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Research Article

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Studies on Derivatives Uracil stability in various solvents and different functional groups: A DFT Study

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ABSTRACT

We have studied the Uracil system with a set of 4,12b-Dihydro-3-thioxo-1H,7H-chromeno [4/,3/:4,5]pyrano[2,3-d]pyrimidine-1(2H)-one of different electronic features using several methods. Calculations based on density functional theory(DFT)have been performed to investigate the stabilities. Our aim is to find the lowest energy uracil derivatives in different solvents. Also recognize the stability of different functional groups in the biological molecules is important. The investigated models have been relaxed to minimum energy structures. The combined IR , NBO and physical properties of the molecule have been evaluated. The solution changes caused that significant amount is changed Energy and properties of these molecules. Different functional groups can have various effects on Stability of the molecule and cell receptor. So by replacing the different functional groups, The calculations were carried out and optimal energy Was obtained.

Keywords: Density Functional Theory, Uracil, Solvent, functional groups, dipole moments

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INTRODUCTION

Uracil (U) is one of the four nucleobases in the nucleic acid of RNA that are represented by the letters A, G, C and U. The others are adenine (A), cytosine (C), and guanine (G). In RNA, uracil binds to adenine via two hydrogen bonds. In DNA, the uracil nucleobase is replaced by thymine. Uracil is a demethylated form of thymine. Uracil is a common and naturally occurring pyrimidine derivative[1]. Uracil is one of the most common lesions in DNA, and holds a rather special position among the various aberrant DNA bases described in the literature. First, uracil is a natural component of RNA, which likely was the dominating molecule for storage of genetic information early in evolution[2]. The name "uracil" was coined in 1885 by the German chemist Robert Behrend, who was attempting to synthesize derivatives of uric acid[3]. Originally discovered in 1900 by Alberto Ascoli, it was isolated by hydrolysis of yeast nuclein [4].

In RNA, uracil base-pairs with adenine and replaces thymine during DNA transcription. Methylation of uracil produces thymine. In DNA, the evolutionary substitution of thymine for uracil may have increased DNA stability and improved the efficiency of DNA replication. Uracil pairs with adenine through hydrogen bonding. When base pairing with adenine, uracil acts as both a hydrogen bond acceptor and a hydrogen bond donor. In RNA, uracil binds with a ribose sugar to form the ribonucleoside uridine. When a phosphate attaches to uridine, uridine 5'-monophosphate is produced [5]. Uracil can be used for drug delivery and as a pharmaceutical. When elemental fluorine is reacted with uracil, 5-fluorouracil is produced. 5-Fluorouracil is an anticancer drug (antimetabolite) used to masquerade as uracil during the nucleic acid replication process. Because 5-Fluorouracil is similar in shape to, but does not undergo the same chemistry as, uracil, the drug inhibits RNA replication enzymes, thereby blocking RNA

synthesis and stopping the growth of cancerous cells[6] . The derivatives uracil that has been studied is similar to thiouracil. The substance is a historically relevant anti-thyroid preparation. Astwood E.B. used it in 1943 as therapy of Graves' disease for the first time [7]. Thiouracil inhibits thyroid activity by blocking the enzyme thyroid peroxidase[8] . It's use in recent times has been replaced by advent of more potent and safer antithyroid drugs.

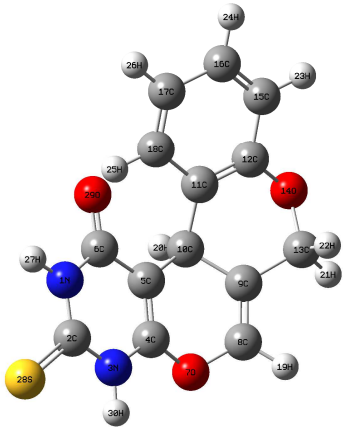

Fig. 1. 4,12b-Dihydro-3-thioxo-1H,7H-chromeno[4′,3′:4,5]pyrano[2,3-d]pyrimidine-1(2H)-one

