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Synthesis and characterization of substituted 5 bromo 2-benzylidine-1-benzofuran-3-one and its structural determination

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ABSTRACT

As the halogen substituted aurones having various biological activity thus A series of 5 bromo 2-hydroxy-chalcones and their oxidative cyclization products aurones by using $HgCl_2$ or mercuric acetate , aurones, have been synthesized and tested for their purity by melting point method and by spectral interpretation technique specially by FTIR and H^1NMR

Keywords: Aurones , Chalcones, Plant pigment.

1. INTRODUCTION

Chalcones (1,3-diaryl-2-propen-1-ones) are flavonoid and isoflavonoid precursors (aurone) which are abundant in edible plants and display a wide spectrum of biological activities including antioxida-nt [1–5], antibacterial [6,7] antileishmanial [8–10], anticancer [11–13], antiangiogenic [14] anti-infective and anti-inflammatory activities [15–19]. The growing interest in these compounds and their potential use inmedicinal applications are proved by the growing number of publications concerning the synthesis and biological evaluation of chalcones analogues. Aurones, (Z)-2-benzylidenebenzofuran-3-(2H)-ones constitute a less studied subclass of flavonoids, which occur rarely in nature: to date approximately 100 aurones have been reported from natural sources, mainly flowering plants, and a few ferns, mosses and marine brown algae [20]. Aurones are responsible forthe bright yellow color of some popular ornamental flowers suchas snapdragon, cosmos and dahlia and are biosynthesized from chalcones by the key enzyme aureusidin synthase [21]. Representative naturally occurring aurones are aureusidin [22], sulfuretin [23] and maritimetin [24] possessing various hydroxylation patterns. A few natural aurones bearing methoxy substituents on either or both rings have been reported [25-31].

2. MATERIAL AND METHODS

2.1. Materials

2.1.1. Chemical reagents

5- bromo 2 hydroxy –acetophenones, anisaldehyde benzaldehyde,cinnamaldehyde, furfuraldehyde salysilaldehyde, $HgCl_2$

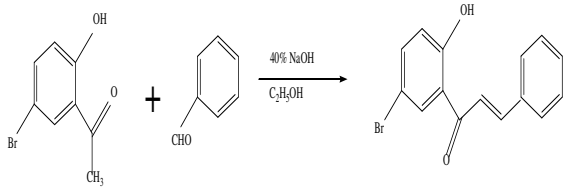
2.1.2. Instrument

MAC- melting points apparatus , FTIR IR spectrophotometr .

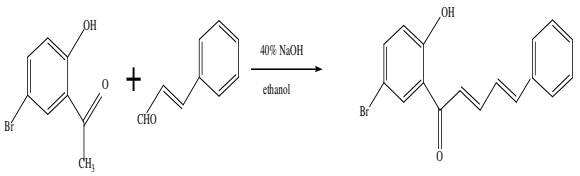
2.2. Synthesis of chalcone

chalcones have been synthesized via the Claisen–Schmidt condensation reaction between appropriately substituted acetophenone i.e 5-bromo 2 hydroxy -acetophenones and aldehydes like (anisaldehyde benzaldehyde,cinnamaldehyde, furfuraldehyde, salysilaldehyde) in ethanol both the compound should dissolve in it, after that 40% NaOH added dropwise until the solid mass is obtained then it keep for the next laboratory period then filtration followed by washing is done then compound was recrystalized from ethanol we get the corresponding chalcones . purity was checked by spectral interpretation and melting point .

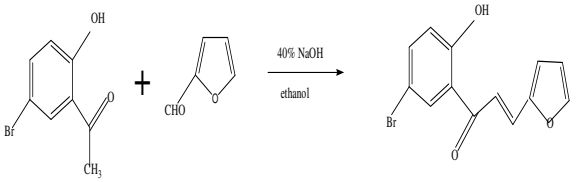
2.2.1. Synthesis of 5-bromo2-hydroxy(1,3)diphenyl-2 propen-1 one (C1)



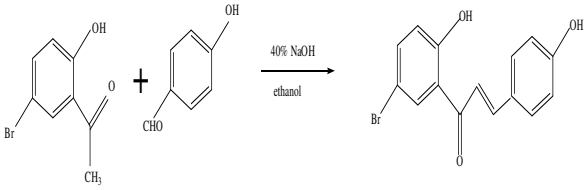
2.2.2. Synthesis of 5-bromo2-hydroxy(1,5)diphenyl-2 ,4 -butadien-1 one (C2)



