

تحضير و تشخيص مركب-2,2-diamino-2,5-di(4-hydroxyphenyl)-4-oxo-5-thiourayl-(1,2,4)Oxadizolidine(Oxa.) الفعالية البيولوجية

عواطف حميد عيسى المحيسن ، بلسم أنيس مارينا ، شروق شبرغالب الموسوي * ، إسرائ عبد علي
حسن الحواتي .
قسم علوم الحياة / كلية العلوم / جامعة البصرة .
* قسم الهندسة الكيماوية / كلية الهندسة/جامعة البصرة .

2,2-diamino-2.5-di(4-hydroxyphenyl)-4-oxo-5-thioureayl-(1,2,4) Oxadizolidine (Oxa.)
 α -(4-hydroxy phenyl)-N-benzyl Thiourea
 IR (Oxa.)
 -299 c UV
 Oxa. 297
Escherichia coli ATCC 25922
Staphylococcus aureus , *Pseudomonas aeruginosa* ATCC 27853
 100 μ g ATCC 25923
 (11.7 g/kg) LD₅₀
 (0.117 g/kg)

Synthesis and characterization of the compound
 2,2-diamino-2,5-di(4-hydroxyphenyl)-4-oxo-5-thiourayl-(1,2,4) Oxadizolidine (Oxa.)
 that had a biological activity
 Awatif H.I Al-Mohasin , Balsam A. Marina ,* Shurooq S. G. Al – Mosa wi,
 Israa A. H. Al- Hawani
 Biology department / College of Science / Basrah university .
 Chemical engineering department / College of Engineering \ Basrah university .

Asstract

The compound 2,2-diamino-2.5-di(4-hydroxyphenyl)-4-oxo-5-thioureayl-(1,2,4) oxadizolidene (Oxa.) was prepared by 1,3 dipolar cycloaddition reaction between α -(4-hydroxy phenyl)-N-benzyl and thiourea alken.

The compound Oxa. was purified by colum chromatography techniques. It's purity tested by using thin layer chromatography technique and showed single spot. The compound Oxa. was characterized by using spectroscopic techniques like IR , UV , Ms spectrum

The in correct melting point for Oxa. was 295-297 °C. The spectrum of biological activity of Oxa. Was broad , it was effective against reference strains of gram negative *Escherichia coli* ATCC 25922 , *Pseudomonas aeruginosa* ATCC 27853 and gram

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2,2-diamino-2.5-di(4-hydroxyphenyl)-4-oxo-5-thioiureayl-(1,2,4) C1=NC(=O)N(C1)C2=CC=C(O)C=C2 : Oxadizolidine (Oxa.)

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 Oxa. C1=NC(=O)N(C1)C2=CC=C(O)C=C2

1,3-dipolar C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (Hamer & Macaluso, 1964) C1=NC(=O)N(C1)C2=CC=C(O)C=C2 cycloaddition

0.2) C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (Hamer & Macaluso, 1964) C1=NC(=O)N(C1)C2=CC=C(O)C=C2 cycloaddition

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 2,2-diamino-4-(4-hydroxyphenyl)-(1,3,5)Oxathiozoline C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (Û 0.01

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 Û 100 (2001) C1=NC(=O)N(C1)C2=CC=C(O)C=C2

(α -4-hydroxyphenyl)-N-benzyl Nitron C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (Û 0.01, 2.27) C1=NC(=O)N(C1)C2=CC=C(O)C=C2

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 3, 30 °C Õ Reflex

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 Û Û

Oxa.

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (Al-Timari, 1991) (400-230) C1=NC(=O)N(C1)C2=CC=C(O)C=C2

Thin Layer Chromatography (TLC)

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (TLC) C1=NC(=O)N(C1)C2=CC=C(O)C=C2 C1=NC(=O)N(C1)C2=CC=C(O)C=C2

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (3:7) C1=NC(=O)N(C1)C2=CC=C(O)C=C2 (CHCl₃:CH₃OH)

(Huber & Vasella, 1989¹ Fried & Sherma, 1986)

Oxa.

Noto Û -

Infrared Spectroscopy (IR)

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 KBr Û (Shimadzu FT IR-8300)

Ultraviolet Spectroscopy (UV)

C1=NC(=O)N(C1)C2=CC=C(O)C=C2 Û (Pye, Unicam SP 8-100S Ultraviolet visible spectrophotometer, UK)

Mass spectrum (MS)

- Varian star 3400 CX – Sturn 2000 Û

Melting point (MP)

0 0 0 0 0 0 (0 0) 0 0

(Gallenkampherthermal apparatus, UK)

Oxa.