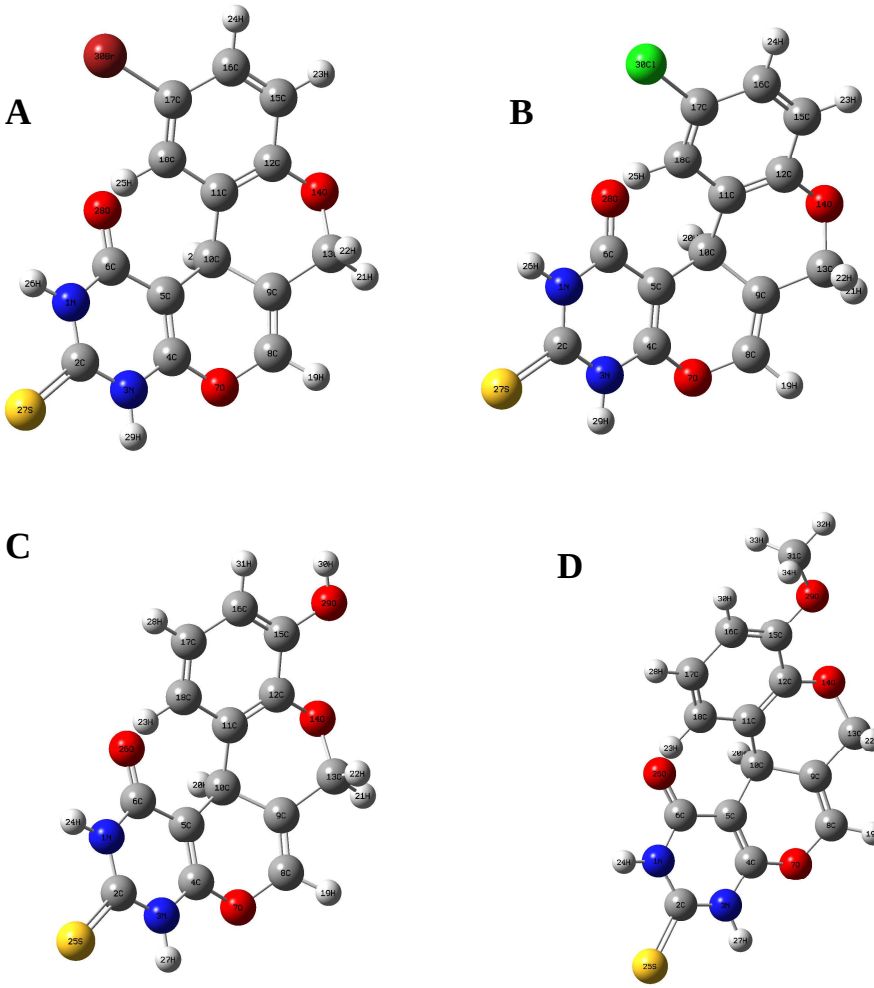

Fig. 2. The optimized molecular structures of 4,12b-Dihydro-3-thioxo-1H,7H-chromeno [4′,3′:4,5]pyrano[2,3-d]pyrimidine-1(2H)-one by different functional groups

Quantum mechanical geometry optimizations, dipole moments and frontier molecular orbital properties of all compounds were performed with the Gaussian09 program package. They were carried out by using the 6-311++G(d) basis set. The molecular structure, vibrational frequencies and NBO have been calculated. In organic chemistry, functional groups are specific groups (moieties) of atoms or bonds within molecules that are responsible for the characteristic chemical reactions of those molecules. The same functional group will undergo the same or similar chemical reaction(s) regardless of the size of the molecule it is a part of [9,10] . In this research, Also Effective functional groups on the drug were studied and to provide some initial examples of how these properties or characteristics are important for This molecule.

Computational details and discussion:

In this study, the 4,12b-Dihydro-3-thioxo-1H,7H-chromeno[4/,3/:4,5]pyrano[2,3-d]pyrimidine-1(2H)-one (fig1) are investigated density functional theory(DFT) . All the calculations have been performed using the B3LYP exchange correlation functional and the 6-311++G(d) basis set as implemented in the Gaussian 09 program. First, all model structures of this work including Water solvent, acetone, ethanol and ether individual compounds and Different functional groups include: Br, Cl, OH and Methoxy have been fully optimized to reach their minimum energies (fig2). As described previously, the values of total energies, binding energies, IR spectroscopy and dipole moments have been evaluated for the model structures with this optimization process.

Initially, optimized molecules was investigated by different solvents and after the calculation, This result obtained That by changing the solvent, the strength of hydrogen bonds between solvent and molecules is changed (table 1). thus the stability of the molecules changes. due to the physical properties of the uracil, this molecule can show different behaviors.

