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In-vitro evaluation of total reducing property of the synthesized molecule having variable atomic electronegativity

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ABSTRACT

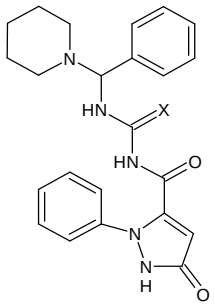
Three different compounds have been synthesized by keeping X as variable: X=O/S/NH for Compound-A/Compound-B/Compound-C respectively. Electronegativity of oxygen for urea X:O=3.5 and of sulfur for thiourea X:S=2.4 and of nitrogen+hydrogen for guanidine X:NH=3.1+2.2=5.3. So the X=NH shows the maximum electronegativity with combined effect of electronegativity of nitrogen and hydrogen, whereas X=O has two lone pairs and X=S has also two pair of electrons, but in case of NH moiety the electronegativity of nitrogen and hydrogen exceeds the electronegativity of oxygen and sulfur: NH (5.3) > O (3.5) > S (2.4). The spectral data for the absorption for the three compounds was compared with gallic acid for the plot was calculated by the equation: y=0.022x-0.1458 (R2=0.982) and found that the antioxidant property of the compounds have the mentioned profle: Compound-C>Compound-B>Compound-A. Compound-C is guanidine moiety having X=NH so according to the highest electronegativity profile this is more potent than other two when compared with the total reducing capacity property. (Compound-A: 272.8µg, Compound-B:317µg, Compound-C:384.9µg) It was expressed as GAE means that reducing power of 10mg of each compound is equivalent to reducing power of µg of gallic acid or expressed as µgGAE/mg of compound.

Key words: Conjugated diamide, Urea/thiourea/guanidine linkage, antioxidant, FRAP assay, Gallic acid, Trichloroacetic acid, Ferric chloride.

INTRODUCTION

An antioxidant is a substance or food, like, red grapes, Rooibos Aspalathox, and black strap molasses, that helps prevent or delay oxidative damage caused by reactive oxygen and or reactive nitrogen species. Oxidative damage to the body, cells and tissues may contribute to diseases like cancer and heart disease. Fruits, vegetables, oils, nuts and whole grains have varying levels of antioxidant compounds like carotenoids, lycopene and the vitamins C and E. Flavonoids and phytochemicals, found in foods of plant origin, also act as antioxidants. Three different compounds have been synthesized by keeping X as variable: X=O/S/NH: Compound-A/Compound-B/Compound-C respectively[1].

Synthesized molecule
X=O: Urea, X=S: Thiourea, X=NH: Guanidine



OBJECTIVE: Electronegativity of oxygen for urea X:O=3.5 and of sulfur for thiourea X:S=2.4 and of nitrogen+hydrogen for guanidine X:NH=3.1+2.2=5.3. So the X=NH shows the maximum electronegativity with combined effect of electronegativity of nitrogen and hydrogen, whereas X=O has two lone pairs and X=S has also two pair of electrons, but in case of NH moiety the electronegativity of nitrogen and hydrogen exceeds the electronegativity of oxygen and sulfur:
NH (5.3) > O (3.5) > S (2.4)

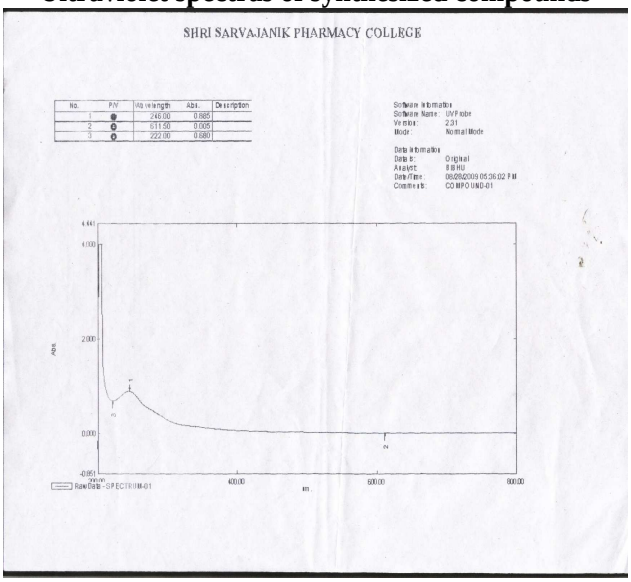
The synthesized molecule (having variable atomic electronegativity) posses CNS depressant activity which is checked by *in-vivo* testing on mice animal[2]. The physicochemical parameters of the synthesised molecules have been shown in Table-1 and the characterisation of the three molecules have been done by N%, UV, IR and Mass spectras. Total antioxidants can be assessed by the reduction of Fe^{+3} to Fe^{+2} (i.e., the FRAP assay), which occurs rapidly with all reductants with half-reaction reduction potentials above that of Fe^{+3}/Fe^{+2}. The values, therefore, expressed the corresponding concentration of electron-donating antioxidants. The FRAP assay is the only assay that directly measures antioxidants or reductants in a sample[3].

