CHAPTER-4 CHARACTERIZATION

4.1 CHARACTERIZATION OF OXAZOLONE COMPOUNDS.

4.1.1 Characterization of 4-benzylidene-2-(3-methylphenyl)-1,3-oxazol-5(4H)-one - {4A}

The compound the molecular formula is C_{17}H_{13}NO_2 and the molecular weight is: 263.29

Assignment of 1H- NMR Chemical shifts to different protons (Figure-4A1) All oxazolone and imidazolone compounds NMR checked in CDCl_3

The ^1H NMR signals were observed at 2.47ppm (s, 3H, - Me), 7.25-8.22ppm (m, 10H, Ar-CH and - C=CH)

Assignment of ^13C NMR Chemical shifts (δ ppm) to different carbons (Figure-4A2): The ^13C NMR signals were observed at 21.37, 125.47, 125.67,128.61, 128.82, 128.87, 128.93, 131.17, 131.57, 132.46, 133.36, 133.58, 134.29, 138.85, 163.74, 167.73ppm

Assignment of the IR spectra (Figure-4A3): Characteristics peaks are observed at 3020 (-CH stretch, aromatic), 1800 (>C=O stretch, cyclic ring), 1650 (>C=N stretch, oxazole ring), 1580 (> C=C <, aromatic), 1320(- C - O stretching)

Fragmentation of mass spectra m/z (GCMS) (Figure-4A4):

The mass spectra display the molecular ion peaks at 263.2(M^+), 234.1, 207, 119.2, 91.1, 65.1 and 39.1. The mass spectra display the molecular ion peaks at 263.2(M^+), 234.1, 207, 119.2, 91.1, 65.1 and 39.1. The compound 4a GCMS fragmentation as 4-benzylidene-2-(3-methylphenyl)-1,3-oxazol-5(4H)-one MW: 263.29, 2-(3-methylbenzylidene)amino)-3-phenylallylium MW: 234.13, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02.

The compound elemental analysis demonstrates the result as Carbon showed 77.57 % and the nitrogen showed 5.36%, The melting point of the compound is 132-137 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4A1

Figure 4A2
4.1.2 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(2-nitrobenzylidene)-1,3-oxazol-5(4H)-one-{4B}

The compound the molecular formula is C\textsubscript{17}H\textsubscript{12}N\textsubscript{2}O\textsubscript{4} and the molecular weight is: 308.08

Assignment of \textsuperscript{1}H- NMR Chemical shifts to different - protons (Figure-4B1):

The \textsuperscript{1}H NMR signals were observed at 2.47ppm (s, 3H, - Me), 7.28-8.67ppm (m, 9H, Ar-CH and -C = CH)

Assignment of \textsuperscript{13}C NMR Chemical shifts (\textdelta ppm) to different carbons (Figure-4B2):

The \textsuperscript{13}C NMR signals were observed at 21.31, 124.44, 124.88, 126, 127.86, 128.98, 129.11, 130.70, 133.06, 133.50, 134.99, 136.32, 139.03, 149.38, 165.72 and 166.45

Assignment of the IR spectra (Figure-4B3):

Characteristics peaks are observed at 3048(-CH stretch, aromatic), 1802 (>C=O stretch, cyclic ring), 1644 (>C=N stretch, oxazole ring), 1515 ( >C=C< , aromatic), 1310 (- C - O stretching), 1402 (>C=C, Stretch, cyclic ring), 1564 (-NO\textsubscript{2}), 1433 (-N=O stretch)

Proposed fragmentation pattern (GCMS) (Figure-4B4):

The mass spectra display the molecular ion peaks at 308.2(M\textsuperscript{+}), 276.2, 235.1, 207.1, 161.1, 119.2, 91.1, 65.1 and 39.1. The compound 4b GCMS fragmentation as 2-(3-methylphenyl)-4-(2-nitrobenzylidene)-1,3-oxazol-5(4H)-one MW: 308.2, 4-benzylidene-2-phenyl-4,5-dihydrooxazol-5-ylium MW: 234.09, N-benzylidyn-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 66.29 % and the nitrogen showed 9.15%

The melting point of the compound is 166-168 °C. Yield: 70 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4B1

Figure 4B2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4B3

Figure 4B4
4.1.3 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(2-chlorobenzylidene)-1,3-oxazol-5(4H)-one-(4C)

The compound the molecular formula is C_{17}H_{12}ClNO_2 and the molecular weight is: 297.73

Assignment of \(^1\)H- NMR Chemical shifts to different - protons (Figure-4C1)

The \(^1\)H NMR signals were observed at 2.50ppm (s, 3H, - Me), 7.28-8.95ppm (m, 9H, Ar-CH and -C = CH)

Assignment of \(^{13}\)C NMR Chemical shifts (\(\delta \) ppm) to different carbons (Figure-4C2): The \(^{13}\)C NMR signals were observed at 21.35, 125.26, 125.84, 126.24, 127.19, 128.93, 129.98, 131.47, 131.81, 133.32, 134.61, 136.63, 138.94, 164.7 and 167.7

Assignment of the IR spectra (Figure-4C3)

Characteristics peaks are observed at 3066 (-CH stretch, aromatic), 1803 (>C=O stretch, cyclic ring), 1657 (>C=N stretch, oxazole ring), 1550 (>C=C< , aromatic), 1321 (-C-O stretching), 1491 (>C=C, Stretch, cyclic ring), 700 (C-Cl).

Proposed fragmentation pattern (GCMS) (Figure-4C4)

The mass spectra display the molecular ion peaks at 297.1(M\(^+\)), 262.1, 233.1, 207.1, 178.1, 150, 119.2, 91.1, 65.1 and 39.1. The compound 4c GCMS fragmentation as 2-(3-methylphenyl)-4-(2-chlorobenzylidene)-1,3-oxazol-5(4H)-one MW: 297.1, 4-benzylidene-2-phenyl-4,5-dihydrooxazol-5-ylium MW: 234.09, N-benzyldyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 68.59 % and the nitrogen showed 4.75 %

The melting point of the compound is 122-145 °C. Yield: 67 %
Synthesis and Characterization of 3-Triazine and Imidazole Heterocycles

Figure 4C1

Figure 4C2
Figure 4C3

Figure 4C4
4.1.4 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(4-chlorobenzylidene -1,3-oxazol-5(4H)-one- {4D}

The compound the molecular formula is C_{17}H_{12}ClNO_{2} and the molecular weight is: 297.73

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-4D1)

The ^1H NMR signals were observed at 2.41 ppm (s, 3H, -Me), 7.10-8.10 ppm (m, 9H, Ar-CH and =C=CH)

Assignment of ^13C NMR Chemical shifts (δ ppm) to different carbons (Figure-4D2): The ^13C NMR signals were observed at 21.37, 125.31, 125.74, 128.87, 128.93, 129.26, 129.82, 132.06, 133.51, 133.71, 134.49, 137.23, 138.93, 164.08 and 167.47

Assignment of the IR spectra (Figure-4D3)

Characteristics peaks are observed at 3487 (-CH stretch, aromatic), 1817 (>C=O stretch, cyclic ring), 1646 (>C=N stretch, oxazole ring), 1581 (>C=C<, aromatic), 1299 (-C-O stretching), 1410 (>C=C, Stretch, cyclic ring), 680 (C-Cl).

Proposed fragmentation pattern (GCMS) (Figure-4D4)

The mass spectra display the molecular ion peaks at 297.1(M^+), 207.1, 177, 150, 119.2, 91.2, 65.1, 39.1. The compound 4d GCMS fragmentation as 2-(3-methylphenyl)-4-(2-chlorobenzylidene)-1,3-oxazol-5(4H)-one MW: 297.1, 4-benzylidene-2-phenyl-4,5-dihydrooxazol-5-ylium MW: 234.09, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 68.65 % and the nitrogen showed 4.75 %

The melting point of the compound is 180-183 °C. Yield: 75 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4D1

Figure 4D2
4.1.5 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(4-methoxybenzylidene)- 1,3-oxazol-5(4H)-one- {4E}

The compound the molecular formula is C_{18}H_{15}NO_{3} and the molecular weight is: 293.31

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-4E1)
The ¹H NMR signals were observed at 2.36 ppm (s, 3H, - Me), 3.80 ppm (s, 3H, - OMe), 6.93-8.09 ppm (m, 9H, Ar-CH and -C = CH)

Assignment of ¹³C NMR Chemical shifts (δ ppm) to different carbons (Figure-4E2)
The ¹³C NMR signals were observed at 21.36, 55.47, 114.54, 125.42, 125.73, 126.62, 128.58, 128.81, 131.68, 133.9, 134.56, 138.77, 162.16, 162.67 and 168.05

Assignment of the IR spectra (Figure-4E3)
Characteristics peaks are observed at 3083 (-CH stretch, aromatic), 1827 (>C=O stretch, cyclic ring), 1643 (>C=N stretch, oxazole ring), 1566 (>C=C< , aromatic), 1382 (- C - O stretching), 1409 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-4E4)
The mass spectra display the molecular ion peaks at 293.2(M⁺), 207.1, 177, 146.1, 119.2, 91.2, 65.1, 39.1. The compound 4e GCMS fragmentation as 2-(3-methylphenyl)-4-(4-methoxybenzylidene)- 1,3-oxazol-5(4H)-one MW: 293.2, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylamium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 73.79 % and the nitrogen showed 4.85 %
The melting point of the compound is 166-173 °C.
Yield: 77 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4E1

Figure 4E2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4E3

Figure 4E4
4.1.6 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(3, 4-dimethoxybenzylidene)-1, 3-oxazol-5(4H)-one- {4F}

The compound the molecular formula is C_{19}H_{17}NO_{4} and the molecular weight is: 323.34

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-4F1)
The $^1$H NMR signals were observed at 2.44ppm (s, 3H, - Me), 3.98ppm (s, 3H, - OMe), 4.05ppm (s, 3H, - OMe), 6.93-8.09ppm (m, 8H, Ar-CH and -C = CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-4F2):The $^{13}$C NMR signals were observed at 21.40, 55.87, 56.02, 110.92, 114.04, 125.25, 125.69, 126.9, 127.64, 128.55, 128.85, 131.26, 131.79, 133.92, 138.76, 149.13, 152.02, 162.6 and 167.89

Assignment of the IR spectra (Figure-4F3)
Characteristics peaks are observed at 3067 (-CH stretch, aromatic), 1814 (>C=O stretch, cyclic ring), 1638 (>C=N stretch, oxazole ring), 1515 (>C=C< , aromatic), 1398 (- C - O stretching), 1489 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-4F4)
The mass spectra display the molecular ion peaks at 323.2(M$^+$), 207.1, 176.1, 147.1, 119.2, 91.2, 65.1, 39.1. The compound 4f GCMS fragmentation as 2-(3-methylphenyl)-4-(3, 4-dimethoxybenzylidene)-1, 3-oxazol-5(4H)-one MW: 323.2, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yln-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 70.65 % and the nitrogen showed 4.39 %
The melting point of the compound is 146-149 °C.
Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4F1

Figure 4F2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4F3

Figure 4F4
4.1.7 CHARACTERIZATION OF 4-(2-methoxybenzylidene)-2-(3-methylphenyl) - 1, 3 - oxazol-5(4H) - one- {4G}

The compound the molecular formula is C\textsubscript{18}H\textsubscript{15}NO\textsubscript{3} and the molecular weight is: 293.31

**Assignment of \textsuperscript{1}H- NMR Chemical shifts to different - protons (Figure-4G1)**

The \textsuperscript{1}H NMR signals were observed at 2.34ppm (s, 3H, - Me), 3.81ppm (s, 3H, - OMe), 6.82-8.76ppm (m, 9H, Ar-CH and -C = CH)

