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"Synthesis, Molecular Docking, SwissADME Evaluation and Biological Activities of Novel Benzothiazole–Triazole Derivatives"

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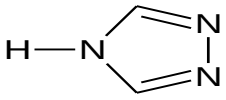
ABSTRACT
The present study was aimed to synthesize a series of novel 5-(1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione and to evaluate their *in-vitro* anti-inflammatory activity and in vitro on panel of 60 different human tumor cell lines derived from nine neoplastic cancer types at NCI. The compounds were evaluated using inhibition of bovine serum albumin denaturation method have shown significant *in-vitro* anti-inflammatory activity. The findings of present study clearly demonstrate that chloro functional group possess inhibition of bovine serum albumin denaturation capacity and has *in-vitro* anti-inflammatory activity. However methoxy and dimethyl derivatives show mild to moderate *in-vitro* anti-inflammatory activity. The compounds were evaluated at single concentration of 10^{-5} M towards the panel of 60 cancer cell lines derived from nine different cancer types: leukemia, lung, colon, CNS, melanoma, Ovarian, Renal, prostate and breast cancer.The compound 7a,7b,7f shows moderate anticancer activity. structural assignments are based on spectroscopic data (FT-IR, ^{1}HNMR, MASS spectra).

KEYWORDS: 2-aminobenzothiazoles,1,2,4-triazole-3-thione, anticancer activity, national Cancer Institute.

INTRODUCTION

In recent years, maintaining good health has become one of the major concerns worldwide. Among various diseases, cancer remains one of the leading causes of death and has become a serious global health problem. Due to the increasing number of cancer cases, continuous research is being carried out to develop new anticancer drugs that are more effective, selective, and less toxic. One of the major challenges for medicinal chemists is to discover novel chemical compounds that can selectively destroy cancer cells without causing severe side effects to normal cells. The use of drugs with different mechanisms of action may also help in reducing drug resistance and improving therapeutic effectiveness. Benzothiazole derivatives are an important class of heterocyclic compounds known for their wide range of biological activities such as anticancer, antimicrobial, antitubercular, antimalarial, anticonvulsant, anthelmintic, analgesic, and anti-inflammatory properties. Previous studies reported by researchers such as Malleshapa N. Noolvi have shown that benzothiazole derivatives possess promising pharmacological potential. Because of their diverse biological activities and chemical reactivity, benzothiazole-containing compounds have gained significant attention in medicinal chemistry and drug discovery research.Heterocyclic compounds are cyclic compounds that contain at least one hetero atom such as nitrogen, oxygen, or sulphur in their ring structure. These heteroatoms play an important role in determining the chemical and biological properties of the compounds. Nitrogen- and sulphur-containing heterocycles are especially important because they serve as versatile scaffolds for the development of biologically active molecules. These compounds participate in various chemical reactions and exhibit a broad spectrum of pharmacological activities.Among different heterocyclic systems, 1,2,4-triazole derivatives are well known for their therapeutic importance. Compounds containing the 1,2,4-triazole nucleus have been reported to possess several biological activities including analgesic, antiasthmatic, diuretic, antihypertensive, anticholinergic, antibacterial, antifungal, and anti-inflammatory properties. Due to these significant medicinal applications, benzothiazole and triazole derivatives continue to attract attention for the development of new potential therapeutic agents.

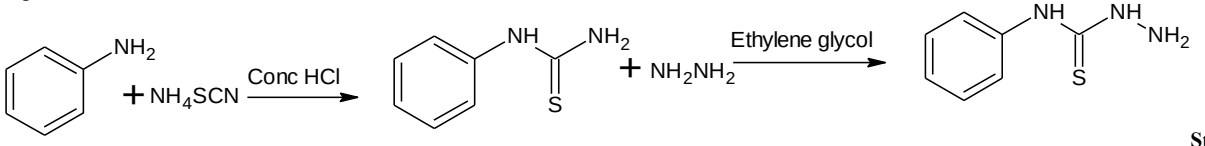


The derivatization of Triazole ring is based on the phenomenon of bioisosterism in which replacement of oxygen of oxadiazole nucleus with nitrogen triazole analogue.Out of the two triazoles 1, 2, 4- triazole has wide variety of activity. Triazole moiety is an important and frequent insecticide, agrochemical structure feature of many biological active compound as cytocrome p450 enzyme inhibitors and peptide analog inhibitor.[6]

EXPERIMENTAL

SCEHME:

Step:1



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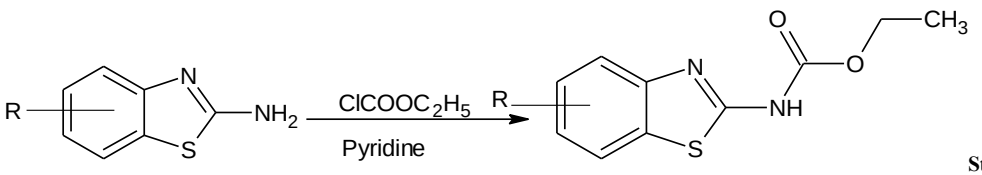

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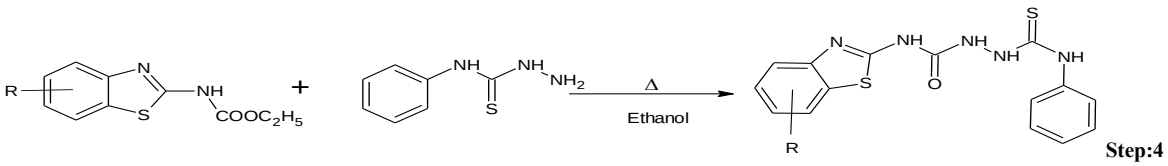

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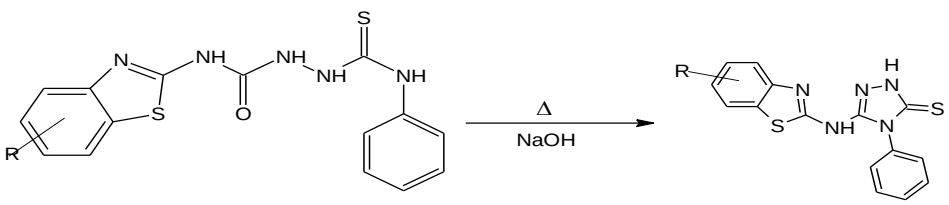

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MATERIALS AND METHODS:

Materials: The melting points of the synthesized compounds were determined using the open capillary tube method. The progress of the reactions was monitored by thin layer chromatography (TLC) using silica gel-G as the adsorbent and benzene as the mobile phase.The infrared (IR) spectra of the synthesized compounds were recorded using KBr pellets on a Bruker α FT-IR spectrometer. The ^1H NMR spectra were obtained in DMSO-d6 solvent using a Bruker Avance II 400 MHz NMR spectrometer at Punjab University, Chandigarh.

GENERAL SYNTHESIS PROCEDURE

Synthesis of starting material was done by as per reported method.[7-9]

Synthesis of N-1,3-benzthiazol-2-yl -2(phenylcarbamothioyl)hyddazinecarboxamide

The solution of carbamates (0.01mol) and hydrazine carbothioamides(0.01 mol) in ethanol (25 ml) refluxed for 4 hr. The residue was concentrated, cooled and poured over crushed ice to the precipitate which was filtered, wash with water.[10]

Synthesis and Biological activities of 5-(1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione

A mixture of substituted hydrazine carboxamides (0.001) and 30 ml of 2 % aq. sodium hydroxide solution was refluxed for 6 hr. After completion of reaction mixture was filtered and filtrate was neutralized with conc. HCl drop wise till pH was adjusted to 7. The mixture was kept aside for few minutes and filter. Recrystallized from ethanol.[11]

TABLE 1. : PHYSICAL CONSTANTS OF SYNTHESIZED COMPOUNDS

Comp. Id.	R	Mol. Formula	Mol. Wt	m.p.°C	*Rf Value	%Yield
7a	4Cl	$C_{15}H_{10}ClN_5OS_2$	359.85	232-234	0.73	55
7b	5Cl	$C_{15}H_{10}ClN_5OS_2$	359.85	244-246	0.67	53.83
7c	6Cl	$C_{15}H_{10}ClN_5OS_2$	359.85	240-242	0.68	55.23
7d	$4OCH_3$	$C_{16}H_{13}N_5OS_2$	355.43	262-264	0.70	51.11
7e	$5OCH_3$	$C_{16}H_{13}N_5OS_2$	355.43	232-234	0.62	52.87
7f	$6OCH_3$	$C_{16}H_{13}N_5OS_2$	355.43	220-222	0.66	52.42
7g	$6NO_2$	$C_{15}H_{12}N_6O_3S2$	388.85	180-182	0.64	60.11
7h	$6Br_2$	$C_{15}H_{10}N_5S_2$ Br	404.30	192-194	0.72	58.69
7i	7-Cl 6-F	$C_{15}H_9ClFN_5S_2$	377.86	226-228	0.76	49.15
7j	4-7 CH_3	$C_{21}H_{20}ClFN_4O_2S$	446.92	238-240	0.65	45.28