Table 1: Molecular properties In different solvents

Water		Ethanol		Acetone		Ether	
Bond length (A0)/N1-C2	1.3611	N1-C2	1.3614	N1-C2	1.3615	N1-C2	1.3631
N1-C6	1.4121	N1-C6	1.4124	N1-C6	1.4124	N1-C6	1.4134
N1-H30	1.0125	N1-H30	1.0125	N1-H30	1.0125	N1-H30	1.0124
C2-N3	1.3665	C2-N3	1.3671	C2-N3	1.3672	C2-N3	1.3699
C2-S27	1.6757	C2-S27	1.6749	C2-S27	1.6747	C2-S27	1.6705
N3-C4	1.3713	N3-C4	1.3713	N3-C4	1.3714	N3-C4	1.3715
N3-H29	1.0121	N3-H29	1.0121	N3-H29	1.0121	N3-H29	1.0117
C4-C5	1.3611	C4-C5	1.3609	C4-C5	1.3609	C4-C5	1.3601
C4-O7	1.3405	C4-O7	1.3408	C4-O7	1.3409	C4-O7	1.3428
C5-C6	1.4456	C5-C6	1.446	C5-C6	1.4462	C5-C6	1.4486
C5-C10	1.5127	C5-C10	1.5129	C5-C10	1.513	C5-C10	1.514
C6-O28	1.2248	C6-O28	1.2244	C6-O28	1.2243	C6-O28	1.2223
O7-C8	1.3935	O7-C8	1.3934	O7-C8	1.3934	O7-C8	1.3929
C8-C9	1.3256	C8-C9	1.3256	C8-C9	1.3256	C8-C9	1.3257
C8-H19	1.0802	C8-H19	1.0802	C8-H19	1.0802	C8-H19	1.0804
C9-C10	1.5097	C9-C10	1.5097	C9-C10	1.5097	C9-C10	1.5097
C9-C13	1.49	C9-C13	1.4902	C9-C13	1.4902	C9-C13	1.4909
C10-C11	1.5352	C10-C11	1.5354	C10-C11	1.5355	C10-C11	1.5364
C10-H20	1.0989	C10-H20	1.099	C10-H20	1.099	C10-H20	1.0991
C11-C12	1.4074	C11-C12	1.4073	C11-C12	1.4073	C11-C12	1.407
C11-C18	1.3984	C11-C18	1.3984	C11-C18	1.3984	C11-C18	1.407
C12-O14	1.3721	C12-O14	1.3723	C12-O14	1.3724	C12-O14	1.3987
C12-C15	1.3993	C12-C15	1.3992	C12-C15	1.3992	C12-C15	1.3987
C13-O14	1.4468	C13-O14	1.4461	C13-O14	1.4459	C13-O14	1.4423
C13-H21	1.0954	C13-H21	1.0955	C13-H21	1.0955	C13-H21	1.0962
C13-H22	1.0892	C13-H22	1.0892	C13-H22	1.0893	C13-H22	1.0896
C15-C16	1.3893	C15-C16	1.3892	C15-C16	1.3892	C15-C16	1.3886
C15-H23	1.0848	C15-H23	1.0848	C15-H23	1.0848	C15-H23	1.0847
C16-C17	1.3957	C16-C17	1.3957	C16-C17	1.3957	C16-C17	1.3954
C16-H24	1.0851	C16-H24	1.0851	C16-H24	1.0851	C16-H24	1.0852
C17-C18	1.3927	C17-C18	1.3925	C17-C18	1.3925	C17-C18	1.3919
C17-H26	1.0846	C17-H26	1.0846	C17-H26	1.0846	C17-H26	1.0846
C18-H25	1.0825	C18-H25	1.0824	C18-H25	1.0824	C18-H25	1.0821
Bond Angel/C2N1C6	127.4098	C2N1C6	127.4359	C2N1C6	127.4429	C2N1C6	127.5936
C2N1H30	116.7953	C2N1H30	116.7844	C2N1H30	116.7777	C2N1H30	116.6917
C6N1H30	115.7778	C6N1H30	115.7631	C6N1H30	115.761	C6N1H30	115.6919

