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# Esters of Benzoic, 5-Arylisoxazole-3-carboxylic and 4,5-Dichloroisothiazole-3-carboxylic Acids

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**Abstract**—The method of synthesis was developed of esters of benzoic, 2-chlorobenzoic, 5-phenylisoxazole-3-carboxylic, 5-tolylisoxazole-3-carboxylic, and 4,5-dichloroisothiazole-3-carboxylic acids with some aliphatic and substituted aromatic alcohols. The latter were obtained by reduction of aldehydes used in perfumery.

**Keywords:** esters of carboxylic acids, aldehydes, alcohols

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Aliphatic and substituted aromatic aldehydes such as lauric aldehyde (*n*-dodecanal) **I**, jasmorange [2-methyl-3-(4-methylphenyl)propanal] **II**, cyclamen aldehyde [2-(4-isopropylbenzyl)propanal] **III**, anisic aldehyde (4-dehydromethoxybenzaldehyde) **IV**, veratric aldehyde (3,4-dimethoxybenzaldehyde) **V**, 4-(*n*-hexyloxy)-3-methoxybenzylaldehyde **VI**, 4-benzyloxy-3-methoxybenzaldehyde **VII**, 4-(*n*-hexyloxy)-3-ethoxybenzaldehyde **VIII**, 4-(*n*-octyloxy)-3-ethoxybenzaldehyde **IX**, 3,4-di(*n*-butyloxy)benzaldehyde **X** are present in essential oils of some plants. They are widely used in the perfume industry as odoriferous substances [1–3], and may also be used as starting compounds accessible for chemical modification for the purpose of synthesis of biologically active compounds [4–6].

The aim of this work was to develop a method for the synthesis of esters of benzoic, 2-chlorobenzoic, 5-phenylisoxazole-3carboxylic, 5-tolylisoxazole-3-carboxylic, and 4,5-dichloroisothiazole-3-carboxylic acids **XXI**–**XXV** with a series of aliphatic and substituted aromatic alcohols **XI**–**XX** obtained by reduction of the available aldehydes **I**–**X**. The latter were converted to alcohols **XI**–**XX** by the reduction with sodium borohydride in 2-propanol with 68–84% yields. The esterification of aliphatic and substituted aromatic alcohols **XI**–**XX** with chlorides of benzoic **XXI**, 2-chlorobenzoic **XXII**, 5-phenylisoxazole-3-carboxylic **XXIII**, 5-tolylisoxazole-3-carboxylic **XXIV** or 4,5-dichloroisothiazole-3-carboxylic acid **XXV** in ahydrous diethyl ether in the presence of triethylamine afforded the corresponding esters **XXVI**–**LVI** with 88–92% yields (Scheme 1).

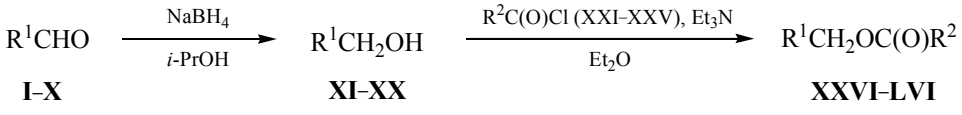
Physicochemical characteristics of alcohols **XI**, **XIV**, **XV** have been reported in [7]. The composition and structure of the rest of the synthesized compounds **XII**, **XIII**, **XVI**–**XX**, **XXVI**–**LVI** was proved by elemental analysis, gas chromatography-mass spectrometry, IR and $^1$H NMR spectroscopy data (Tables 1, 2). The resulting compounds are colorless or lightly colored crystalline solids or liquids which did not require additional purification and did not contain impurities of the starting compounds.

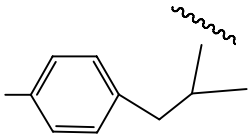
Due to the presence of aromatic and heterocyclic moieties in the molecules esters **XXVI**–**LVI** are of interest for the study of biological activity to detect the correlation between the biological activity and organoleptic analysis of odors and flavors of the starting aldehydes **I**–**X**. This is one of new and promising approaches to the creation of effective drugs for medical and agricultural purposes [8].

