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A novel and facile synthesis of fatty acid chain substituted benzoxadiazepine and naphthoxadiazepine derivatives

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ABSTRACT

*A series of novel benzoxadiazepine and naphthoxadiazepine (**4a-e** and **5a-e**) were synthesized by nucleophilic attack of selected fatty acid hydrazides (**1a-e**) on 2,3,5,6-Tetrachloro-1,4-benzoquinone and 2,3-dichlor-1,4-naphthoquinone in appreciable yield.*

Key words: Fatty acid hydrazides, 2,3,5,6-Tetrachloro-1,4-benzoquinone, 2,3-dichlor-1,4-naphthoquinone, benzoxadiazepine, naphthoxadiazepine.

INTRODUCTION

Modern organic chemistry is more and more related to heterocycles. Developing novel heterocycles and relating synthetic methods is the eternal goal in synthetic chemistry [1]. Particular interest on nitrogen-containing heterocycles is due to their existence in many natural or synthetic molecules [2]. Despite diverse synthetic utility, exploring novel synthetic methods to meet increasing scientific and practical demands is still an active area. Fused ring systems are very well-known and interesting molecules from several points of view [3-5]. The addition of nitrogen nucleophiles to benzo- and naphthoquinones represents a common synthetic route to many fused heterocyclic rings which have been used as synthetic intermediates in medicinal chemistry [6-7] and for food science [8]. Numerous studies have been reported [9-11] on the synthesis of a variety of oxadiazepine derivatives covering a wide range of bioorganic, natural products and medicinal chemistry. Considering potential safety risk implications of a compound with even further medicinal chemistry effort was focused towards design of novel fatty acid chain substituted naphthoxadiazepine and benzoxadiazepine derivatives using fatty acids. In present work, we developed a method for preparing fatty acid chain substituted benzoxadiazepine (**4a-e**) and naphthoxadiazepine (**5a-e**) derivatives using readily available 2,3,5,6-Tetrachloro-1,4-benzoquinone (**2**) and 2,3-dichloro-1,4-naphthoquinone (**3)** .Compounds (**4a-e**) and (**5a-e**) were prepared by using procedure [12].

MATERIALS AND METHODS

1. Experimental

1.1. Chemicals and Instruments

Undec-10-enoic (purity 98%), (9*Z*)-octadec-9-enoic (purity 97%), octadecanoic (stearic) and hexadecanoic (palmitic) acids were purchased commercially from Fluka Chemicals, (Buck: Switzerland). (9*Z*, 12*R*)-12-Hydroxyoctadec-9-enoic (ricinolic) acid was isolated from *Ricinus communis* (castor) oil following Gunstone's partition procedure.[16] Melting points were determined on a Kofler apparatus and are uncorrected. IR spectra were

recorded on Perkin Elmer FTIR spectrophotometer. ^{1}H NMR spectra were recorded on a Bruker Avance II 400 spectrometer (400 MHz) in $CDCl_3$ using TMS as internal standard. Chemical shifts (δ) are quoted in ppm and coupling constant (*J*) are expressed in Hz. ^{13}C NMR spectra were recorded on Bruker Avance II at 100 MHz spectrometer in $CDCl_3$ (δ = 77.00). The mass spectra were obtained on LC–MS spectrometer Model Q-TOF Micro waters. Reaction progress was monitored using TLC (glass plates- 0.5 mm thickness, silica gel G, Merck). Mixture of petroleum ether: acetone: acetic acid (80:20:1; v/v) were used as developing solvent. Silica gel (60-120 mesh, Merck) was used to carry out column chromatography.

1.2. General procedure for the synthesis of fatty acid hydrazides (1a-e) as starting material:
The fatty acid hydrazides (**1a-e**) were prepared from the literature reported [13] method.

