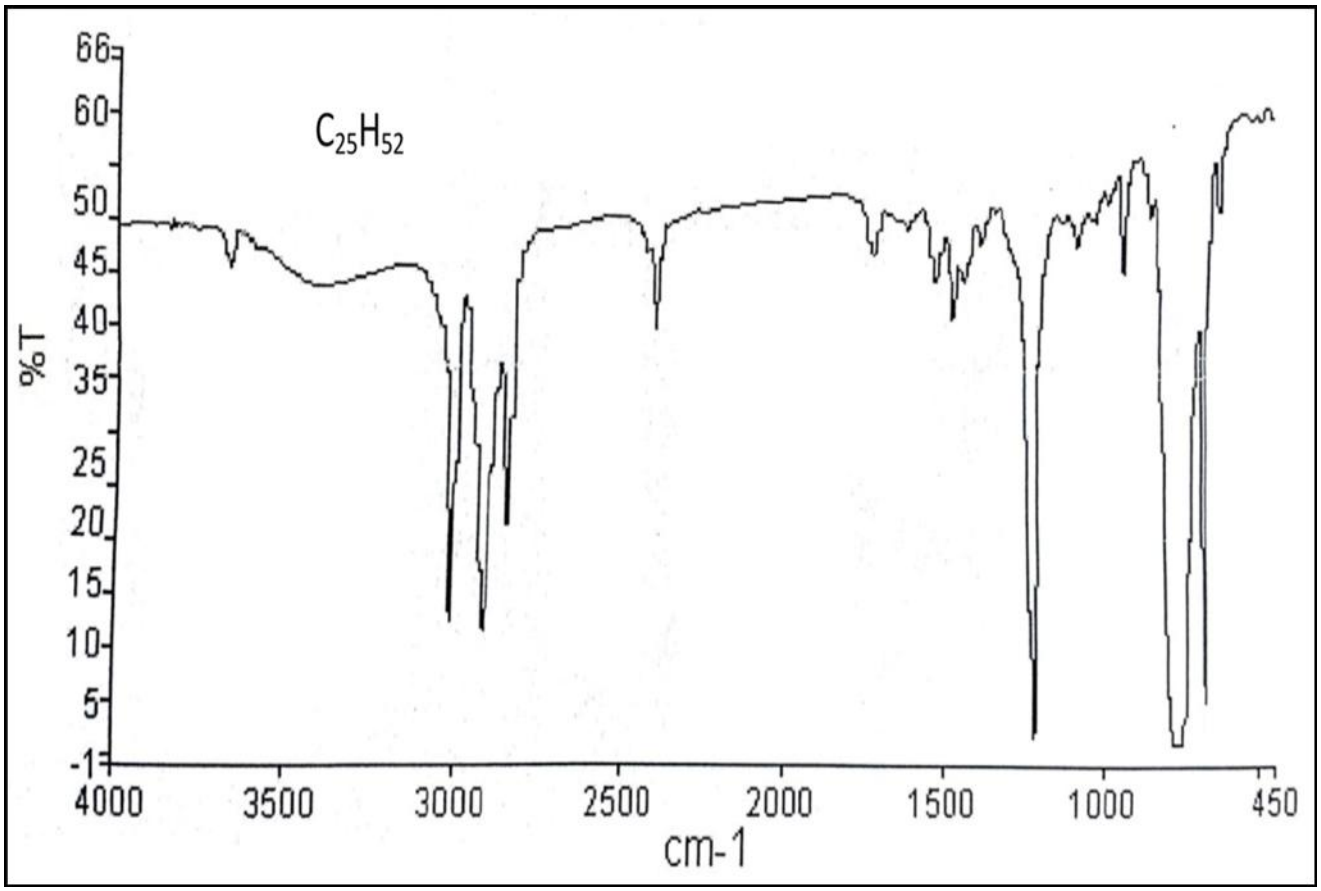

Figure S5: IR spectrum of *n*-Pentacosane (MC-2)

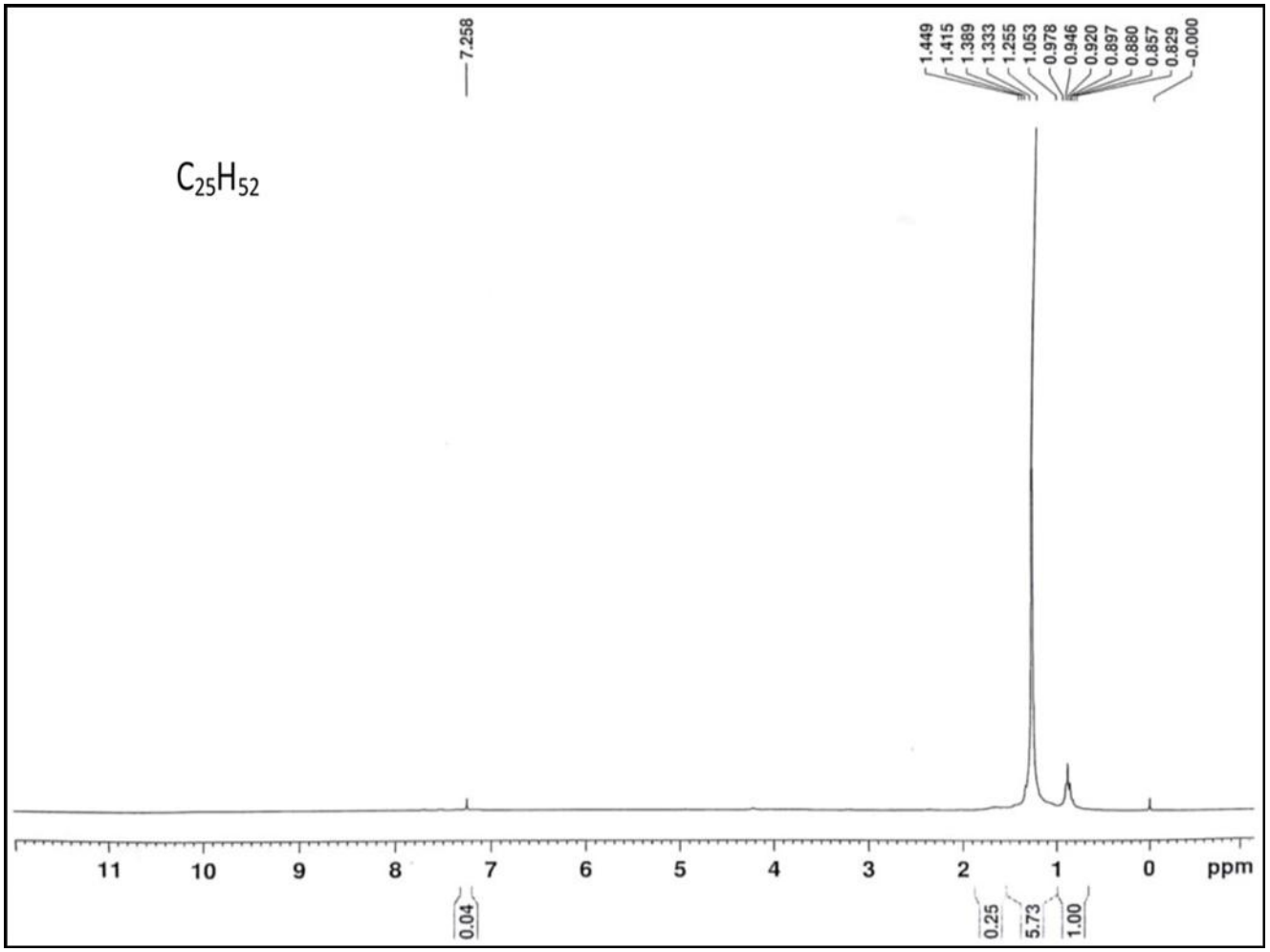

Figure S6: ^{1}H-NMR spectrum of *n*-Pentacosane (MC-2)