(0.1-500 µg/ml) 00 00 00 00 00 00 00 00

0 0 0 (Collee *et al.*, 1996) 00000000000000

Escherichia coli ATCC 25922

(WHO, 1987)

Staphylococcus aureus ATCC 25923 , *Pseudomonas aeruginosa* ATCC 27853

0 0

2 2 4 0 () Balb/c mice

0 0 0 0 0 0 0 0 0 0
(Klassen & Doull, 1980) 00000000000000

0 0 (75-70) (28-19gm) 000000000000

0 (8 ,10 ,12 ,14 ,16 gm/kg) Stomach tube

0 0 72

0 0 30 °C

0

2,2-diamino-2.5-di(4-hydroxyphenyl)-4-oxo-5-thioiureayl-(1,2,4)

Oxadizolidine (Oxa.)

0 0 0 Oxa. 0 0

(2001 ,) 00 80% 0 0000000000

Oxa.

TLC 0

CHCl₃:CH₃OH 0 0

(1 0) 0.7 Retardation Factor (Rf) 0

00 0

(Fried & Sherma , 1986; Fieser & Williamson , 1983)

Oxa.

IR

00 00 00 00 00 00 00 00 00

NH₂

(3450-3350)cm⁻¹

0 0

OH

(3500) cm⁻¹

$\tilde{\nu}$ (1377.1-1274.9) cm^{-1}
 $\tilde{\nu}$ $\tilde{\nu}$ (3030-3070.5) cm^{-1} $\tilde{\nu}$ (C-N)
 $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ CH_2
 $\tilde{\nu}$ (2A, $\tilde{\nu}$, 2A $\tilde{\nu}$) (2000-1750) cm^{-1} $\tilde{\nu}$
 $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$
 $\tilde{\nu}$ $\tilde{\nu}$ (N \rightarrow O) $\tilde{\nu}$
 $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$ (1160-1140) cm^{-1} $\tilde{\nu}$
 (2 B) $\tilde{\nu}$ (α -(4-Hydroxyphenyl)-N-benzyl nitron)
) cm^{-1} (C=N) $\tilde{\nu}$ $\tilde{\nu}$
 (1288.4) cm^{-1} C-O (1590-1570)
 (1988, $\tilde{\nu}$ 1 Silverstein *et al.*, 1981) (1) $\tilde{\nu}$
 UV

250
 $\tilde{\nu}$) (π - π^*) $\tilde{\nu}$ 270 nm
 α -(4-) (1991,) (3A
 $\tilde{\nu}$) 280,310,350nm (Hydroxyphenyl)-N-benzyl nitron
 . (2001,) $\tilde{\nu}$ (3B

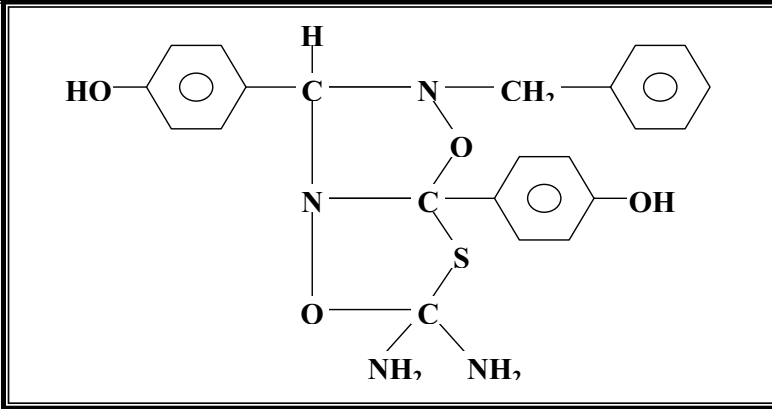
(430) M^+
 (3) $\tilde{\nu}$ (4) $\tilde{\nu}$ %30
 $(\text{CH}_4\text{N}_2\text{S})^+$ (M/Z= 76) $\tilde{\nu}$
 $(\text{C}_7\text{H}_7)^+$ (M/Z= 91)
 $(\text{C}_7\text{H}_7\text{NO})^+$ $\tilde{\nu}$ (M/Z= 121)
 . (1988, $\tilde{\nu}$ 1 2001,) . (1 $\tilde{\nu}$) ($\text{C}_{22}\text{H}_{22}\text{N}_4\text{SO}_4$)

$^0\text{C}\tilde{\nu}$ $\tilde{\nu}$ $\tilde{\nu}$,
 $\tilde{\nu}$ $\tilde{\nu}$ Oxa. , 297-299
 $\tilde{\nu}$ $\tilde{\nu}$. (1) $\tilde{\nu}$