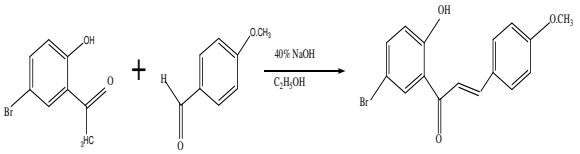
2.2.3. Synthesis of 5-bromo2-hydroxy-3furan 1-phenyl -2 propen-1 one (C3)



2.2.4. Synthesis of 5-bromo2-hydroxy 4 hydroxy (1,3)diphenyl-2 propen-1 one (C4)



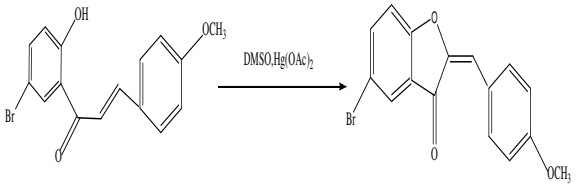
2.2.5. 5-bromo2-hydroxy 4- methoxy (1,3)diphenyl-2 propen-1 one (C5)



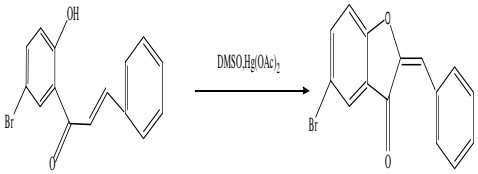
2.3. Synthesis of Aurones from chalcones

About 3.35 gm (0.01 M) of chalcones , 2.35 gm of (0.01M) mercuric chloride in 20 ml DMSO dissolved in round bottom flask. Reflux the reaction mixture for 3 hours, then reaction mixture was hydrolysed by using acidified ice cold water, filter the crude product and wash it 3-4 times by distilled water, dried, and crystallized by ethanol, solid product was obtained i.e aurone .

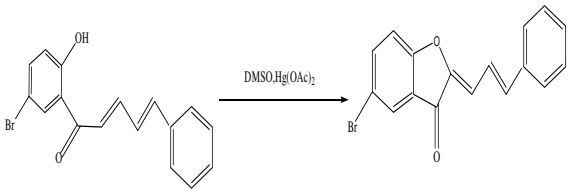
2.3.1. Synthesis of 5- bromo 4- methoxy 2-Benzylidene-1-benzofuran-3-one (A1)-



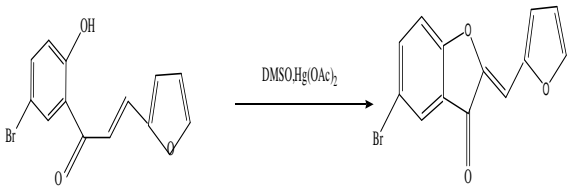
2.3.2. Synthesis of 5- bromo 2-Benzylidene-1-benzofuran-3-one (A2)



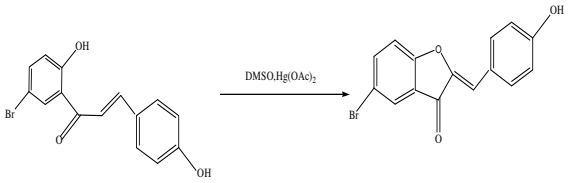
2.3.3. Synthesis of 5- bromo(1,3)butadiene- 3-Benzylidene-1-benzofuran-3-one (A3)



2.3.4. Synthesis of 5- bromo 2-furane -1-benzofuran-3-one (A4)



2.3.5. Synthesis of 5- bromo 4-hydroxy -2-Benzylidene-1-benzofuran-3-one (A5)



3. RESULTS AND DISCUSSION

The compounds prepared by using the described procedure are prepared correctly which is confirmed by the colour, melting point and from the spectral data i.e IR and H1 NMR spectroscopy.