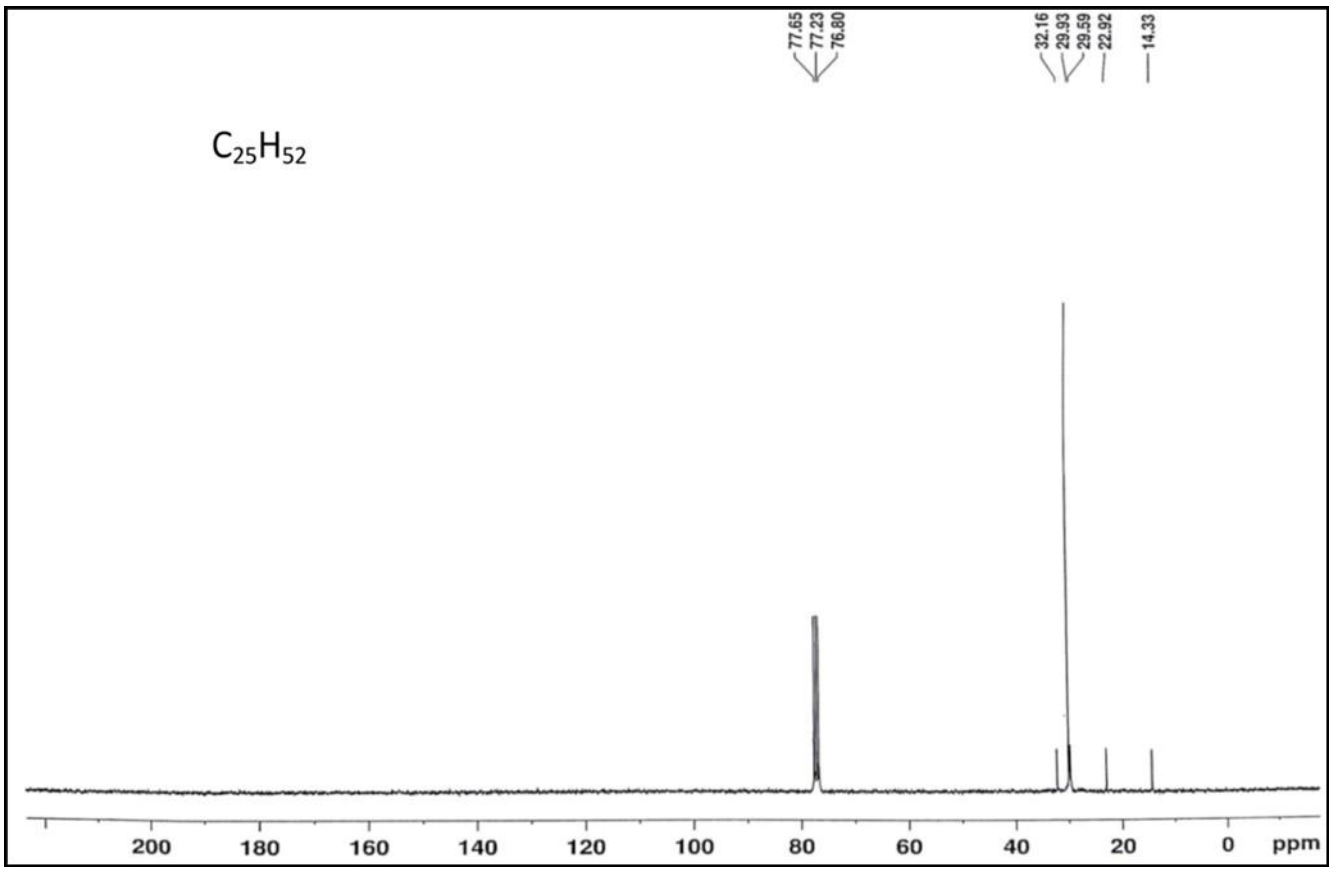

Figure S7: ^{13}C-NMR spectrum of *n*-Pentacosane (MC-2)

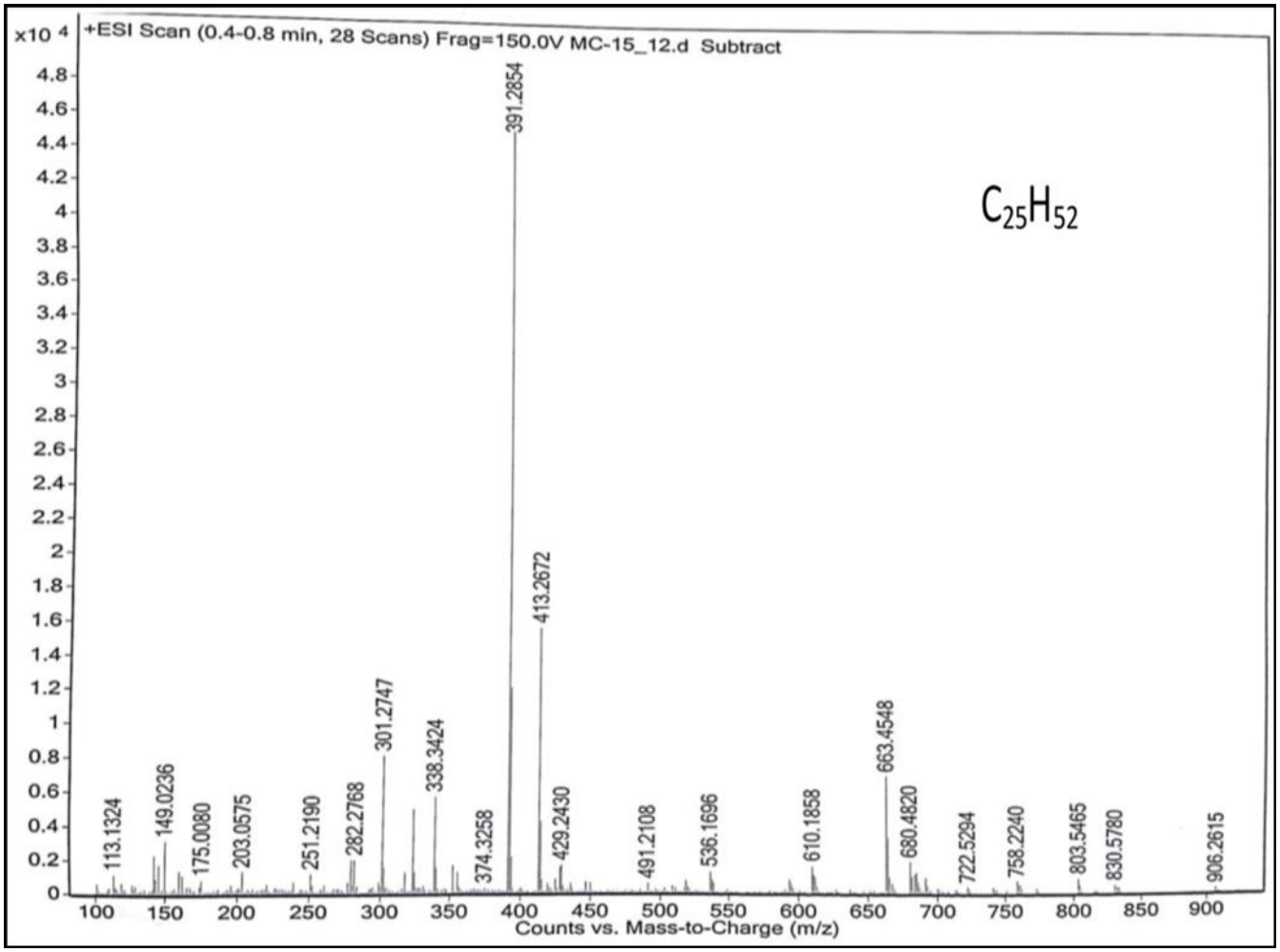

Figure S8: Mass spectrum of *n*-Pentacosane (MC-2)

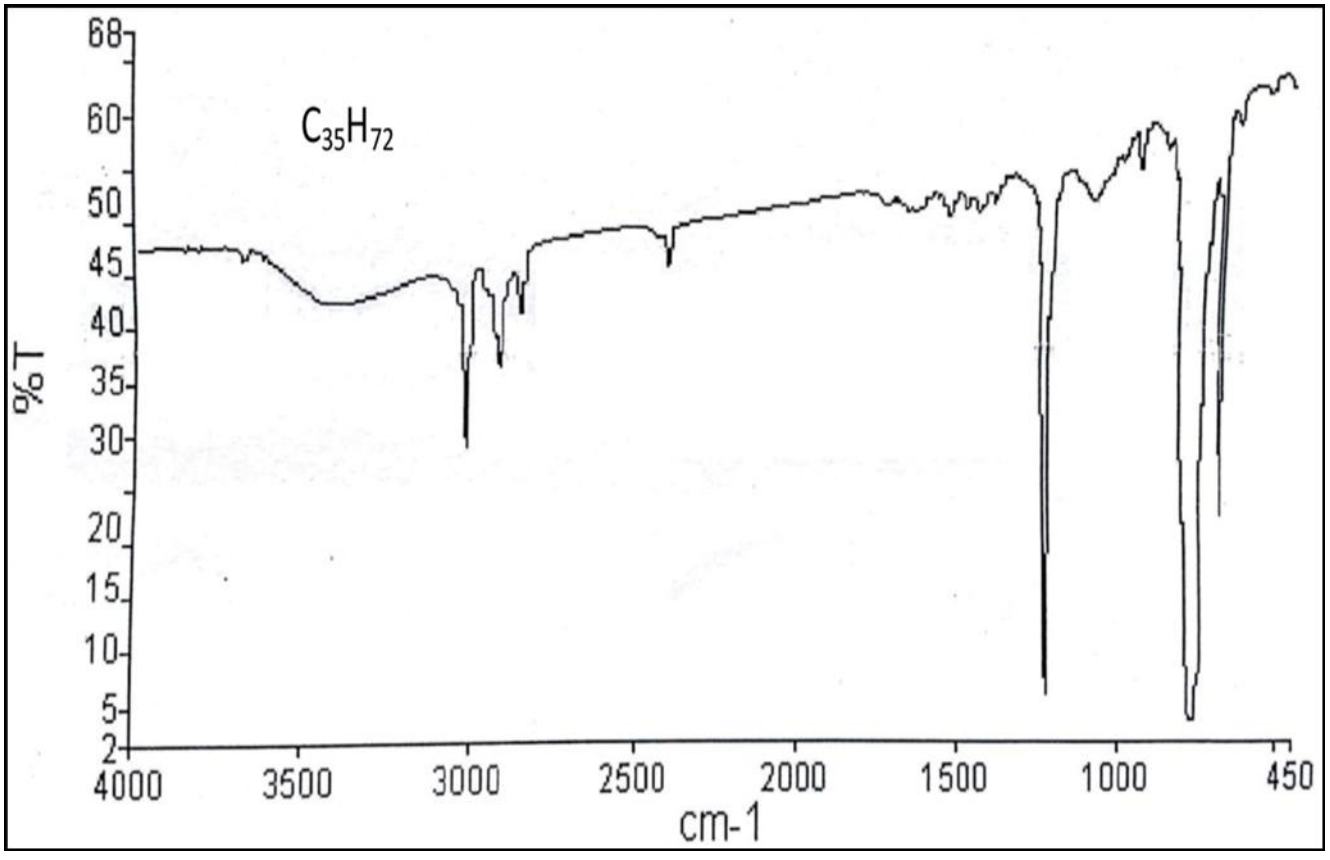

Figure S9: IR spectrum of *n*-Pentatriacontane (MC-3)