(1) $\tilde{\nu}$

%	Rf	$\tilde{\nu}$	$\tilde{\nu}$ $\tilde{\nu}$	
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80	0.7	CHCl ₃ :CH ₃ OH 3:7	C ₂₂ H ₂₂ N ₄ SO ₄
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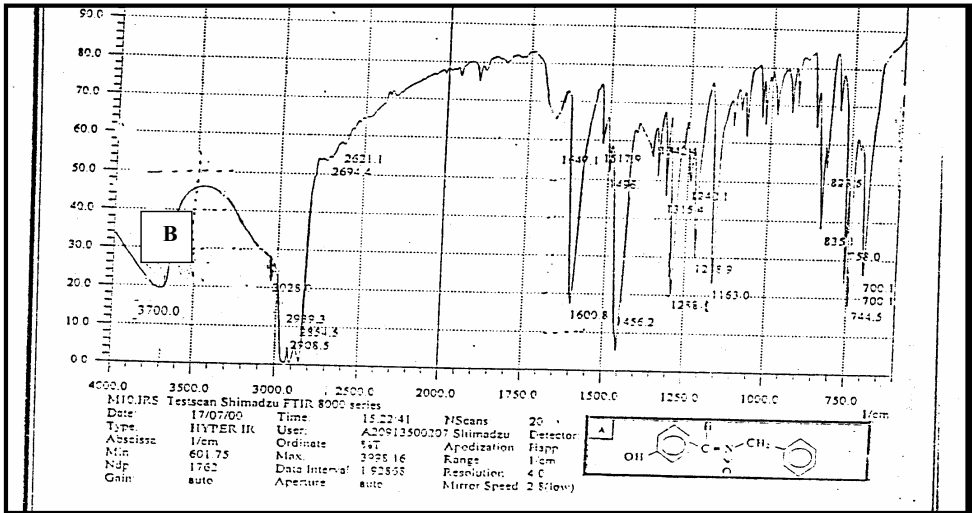
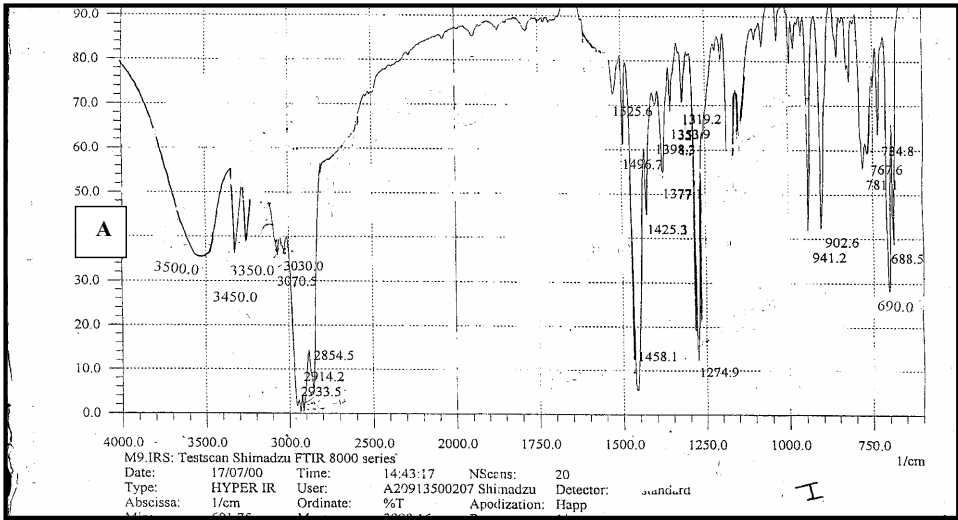
شكل (1) التركيب الفراغي لمركب Oxa.

