5.1 RESULT AND DISCUSSION OF EXPERIMENTAL SECTION OF SYNTHESIZED COMPOUNDS:

5.1.1(a) Result and discussion of experimental section of pyrazoline compounds of scheme-1.

*Ethyl-2-substituted phenylhydrazono-3-oxobutyrate(1a-j)*

The purity of the compounds was checked by TLC and its characterization on the basis of IR and NMR spectral data.
The IR spectrum of the compounds (1a-j) showed peaks at 3418-3386 cm\(^{-1}\), NH stretching; 2993-2982 cm\(^{-1}\), CH stretching; 1705-1686 cm\(^{-1}\), C=O stretching and 1583-1571 cm\(^{-1}\), C=C stretching vibrations of aromatic rings.

The NMR spectrum of the compounds:

Compound 1b showed a triplet at \(\delta\) 1.20-1.25 and a quartet at \(\delta\) 4.22-4.29 for CH\(_3\) and OCH\(_2\) protons of ethoxy group, a singlet at \(\delta\) 2.39 was noticed and point out the existence of COCH\(_3\) protons. A signal of NH proton was observed as a singlet at \(\delta\) 8.28 whereas, the singlet of COOH proton observed down field at \(\delta\) 15.25. In the aromatic region a multiplet of four protons was observed at \(\delta\) 7.00-7.99 indicating the presence of phenyl protons.

Compound 1d showed a triplet at \(\delta\) 1.41-1.43 and a quartet at \(\delta\) 4.38-4.41 for CH\(_3\) and OCH\(_2\) protons of ethoxy group, two singlets were observed at \(\delta\) 2.60 and \(\delta\) 3.95 for COCH\(_3\) and OCH\(_3\) protons respectively. A multiplet for four aromatic protons was observed at \(\delta\) 6.92-7.27. Furthermore, the singlet of NH proton was observed at \(\delta\) 11.88.

Compound 1g showed a triplet at \(\delta\) 1.24-1.26 and a quartet at \(\delta\) 4.27-4.29 for CH\(_3\) and OCH\(_2\) protons of ethoxy group, a singlet at \(\delta\) 2.35 was noticed and point out the existence of COCH\(_3\) protons. The multiplet for four aromatic protons was observed at \(\delta\) 7.39-7.40. Furthermore, the singlet of NH proton was observed at \(\delta\) 11.62.

Compound 1j showed a triplet at \(\delta\) 1.31-1.35 and a quartet at \(\delta\) 4.20-4.26 for CH\(_3\) and OCH\(_2\) protons of ethoxy group, the singlet for COCH\(_3\) protons was observed at \(\delta\) 2.70, whereas, the singlet for CH\(_3\) protons attached to the phenyl ring was observed at \(\delta\) 2.50. The multiplet for four aromatic protons was observed at \(\delta\) 7.39-7.40. Furthermore, the singlet of NH proton was observed at \(\delta\) 11.62. In the aromatic region a multiplet of five protons was observed at \(\delta\) 7.10-7.90 point out the existence of four phenyl protons and one NH proton.

On the basis of these spectral data the following structure was assigned to the compounds.
8-Quinolinoxyacetic acid hydrazide (3)

The IR spectrum of the compound (3) showed peaks at 3225 cm\(^{-1}\), NH stretching; 2980 cm\(^{-1}\), CH stretching; 1689 cm\(^{-1}\), C=O stretching and 1578 cm\(^{-1}\), C=C stretching vibrations of aromatic ring. The structure of the compound was further supported by its NMR spectrum which showed a singlet at \(\delta\) 4.90 OCH\(_2\) protons. In the aromatic region a multiplet of eight protons at \(\delta\) 7.15-6.23 was noticed and point out the existence of six aromatic and two NH\(_2\) protons. The broad singlet of CONH proton was observed at \(\delta\) 8.95. On the basis of these spectral data the following structure was assigned to the compounds.

1-(8-Quinolinoxyacetyl)-3-methyl-4-(substitutedphenylhydrazono)-2-pyrazoline-5-ones (4a-j)

The IR spectrum of the compounds (4a-j) showed peaks at 3012-2969 cm\(^{-1}\), CH stretching; 1691-1682 cm\(^{-1}\), C=O stretching of pyrazoline ring; 1673-1657 cm\(^{-1}\), C=N stretching and 1599-1568 cm\(^{-1}\), C=C stretching vibrations of aromatic rings.

The NMR and Mass spectrum of compounds:

Compound 4a showed a singlet for CH\(_3\) protons at \(\delta\) 2.16, the OCH\(_2\) protons attached to the quinoline ring was obtained as a singlet at \(\delta\) 3.34. A multiplet was obtained at \(\delta\) 7.30-8.26 indicating the presence of 10 aromatic protons. The NH proton was obtained as a singlet at \(\delta\) 11.52, whereas the singlet of COOH proton was obtained at \(\delta\) 12.40.
Compound 4d showed a singlet at $\delta$ 2.27, showing the presence of methyl protons. The singlet of OCH$_2$ protons attached to the quinoline ring was observed at $\delta$ 3.50, whereas the singlet of methoxy protons attached to the phenyl ring was observed at $\delta$ 3.85. A multiplet at $\delta$ 6.95-7.39 was noticed and point out the existence of of 10 aromatic protons. Singlet for NH proton was observed at $\delta$ 8.53. Its mass spectral data, showed molecular ion peak M$^+$ at m/z 417, having molecular formula C$_{22}$H$_{19}$N$_5$O$_4$. Further peaks were obtained at m/z 232, 186, 125 and 97.