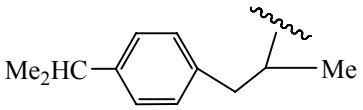
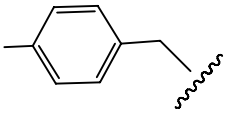
## EXPERIMENTAL

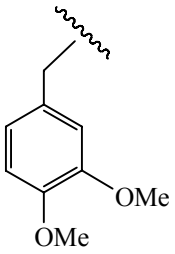
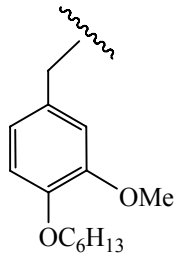
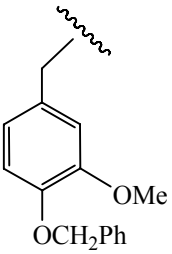
The IR spectra were recorded on a Nicolet Protégé-460 FTIR spectrophotometer from KBr pellets or thin

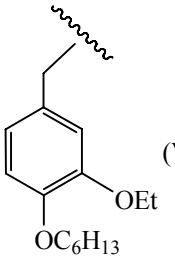
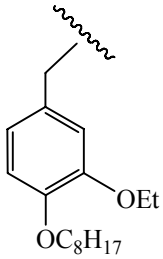
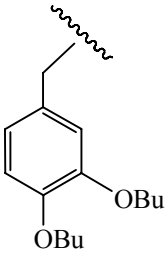
**Scheme 1.**

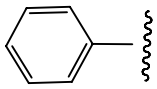
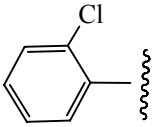


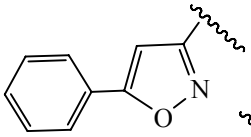

R = $Me(CH_2)_{10}$ (**I, XI, XXVI–XXVIII**),  (**II, XII, XXIX–XXXII**),

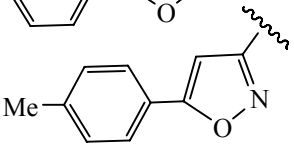
 (**III, XIII, XXXIII–XXXV**),  (**IV, XIV, XXXVI–XXXIX**),

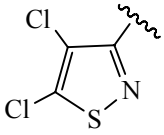
 (**V, XV, XL–XLII**),  (**VI, XVI, XLIII–XLVI**),  (**VII, XVII, XLVII–XLIX**),

 (**VIII, XVIII, L, LI**),  (**IX, XIX, LII, LIII**),  (**X, XX, LIV–LVI**);

$R^2$ =  (**XXI, XXIX, XXXVI, XL, XLIII, XLVII, LIV**),  (**XXII, XLIV**),

 (**XXIII, XXVI, XXX, XXXIII, XXXVII, XLI, XLV, XLVIII, L, LII, LV**),

 (**XXIV, XXVII, XXXI, XXXIV, XXXVIII**),

 (**XXV, XXVIII, XXXII, XXXV, XXXIX, XLII, XLVI, XLIX, LI, LIII, LVI**).

All alkoxy substituents (BuO, $C_6H_{13}O$ and $C_8H_{17}O$) have linear structure.

films. The $^1H$ NMR spectra were registered on a Bruker Avance-500 spectrometer from 5% solutions in $CDCl_3$. Mass spectra were obtained on a Hewlett Packard 5890/5972 instrument operating at electron impact ionization mode with ionizing electrons energy of 70 eV; capillary column HP-5MS 30 m × 0.25 mm, phase (5% PhMe Silicone) 0.25 microns, the evaporator temperature 250°C.