*Mobile phase-benzene

SPECTRAL DATA

5-(4-chloro-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7a)

FT-IR- 3430(N-H str.); 3025(C-H str); 1620(C=N str); 1540(C=C str); 1266(C-S str); 730(C-Cl str) ,^{1}H NMR δ: δ4.56(s,1H,NH); 7.12-8.32 (m,8H,Ar-H);δ7.12 (s,1H,NH), % Anal calculated; C-50.06, H-2.80%;N- 19.46%,Found: C -49.90%;H -2.75%;N-19.53%,

5-(5-chloro-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7b)

FT-IR: 3413(N-H str); 3032(C-H str); 1718(C=O str); 1601(C=N str);1530(C=C str); 1277(C-S str); 733(C-Cl str),^{1}H NMR δ ppm:, 4.12(s,1H,NH),6.89 (s,1H,NH),7.05-8.30(m,8H,ArH), % Anal.calculated:C-50.06%;H-2.80%; N- 19.46%; Found: C 50.13%;H-2.88%; N- 19.39%.

5-(6-chloro-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7c)

FT-IR: 3445(N-H str);3031(C-H str);1655(C=N str);1533(C=C str);1250(C-S str) ;740(C-Cl str), ^{1}H NMR δ ppm: 4.02(s,1H,NH);6.78(s,1H,NH);7.02-8.24(m,8H,ArH)Anal.calculated:C-50.06;H-2.80%;N- 19.46%, Found: C -50.01;H-2.85%;N- 19.40%.

5-(4-methoxy-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7d)

FT-IR: 3355(N-H str); 2987(C-H str); 1585(C=N str); 1543(C=C str);1270(C-S str);1092(C-0-C str), ^{1}H NMR δ 3.49(s,1H,OCH_3); 4.11(s,1H, NH); 6.98(s,1H,NH); (7.12-8.51(m,8H,Ar H), % Anal. Calculated C 54.07%,H 3.69%, N 19.70%, Found: C-54.14 %, H-3.66 %.N-19.68%.

5-(5-methoxy-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7e)

FT-IR:3440(N-H-str);3095(C-H-str);1590(C=N-str);1524(C=C-str);1272(C-S-str); 1099(C-O-C-Str) ^{1}H-NMR,δ-ppm3.73(s,1H,OCH_3);4.35(s,1H,NH_1);6.26(s,1H,NH);6.92-8.41(m,8H,Ar-H),% Anal. calculated:C 54.07%; H 3.69%;N 19.70%,Found:C 54.06%;H 3.56%.; N 19.54%.

5-(6-methoxy-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7f)

FT-IR: , 3385(N-H str); 2943(C-H str); 1675(C=N str); 1519(C=C str); 1288(C-S str);1092(C-O-C Str) ^{1}H NMR δ-ppm3.73(s,1H,OCH_3);4.35(s,1H,NH_1);6.26(s,1H,NH);6.92-8.41(m,8H,Ar-H),% Anal. calculated:C 54.07%; H 3.69%;N 19.70%,Found:C 54.06%;H 3.56%.; N 19.54%.

5-(6-nitro-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7g)

FT-IR: 3424(N-H str); 3022(C-H str); 1630(C=N str);1529(-NO_2str); 1520(C=C str); 1264(C-S str) , ^{1}H NMR δ ppm:, 4.32(s,1H,NH);6.69 (s,1H,NH);7.05-8.30(m,8H,ArH), % Anal.calculated:C-48.64%;H-2.72%; N- 22.69%; Found: C 48.74%;H-2.68%; N- 22.59%.

5-(6-bromo-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione(7h)

FT-IR: , 3414(N-H str); 2979(C-H str); 1602(C=N str), 1530(C=C str), 1265(C-S str), ^{1}H NMR δ ppm:, 4.02(s,1H,NH);6.89 (s,1H,NH);7.05-8.30(m,8H,ArH), % Anal.calculated:C-44.56%;H-2.89%; N- 17.32%; Found: C 44.54%;H-2.83%; N- 17.39%.