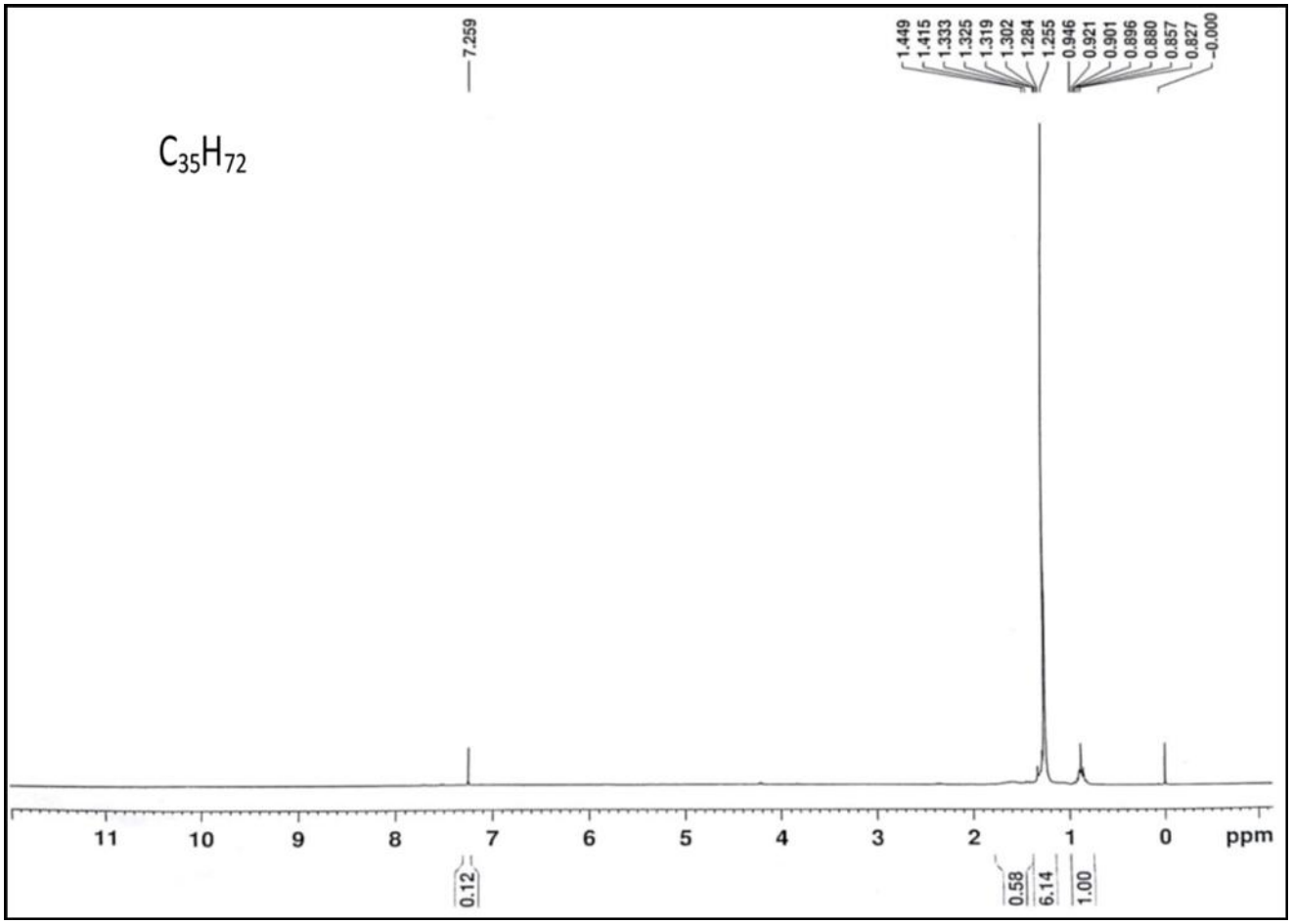

Figure S10: ^{1}H-NMR spectrum of *n*-Pentatriacontane (MC-3)

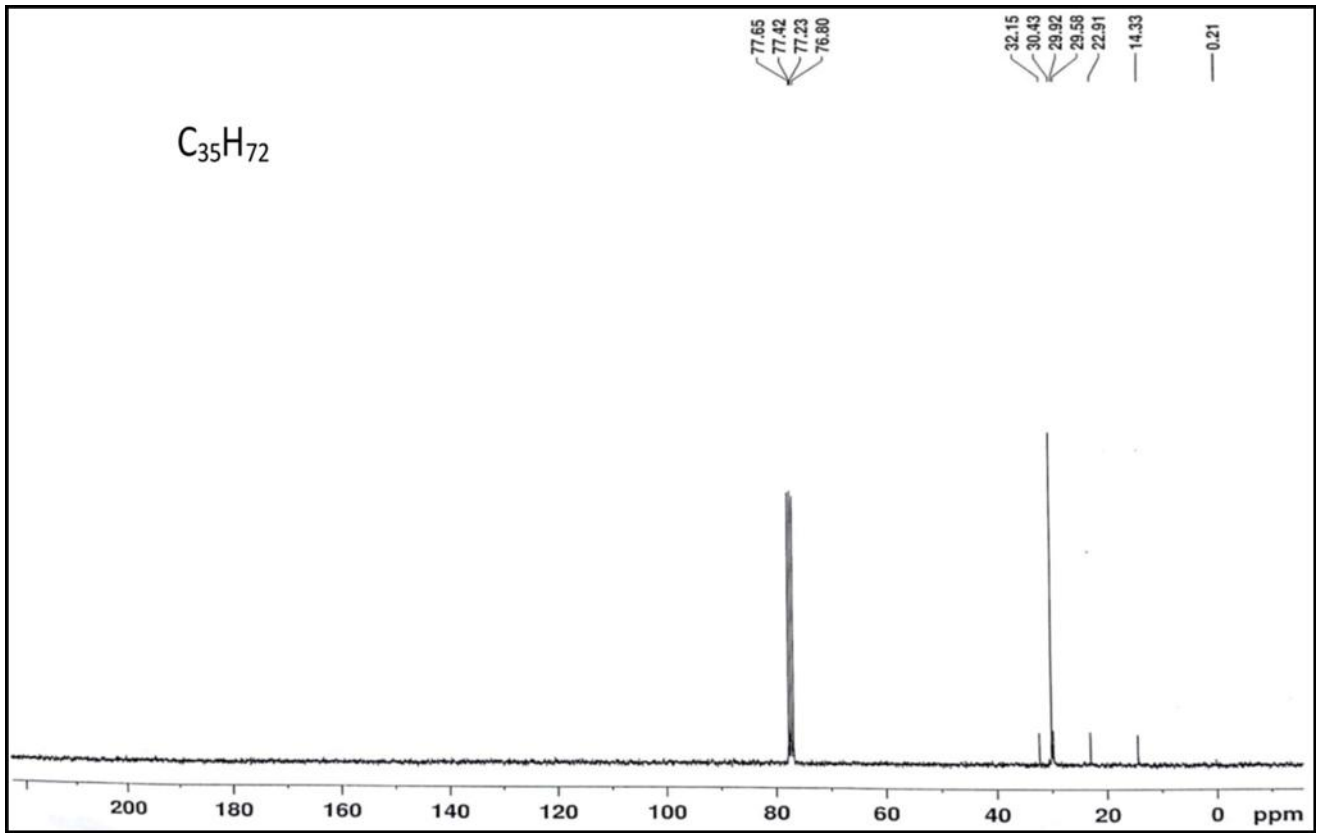

Figure S11: ^{13}C-NMR spectrum of *n*-Pentatriacontane (MC-3)

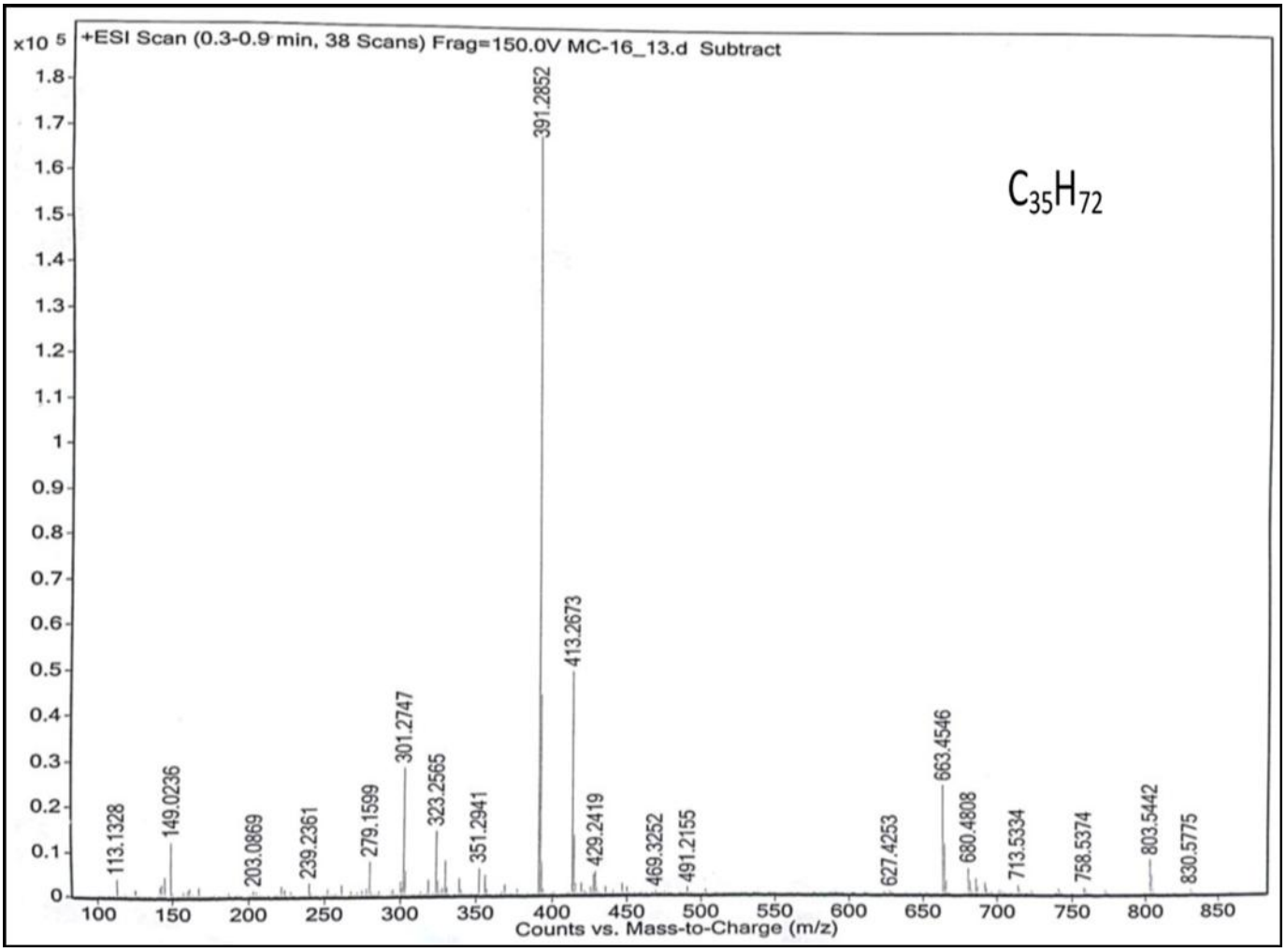

Figure S12: Mass spectrum of *n*-Pentatriacontane (MC-3)