N1C2N3	113.7241	N1C2N3	113.6801	N1C2N3	113.6679	N1C2N3	113.4268
N1C2S27	123.7445	N1C2S27	123.788	N1C2S27	123.7981	N1C2S27	124.024
N3C2S27	122.5288	N3C2S27	122.529	N3C2S27	122.5312	N3C2S27	122.5459
C2N3C4	123.3908	C2N3C4	123.4062	C2N3C4	123.4113	C2N3C4	123.497
C2N3H29	117.9021	C2N3H29	117.87	C2N3H29	117.8603	C2N3H29	117.6705
C4N3H29	118.6951	C4N3H29	118.713	C4N3H29	118.7176	C4N3H29	118.8238
N3C4C5	122.8306	N3C4C5	122.8514	N3C4C5	122.8572	N3C4C5	122.9639
N3C4O7	111.7089	N3C4O7	111.6839	N3C4O7	111.6743	N3C4O7	111.5399
C5C4O7	125.4425	C5C4O7	125.4463	C5C4O7	125.45	C5C4O7	125.4763
C4C5C6	117.1795	C4C5C6	117.1653	C4C5C6	117.1583	C4C5C6	117.0881
C4C5C10	120.5928	C4C5C10	120.6163	C4C5C10	120.6231	C4C5C10	120.7187
C6C5C10	121.755	C6C5C10	121.738	C6C5C10	121.7359	C6C5C10	121.6851
N1C6C5	115.0682	N1C6C5	115.0585	N1C6C5	115.0584	N1C6C5	115.0059
N1C6O28	119.0759	N1C6O28	119.0903	N1C6O28	119.0953	N1C6O28	119.167
C5C6O28	125.8547	C5C6O28	125.8499	C5C6O28	125.8449	C5C6O28	125.8251
C4O7C8	116.8639	C4O7C8	116.8394	C4O7C8	116.8306	C4O7C8	116.7007
O7C8C9	123.257	O7C8C9	123.2792	O7C8C9	123.2866	O7C8C9	123.3979
O7C8H19	110.1911	O7C8H19	110.1817	O7C8H19	110.1809	O7C8H19	123.3979
C9C8H19	126.551	C9C8H19	126.5384	C9C8H19	126.5319	C9C8H19	126.46
C8C9C10	122.9964	C8C9C10	123.0136	C8C9C10	123.0205	C8C9C10	123.0839
C8C9C13	122.8654	C8C9C13	122.8388	C8C9C13	122.8281	C8C9C13	122.7111
C10C9C13	113.6876	C10C9C13	113.6811	C10C9C13	113.6789	C10C9C13	113.6547
C5C10C9	109.4929	C5C10C9	109.4709	C5C10C9	109.4616	C5C10C9	109.3596
C5C10C11	117.3043	C5C10C11	117.307	C5C10C11	117.3065	C5C10C11	117.3325
C5C10H20	107.6987	C5C10H20	107.6698	C5C10H20	107.6639	C5C10H20	107.5615
C9C10C11	106.0416	C9C10C11	106.0853	C9C10C11	106.0958	C9C10C11	106.2263
C9C10H20	108.6749	C9C10H20	108.6938	C9C10H20	108.7015	C9C10H20	108.8034
C11C10H20	107.3704	C11C10H20	107.3587	C11C10H20	107.3573	C11C10H20	107.3163
C10C11C12	118.4095	C10C11C12	118.4693	C10C11C12	118.4896	C10C11C12	118.7153
C10C11C18	123.5471	C10C11C18	123.4972	C10C11C18	123.4821	C10C11C18	123.2978
C12C11C18	118.0433	C12C11C18	118.0334	C12C11C18	118.0283	C12C11C18	117.9859
C11C12O14	124.2827	C11C12O14	124.2973	C11C12O14	124.3015	C11C12O14	124.3396
C11C12C15	120.5426	C11C12C15	120.5521	C11C12C15	120.5558	C11C12C15	120.6077
O14C12C15	115.1665	O14C12C15	115.1417	O14C12C15	115.1336	O14C12C15	115.0421
C9C13O14	110.9269	C9C13O14	110.8732	C9C13O14	110.8546	C9C13O14	110.6785
C9C13H21	110.5926	C9C13H21	110.6015	C9C13H21	110.6049	C9C13H21	110.6167
C9C13H22	112.7654	C9C13H22	112.7778	C9C13H22	112.7814	C9C13H22	112.8124
O14C13H21	107.7291	O14C13H21	107.7897	O14C13H21	107.8102	O14C13H21	108.0565
O14C13H22	105.8484	O14C13H22	105.8325	O14C13H22	105.828	O14C13H22	105.7945
H21C13H22	108.7463	H21C13H22	108.736	H21C13H22	108.7324	H21C13H22	108.663
C12O14C13	119.2788	C12O14C13	119.2029	C12O14C13	119.1773	C12O14C13	118.8603
C12C15C16	120.2542	C12C15C16	120.2528	C12C15C16	120.253	C12C15C16	120.2339
C12C15H23	118.5685	C12C15H23	118.5523	C12C15H23	118.5473	C12C15H23	118.4713
C16C15H23	121.1762	C16C15H23	121.194	C16C15H23	121.1988	C16C15H23	121.2945
C15C16C17	119.974	C15C16C17	119.9708	C15C16C17	119.9691	C15C16C17	119.9613
C15C16H24	119.6028	C15C16H24	119.6062	C15C16H24	119.6067	C15C16H24	119.6186
C17C16H24	120.4224	C17C16H24	120.4224	C17C16H24	120.4236	C17C16H24	120.4201
C16C17C18	119.5189	C16C17C18	119.5259	C16C17C18	119.528	C16C17C18	119.5629
C16C17H26	120.522	C16C17H26	120.5201	C16C17H26	120.5216	C16C17H26	120.518
C18C17H26	119.9591	C18C17H26	119.954	C18C17H26	119.9504	C18C17H26	119.9188
C11C18C17	121.6611	C11C18C17	121.6604	C11C18C17	121.6617	C11C18C17	121.6477
C11C18H25	119.2277	C11C18H25	119.2225	C11C18H25	119.2246	C11C18H25	119.2024
C17C18H25	119.1083	C17C18H25	119.1137	C17C18H25	119.1101	C17C18H25	119.1429
E(Kev)	-34.6453	-34.6452		-34.6443		-34.6440	
Dipol Moment (Debay)	6.4929	6.3722		6.3360		5.7033	

In the next step, the stability of the molecule by replacing functional groups in the Orto and Para positions were studied (fig2). functional groups have different Electronegative properties that can be changed dipole moment of the molecule. And thus the stability of the molecules change. Calculations show that different functional groups have a profound impact on bond length and bond angles (table 2). The effect of a drug depends on proper functional group. By selecting suitable functional groups can be increased the stability and potential a drug.