5-(7-chloro-6-fluro-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione

FT-IR: 3389(N-H str);2973(C-H str);1632(C=N str);1539 (C=C str); 1263(C-S,str) 1100 (C-F str), ^{1}H NMR δ ppm:, 4.18(s,1H,NH);6.73 (s,1H,NH);7.05-8.30(m,7H,ArH), % Anal.calculated:C-47.68%;H-2.40%; N- 18.53%; Found: C 47.54%;H-2.43%; N- 18.49%.

5-(4-7-dimethyl-1,3-benzthiazol-2-ylamino)-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione

FT-IR: 3390(N-H str); 2954(C-H str); 1614(C=N str), 1509 (C=C str), 1272(C-S str),), ^{1}H NMR δ ppm:, 2.35(s,6H,CH_3);4.18(s,1H,NH);6.73 (s,1H,NH);7.05-8.30(m,7H,ArH), % Anal.calculated:C-57.77%;H-4.28%; N- 19.81%; Found: C 57.64%;H-4.33%; N- 19.89%.

Molecular Docking Studies

The chemical structures of the synthesized compounds were initially drawn using ChemSketch software and subsequently converted into PDB format with the help of PyMOL software for molecular docking analysis.Molecular docking studies were carried out using AutoDock software developed by The Scripps Research Institute to evaluate the binding interactions of the synthesized compounds with the selected target protein. The best docking conformations and binding poses were further analyzed and visualized using Discovery Studio Visualizer v21.1.0.20298.For docking calculations, the grid box dimensions were set at 22.508 Å, 5.554 Å, and 22.033 Å along the X, Y, and Z axes, respectively, with a grid spacing of 0.375 Å. These parameters were selected to appropriately cover the active binding site of the target protein and to ensure accurate ligand–protein interaction analysis.

Table No 1: Molecular Docking Study

Sr. No	Compound	Affinity (Kcal/mol)	Amino Acid interaction
1	STD	-8.4	A:MET,A:LYS, :ASN,A:GLU,A:TYR
2	BZT1	-8.3	A:ARG , A:LEU,
3	BZT2	-8.1	A:TRP,A:GLU, A:MET, A:LEU
4	BZT3	-7.8	A:HIS, A:ARG, A:ALA
5	BZT4	-7.6	A:ARG,:A:PRO, A:LEU, A:ASP
6	BZT5	-7.9	A:GLY,:A:ALA, A:ASP
7	BZT6	-7.7	A:ARG,:A:GLU, A:ALA, A:LEU
8	BZT7	-7.4	A:CYS, A:TYR, A:MET, A:LYS
9	BZT8	-8.1	A:ARG, A:ALA, A:PRO, A:LEU
10	BZT9	-8.2	A:HIS, A:ARG, A:LEU, A:ILE
11	BZT10	-8.3	A:TRP, A:LYS, A:GLU, A:LEU

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Swiss ADME Study: SwissADME analysis was carried out to study the drug-likeness and pharmacokinetic properties of the synthesized benzothiazole incorporated 1,2,4-triazole derivatives. This study helps in predicting whether the synthesized compounds can behave like suitable drug molecules in the human body. The structures of all synthesized compounds were first drawn using ChemSketch software and then converted into appropriate molecular formats for computational analysis. The prepared structures were uploaded to the Swiss ADME online tool to evaluate important parameters such as molecular weight, lipophilicity (LogP), hydrogen bond donor and acceptor count, topological polar surface area (TPSA), gastrointestinal absorption, blood-brain barrier permeability, and Lipinski's Rule of Five. The results obtained from the Swiss ADME study showed that most of the synthesized compounds possessed acceptable physicochemical properties and followed Lipinski's Rule of Five, indicating good oral bioavailability and drug-like nature. These findings suggest that the synthesized compounds may exhibit favorable pharmacokinetic behavior and can be considered as potential candidates for further biological studies.Overall, the SwissADME analysis supported the biological activity results and helped in identifying promising compounds with suitable drug-like properties.

Table No 2: SwissADME analysis

Compound No	Mol. Wt	H-Bond acceptor	H-bond Donors	Log P	Violation of Lipin ski's Rule
STD	371.51	2	2	4.63	0
BZT1	359.86	2	2	2.49	0
BZT2	359.86	2	2	2.58	0
BZT3	359.86	2	2	2.58	0
BZT4	355.44	3	2	2.61	0
BZT5	355.44	3	2	2.7	0
BZT6	355.44	3	2	2.64	0
BZT7	404.31	2	2	2.69	0
BZT8	353.46	2	2	2.78	0
BZT9	377.85	3	2	2.62	0
BZT10	370.41	4	2	2.02	0

ANTICANCER ACTIVITY

The compounds (7a,7b, 7h) were screened for preliminary anticancer assay by National Cancer Institute(NCI),Bethesda, Maryland, USA in an in *vitro* 60 human tumor cell panel derived from nine neoplastic cancer types.