**Assignment of \textsuperscript{13}C NMR Chemical shifts (\delta ppm) to different carbons (Figure-4G2)**

The \textsuperscript{13}C NMR signals were observed at 21.36, 55.66, 110.74, 121.02, 122.66, 125.53, 125.68, 125.72, 128.69, 128.82, 132.52, 132.92, 132.94, 134.02, 138.77, 159.26, 163.19 and 167.95

**Assignment of the IR spectra (Figure-4G3)**

Characteristics peaks are observed at 3067 (-CH stretch, aromatic), 1818 (>-C=O stretch, cyclic ring), 1653 (>-C=N stretch, oxazole ring), 1515 (>C=C< , aromatic)

**Proposed fragmentation pattern (GCMS) (Figure-4G4)**

The mass spectra display the molecular ion peaks at 293.2(M^+) , 265.2, 207.1, 177.1, 146.1, 119.2, 91.2, 65.1, 39.1. The compound \textsuperscript{4g} GCMS fragmentation as 4-(2-methoxybenzylidene)-2-(3-methylphenyl)-1,3-oxazol-5(4H)-one MW: 293.2, 4-(2-methoxybenzylidene)-2-phenyl-4,5-dihydrooxazol-5-ylium MW: 264.10 , N-benzylidyne-2- phenylethlenaminium MW: 206.10, 2-phenylethlenaminium MW: 120.08, phenethylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 73.79 % and the nitrogen showed 4.85 %

The melting point of the compound is 162-166 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4G1

Figure 4G2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4G3

Figure 4G4
4.1.8 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(4-methylbenzylidene)-1,3-oxazol-5(4H)-one - {4H}

The compound the molecular formula is C_{18}H_{15}NO_{2} and the molecular weight is: 277.31

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-4H1)
The $^1$H NMR signals were observed at 2.30ppm (s, 3H, - Me), 2.37ppm (s, 3H, - OMe), 7.12 - 8.0ppm (m, 9H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-4H2)
The $^{13}$C NMR signals were observed at 21.37, 21.83, 125.56, 125.6, 128.71, 128.84, 129.75, 130.95, 131.83, 132.52, 134.09, 138.80, 142.05, 163.20 and 167.89

Assignment of the IR spectra (Figure-4H3)
Characteristics peaks are observed at 3053 (-CH stretch, aromatic), 1804 (>C=O stretch, cyclic ring), 1647 (>C=N stretch, oxazole ring), 1550 (>C=C<, aromatic), 1491 (>C=C, Stretch, cyclic ring), 1475 (-methyl group)

Proposed fragmentation pattern (GCMS) (Figure-4H4)
The mass spectra display the molecular ion peaks at 277.2(M+), 232.2, 207.1, 178.1, 152.1, 119.2, 91.2, 65.1, 39.1. The compound 4h GCMS fragmentation as 2-(3-methylphenyl)-4-(4-methylbenzylidene)-1,3-oxazol-5(4H)-one MW: 277.2, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 77.99 % and the nitrogen showed 5.16 %
The melting point of the compound is 157-161 °C.
Yield: 68 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4H1

Figure 4H2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4H3

Figure 4H4
4.1.9 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(3-bromobenzylidene)-1,3-oxazol-5(4H)-one- {4I}

The compound the molecular formula is C_{17}H_{12}BrNO_{2} and the molecular weight is: 342.18

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-4I1)

The 1H NMR signals were observed at 2.48ppm (s, 3H, - Me), 7.11-8.40ppm (m, 9H, Ar-CH and -C = CH)

Assignment of 13C NMR Chemical shifts (δ ppm) to different carbons (Figure-4I2): The 13C NMR signals were observed at 21.37, 122.93, 125.15, 125.84, 128.94, 128.96, 129.23, 130.31, 130.81, 133.75, 134.37, 134.62, 134.75, 135.46, 138.92, 164.43 and 167.22

Assignment of the IR spectra (Figure-4I3)

Characteristics peaks are observed at 3067 (-CH stretch, aromatic), 1803 (>C=O stretch, cyclic ring), 1643 (>C=N stretch, oxazole ring), 1581 (> C=C < , aromatic), 1312 (-C - O stretching), 1410 ( >C=C, Stretch, cyclic ring), 694 (C-Br stretch, aromatic)

Proposed fragmentation pattern (GCMS) (Figure-4I4)

The mass spectra display the molecular ion peaks at 343.1(M^+), 233.1, 207.1, 167.0, 143, 119.2, 91.2, 65.1, 39.1. The compound 4I GCMS fragmentation as 2-(3-methylphenyl)-4-(3-bromobenzylidene)-1,3-oxazol-5(4H)-one MW: 342.1, 4-benzylidene-2-phenyl-4,5-dihydrooxazol-5-ylium MW: 234.09, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 59.75 % and the nitrogen showed 4.11 %
The melting point of the compound is 147-150 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4I1

Figure 4I2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4I3

Figure 4I4
The compound the molecular formula is $C_{20}H_{19}NO_5$ and the molecular weight is: 353.36

**Assignment of $^1$H- NMR Chemical shifts to different - protons (Figure-4J1)**

The $^1$H NMR signals were observed at 2.36ppm (s, 3H, - Me), 3.90ppm (s, 9H, - OMe), 7.07-7.85ppm (m, 7H, Ar-CH and -C = CH)

**Assignment of $^{13}$C NMR Chemical shifts ($\delta$ ppm) to different carbons (Figure-4J2)**

The $^{13}$C NMR signals were observed at 21.37, 56.15, 61.09, 109.77, 125.34, 125.5, 128.68, 128.92, 128.94, 131.48, 132.43, 134.17, 138.82, 141.12, 153.2, 163.27 and 167.64

**Assignment of the IR spectra (Figure-4J3)**

Characteristics peaks are observed at 3048 (-CH stretch, aromatic), 1801 (>C=O stretch, cyclic ring), 1638 (>C=N stretch, oxazole ring), 1566 (>C=C< , aromatic), 1311 (- C - O stretching), 1409 (>C=C, Stretch, cyclic ring)

**Proposed fragmentation pattern (GCMS) (Figure-4J4)**

The mass spectra display the molecular ion peaks at 353.2($M^+$), 308.1, 281.1, 206.1, 173.1, 146.1, 119.2, 91.2, 65.1, 39.1. The compound 4j GCMS fragmentation as 2-(3-methylphenyl)-4-(3,4,5-trimethoxy- benzylidene)-1,3-oxazol-5(4h)-one MW: 353.6, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 68.05 % and the nitrogen showed 3.99 %

The melting point of the compound is 133-136 °C.

Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4J1

Figure 4J2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 4J3

Figure 4J4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.1.11 CHARACTERIZATION OF 4-benzylidene-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one - {7A}

The compound the molecular formula is C₁₆H₁₀ClNO₂ and the molecular weight is: 283.70

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-7A1)
The ¹H NMR signals were observed at 7.20-8.11ppm (m, 10H, Ar-CH and -C = CH)

Assignment of ¹³C NMR Chemical shifts (δ ppm) to different carbons (Figure-7A2)
The ¹³C NMR signals were observed at 124.09, 128.98, 129.43, 129.60, 131.42, 132.35, 132.54, 133.03, 133.42, 139.83, 162.68 and 167.38

Assignment of the IR spectra (Figure-7A3)
Characteristics peaks are observed at 3050 (-CH stretch, aromatic), 1800 (>C=O stretch, cyclic ring), 1640 (~C=N stretch, oxazole ring), 1500 (~C=C<, aromatic), 1310(- C - O stretching), 750 (-C-Cl)

Fragmentation of mass spectra m/z (GCMS) (Figure-7A4)
The mass spectra display the molecular ion peaks at 283.1(M⁺), 207.1, 139.1, 111.1, 75.1, 39.1. The compound 7a GCMS fragmentation as 4-benzylidene-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one MW: 283.70, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylium MW: 206.00, (4-chlorobenzylidyne) ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 67.76 % and the nitrogen showed 4.96 %
The melting point of the compound is 180-183 °C. Yield: 76 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7A1

Figure 7A2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7A3

Figure 7A4
4.1.12 CHARACTERIZATION OF 4-(2-nitrobenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one -{7B}

The compound the molecular formula is C\textsubscript{19}H\textsubscript{9}ClN\textsubscript{2}O\textsubscript{4} and the molecular weight is: 328.70

Assignment of \textsuperscript{1}H NMR Chemical shifts to different - protons (Figure-7B1)
The \textsuperscript{1}H NMR signals were observed at 7.27-8.62ppm (m, 9H, Ar-CH and -C = CH)

Assignment of \textsuperscript{13}C NMR Chemical shifts (δ ppm) to different carbons (Figure-7B2): The \textsuperscript{13}C NMR signals were observed at 123.55, 124.98, 125.48, 127.78, 129.56, 129.94, 130.88, 133.06, 133.46, 136.04, 140.61, 149.41, 164.67 and 166.1

Assignment of the IR spectra (Figure-7B3)
Characteristics peaks are observed at 3048 (-CH stretch, aromatic), 1802 (\(\text{>C}=\text{O}\) stretch, cyclic ring), 1649 (\(\text{>C}=\text{N}\) stretch, oxazole ring), 1516 (\(\text{>C}=\text{C}<\), aromatic), 1310 (-C – O – stretching), 750 (-C-Cl), 1402 (\(\text{>C}=\text{C}<\), Stretch, cyclic ring), 1565 (-\(\text{NO}_2\)), 1439 (-\(\text{N}=\text{O}\) stretch), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-7B4)
The mass spectra display the molecular ion peaks at 327.9(M\textsuperscript{+}), 280.9, 248.2, 207.1, 181.8, 161, 139, 111,75.1, 50.1. The compound 7b GCMS fragmentation as 4-(2-nitrobenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one MW: 328.70, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) (phenyl) methylium MW: 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylium MW: 206.00, (4-chlorobenzylidyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 58.49 % and the nitrogen showed 5.54 %
The melting point of the compound is 228-230 °C. Yield: 74 %
Figure 7B 1

Figure 7B 2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
The compound the molecular formula is C_{16}H_{9}Cl_{2}NO_{2} and the molecular weight is: 318.15

**Assignment of 1H- NMR Chemical shifts to different - protons (Figure-7C1)**
The $^1$H NMR signals were observed at 7.19-8.81 ppm (m, 10H, Ar-CH and -C= CH)

**Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-7C2)**
The $^{13}$C NMR signals were observed at 123.86, 127.01, 127.20, 129.50, 129.76, 130.06, 131.32, 132.06, 133.30, 134.28, 136.79, 140.19, 163.62 and 166.95

**Assignment of the IR spectra (Figure-7C3)**
Characteristics peaks are observed at 3068 (-CH stretch, aromatic), 1805 (>C=O stretch, cyclic ring), 1652 (>C=N stretch, oxazole ring), 1550 (>C=C<, aromatic), 812 (-C-Cl), 1491 (>C=C, Stretch, cyclic ring), 750 (-C-Cl)

**Proposed fragmentation pattern (GCMS) (Figure-7C4)**
The mass spectra display the molecular ion peaks at 317.1(M$^+$), 282.1, 253.1, 207.1, 177.1, 139.1, 111.1, 75.1, 50.1. The compound 7c GCMS fragmentation as 2-(4-chlorophenyl)-4-(2-chlorobenzylidene)-1,3-oxazol-5(4H)-one MW: 317.1, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) (phenyl)methylum MW: 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylium MW: 206.00, (4-chlorobenzylidyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 60.44 % and the nitrogen showed 4.44 %
The melting point of the compound is 226-230 °C. Yield: 73 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7C 3