Table 2: Molecular properties of the Uracil derivatives with different functional groups

Br(A)		Cl(B)		OH(C)		OMe(D)	
Bond length (A0)/N1-C2	1.3675	N1-C2	1.3675	N1-C2	1.3668	N1-C2	1.3666
N1-C6	1.4139	N1-C6	1.414	N1-C6	1.4154	N1-C6	1.4156
N1-H26	1.0121	N1-H26	1.0121	N1-H24	1.012	N1-H24	1.0120
C2-N3	1.3774	C2-N3	1.3775	C2-N3	1.376	C2-N3	1.3758
C2-S27	1.6593	C2-S27	1.6592	C2-S25	1.6607	C2-S25	1.6609
N3-C4	1.3706	N3-C4	1.3706	N3-C4	1.3717	N3-C4	1.3718
N3-H29	1.0108	N3-H29	1.0108	N3-H27	1.0107	N3-H27	1.0107
C4-C5	1.3583	C4-C5	1.3582	C4-C5	1.3584	C4-C5	1.3585
C4-O7	1.3476	C4-O7	1.3476	C4-O7	1.3468	C4-O7	1.3469
C5-C6	1.4539	C5-C6	1.4538	C5-C6	1.4538	C5-C6	1.4539
C5-C10	1.5151	C5-C10	1.515	C5-C10	1.5158	C5-C10	1.5162
C6-O28	1.2179	C6-O28	1.218	C6-O26	1.2179	C6-O26	1.2179
O7-C8	1.3896	O7-C8	1.3898	O7-C8	1.3913	O7-C8	1.3914
C8-C9	1.326	C8-C9	1.326	C8-C9	1.3256	C8-C9	1.3255
C8-H19	1.0809	C8-H19	1.0809	C8-H19	1.0808	C8-H19	1.0808
C9-C10	1.5102	C9-C10	1.51	C9-C10	1.5094	C9-C10	1.5091
C9-C13	1.4918	C9-C13	1.492	C9-C13	1.4918	C9-C13	1.4916
C10-C11	1.5383	C10-C11	1.5385	C10-C11	1.5392	C10-C11	1.5398
C10-H20	1.0996	C10-H20	1.0996	C10-H20	1.0994	C10-H20	1.0994
C11-C12	1.4062	C11-C12	1.4061	C11-C12	1.4036	C11-C12	1.4013
C11-C18	1.3992	C11-C18	1.3987	C11-C18	1.4002	C11-C18	1.4018
C12-O14	1.3729	C12-O14	1.3735	C12-O14	1.3705	C12-O14	1.3711
C12-C15	1.3972	C12-C15	1.3972	C12-C15	1.4082	C12-C15	1.4148
C13-O14	1.436	C13-O14	1.4357	C13-O14	1.4332	C13-O14	1.4324
C13-H21	1.0973	C13-H21	1.0973	C13-H21	1.0976	C13-H21	1.0976
C13-H22	1.0901	C13-H22	1.0901	C13-H22	1.0903	C13-H22	1.0903
C15-C16	1.3869	C15-C16	1.3866	C15-C16	1.3887	C15-C16	1.3905
C15-H23	1.0842	C15-H23	1.0841	C15-O29	1.3673	C15-O29	1.3620
C16-C17	1.3922	C16-C17	1.3919	C16-C17	1.3943	C16-C17	1.3970
C16-H24	1.0831	C16-H24	1.0833	C16-H31	1.0875	C16-H34	1.0826
C17-C18	1.3878	C17-C18	1.3875	C17-C18	1.3878	C17-C18	1.3851
C17-Br30	1.9188	C17-Br30	1.7606	C17-H28	1.0844	C17-H28	1.0847
C18-H25	1.0804	C18-H25	1.0806	C18-H23	1.0808	C18-H23	1.0809
Bond Angel/C2N1C6	127.9311	C2N1C6	127.937	O29-H30	0.9646	O29-C30	1.4181
C2N1H26	116.5012	C2N1H26	116.5075	C2N1C6	127.9635	C30-H31	1.0886
C6N1H26	115.5385	C6N1H26	115.5249	C2N1H24	116.4904	C30-H32	1.0953
N1C2N3	112.8482	N1C2N3	112.8384	C6N1H24	115.5065	C30-H33	1.0953
N1C2S27	124.5768	N1C2S27	124.5848	N1C2N3	112.8426	C2N1C6	127.9680
N3C2S27	122.571	N3C2S27	122.5728	N1C2S25	124.5405	C2N1H24	116.4980
C2N3C4	123.7187	C2N3C4	123.7224	N3C2S25	122.6126	C6N1H24	115.4859
C2N3H29	117.1303	C2N3H29	117.1279	C2N3C4	123.7184	N1C2N3	112.8375
C4N3H29	119.1368	C4N3H29	119.135	C2N3H27	117.1931	N1C2S25	124.5374
N3C4C5	123.1523	N3C4C5	123.1539	C4N3H27	119.0786	N3C2S25	122.6209
N3C4O7	111.3533	N3C4O7	111.3561	N3C4C5	123.1926	C2N3C4	123.7236
C5C4O7	125.4747	C5C4O7	125.4689	N3C4O7	111.2453	C2N3H27	117.1967
C4C5C6	116.9896	C4C5C6	116.9987	C5C4O7	125.541	C4N3H27	119.0636
C4C5C10	120.9687	C4C5C10	120.9616	C4C5C6	116.9149	N3C4C5	123.2082
C6C5C10	121.4496	C6C5C10	121.4526	C4C5C10	120.8853	N3C4O7	111.2135
N1C6C5	114.9269	N1C6C5	114.9261	C6C5C10	121.617	C5C4O7	125.5571
N1C6O28	119.4517	N1C6O28	119.4467	N1C6C5	114.8927	C4C5C6	116.8755
C5C6O28	125.6187	C5C6O28	125.6246	N1C6O26	119.2611	C4C5C10	120.8980
C4O7C8	116.4203	C4O7C8	116.4256	C5C6O26	125.843	C6C5C10	121.6284
O7C8C9	123.7378	O7C8C9	123.7288	C4O7C8	116.3817	N1C6C5	114.9009
O7C8H19	110.1525	O7C8H19	110.1446	O7C8C9	123.6454	N1C6O26	119.2210
C9C8H19	126.1096	C9C8H19	126.1263	O7C8H19	110.1438	C5C6O26	125.8747
C8C9C10	123.1286	C8C9C10	123.1179	C9C8H19	126.2099	C4O7C8	116.3585
C8C9C13	122.4415	C8C9C13	122.4779	C8C9C10	123.1955	O7C8C9	123.6425
C10C9C13	113.7471	C10C9C13	113.7163	C8C9C13	122.5473	O7C8H19	110.1538
C5C10C9	109.1725	C5C10C9	109.1877	C10C9C13	113.5226	C9C8H19	126.2024
C5C10C11	117.577	C5C10C11	117.5757	C5C10C9	109.1316	C8C9C10	123.2572
C5C10H20	107.4628	C5C10H20	107.4056	C5C10C11	117.3771	C8C9C13	122.5116
C9C10C11	106.3817	C9C10C11	106.3765	C5C10H20	107.3709	C10C9C13	113.4535
C9C10H20	109.0271	C9C10H20	109.0323	C9C10C11	106.6279	C5C10C9	109.0923