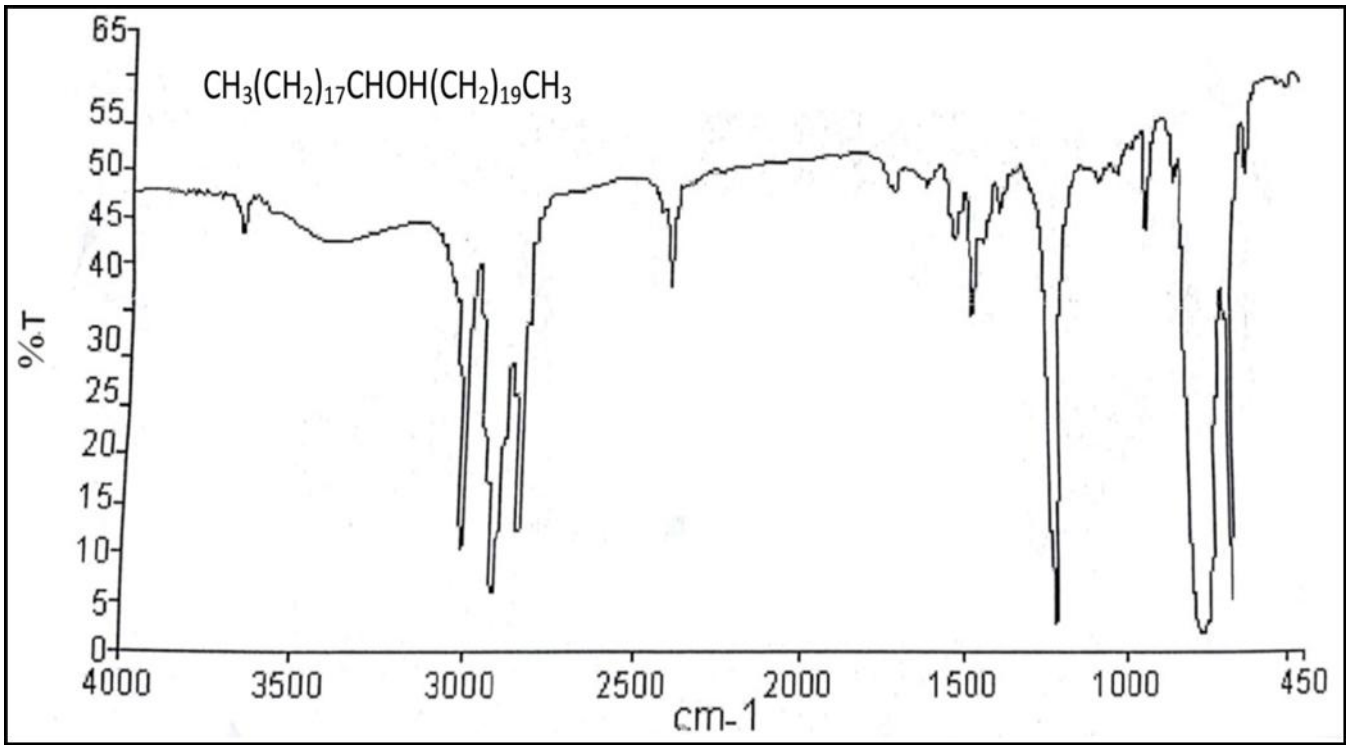

Figure S13: IR spectrum of *n*-Nonatriacontan-19*α*-ol (MC-4)

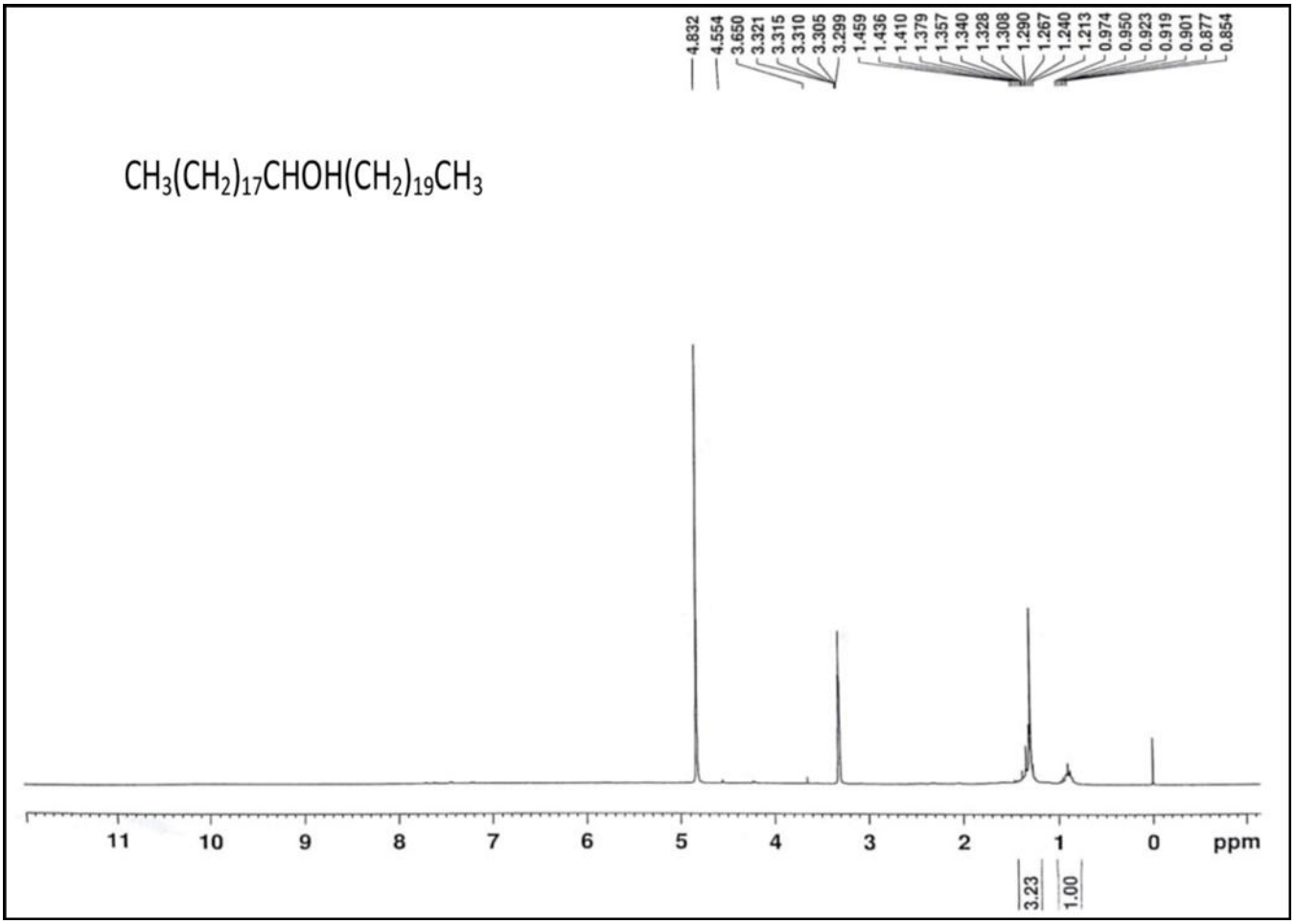

Figure S14: ^{1}H-NMR spectrum of *n*-Nonatriacontan-19*α*-ol (MC-4)