Figure 7C 4
The compound the molecular formula is C_{16}H_{10}ClNO_2 and the molecular weight is: 318.15

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-7D1)
The 1H NMR signals were observed at 7.14-8.06 ppm (m, 10H, Ar-CH and -C= CH)

Assignment of 13C NMR Chemical shifts (δ ppm) to different carbons (Figure-7D2): The 13C NMR signals were observed at 123.93, 129.31, 129.48, 129.66, 130.57, 131.90, 133.39, 133.57, 137.51, 140.06, 163.02 and 167.33

Assignment of the IR spectra (Figure-7D3)
Characteristics peaks are observed at 3082 (-CH stretch, aromatic), 1815 (>C=O stretch, cyclic ring), 1649 (>C=N stretch, oxazole ring), 1580 (>C=C<, aromatic), 1299 (- C - O stretching), 639(-C-Cl), 1409 (>C=C, Stretch, cyclic ring), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-7D4)
The mass spectra display the molecular ion peaks at 317(M+), 281.1, 249.1, 207, 176.2, 139, 111,75.1, 39.1. The compound 7d GCMS fragmentation as 2-(4-chlorophenyl)-4-(4-chlorobenzylidene)-1,3-oxazol-5(4H)-one MW: 317, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene)(phenyl)methylum MW: 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylum MW: 206.00, (4-chlorobenzylidyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylum MW: 110.96, hexa-1,3,5-triyn-1-ylum MW: 73.01, buta-1,3-diyn-1-ylum MW: 49.01, prop-2-yn-1-ylum MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 60.44 % and the nitrogen showed 4.44 %
The melting point of the compound is 226-230 °C. Yield: 67 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7D 1

Figure 7D 2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7D 3

Figure 7D 4
4.1.15 CHARACTERIZATION OF 4-(4-methoxybenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one - {7E}

The compound the molecular formula is C_{17}H_{12}ClNO_{3} and the molecular weight is: 313.73

Assignment of 1H NMR Chemical shifts (δ ppm) to different protons (Figure-7E1): The 1H NMR signals were observed at 3.81ppm (s, 3H, -methoxy), 6.94-8.10 ppm (m, 9H, Ar-CH and -C= CH)

Assignment of 13C NMR Chemical shifts (δ ppm) to different carbons (Figure-7E2): The 13C NMR signals were observed at 55.51, 114.58, 124.34, 126.46, 129.35, 130.83, 132.43, 134.69, 139.36, 161.54, 162.35 and 167.71

Assignment of the IR spectra (Figure-7E3)

Characteristics peaks are observed at 3482 (-CH stretch, aromatic), 1821 (>C=O stretch, cyclic ring), 1641 (>C=N stretch, oxazole ring), 1566 (>C=C< , aromatic),765 (-C-Cl), 1409 (>C=C, Stretch, cyclic ring), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-7E4)

The mass spectra display the molecular ion peaks at 313.2(M^{+}), 281.1, 254.1, 207.1, 177.1, 139.2, 111.1,75.2, 39.2. The compound 7e GCMS fragmentation as 4-(4-methoxybenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one MW: 313.2, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene)(phenyl)methylmum MW: 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene)methylmum MW: 206.00, (4-chlorobenzylidyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 65.09 % and the nitrogen showed 4.49 %
The melting point of the compound is 178-182 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7E 1

Figure 7E 2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7E 3

Figure 7E 4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.1.16 CHARACTERIZATION OF 4-(3,4 dimethoxybenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one {7F}

The compound the molecular formula is C_{18}H_{14}ClNO_{4} and the molecular weight is: 343.76

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-7F1)

The ^1H NMR signals were observed at 3.88ppm (s, 3H, -methoxy), 3.94ppm (s, 3H, -methoxy), 6.87-8.02ppm (m, 8H, Ar-CH and - C= CH)

Assignment of ^13C NMR Chemical shifts (δ ppm) to different carbons (Figure-7F2): The ^13C NMR signals were observed at 55.91, 56.06, 110.92, 113.94, 124.28, 126.72, 127.90, 129.40, 130.88, 132.58, 139.41, 149.15, 152.24, 161.51 and 167.57

Assignment of the IR spectra (Figure-7F3): Characteristics peaks are observed at 3065 (-CH stretch, aromatic), 1814 (>C=O stretch, cyclic ring), 1369 (>C=N stretch, oxazole ring), 1514 (>C=C< , -aromatic), 1298 (-C–O stretching), 809 (-C–Cl), 1489 (>C=C, Stretch, cyclic ring), 750 (-C–Cl)

Proposed fragmentation pattern (LCMS) (Figure-7F4): The mass spectra display the molecular ion peaks at 343.1(M^+), 313.1, 281.1, 252.1, 207.1, 176.1, 139, 111,75.1, 50.1. The compound 7f GCMS fragmentation as 4-(3,4-dimethoxybenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one MW: 343.1, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene)(phenyl)methylium MW: 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylium MW: 206.00, (4-chlorobenzylidyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 62.92 % and the nitrogen showed 4.09 %

The melting point of the compound is 205-208 °C. Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7F 1

Figure 7F 2
Synthesis and Characterization of $\text{a-Triazine}$ and Imidazole Heterocycles

**Figure 7F 3**

**Figure 7F 4**
4.1.17 CHARACTERIZATION OF 4-(2-methoxybenzylidene) - 2-(4-chlorophenyl) - 1,3-oxazol - 5(4H) - one - {7G}

The compound the molecular formula is $C_{17}H_{12}ClNO_3$ and the molecular weight is: 313.73

**Assignment of 1H- NMR Chemical shifts to different - protons (Figure-7G1)**

The $^1$H NMR signals were observed at 3.93ppm (s, 3H, -methoxy), 6.98-8.84ppm (m, 9H, Ar-CH and - C= CH)

**Assignment of 13C NMR Chemical shifts (δ ppm) to different carbons (Figure-7G2):** The $^{13}$C NMR signals were observed at 55.69, 110.82, 121.02, 122.53, 124.32, 126.53, 129.47, 132.19, 132.90, 133.22, 139.51, 159.38, 162.12 and 167.61

**Assignment of the IR spectra (Figure-7G3)**

Characteristics peaks are observed at 3050 (-CH stretch, aromatic), 1810 (>C=O stretch, cyclic ring), 1652 (>C=N stretch, oxazole ring), 777 (-C-Cl)

**Proposed fragmentation pattern (LCMS) (Figure-7G4)**

The mass spectra display the molecular ion peaks at 313.1(M$^+$), 281.1, 248.9, 207.1, 176.1, 139.1, 111.1, 75.1, 50.1, 39.1. The compound 7g GCMS fragmentation as 4-(2-methoxybenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one MW: 313.1, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene)(phenyl)methylium MW: 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylium MW: 206.00, (4-chlorobenzylidyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 65.12 % and the nitrogen showed 4.49 %

The melting point of the compound is 178-182 °C. Yield: 73 %

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Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7G 1

Figure 7G 2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7G 3

Figure 7G 4
4.1.18 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(4-methylbenzylidene)-1,3-oxazol-5(4H)-one - {7H}

The compound the molecular formula is C_{17}H_{12}ClNO_{2} and the molecular weight is: 297.73

Assignment of 1H- NMR Chemical shifts to different - protons (Figure-7H1)
The 1H NMR signals were observed at 2.35ppm (s, 3H, -methyl), 7.13-8.00ppm (m, 9H, Ar-CH and - C= CH)

Assignment of 13C NMR Chemical shifts (δ ppm) to different carbons (Figure-7H2): The 13C NMR signals were observed at 13C NMR(CDCl_{3}): 21.85, 124.23, 129.37, 129.49, 129.79, 130.80, 132.18, 132.6, 139.6, 142.36, 162.12 and 167.52

Assignment of the IR spectra (Figure-7H3 ): Characteristics peaks are observed at 3055 (-CH stretch, aromatic), 1809 (>C=O stretch, cyclic ring), 1649 (>C=N stretch, oxazole ring), 1550 (>C=C< , aromatic), 754 (-C-Cl), 1491 (>C=C, Stretch, cyclic ring), 1475 (-methyl group), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-7H4)
The mass spectra display the molecular ion peaks at 297.2(M^+), 253.1, 207.1, 178.2, 139.1, 111.2,75.2, 50.1, 39.2. The compound 7h GCMS fragmentation as 2-(4-chlorophenyl)-4-(4-methylbenzylidene)-1,3-oxazol-5(4H)-one MW: 297.2, (2-((4-chlorobenzoyl)imino)-1-phenylethen-1-ylium MW: 254.04, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylium MW: 206.00, (4-chlorobenzylidyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yln-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 68.62 % and the nitrogen showed 4.72 %
The melting point of the compound is 201-205 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7H1

Figure 7H2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7H3

Figure 7H4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

**4.1.19 CHARACTERIZATION OF 4-(3-bromobenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one-{7I}**

The compound the molecular formula is $\text{C}_{16}\text{H}_9\text{BrClNO}_2$ and the molecular weight is: 362.60

**Assignment of $^1$H- NMR Chemical shifts to different - protons (Figure-7I1)**

The $^1$H NMR signals were observed at 7.07-8.32ppm (m, 9H, Ar-CH and - C=CH)

**Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-7I2):** The $^{13}$C NMR signals were observed at 123, 123.77, 129.51, 129.76, 130.03, 130.36, 130.92, 134.0, 134.07, 134.8, 135.3, 140.22, 163.41 and 166.89

**Assignment of the IR spectra (Figure-7I3):** Characteristics peaks are observed at 3064(-CH stretch, aromatic), 1802 (>C=O stretch, cyclic ring), 1641 ( >C=N stretch, oxazole ring), 1581 ( >C = C< , aromatic), 1312 (-C–O, -stretching), 654 (-C-Cl), 1409 ( >C=C–, Stretch, cyclic ring), 690 (C-Br stretch, aromatic), 750 (-C-Cl)

**Proposed fragmentation pattern (LCMS) (Figure-7I4)**

The mass spectra display the molecular ion peaks at 363(M$^+$), 313.1, 281.1, 194, 167, 139, 111.75, 50, 39.1. The compound 7I GCMS fragmentation as 4-(3-bromobenzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one MW: 363, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene)(phenyl)methylonium MW : 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylonium MW: 206.00, (4-chlorobenzylidylyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylium MW: 110.96, hexa-1,3,5-triyn-1-ylium MW: 73.01, buta-1,3-diyn-1-ylium MW: 49.01, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 53.05 % and the nitrogen showed 3.89 %

The melting point of the compound is 181-185 °C. Yield: 67 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 7I3

Figure 7I4
The compound the molecular formula is C_{19}H_{16}ClNO_5 and the molecular weight is 373.78

**Assignment of 1H- NMR Chemical shifts to different - protons (Figure-7J1)**

The \(^1\)H NMR signals were observed at 3.89 ppm (s, 9H, -methoxy), 7.07-7.95 ppm (m, 7H, Ar-CH and - C= CH)

**Assignment of \(^{13}\)C NMR Chemical shifts (δ ppm) to different carbons (Figure-7J2):**

The \(^{13}\)C NMR signals were observed at 56.19, 61.12, 109.83, 124.10, 128.75, 129.31, 129.48, 132.06, 132.28, 139.72, 141.34, 153.23, 162.21 and 167.32

**Assignment of the IR spectra (Figure-7J3) :** Characteristics peaks are observed at 3045 (-CH stretch, aromatic), 1801 (\(>\)C=O stretch, cyclic ring), 1639 (\(>\)C=N stretch, oxazole ring), 1566 (\(>\)C=C\(\_\) , -aromatic), 1311 (-C-O , -stretching), 654 (-C-Cl), 1409 (\(>\)C=C, Stretch, cyclic ring), 750 (-C-Cl)