Compound 4e showed a singlet at $\delta$ 2.24, indicating the presence of methyl protons. The signal for OCH$_2$ protons was observed as a singlet at $\delta$ 3.47. A multiplet at $\delta$ 7.24-7.52 was noticed and point out the existence of of 10 aromatic protons. Singlet was observed at $\delta$ 8.54 indicating the presence of NH proton. Its mass spectral data, showed M$^+$ at m/z 466, having molecular formula C$_{21}$H$_{16}$N$_5$O$_3$Br. Other peaks were obtained at m/z 281, 186, 125 and 97.

Compound 4g showed a singlet at $\delta$ 2.46, indicating the presence of methyl protons. The signal for OCH$_2$ protons was obtained as a singlet at $\delta$ 3.79. A multiplet at $\delta$ 7.44-7.69 was noticed and point out the existence of of 10 aromatic protons. Singlet was obtained at $\delta$ 8.87 indicating the presence of NH proton.

Compound 4j showed a singlet at $\delta$ 2.32, indicating the presence of methyl protons attached to the pyrazoline ring. The methyl protons attached to the phenyl ring were obtained as a singlet at $\delta$ 2.50. Furthermore, a singlet was observed at $\delta$ 3.76 indicating the presence of OCH$_2$ protons attached to the quinoline ring. A multiplet at $\delta$ 7.03-7.37 was noticed and point out the existence of 10 aromatic protons. The singlet of NH proton was also observed at $\delta$ 8.39.

On the basis of these spectral data the following structure was assigned to the compounds.
5.1.1(b) Result and discussion of experimental section of pyrazoline compounds of scheme-2.

2-Hydrazino-6-chlorobenzothiazole (6)

The structure of the compound (6) was confirmed by its NMR spectral data which showed a multiplet for 3 aromatic protons at δ 7.17-7.38. The NH proton was observed as a singlet at δ 7.74, whereas the singlet of NH$_2$ protons was observed at δ 9.03

On the basis of these spectral data the following structure was assigned to the compound (6).
1-(6-Chlorobenzothiazol-2-yl)-3-methyl-4-(substituted phenylhydrazono)-2-pyrazoline-5-ones (7a-j)

The IR spectrum of the compounds (7a-j) exhibit peaks at 3013-2970 cm$^{-1}$, CH stretching; 1696-1680 cm$^{-1}$, C=O stretching; 1676-1658 cm$^{-1}$, C=N stretching; 1595-1562 cm$^{-1}$, C=C stretching of aromatic rings and 755-738 cm$^{-1}$, stretching vibrations.

The NMR and Mass spectrum of compounds:

Compound 7c showed a singlet at $\delta$ 2.38 for CH$_3$ protons. A multiplet at $\delta$ 6.95-7.87 was noticed and point out the existence of 7 aromatic protons. The two NH protons were obtained as a singlet at $\delta$ 10.63. Furthermore a broad singlet was obtained at $\delta$13.31 indicating the presence of OH group attached to the phenyl ring.

Compound 7d showed two singlets at $\delta$ 2.44 and $\delta$ 3.84 indicating the presence of methyl and methoxy group respectively. The 7 aromatic protons were obtained as a multiplet at $\delta$ 6.99-7.92. Furthermore, the singlet of NH proton was obtained at $\delta$ 13.38. Its mass spectra showed M$^+$ at m/z 399, having molecular formula C$_{18}$H$_{14}$N$_5$O$_2$ScI. Other peaks were observed at m/z 232, 186 and 97.

Compound 7e showed a singlet at $\delta$ 2.38 indicating the presence of methyl protons, a multiplet at $\delta$ 7.24-7.87 was noticed and point out the existence of 7 aromatic protons. The NH proton was observed as a singlet at $\delta$ 10.74.

Compound 7g showed a singlet at $\delta$ 2.36 indicating the presence of CH$_3$ protons. A multiplet of 7 protons was obtained at $\delta$ 7.33-8.05 indicating the presence of 7 aromatic protons. The NH proton was observed as a singlet at $\delta$ 10.82.

Compound 7i showed a singlet at $\delta$ 2.38 indicating the presence of methyl protons attached to the pyrazoline ring. The singlet of methyl proton attached to the phenyl ring was observed at $\delta$ 2.45. In the aromatic region a multiplet at $\delta$ 7.23-7.92 was noticed and point out the existence of 7 aromatic protons, the singlet of NH proton was obtained at $\delta$ 10.27. Its mass spectral data showed molecular ion peak M$^+$ at m/z 383, with the molecular formula C$_{18}$H$_{14}$N$_5$OScI. Further peaks were observed at m/z 216, 168, 125 and 97. On the basis of these spectral data the following structure was assigned to the compounds.
5.1.2 Result and discussion of experimental section of pyrazole compounds of scheme-3:

2,4-Diketo-3-(arylazo)-propane (8a-j)

The IR spectrum of the compounds (8a-j) showed peaks at 3012-2993 cm\(^{-1}\), CH stretching; 1693-1661 cm\(^{-1}\), C=O stretching and 1573-1536 cm\(^{-1}\), -N=N- stretching vibrations.