Physicochemical Parameters

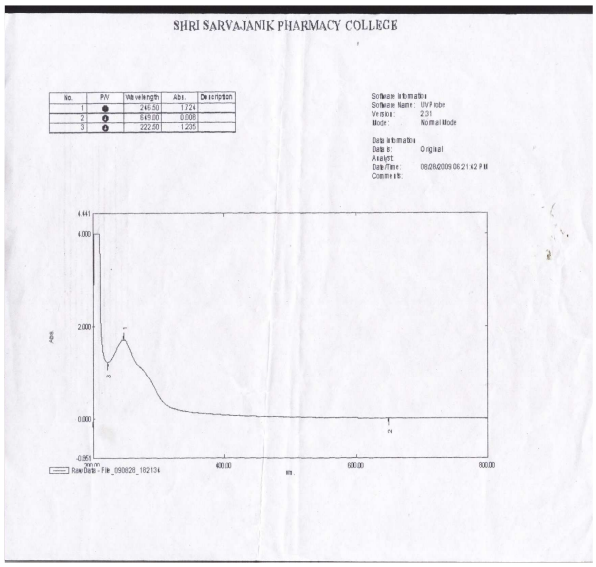
COMPOUNDS	% YIELD	M.P. ºC	POLARITY	MOL. FORMULA	N% CALCD	N% FOUND
Compound-A : X=O	87.71	220	Semipolar	$C_{23}H_{25}N_5O_3$	16.70	17.06
Compound-B : X=S	42.89	235-238	Semipolar	$C_{23}H_{25}N_5O_2S$	16.08	16.68
Compound-C : X=NH	33.83	80-82	Semipolar	$C_{23}H_{26}N_6O_2$	20.08	20.52

Table-1

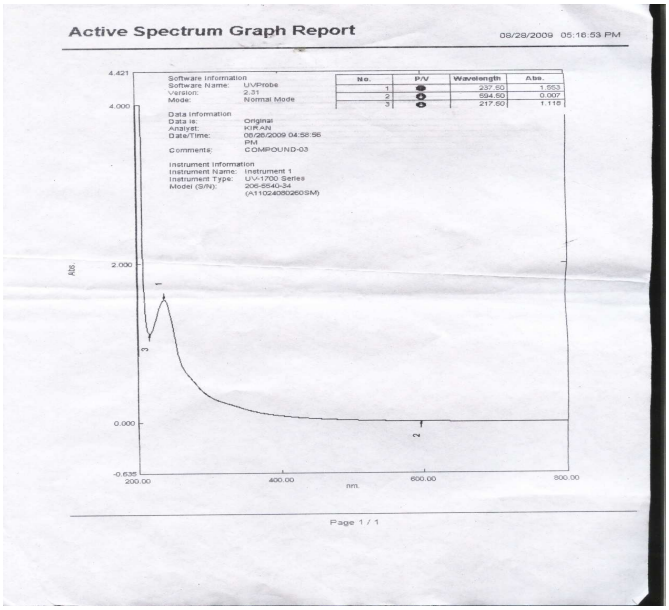
Ultraviolet spectras of synthesized compounds