**Table 1.** Yields, melting points, and elemental analysis data for compounds **XII**, **XIII**, **XVI–XX**, **XXVI–LVI**

| Comp. no. | Yield, % | mp, °C | | Found, % | | | | | Formula | Calculated, % | | | | | $[M]^+$ | $M$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $d_{20}^{20}$ | $n_D^{20}$ | C | H | Cl | N | S | | C | H | Cl | N | S | | |
| **XII** | 79 | 0.9974 | 1.5185 | 80.67 | 9.95 | – | – | – | $C_{11}H_{16}O$ | 80.44 | 9.82 | – | – | – | 164 | 164.24 |
| **XIII** | 68 | 0.9292 | 1.5120 | 81.44 | 10.63 | – | – | – | $C_{13}H_{20}O$ | 81.20 | 10.48 | – | – | – | 192 | 192.30 |
| **XVI** | 84 | 41–42 | | 70.80 | 9.45 | – | – | – | $C_{14}H_{22}O_3$ | 70.56 | 9.30 | – | – | – | 238 | 238.32 |
| **XVII** | 82 | 64–65 | | 74.08 | 6.72 | – | – | – | $C_{15}H_{16}O_3$ | 73.75 | 6.60 | – | – | – | 244 | 244.29 |
| **XVIII** | 70 | 20–21 | | 71.77 | 9.55 | – | – | – | $C_{15}H_{24}O_3$ | 71.39 | 9.59 | – | – | – | 252 | 252.35 |
| **XIX** | 76 | 22–23 | | 73.14 | 10.24 | – | – | – | $C_{17}H_{28}O_3$ | 72.82 | 10.06 | – | – | – | 280 | 280.40 |
| **XX** | 83 | 34–35 | | 71.73 | 9.70 | – | – | – | $C_{15}H_{24}O_3$ | 71.39 | 9.59 | – | – | – | 252 | 252.35 |
| **XXVI** | 89 | 46–47 | | 74.25 | 8.99 | – | 3.58 | – | $C_{22}H_{31}NO_3$ | 73.91 | 8.74 | – | 3.92 | – | 357 | 357.49 |
| **XXVII** | 92 | 52–53 | | 74.73 | 9.12 | – | 3.46 | – | $C_{23}H_{33}NO_3$ | 74.36 | 8.95 | – | 3.77 | – | 371 | 371.51 |
| **XXVIII** | 90 | 32–33 | | 52.84 | 7.03 | 19.10 | 3.46 | 8.29 | $C_{16}H_{25}Cl_2NO_2S$ | 52.46 | 6.88 | 19.35 | 3.82 | 8.75 | 365 | 366.35 |
| **XXIX** | 90 | 1.0145 | 1.5495 | 80.91 | 7.35 | – | – | – | $C_{18}H_{20}O_2$ | 80.56 | 7.51 | – | – | – | 268 | 268.15 |
| **XXX** | 92 | 56–57 | | 75.64 | 6.50 | – | 3.87 | – | $C_{21}H_{21}NO_3$ | 75.20 | 6.31 | – | 4.18 | – | 335 | 335.40 |
| **XXXI** | 91 | 36–37 | | 75.89 | 6.74 | – | 3.65 | – | $C_{22}H_{23}NO_3$ | 75.62 | 6.63 | – | 4.01 | – | 349 | 349.42 |
| **XXXII** | 88 | 1.2350 | 1.5690 | 52.68 | 4.15 | 20.27 | 3.84 | 8.86 | $C_{15}H_{55}Cl_2NO_2S$ | 52.33 | 4.39 | 20.60 | 4.07 | 9.31 | 343 | 344.26 |
| **XXXIII** | 88 | 52–53 | | 76.42 | 7.16 | – | – | – | $C_{23}H_{25}O_3$ | 76.01 | 6.93 | – | – | – | 363 | 363.45 |
| **XXXIV** | 90 | 54–55 | | 76.67 | 7.38 | – | 3.49 | – | $C_{24}H_{27}NO_3$ | 76.36 | 7.21 | – | 3.71 | – | 277 | 377.48 |
| **XXXV** | 91 | 1.3425 | 1.5545 | 55.12 | 5.25 | 18.79 | 3.32 | 8.16 | $C_{17}H_{19}Cl_2NO_2S$ | 54.84 | 5.14 | 19.04 | 3.76 | 8.61 | 371 | 372.31 |
| **XXXVI** | 89 | 1.0345 | 1.5695 | 74.66 | 6.01 | – | – | – | $C_{15}H_{14}O_3$ | 74.36 | 5.82 | – | – | – | 242 | 242.27 |
| **XXXVII** | 89 | 77–78 | | 70.10 | 4.98 | – | 4.08 | – | $C_{18}H_{15}NO_4$ | 69.89 | 4.89 | – | 4.53 | – | 309 | 309.32 |
| **XXXVIII** | 88 | 104–105 | | 70.87 | 5.43 | – | 4.14 | – | $C_{19}H_{17}NO_4$ | 70.58 | 5.30 | – | 4.33 | – | 323 | 323.34 |