**Proposed fragmentation pattern (LCMS) (Figure-7J4):** The mass spectra display the molecular ion peaks at 373.1(M^+), 341.1, 311.2, 281.1, 206.2, 173.1, 139, 111,75.1, 50.1. The compound 7j GCMS fragmentation as 4-(3,4,5-trimethoxy-benzylidene)-2-(4-chlorophenyl)-1,3-oxazol-5(4H)-one MW: 373.1, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) (phenyl)methylammonium MW: 282.03, (2-(4-chlorophenyl)-5-oxooxazol-4(5H)-ylidene) methylammonium MW: 206.00, (4-chlorobenzyldyne)ammonium MW: 138.01, 1-chloro-5-oxopenta-1,2,3,4-tetraen-1-ylum MW: 110.96, hexa-1,3,5-triyn-1-ylum MW: 73.01, buta-1,3-diyn-1-ylum MW: 49.01, prop-2-yn-1-ylum MW: 39.02

**The compound elemental analysis demonstrates the result as**

Carbon showed 61.06 % and the nitrogen showed 3.76 %

The melting point of the compound is 186-190 °C. Yield: 70 %
Figure 7J1

Figure 7J2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

**Figure 7J3**

**Figure 7J4**
4.2. CHARACTERIZATION OF IMIDAZOLONE COMPOUNDS.

4.2.1 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(benzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one- {5A}

The compound the molecular formula is C_{24}H_{20}N_{2}O and the molecular weight is: 352.42

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-5A1): The $^1$H NMR signals were observed at 2.25ppm (s, 3H, - Me), 2.31ppm (s, 3H, - Me), 6.97-8.22ppm (m,14H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-5A2): The $^{13}$C NMR signals were observed at $^{13}$C NMR(CDCl$_3$) δ(ppm): 21.25, 21.41,126.42, 127.13, 128.05, 128.80, 129.03, 129.89, 130.40, 132.11, 132.19, 132.60, 134.45, 138.25, 138.34, 138.69, 160.96 and 170.80

Assignment of the IR spectra (Figure-5A3)

Characteristics peaks are observed at 3000 (-CH stretch, aromatic), 1720 (>C=O stretch, cyclic ring), 1620 (>C=N stretch, imidazole ring), 1510 (>C=C<, aromatic), 1250(-C-N tertiary amine)

Fragmentation of mass spectra m/z (GCMS) (Figure-5A4)

The mass spectra display the molecular ion peaks at 352.2 (M$^+$), 261.1, 208.1, 165.1, 119.1, 91.1, 65.1, 39.1. The compound 5a GCMS fragmentation as 2-(3-methylphenyl)-4-(benzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 352.2, (5-(5-(cyclohexa-2,4-dien-1-ylidenemethyl)-4-oxo-4H-imidazol-2-yl)cyclohexa-2,4-dien-1-ylidene)methylum MW: 261.10, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 81.82 % and the nitrogen showed 7.96 %
The melting point of the compound is 208-212 °C. Yield: 68 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5A1

Figure 5A2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5A3

Figure 5A4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.2 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(2-nitrobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one - {5B}

The compound the molecular formula is C_{24}H_{19}N_{3}O_{3} and The molecular weight is: 397.42

Assignment of \(^1\)H NMR Chemical shifts (δ ppm) to different protons (Figure-5B1) : The \(^1\)H NMR signals were observed at 2.23ppm (s, 3H, - Me), 2.31ppm (s, 3H, - Me), 6.99-8.65ppm (m,13H, Ar-CH and - C= CH)

Assignment of \(^{13}\)C NMR Chemical shifts (δ ppm) to different carbons (Figure-5B2) : The \(^{13}\)C NMR signals were observed at 21.26, 21.38, 119.77, 122.10, 124.74, 126.52, 127.06, 128.15, 128.31, 128.90, 129.56, 129.8, 129.93, 129.95, 130.11, 131.68, 132.71, 132.92, 133.99, 138.39, 138.61, 141.15, 149.63, 163.34 and 170.02

Assignment of the IR spectra (Figure-5B3)
Characteristics peaks are observed at 2925 (-CH stretch, aromatic), 1718 (>C=O stretch, cyclic ring), 1620 (>C=N stretch, imidazole ring), 1518 (>C=C< , aromatic), 1313 (-C - O stretching), 1293 (-C-N tertiary amine), 1411 (>C=C, Stretch, cyclic ring), 1565 (-NO\(_2\)), 1439 (-N=O stretch)

Proposed fragmentation pattern (GCMS) (Figure-5B4)
The mass spectra display the molecular ion peaks at 396.1(M\(^{+}\)), 354.9, 327, 280.9, 236.1, 207.1, 165, 132, 104, 77, 50.9. The compound 5b GCMS fragmentation as 2-(3-methylphenyl)-4-(2-nitrobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 397.42, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 72.56 % and the nitrogen showed 10.59 %
The melting point of the compound is 165-169 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5B1

Figure 5B2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5B3

Figure 5B4
The compound the molecular formula is $C_{24}H_{19}ClN_2O$ and the molecular weight is: 386.87

**Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-5C1):**
The $^1$H NMR signals were observed at 2.25ppm (s, 3H, - Me), 2.31ppm (s, 3H, - Me), 6.99-8.95ppm (m, 13H, Ar-CH and - C= CH)

**Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-5C2):**
The $^{13}$C NMR signals were observed at 21.26, 21.40, 123.7, 126.47, 127.08, 127.11, 128.09, 128.62, 129.81, 129.91, 130.06, 131.0, 131.96, 132.34, 132.41, 133.76, 136.52, 138.30, 138.42, 139.82, 163.10 and 170.50

**Assignment of the IR spectra (Figure-5C3):**
Characteristics peaks are observed at 2926 (-CH stretch, aromatic), 1716 (>C=O stretch, cyclic ring), 1638 (>C=N stretch, imidazole ring), 1544 (>C=C<, -aromatic), 1298 (-C=O stretching), 1403 (>C=C, Stretch, cyclic ring), 750 (-C-Cl)

**Proposed fragmentation pattern (GCMS) (Figure-5C4):**
The mass spectra display the molecular ion peaks at 386.2(M$^+$), 351.2, 208.2, 175.3, 119.1, 91.1, 65.1, 39.1. The compound 5c GCMS fragmentation as 2-(3-methylphenyl)-4-(2-chlorobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 386.87, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The mass spectra display the molecular ion peaks at 386.2(M$^+$), 351.2, 208.2, 175.3, 119.1, 91.1, 65.1, 39.1. The compound 5c GCMS fragmentation as 2-(3-methylphenyl)-4-(2-chlorobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 386.87, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

**The compound elemental analysis demonstrates the result as:**
Carbon showed 74.55 % and the nitrogen showed 7.26 %
The melting point of the compound is 182-186 °C.

Yield: 74 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5C1

Figure 5C2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5C3

Figure 5C4
4.2.4 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(4-chlorobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one - {5D}

The compound the molecular formula is C_{24}H_{19}ClN_{2}O and the molecular weight is: 386.87

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-5D1): The $^1$H NMR signals were observed at 2.25ppm (s, 3H, - Me), 2.31ppm (s, 3H, - Me), 6.96-8.14ppm (m,13H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-5D2): The $^{13}$C NMR signals were observed at 21.24, 21.40, 126.42, 127.1, 127.25, 128.10, 128.64, 129.08, 129.87, 130.06, 131.98, 132.34, 132.96, 133.66, 136.34, 138.31, 138.44, 138.98, 161.33 and 170.63

Assignment of the IR spectra (Figure-5D3)
Characteristics peaks are observed at 2900 (-CH stretch, aromatic), 1779 (>C=O stretch, cyclic ring), 1640 (>C=N stretch, imidazole ring), 1518 (>C=C <, -aromatic), 1395 (-C-O stretching), 1280 (-C-N tertiary amine), 1491 (>C=C<, Stretch, cyclic ring), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-5D4)
The mass spectra display the molecular ion peaks at 386.2(M$^+$), 351.2, 208.2, 178.1,150.1, 119, 91.1, 65.1, 39.1. The compound 5d GCMS fragmentation as 2-(3-methylphenyl)-4-(4-chlorobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 386.87, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 74.55 % and the nitrogen showed 7.26 %
The melting point of the compound is 188-192 °C.
Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5D3

Figure 5D4
4.2.5 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(4-methoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one- {5E}

The compound the molecular formula is C_{25}H_{22}N_{2}O_{2} and the molecular weight is: 382.45

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-5E1): The $^1$H NMR signals were observed at 2.24ppm (s, 3H, - Me), 2.30ppm (s, 3H, - Me), 3.79ppm (s, 3H, –OMe), and 6.90-8.20ppm (m,13H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-5E2): The $^{13}$C NMR signals were observed at 21.25, 21.42, 55.42, 114.40, 114.55, 125.43, 126.31, 127.15, 127.46, 128.01, 129.01,129.14, 129.42, 129.78, 129.99, 131.72, 131.91, 132.27, 133.93, 134.59, 136.88, 138.19, 159.68, 161.57, 162.17 and 170.78

Assignment of the IR spectra (Figure-5E3): Characteristics peaks are observed at 2924(-CH stretch, aromatic), 1717 (>C=O stretch, cyclic ring), 1642 (>C=N stretch, imidazole ring), 1517 (>C=C< , -aromatic), 1343 (-C– O stretching), 1279 (-C-N tertiary amine), 1409 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-5E4)
The mass spectra display the molecular ion peaks at 382.1(M$^+$), 208.2, 174.1,146.1, 119, 91, 65, 39. The compound 5e GCMS fragmentation as 2-(3-methylphenyl)-4-(4-methoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 382.45, N-benzyldidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylum MW: 65.04 , prop-2-yn-1-ylum MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 78.56 % and the nitrogen showed 7.36 %
The melting point of the compound is 168-172 °C. Yield: 67 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5E1

Figure 5E2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5E3

Figure 5E4
4.2.6 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(3,4-dimethoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one - {5F}

The compound the molecular formula is $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_3$ and the molecular weight is: 412.48

Assignment of $^1$H NMR Chemical shifts ($\delta$ ppm) to different protons (Figure-5F1) : The $^1$H NMR signals were observed at 2.21ppm (s, 3H, –methyl), 2.30ppm (s, 3H, –Me), 3.87ppm (s, 3H, - Me), 3.93ppm (s, 3H, - OMe), and 6.87-8.21ppm (m,12H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts ($\delta$ ppm) to different carbons (Figure-5F2) : The $^{13}$C NMR signals were observed at 21.25, 21.42, 55.82, 55.98, 110.90, 114.44, 126.18, 127.18, 127.42, 127.80, 128.06, 129.02, 129.18, 129.74, 130.03, 131.92, 132.29, 137.01, 138.09, 138.28, 149.01, 151.36, 159.36 and 170.75

Assignment of the IR spectra (Figure-5F3) : Characteristics peaks are observed at 2924 (-CH stretch, aromatic), 1647 (>C=O stretch, cyclic ring), 1559 (>C=N stretch, imidazole ring), 1280(-C-N tertiary amine), 1409 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-5F4) : The mass spectra display the molecular ion peaks at 412.1(M$^+$), 382, 355, 325.1, 281.1, 228.1, 193, 165, 139, 91, 65, 39. The compound 5f GCMS fragmentation as 2-(3-methylphenyl)-4-(3,4-dimethoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 412.48, N-benzyldyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethyl, MW: 91.05, cyclopenta-2,4-dien-1-ylum MW: 65.04 , prop-2-yn-1-ylum MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 75.73 % and the nitrogen showed 6.81 %