Criterion for submission and selection of compounds for testing in the NCI screens

The compounds (7a,7b,7f) were submitted to NCI under the Developmental Therapeutic Program (DTP) which operates a tiered anticancer compound screening course for the benefit of the general research community with the goal of identifying novel chemical leads and biological mechanisms. Structures of the compounds were selected for screening based on their ability to add diversity to the NCI small molecule compound collection. In addition, the submission of compounds with drug-like properties utilizing the concept of privileged scaffold or structures based on computer-aided design were preferred.

Fig.1.Selected NCI sixty cell lines data highlighting the potency of compound(NSC:D-771857z) against non small cell lung cancer cell line(HOP-92).

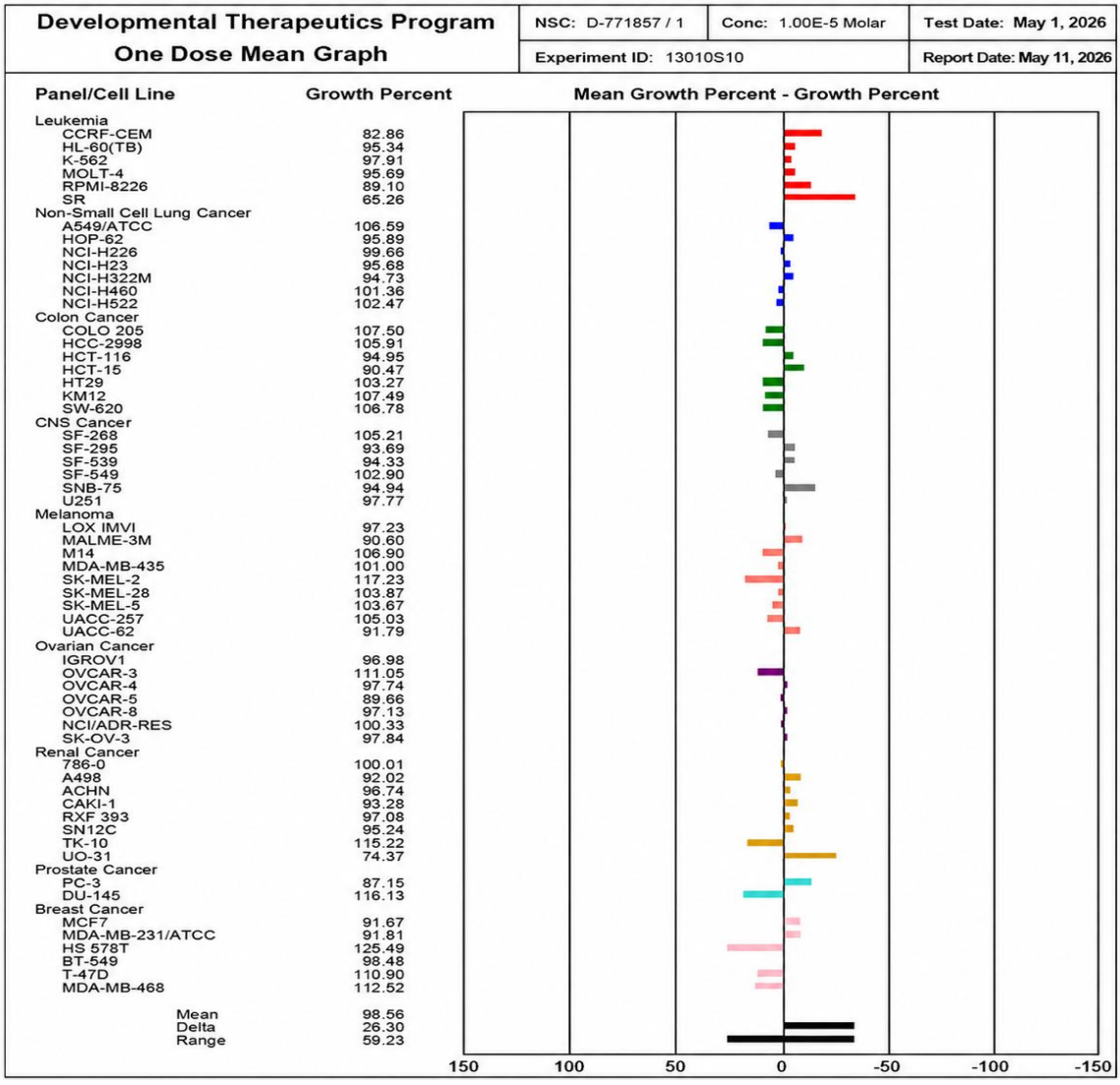

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Table No 2.Anticancer screening data of tested compounds