**Table 1.** (Contd.)

| Comp. no. | Yield, % | mp, °C | | Found, % | | | | | Formula | Calculated, % | | | | | $[M]^+$ | $M$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $d_{20}^{20}$ | $n_D^{20}$ | C | H | Cl | N | S | | C | H | Cl | N | S | | |
| **XXXIX** | 90 | 55–56 | 55–56 | 45.69 | 3.02 | 21.95 | 4.06 | 9.88 | $C_{12}H_9Cl_2NO_3S$ | 45.30 | 2.85 | 22.29 | 4.40 | 10.08 | 317 | 318.18 |
| **XLI** | 88 | 82–83 | | 67.41 | 5.25 | – | 3.76 | – | $C_{19}H_{17}NO_5$ | 67.25 | 5.05 | – | 4.13 | – | 339 | 339.34 |
| **XLII** | 89 | 83-84 | | 45.10 | 3.37 | 20.00 | 3.65 | 8.85 | $C_{13}H_{11}Cl_2NO_4S$ | 44.84 | 3.18 | 20.36 | 4.02 | 9.21 | 347 | 348.20 |
| **XLIII** | 90 | 1.0108 | 1.5415 | 73.82 | 7.79 | – | – | – | $C_{21}H_{26}O_4$ | 73.66 | 7.65 | – | – | – | 342 | 342.43 |
| **XLIV** | 89 | 1.0234 | 1.5505 | 67.29 | 6.88 | 9.65 | – | – | $C_{21}H_{25}ClO_4$ | 66.93 | 6.69 | 9.41 | – | – | 376 | 376.87 |
| **XLV** | 90 | 63–64 | | 70.85 | 6.18 | – | 3.11 | – | $C_{24}H_{27}NO_5$ | 70.40 | 6.65 | – | 3.42 | – | 409 | 409.47 |
| **XLVI** | 91 | 57–58 | | 52.08 | 5.23 | 16.56 | 3.05 | 7.28 | $C_{18}H_{21}Cl_2NO_4S$ | 51.68 | 5.06 | 16.95 | 3.35 | 7.66 | 417 | 418.33 |
| **XLVII** | 90 | 55–56 | | 76.24 | 5.90 | – | – | – | $C_{22}H_{20}O_4$ | 75.84 | 5.79 | – | – | – | 348 | 348.39 |
| **XLVIII** | 88 | 111–112 | | 72.60 | 5.27 | – | 3.11 | – | $C_{25}H_{21}NO_5$ | 72.28 | 5.10 | – | 3.37 | – | 415 | 415.44 |
| **XLIX** | 88 | 88–89 | | 53.99 | 3.86 | 16.35 | 2.94 | 7.20 | $C_{19}H_{15}Cl_2NO_4S$ | 53.78 | 3.56 | 16.71 | 3.30 | 7.56 | 423 | 424.30 |
| **L** | 90 | 73–74 | | 71.26 | 7.14 | – | 3.10 | – | $C_{25}H_{29}NO_5$ | 70.90 | 6.90 | – | 3.31 | – | 423 | 423.50 |
| **LI** | 91 | 57–58 | | 53.05 | 5.21 | 16.04 | 3.00 | 7.11 | $C_{19}H_{23}Cl_2NO_4S$ | 52.78 | 5.36 | 16.40 | 3.24 | 7.42 | 431 | 432.36 |
| **LII** | 91 | 71–72 | | 72.07 | 7.24 | – | 2.85 | – | $C_{27}H_{33}NO_5$ | 71.82 | 7.37 | – | 3.10 | – | 451 | 451.55 |
| **LIII** | 89 | 55–56 | | 55.07 | 6.07 | 15.12 | 2.74 | 6.45 | $C_{21}H_{27}Cl_2NO_4S$ | 54.78 | 5.91 | 15.40 | 3.04 | 6.96 | 459 | 460.41 |
| **LIV** | 90 | 28–29 | | 74.62 | 8.16 | – | – | – | $C_{22}H_{28}O_4$ | 74.13 | 7.92 | – | – | – | 356 | 356.46 |
| **LV** | 92 | 86–87 | | 71.28 | 7.12 | – | 3.03 | – | $C_{25}H_{29}NO_5$ | 70.90 | 6.90 | – | 3.31 | – | 423 | 423.50 |
| **LVI** | 89 | 67–68 | | 52.98 | 5.08 | 16.10 | 2.91 | 7.23 | $C_{19}H_{23}Cl_2NO_4S$ | 52.78 | 5.36 | 16.40 | 3.24 | 7.42 | 431 | 432.36 |