Compound-A : X=O; λmax= 246nm

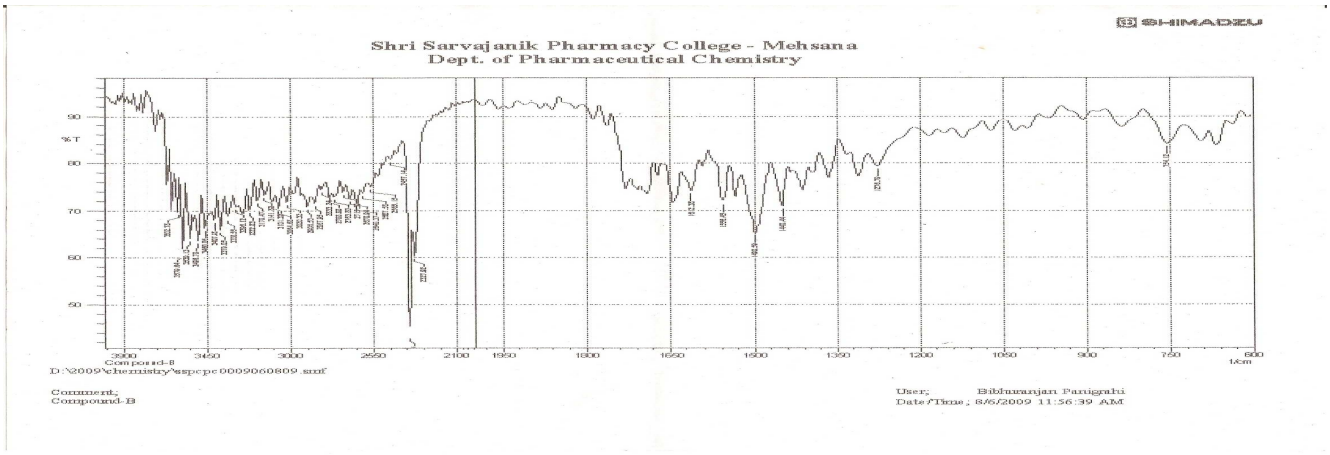


Compound-B : X=S; λmax= 246.50nm

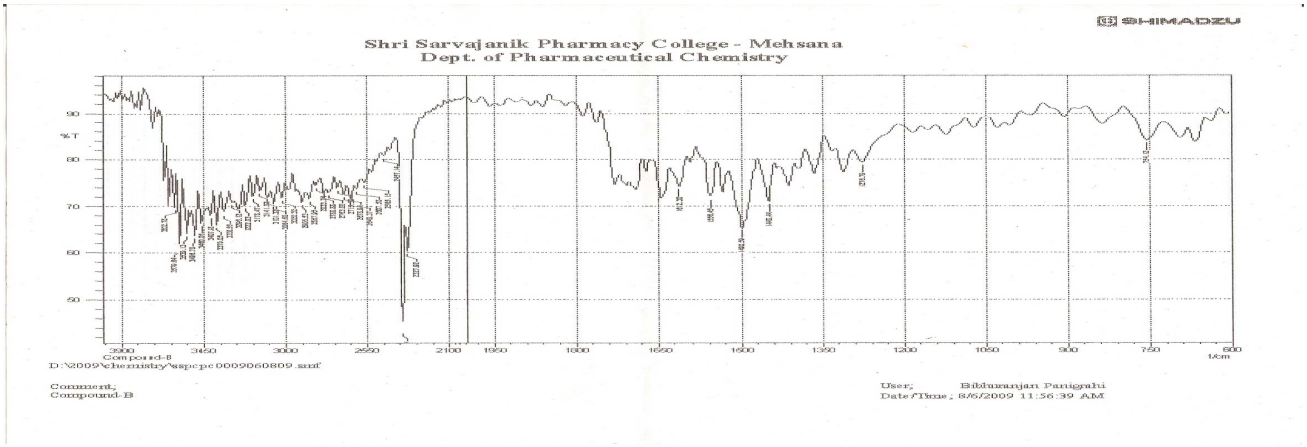


Compound-C : X=NH; λmax= 237.50nm

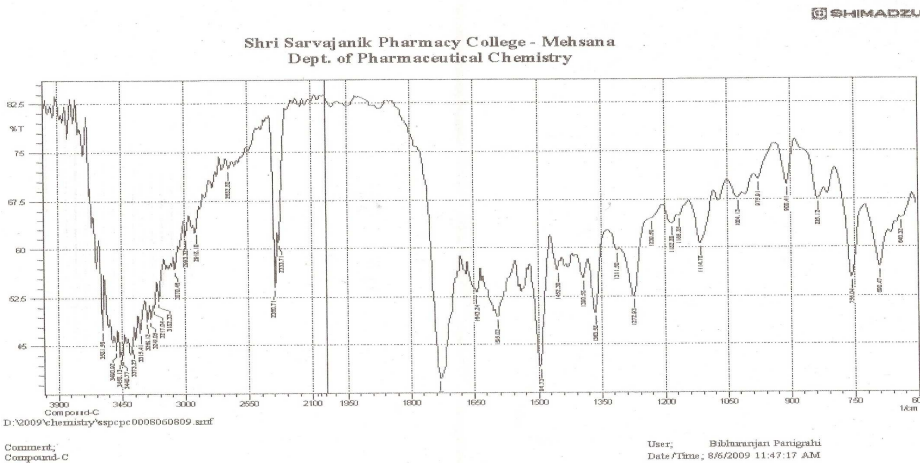
Infra Red spectras of synthesized compounds