The melting point of the compound is 194-197 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5F1

Figure 5F2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5F3

Figure 5F4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.7 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(2-methoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one- {5g}

The compound the molecular formula is \( \text{C}_{25}\text{H}_{22}\text{N}_{2}\text{O}_{2} \) and the molecular weight is: 382.45

Assignment of \(^1\text{H}\) NMR Chemical shifts (\( \delta \) ppm) to different protons (Figure-5G1): The \(^1\text{H}\) NMR signals were observed at 2.23ppm (s, 3H, - Me), 2.30ppm (s, 3H, - Me), 3.82ppm (s, 3H, - OMe), and 6.84-8.90ppm (m,13H, Ar-CH and - C= CH)

Assignment of \(^{13}\text{C}\) NMR Chemical shifts (\( \delta \) ppm) to different carbons (Figure-5G2): The \(^{13}\text{C}\) NMR signals were observed at 21.24, 21.40, 55.62, 110.63, 120.97, 123.12, 123.51, 126.36, 127.17, 128, 129, 129.84, 129.98, 131.97, 132.03, 132.28, 133.35, 138.14, 138.16, 138.18, 159.35, 160.34 and 170.72

Assignment of the IR spectra (Figure-5G3): Characteristics peaks are observed at 2927 (-CH stretch, aromatic), 1770 (>C=O stretch, cyclic ring), 1648 (>C=N stretch, imidazole ring), 1581 ( >C=C< , -aromatic), 1349 (-C-O -stretching), 1291 (-C-N tertiary amine), 1490 ( >C=C< , Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-5F4)

The mass spectra display the molecular ion peaks at 412.1(M\(^{+}\)), 382, 355, 325.1, 281.1, 228.1, 193, 165, 139, 91, 65, 39. The compound \( 5g \) GCMS fragmentation as 2-(3-methylphenyl)-4-(2-methoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 382.45 , N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 75.73 % and the nitrogen showed 6.81 %

The melting point of the compound is 194-197 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5G3

Figure 5G4
4.2.8 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(4-methylbenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one- {5H}

The compound the molecular formula is $\text{C}_{25}\text{H}_{22}\text{N}_2\text{O}$ and the molecular weight is: 366.45

Assignment of $^1$H NMR Chemical shifts ($\delta$ ppm) to different protons (Figure-5H1): The $^1$H NMR signals were observed at 2.24 ppm (s, 3H, - Me), 2.30 ppm (s, 3H, - Me), 2.33 ppm (s, 3H, - Me), 6.98-8.10 ppm (m, 13H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts ($\delta$ ppm) to different carbons (Figure-5H2): The $^{13}$C NMR signals were observed at 21.24, 21.41, 21.78, 126.37, 127.14, 128.03, 128.92, 129.30, 129.62, 129.85, 130.01, 131.78, 132.04, 132.20, 132.65, 137.99, 138.21, 138.25, 141.08, 160.33 and 170.81

Assignment of the IR spectra (Figure-5H3)

Characteristics peaks are observed at 2928 (-CH stretch, aromatic), 1729 (>C=O stretch, cyclic ring), 1729 (>C=N stretch, imidazole ring), 1569 (>C=C<, aromatic), 1359 (- C - O stretching), 692 (-methyl group )

Proposed fragmentation pattern (GCMS) (Figure-5H4)

The mass spectra display the molecular ion peaks at 366.3 (M$^+$), 337.2, 307.1, 275.1, 247.1, 208.2, 165.1, 119.1, 91.1, 65.1, 39.1. The compound 5h GCMS fragmentation as 2-(3-methylphenyl)-4-(4-methylbenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 366.45, N-benzyldyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 81.95 % and the nitrogen showed 7.66 %

The melting point of the compound is 188-191 °C. Yield: 68 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5H1

Figure 5H2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5H3

Figure 5H4
4.2.9 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(3-bromobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one- {5I}

The compound the molecular formula is C$_{24}$H$_{19}$BrN$_{2}$O and The molecular weight is: 431.32

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-5I1):
The $^1$H NMR signals were observed at 2.23ppm (s, 3H, - Me), 2.30ppm (s, 3H, - Me), 6.96-8.36ppm (m,13H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-5I2):
The $^{13}$C NMR signals were observed at 21.26, 21.42, 122.79, 126.5, 126.71, 127.11, 128.13, 128.52, 129.98, 130.08, 130.22, 130.95, 131.96, 132.46, 133, 134.93, 136.47, 138.29, 138.48, 139.6, 161.76 and 170.58

Assignment of the IR spectra (Figure-5I3):
Characteristics peaks are observed at 2964 (-CH stretch, aromatic), 1717 (>C=O stretch, cyclic ring), 1512 ( >C=C<, aromatic), 1312 ( - C - O stretching), 1290 (-C-N tertiary amine), 1491 (>C=C, Stretch, cyclic ring), 692 (C-Br stretch, aromatic)

Proposed fragmentation pattern (GCMS) (Figure-5I4):
The mass spectra display the molecular ion peaks at 432(M$^+$), 351, 208.1, 168, 119, 91.1, 65, 39. The compound 5I GCMS fragmentation as 2-(3-methylphenyl)-4-(3-bromobenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 431.32 , N-benzyldiyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 66.85 % and the nitrogen showed 6.51 %
The melting point of the compound is 168-172 °C. Yield: 74 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5I1

Figure 5I2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5I3

Figure 5I4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.10 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(3, 4, 5-trimethoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one - {5J}

The compound the molecular formula is C$_{27}$H$_{26}$N$_2$O$_4$ and the molecular weight is: 442.50

**Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-5J1):** The $^1$H NMR signals were observed at 2.2ppm (s, 3H, - Me), 2.31ppm (s, 3H, - Me), 3.85ppm (s, 3H, - OMe), 3.87ppm (s, 6H, - OMe), 6.99-7.59ppm (m, 11H, Ar-CH and - C= CH)

**Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-5J2):** The $^{13}$C NMR signals were observed at 21.25, 21.42, 38.42, 56.10, 61.06, 109.88, 119.93, 126.21, 127.17, 128.12, 128.82, 128.87, 129.43, 129.79, 129.96, 130.07, 132.11, 132.19, 138.02, 138.08, 138.41, 140.44, 153.15, 160.18 and 170.41

**Assignment of the IR spectra (Figure-5J3):** Characteristics peaks are observed at 2449 (-CH stretch, aromatic), 1727 (>C=O stretch, cyclic ring), 1642 (>C=N stretch, imidazole ring), 1517 (>C=C<, aromatic), 1311 (- C - O stretching), 1291 (-C-N tertiary amine), 1409 (>C=C, Stretch, cyclic ring)

**Proposed fragmentation pattern (GCMS) (Figure-5J4):** The mass spectra display the molecular ion peaks at 442.1(M$^+$), 396.1, 355, 324.8, 281, 234.1, 208.2, 173, 146, 119, 91, 65, 39. The compound 5i GCMS fragmentation as 2-(3-methylphenyl)-4-(3, 4, 5-trimethoxybenzylidene)-1-(4-methylphenyl)-4H-imidazol-5-one MW: 442.50 , N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 73.32 % and the nitrogen showed 6.33 %

The melting point of the compound is 212-217 °C. Yield: 74 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5J1

Figure 5J2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 5J3

Figure 5J4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.11 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(benzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6A}

The compound the molecular formula is C_{26}H_{24}N_{2}O and the molecular weight is: 380.48

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-6A1): The $^1$H NMR signals were observed at 1.98 (s, 6H, - Me), 2.22ppm (s, 3H, - Me), 2.25ppm (s, 3H, - Me), 6.88ppm - 8.25ppm (m,12H, Ar-CH and -C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-6A2): The $^{13}$C NMR signals were observed at 18.12, 18.39, 21.2, 21.47, 124.97, 128.34, 128.75, 128.84, 128.92, 129.07, 129.63, 130.41, 130.67, 132.55, 132.62, 134.48, 135.48, 135.34, 135.97, 138.35, 138.62, 139.22, 160.74 and 170.75

Assignment of the IR spectra (Figure-6A3): Characteristics peaks are observed at 2880 (-CH stretch, aromatic), 1720 (>C=O stretch, cyclic ring), 1620 (>C=N stretch, imidazole ring), 1500 (>C=C< , aromatic), 1250(-C-N tertiary amine)

Fragmentation of mass spectra m/z (GCMS) (Figure-6A4): The mass spectra display the molecular ion peaks at 380.3(M$^+$), 281.1, 236.2, 207.1, 177, 147.1, 119.1, 91.1, 65.1, 39.1 The compound 6a GCMS fragmentation as 2-(3-methylphenyl)-4-(benzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 380.48, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 82.09 % and the nitrogen showed 7.39 % The melting point of the compound is 128-132 °C. Yield: 68 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
Synthesis and Characterization of S-Triazine and Imidazole Heterocycles

4.2.12 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(2-nitrobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one -{6B}

The compound the molecular formula is C_{28}H_{31}N_{3}O_{3} and the molecular weight is: 425.47

Assignment of ^1H NMR Chemical shifts (δ ppm) to different protons (Figure-6B1): The ^1H NMR signals were observed at 1.99 (s, 6H, -Me), 2.2ppm (s, 3H, - Me), 2.27ppm (s, 3H, - Me), 6.9-8.77ppm (m,11H, Ar-CH and - C= CH)

Assignment of ^13C NMR Chemical shifts (δ ppm) to different carbons (Figure-6B2): The ^13C NMR signals were observed at 18.13, 21.19, 21.43, 121.29, 124.73, 125.16, 128.43, 128.58, 128.78, 129.06, 129.57, 129.69, 129.92, 130.29, 132.68, 132.81, 133.12, 134.03, 135.81, 135.89, 138.50, 139.43, 141.12, 149.85, 163.19 and 169.97

Assignment of the IR spectra (Figure-6B3)
Characteristics peaks are observed at 2925 (-CH stretch, aromatic), 1725 (>C=O stretch, cyclic ring), 1521 (>C=C<, aromatic), 1424 (>C=C, Stretch, cyclic ring), 1567 (-NO2), 1451 (-N=O), 1369 (-methyl group)

Assignment of HSQC NMR (Figure-6B4)
The compound 6b HSQC NMR showed ^1H NMR singlet at 1.99 ppm for the m-methyl group (6H)protons attached to N-phenyl ring and related to peak at 18.3ppm in ^13C NMR, singlet at 2.20ppm for the p-methyl group protons attached to 2-phenyl ring and related to peak at 21.19ppm in ^13C NMR, singlet at 2.27ppm for the m-methyl group protons attached to N-phenyl ring and related to peak at 21.43ppm in ^13C NMR, multiplet of ten protons and singlet for one proton -C=CH was observed at 6.9-8.77 ppm indication the presence of phenyl protons and related to peak at 121.29 to 169.97ppm in ^13C NMR.