The NMR spectrum of the compounds:

Compound 8d showed a singlet at \(\delta\) 1.65 indicating the presence of N-CH proton. The signals of two COCH\(_3\) were obtained as singlets at \(\delta\) 2.47 and \(\delta\) 2.59. Furthermore the singlet of OCH\(_3\) protons attached to the phenyl ring was obtained at \(\delta\) 3.83. In the aromatic region two doublets were obtained at \(\delta\) 6.93 and \(\delta\) 7.35 indicating the presence of 2′,6′- and 3′,5′- aromatic protons respectively.

Compound 8g showed a singlet at \(\delta\) 1.78 indicating the presence of N-CH proton. The protons of two COCH\(_3\) were obtained as singlets at \(\delta\) 2.35 and \(\delta\) 2.43. Furthermore two doublets were obtained at \(\delta\) 7.37 and \(\delta\) 7.51 indicating the presence of 2′,6′- and 3′,5′- aromatic protons respectively.
On the basis of these spectral data the following structure was assigned to the compound.

![Chemical structure](image)

(8a-j)

R = a: 4-COOH, b: 2-COOH, c: 2-OH, d: 4-OCH₃, e: 4-Br, f: 4-F, g: 4-Cl, h: 2-Cl, i: 4-CH₃, j: 2-CH₃
1-(8-Quinolinoxyacetyl)-3,5-dimethyl-4-(substituted phenylazo) pyrazoles (9a-j)

The IR spectrum of the compounds (9a-j) showed peaks at 3008-2972 cm\(^{-1}\), CH stretching; 1693-1658 cm\(^{-1}\), C=O stretching of pyrazoline ring; 1681-1664 cm\(^{-1}\), C=N stretching; 1556-1530 cm\(^{-1}\), -N=N- stretching and 1603-1578 cm\(^{-1}\), C=C stretching vibrations of aromatic rings.

The NMR and Mass spectrum of compounds:

Compound 9a showed a merged singlet observed at \(\delta\) 2.46, indicating the presence of 3 and 5 methyl groups attached to the pyrazole ring. The OCH\(_2\) protons were observed as a singlet at \(\delta\) 3.42. In the aromatic region a multiplet of 10 protons was observed at \(\delta\) 7.62-8.08. Furthermore, the COOH proton was obtained as a singlet at \(\delta\) 13.69.

Compound 9e showed a singlet of methyl protons attached to the 3\(^{rd}\) position of the pyrazole ring at \(\delta\) 2.17. The signals of OCH\(_2\) protons and 5-CH\(_3\) protons were merged together and obtained as a singlet at \(\delta\) 2.58. In the aromatic region a multiplet at \(\delta\) 7.56-7.68 was noticed and point out the existence of 10 aromatic protons.

Compound 9g showed a singlet of methyl protons attached to the 3\(^{rd}\) position of the pyrazole ring at \(\delta\) 2.17. The signals of OCH\(_2\) protons and 5-CH\(_3\) protons were merged together and obtained as a singlet at \(\delta\) 2.58. In the aromatic region a multiplet at \(\delta\) 7.36-7.75 was noticed and point out the existence of 10 aromatic protons. Its mass spectral data showed M\(^+\) at m/z 420, having molecular formula C\(_{22}\)H\(_{18}\)N\(_5\)O\(_2\)Cl. Other peaks were observed at m/z 233, 186 and 139.

Compound 9j showed a singlet at \(\delta\) 2.39, indicating the presence of methyl group attached to the phenyl ring. Two singlets were also observed at \(\delta\) 2.57 and 2.58 indicating the presence of methyl groups attached to the 3\(^{rd}\) and 5\(^{th}\) position of the pyrazole ring. The OCH\(_2\) protons were observed as a singlet at \(\delta\) 2.62. In the aromatic region a multiplet at \(\delta\) 7.24-7.60 was noticed and point out the existence of 10 aromatic protons.

On the basis of these spectral data the following structure was assigned to the compounds (9a-j).
5.1.3(a) Result and discussion of experimental section of 1,3,4 oxadiazole compounds of scheme-4:

2,4,6-Trichlorophenoxymethyl acetic acid Hydrazide (2)

The IR spectrum of the compound (2) showed peaks at 3359 cm\(^{-1}\), NH stretching; 3072 cm\(^{-1}\), CH stretching; 1669 cm\(^{-1}\), C=O stretching; 1580 cm\(^{-1}\), C=C stretching of aromatic rings and 757 cm\(^{-1}\), C-Cl stretching vibrations. Its NMR spectrum which showed a singlet at \(\delta\) 3.99 for OCH\(_2\) protons, a singlet at \(\delta\) 4.58 was also observed for NH\(_2\) protons. In the aromatic region a singlet at \(\delta\) 7.35 was noticed and point out the existence of 3 & 5 aromatic protons. A broad singlet at \(\delta\) 8.06 was noticed and point out the existence of CONH proton. On the basis of these spectral data the following structure was assigned to the compound (2)

5-(2,4,6-Trichlorophenoxymethyl)-2-(aryl)-1,3,4-oxadiazoles (3a-p)

The IR spectrum of the compounds (3a-p) showed peaks at 3016-2970 cm\(^{-1}\), CH stretching; 1680-1650 cm\(^{-1}\), C=N stretching; 1600-1560 cm\(^{-1}\), C=C stretching of aromatic rings and 800-740 cm\(^{-1}\), C-Cl stretching vibrations.