1.3. General procedure for the synthesis of benzoxadiazepine (4a-e) derivatives:
A solution of **1a-e** (1.0 mmol) in 5 mL DMF was added drop-wise to a solution of **2** (1.0 mmol) in DMF (15 mL) over 5 min at room temperature with continuous stirring. The stirring was continued for 45-48 h, during which it turned yellowish to deep red. The progress of the reaction was being monitored by TLC. Upon the completion of reaction, the reaction mixture was filtered, washed with cold water, dried and then evaporated under high pressure vacuum pump to remove any residual DMF. The purified products (**4a-e)** were obtained by silica gel column chromatography with a mixture of n-hexane-ethyl acetate (89:11; v/v) as eluent. The characterization data of compounds (**4a-e**) are summarized below:

1.3.1. 6,8,9-Trichloro-2-(dec-9′-enyl)-7-hydroxybenzo[f][1,3,4]oxadiazepin-5(4H)-one (4a): Reddish brown, Yield 71%, mp 148˚C. IR (KBr, *ν*, cm^{-1}): 1080 (C-O-C), 1590 (Ar-C=C), 1625 (C=N), 1710 (C=O), 3320 (NH), 3455 (OH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 1.21 (br.s, 10H, $CH_2(CH_2)_5$), 1.65 (m, 2H, CH_2CH_2C=N), 2.05 (m, 2H, =$CHCH_2$), 2.20 (t, 2H, *J* = 7.50, CH_2C=N), 4.70 (dd, 1H, J_{H_b-H} = 16.80, $J_{H_b-H_a}$ = 2.70, H_bC=CH), 4.85 (dd, 1H, J_{H_a-H} = 10.10, $J_{H_a-H_b}$ = 2.70, H_aC=CH), 5.85 (tdd, 1H, $J_{H-^8CH_2}$ = 6.70, J_{H-H_a} = 10.10, J_{H-H_b} = 16.80, CH_2=CH), 7.78 (br, 1H, oxadiazepine-NH), 8.58 (br. 1H, Ar-OH). ^{13}C NMR ($CDCl_3$, δ_C): 24.5, 28.1, 28.4, 28.7, 29.2, 29.7, 30.2, 33.8 (chain CH_2, C-7′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′, C-8′), 115.2, (CH_2=CH, C-10′,), 121.1 (C-5a), 122.2, 122.9, 124.3 (C-9, 8 and 6), 139.0 (CH_2=CH, C-9′), 146.6 (C-9a), 152.5 (C-7), 155.8 (C=N, C-2), 167.2 (C=O). MS (ESI): Found, *m/z*: 419.61 M^+. $C_{18}H_{21}Cl_3N_2O_3$. Calculated, *m/z*: 419.68.

1.3.2. (Z)-6,8,9-Trichloro-2-(heptadec-8′-enyl)-7-hydroxybenzo[f][1,3,4]oxadiazepin-5(4H)-one (4b): Reddish brown, Yield 68%, mp 155˚C. IR (KBr, *ν*, cm^{-1}): 1090 (C-O-C), 1585 (Ar-C=C), 1630 (C=N), 1700 (C=O), 3330 (NH), 3470 (OH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.85 (dist.t , 3H, terminal-CH_3), 1.25 (br.s, 20H, $(CH_2)_{10}$), 1.52 (m, 2H, CH_2CH_2C=N), 2.07 (t, 2H, *J*=7.42, CH_2C=N), 2.28 (m, 4H, CH_2CH=$CHCH_2$), 5.28 (m, 2H, CH=CH), 7.72 (br, 1H, oxadiazepine-NH), 8.75 (m, 4H, Ar-OH). ^{13}C NMR ($CDCl_3$, δ_C): 14.1 (terminal-CH_3, C-17′), 22.5, 26.9, 27.2, 27.5, 28.1, 28.6, 28.7, 29.0, 29.2, 29.7, 29.8, 31.9 (chain CH_2, C-16′, C-15′, C-14′, C-13′, C-12′, C-11′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 34.1, 34.8 (CH_2, C-7′, C-10′), 120.9 (C-5a), 121.8, 123.2, 123.9 (C-9, 8 and 6), 128.5, 129.8 (CH=CH, C-8′, C-9′), 147.8 (C-9a), 152.7 (C-7), 156.2 (C=N, C-2), 169.4 (C=O). MS (ESI): Found, *m/z*: 516.97 M^+. $C_{25}H_{35}Cl_3N_2O_3$. Calculated, *m/z*: 517.83.