The compound elemental analysis demonstrates the result as
Carbon showed 73.71 % and the nitrogen showed 9.94 %
The melting point of the compound is 163-167 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6B1

Figure 6B2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6B3

Figure 6B4
4.2.13 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(2-chlorobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6c}

The compound the molecular formula is C_{26}H_{23}ClN_{2}O
and The molecular weight is: 414.92

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-6C1)
The $^1$H NMR signals were observed at 1.98 (s, 6H, -Me), 2.20ppm (s, 3H, -Me), 2.25ppm (s, 3H, -Me), 6.88ppm-9.02ppm (m,11H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-6C2)
The $^{13}$C NMR signals were observed at 18.13, 21.21, 21.46, 123.31, 125.07, 127.1, 128.38, 128.88, 128.98, 129.65, 129.87, 130.53, 131.03, 132.36, 132.8, 133.78, 135.95, 136.64, 138.41, 139.29, 139.71, 161.9 and 170.47

Assignment of the IR spectra (Figure-6C3)
Characteristics peaks are observed at 2926 (-CH stretch, aromatic), 1725 (>C=O stretch, cyclic ring), 1641 (>C=N stretch, imidazole ring), 1518 (>C=C< , aromatic), 1280 (-C-N tertiary amine), 1370 (-methyl group), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-6C4)
The mass spectra display the molecular ion peaks at 414.1 (M+), 379.3, 295.1, 262.1, 236.1, 220, 150, 119, 91.1, 65.1 and 39.1

The compound 6c GCMS fragmentation as 2-(3-methylphenyl)-4-(2-chlorobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 414.92, N-benzyldyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-yl um MW: 65.04 , prop-2-yn-1-yl um MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 75.29 % and the nitrogen showed 6.78 %
The melting point of the compound is 154-157 °C. Yield: 73 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6C1

Figure 6C6
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6C3

Figure 6C4
4.2.14 CHARACTERIZATION OF 2-(3-methylphenyl)-4-(4-chlorobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one - {6D}

The compound the molecular formula is C_{26}H_{23}ClN_{3}O and the molecular weight is: 414.92

Assignment of \(^1\)H NMR Chemical shifts (\(\delta\) ppm) to different protons (Figure-6D1)

The \(^1\)H NMR signals were observed at 1.97 (s, 6H, -Me), 2.22ppm (s, 3H, -Me), 2.25ppm (s, 3H, -Me), 6.88ppm- 8.18ppm (m,11H, Ar-CH and -C= CH)

Assignment of \(^{13}\)C NMR Chemical shifts (\(\delta\) ppm) to different carbons (Figure-6D2)

The \(^{13}\)C NMR signals were observed at 18.1, 18.33, 21.20, 21.47, 125, 126.99, 128.39, 128.91, 129.12, 129.65, 130.54, 132.72, 133, 133.69, 135.93, 136.33, 138.41, 138.90, 139.3, 161.12 and 170.58

Assignment of the IR spectra (Figure-6D3)

Characteristics peaks are observed at 2916(-CH stretch, aromatic), 1736 (>C=O stretch, cyclic ring), 1649 >C=N stretch, imidazole ring), 1538 (>C=C< , aromatic), 1425 (>C=C, Stretch, cyclic ring), 797 (-NO₂), 1279 (-C-N tertiary amine), 1319 (- Me group ), 750 (-C-Cl)

Assignment of HSQC NMR (Figure-6D4)

The compound 6d HSQC NMR showed \(^1\)H NMR singlet at 1.97 ppm for the \(m\)-Me group (6H)protons attached to N-phenyl ring and related to peak at 18.11ppm in \(^{13}\)C NMR , singlet at 2.22ppm for the \(p\)-Me group protons attached to 2-phenyl ring and related to peak at 21.20ppm in \(^{13}\)C NMR, singlet at 2.25ppm for the \(m\)-Me group protons attached to N-phenyl ring and related to peak at 21.47ppm in \(^{13}\)C NMR, multiplet of ten protons and singlet for one proton -C=CH was observed at 6.88-8.18 ppm indication the presence of phenyl protons and related to peak at 125 to 170.58 ppm in \(^{13}\)C NMR.

The compound elemental analysis demonstrates the result as

Carbon showed 75.29 % and the nitrogen showed 6.78 %

The melting point of the compound is 146-150 °C. Yield: 69 %
Synthesis and Characterization of $s$-Triazine and Imidazole Heterocycles

Figure 6D1

Figure 6D2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6D1

Figure 6D4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.216 CHARACTERIZATION OF 2-(3-Methylphenyl)-4-(4-methoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6E}

The compound the molecular formula is C$_{27}$H$_{26}$N$_2$O$_2$ and the molecular weight is 410.50.

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-6E1)
The $^1$H NMR signals were observed at 1.98ppm (s, 6H, - Me), 2.22ppm (s, 3H, - Me), 2.25ppm (s, 3H, - Me), 3.81ppm (s, 3H, -OMe), 6.88-8.24ppm (m, 11 H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-6E2)
The $^{13}$C NMR signals were observed at 18.13, 21.20, 21.47, 55.44, 114.44, 124.82, 127.47, 128.28, 128.79, 128.88, 129.26, 129.58, 130.81, 132.24, 134.60, 135.99, 136.83, 138.28, 139.10, 159.43, 161.57 and 170.71

Assignment of the IR spectra (Figure-6E3)
Characteristics peaks are observed at 2937 (-CH stretch, aromatic), 1722 (>C=O stretch, cyclic ring), 1640 (>C=N stretch, imidazole ring), 1529 (>C=C<, aromatic), 1419 (>C=C, Stretch, cyclic ring), 1280 (-C-N tertiary amine), 1312 (- Me group)

Proposed fragmentation pattern (GCMS) (Figure-6E4)
The mass spectra display the molecular ion peaks at 410.1 (M$^+$), 382.1, 351.1, 236.1, 220, 208.1, 146, 119, 91, 65 and 39

The compound 6e GCMS fragmentation as 2-(3-Methylphenyl)-4-(4-methoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 410.50, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 79.02 % and the nitrogen showed 6.85 %
The melting point of the compound is 153-157°C. Yield: 73 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6E3

Figure 6E4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.16 CHARACTERIZATION OF 2-(3- Mephenyl)-4-(3,4-dimethoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6F}

The compound the molecular formula is C_{28}H_{28}N_{2}O_{3} and the molecular weight is 440.53

Assignment of \(^1\)H NMR Chemical shifts (δ ppm) to different protons (Figure-6F1): The \(^1\)H NMR signals were observed at 1.99ppm (s, 6H, - Me), 2.19ppm (s, 3H, - Me), 2.25ppm (s, 3H, - Me), 3.9ppm (s, 3H, -OMe), 3.97ppm (s, 3H, - OMe), 6.9-8.32ppm (m,10 H, Ar-CH and - C= CH)

Assignment of \(^{13}\)C NMR Chemical shifts (δ ppm) to different carbons (Figure-6F2): The \(^{13}\)C NMR signals were observed at 18.13, 21.20, 21.47, 55.77, 55.99, 110.87, 114.29, 124.65, 127.52, 127.81, 128.37, 128.72, 128.91, 129.25, 129.61, 130.81, 132.27, 136.0, 136.91, 138.21, 139.17, 149.05, 151.35, 159.14 and 170.64

Assignment of the IR spectra (Figure-6F3): Characteristics peaks are observed at 2918 (-CH stretch, aromatic), 1726 (>C=O stretch, cyclic ring), 1639 (>C=N stretch, imidazole ring), 1519 (>C=C< , aromatic), 1400-1300 (Ar-CH=C< ), 1412 (>C=C, Stretch, cyclic ring), 1291 (-C-N tertiary amine), 1310 (- Me group)

Proposed fragmentation pattern (GCMS) (Figure-6F4): The mass spectra display the molecular ion peaks at 440.1 (M\(^+\)), 409.1, 349.1, 236.1, 220, 204, 146,176, 146, 119, 91, 65 and 39. The compound 6f GCMS fragmentation as 2-(3- Mephenyl)-4-(3,4-dimethoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 440.53, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 76.36 % and the nitrogen showed 6.39 %

The melting point of the compound is 166-170 °C. Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6F1

Figure 6F2
Synthesis and Characterization of σ-Triazine and Imidazole Heterocycles

Figure 6F3

Figure 6F4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.17 CHARACTERIZATION OF 2-(3-Mephenyl)-4-(2-methoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6G}

The compound the molecular formula is C_{27}H_{26}N_{2}O_{2} and the molecular weight is: 410.50

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure-6G1): The $^1$H NMR signals were observed at 1.97ppm (s, 6H, -Me), 2.21ppm (s, 3H, -Me), 2.27ppm (s, 3H, -Me), 3.83ppm (s, 3H, -OMe), 6.89-8.96ppm (m, 11 H, Ar-CH and -C=CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-6G2): The $^{13}$C NMR signals were observed at 18.12, 21.19, 21.45, 55.60, 110.64, 120.99, 122.76, 123.51, 124.89, 128.27, 128.87, 129.25, 129.57, 130.82, 132.04, 132.31, 133.31, 136.01, 138.07, 138.27, 139.07, 159.41, 160.11 and 170.66

Assignment of the IR spectra (Figure-6G3): Characteristics peaks are observed at 2948 (-CH stretch, aromatic), 1727 (>C=O stretch, cyclic ring), 1653 (>C=N stretch, imidazole ring), 1515 (>C=C<, aromatic), 1431 (>C=C, Stretch, cyclic ring), 1280 (-C-N tertiary amine), 1389 (-Me group)

Proposed fragmentation pattern (GCMS) (Figure-6G4): The mass spectra display the molecular ion peaks at 410.2 (M$^+$), 382.1, 351.1, 236.1, 220, 208, 146, 174, 146, 119, 91, 65 and 39. The compound 6g GCMS fragmentation as 2-(3-Mephenyl)-4-(2-methoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 410.50, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 79.02 % and the nitrogen showed 6.85 %

The melting point of the compound is 156-159 °C. Yield: 74 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6G1

Figure 6G2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6G3

Figure 6G4
4.2.18 CHARACTERIZATION OF 2-(3-Mephenyl)-4-(4-Mebenzyldene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6H}

The compound the molecular formula is C\textsubscript{27}H\textsubscript{26}N\textsubscript{2}O and the molecular weight is: 394.50

Assignment of \textsuperscript{1}H NMR Chemical shifts (δ ppm) to different protons (Figure-6H1):
The \textsuperscript{1}H NMR signals were observed at 1.98ppm (s, 6H, - Me), 2.23ppm (s, 3H, - Me), 2.25ppm (s, 3H, - Me), 2.34ppm (s, 3H, - Me), 6.88-8.12ppm (m,11 H, Ar-CH and - C= CH)

Assignment of \textsuperscript{13}C NMR Chemical shifts (δ ppm) to different carbons (Figure-6H2) : The \textsuperscript{13}C NMR signals were observed at 18.13, 21.20, 21.47, 21.81, 124.9, 128.31, 128.88, 129.04, 129.17, 129.30, 129.60, 129.67, 130.74, 131.79, 132.40, 132.66, 135.98, 137.91, 138.31, 139.15, 141.08, 160.09 and 170.76

Assignment of the IR spectra (Figure-6H3) : Characteristics peaks are observed at 2932 (-CH stretch, aromatic), 1731 (>C=O stretch, cyclic ring), 1639 (>C=N stretch, imidazole ring), 1498 (>C=C< , aromatic), 1412 (>C=C, Stretch, cyclic ring), 1279 (-C-N tertiary amine), 1383 (- Me group)

Proposed fragmentation pattern (GCMS) (Figure-6H4)
The mass spectra display the molecular ion peaks at 394.3 (M\textsuperscript{+}), 380, 335, 275.1, 236.1, 220, 197.2, 158.1, 130, 119.1, 91.1, 65.1 and 39.1. The compound 6h GCMS fragmentation as 2-(3- Mephenyl)-4-(4- Mebenzyldiene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 394.50, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylum MW: 65.04 , prop-2-yn-1-ylum MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 82.22 % and the nitrogen showed 7.12 %
The melting point of the compound is 158-161 °C. Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6H1

Figure 6H2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6H3

Figure 6H4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.19 CHARACTERIZATION OF 2-(3-Mephenyl)-4-(3-bromobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6l}