The NMR and Mass spectrum of compounds:
Compound 3a showed a singlet at $\delta$ 5.18 and point out the existence of OCH$_2$ protons, in the aromatic region a multiplet was observed at $\delta$ 7.21-7.58 for 7 aromatic protons.

Compound 3d showed a singlet at $\delta$ 5.35 and point out the existence of OCH$_2$ protons. The presence of 5 aromatic protons was confirmed by the appearance of the multiplet at $\delta$ 7.26-7.96.

Compound 3e showed two singlets centred at $\delta$ 5.21 and $\delta$ 5.35 indicating the presence of OCH$_2$ protons attached to the 2,4-dichlorophenyl and 2,4,6-trichlorophenyl rings respectively. In the aromatic region a multiplet at $\delta$ 7.06-7.41 was noticed and point out the existence of 5 aromatic protons. Its mass spectral data showed M$^+$ at m/z 452, consistent with the expected molecular formula C$_{16}$H$_9$N$_2$O$_2$Cl$_5$. Further fragments were obtained at m/z 237, 209 and 195.

Compound 3f showed a singlet at $\delta$ 4.59 indicating the presence of OCH$_2$ protons. The singlet for NH$_2$ protons was observed at $\delta$ 5.08. In the aromatic region a multiplet of 6 protons was observed at $\delta$ 7.67-7.87 indicating the presence of phenyl protons.

Compound 3h showed a singlet at $\delta$ 5.36 for OCH$_2$ protons. A complex multiplet was observed at $\delta$ 7.36-8.40 indicating the presence of 6 aromatic protons. Its mass spectral data showed M$^+$ at m/z 400, having molecular formula C$_{15}$H$_8$N$_3$O$_4$Cl$_3$. Further fragments were obtained at m/z 249, 150 and 122.

The compound 3j was identified by its NMR spectral data, which showed a double doublet at $\delta$ 0.88 for six (CH$_3$)$_2$ protons. A doublet and a quartet were also observed at $\delta$ 1.56 and 3.69-3.74 for CH$_3$ and CH$_3$CH protons respectively. Moreover a doublet and a multiplet of CH$_2$ and CH protons of isobutyl group were observed at $\delta$ 2.45 and $\delta$ 1.84-1.89 respectively. The singlet of OCH$_2$ protons was also observed at $\delta$ 4.64, a complex multiplet of 6 phenyl protons was observed in the aromatic region at $\delta$ 7.11-7.61. Its mass spectral data showed M$^+$ at m/z 439, having molecular formula C$_{21}$H$_{21}$N$_2$O$_2$Cl$_3$. Further fragments were obtained at m/z 395, 189 and 161.

Compound 3k showed a doublet and a quartet for CH$_3$ and CH protons at $\delta$ 1.60 and 3.78-3.86 respectively. A singlet of OCH$_2$ protons was observed at $\delta$ 4.61, in the aromatic region a complex multiplet of 10 protons was obtained at $\delta$ 7.18-7.53 and point out the
existence of phenyl protons. Its mass spectral data showed \( M^+ \) at \( m/z \) 477, having molecular formula \( \text{C}_{22}\text{H}_{16}\text{N}_{2}\text{O}_{2}\text{Cl}_{3}\text{F} \). Further peaks were observed at \( m/z \) 249, 227, 199 and 185.

Compound 3l showed a doublet and a quartet at \( \delta \) 1.58 and 3.80-3.84 for the presence of \( \text{CH}_3 \) and \( \text{CH} \) protons respectively. A singlet for the meyhoxy protons in the naphthyl ring was observed at \( \delta \) 3.87. The singlet of \( \text{OCH}_2 \) protons attached to the oxadiazole ring was also observed at \( \delta \) 4.62. A multiplet of 6 naphthyl protons was observed in the aromatic region at \( \delta \) 7.10-7.43, whereas the two protons of trichlorophenyl ring were obtained as a singlet at \( \delta \) 7.68.

5-(2,4,6-Trichlorophenoxy)methyl)-2-mercapto-1,3,4-oxadiazole (3q)

The IR spectrum of the compound (3q) showed peaks at 3049 cm\(^{-1}\), \( \text{CH} \) stretching; 1632 cm\(^{-1}\), \( \text{C}=\text{N} \) stretching; 1586 cm\(^{-1}\), \( \text{C}=\text{C} \) stretching of aromatic rings; 1160 cm\(^{-1}\), \( \text{C}=-\text{S} \) stretching and 734 cm\(^{-1}\), \( \text{C}-\text{Cl} \) stretching vibrations.

