Novel Dibenz[b,e]Oxepins Derivatives

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By chemical modeling we combined in the same molecule the dibenz[b,e]oxepinic system and the oximinic group double bound with the carbon from 11-position of the dibenz[b,e]oxepinic nucleus. The synthesis of the new compounds contains three stages. In the first stage, the 2-phenoxymethylbenzoic acid was prepared by treating the phtalide with potassium phenoxyde in xylene. The resulting 2-phenoxymethylbenzoic acid potassium salt shows a good solubility in a sodium hydroxide aqueous solution and thus was separated from xylene. The aforementioned acid was precipitated using a mineral acid solution. The potassium salt of phenol was obtained using phenol and potassium hydroxide in xylene, the resulting water being removed by azeotropic distillation. The 6,11-dihydro-dibenz[b,e]oxepin-11(6H)-one was synthesized in the second stage by a Friedel-Crafts cyclization of the 2-phenoxymethylbenzoic acid chloride in dry 1,2-dichloroethane. The acid chloride was obtained by refluxing the coresponding acid with thionyl chloride in excess, but it could also be obtained using different anhydrous solvents as reaction medium, such as 1,2-dichloroethane. The desired ketone was also prepared directly from the 2-phenoxymethylbenzoic acid by using various agents for anhydrization (e.g. poliphosporic acid), but the yields were smaller. The new compounds were prepared by acylation of the 11-hydroximino-6,11-dihydro-dibenz[b,e]oxepin with various substituted benzoic acid chlorides, in dry benzene and in the presence of anhydrous pyridine as a proton fixator. The oxime was obtained by treating the 6,11-dihydro-dibenz[b,e]oxepin-11(6H)-one with hydroxylamine hydrochloride in presence of pyridine. We established the optimal reaction conditions in the synthesizing process of the new compounds to achive high purity and yields. The new compounds, which have not been mentioned in the literature concerning this domain, have been characterized by their physical constants (melting point, solubility) and the structures were confirmed by ¹H-NMR, ¹³C-NMR and IR spectral methods.

Keywords: dibenz[b,e]oxepin, ¹H-NMR, ¹³C-NMR

The present application is a continuation of our research concerning the synthesis and characterization of new O-acyl-oximino-dibenz[b,e]oxepins.

Dibenz[b,e]oxepins are known for their biological activities such as antidepressant, antipsychotic and antiinflammatory activity. In previous papers[1-12] we presented the synthesis, structural and pharmacological characterization of some O-acyl-oximino-dibenz[b,e] oxepins unsubstituted or substituted with a methyl or methoxy group.

In order to continue our work on the synthesis of new compounds with dibenz[b,e]oxepin structure and having potential biological properties, we made some chemical modeling and we combined in the same molecule the dibenz[b,e]oxepinic system and the oximinic group double bound with the carbon from 11-position of the dibenz[b,e]oxepinic nucleus.

Experimental part

The compounds melting points were measured on an Electrothermal 9100 apparatus and are uncorrected and the elemental analysis was realized using a Perkin Elmer CHNS/O Analyser Series II 2400 apparatus.

The NMR spectra were recorded on a Gemini 300BB instrument, at room temperature, operating at 300MHz for ¹H and 75MHz for ¹³C and a Unity Inova 400 instrument, operating at 400 MHz for ¹H and 100 MHz for ¹³C. The new dibenz[b,e]]oxepines were dissolved in chloroform-d1 and the chemical shifts were recorded as β values in parts per

million (ppm) relative with tetramethylsilane used as internal standard.

Infrared spectra were performed with FT-IR Bruker Vertex 70 apparatus.

The synthesis of 2-phenoxymethylbenzoic acid

A solution containing 0.05 mol of freshly distilled phenol in 30 mL xylene was placed in a round-bottom flask equipped with a Dean-Stark trap device. Subsequently, 0.055 mol of potassium hydroxide were added.

The reaction mixture was refluxed until the resulting water was removed by azeotropic distillation while potassium phenoxide precipitated at the bottom. Afterwards 0.05 Mol of phtalide were added and the mixture was refluxed until it became solid.

The precipitate was solubilisated with a 10% potassium hydroxide solution and then was diluted with 50 mL of water.

The aqueous phase was separated and acidulated with 1M hydrochloric acid solution until the mixture became acidic (pH 3) and the 2-phenoxymethylbenzoic acid precipited. The resulting precipitate was crystallized from water and presents a m.p. 126.5-128.5°C. 4.5 g 2-Phenoxymethylbenzoic acid (Mol wt 228.24) resulted (39.5% yield).