. Oxa. IR (2 A) \ddot{U}

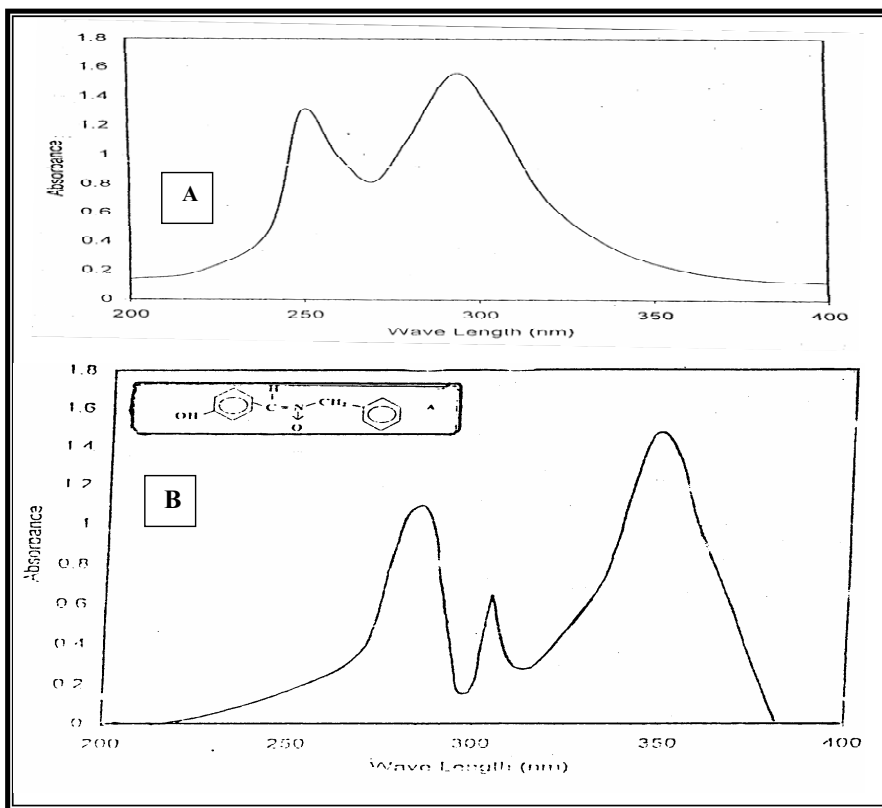
	(cm ⁻¹)	(cm ⁻¹)
OH	3500.0(S)	1398.0
NH ₂	3350.0(S)	1525.6
	3450.0(S)	
CH ₂	3070.0(W)	
(arom.)	3030.5(W)	
	2933.5(S)	
—C—H	2914.2(S)	902.0(S)
(alif.)	2000.0-1750.0(W)	941.2(S)
COMB. BAND	1458.1(S)	
N-O	1377.11(S)	
C-N(ter)	1178.4	
	1274.9(S)	
	690.0	
C-N		
C-S		

IR (2B) \hat{U}		
	(Cm^{-1})	(Cm^{-1})
-OH	3700.0 (S)	700.1 (IN)
H-C=	3000-3168.8 (S)	700-835.1 (S)
-CH ₂	2908.5(S)(s)2854.5(S)(s)	1240-1230 (S)
HC=N	2621.1(S)(s)- 2694(S)(as)	
COMB. BAND (over tone)	2000.0-1750.0	
C=N	1600.8-1590.0 (S)	
C-C	1530-1400 (S)	
C-N	1300.0-1200.0 (S)	
C-O	1288.4 (S)	1640.1 (S)
N→O	1165.0-1140.0 (S)	