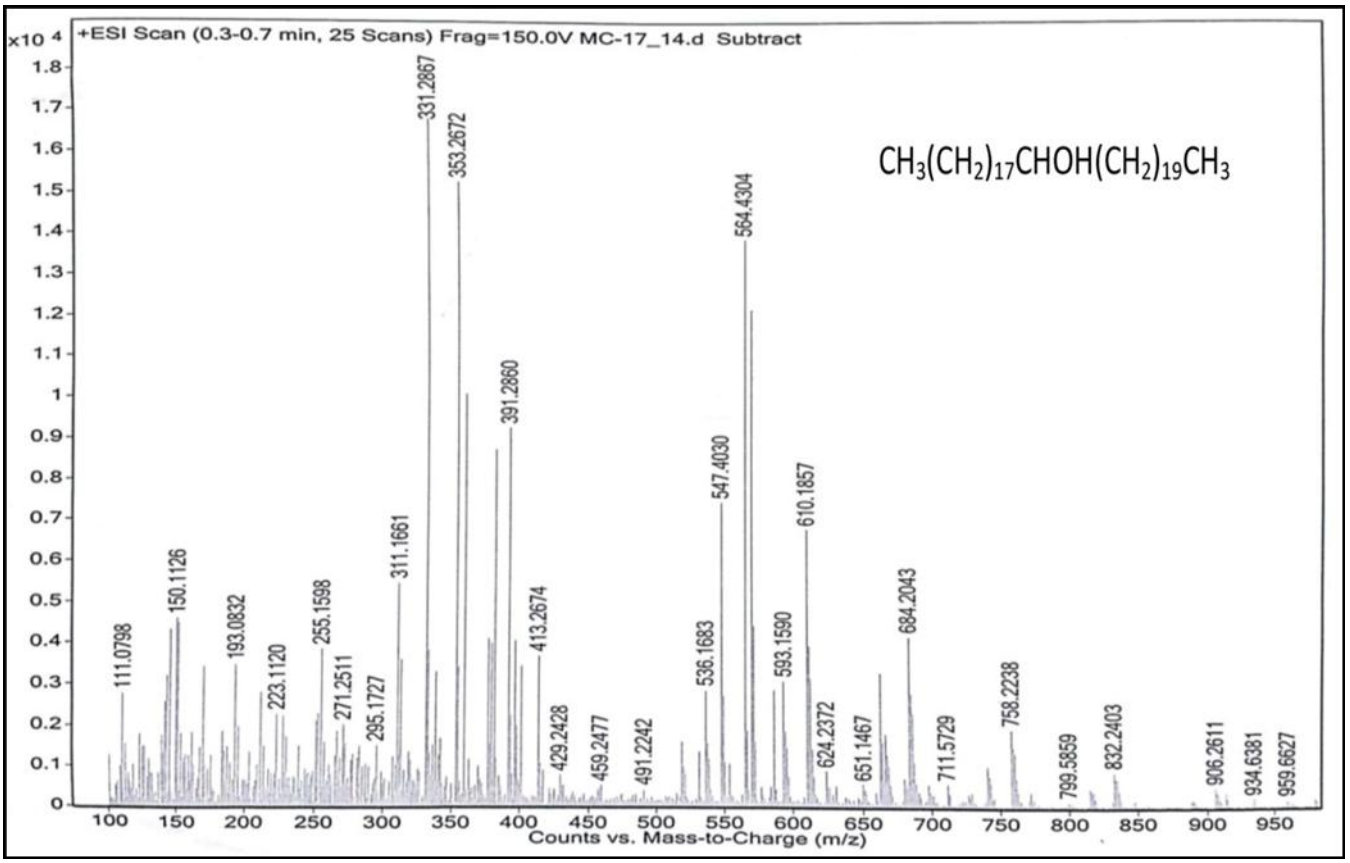

Figure S15: Mass spectrum of *n*-Nonatriacontan-19*α*-ol (MC-4)

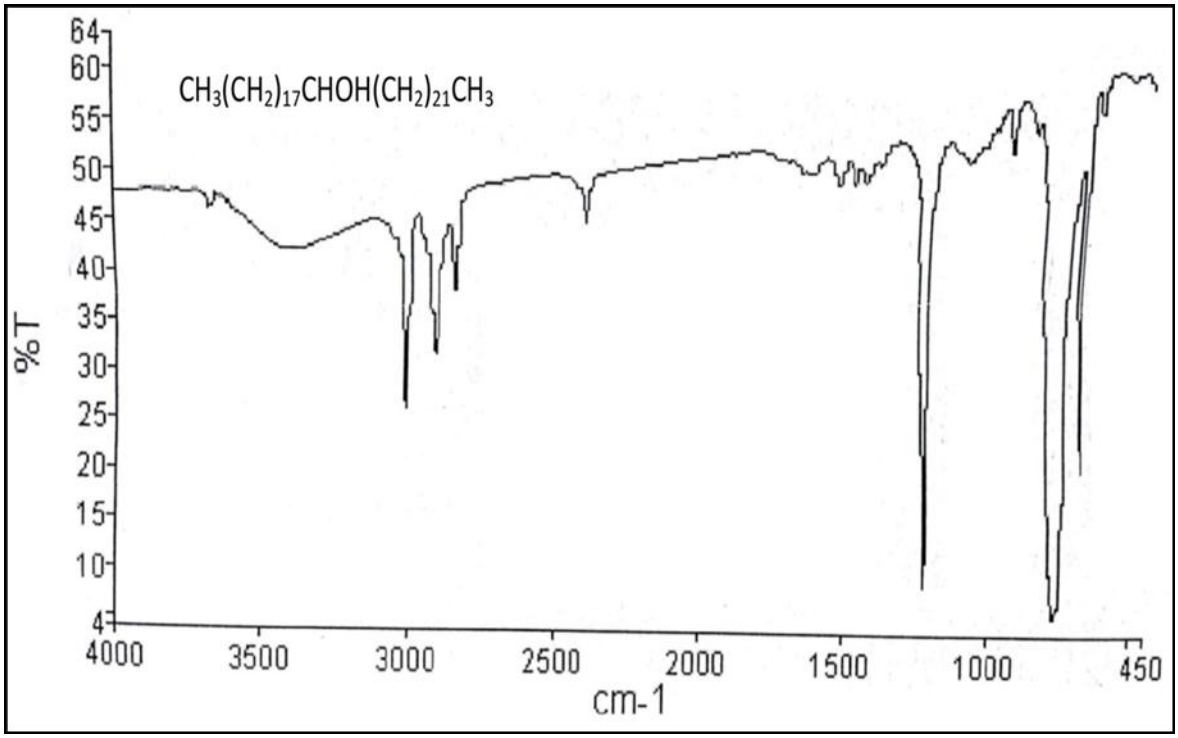

Figure S16: IR spectrum of *n*-Henetetracontan-19*α*-ol (MC-5)

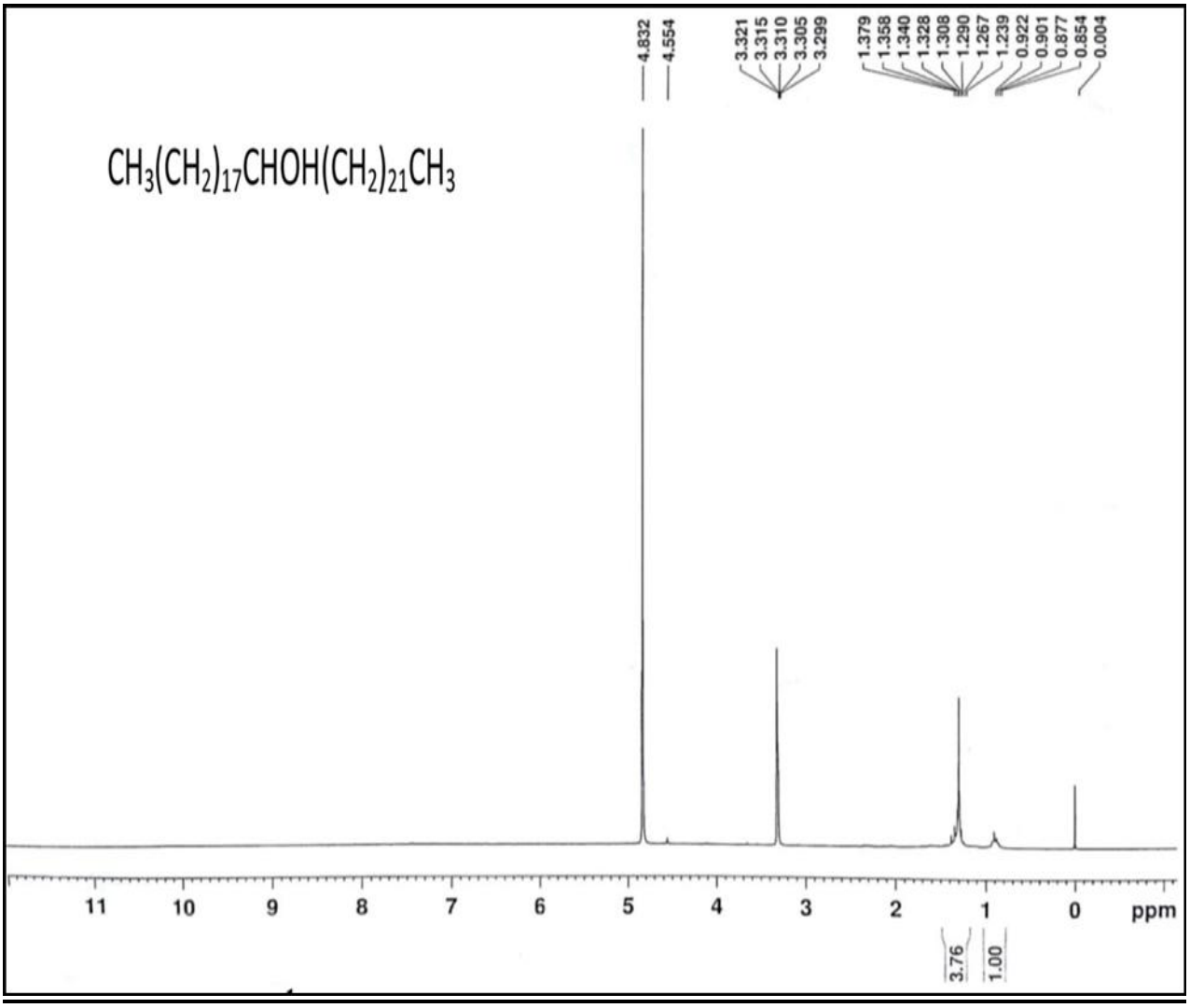

Figure S17: ^{1}H-NMR spectrum of *n*-Henetetracontan-19*α*-ol (MC-5)