NSC code (Comp No)	60 cell line assay in 1-dose 10^{-5} M concentration					
	Most sensitive cell lines	Mean growth %	Range	Delta	% Growth	%GI
D-771857 (7a)	Leukemia SR	99.16	59.23	32.90	66.36	33.64
D-773070 (7b)	Renal cancer UO-31	101.71	57.76	29.26	72.45	17.99
D-773069 (7h)	Prostate Cancer PC-3	102.30	58.75	23.75	78.55	27.55

IN VITRO ANTI-INFLAMMATORY ACTIVITY

The synthesized compounds are screened for anti-inflammatory activity dy using inhibition of albumin denaturation technique. The standard drug and test compounds were dissolved in minimum amount of dimethyl formamide (DMF) and diluted with phosphate buffer (0.2 M, pH 7.4). Final concentration of DMF in all solusions was less than 2.0%. Test solution (1 ml) containing different concentrations of drug was mixed with 1 ml of 1% mM albumin solution in phosphate buffer and incubated at 27°±1°C in BOD incubator for 15 min. Denaturation was induced by keeping the reaction mixture at 60°±1°C in water bath for 10 min. After cooling the turbidity was measured at 660 nm (UV-Visible Spectrophotometer SCHIMATZU 1800). Percentage of inhibition of denaturation was calculated from control where no drug was added. Each experiment was done in triplicate and average was taken. The diclofenac sodium was used as standard drug.

% of inhibition = 100 x ((Vc/Vt)-1) Where, Vt and Vc are mean absorbance value of test group and control group.

TABLE NO 3. IN VITRO ANTI-INFLAMMATORY ACTIVITY

Sr.no.	Name of compound	Absorbance value (mean±SE)	Inhibition of denaturation (in %)
1.	Control	0.089	--
2.	7a	0.162	82.02
3	7b	0.153	71.91
4.	7c	0.158	77.52
5.	7d	0.112	25.84
6.	7e	0.126	41.57
7.	7f	0.121	35.95
8.	7g	0.137	53.93
9	7h	0.159	78.64
10	7i	0.118	32.58
11	7j	0.132	48.48
12	Standard (Diclofenac sodium)	0.173	94.38

RESULT AND DISCUSSION

The compounds were evaluated at single concentration of 10^{-5} M towards the panel of approximately 60 cancer cell lines derived from nine different cancer types: leukemia, lung, colon, CNS, melanoma, ovarian, renal, prostrate and breast cancers. Preliminary anticancer assay was performed according to the US NCI protocol. All the compounds (7a, 7g, and 7h) were added to a previously prepared cell culture at a single concentration. The cell culture was incubated for 48 h. End point determinations were made with a protein binding dye, sulforhodamine B (SRB).

The mean growth %, range of growth % and % growth inhibition is depicted in Table 1. The tested compounds showed a broad spectrum of growth inhibitory activity against human tumor cells, as well as some distinctive patterns of selectivity Fig.1. Compound (7a) was found to have good growth inhibitor activity against Leukemia (SR) with a growth % of most sensitive cell line to be 64.93, whilst least active over other cell lines. The mean growth % for compound (7a) was observed 99.16 and fall in a range of 59.23. Compounds (7g) and (7h) showed selectivity on renal cancer (UO-31) with a growth % of most sensitive cell line to be 78.91, 74.74 and respectively.

All the newly synthesized compounds 7a-7j was tested for *in vitro* anti-inflammatory activity. Compared to the standard, Diclofenac sodium, they have shown acceptable anti-inflammatory activity of synthesized compounds. Amongst all the tested compounds 4g found with most potent activity.

CONCLUSIONS

In the present paper ten compounds were tested and three of them displayed antitumor activity on renal cancer, lung cancer cell lines. compound **7a,7b,7c** was found to potent anti-inflammatory activity and all are showing good anti-inflammatory activity. The most efficient anticancer compound (**7a**) was found to be active with selective influence on non small cell lung cancer cell lines, especially on Leukemia SR with a % growth inhibition of 33.64. The obtained results prove the necessity for further investigations to clarify the features underlying the antitumor potential of tested compounds.

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