Table 1: Physical data of chalcones (melting point & colour)

Symbol	Name of compound	Melting point	Colour
C1	5-bromo2-hydroxy(1,3)diphenyl-2 propen-1 one	79^0c	Brown
C2	5-bromo2-hydroxy(1,5)diphenyl-2 ,4 -butadien-1 one	80^0c	yellow
C3	5-bromo2-hydroxy-3furan 1-phenyl -2 propen-1 one	69^0c	Yellowish brown
C4	5-bromo2-hydroxy 4 hydroxy(1,3)diphenyl-2 propen-1 one	128^0c	Greenish yellow
C5	5-bromo2-hydroxy 4- methoxy(1,3)diphenyl-2 propen-1 one	72^0c	Golden yellow

Table - 2: Physical data of substituted benzofuran i.e. Aurone

Symbol	Name	Melting point	Colour
A1	5- bromo 4- methoxy 2-Benzylidene-1-benzofuran-3-one	79 °c	Greenish yellow
A2	5- bromo 2-Benzylidene-1-benzofuran-3-one	85 °c	Greenish yellow
A3	5- bromo(1,3)butadiene- 3-Benzylidene-1-benzofuran-3-one	78 °c	Golden yellow
A4	5- bromo 2-furane -1-benzofuran-3-one	92 °c	yellow
A5	5- bromo 4-hydroxy -2-Benzylidene-1-benzofuran-3-one	75 °c	Yellowish brown

Table - 3: The IR spectral analysis of compound shows the presence of following absorption bands

Name of compound	V (C=O)cm-1 Cyclic	V(c-o-c)cm1	V(c=c) cm1 aliphatic	V(-Br) cm1 Para substituted	Any special substituent	V(c=c) cm1 Aromatic
A-1	1692	1302	1636	694	V –OCH3 2835	1562
A-2	1681	1274	1640	700	-	1596
A-3	1694	1216	1636	684	1636 conjugated diene	1556
A-4	1690	1019	1641	628	1208 furan ring –O-	1579
A- 5	1636	1306	1670	664	3236 (-OH)	1598

Table - 4: The H^1 NMR spectral analysis of compound aurone showed the presence of following absorption bands

Name of compound	(δ ppm)	No.of potons	Assignment
A-1	3.33,7.6 7.84, 3.8 ,8.36 ,8.37	3H ,1H 1H,1H 1H,1H 1H	Ar-O-CH_3, Ar-H Ar-H, C=C-H, Br-Ar-H, Br-Ar-H
A-2	7.13, 3.24, 8.17	1H, 1H, 1H,	Ar-H, C=C-H, Br-Ar-H
A-3	7.16, 2.5, 8.14	1H, 1H, 1H,	Ar-H, C=C-H, Br-Ar-H
A-4	6.64, 3.3260 8.21, 8.07	1H, 1H, 1H, 1H	Ar-H Ar-H, , Ar-H, Br-Ar-H
A- 5	5.80, 7.44, 3.32 8.210	1H, 1H, 1H, 1H	Ar-O-H, Ar-H, C=C-H , Br-Ar-H

4. CONCLUSION

The compound i.e substituted aurones was successfully synthesized and their purity and conformation was checked by melting point and from spectral data .These aurones can be prove a good biological activities.