NMR spectra of (3q) showed a singlet at \( \delta \) 5.17 for \( \text{OCH}_2 \) protons. The two trichlorophenyl protons were obtained as a singlet at \( \delta \) 7.50. Furthermore a broad singlet was observed at \( \delta \) 10.84 indicating the presence of \( \text{SH} \) protons. On the basis of these spectral data the following structure was assigned to the compounds.
5.1.3(b) Result and discussion of experimental section of 1,3,4 oxadiazole compounds of scheme-5:

4-Hydroxyphenyl acetic acid hydrazide (5)

The IR spectrum of the compound (5) showed peaks at 3596 cm\(^{-1}\), OH stretching; 3406 cm\(^{-1}\), NH stretching; 2981 cm\(^{-1}\), CH stretching; 1690 cm\(^{-1}\), C=O stretching and 1582 cm\(^{-1}\), C=C stretching vibrations of aromatic rings.

The structure of the compound (5) was further supported by its NMR spectral data which showed two singlets at \(\delta\) 3.20 and \(\delta\) 4.19 for CH\(_2\) and NH\(_2\) protons respectively. In the aromatic region two doublets centered at \(\delta\) 6.65 and \(\delta\) 7.05 were observed indicating the presence of 2,6- and 3,5- aromatic protons respectively. A singlet was observed at \(\delta\) 9.13 indicating the presence of CONH proton. Furthermore the phenolic OH proton was observed as broad singlet at \(\delta\) 9.22.

On the basis of these spectral data the following structure was assigned to the compound (5).

\[
\text{HO-} \begin{array}{c}
\text{CH}_2\text{CONHNH}_2
\end{array} \\
(5)
\]

N\(^1\)-[2-(4-Hydroxyphenyl) acetyl]-N\(^4\)-alkyl/aryl-3-thiosemicarbazides (6a-i)

The IR spectrum of the compounds (6a-i) showed peaks at 3612-3571 cm\(^{-1}\), OH stretching; 3392-3237 cm\(^{-1}\), NH stretching; 3028-2963 cm\(^{-1}\), CH stretching; 1695-1660 cm\(^{-1}\), C=O stretching and 1183-1146 cm\(^{-1}\), C=S stretching vibrations.

The NMR and Mass spectrum of compounds:

Compound 6c showed a singlet at \(\delta\) 2.50 for CH\(_2\) protons. Two broad singlets were observed at \(\delta\) 9.69 and \(\delta\) 10.09 indicating the presence of CONH-NH-C=S and OH proton respectively. The other NH attached to p-chlorophenyl ring was also observed as a singlet at \(\delta\) 9.27. In the aromatic region two doublets centered at \(\delta\) 6.67 and \(\delta\) 7.08 were observed indicating the presence of 2,6- and 3,5- phenolic protons respectively. The four protons of p-
chlorophenyl ring were also observed as doublets centered at $\delta$ 7.37 and $\delta$ 7.46 indicating the presence of 2',6'- and 3',5'- aromatic protons. Its mass spectral data showed M$^+$ at m/z 335, having molecular formula C$_{15}$H$_{14}$N$_3$O$_2$SCl. Further peaks were observed at m/z 166, 135 and 107.

Compound 6h showed two singlets at $\delta$ 2.50 and $\delta$ 3.81 for CH$_2$ and OCH$_3$ protons respectively. The signals of CONH-NH-C=S protons was observed as a broad singlet at $\delta$ 9.58, whereas the signal of OH proton was observed at $\delta$ 10.02 as a broad singlet. The NH proton attached to p-methoxyphenyl ring was also observed as a singlet at $\delta$ 9.23. In the aromatic region two doublets centered at $\delta$ 6.65 and $\delta$ 7.01 were observed indicating the presence of 2,6- and 3,5- phenolic protons respectively. The four protons of p-methoxyphenyl ring were also observed as doublets centered at $\delta$ 7.32 and $\delta$ 7.45 indicating the presence of 2',6'- and 3',5'- aromatic protons. On the basis of these spectral data the following structure was assigned to the compounds.

\[
\text{HO-CH}_2\text{CONHNH-C-NHR}
\]

\[
\text{(6a-i)}
\]

R = a: , b: Br , c: Cl , d: , e: , f: H$_2$C , g: , h: CH$_3$O , i: n-CH$_3$CH$_2$CH$_2$CH$_2$

5-(Hydroxyphenyl)methyl-2-alkyl/arylamino-1,3,4-oxadiazoles (7a-i)

The IR spectrum of the compounds (7a-i) showed peaks at 3580-3560 cm$^{-1}$, OH stretching; 3382-3294 cm$^{-1}$, NH stretching; 2988-2960 cm$^{-1}$, CH stretching; 1670-1630 cm$^{-1}$, C=N stretching and 1591-1560 cm$^{-1}$, C=C stretching vibrations of aromatic rings.