**Table 2.** IR and $^1$H NMR spectral data of compounds **XII–XX**, **XXVI–LVI**

| Comp. no. | IR spectrum, ν, $cm^{-1}$ | $^1$H NMR spectrum, δ, ppm (*J*, Hz) |
|---|---|---|
| **XII** | 3343 (OH); 1515 (Ar); 1035 (C–O) | 0.94 d (3H, Me, *J* 6.6), 2.36 s (3H, Me$C_6H_4$), 3.51 d (2H, $CH_2O$, *J* 6.6), 7.11 s (4H, $C_6H_4$) |
| **XIII** | 3333 (OH); 1512 (Ar); 1035 (C–O) | 0.95 d (3H, Me, *J* 6.5), 1.29 d (6H, $Me_2C$, *J* 6.3), 3.52 d (2H, $CH_2O$, *J* 5.6), 7.16 s (4H, $C_6H_4$) |
| **XIV** | 3384 (OH); 1612, 1514 (Ar); 1251, 1180, 1033 (C–O) | 3.82 s (3H, Me), 4.63 s (2H, $CH_2O$) |
| **XV** | 3477, 3386 (OH); 1608, 1594, 1516 (Ar); 1262, 1237, 1155, 1138, 1027(C–O) | 3.71 s (6H, 2Me), 4.42 s (2H, $CH_2O$) |
| **XVI** | 3418 (OH); 1608, 1592, 1515 (Ar); 1263, 1236, 1159, 1138, 1036 (C–O) | 0.91 t (3H, Me, *J* 6.6), 3.88 s (3H, MeO), 4.61 d (2H, $CH_2O$, *J* 5.8) |
| **XVII** | 3410 (OH); 1609, 1590, 1515 (Ar); 1260, 1235, 1160, 1134, 1032, 1004 (C–O) | 3.89 s (3H, MeO), 4.60 d (2H, $CH_2O$, *J* 5.8), 5.15 s (2H, Ph$CH_2O$) |
| **XVIII** | 3405 (OH); 1607, 1591, 1514 (Ar); 1261, 1234, 1164, 1137, 1045 (C–O) | 0.90 t (3H, Me, *J* 6.5), 4.44 s (2H, $CH_2O$) |
| **XIX** | 3335, 3252 (OH); 1606, 1591, 1517 (Ar); 1258, 1234, 1136, 1041 (C–O) | 0.89 t (3H, Me, *J* 6.5), 4.60 s (2H, $CH_2O$) |
| **XX** | 3414 (OH); 1608, 1592, 1515 (Ar); 1263, 1236, 1165, 1136, 1066, 1025 (C–O) | 0.98 t (6H, 2Me, *J* 6.4), 4.00 t (4H, $2CH_2O$, *J* 6.3), 4.56 d (2H, $CH_2O$, *J* 5.9) |
| **XXVI** | 3150 ($CH_{isoxazole}$); 1737, 1728 (C=O); 1611, 1589, 1571 (Ar); 1449 (C=N); 1246, 1144 (C–O) | 0.95 t (3H, Me, *J* 6.4), 4.42 t (2H, $CH_2O$, *J* 5.8), 6.92 s (1H, $CH_{isoxazole}$) |
| **XXVII** | 3138 ($CH_{isoxazole}$); 1728 (C=O); 1616 (Ar); 1449 (C=N); 1245, 1140 (C–O) | 0.96 t (3H, Me, *J* 6.4), 3.93 s (3H, Me), 4.42 t (2H, $CH_2O$, *J* 5.8), 7.02 s (1H, $CH_{isoxazole}$) |