The compound the molecular formula is C_{26}H_{23}BrN_{2}O and the molecular weight is: 459.37

Assignment of \(^1\)H NMR Chemical shifts to different - protons (Figure-6l1)

The \(^1\)H NMR signals were observed at 1.97 (s, 6H, - Me), 2.22ppm (s, 3H, - Me), 2.25ppm (s, 3H, - Me), 6.89ppm-8.44ppm (m, 11H, Ar-CH and - C= CH)

Assignment of \(^{13}\)C NMR Chemical shifts (\(\delta \) ppm) to different carbons (Figure-6l2): The \(^{13}\)C NMR signals were observed at 18.11, 21.21, 21.48, 122.85, 125.07, 126.45, 128.43, 128.78, 129.02, 129.68, 130.24, 130.52, 131.0, 132.85, 133.0, 134.95, 135.93, 136.50, 138.42, 139.35, 139.49, 161.56 and 170.53

Assignment of the IR spectra (Figure-6l3): Characteristics peaks are observed at 2959 (-CH stretch, aromatic), 1721 (>C=O stretch, cyclic ring), 1512 (>C=C< , aromatic), 1415 (>C=C, Stretch, cyclic ring), 671 (C-Br stretch, aromatic), 1280 (-C-N tertiary amine), 1319 (- Me group)

Proposed fragmentation pattern (GCMS) (Figure-6l4): The mass spectra display the molecular ion peaks at 460 (M+), 410.1, 379.2, 340.9, 291.1, 236.1, 220, 196, 168.9, 119.1, 91.1, 65.1 and 39.1. The compound 6i GCMS fragmentation as 2-(3- Mephenyl)-4-(3-bromobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 459.39, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 67.99 % and the nitrogen showed 6.12 %
The melting point of the compound is 180-185 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6I3

Figure 6I4
4.2.20 CHARACTERIZATION OF 2-(3-Methylphenyl)-4-(3, 4, 5-trimethoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {6J}

The compound the molecular formula is \( \text{C}_{29}\text{H}_{30}\text{N}_{2}\text{O}_{4} \) and the molecular weight is: 470.55

Assignment of \(^1\text{H} \) NMR Chemical shifts (\( \delta \ \text{ppm} \)) to different protons (Figure-6J1) : The \(^1\text{H} \) NMR signals were observed at 1.98ppm (s, 6H, - Me), 2.19ppm (s, 3H, - Me), 2.26ppm (s, 3H, - Me), 3.86ppm (s, 3H, - OMe), 3.91ppm (s, 6H, - OMe), 6.91-7.62ppm (m, 9H, Ar-CH and - C= CH)

Assignment of \(^{13}\text{C} \) NMR Chemical shifts (\( \delta \ \text{ppm} \)) to different carbons (Figure-6J2) : The \(^{13}\text{C} \) NMR signals were observed at 18.09, 21.20, 21.47, 56.08, 61.09, 109.83, 124.7, 128.42, 128.52, 128.78, 129.10, 129.64, 129.97, 130.7, 132.47, 135.97, 137.93, 138.23, 139.27, 140.42, 153.17, 159.92 and 170.62

Assignment of the IR spectra (Figure-6J3) : Characteristics peaks are observed at 2980 (-CH stretch, aromatic), 1725 (>C=O stretch, cyclic ring), 1642 (>C=N stretch, imidazole ring), 1510 (>C=C< , aromatic), 1431 (>C=C, Stretch, cyclic ring), 1291 (-C-N tertiary amine), 1312 (- Me group)

Proposed fragmentation pattern (GCMS) (Figure-6J4)

The mass spectra display the molecular ion peaks at 470.3 (\( \text{M}^+ \)), 455, 424.2, 379.2, 236.2, 220, 206.1, 173, 146, 119.1, 91.1, 65.1 and 41.2

The compound 6j GCMS fragmentation as 2-(3-Methylphenyl)-4-(3, 4, 5-trimethoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 470.55, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 74.03 % and the nitrogen showed 5.98 %

The melting point of the compound is 263-267 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 6J1

Figure 6J2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

**Figure 6J3**

**Figure 6J4**
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.21 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(benzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one- {8A}

The compound the molecular formula is C_{23}H_{17}ClN_{2}O and the molecular weight is: 372.84

Assignment of \(^1\)H NMR Chemical shifts (δ ppm) to different protons (Figure-8A1): The \(^1\)H NMR signals were observed at 2.32ppm (s, 3H, -Me), 6.99-8.19ppm (m, 14H, Ar-CH and -C=CH)

Assignment of \(^13\)C NMR Chemical shifts (δ ppm) to different carbons (Figure-8A2): The \(^13\)C NMR signals were observed at 21.27, 119.78, 127.13, 127.34, 128.71, 128.84, 129.64, 129.80, 130.28, 130.55, 130.61, 131.84, 132.66, 134.33, 137.70, 138.44, 138.72, 159.57 and 170.61

Assignment of the IR spectra (Figure-8A3)
Characteristics peaks are observed at 2922 (-CH stretch, aromatic), 1720 (>C=O stretch, cyclic ring), 1638 (>C=N stretch, imidazole ring), 1514 (>C=C< , aromatic), 1293(-C-N tertiary amine), 757 (-C-Cl)

Fragmentation of mass spectra m/z (GCMS) (Figure-8A4)
The mass spectra display the molecular ion peaks at 372.2(M\(^+\)), 281.1, 207.1, 177.0, 139.0, 91.1, 65.1, 39.1

The compound 8a GCMS fragmentation as 2-(4-chlorophenyl)-4-(benzylidene)-1-(4- Mephenyl)-4H-imidazol-5-one: MW: 372.84, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 74.12 % and the nitrogen showed 7.53 %
The melting point of the compound is 197-202 °C. Yield: 75 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8A1

Figure 8A2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
4.2.22 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(2-nitrobenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one- {8B}

The compound the molecular formula is C_{23}H_{16}ClN_{3}O_{3} and the molecular weight is: 417.84

**Assignment of ^1H NMR Chemical shifts to different - protons (Figure-8B1)**

The ^1H NMR signals were observed at 2.32ppm (s, 3H, - Me), 7.27-8.62ppm (m, 9H, Ar-CH and - C= CH)

**Assignment of ^13C NMR Chemical shifts (δ ppm) to different carbons (Figure-8B2)**

The ^13C NMR signals were observed at 21.27, 119.78, 122.73, 124.78, 126.85, 127.06, 128.74, 128.81, 129.79, 130.10, 130.35, 130.67, 131.43, 132.86, 133.91, 138.29, 138.99, 140.91, 149.70, 161.94 and 169.81

**Assignment of the IR spectra (Figure-8B3)**

Characteristics peaks are observed at 2924 (-CH stretch, aromatic), 1718 (>C=O stretch, cyclic ring), 1640 (>C=N stretch, imidazole ring), 1298 (> C - O stretching), 776 (-C-Cl), 1402 (>C=C, Stretch, cyclic ring), 1565 (-NO_{2}), 1443 (N=O stretch) 1565 (-NO_{2}), 750 (-C-Cl)

**Assignment of HSQC NMR (Figure-8B4)**

The compound 8b HSQC NMR showed ^1H NMR singlet at 2.32 ppm for the p-Me group (3H)protons attached to N- phenyl ring and related to peak at 21.27ppm in ^13C NMR , multiplet of twelve protons and singlet for one proton -C=CH was observed at 7.27-8.62 ppm indication the presence of phenyl protons and related to peak at 119.78 to 169.81 ppm in ^13C NMR.

The compound elemental analysis demonstrates the result as

Carbon showed 66.13 % and the nitrogen showed 10.08 %

The melting point of the compound is 161-166 °C. Yield: 73 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8B1

Figure 8B2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8B3

Figure 8B4
4.2.23 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(2-chlorobenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one- \{8C\}

The compound the molecular formula is \( C_{23}H_{16}Cl_2N_2O \) and the molecular weight is: 407.29

Assignment of \( ^1H \) NMR Chemical shifts to different - protons (Figure-8C1)
The \( ^1H \) NMR signals were observed at 2.05ppm (s, 3H, - Me), 6.76- 9.49ppm (m, 13H, Ar-CH and - C= CH)

Assignment of \( ^{13}C \) NMR Chemical shifts (\( \delta \) ppm) to different carbons (Figure-8C2): The \( ^{13}C \) NMR signals were observed at 20.67, 123.02, 126.84, 127.14, 127.54, 127.66, 127.78, 128.02, 128.42, 129.79, 129.85, 130.71, 130.94, 132.08, 132.74, 133.84, 136.72, 137.52, 137.93, 140.34, 160.91 and 169.62

Assignment of the IR spectra (Figure-8C3)
Characteristics peaks are observed at 2924(-CH stretch, aromatic), 1779 (>C=O stretch, cyclic ring), 1640 (>C=N stretch, imidazole ring), 1298 (- C - O stretching), 1280 (-C-N tertiary amine), 776 (-C-Cl), 1491 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-8C4)
The mass spectra display the molecular ion peaks at 406 (M\(^+\)), 371.1, 341.1, 280.9, 228, 178.1, 150, 123, 91.1, 65.1, 39.1

The compound \( 8c \) GCMS fragmentation as 2-(4-chlorophenyl)-4-(2-chlorobenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one MW: 407.29, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 67.85 % and the nitrogen showed 6.89 %
The melting point of the compound is 175-179 °C. Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8C1

Figure 8C2
Figure 8C3

Figure 8C4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.24 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(4-chlorobenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one-{8d}

The compound the molecular formula is C_{23}H_{16}Cl_{2}N_{2}O and the molecular weight is: 407.29

Assignment of \(^1\)H NMR Chemical shifts to different - protons (Figure-8D1)

The \(^1\)H NMR signals were observed at 2.31ppm (s, 3H, - Me), 6.98- 8.12ppm (m, 13H, Ar-CH and - C= CH)

Assignment of \(^{13}\)C NMR Chemical shifts (δ ppm) to different carbons (Figure-8D2): The \(^{13}\)C NMR signals were observed at 21.27, 127.10, 127.16, 127.87, 128.76, 129.13, 130.31, 130.56, 131.70, 132.83, 133.72, 136.60, 137.89, 138.71, 138.82, 159.94 and 170.45

Assignment of the IR spectra (Figure-8D3)

Characteristics peaks are observed at 2924 (-CH stretch, aromatic), 1780 (>C=O stretch, cyclic ring), 1512 (>C=C<, aromatic), 1343 (- C - O stretching), 1279 (-C-N tertiary amine), 711 (-C-Cl), 1409 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-8D4)

The mass spectra display the molecular ion peaks at 406 (M^+), 371.1, 341.1, 280.9, 228, 178, 150, 138.9, 91, 65, 39

The compound 8d GCMS fragmentation as 2-(4-chlorophenyl)-4-(4-chlorobenzylidene)-1-(4- Mephenyl)-4H-imidazol-5-one MW: 407.29, N-benzyldyde-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 67.85 % and the nitrogen showed 6.89 %
The melting point of the compound is 234-238 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8D1

Figure 8D2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8D3

Figure 8D4
Characterization of 2-(4-chlorophenyl)-4-(4-methoxybenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one-{8E}

The compound the molecular formula is $C_{24}H_{19}ClN_2O_2$ and the molecular weight is 402.87.

Assignment of $^1H$ NMR Chemical shifts to different - protons (Figure-8E1)
The $^1H$ NMR signals were observed at 2.31ppm (s, 3H, -Me), 3.8ppm (s, 3H, -OMe) 6.89-8.19ppm (m, 13H, Ar-CH and -C=CH).