Compound-A: X=O

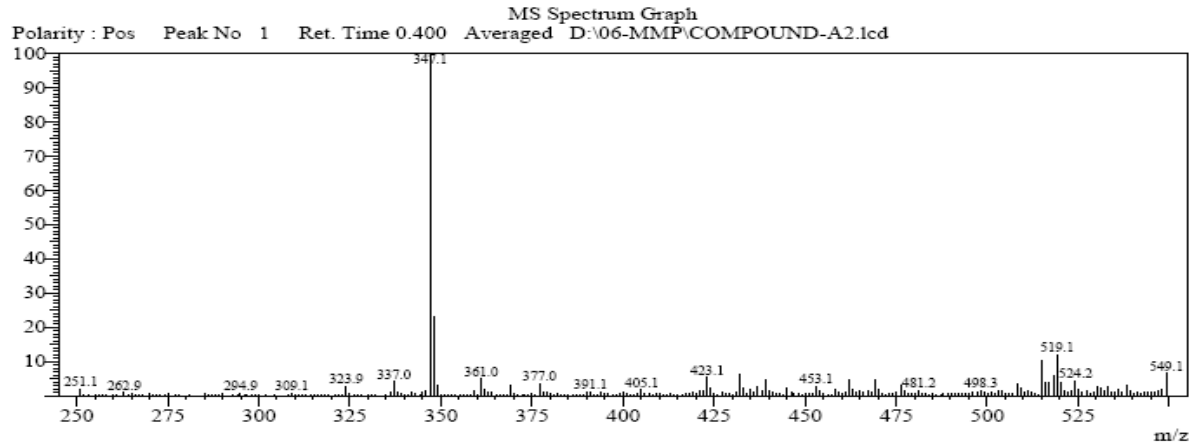


Compound-B : X=S

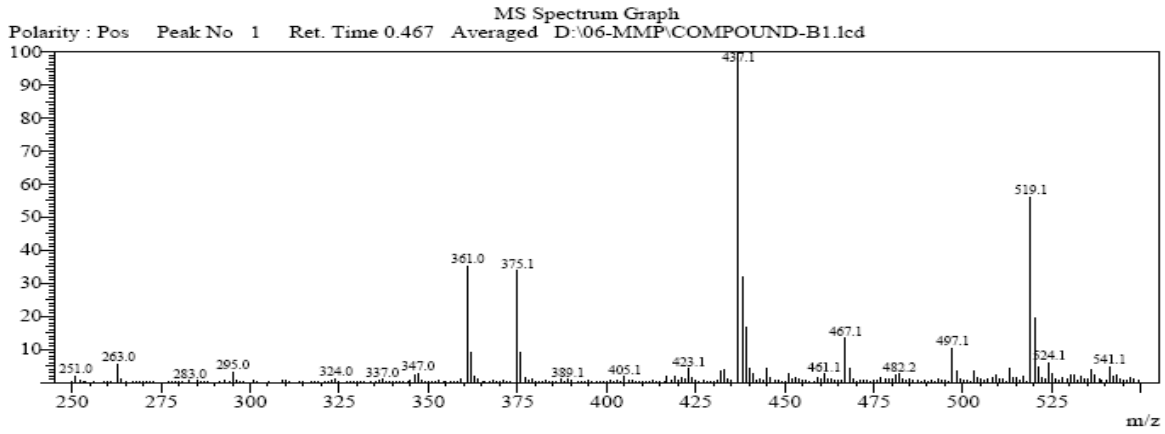


Compound-C: X=NH

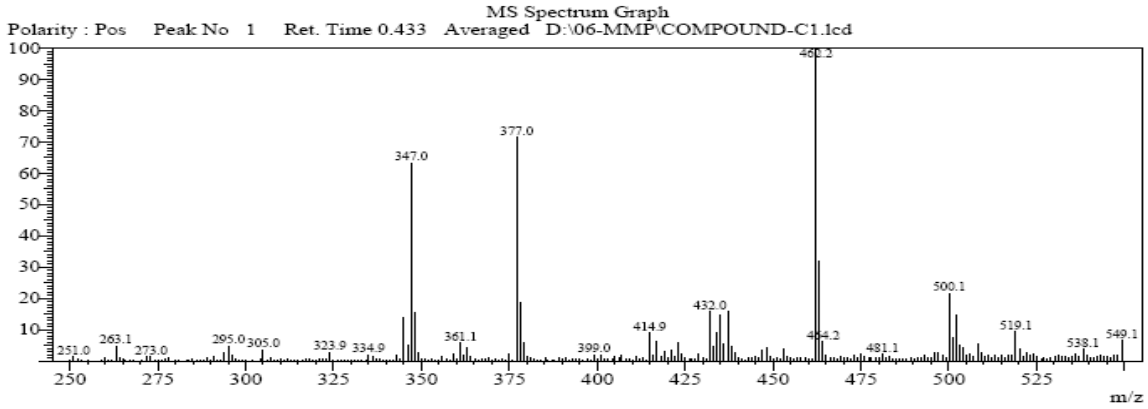
Mass spectras of synthesized compounds



Compound-A: X=O



Compound-B : X=S



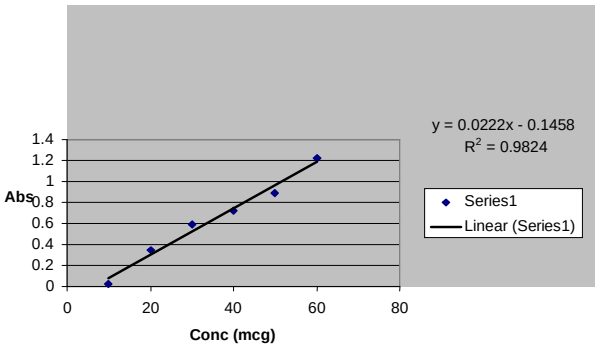
Compound-C: X=NH

EXPERIMENTAL SECTION

Ferric reducing antioxidant power

Serially diluted compounds (10-100µg/ml) were mixed with 2.5 ml of potassium phosphate buffer (0.2M, pH 6.6) & 2.5 ml of potassium ferricyanide (1g/100ml) the mix was incubated at 50 for 20 minute. A total of 2.5 ml of 10% trichloroacetic acid was added to the mixture to stop the reaction. Equal volume of ultra pure water was added to 2.5 ml of the mixture before the addition of 0.5 ml of $FeCl_3$(0.1g/100 ml) The sample was allowed to stand for 30 min. before measuring the absorbance at 700nm. The absorbance obtained was converted to Gallic acid equivalents in mg/gram compound (mgGAE/g) using a Gallic acid standard curve[4].

STD Gallic acid curve for (FRAP Assay)



RESULTS AND DISCUSSION

The preliminary chemical screening investigation shows that synthesized compounds have enolic groups. The spectral data for the absorption for the three compounds was compared with gallic acid for the plot was calculated by the equation: y=0.022x-0.1458 (R2=0.982) and found that the antioxidant property of the compounds have the mentioned profle: Compound-C>Compound-B>Compound-A.