The NMR spectrum of compounds:

Compound 7b showed a singlet at $\delta$ 2.51 for CH$_2$ protons. In the aromatic region two doublets centered at $\delta$ 6.57 and $\delta$ 6.70 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-bromophenyl ring were also observed
as doublets centered at δ 7.18 and δ 7.48 indicating the presence of 2’, 6’- and 3’, 5’- aromatic protons. Furthermore two singlets were also observed at δ 9.29 and δ 10.41 indicating the presence of NH and OH protons respectively. Its mass spectral data, showed M⁺ at m/z 346, having molecular formula C₁₅H₁₂N₃O₂ClBr. Further peaks were observed at m/z 211, 135 and 107.

Compound 7e showed a singlet at δ 2.50 for CH₂ protons. In the aromatic region two doublets centered at δ 6.56 and δ 6.69 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-chlorophenyl ring were also observed as doublets centered at δ 7.23 and δ 7.53 indicating the presence of 2’, 6’- and 3’, 5’- aromatic protons. Furthermore two singlets were also observed at δ 9.33 and δ 10.55 indicating the presence of NH and OH protons respectively. Its mass spectral data showed M⁺ at m/z 301, having molecular formula C₁₅H₁₂N₃O₂Cl. Further peaks were observed at m/z 166, 135 and 107.

Compound 7f showed two singlets at δ 2.36 and δ 2.50 for CH₃ and CH₂ protons respectively. In the aromatic region two doublets centered at δ 6.57 and δ 6.69 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-methylphenyl ring were also observed as doublets centered at δ 7.06 and δ 7.26 indicating the presence of 2’, 6’- and 3’, 5’- aromatic protons. Furthermore a singlet at δ 9.26 and a broad singlet at δ 13.25 were also observed for NH and OH protons respectively. Its mass spectral data showed M⁺ at m/z 281, having molecular formula C₁₆H₁₅N₃O₂. Further peaks were observed at m/z 135 and 107.

Compound 7h showed two singlets at δ 2.50 and δ 3.80 for CH₂ and OCH₃ protons respectively. In the aromatic region two doublets centered at δ 6.57 and δ 6.69 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-methoxyphenyl ring were also observed as doublets centered at δ 6.99 and δ 7.10 indicating the presence of 2’, 6’- and 3’, 5’- aromatic protons. Furthermore a singlet at δ 9.29 and a broad singlet at δ 13.79 were also observed for NH and OH protons respectively.

Compound 7i showed a triplet at δ 0.76-0.78 indicating the presence of methyl protons of n-butyl group. The CH₃-CH₂CH₂ protons of n-butyl group were merged together and obtained as a multiplet at δ 1.16-1.22. The NH-CH₂ protons of n-butyl group was
obtained as a triplet at $\delta$ 3.74. A singlet at $\delta$ 2.48 was also obtained indicating the presence of CH$_2$ protons attached to oxadiazole ring. In the aromatic region two doublets centered at $\delta$ 6.68 and $\delta$ 7.03 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. Furthermore a singlet at $\delta$ 9.38 and a broad singlet at $\delta$ 13.53 were also observed for NH and OH protons respectively. Its mass spectral data, showed M$^+$ at m/z 247, having molecular formula C$_{13}$H$_{17}$N$_3$O$_2$. Further peaks were observed at m/z 175, 135 and 107.

5-(Hydroxyphenyl) methyl-2-mercapto-1,3,4-oxadiazoles (7j)

The IR spectrum of the compound (7j) showed peaks at 3611 cm$^{-1}$, OH stretching; 2987 cm$^{-1}$, CH stretching; 1662 cm$^{-1}$, C=N stretching; 1586 cm$^{-1}$, C=C stretching of aromatic rings and 1165 cm$^{-1}$, C=S stretching vibrations.

On the basis of spectral data the following structure of the compounds (7a-j) was assigned.

(7a-i)

R = a: , b: Br, c: Cl, d: , e: F, f: H, g: , h: CH$_3$O, i: n-CH$_2$CH$_2$CH$_2$CH$_2$-

(7j)
5.1.4 Result and discussion of experimental section of 1,2,4 triazole compounds of scheme-6:

5-(Hydroxyphenyl) methyl-4-alkyl/aryl-2-mercepto-1,2,4(H)-triazoles (8a-i):

The IR spectrum of the compounds (8a-i) showed peaks at 3576-3545 cm\(^{-1}\), OH stretching; 2992-2963 cm\(^{-1}\), CH stretching; 1657-1620 cm\(^{-1}\), C=N stretching; 1596-1578 cm\(^{-1}\), C=C stretching of aromatic rings and 1186-1145 cm\(^{-1}\), C=S stretching vibrations.

The NMR and mass spectrum of compounds:

Compound 8b showed a singlet at \(\delta\) 2.48 and point out the existence of CH\(_2\) protons. In the aromatic region two doublets centered at \(\delta\) 6.54 and \(\delta\) 6.68 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-bromophenyl ring were also observed as doublets centered at \(\delta\) 7.21 and \(\delta\) 7.50 indicating the presence of 2’, 6’- and 3’, 5’- aromatic protons. Furthermore a singlet at \(\delta\) 9.29 and a broad singlet at \(\delta\) 13.70 were also observed for SH and OH protons respectively. Its mass spectral data showed M\(^+\) at m/z 362, having molecular formula C\(_{15}\)H\(_{12}\)N\(_3\)OSBr. Further peaks were observed at m/z 329, 303, 133 and 107.