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5. REFERENCES

1. Stevens JF, Miranda CL, Frei B and Buhler DR. **Chem. Res. Toxicol.** 2003; 16: 1277.
2. Nishida J and Kawabata J. **Biosci. Biotechnol. Biochem.,** 2006; 70: 193.
3. Gacche RN, Dhole NA, Kamble SG and Bandgar BP. **J. Enzyme Inhib. Med. Chem.** 2007; 23: 28.
4. Vogel S, Ohmayer S, Brunner G and Heilmann, J. **Bioorg. Med. Chem.** 2008; 16; 4286.
5. Jung JC, Jang S, Lee Y, Min Y, Lim E, Jung H, Oh M, Oh S and Jung M. **J. Med. Chem.** 2008; 51: 4054.
6. Sugamoto K, Kurogi C, Matsushita Y and Matsui T. **Tetrahedron Lett.** 2008; 49: 6639.
7. Fvila HP, Smania E, Monache FD and Smania A. **Bioorg. Med. Chem.** 2008; 16: 9790.
8. Quintin J, Desrivot J, Thoret S, Le Menez P, Cresteil T and Lewin G. Bioorg. **Med. Chem. Lett.** 2009, 19, 167.
9. Suryawanshi SN, Chandra N, Kumar P, Porwal J and Gupta S. **Eur. J. Med. Chem.** 2008; 43: 2473.
10. Boeck P, Falcao CAB, Leal PC, Yunes RA, Filho VC, Torres-Santos EC and Rossi-Bergmann B. **Bioorg. Med. Chem.** 2006; 14: 1538.
11. Lawrence NJ, Patterson RP, Ooi LL, Cook D and Ducki S. **Bioorg. Med. Chem. Lett.** 2006; 16: 5844.
12. Cabrera M, Simoens M, Falchi G, Lavaggi ML, Piro OE, Castellano EE, Vidal A, Azqueta A, Monge A, De Cerain AL, Sagrera G, Seoane G, Cerecetto H and Gonzalez M. **Bioorg. Med. Chem.** 2007; 15: 3356.
13. Boumendjel A, Boccard J, Carrupt PA, Nicolle E, Blanc M, Geze A, Choisnard L, Wouessidjewe D, Matera EL and Dumontet C. **J. Med. Chem.** 2008; 51: 2307.
14. Mojzis J, Varinska L, Mojzisova G, Kostova I and Mirossay L. **Pharmacol. Res.** 2008; 57: 259.
15. Nowakowska Z. **Eur. J. Med. Chem.** 2007; 42, 125.
16. Meng CQ, Ni L, Worsencroft KJ, Ye Z, Weingarten MD, Simpson JE, Skudlarek JW, Marino EM, Suen KL, Kunsch C, Souder A, Howard RB, Sundell CL, Wasserman MA and Sikorski J. **A. J. Med. Chem.** 2007; 50: 1304.
17. Kim YH, Kim J, Park H and Kim HP. **Biol. Pharm. Bull.** 2007, 30, 1450.
18. Lee SH, Seo GS, Kim JY, Jin XY, Kim HD and Sohn DH. **Eur. J. Pharmacol.** 2006; 532: 178.
19. Cheng JH, Hung CF, Yang SC, Wang JP, Won SJ and Lin CN. **Bioorg. Med. Chem.** 2008, 16, 7270.
20. Stevens JF and Page JE. **Phytochemistry** 2004; 65: 1317.
21. Lee JH, Jung HS, Giang PM, Jin X, Lee S, Son PT, Lee D, Hong YS, Lee K and Lee JJ. **J. Pharmacol. Exp. Ther.** 2006, 316, 271.
22. Ahmad S, Israf DA, Lajis NH, Shaari K, Mohamed H, Wahab AA, Ariffin KT, Hoo WY, Aziz NA, Kadir AA, Sulaiman MR and Somchit MN. **Eur. J. Pharmacol.** 2006; 538: 188.
23. Cote CS, Kor C, Cohen J and Auclair K. **Biochem. Biophys. Res. Commun.** 2004; 10: 147.
24. Huang, HQ, Li HL, Tang J, Lv YF and Zhang WD. **Biochem. Syst. Ecol.** 2008; 36: 590.
25. Ono E, Fukuchi-Mizutani M, Nakamura N, Fukui Y, Yonekura-Sakakibara K, Yamaguch M, Nakayama T, Tanaka T, Kusumi T and Tanaka Y. **Proc. Natl. Acad. Sci.** U.S.A. 2006; 103: 11075.
26. Mohan P and Joshi T. **Phytochemistry**, 1989; 28: 2529.
27. Magela V, Junior G, Sousa CM de M, Cavalheiro AJ, Lago JHG and Chaves MH. **Helv. Chim. Acta** 2008; 91: 2159.
28. Romussi G and Pagani F. **Boll. Chim. Pharm.** 1970; 109: 467.
29. Seabra RM, Andrade PB, Ferreres F and Moreira MM. **Phytochemistry**, 1997; 45: 839.
30. Ferreira E, Salvador M, Pral EMF, Alfieri SC, Ito IY and Dias DAZ. **Naturforsch.** 2004; 59c: 499.
31. Morimoto M, Fukumoto H, Nozoe T, Hag Ur Rehaman A, Choudhary MI, Hayat S, Khan AH and Ahmed A. **Chem. Pharma. Bull.** 2001; 49: 105.