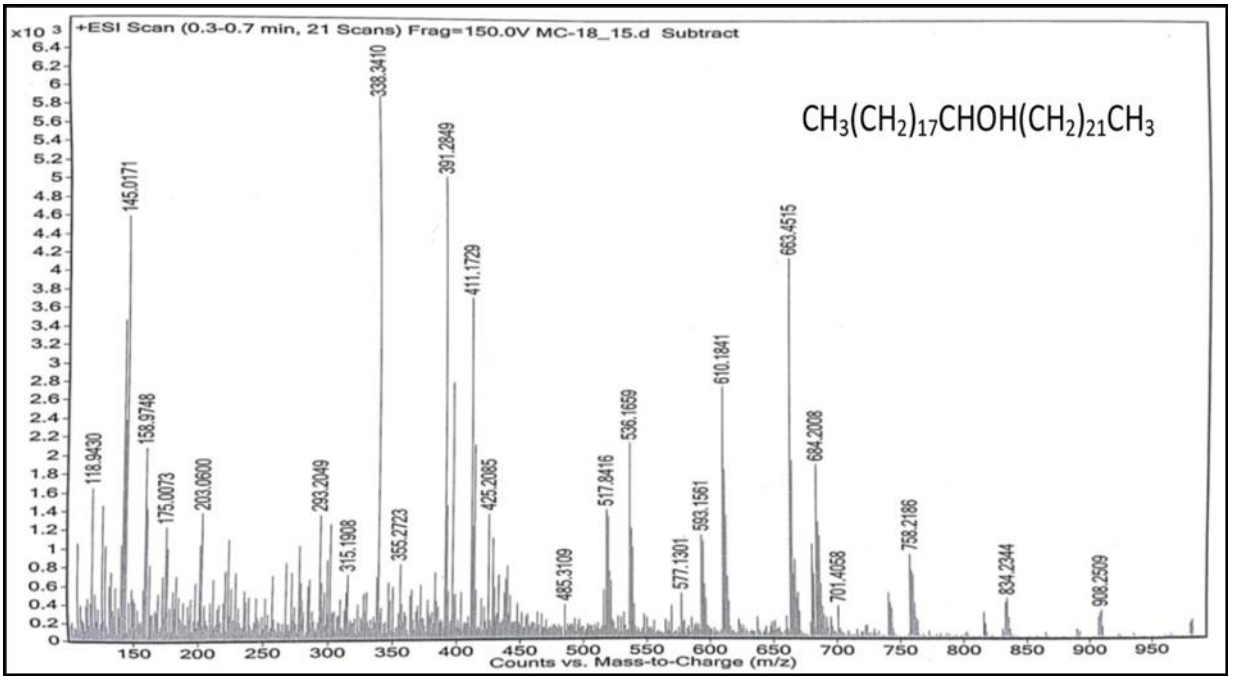

Figure S18: Mass spectrum of *n*-Henetetracontan-19*α*-ol (MC-5)

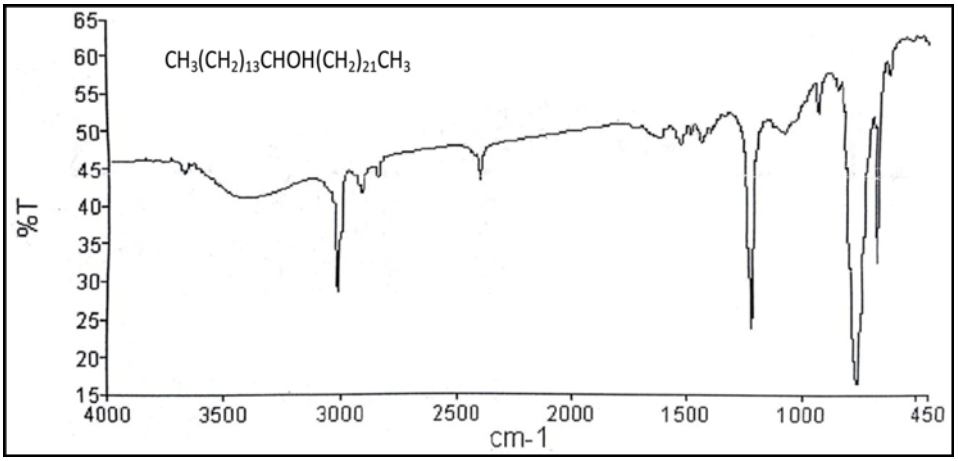

Figure S19: IR spectrum of *n*-Heptatriacontan-15*α*-ol (MC-6)

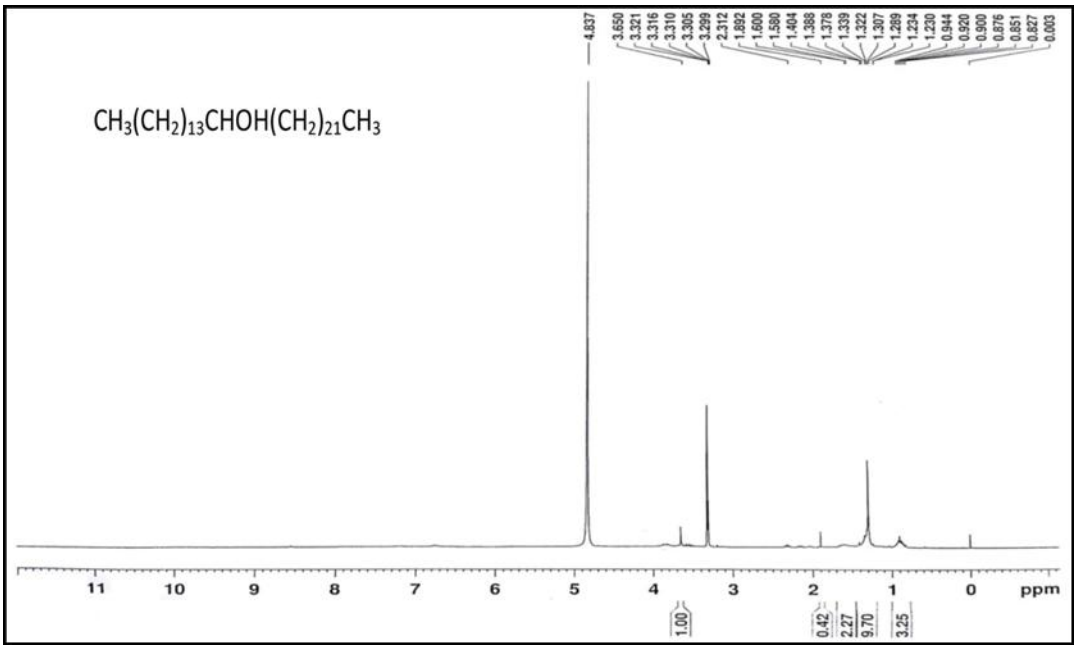

Figure S20: ^{1}H-NMR spectrum of *n*-Heptatriacontan-15*α*-ol (MC-6)

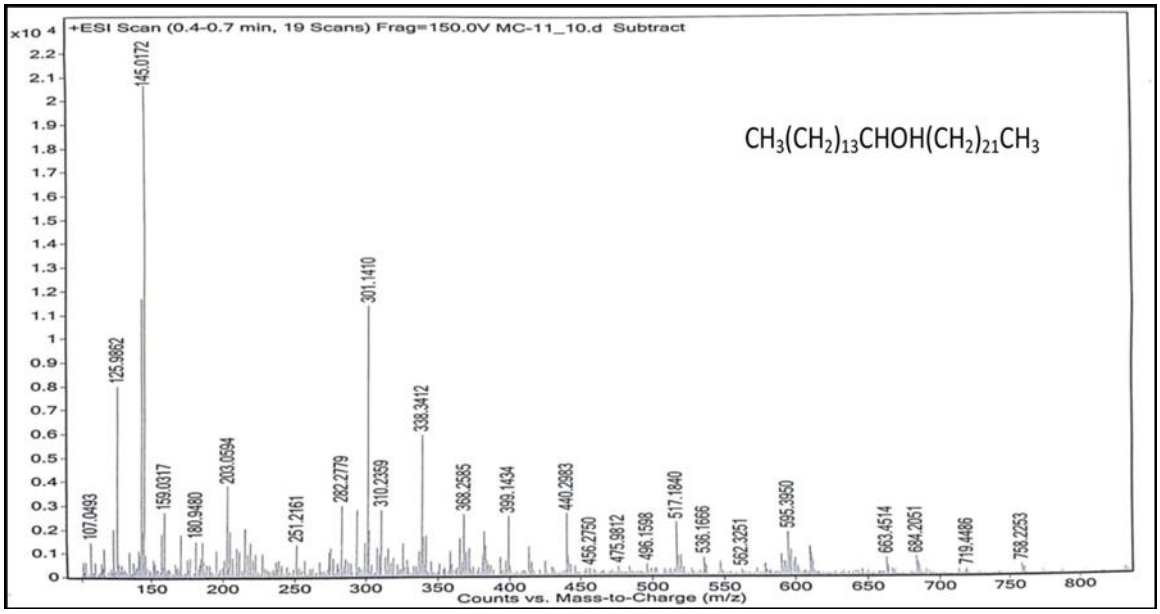

Figure S21: Mass spectrum of *n*-Heptatriacontan-15*α*-ol (MC-6)

Tables for prediction of biological activity (Tables S1- S6)

Table S1: Biological Activity for *n*-tetracosane

Percentage Activity	Percentage Inactivity	Name of Activity
95.4	0.2	Sugar-phosphatase inhibitor
95	0.2	Acrocylindropepsin inhibitor
95	0.2	Chymosin inhibitor
95	0.2	Saccharopepsin inhibitor
94.2	0.2	Acylcarnitine hydrolase inhibitor
94.1	0.2	Alkylacetylglycerophosphatase inhibitor
94	0.2	CarboxypeptidaseTaq inhibitor
93.7	0.2	IgA-specific serine endopeptidase inhibitor
93.5	0.2	Cutinase inhibitor
93	0.2	Pullulanase inhibitor
92.6	0.3	CYP2J substrate
92.5	0.3	Taurine dehydrogenase inhibitor
92.9	0.6	CYP2C12 substrate
92.4	0.4	Phobic disorders treatment
91.8	0.3	CYP2J2 substrate
91.5	0.2	Poly(alpha-L-guluronate) lyase inhibitor
91.3	0.2	Exoribonuclease II inhibitor
91	0.2	Xylan endo-1,3-beta-xylosidase inhibitor
90.7	0.3	Dextranase inhibitor
90.4	0.2	Poly(beta-D-mannuronate) lyase inhibitor
89.5	0.5	Antieczematic
89.2	0.3	Sarcosine oxidase inhibitor
88.8	0.2	Anthranilate-CoA ligase inhibitor
88.1	0.4	Glutamylendopeptidase II inhibitor
87	0.4	5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor
86	0.4	Phosphatidylcholine-retinol O-acyltransferase inhibitor
86.4	0.9	Chlordeconereductase inhibitor
86.9	1.9	Membrane integrity agonist