Compound 8c showed a singlet at \(\delta\) 2.50 and point out the existence of CH\(_2\) protons. In the aromatic region two doublets centered at \(\delta\) 6.56 and \(\delta\) 6.69 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-chlorophenyl ring were also observed as doublets centered at \(\delta\) 7.23 and \(\delta\) 7.53 indicating the presence of 2’, 6’- and 3’, 5’- aromatic protons. Furthermore a singlet at \(\delta\) 9.32 and a broad singlet at \(\delta\) 13.83 were also observed for SH and OH protons respectively. Its mass spectral data showed M\(^+\) at m/z 317, having molecular formula C\(_{15}\)H\(_{12}\)N\(_3\)OSCl. Further peaks were observed at m/z 284, 258, 133 and 107.

Compound 8f showed two singlets at \(\delta\) 2.36 and \(\delta\) 2.50 for CH\(_3\) and CH\(_2\) protons respectively. In the aromatic region two doublets centered at \(\delta\) 6.56 and \(\delta\) 6.69 were observed
indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-methylphenyl ring were also observed as doublets centered at $\delta$ 7.07 and $\delta$ 7.27 indicating the presence of 2', 6'- and 3', 5'- aromatic protons. Furthermore a singlet at $\delta$ 9.31 and a broad singlet at $\delta$ 13.64 were also observed for SH and OH protons respectively. Its mass spectral data showed $M^+$ at m/z 297, having molecular formula $C_{16}H_{15}N_3OS$. Further peaks were observed at m/z 264, 238, 133 and 107.

Compound 8h showed two singlets at $\delta$ 2.50 and $\delta$ 3.80 for CH$_2$ and OCH$_3$ protons respectively. In the aromatic region two doublets centered at $\delta$ 6.57 and $\delta$ 6.69 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. The four protons of p-methoxyphenyl ring were also observed as doublets centered at $\delta$ 6.99 and $\delta$ 7.09 indicating the presence of 2', 6'- and 3', 5'- aromatic protons. Furthermore a singlet at $\delta$ 9.29 and a broad singlet at $\delta$ 13.25 were also observed for SH and OH protons respectively.

Compound 8i showed a triplet at $\delta$ 0.76-0.80 indicating the presence of methyl protons of n-butyl group. The CH$_3$-CH$_2$CH$_2$ protons of n-butyl group were merged together and obtained as a multiplet at $\delta$ 1.16-1.27. The NH-CH$_2$ protons of n-butyl group was obtained as a triplet at $\delta$ 3.74-3.78, a singlet at $\delta$ 2.50 was also obtained indicating the presence of CH$_2$ protons attached to oxadiazole ring. In the aromatic region two doublets centered at $\delta$ 6.67 and $\delta$ 7.02 were observed indicating the presence of 2, 6- and 3, 5- phenolic protons respectively. Furthermore a singlet at $\delta$ 9.11 and a broad singlet at $\delta$ 13.55 were also observed for SH and OH protons respectively. Its mass spectral data showed $M^+$ at m/z 263, having molecular formula $C_{13}H_{17}N_3OS$. Further peaks were observed at m/z 230 and 204.

On the basis of these spectral data the following structure was assigned to the compounds (8a-i).
5.2 Result and discussion of biologically screened compounds:

5.2.1 Result and discussion of biologically screened pyrazoline derivatives of scheme-1 and scheme-2 has been explained as:

Compounds (4a-j, 7a-j) have been evaluated for their in-vitro anti-microbial activity against Staphylococcus aureus (S. aureus, ATCC-29737), as an example of gram positive bacteria, Escherchia coli (E. coli, ATCC-8739) as an example of gram negative bacteria and Aspergillus niger (A. niger) as a representative of fungi. The microdilution susceptibility test in nutrient agar media (Hi-Media), Sabroaud’s dextrose agar media were used for determination of antibacterial and antifungal activities respectively. The minimal inhibitory concentration (MICs, µgmL\(^{-1}\)) of the tested compounds were recorded.

The results revealed that most of the newly synthesized pyrazoline derivatives bearing quinoline moiety (4a-j) exhibited promising anti-bacterial activity. Out of the compound tested, compound 4i and 4j having 2 & 4 methyl groups in the phenyl ring exhibited remarkable antibacterial activity (MIC 25 µgmL\(^{-1}\)) against E. coli (gram negative bacteria) whereas compound 4a having COOH group at 4\(^{th}\) position of the phenyl ring showed the similar antibacterial potency (MIC 25 µgmL\(^{-1}\)) against S. aureus (gram positive bacteria) as compared with the broad spectrum antibiotics ofloxacin (MIC 10.0 µgmL\(^{-1}\) against S. aureus and 12.5 µgmL\(^{-1}\) against E. coli). The results have shown in table-4.