| **XXVIII** | 1728 (C=O); 1228, 1084 (C–O) | 0.95 t (3H, Me, *J* 6.4), 4.42 t (2H, $CH_2O$, *J* 5.8) |
| **XXIX** | 1720 (C=O); 1600, 1585, 1515 (Ar); 1274, 1213, 1112 (C–O) | 1.06 d (3H, Me, *J* 6.6), 2.35 s (3H, Me$C_6H_4$), 4.23 d (2H, $CH_2O$, *J* 5.6), 7.12 s (4H, $C_6H_4$) |
| **XXX** | 3134 ($CH_{isoxazole}$); 1729 (C=O); 1612, 1585, 1572, 1514 (Ar); 1254, 1146, 1005 (C–O) | 1.04 d (3H, Me, *J* 6.6), 2.32 s (3H, Me$C_6H_4$), 4.28 d (2H, $CH_2O$, *J* 5.6), 6.82 s (1H, $CH_{isoxazole}$), 7.10 s (4H, $C_6H_4$) |
| **XXXI** | 3139 ($CH_{isoxazole}$); 1733 (C=O); 1616, 1595, 1574, 1513 (Ar); 1240, 1140, 1005 (C–O) | 1.04 d (3H, Me, *J* 6.6), 2.32 s and 2.43 s (6H, Me$C_6H_4$), 4.27 d (2H, $CH_2O$, *J* 5.6), 6.83 s (1H, $CH_{isoxazole}$), 7.10 s (4H, $C_6H_4$) |
| **XXXII** | 1735 (C=O); 1515 (Ar); 1223, 1084, 986 (C–O) | 1.04 d (3H, Me, *J* 6.6), 2.32 s (3H, Me$C_6H_4$), 4.32 d (2H, $CH_2O$, *J* 5.6), 7.09 s (4H, $C_6H_4$) |
| **XXXIII** | 1732 (C=O); 1612, 1591, 1573, 1512 (Ar); 1239, 1140, 1004 (C–O) | 1.05 d (3H, Me, *J* 6.5), 1.24 d (6H, $Me_2C$, *J* 6.9), 4.29 d (2H, $CH_2O$, *J* 5.6), 7.14 s (4H, $C_6H_4$) |
| **XXXIV** | 3140 ($CH_{isoxazole}$); 1733 (C=O); 1615, 1595, 1572, 1511 (Ar); 1240, 1139, 1004 (C–O) | 1.05 d (3H, Me, *J* 6.5), 1.24 d (6H, $Me_2C$, *J* 6.3), 2.43 s (3H, Me$C_6H_4$), 4.27 d (2H, $CH_2O$, *J* 5.6), 6.85 s (1H, $CH_{isoxazole}$), 7.14 s (4H, $C_6H_4$) |
| **XXXV** | 1736 (C=O); 1512 (Ar); 1223, 1084, 986 (C–O) | 1.02 d (3H, Me, *J* 6.5), 1.24 d (6H, $Me_2C$, *J* 6.3), 4.24 d (2H, $CH_2O$, *J* 5.6), 7.11 s (4H, $C_6H_4$) |
| **XXXVI** | 1717 (C=O); 1613, 1601, 1585, 1515 (Ar); 1272, 1249, 1175, 1109, 1070, 1035, 1027 (C–O) | 3.83 s (3H, Me), 5.32 s (2H, $CH_2O$) |
| **XXXVII** | 3129 ($CH_{isoxazole}$); 1727 (C=O); 1613, 1571, 1516 (Ar); 1257, 1231, 1182, 1137, 1032, 1005, 979 (C–O) | 3.83 s (3H, Me), 5.39 s (2H, $CH_2O$), 6.91 s (1H, $CH_{isoxazole}$) |