1.3.3. 6,8,9-Trichloro-7-hydroxy-2-pentadecylbenzo[f][1,3,4]oxadiazepin-5(4H)-one (4c): Brown, Yield 74%, mp 142˚C. IR (KBr, *ν*, cm^{-1}): 1085 (C-O-C), 1590 (Ar-C=C), 1620 (C=N), 1705 (C=O), 3285 (NH), 3465 (OH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.90 (dist. t, 3H, terminal-CH_3), 1.27 (m, 24H, $(CH_2)_{12}$), 1.65 (m, 2H, CH_2CH_2C=N), 1.95 (t, 2H, *J*=7.35, CH_2C=N), 7.75 (br, 1H, oxadiazepine-NH), 8.68 (m, 4H, Ar-OH). ^{13}C NMR ($CDCl_3$, δ_C): 14.7 (ter-CH_3, C-15′), 23.0, 25.4, 26.9, 27.2, 27.7, 28.5, 28.8, 29.1, 29.6, 29.8, 30.2, 31.7, 32.8, 32.9 (chain CH_2, C-14′, C-13′, C-12′, C-11′, C-10′, C-9′, C-8′, C-7′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 121.2 (C-5a), 122.7, 123.6, 124.5 (C-9, 8 and 6), 148.1 (C-9a), 152.6 (C-7), 156.9 (C=N, C-2), 168.8 (C=O). MS (ESI): Found, *m/z*: 491.25 M^+. $C_{23}H_{33}Cl_3N_2O_3$. Calculated, *m/z*: 491.81.

1.3.4. (Z)-6,8,9-Trichloro-7-hydroxy-2(11-hydroxyheptadec-8′-enyl)-benzo[f][1,3,4]oxadiazepin-5(4H)-one (4d): Reddish brown, Yield 67%, mp 157˚C. IR (KBr, *ν*, cm^{-1}): 1090 (C-O-C), 1595 (Ar-C=C), 1630 (C=N), 1710 (C=O), 3315 (NH), 3485 (OH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.85 (dist.t , 3H, -CH_3), 1.29 (br.s, 18H, $(CH_2)_9$), 1.33 (m , 2H, CH_2CHOH), 1.8 (m, 2H, CH_2CH_2C=N), 1.90 (m, 4H, -CH_2-C=C-CH_2), 1.97 (t, 2H, *J*=7.30, CH_2C=N), 2.30 (s, 1H, CH-OH), 3.60 (m, 1H, -CH-OH), 5.35 (m, 2H, -CH=CH-), 7.81 (br, 1H, oxadiazepine-NH),

8.72 (m, 4H, Ar-OH). ^{13}C NMR ($CDCl_3$, δ_C): 13.8 (ter-CH_3, C-17′), 25.2, 27.1, 27.7, 28.2, 28.9, 29.2, 29.6, 29.8, 30.2, 31.5 (chain CH_2, C-16′, C-15′, C-14′, C-13′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 35.4 (CH_2, C-7′), 37.6 (CH_2, C-12′), 39.7 (CH_2, C-10′), 72.2 (CH-OH, C-11′), 120.8 (C-5a), 121.1, 122.9, 124.5 (C-9, 8 and 6), 127.3, 131.2 (CH=CH, C-9′, C-8′), 146.6 (C-9a), 152.4 (C-7), 156.3 (C=N, C-2), 169.6 (C=O). MS (ESI): Found, *m/z*: 532.97 M^+. $C_{25}H_{35}Cl_3N_2O_4$. Calculated, *m/z*: 533.85.