The synthesis of 2-phenoxymethylbenzoyl chloride

0.02 Mol of 2-phenoxymethylbenzoic acid, 30 mL of dry 1,2-dichloroethane and 0.042 mol of thionyl chloride

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were placed in a round-bottom flask equipped with a condenser and drying tube. The mixture was refluxed for 3 h. The surplus of thionyl chloride and the solvent were removed by reduced pressure distillation. For the next step the acid chloride was used in raw state.

1,2-Dichloroethane was anhydrized over calcium chloride and distillated at normal pressure.

The synthesis of 6,11-dihydro-dibenz[b,e]oxepin-11(6H)-one

0.02 Mol of anhydrous aluminium chloride and 15 mL of 1,2-dichloroethane were placed in a round-bottom flask equipped with stirrer, condenser with a drying tube, thermometer and an addition funnel.

The suspension was cooled to 0° C while stirring. The 0.02 mol of 2-phenoxymethylbenzoyl chloride solubilised in 25 mL of 1,2-dichloroethane was added in portions, with the mixture maintained at 0 to 5°C, during the addition period.

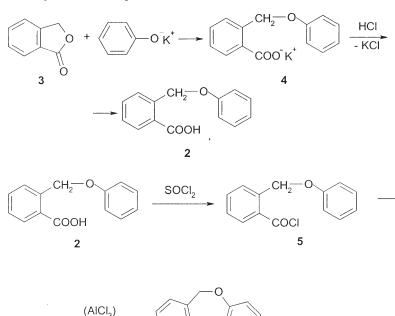
After the acid chloride was added, the reaction mixture was stirred one hour at 5 to 20°C and afterwards, for another hour at 20°C.

The reaction mixture was poured into a 5% hydrochloric acid solution and stirred until the aluminium chloride: ketone complex was decomposed.

The organic and aqueous layers were then separated and the organic layer was washed once with a 5% sodium hydroxide solution and twice with water, dried (anhyd. calcium chloride), treated with decolorizing charcoal and evaporated under vacum to yield the 6,11-dihydrodibenz[b,e]oxepin-11(6H)-one (Mol wt 210.24) which was recrystallized from hexane (4 g-ketone; 94% yield; m.p.67-68°C).

The synthesis of 11-hydroximino-6,11-dihydrodibenz[b,e]oxepin

0.05 Mol of 6,11-dihydro-dibenz[b,e]oxepin-11(6H)-one and 0.15 mol of hydroxylamine hydrochloride were boiled under reflux in 100 mL of pyridine for 72 h. The pyridine is subsequently distilled off in vacuum, the residue is triturated with water, filtered, dried and recrystallized from isopropanol. It resulted 8 g of compound, Mol wt 225.24, 71.1% yield and a m.p. 208- 210°C.



Ö 1 *The synthesis of the new O-acyl-oximinodibenz[b,e]oxepins (general procedure)*

0.016 Mol of oxime was solubilised in anhydrous benzene by refluxing in a round-bottom flask equipped with condenser and drying tube. To this solution it was added dropwise a solution of 0.016 mol acyl chloride in 10 mL anhydrous benzene and 0.016 mol of dry pyridine and the mixture was refluxed two hours.

After cooling and filtration, the solvent was removed by distillation and the residue was triturated with isopropanol. The resulting solid was recrystallized from isopropanol to yield the new O-acyl-oximino-dibenz[b,e]oxepins.

Results and discussion

For the new compounds synthesis we used 6,11-dihydrodibenz[b,e]oxepin-11(6H)-one (1) as intermediate substance.

The synthesis contains three stages.

<u>The synthesis of 2-phenoxymethylbenzoic acid (scheme</u> 1)

In the first stage, the 2-phenoxymethylbenzoic acid (2) was prepared by treating the phtalide (3) with potassium phenoxide in xylene.

The resulted potassium salts of 2-phenoxymethylbenzoic acid (4) shows a good solubility in an aqueous solution of 10% sodium hydroxide and was separated from xylene. The acid 2 was precipitated using a mineral acid solution.

The phenol potassium salt was obtained reacting phenol with potassium hydroxide in xylene, the resulting water being removed by azeotropic distillation.

The reactions are presented in the scheme 1.