**Table 2.** (Contd.)

| Comp. no. | IR spectrum, ν, $cm^{-1}$ | $^1H$ NMR spectrum, δ, ppm (*J*, Hz) |
|---|---|---|
| **XXXVIII** | 3138 ($CH_{isoxazole}$); 1727 (C=O); 1613, 1515 (Ar); 1256, 1232, 1179, 1135, 1035, 1006, 980 (C–O) | 3.82 s (3H, MeO), 3.94 s (3H, Me), 5.38 s (2H, $CH_2O$), 6.86 s (1H, $CH_{isoxazole}$) |
| **XXXIX** | 1727 (C=O); 1614, 1582, 1516 (Ar); 1239, 1228, 1176, 1085, 1034, 971 (C–O) | 3.82 s (3H, Me), 5.38 s (2H, $CH_2O$) |
| **XL** | 1718 (C=O); 1598, 1518 (Ar); 1266, 1213, 1161, 1141, 1109, 1070, 1028 (C–O) | 3.90 s and 3.91 s (6H, 2Me), 5.31 s (2H, $CH_2O$) |
| **XLI** | 3130 ($CH_{isoxazole}$); 1730 (C=O); 1611, 1595, 1573, 1525 (Ar); 1241, 1166, 1136, 1037, 1022, 1001 (C–O) | 3.90 s and 3.92 s (6H, 2Me), 5.39 s (2H, $CH_2O$), 6.92 s (1H, $CH_{isoxazole}$) |
| **XLII** | 1724 (C=O); 1593, 1519 (Ar); 1256, 1225, 1138, 1092, 1031, 1012, 969 (C–O) | 3.89 s (6H, 2Me), 5.37 s (2H, $CH_2O$) |
| **XLIII** | 1719 (C=O); 1595, 1516 (Ar); 1267, 1238, 1213, 1164, 1140, 1109, 1070, 1038 (C–O) | 0.91 t (3H, Me, *J* 6.6), 3.87 s (3H, MeO), 5.30 s (2H, $CH_2O$) |
| **XLIV** | 1729 (C=O); 1608, 1592, 1517 (Ar); 1290, 1266, 1249, 1164, 1139, 1121, 1075, 1049, 1040 (C–O) | 0.89 t (3H, Me, *J* 6.6), 3.85 s (3H, MeO), 5.29 s (2H, $CH_2O$) |
| **XLV** | 3130 ($CH_{isoxazole}$); 1727 (C=O); 1607, 1592, 1573, 1518 (Ar); 1274, 1253, 1234, 1138, 1027, 993 (C–O) | 0.88 t (3H, Me, *J* 6.6), 3.90 s (3H, MeO), 5.38 s (2H, $CH_2O$), 6.92 s (1H, $CH_{isoxazole}$) |
| **XLVI** | 1731 (C=O); 1593, 1519 (Ar); 1260, 1217, 1164, 1139, 1085, 1037, 1022, 993, 965 (C–O) | 0.90 t (3H, Me, *J* 6.6), 3.88 s (3H, MeO), 5.37 s (2H, $CH_2O$) |
| **XLVII** | 1716 (C=O); 1595, 1515 (Ar); 1267, 1233, 1162, 1140, 1109, 1070, 1025 (C–O) | 3.92 s (6H, 2Me), 5.18 s and 5.31 s (4H, $CH_2O$) |
| **XLVIII** | 3132 ($CH_{isoxazole}$); 1729 (C=O); 1609, 1590, 1581, 1518 (Ar); 1253, 1227, 1167, 1130, 1028, 1000, 986 (C–O) | 3.93 s (6H, 2Me), 5.18 s and 5.37 s (4H, $CH_2O$), 6.92 s (1H, $CH_{isoxazole}$) |
| **XLIX** | 1723 (C=O); 1608, 1593, 1517 (Ar); 1270, 1233, 1165, 1147, 1083, 1036, 1012, 973(C–O) | 3.90 s (6H, 2Me), 5.16 s and 5.36 s (4H, $CH_2O$) |
| **L** | 3133 ($CH_{isoxazole}$); 1729 (C=O); 1608, 1591, 1573, 1519 (Ar); 1274, 1260, 1235, 1136, 1040, 995 (C–O) | 0.91 t (3H, Me, *J* 6.6), 5.36 s (2H, $CH_2O$), 6.92 s (1H, $CH_{isoxazole}$) |
| **LI** | 1727 (C=O); 1608, 1594, 1522 (Ar); 1273, 1239, 1178, 1145, 1085, 1050, 973 (C–O) | 0.91 t (3H, Me, *J* 6.6), 5.36 s (2H, $CH_2O$) |
| **LII** | 3133 ($CH_{isoxazole}$); 1729 (C=O); 1606, 1592, 1573, 1518 (Ar); 1274, 1254, 1232, 1137, 1043, 999 (C–O) | 0.91 t (3H, Me, *J* 6.7), 5.36 s (2H, $CH_2O$), 6.92 s (1H, $CH_{isoxazole}$) |
| **LIII** | 1726 (C=O); 1607, 1594, 1523 (Ar); 1274, 1239, 1179, 1146, 1084, 1052, 972 (C–O) | 0.89 t (3H, Me, *J* 6.7), 5.36 s (2H, $CH_2O$) |
| **LIV** | 1717, 1708 (C=O); 1594, 1515 (Ar); 1275, 1266, 1241, 1179, 1140, 1118, 1068, 1026, 972 (C–O) | 0.99 t (6H, 2Me, *J* 6.3), 4.02 t (4H, $2CH_2$, *J* 6.1), 5.29 s (2H, $CH_2O$) |
| **LV** | 3133 ($CH_{isoxazole}$); 1728 (C=O); 1608, 1591, 1576, 1520 (Ar); 1276, 1258, 1235, 1135, 1069, 1024, 999, 978 (C–O) | 0.98 t (6H, 2Me, *J* 6.3), 4.03 t (4H, $2CH_2$, *J* 6.1), 5.36 s (2H, $CH_2O$), 6.92 s (1H, $CH_{isoxazole}$) |
| **LVI** | 1726 (C=O); 1608, 1594, 1522 (Ar); 1275, 1241, 1178, 1145, 1083, 1070, 1041, 972 (C–O) | 0.98 t (6H, 2Me, *J* 6.3), 4.01 t (4H, $2CH_2$, *J* 6.1), 5.35 s (2H, $CH_2O$) |