1.3.5. 6,8,9-Trichloro-2-heptadecyl-7-hydroxybenzo[f][1,3,4]oxadiazepin-5(4H)-one (4e): Brown, Yield 72%, mp 145˚C. IR (KBr, *v*, cm^{-1}): 1080 (C-O-C), 1590 (Ar-C=C), 1625 (C=N), 1705(C=O), 3295 (NH), 3460 (OH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.89 (dist. t, 3H, terminal-CH_3), 1.31 (m, 28H, $(CH_2)_{14}$), 1.45 (m, 2H, CH_2CH_2C=N), 1.97 (t, 2H, *J*=7.45, CH_2C=N), 7.85 (br, 1H, oxadiazepine-NH), 8.71 (m, 4H, Ar-OH). ^{13}C NMR ($CDCl_3$, δ_C): 14.0 (ter-CH_3, C-17′), 22.9, 25.4, 26.9, 27.2, 27.7, 28.5, 28.8, 29.1, 29.4, 29.7, 30.6, 31.5, 31.9, 32.5, 32.8, 33.2 (chain CH_2, C-16′, C-15′, C-14′, C-13′, C-12′, C-11′, C-10′, C-9′, C-8′, C-7′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 119.7 (C-5a), 122.2, 123.7, 124.1 (C-9, 8 and 6), 148.3 (C-9a), 152.8 (C-7), 156.7 (C=N, C-2), 169.4 (C=O). MS (ESI): Found, *m/z*: 519.45 M^+. $C_{25}H_{37}Cl_3N_2O_3$. Calculated, *m/z*: 519.86.

1.4. General procedure for the synthesis of naphthoxadiazepine (5a-e) derivatives:

A solution of **1a-e** (1.0 mmol) in DMF (15 mL) was added drop-wise with continuous stirring to a solution of **3** (1.0 mmol) in 10 mL DMF over 10 min at room temperature. The reaction mixture undergo continuous stirring for 70-72 h, during which it turned orange to deep red. The progress of the reaction was being monitored by TLC. Once the reaction completed, the reaction mixture was filtered, washed with cold water, dried and then evaporated under high pressure vacuum pump to remove any residual DMF. The isolated products (**5a-e)** were further purified by silica gel column chromatography using a mixture of n-hexane-ethyl acetate (87:13; v/v) as eluent. The characterization data of compounds (**5a-e**) are summarized below:

1.4.1. 2-(Dec-9′-enyl)naphtho[2,3-f][1,3,4]oxadiazepine-5,6,11(4H)-trione (5a): Reddish brown, Yield 67%, mp 198˚C. IR (KBr, *v*, cm^{-1}): 1085 (C-O-C), 1580 (Ar-C=C), 1625 (C=N), 1690, 1710 (C=O), 3240 (NH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 1.24 (br.s, 10H, $CH_2(CH_2)_5$), 1.70 (m, 2H, CH_2CH_2C=N), 2.12 (m, 2H, =$CHCH_2$), 2.30 (t, 2H, *J* = 7.50, C*H*$_2$C=N), 4.90 (dd, 1H, J_{H_b-H} = 16.90, $J_{H_b-H_a}$ = 2.80, H_bC=CH), 4.98 (dd, 1H, J_{H_a-H} = 10.0, $J_{H_a-H_b}$ = 2.80, H_aC=CH), 5.81 (tdd, 1H, $J_{H-^8CH_2}$ = 6.65, J_{H-H_a} = 10.0, J_{H-H_b} = 16.90, CH_2=CH), 7.84 (br, 1H, oxadiazepine-NH), 7.90-8.15 (m, 4H, Ar-H). ^{13}C NMR ($CDCl_3$, δ_C): 25.4, 28.1, 28.7, 29.2, 29.6, 29.9, 31.2, 33.6 (chain CH_2, C-7′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′, C-8′), 114.4 (CH_2=CH, C-10′), 126.6, 127.3, 134.8, 136.2 (Ar-CH), 131.6, 132.1, 132.4, 141.5 (Ar-C), 138.6 (CH_2=CH, C-9′), 156.3 (C-2), 187.2, 187.3 (C-6 and C-11). MS (ESI): Found, *m/z*: 380.11 M^+. $C_{22}H_{24}N_2O_4$. Calculated, *m/z*: 380.42.