C11C10H20	106.9911	C11C10H20	107.036	C9C10H20	109.0011	C5C10C11	117.4238
C10C11C12	119.1232	C10C11C12	119.1205	C11C10H20	107.1129	C5C10H20	107.3167
C10C11C18	122.597	C10C11C18	122.5957	C10C11C12	118.4213	C9C10C11	106.6390
C12C11C18	118.2732	C12C11C18	118.2787	C10C11C18	122.5753	C9C10H20	109.0170
C11C12O14	124.4661	C11C12O14	124.4749	C12C11C18	118.9984	C11C10H20	107.1337
C11C12C15	120.5124	C11C12C15	120.5021	C11C12O14	125.1393	C10C11C12	118.6702
O14C12C15	115.0102	O14C12C15	115.0105	C11C12C15	120.0461	C10C11C18	122.4436
C9C13O14	110.3871	C9C13O14	110.3719	O14C12C15	114.8006	C12C11C18	118.8796
C9C13H21	110.7034	C9C13H21	110.6754	C9C13O14	110.352	C11C12O14	124.9558
C9C13H22	112.8725	C9C13H22	112.8864	C9C13H21	110.5907	C11C12C15	120.3996
O14C13H21	108.37	O14C13H21	108.3911	C9C13H22	112.9374	O14C12C15	114.6302
O14C13H22	105.7364	O14C13H22	105.7561	O14C13H21	108.4863	C9C13O14	110.2722
H21C13H22	108.5608	H21C13H22	108.552	O14C13H22	105.7112	C9C13H21	110.6056
C12O14C13	118.1951	C12O14C13	118.1354	H21C13H22	108.5613	C9C13H22	112.9343
C12C15C16	120.6443	C12C15C16	120.6294	C12O14C13	117.9632	O14C13H21	108.5395
C12C15H23	118.4979	C12C15H23	118.4831	C12C15C16	119.9114	O14C13H22	105.7138
C16C15H23	120.8577	C16C15H23	120.8873	C12C15O29	116.9115	H21C13H22	108.5766
C15C16C17	118.9138	C15C16C17	118.9351	C16C15O29	123.1769	C12O14C13	117.9016
C15C16H24	120.3219	C15C16H24	120.5721	C15C16C17	120.1591	C12C15C16	119.5654
C17C16H24	120.7641	C17C16H24	120.4927	C15C16H31	119.44	C12C15O29	115.5313
C16C17C18	121.0427	C16C17C18	121.0324	C17C16H31	120.4003	C16C15O29	124.9032
C16C17Br30	119.5206	C16C17Br30	119.5031	C16C17C18	120.0829	C15C16C17	119.9427
C18C17Br30	119.4363	C18C17Br30	119.4642	C16C17H28	119.834	C15C16H34	120.4280
C11C18C17	120.6093	C11C18C17	120.6187	C18C17H28	120.0818	C17C16H34	119.6282
C11C18H25	119.7481	C11C18H25	119.9708	C11C18C17	120.798	C16C17C18	120.5118
C17C18H25	119.6217	C17C18H25	119.3903	C11C18H23	119.5709	C16C17H28	119.5272
				C17C18H23	119.6065	C18C17H28	119.9600
				C15O29H30	109.5506	C11C18C17	120.6949
						C11C18H23	119.5952
						C17C18H23	119.6853
						C15O29H30	118.2532
						O29C30C31	105.7516
						O29C30C32	111.5158
						O29C30C33	111.5076
						H31C30H32	109.2757
						H31C30H33	109.2983
						H32C30H33	109.3989
E(Kev)	-104.671	-47.149		-36.690		-37.759	
Dipol Moment (Debay)	6.0678	6.616		3.7967		4.4483	