85.7	0.9	Antiseborrheic
85.1	0.3	Electron-transferring-flavoprotein dehydrogenase inhibitor
85.2	0.4	2-Hydroxymuconate-semialdehyde hydrolase inhibitor
85	0.5	Dehydro-L-gulonate decarboxylase inhibitor
85.3	0.8	Beta-adrenergic receptor kinase inhibitor
84.5	0.9	Protein-glutamate methylesterase inhibitor
84	0.4	Creatininase inhibitor
83.9	0.5	Fragilysin inhibitor
83.8	0.4	UDP-N-acetylglucosamine 4-epimerase inhibitor
83.7	0.8	Feruloyl esterase inhibitor
82.9	0.5	Omptin inhibitor
82.3	0.2	Oryzin inhibitor
82.7	0.7	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
82.9	0.9	NADPH peroxidase inhibitor
82.3	0.3	Leukopoiesis stimulant
82.7	0.9	Glucose oxidase inhibitor
81.5	0.5	Vasoprotector
81	0.6	Glutathione thiolesterase inhibitor
81.5	1.2	Mucositis treatment
80.2	0.6	Pseudolysin inhibitor
79.5	0.3	Licheninase inhibitor
79.4	0.2	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
80.1	1	Nicotinic alpha2beta2 receptor antagonist
79.2	0.5	N-benzyloxycarbonylglycine hydrolase inhibitor
79.1	0.4	NADH kinase inhibitor
79	0.4	Coccolysin inhibitor
78.9	0.3	Polyneuridine-aldehyde esterase inhibitor
78.9	0.3	Oxygen scavenger
78.5	0.5	L-glutamate oxidase inhibitor
78	0.6	2-Hydroxyquinoline 8-monooxygenase inhibitor
78	1.2	Arylacetonitrilase inhibitor
77	0.4	Laccase inhibitor
76.5	1.2	Prostaglandin-E2 9-reductase inhibitor
75.5	0.4	Kidney function stimulant
75	0.3	Glycolate dehydrogenase inhibitor
74.4	0.3	2-Hydroxy-3-oxoadipate synthase inhibitor
74.2	0.5	Sulfite reductase inhibitor
73.1	0.7	Hydrogen dehydrogenase inhibitor
72.9	1.4	Peptidyl-dipeptidaseDcp inhibitor
71	0.8	Histidine N-acetyltransferase inhibitor
70	0.2	N-methyl-2-oxoglutaramate hydrolase inhibitor

Table S2: Biological Activity for *n*-pentacosane

Percentage Activity	Percentage Inactivity	Name of Activity
95.4	0.2	Sugar-phosphatase inhibitor
95	0.2	Acrocylindropepsin inhibitor
95	0.2	Chymosin inhibitor

95	0.2	Saccharopepsin inhibitor
94	0.2	CarboxypeptidaseTaq inhibitor
93	0.2	Pullulanase inhibitor
92.9	0.6	CYP2C12 substrate
91	0.2	Xylan endo-1,3-beta-xylosidase inhibitor
90.4	0.2	Poly(beta-D-mannuronate) lyase inhibitor
89	0.3	Cl--transporting ATPase inhibitor
89	0.3	Lysine 2,3-aminomutase inhibitor
88.8	0.2	Anthranilate-CoA ligase inhibitor
87	0.3	Thioredoxin inhibitor
86.9	0.4	Complement factor D inhibitor
86.7	0.3	Polyamine-transporting ATPase inhibitor
86.8	0.4	Cardiovascular analeptic
86.7	0.4	Ribulose-phosphate 3-epimerase inhibitor
86.6	0.4	Nitrate reductase (cytochrome) inhibitor
86.4	0.3	Amine dehydrogenase inhibitor
86.3	0.3	Phosphatidylglycerophosphatase inhibitor
86.3	0.3	Levanase inhibitor
86.4	0.4	GST A substrate
86.2	0.4	Venombin AB inhibitor
86.4	0.9	Chlordeconereductase inhibitor
85.8	0.4	Fusarinine-C ornithinesterase inhibitor
85.5	0.3	Trimethylamine-oxide aldolase inhibitor
85.3	0.2	Endopeptidase So inhibitor
85.3	0.3	Urethanase inhibitor
85.8	0.8	Mucomembranous protector
86.9	1.9	Membrane integrity agonist
85.7	0.9	Antiseborrheic
85.1	0.3	Electron-transferring-flavoprotein dehydrogenase inhibitor
85.2	0.4	2-Hydroxymuconate-semialdehyde hydrolase inhibitor
85	0.5	Dehydro-L-gulonate decarboxylase inhibitor
85.3	0.8	Beta-adrenergic receptor kinase inhibitor
85.3	0.8	G-protein-coupled receptor kinase inhibitor
84.8	0.4	Dimethylargininase inhibitor
85	0.6	Glycosylphosphatidylinositol phospholipase D inhibitor
84.6	0.3	Rhamnulose-1-phosphate aldolase inhibitor
84.7	0.4	Glyceryl-ether monooxygenase inhibitor
84.6	0.2	Prostaglandin-A1 DELTA-isomerase inhibitor
84.8	0.5	Glucan endo-1,6-beta-glucosidase inhibitor
84.6	0.3	Methylamine-glutamate N-methyltransferase inhibitor
84.4	0.2	BRAF expression inhibitor
84	0.2	2-Haloacid dehalogenase inhibitor
84.5	0.9	Protein-glutamate methylesterase inhibitor
83.2	1.4	Methylenetetrahydrofolatereductase (NADPH) inhibitor
81.9	0.3	2-Haloacid dehalogenase (configuration-inverting) inhibitor
81	0.6	Glutathione thiolesterase inhibitor
81.5	1.2	Mucositis treatment

80.4	0.5	Lipoprotein lipase inhibitor
80	0.3	Procollagen N-endopeptidase inhibitor
80.1	1	Nicotinic alpha2beta2 receptor antagonist
79	0.4	Coccolysin inhibitor
78.9	0.3	Polyneuridine-aldehyde esterase inhibitor
78.9	0.3	Oxygen scavenger
79	0.4	1, 4-Lactonase inhibitor
79	0.5	Limulus clotting factor C inhibitor
78	1.2	Arylacetonitrilase inhibitor
77	0.4	Laccase inhibitor
76	0.4	Tpr proteinase (Porphyromonasgingivalis) inhibitor
76.1	0.7	Phthalate 4, 5-dioxygenase inhibitor
76.5	1.2	Prostaglandin-E2 9-reductase inhibitor
75	0.3	Glycolate dehydrogenase inhibitor
75.1	0.4	Opheline kinase inhibitor
75.1	0.4	Taurocyamine kinase inhibitor
75.3	2.7	Antineurotic
73	0.4	Carbon-monoxide dehydrogenase inhibitor
72.5	0.3	Plastoquinol-plastocyaninreductase inhibitor
72.1	1.5	Aldehyde oxidase inhibitor
71	0.8	Histidine N-acetyltransferase inhibitor
70	0.2	N-methyl-2-oxoglutaramate hydrolase inhibitor

Table S3: Biological Activity for *n*-pentatriacontane

Percentage Activity	Percentage Inactivity	Name of Activity
95.4	0.2	Sugar-phosphatase inhibitor
95	0.2	Acrocylindropepsin inhibitor
95	0.2	Chymosin inhibitor
95	0.2	Saccharopepsin inhibitor
94	0.2	CarboxypeptidaseTaq inhibitor
93.5	0.3	Alkenylglycerophosphocholine hydrolase inhibitor
93	0.2	Pullulanase inhibitor
91.8	0.3	CYP2J2 substrate
91.5	0.4	Sphinganine kinase inhibitor
91	0.2	Xylan endo-1,3-beta-xylosidase inhibitor
90.7	0.3	Dextranase inhibitor
90.4	0.2	Poly(beta-D-mannuronate) lyase inhibitor
8.9	0.3	Lysine 2,3-aminomutase inhibitor
88.8	0.2	Anthranilate-CoA ligase inhibitor
87	0.4	5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor
86.9	1.9	Membrane integrity agonist
85	0.6	Glycosylphosphatidylinositol phospholipase D inhibitor
84.5	0.9	Protein-glutamate methylesterase inhibitor
83.5	0.2	Hydroxylamine oxidase inhibitor
83.5	0.6	Membrane permeability inhibitor
83.2	0.3	Beta-mannosidase inhibitor
83.7	0.8	Feruloyl esterase inhibitor

82.9	0.5	Omptin inhibitor
82.8	0.5	Bisphosphoglycerate phosphatase inhibitor
82.5	0.2	Phenylacetate-CoA ligase inhibitor
82.7	0.4	3-Hydroxybenzoate 6-monooxygenase inhibitor
82.3	0.3	Leukopoiesis stimulant
82.3	0.5	NADPH-cytochrome-c2 reductase inhibitor
81	0.4	Lysostaphin inhibitor
80	0.3	Procollagen N-endopeptidase inhibitor
80.2	0.6	Pseudolysin inhibitor
79.2	0.5	N-benzyloxycarbonylglycine hydrolase inhibitor
79.1	0.4	NADH kinase inhibitor
79	0.4	1,4-Lactonase inhibitor
79	0.5	Limulus clotting factor C inhibitor
78	1.2	Arylacetonitrilase inhibitor
77.2	0.4	Carminative
77	0.4	Laccase inhibitor
76.1	0.7	Phthalate 4,5-dioxygenase inhibitor
76.5	1.2	Prostaglandin-E2 9-reductase inhibitor
75	0.3	Glycolate dehydrogenase inhibitor
75.1	0.4	Opheline kinase inhibitor
75.2	1	ADP-thymidine kinase inhibitor
74.4	0.4	Di-trans,poly-cis-decaprenylcistransferase inhibitor
74.4	0.4	Adenomatous polyposis treatment
73	0.5	Tryptophanamidase inhibitor
72.9	1.4	Peptidyl-dipeptidaseDcp inhibitor
72	1.4	2-Dehydropantoate 2-reductase inhibitor
71	0.4	Acylaminoacyl-peptidase inhibitor
72.1	1.5	Aldehyde oxidase inhibitor
71	0.8	Histidine N-acetyltransferase inhibitor
70	0.2	N-methyl-2-oxoglutaramate hydrolase inhibitor