<u>The synthesis of 6,11-dihydro-dibenz[b,e]oxepin-</u> <u>11(6H)-one</u>

The 6,11-dihydro-dibenz[b,e]oxepin-11(6H)-one (1) was synthesized by a Friedel-Crafts cyclization of the 2-phenoxymethylbenzoic acid chloride (5) in dry 1,2-dichloroethane.

The acid chloride 5 was obtained by refluxing the acid 2 with thionyl chloride in excess (the most favorable ratio is 1: 1,25), but could also be obtained using different anhydrous solvents as reaction medium, such as 1,2-dichloroethane.

Scheme 1. Synthesis of 2phenoxymethylbenzoic acid

Scheme 2. Synthesis of 6,11-dihydrodibenz[b,e]oxepin-11(6H)-one

- HCI

The desired ketone was also directly prepared from acid 2 using various agents for anhydrization (e.g. polyphosphoric acid), but the yields were smaller.

The acid chloride was used in the next step without further purification.

<u>The synthesis of the new O-acyl-oximino-</u> <u>dibenz[b,e]oxepins (scheme 3)</u>

The new compounds (**6a**-**h**) were prepared by acylation of the 11-hydroximino-6,11-dihydro-dibenz[b,e]oxepin (**7**)

Py

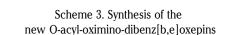
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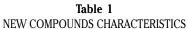
CI H₃N-OH Pv with various substituted benzoic acid chlorides in dry benzene using anhydrous pyridine as a proton fixator.

The oxime 7 resulted by treating the ketone 1 with hydroxylamine hydrochloride in the presence of pyridine. The reactions are presented in the scheme 3 and the

The reactions are presented in the scheme 3 and the structures of the new compounds (6a- h) are presented in the table 1.

The structure, molecular weight, melting point and yield of the new O-acyl-oximino-dibenz[b,e]oxepins are presented in table 1.





6(a-h)

N-OH

7

N-O-C-R

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		NEW C	COMPOUNDS C		ERISTIC	.5				
$\begin{array}{c} & & 5 \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & &$										
No.	R	Molecular weight	Melting point (⁰ C)	Yield (%)	C%		Н%		N%	
				(70)	c.	e.	с. е.		с. е.	
6a.	18 17 16 15 14 19 CH ₃	343.368	132.9- 135.7	72	76.95	76.78	4.99	4.87	4.08	4.03
6b.	CI 18 17 16 CI 14 15	398.24	129.7- 131	69	63.34	63.19	3.29	3.30	3.52	3.54
6c.	CI 18 17 16 CI 14 15	398.24	156- 157.4	75	63.34	63.39	3.29	3.25	3.52	3.48
6d.	$\begin{array}{c} 18 & 17 \\ \hline 13 & 16 \\ 14 & 15 \\ CI \end{array}$	398.24	140.2- 142.8	64	63.34	63.40	3.29	3.29	3.52	3.55
6e.	$ \begin{array}{c} 18 & 17 \\ 13 & 16 \\ 14 & 15 \end{array} $	455.242	168.9- 171.6	61	55.40	55.29	3.10	3.07	3.08	3.10
6f.	18 17 16 19 14 15 H ₃ C-O	359.368	119.4- 122.7	71	73.53	73.59	4.77	4.71	3.90	3.91
6g.	18 17 13 16 15 19 0-CH ₃	359.368	134.9- 138.4	71	73.53	73.63	4.77	4.59	3.90	3.95
6h.	$\begin{array}{c} \begin{array}{c} & 19 \\ O-CH_3 \\ \hline \\ & 18 & 17 \\ \hline \\ & 14 & 16 \\ 14 & 15 \\ \end{array} \begin{array}{c} O-CH_3 \\ \hline \\ & 14 & 15 \\ O-CH_3 \end{array}$	419.414	182.4- 185.1	' 63	68.72	68.58	5.05	5.14	3.34	3.30

The new compounds are solid, crystallized, white or light yellow, soluble at normal temperature in acetone, benzene, toluene, xylene, chloroform, dichloromethane and dichloroethane, by heating in inferior alcohols, insoluble in water.

Spectral data

The structures of the new O-acyl-oximino-dibenz[b,e] oxepins were established through NMR and IR spectroscopy.

The NMR spectra of the new dibenz[b,e]oxepins can be theoretically divided into two spectra, one corresponding to the oxepinic system and the other to the acyl attached to the oximino group.