In quantum chemistry, a natural bond orbital or NBO is a calculated bonding orbital with maximum electron density. NBO analysis is a useful tool enabling chemists to see an intuitive picture of both electron orbitals and population analysis. In the NBO method, delocalization of electrondensity between occupied Lewis-typeorbitals and formally unoccupied non-Lewis NBOs corresponds to a stabilizing donor–acceptor interaction. The strength of this interaction can be estimated by the second order perturbation theory. Thus, the results obtained from NBO analysis provide convenient basis for investigating conjugative interactions in molecular systems. The calculated values of NBO charges of optimized structures of uracil derivatives are listed (table 3).

Table3: parameters NBO analysis

Atom Number	Charge	Core	Valence	Rydberg	Total
N1	-0.61073	1.99923	5.58911	0.02239	7.61073
C2	0.26250	1.99939	3.69631	0.04181	5.73750
N3	-0.58180	1.99919	5.56344	0.01917	7.58180
C4	0.58628	1.99871	3.38765	0.02736	5.41372
C5	-0.22861	1.99881	4.21190	0.01790	6.22861
C6	0.65871	1.99921	3.29989	0.04220	5.34129
O7	-0.50767	1.99969	6.49076	0.01723	8.50767
C8	0.16535	1.99863	3.81176	0.02427	5.83465
C9	-0.09159	1.99898	4.07608	0.01653	6.09159
C 10	-0.24632	1.99904	4.22474	0.02254	6.24632
C 11	-0.07691	1.99892	4.06161	0.01639	6.07691
C 12	0.31460	1.99866	3.66350	0.02324	5.68540
C 13	-0.02492	1.99908	4.00361	0.02223	6.02492

O 14	-0.54701	1.99973	6.52843	0.01886	8.54701
C 15	-0.21751	1.99906	4.20042	0.01803	6.21751
C 16	-0.20577	1.99896	4.18739	0.01942	6.20577
C 17	-0.11726	1.99860	4.09619	0.02247	6.11726
C 18	-0.20285	1.99886	4.18400	0.01999	6.20285
H 19	0.20426	0.00000	0.79483	0.00091	0.79574
H 20	0.24029	0.00000	0.75669	0.00303	0.75971
H 21	0.18429	0.00000	0.81402	0.00169	0.81571
H 22	0.19773	0.00000	0.80118	0.00109	0.80227
H 23	0.22215	0.00000	0.77675	0.00111	0.77785
H 24	0.22225	0.00000	0.77695	0.00081	0.77775
H 25	0.23853	0.00000	0.75995	0.00151	0.76147
H 26	0.42849	0.00000	0.56892	0.00260	0.57151
S27	-0.15739	9.99915	6.12883	0.02941	16.15739
O28	-0.60039	1.99976	6.58847	0.01216	8.60039
H29	0.43203	0.00000	0.56450	0.00347	0.56797
Br30	0.05930	27.99927	6.92254	0.01890	34.94070
* Total *	0.00000	75.98091	105.53040	0.48869	182.0000