1.4.2. (Z)-2-(Heptadec-8′-enyl)-naphtho[2,3,-f][1,3,4]oxadiazepine-5,6,11(4H)-trione (5b): Brown, Yield 69%, mp 195˚C. IR (KBr, *v*, cm^{-1}): 1080 (C-O-C), 1585 (Ar-C=C), 1620 (C=N), 1680, 1705 (C=O), 3235 (NH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.88 (dist. t, 3H, terminal-CH_3), 1.29 (br.s, 20H, $(CH_2)_{10}$), 1.55 (m, 2H, CH_2CH_2C=N), 2.04 (t, 2H, *J*=7.42, CH_2C=N), 2.32 (m, 4H, CH_2CH=$CHCH_2$), 5.40 (m, 2H, CH=CH), 7.78 (br, 1H, oxadiazepine-NH), 8.00-8.20 (m, 4H, Ar-H). ^{13}C NMR ($CDCl_3$, δ_C): 14.5 (ter-CH_3, C-17′), 23.6, 25.9, 26.2, 27.3, 27.8, 28.0, 28.5, 28.8, 29.2, 29.6, 30.1, 31.9 (chain CH_2, C-16′, C-15′, C-14′, C-13′, C-12′, C-11′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 129.5, 130.1 (CH=CH, C-8′, C-9′), 125.8, 126.6, 135.3, 136.2 (Ar-CH), 131.4, 131.9, 132.2, 142.6 (Ar-C), 156.5 (C-2), 169.8 (oxadiazepine-C=O), 187.3, 187.8 (C-6 and C-11). MS (ESI): Found, *m/z*: 477.92. M^+. $C_{29}H_{38}N_2O_4$. Calculated, *m/z*: 478.59.

1.4.3. 2-Pentadecylnaphtha[2,3-f][1,3,4]oxadiazepine-5,6,11(4H)-trione (5c): Brown, Yield 73%, mp 182˚C. IR (KBr, *v*, cm^{-1}): 1090 (C-O-C), 1585 (Ar-C=C), 1625 (C=N), 1690, 1705 (C=O), 3245 (NH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.92 (dist.t, 3H, terminal-CH_3), 1.28 (br. s, 24H, $(CH_2)_{12}$), 1.60 (m, 2H, CH_2CH_2C=N), 1.90 (t, 2H, *J*=7.30, CH_2C=N), 7.82 (br, 1H, oxadiazepine-NH), 7.90-8.20 (m, 4H, Ar-H). ^{13}C NMR ($CDCl_3$, δ_C): 14.6 (ter-CH_3, C-15′), 23.4, 26.2, 26.6, 27.2, 27.9, 28.3, 28.6, 29.1, 29.4, 29.8, 30.3, 31.5, 31.9, 33.0 (chain CH_2, C-14′, C-13′, C-12′, C-11′, C-10′, C-9′, C-8′, C-7′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 126.8, 129.6, 136.3, 136.9 (Ar-CH), 131.5, 131.8, 133.2, 140.8 (Ar-C), 156.8 (C-2), 169.6 (oxadiazepine-C=O), 187.1, 187.5 (C-6 and C-11). MS (ESI): Found, *m/z*: 452.40 M^+. $C_{27}H_{36}N_2O_4$. Calculated, *m/z*: 452.56.