The presence of an oxygen in the 5th position makes possible the existence of sin-anti isomery, materialised in our spectra through the dedoublation of the protons and the carbons signals, but the diference between chemical shifts of methylene group is insignificant. The ratio of *sin* and *anti* isomers has been evaluated comparing the ratio of H-19 and H-6 signals square integral, signal that can be isolated from the rest of the molecule protons signals and they provide a good confidence interpretation. Prior determinations on other compounds show that the two isomers result from the reaction in aproximately constant ratio.

The spectral data using ¹H-NMR, ¹³C-NMR and IR spectroscopy confirmed the structure of the obtained compounds.

O-(3-methylbenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin(6a)

¹**H-NMR** (CDCl₃, δ ppm, *J* Hz): 7.92 (dd, 1H, 1.7, 8.0); 7.74 (t, 1H, H-14, 1.5); 7.70÷7.60 (m, 2H, H-arom); 7.52÷7.32 (m, 5H, H-arom); 7.28 (t, 1H, H-17, 7.5); 7.10 (td, 1H, H-8, 1.1, 8.2); 6.91 (dd, 1H, H-4, 1.1, 8.2); 5.26 (s, 0.2*2H, H-6^m); 5.21 (s, 0.8*2H, H-6^M); 2.39 (s, 0.2*3H, H-19^m); 2.35 (s, 0.8*3H, H-19^M).

¹³C-NMR (CDCl., S ppm): 164.07 (C-12); 163.80 (C-11); 157.45 (C-4a); 138.36 (Cq); 134.14 (CH); 132.95 (Cq); 132.65 (CH); 131.00 (CH); 130.53 (Cq); 130.45 (CH); 130.40 (CH); 129.36 (Cq); 128.52 (CH); 128.40 (CH); 128.33 (CH); 128.20 (CH); 126.78 (CH); 121.47 (CH); 119.88 (CH); 119.72 (Cq); 70.56 (C-6^M); 70.42 (C-6^m); 21.25 (C-19).

FT-IR(solid in ATR, v cm⁻¹): 3056w; 2985w; 2930w; 2878w; 1755vs; 1602m; 1479m; 1439m; 1370w; 1329w; 1301m; 1263vs; 1222w; 1205w; 1174vs; 1109w; 1083s; 1047m; 1004w; 977m; 906s; 815w; 778w; 754m; 731s; 682w; 635w; 591w.

O-(2,5-dichlorobenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin (6b)

¹**H-NMR** (CDCl₃, δ ppm, *J* Hz): 7.88 (dd, 1H, 1.7, 8.0); 7.67 (dd, 1H, H-7, 1.0, 7.8); 7.60 (d, 1H, H-18, 1.1); 7.55 (dd, 1H, 1.2, 8.2); 7.50 ÷ 7.30 (m, 5H, H-arom); 7.02 (td, 1H, H-8, 1.0, 8.2); 6.91 (dd, 1H, H-2, 1.0, 8.2); 5.26 (s, 0.2*2H, H-6^m); 5.20 (s, 0.8*2H, H-6^M).

6^m); 5.20 (s, 0.8*2H, H-6^M). ¹³C-NMR (CDCl₂, δ ppm): 165.47 (C-12); 161.84 (C-11); 157.53 (C-4a); 134.27 (Cq); 134.07 (Cq); 132.89 (CH); 132.78 (CH); 132.72 (Cq); 132.24 (CH); 131.21 (CH); 130.80 (CH); 130.62 (CH); 130.06 (Cq); 128.54 (CH); 128.46 (CH); 128.05 (CH); 127.12(Cq); 121.48 (CH); 119.98 (CH); 119.30 (Cq); 70.53 (C-6^M); 70.44 (C-6^m).

FT-IR (solid in ATR, v cm⁻¹): 3063w; 2982w; 2881w; 1757vs; 1602m; 1575w; 1464m; 1439m; 1380w; 1328m; 1304m; 1285m; 1254m; 1221s; 1151m; 1104m; 1034s;

1005s; 975m; 895m; 830m; 803w; 752s; 727w; 700w; 678w; 635w; 595w.

O-(2,6-dichlorobenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin (6c)

¹**H-NMR** (CDCl₃, δ ppm, *J* Hz): 7.81 (dd, 1H, 1.4, 8.0); 7.67 (dd, 1H, H-7, 1.0, 7.8); 7.54 (dd, 1H, 1.2, 8.2); 7.46÷7.22 (m, 6H, H-arom); 6.99 (td, 1H, H-8, 1.0, 8.2); 6.90 (dd, 1H, H-2, 1.0, 8.2); 5.23 (s, 0.2*2H, H-6^m); 5.18 (s, 0.8*2H, H-6^M).