W= Weak , S= Strong , IN= inplain , s= symmetric , as = asymmetric



IR (2) $\bar{\nu}$
 (2001,) α -(4-Hydroxyphenyl)-N-benzyl nitron :B, Oxa. :A



UV (3) Ū

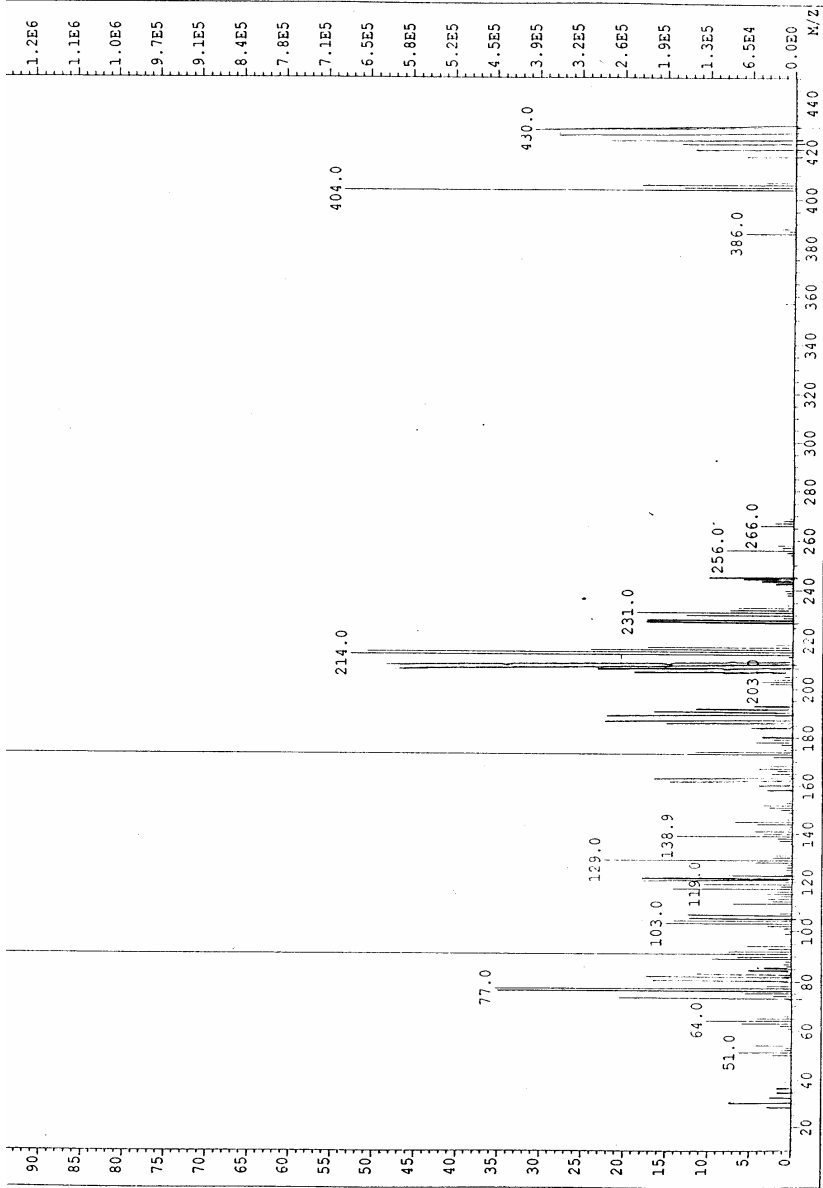
(2001) α-(4-Hydroxyphenyl)-N-benzyl nitron :B , Oxa. :A

.3 Ū

		(m/z)
30	430	M ⁺
47	227	[C ₁₄ H ₁₃ NO ₂]
50/49	211/210	[C ₁₄ H ₁₂ NO] ⁺
18/17	122/121	[C ₇ H ₇ NO] ⁺
15	106	[C ₇ H ₆ O] ⁺
100	91	[C ₇ H ₇] ⁺
35	76	[CH ₄ N ₂ S] ⁺

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2.12



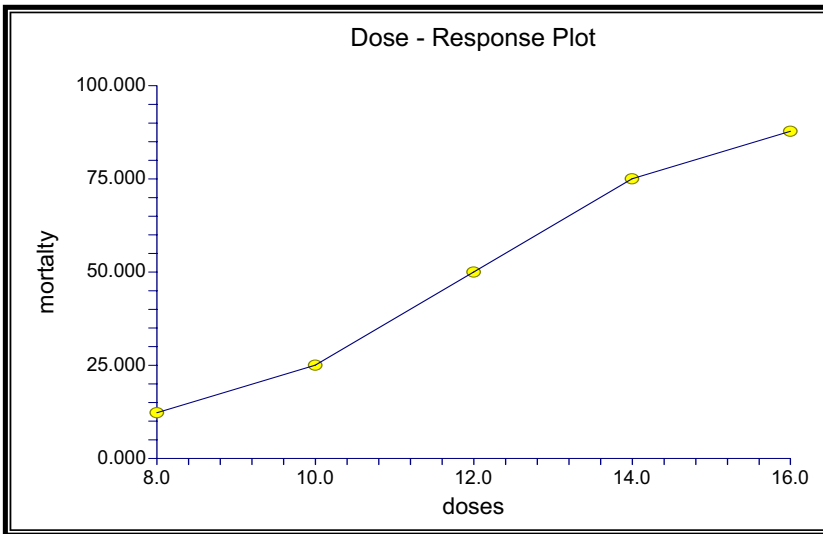
شكل (4) وضع طيف الكتلة المركب Oxa.

(4) \hat{U}

	λ	
C	0	0
T1	8	0
T2	10	25
T3	12	50
T4	14	75
T5	16	100

C = Control , T =

(Treatment) , N= 4



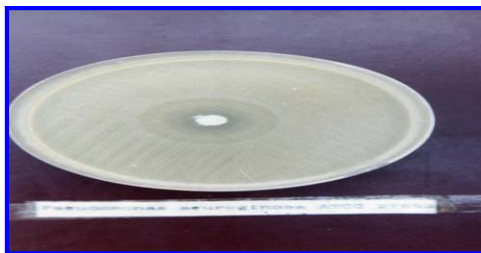
Oxa.

(5) \hat{U}



Oxa. .1

E. coli ATCC 25922



Oxa. .2

Pseudo. aeruginosa ATCC 27853



Oxa. .3

Staph. aureus ATCC 25923

-	Noto
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