Compound-C is guanidine moiety having X=NH so according to the highest electronegativity profile this is more potent than other two when compared with the total reducing capacity property[5]. It was expressed as GAE means that reducing power of 10mg of each compound is equivalent to reducing power of µg of gallic acid or expressed as µgGAE/mg of compound(Compound-A: 272.8µg, Compound-B:317µg, Compound-C:384.9µg)

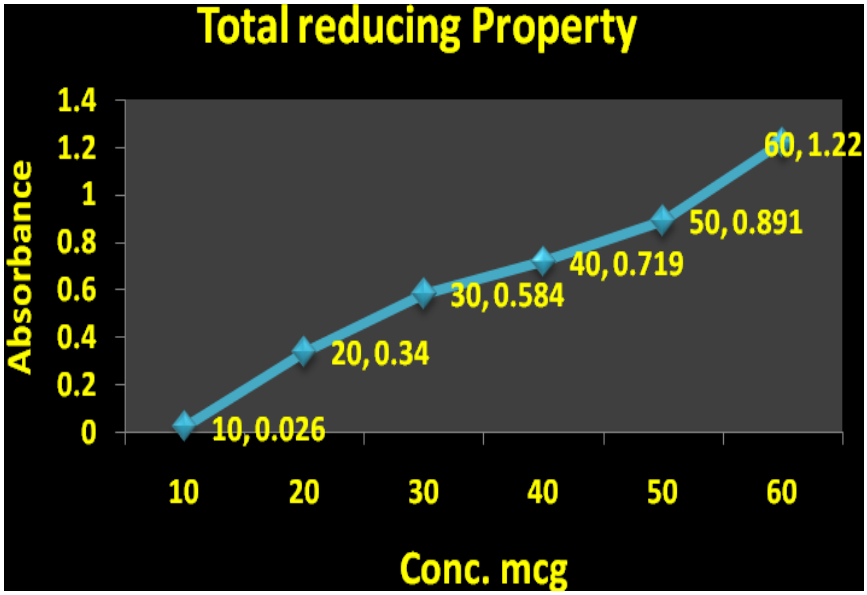
POTENTIATION OF COMPOUND

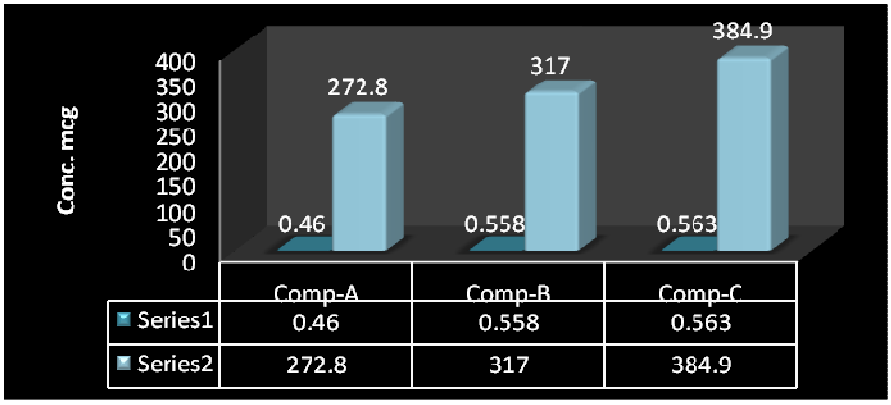
Compound	Concentration (µg)
Compound-1	272.8
Compound-2	317
Compound-3	384.9

Table-2

Std. Gallic acid (µg)	Absorbance
10	**0.026**
20	**0.34**
30	**0.584**
40	**0.719**
50	**0.891**
60	**1.22**

Table-3





CONCLUSION

In-vitro antioxidant activity by Reducing Power indicated that incresed absorbance with concentration of showed that synthesized compounds have reducing power. By Ferric reducing antioxidant power (FRAP) assay method, it is concluded that the three synthesized compound are responsible for the antioxidant potency. The spectral data for the absorption for the three compounds was compared with gallic acid for the plot was calculated by the equation: y=0.022x-0.1458 (R2=0.982) and found that the antioxidant property of the compounds have the mentioned profle: Compound-C>Compound-B>Compound-A. Compound-C is guanidine moiety having X=NH so according to the highest electronegativity profile this is more potent than other two when compared with the total reducing capacity property. (Compound-A: 272.8µg, Compound-B: 317µg, Compound-C: 384.9µg) It was expressed as GAE means that reducing power of 10mg of each compound is equivalent to reducing power of µg of gallic acid or expressed as µgGAE/mg of compound.

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