¹³C-NMR (CDCl₃, δ ppm): 165.56 (C-12); 164.56 (C-11); 157.63 (C-4a); 155.88 (Cq); 134.16 (Cq); 132.94 (CH); 132.67 (Cq); 131.40 (CH); 132.40 (Cq); 130.89 (CH); 130.64 (CH); 128.76 (CH); 128.41 (CH); 128.35 (CH); 127.98 (CH); 121.50 (CH); 120.09 (CH); 119.36 (Cq); 70.60 (C-6^M); 70.41 (C-6^m).

FT-IR (solid in ATR, v cm⁻¹): 3084w; 2986w; 2868w; 1755vs; 1595w; 1579m; 1584m; 1481m; 1436vs; 1307m; 1241vs; 1200m; 1163w; 1154m; 1124vs; 1079m; 1039s; 1015m; 971s; 876m; 863m; 799m; 777vs; 756s; 736m; 692m; 568w; 551w; 517w; 465w.

O-(3,4-dichlorobenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin (6d)

¹**H**-NMR (CDCl₃, δ ppm, *J* Hz): 7.87 (d, 1H, 1.2); 7.81 (dd, 1H, H-10, 1.6, 8.4); 7.63 (dd, 1H, H-7, 1.2, 8.5); 7.52 ÷ 7.26 (m, 6H, H-arom); 6.95 (td, 1H, H-8, 8.0, 1.3); 6.84 (dd, 1H, H-2, 1.0, 8.2); 5.18 (s, 0.2*2H, H-6^m); 5.12 (s, 0.8*2H, H-6^M).

6^M). ¹³C-NMR (CDCl₃, δ ppm): 165.05 (C-12); 161.93 (C-11); 157.65 (C-4a); 156.00 (Cq); 138.20 (Cq); 134.39 (Cq); 133.28 (Cq); 134.14 (CH); 133.01(CH); 131.73 (CH); 130.96 (CH); 130.83 (CH); 128.78 (CH); 128.55 (CH); 127.97 (CH); 127.26 (Cq); 121.63 (CH); 120.94 (CH); 120.08 (CH); 119.42 (Cq); 70.65 (C-6).

FT-IR (solid in ATR, v cm⁻¹): 3065w; 2988w; 2886w; 1751vs; 1596m; 1562w; 1481m; 1463m; 1441m; 1383w; 1336w; 1302w; 1264m; 1224vs; 1153w; 1109w; 1077s; 1038s; 978s; 882m; 834w; 804w; 751vs; 678w; 632w.

O-(4-iodobenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin (6e)

¹**H-NMR** (CDCl₃, δ ppm, *J* Hz): 7.91 (dd, 1H, H-1, 1.8, 7.9); 7.8 (d, 2H, H-14, H-18, 8.7); 7.56÷7.59 (m, 2H, H-arom); 7.32÷7.48 (m, 3H, H-arom); 7.46 (d, 2H, H-15, H-17, 8.6); 7.02 (ddd, 1H, H-2, 7.7, 7.3, 1.2); 6.91 (dd, 1H, H-4, 1.1, 8.4); 5.25 (s, 2H, H-6^M); 5.19 (s, 2H, H-6^m)

¹³**C**-**NMR** (CDCl, δ ppm): 164.5 (C-12); 163.3 (C-11); 157.5 (C-4a); 137.9 (C-15; C-17); 136.9 (Cq); 133.0 (Cq); 132.6 (CH); 131.2 (C14; C-18); 130.6 (CH); 128.1 (CH); 127.9 (CH); 121.5 (CH); 120.0 (CH); 119.5 (Cq); 70.52 ^M, 70.45^m (C-6). 101.3 (Cq).

O-(2-methoxybenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin (6f)

¹**H**-NMR (CDCl₃, δ ppm, *J* Hz): 7.82 (dd, 1H, 1.7, 8.0); 7.72 (dd, 1H, H-7, 1.7, 8.0); 7.59 (dd, 1H, H-14, 1.9, 8.1); 7.52 (dd, 1H, 1.4, 7.8); 7.43 ÷ 7.18 (m, 4H, H-arom); 6.96 ÷ 6.80 (m, 4H, H-2, H-8, H-15, H-17); 5.17 (s, 0.3*2H, H-6^m); 5.12 (s, 0.7*2H, H-6^M); 3.76 (s, 0.3*2H, H-6^m); 3.69 (s, 0.7*2H, H-6^M).