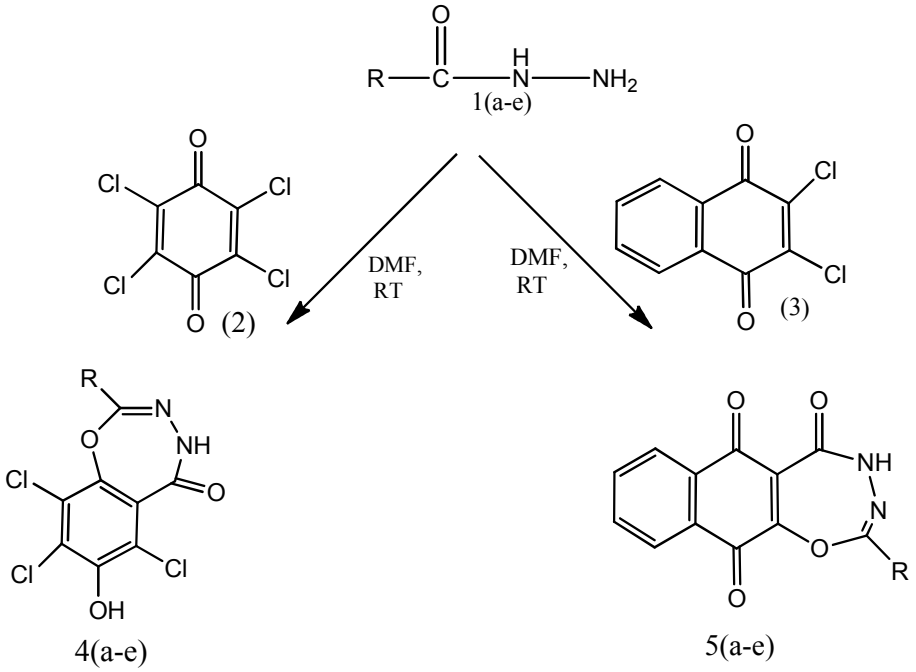
1.4.4. 2-[(8′*Z*,11′*R*)-11′-Hydroxyheptadec-8′-enyl]-naphtho[2,3-f][1,3,4]oxadiazepine-5,6,11(4H)-trione (5d): Reddish brown, Yield 65%, mp 197°C. IR (KBr, *v*, cm^{-1}): 1075 (C-O-C), 1590 (Ar-C=C), 1630 (C=N), 1695, 1715 (C=O), 3245 (NH), 3345 (OH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.87 (dist.t, 3H, $-CH_3$), 1.32 (br.s, 18H, $(CH_2)_9$), 1.50 (m, 2H, CH_2CHOH), 1.85 (m, 2H, $CH_2CH_2C=N$), 1.92 (m, 4H, $-CH_2-C=C-CH_2$), 1.95 (t, 2H, *J*=7.40, $CH_2C=N$), 2.40 (s, 1H, CH-OH), 3.52 (m, 1H, -CH-OH), 5.45 (m, 2H, -CH=CH-), 7.85 (br, 1H, oxadiazepine-NH), 7.75-8.05 (m, 4H, Ar-H). ^{13}C NMR ($CDCl_3$, δ_C): 13.6 (ter-CH_3, C-17′), 24.8, 26.9, 27.5, 28.3, 28.7, 29.1, 29.8, 31.2, 31.7, 32.3 (chain CH_2, C-16′, C-15′, C-14′, C-13′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 35.8 (CH_2, C-7′), 37.4 (CH_2, C-12′), 38.7 (CH_2, C-10′), 73.3 (CH-OH, C-11′), 126.7, 132.2 (CH=CH, C-9′, C-8′), 126.7, 129.3, 135.2, 136.6 (Ar-CH), 131.3, 131.6, 134.2, 141.7 (Ar-C), 156.4 (C-2), 169.5 (oxadiazepine-C=O), 187.3, 187.6 (C-6 and C-11). MS (ESI): Found, *m/z*: 494.07 M^+. $C_{29}H_{38}N_2O_5$. Calculated, *m/z*: 494.59.

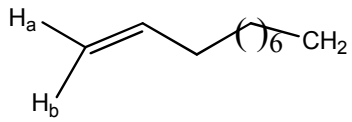
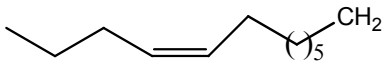
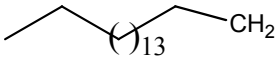
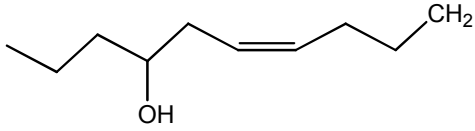
1.4.5. 2-Heptadecylnaphtho[2,3-f][1,3,4]oxadiazepine-5,6,11(4H)-trione (5e): Brown, Yield 70%, mp 182°C. IR (KBr, *v*, cm^{-1}): 1085 (C-O-C), 1595 (Ar-C=C), 1630 (C=N), 1685, 1720 (C=O), 3255 (NH). ^{1}H NMR (400MHz, $CDCl_3$, δ_H): 0.92 (dist. t, 3H, terminal-CH_3), 1.28 (br. s, 28H, $(CH_2)_{14}$), 1.55 (m, 2H, $CH_2CH_2C=N$), 1.92 (t, 2H, *J*=7.30, $CH_2C=N$), 7.76 (br, 1H, oxadiazepine-NH), 8.00-8.19 (m, 4H, Ar-H). ^{13}C NMR ($CDCl_3$, δ_C): 13.7 (ter-CH_3, C-17′), 22.3, 24.8, 26.9, 27.1, 27.8, 28.0, 28.7, 29.1, 29.5, 29.7, 30.2, 31.5, 31.7, 32.5, 32.9, 33.8 (chain CH_2, C-16′, C-15′, C-14′, C-13′, C-12′, C-11′, C-10′, C-9′, C-8′, C-7′, C-6′, C-5′, C-4′, C-3′, C-2′, C-1′), 127.1, 129.4, 136.2, 137.3 (Ar-CH), 130.7, 131.2, 134.6, 139.8 (Ar-C), 156.7 (C-2), 169.7 (oxadiazepine-C=O), 187.5, 187.7 (C-6 and C-11). MS (ESI): Found, *m/z*: 480.55 M^+. $C_{29}H_{40}N_2O_4$. Calculated, *m/z*: 480.61.