Table S4: Biological Activity for *n*-nonatriacontan-19*α*-ol

Percentage Activity	Percentage Inactivity	Name of Activity
95.5	0.2	Alkylacetylglycerophosphatase inhibitor
95.3	0.2	Acrocylindropepsin inhibitor
95.3	0.2	Chymosin inhibitor
95.3	0.2	Saccharopepsin inhibitor
94.8	0.3	Sphinganine kinase inhibitor
94.4	0.2	Sugar-phosphatase inhibitor
94.3	0.2	Acylcarnitine hydrolase inhibitor
93.7	0.3	Polyporopepsin inhibitor
93	0.1	Beta-mannosidase inhibitor
92.9	0.6	CYP2C12 substrate
92.1	0.3	Fucosterol-epoxide lyase inhibitor
91.9	0.4	Alkenylglycerophosphocholine hydrolase inhibitor
91.1	0.2	Glucan 1,4-alpha-maltotriohydrolase inhibitor
91	0.3	CarboxypeptidaseTaq inhibitor

90.1	0.4	CYP2J2 substrate
90	0.3	Cutinase inhibitor
89.9	0.3	IgA-specific metalloendopeptidase inhibitor
87.1	0.5	Feruloyl esterase inhibitor
86.6	0.2	Alcohol dehydrogenase (acceptor) inhibitor
86.4	0.3	Trimethylamine-oxide aldolase inhibitor
86.5	0.3	All-trans-retinyl-palmitate hydrolase inhibitor
86	0.2	Anthranilate-CoA ligase inhibitor
86.1	0.3	Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
85.9	0.3	Poly(beta-D-mannuronate) lyase inhibitor
85.1	0.4	Vasoprotector
84.9	0.2	CYP4A11 substrate
85.3	0.7	Prostaglandin-E2 9-reductase inhibitor
84.7	0.1	Sclerosant
84	0.4	Venombin AB inhibitor
83	0.3	Endopeptidase So inhibitor
82.1	0.4	Allyl-alcohol dehydrogenase inhibitor
81.5	0.8	Membrane permeability inhibitor
81	0.3	Alkylglycerone-phosphate synthase inhibitor
80.7	0.2	Oryzin inhibitor
80.1	0.8	5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor
79.4	0.4	Lactase inhibitor
79.6	0.7	Superoxide dismutase inhibitor
79	0.3	Aspergillopepsin I inhibitor
79.1	0.5	Polyamine-transporting ATPase inhibitor
78.4	0.2	Sphinganine-1-phosphate aldolase inhibitor
80.1	2	Chlordeconereductase inhibitor
79	2	Methylenetetrahydrofolatereductase (NADPH) inhibitor
78	2.3	Antieczematic
77.4	2.4	Antiseborrheic
76	0.9	Bisphosphoglycerate phosphatase inhibitor
75	0.3	CYP4A substrate
75	0.4	Hydroxylamine oxidase inhibitor
76.4	2.9	Mucomembranous protector
74.1	1.5	Protein-disulfide reductase (glutathione) inhibitor
73.3	1.3	Fibrinolytic
72	0.5	N-formylmethionyl-peptidase inhibitor
71.5	0.4	Phosphatidylcholine-sterol O-acyltransferase inhibitor
71	0.5	Long-chain-aldehyde dehydrogenase inhibitor
70.6	0.4	Polygalacturonase inhibitor

Table S5: Biological Activity for *n*-henetetracontan-19*α*-ol

Percentage Activity	Percentage Inactivity	Name of Activity
95.5	0.2	Alkylacetylglycerophosphatase inhibitor
95.3	0.2	Acrocylindropepsin inhibitor
95.3	0.2	Chymosin inhibitor
95.3	0.2	Saccharopepsin inhibitor

94.8	0.3	Sphinganine kinase inhibitor
94.4	0.2	Sugar-phosphatase inhibitor
94.3	0.2	Acylcarnitine hydrolase inhibitor
93.7	0.3	Polyporopepsin inhibitor
93.6	0.4	5 Hydroxytryptamine release stimulant
93.4	0.1	Xylan endo-1,3-beta-xylosidase inhibitor
93	0.1	Beta-mannosidase inhibitor
92.6	0.4	Ubiquinol-cytochrome-c reductase inhibitor
92.4	0.2	Acetylesterase inhibitor
91.9	0.4	Alkenylglycerophosphocholine hydrolase inhibitor
90.9	0.4	CYP2J substrate
89.3	0.3	Exoribonuclease II inhibitor
88.6	0.6	Benzoate-CoA ligase inhibitor
87.6	0.4	Dextranase inhibitor
88.3	1.5	Membrane integrity agonist
86.6	1.3	Phobic disorders treatment
85.1	0.4	Vasoprotector
85.3	0.7	Prostaglandin-E2 9-reductase inhibitor
84.7	0.1	Sclerosant
84.6	0.2	Leukopoiesis stimulant
84.3	0.3	Alcohol oxidase inhibitor
84.4	0.4	Lipoprotein lipase inhibitor
83.9	0.2	Galactolipase inhibitor
84	0.4	Venombin AB inhibitor
83.7	0.3	N-Acyl-D-aspartate deacylase inhibitor
83.6	0.3	1,4-Lactonase inhibitor
83.6	0.5	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
83.2	0.5	Ribulose-phosphate 3-epimerase inhibitor
82.4	0.4	Levanase inhibitor
82.1	0.4	Allyl-alcohol dehydrogenase inhibitor
81.7	0.2	Protein-tyrosine sulfotransferase inhibitor
81.5	0.3	Phosphatidylglycerophosphatase inhibitor
80.7	0.2	Oryzin inhibitor
80.1	0.4	Phenol O-methyltransferase inhibitor
80.4	0.7	Omptin inhibitor
80.5	0.8	Arginine 2-monooxygenase inhibitor
79.9	0.2	Platelet aggregation stimulant
80.1	0.8	5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor
79.4	0.4	Lactase inhibitor
79.6	0.7	Superoxide dismutase inhibitor
79	0.3	Aspergillopepsin I inhibitor
78	2.3	Antieczematic
76.4	2.9	Mucomembranous protector
75.4	2	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
73.5	0.9	Lipid metabolism regulator
72.7	0.4	Transketolase inhibitor

72.7	0.5	Oxygen scavenger
73.3	1.3	Fibrinolytic
73.2	1.2	Membrane integrity antagonist
72	0.5	N-formylmethionyl-peptidase inhibitor
71.5	0.2	Antiviral (Rhinovirus)
71.2	0.2	Oxidizing agent
71	0.4	GABA aminotransferase inhibitor
70.5	0.8	Methylumbelliferyl-acetate deacetylase inhibitor

Table S6: Biological Activity for *n*-heptatriacontan-15α-ol

Percentage Activity	Percentage Inactivity	Name of Activity
95.5	0.2	Alkylacetylglycerophosphatase inhibitor
95.3	0.2	Acrocylindropepsin inhibitor
95.3	0.2	Chymosin inhibitor
95.3	0.2	Saccharopepsin inhibitor
94.8	0.3	Sphinganine kinase inhibitor
94.4	0.2	Sugar-phosphatase inhibitor
94.3	0.2	Acylcarnitine hydrolase inhibitor
93.7	0.3	Polyporopepsin inhibitor
93.6	0.4	5 Hydroxytryptamine release stimulant
93.4	0.1	Xylan endo-1,3-beta-xylosidase inhibitor
93	0.1	Beta-mannosidase inhibitor
92.6	0.4	Ubiquinol-cytochrome-c reductase inhibitor
92.4	0.2	Acetylesterase inhibitor
92.9	0.6	CYP2C12 substrate
92.1	0.1	Prostaglandin-A1 DELTA-isomerase inhibitor
92.2	0.3	Pro-opiomelanocortin converting enzyme inhibitor
92.1	0.3	Fucosterol-epoxide lyase inhibitor
90	0.3	Cutinase inhibitor
89.3	0.3	Exoribonuclease II inhibitor
88.9	0.2	Gluconate 5-dehydrogenase inhibitor
89.1	0.8	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
88.2	0.3	D-lactaldehyde dehydrogenase inhibitor
88.6	0.6	Benzoate-CoA ligase inhibitor
88.1	0.3	Nitrate reductase (cytochrome) inhibitor
87.6	0.4	Dextranase inhibitor
88.3	1.5	Membrane integrity agonist
87.1	0.5	Feruloyl esterase inhibitor
86.6	0.2	Alcohol dehydrogenase (acceptor) inhibitor
86.9	1.5	Aspulvinonedimethylallyltransferase inhibitor
85.1	0.4	Vasoprotector
85.3	0.7	Prostaglandin-E2 9-reductase inhibitor
84.7	0.1	Sclerosant
84.6	0.2	Leukopoiesis stimulant
84.3	0.3	Alcohol oxidase inhibitor
84	0.4	Venombin AB inhibitor
83.7	0.3	N-Acyl-D-aspartate deacylase inhibitor

83.6	0.3	1,4-Lactonase inhibitor
82.4	0.4	Levanase inhibitor
81.1	0.3	Snapalysin inhibitor
81.5	0.8	Membrane permeability inhibitor
80.7	0.2	Oryzin inhibitor
80.4	0.6	2-Hydroxymuconate-semialdehyde hydrolase inhibitor
80.1	0.4	Phenol O-methyltransferase inhibitor
80.4	0.7	Omptin inhibitor
79.4	0.4	Lactase inhibitor
79.6	0.7	Superoxide dismutase inhibitor
79	0.3	Aspergillopepsin I inhibitor
79.1	0.5	Polyamine-transporting ATPase inhibitor
78.4	0.2	Sphinganine-1-phosphate aldolase inhibitor
77.7	1.5	NADPH peroxidase inhibitor
78	2.3	Antieczematic
76.4	2.9	Mucomembranous protector
75.4	2	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
73.3	0.6	Carnitinamidase inhibitor
72.7	0.4	Transketolase inhibitor
72.7	0.5	Oxygen scavenger
73.3	1.3	Fibrinolytic
73.2	1.2	Membrane integrity antagonist
72.2	0.4	GST P substrate
71.5	0.2	Antiviral (Rhinovirus)
71.2	0.2	Oxidizing agent
71	0.4	GABA aminotransferase inhibitor
71.2	0.8	Vasodilator, peripheral
71	1.2	Creatininase inhibitor
71.3	1.6	Glutathione thiolesterase inhibitor
70.1	0.5	D-xylulosereductase inhibitor