The antifungal screening results have shown that the compound 4d and 4g having 4-methoxy and 4-chloro respectively groups in the phenyl ring exhibited good activity (MIC 50 µgmL\(^{-1}\)) against A. niger, as compared with the standard drug ketoconazole (MIC 12.5 µgmL\(^{-1}\)).
When the quinoline moiety of the pyrazoline nucleus has been replaced by 6-chlorobenzothiazole moiety (7a-j), they exhibited almost similar activity against S. aureus (gram positive bacteria) but the activity was found to be decreased against E. coli (gram negative bacteria) and fungus A. niger. The compound 7b having a COOH group at 2-position of the phenyl ring was found to be most potent (MIC 25 µg/mL) against S. aureus. None of the compound of the series showed significant activity against E. coli and fungus A. niger. The result have shown in table 5.

5.2.2 Result and discussion of biologically screened pyrazole derivatives of scheme-3 has been explained as:

The antimicrobial screening results of the pyrazole derivatives bearing quinoline moiety (9a-j) showed that some of the compounds exhibited significant antibacterial activity, at the same time, the compounds showed only moderate antifungal activity.

Out of all the synthesized pyrazole derivatives of the series, compound 9g having chloro group at the 4th position of the phenyl ring exhibited remarkable antibacterial activity (MIC 25 µg/mL), against E. coli (gram negative bacteria), whereas the compound 9h having chloro group at the 2nd position of the phenyl ring showed similar antibacterial activity (MIC 25 µg/mL), against S. aureus (gram positive bacteria), as compared with the standard drug ofloxacin (MIC 10.0 µg/mL against S. aureus and 12.5 µg/mL against E. coli). In case of the antifungal activity only the compounds 9a and 9b having COOH group at 4th and 2nd positions of the phenyl ring respectively, have shown moderate activity (MIC 50 µg/mL) against fungus A. niger, as compared with the standard drug ketoconazole (MIC 12.5 µg/mL). The result have shown in table-6.

5.2.3 Result and discussion of biologically screened 1,3,4 oxadiazole derivatives of scheme-4 and scheme-5 has been explained as:

1,3,4-Oxadiazole derivatives were screened for their anti-inflammatory activity by carageenin-induced rat paw edema method of Winter et al. 2,4,6-Trichlorophenol and 4-hydroxyphenyl acetic acid were used to synthesize oxadiazole derivatives and were tested for anti-inflammatory activity.
The oxadiazole derivatives of 2,4,6-trichlorophenol (3a-n & 3q) showed anti-inflammatory activity ranging from 49.99% to 72.72% at 70mg/Kg oral dose after 4 hours, whereas the standard drug Ibuprofen showed 86.35% inhibition of rat paw edema at the same oral dose. The results have shown in table-7.

The oxadiazole derivatives 3d (Ar = 2,4-dichlorophenoxy methyl) and 3j (Ar = 1-(4-isobutylphenyl)ethyl) showed maximum anti-inflammatory activity (72.72%), and when these groups were replaced by 4-aminophenyl (3f) and 4-nitrophenyl (3h) the activity was found to be minimum (51.51% and 49.99% respectively). A good anti-inflammatory activity was also observed when aryl group at 2-position of the oxadiazole nucleus was replaced by mercapto group. Rest of the compounds showed moderate to good activity.

The oxadiazole derivatives of 4-hydroxyphenyl acetic acid (7a-j) showed anti-inflammatory activity ranging from 37.37% to 66.66% at 70mg/Kg oral dose after 4 hours, whereas the standard drug Ibuprofen showed 86.35% inhibition of rat paw edema at the same oral dose. The results have shown in table-8.

The minimum anti-inflammatory activity was found in the compound 7a having phenylamino group at 2nd position of the oxadiazole nucleus (37.37% inhibition). The substitution on the phenyl ring with small groups like chloro, fluoro, bromo, methyl etc. increases the activity. The compound 7h having methoxy group at the 4th position of the phenyl ring was found to be the most potent (66.66% inhibition) of the series. Replacement of the arylamino group at 2nd position of the oxadiazole nucleus with n-butylamino group (7i) results in a compound possessing good anti-inflammatory activity (53.53% inhibition), whereas compound with mercapto group (7j) at the 2nd position showed moderate activity in comparison with the standard drug.

5.2.4 Result and discussion of biologically screened 1,2,4 triazole derivatives of scheme-6 has been explained as:

The anti-inflammatory activity of 1,2,4-triazole derivatives was carried out by the method of Winter et al.180 4-Hydroxyphenyl acetic acid was used to synthesize triazole derivatives and were evaluated for anti-inflammatory activity.

The 1,2,4-triazole derivatives of 4-hydroxyphenyl acetic acid (8a-i) showed anti-inflammatory activity ranging from 45.45% to 68.17% inhibition at 70 mg/Kg oral dose after
4 hours, whereas the standard drug Ibuprofen showed 86.35% inhibition at the same oral dose.

The triazole derivatives having n-butyl group (8i) at the 4th position of the triazole nucleus showed maximum inhibition (68.17%). Replacement of n-butyl group with 4-bromophenyl (8b), 4-chlorophenyl (8c) and 4-methoxyphenyl (8h) results in slight decrease in the activity but when these groups were replaced with 4-methylphenyl (8f) and 2-methylphenyl (8g) groups, a marked decrease in activity have been observed. Rest of the compounds showed moderate activity. The results have shown in table-9.