RESULTS AND DISCUSSION

The syntheses of the newly fatty acid substituted benzoxadiazepine and naphthoxadiazepine derivatives (**4a-e and 5a-e**) were performed by nucleophilic aromatic substitution of the chlorine atoms in 2,3,5,6-Tetrachloro-1,4-benzoquinone (**2**) and 2,3-dichloro-1,4-naphthoquinone(**3)** by different fatty acid hydrazides (**1a-e**) as depicted in Scheme. The fatty acid hydrazides (**1a-e**) being used here as a starting materials were previously prepared in our laboratory [13]. A solution of **1a-e** with **2** and **3** in DMF upon continuous standing for 48 and 72 hours at room temperature formed the derivatives of benzoxadiazepine (**4a-e**) and naphthoxadiazepine (**5a-e**) respectively in appreciable yields. IR spectrum of structures of 6,8,9-trichloro-7-hydroxy-2 (substituted) benzo[f][1,3,4]oxadiazepine-5(H)-ones (**4a-e**) showed a broad bands at 3455–3485 cm^{-1} and 3285–3335 cm^{-1} for OH and NH. A sharp peak at 1700–1710 cm^{-1} for C=O and 1620–1630 cm^{-1} for C=N. The ^{1}H NMR of (**4a-e**) showed two broad singlets at δ_H= 7.72–7.85 ppm and δ_H= 8.58–8.75 ppm for oxadiazepine-NH and phenolic-OH respectively. The ^{13}C NMR of (**4a-e**) showed peak at δ 167.2-169.6 ppm due to presence of one C=O group and at δ 155.8-156.9 ppm for oxadiazepine C-2. The signal at δ 152.4-152.8 ppm for aromatic quaternary carbon atom having hydroxyl group [14].

2-Substituted naphtho [2,3-f][1,3,4]oxadiazepine-5,6,11-(4H)-triones (**5a-e)** showed IR for N-H absorption at 3235-3255 cm^{-1} , C=O at 1705-1720 cm^{-1} and 1680-1695 cm^{-1} respectively and at 1620-1630 cm^{-1} for C=N. The ^{1}H NMR spectra of (**5a-e)** showed one broad signal at 7.76–7.85 ppm for oxadiazepine-NH. In ^{13}C NMR spectra of (**5a-e)** signals around 169.4-169.8 ppm for oxadiazepine C=O, 187.1-187.5 ppm for (C-6) and 187.3-187.8 ppm for (C-11) [15].



Compounds	(R)
1a, 4a, 5a	
1b, 4b, 5b	
1c, 4c, 5c	
1d, 4d, 5d	
1e, 4e, 6e	

Scheme: Synthesis of novel series of fatty acid chain substituted benzoxadiazepine and naphthoxadiazepine derivatives

CONCLUSION

A series of oxadiazepine derivatives **(4a-e and 5a-e)** have been synthesized using different fatty acid hydrazides (**1a-e)** for the first time and their preparation was made easily possible through the use of simple and cheap reagents in appreciable yields. Further studies are underway to extend this synthetic strategy using other fatty acids, with the intention of construction of more complex moiety.

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