Table 4: IR spectra and relative intensity spectra of A

frequency (cm^{-1})	intensity	frequency (cm^{-1})	intensity
560	12.71	1340	9.21
620	5.21	1400	30.62
680	19.39	1460	6.65
740	15.50	1520	3.56
800	37.99	1580	26.10
860	5.36	1640	102.89
920	10.99	1700	60.27
980	8.95	1760	153.11
1040	49.76	1820	9.79
1100	38.57	1880	18.58
1160	10.60	3080	4.46
1220	87.26	3200	9.99
1280	17.01	3620	226.98

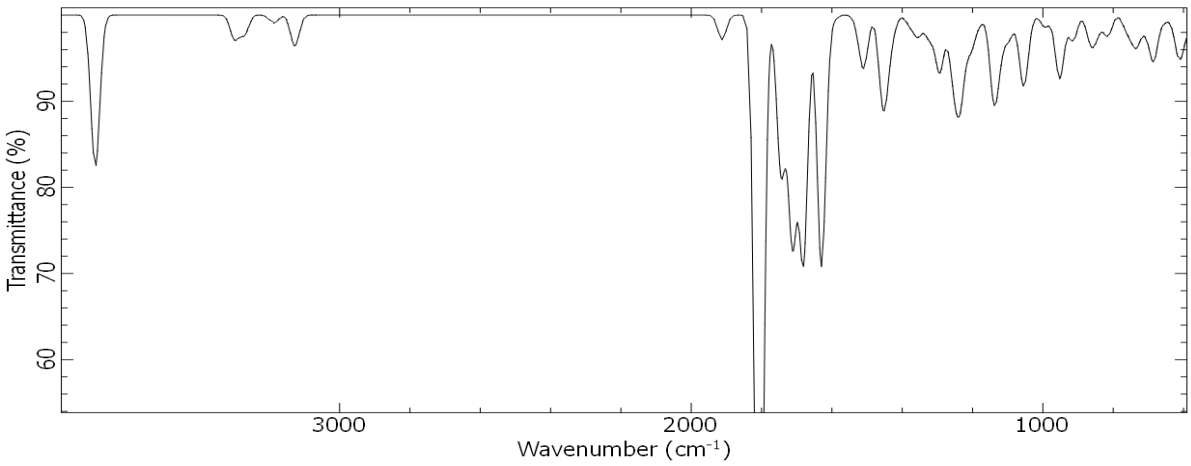

Fig3: spectrum IR Molecule A

The combination of vibrational spectra quantum chemical calculation is effective for understanding The fundamental mode of vibration of the compound. The IR spectra of A (fig 3) have been recorded in the region 4000-400 cm^{-1}. The spectra have been interpreted with the aid of normal coordinate analysis following full structure optimaizion and force field calculation based on the DFT method using 6-311++G(d) basis set. The structural characteristic, stability and energy of compound under investigation are determined by DFT with gaussian 09. In this work, the IR bands observed at 3062 cm^{-1} , 3066 cm^{-1} and 3124 cm^{-1} are assigned to C-H stretching vibration. C-C vibration and C=C stretching vibrations observed at 1567 cm^{-1} and 1207-1232 cm^{-1} . The C-Br stretching

vibrations observed at 550 cm^{-1}. C-N vibration_ to identify the C-N stretching frequency is a rather difficult task from other vibrations. the IR bands observed at 1416-1479 cm^{-1} and 1567-1647 cm^{-1} are assigned to C-N stretching absorption. The interpretation of IR spectra of zero generation allows determining the local changes in the structure. in the IR spectrum of the Uracil derivative is asymmetric and symmetric NH stretching vibrations of amid group. (table 4).

CONCLUSION

Initial quantum mechanic studies and density function theory (DFT) in the level of B3LYP/6-311++G on 4,12b-Dihydro-3-thioxo-1H,7H-chromeno [4′,3′:4,5]pyrano[2,3-d]pyrimidine-1(2H)-one structure. In this study, the uracil derivative was studied in different solvents and according to data obtained, it was concluded that the solvent water is more stable than other Other solvents. By studying the functional groups bromine, chlorine, methoxy, and OH It was found that by replacing bromine atoms in the C17 stability of the molecule too much.

The results of NBO analysis was noticed previously, N1 carry the largest negative charge and Br30 have the largest energy of the core orbital. The values of dipole moment, NBO, HOMO, LUMO, and bond lengths detect the effects of different functional groups. In the solution and with increase of polarity, the molecule were more stable. With increase of polarity, total energies of all compounds were more negative. The dipole moments of all compounds are affected by solvent. With increase of the polarity of solvents the dipole moments of the molecule were increased. The charges of the molecule were affected by functional groups and solvents.

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