**Reduction of aldehydes I–X to alcohols XI–XX.** To a solution of 10 mmol of an appropriate aldehyde **I–X** in 50 mL of anhydrous 2-propanol was added 10 mmol of sodium borohydride. The reaction mixture was stirred for 4 h and then poured into water. The reaction product was extracted with diethyl ether. The extract was dried over sodium sulfate and evaporated. The residue was purified by recrystallization from

diethyl ether–hexane mixture (2 : 1) or by column chromatography on silica gel (100–400 μm, eluent diethyl ether–hexane, 2 : 1).

**Synthesis of esters XXVI–LVI.** To a mixture of 10 mmol of alcohol **XI**–**XX** and 10 mmol of anhydrous triethylamine in 50 mL of anhydrous diethyl ether was added in portions 10 mmol of the corresponding carboxylic acid chloride **XXI**–**XXV**; a 1 : 1 : 1 ratio of the reactants was used. The reaction mixture was maintained at 20–23°C for 24 h. The resulting precipitate of triethylamine hydrochloride was filtered off and washed with small amount of diethyl ether. The ether solution was washed with water and 5% aqueous sodium hydrogen carbonate. Then the solvent was removed, the residue was purified by recrystallization from diethyl ether–hexane (2 : 1) or by column chromatography on silica gel (100–400 μm, diethyl ether–hexane, 2 : 1).

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