¹³C-NMR (CDCl₃, δ ppm): 164.21 (C-12); 163.82 (C-11); 159.27 (C-17); 157.48 (C-4a); 137.62 (Cq); 134.94 (Cq); 134.01 (CH); 132.82 (Cq); 132.62 (CH); 132.16 (CH); 131.96 (CH); 131.17 (CH); 130.30 (CH); 128.59 (CH); 128.35 (CH); 121.49 (CH); 120.33 (CH); 119.90 (CH); 119.99 (Cq); 112.02 (C-17); 70.61 (C-6^M); 70.40 (C-6^m); 55.81 (C-19). **FT-IR** (solid in ATR, v cm⁻¹): 3069w; 2967w; 2920w; 2868w; 2837w; 1747vs; 1600s; 1482s; 1459m; 1436s; 1375w; 1332w; 1301s; 1226vs; 1159m; 1121m; 1071vs; 1039vs; 1020s; 972vs; 880m; 835w; 774m; 751vs; 701m; 660m; 636m.

O-(3-methoxybenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin (6g)

¹**H-NMR** (CDCl₃, δ ppm, *J* Hz): 7.90 (dd, 1H, 1.7, 8.0); 7.62 (m, 1H, H-7); 7.52 ÷ 7.27 (m, 6H, H-arom); 7.40 (t, 1H, H-18, 1.3); 7.09 (dd, 1H, H-16, 1.3, 8.5); 7.02 (td, 1H, H-8, 1.0, 8.2); 6.91 (dd, 1H, H-2, 1.0, 8.2); 5.26 (s, 0.2*2H, H-6^m); 5.20 (s, 0.8*2H, H-6^M); 3.80 (s, 0.2*2H, H-6^m); 3.77 (s, 0.8*2H, H-6^M).

¹³C-ŃMR (CDCl., δ ppm): 165.24 (C-12); 163.56 (C-11); 159.67 (C-17); 157.55 (C-4a); 134.74 (Cq); 133.05 (Cq); 132.80 (CH); 131.06 (CH); 130.54 (CH); 129.92 (Cq); 129.67 (CH); 128.66 (CH); 128.45 (CH); 128.20 (CH); 122.26 (CH); 121.58 (CH); 120.35 (CH); 119.99 (CH); 119.74 (Cq); 113.93 (C-16); 70.65 (C-6); 55.50 (C-19).

FT-IR (solid in ATR, v cm⁻¹): 3069w; 3009w; 2968w; 2939w; 2836w; 1753vs; 1596m; 1482m; 1457m; 1441m; 1329w; 1304w; 1267m; 1207vs; 1176m; 1156m; 1111w; 1090w; 1057s; 1007m; 981m; 877w; 812w; 778m; 758m; 740s; 683w; 664w; 592w.

O-(3,4,5-trimethoxybenzoyl)-11-oximino-6,11-dihydrodibenz[b,e]oxepin (6h)

¹**H-NMR** (CDCl., δ ppm, *J* Hz): 7.85 (dd 1H, H-1, 8.0 1.8); 7.36- 7.63 (m, 4H, H-7- H-10); 7.29 (ddd, 1H, H-3, 8.1 7.8 1.3); 7.21 (s, 2H, H-14, H-18); 6.93-6.99 (m, 1H, H-2); 6.85 (dd, 1H, H-4, 8.3 1.3); 5.14 (s, 2H, H-6^m); 5.20 (s, 2H, H-6^M)

¹³C-NMR (CDCl₃, δ ppm): 163.8 (C-12); 163.0 (C-11); 157.4 (C-4a); 153.0 (C-17; C-15);137.0 (C-7a); 134.8 (C-16); 133.2 (C-10a); 132.7 (CH); 132.4 (CH); 132.3 (CH); 130.5 (CH); 128.0 (CH); 127.8 (CH); 123.3 (CH); 121.5 (CH); 119.9 (CH); 119.6(Cq); 107.1 (CH); 70.53 (C-6); 60.9 (C-20); 56.1 (C-19, C-21).

Conclusions

Following the synthesis of new compounds with potential biological activity, we obtained eight new O-acyl-oximino-dibenz[b,e]oxepins.

The compounds are prepared by acylating 11-oximino-6,11-dihydro-dibenz[b,e]oxepin with different substituted benzoic acid chlorides.

The obtained compounds have been characterized by some physical properties.

The ¹H-NMR, ¹³C-NMR and IR spectral parameters and the elemental analysis confirm the structure of the prepared compounds.

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