Assignment of $^{13}C$ NMR Chemical shifts (δ ppm) to different carbons (Figure-8E2)
The $^{13}C$ NMR signals were observed at 21.26, 55.44, 114.45, 127.15, 127.34, 127.56, 128.56, 128.65, 129.78, 130.23, 130.43, 132.00, 134.69, 136.62, 137.36, 138.57, 158.25, 161.75 and 170.59.

Assignment of the IR spectra (Figure-8E3)
Characteristics peaks are observed at 2924 (-CH stretch, aromatic), 1643 (>C=N stretch, imidazole ring), 1550 (>C=C< , aromatic), 1280 (-C-N tertiary amine), 758 (-C-Cl), 1409 (>C=C, Stretch, cyclic ring).

Proposed fragmentation pattern (GCMS) (Figure-8E4)
The mass spectra display the molecular ion peaks at 402 (M$^+$), 366.1, 281, 228, 174, 138.9, 91, 65, 39.

The compound 8e GCMS fragmentation as 2-(4-chlorophenyl)-4-(4-methoxybenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one MW: 402.87, N-benzyldiyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02.

The compound elemental analysis demonstrates the result as Carbon showed 71.56 % and the nitrogen showed 6.96 %.

The melting point of the compound is 198-202 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8E1

Figure 8E2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8E3

Figure 8E4
4.2.26 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(3,4-dimethoxybenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one- {8F}

The compound the molecular formula is $\text{C}_{25}\text{H}_{21}\text{ClN}_{2}\text{O}_{3}$ and the molecular weight is: 432.89

Assignment of $^1\text{H}$ NMR Chemical shifts to different - protons (Figure-8F1)

The $^1\text{H}$ NMR signals were observed at 2.32ppm (s, 3H, -Me), 3.88ppm (s, 3H, -OMe), 3.92ppm (s, 3H, -OMe), 6.87- 8.18ppm (m, 12H, Ar-CH and -C=CH)

Assignment of $^{13}\text{C}$ NMR Chemical shifts (δ ppm) to different carbons (Figure-8F2 ):
The $^{13}\text{C}$ NMR signals were observed at 21.26, 55.88, 56.0, 110.91, 114.38, 127.14, 127.58, 127.63, 128.69, 129.87, 130.26, 130.27, 131.98, 136.72, 137.40, 138.63, 149.06, 151.58, 158.16 and 170.54

Assignment of the IR spectra (Figure-8F3): Characteristics peaks are observed at 2924(-CH stretch, aromatic), 1782(>C=O stretch, cyclic ring), 1643 (>C=N stretch, imidazole ring), 1580 (>C=C<, aromatic), 1349 ( -C - O stretching), 1291 (-C-N tertiary amine), 776 (-C-Cl), 1490 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-8F4): The mass spectra display the molecular ion peaks at 432.1( M$^+$), 396.1, 280.9, 228, 176.1, 138.9, 91, 65, 39. The compound 8f GCMS fragmentation as 2-(4-chlorophenyl)-4-(3,4-dimethoxybenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one MW: 432.89, N-benzyldyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 69.39 % and the nitrogen showed 6.52 %
The melting point of the compound is 170-175 °C. Yield: 67 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8F1

Figure 8F2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8F3

Figure 8F4
4.2.27 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(2-methoxybenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one - {8G}

The compound the molecular formula is $C_{24}H_{19}ClN_2O_2$ and the molecular weight is: 402.87

Assignment of $^1$H NMR Chemical shifts to different - protons (Figure-8G1)
The $^1$H NMR signals were observed at 2.32ppm (s, 3H, - Me), 3.83ppm (s, 3H, - OMe), 6.86- 8.88ppm (m, 13H, Ar-CH and -C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-8G2)
The $^{13}$C NMR signals were observed at 21.18, 55.55, 110.61, 120.88, 123.31, 123.70, 127.08, 127.46, 128.57, 130.13, 130.41, 131.92, 132.19, 133.22, 137.36, 137.77, 138.46, 158.85, 159.38 and 170.46

Assignment of the IR spectra (Figure-8G3)
Characteristics peaks are observed at 2924 (-CH stretch, aromatic), 1635 (>C=N stretch, imidazole ring), 1566 (>C=C<, aromatic), 1359 (- C - O stretching), 776 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-8G4)
The mass spectra display the molecular ion peaks at 402(M$^+$), 371, 345.1, 283, 228, 201.1, 174, 146, 116, 91, 65, 39

The compound 8g GCMS fragmentation as 2-(4-chlorophenyl)-4-(2-methoxybenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one MW: 402.87, N-benzyldiene-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 71.56 % and the nitrogen showed 6.98 %
The melting point of the compound is 202-206 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8G1

Figure 8G2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8G3

Figure 8G4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.2.28 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(4-Mebenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one {8H}

The compound the molecular formula is C24H19ClN2O and the molecular weight is: 386.87

Assignment of 1H NMR Chemical shifts to different protons (Figure-8H1)
The 1H NMR signals were observed at 2.32ppm (s, 3H, -Me), 2.34ppm (s, 3H, -Me), 6.96- 8.09ppm (m, 13H, Ar-CH and -C=CH)

Assignment of 13C NMR Chemical shifts (δ ppm) to different carbons (Figure-8H2): The 13C NMR signals were observed at 21.26, 21.80, 127.13, 127.46, 128.68, 129.67, 129.92, 130.25, 130.50, 131.66, 131.92, 132.71, 137.53, 137.72, 138.63, 141.37, 158.94 and 170.62

Assignment of the IR spectra (Figure-8H3)
Characteristics peaks are observed at 2969 (-CH stretch, aromatic), 1719 (>C=O stretch, cyclic ring), 1515 (>C=C<, aromatic), 1312 (-C - O stretching), 1290 (-C-N tertiary amine), 711 (-C-Cl), 1491 (>C=C, Stretch, cyclic ring), 1485 (-Me group), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-8H4)
The mass spectra display the molecular ion peaks at 386.1(M⁺), 350.1, 321.1, 295.1, 228, 193, 165, 138.9, 116, 91, 65, 39

The compound 8h GCMS fragmentation as 2-(4-chlorophenyl)-4-(4-Mebenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one MW: 386.87, N-benzyldyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 74.56 % and the nitrogen showed 7.26 %
The melting point of the compound is 190-195 °C. Yield: 76 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8H1

Figure 8H2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
The compound the molecular formula is C_{23}H_{16}BrClN_{2}O and the molecular weight is 451.74.

**Assignment of $^1$H NMR Chemical shifts to different - protons (Figure-8I1)**

The $^1$H NMR signals were observed at 2.33 ppm (s, 3H, - Me), 6.98 - 8.40 ppm (m, 13H, Ar-CH and - C= CH)

**Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-8I2)**

The $^{13}$C NMR signals were observed at 21.27, 122.85, 127.04, 127.10, 127.35, 128.79, 130.24, 130.33, 130.62, 131.03, 131.67, 133.21, 134.97, 136.30, 138.02, 138.88, 139.32, 160.41 and 170.41

**Assignment of the IR spectra (Figure-8I3)**

Characteristics peaks are observed at 2980 (-CH stretch, aromatic), 1720 (>C=O stretch, cyclic ring), 1642 (>C=N stretch, imidazole ring), 1515 (>C=C<, aromatic), 1311 (-C - O stretching), 1291 (-C-N tertiary amine), 711 (-C-Cl), 1409 (>C=C, Stretch, cyclic ring), 694 (C-Br stretch, aromatic), 750 (-C-Cl)

**Proposed fragmentation pattern (GCMS) (Figure-8I4)**

The mass spectra display the molecular ion peaks at 452 (M$^+$), 371.1, 341, 280.9, 228, 193.9, 165, 138.9, 116, 91, 65, 39. The compound 8i GCMS fragmentation as 2-(4-chlorophenyl)-4-(3-bromobenzylidene)-1-(4-Mephenyl)-4H-imidazol-5-one MW: 451.74, N-benzyliyden-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 61.19 % and the nitrogen showed 6.24 %

The melting point of the compound is 177-181 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8I1

Figure 8I2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8I3

Figure 8I4
4.2.30 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(3, 4, 5-trimethoxybenzylidene)-1-(4-Mphenyl)-4H-imidazol-5-one-{8J}

The compound the molecular formula is $\text{C}_{26}\text{H}_{23}\text{ClN}_{2}\text{O}_{4}$ and the molecular weight is: 462.92

Assignment of $^1\text{H}$ NMR Chemical shifts to different - protons (Figure-8J1)
The $^1\text{H}$ NMR signals were observed at 2.31ppm (s, 3H, - Me), 3.85ppm (s, 9H, -O Me), 6.87 - 8.18ppm (m, 11H, Ar-CH and - C= CH)

Assignment of $^{13}\text{C}$ NMR Chemical shifts (6 ppm) to different carbons (Figure-8J2) :The $^{13}\text{C}$ NMR signals were observed at 21.26, 56.14, 61.06, 109.95, 120.27, 127.13, 127.43, 128.73, 129.50, 129.76, 130.29, 131.88, 137.61, 137.72, 138.72, 140.66, 153.17, 158.93 and 170.50

Assignment of the IR spectra (Figure-8J3) :Characteristics peaks are observed at 2971 (-CH stretch, aromatic), 1720 (>C=O stretch, cyclic ring), 1640 (>C=N stretch, imidazole ring), 1512 (>C=C , aromatic), 1308 ( - C - O stretching),758 (-C-Cl), 1409 (>C=C, Stretch, cyclic ring), 750 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-8J4)
The mass spectra display the molecular ion peaks at 462.1 (M$^+$), 450, 461, 281, 228, 173, 138.9, 116, 91, 65, 39. The compound 8j GCMS fragmentation as 2-(4-chlorophenyl)-4-(3, 4, 5-trimethoxybenzylidene)-1-(4- Mphenyl)-4H-imidazol-5-one MW: 462.92, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 67.49 % and the nitrogen showed 6.07 %
The melting point of the compound is 233-238 °C. Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8J1

Figure 8J2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 8J3

Figure 8J4
The compound the molecular formula is $\text{C}_{25}\text{H}_{21}\text{ClN}_{2}\text{O}$ and the molecular weight is: 400.90

Assignment of $^1\text{H}$ NMR Chemical shifts to different - protons (Figure-9A1)
The $^1\text{H}$ NMR signals were observed at 1.97ppm (s, 6H, - Me), 2.64ppm (s, 3H, - Me), 6.90-8.23ppm (m, 12H, Ar-CH and - C= CH)

Assignment of $^{13}\text{C}$ NMR Chemical shifts (δ ppm) to different carbons (Figure-9A2): The $^{13}\text{C}$ NMR signals were observed at 18.08, 18.32, 21.21, 127.61, 128.87, 128.96, 129.34, 129.38, 129.83, 130.35, 130.62, 132.68, 134.34, 135.94, 138.05, 138.35, 139.54, 159.37 and 170.51

Assignment of the IR spectra (Figure-9A3): Characteristics peaks are observed at 2880 (-CH stretch, aromatic), 1720 (>C=O stretch, cyclic ring), 1640 ( >C=N stretch, imidazole ring), 1510 ( >C=C<, aromatic), 1300(-C-N tertiary amine), 780 (-C-Cl)

Fragmentation of mass spectra m/z (GCMS) (Figure-9A4)
The mass spectra display the molecular ion peaks at 400.3 (M+), 350.2, 309.2, 282.2, 256.2, 207.1, 179.1, 139.1, 91.2, 41.2. The compound 9a GCMS fragmentation as 2-(4-chlorophenyl)-4-(benzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 400.90, N-benzylidyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 74.92 % and the nitrogen showed 7.01 %
The melting point of the compound is 142-145 °C. Yield: 75 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9A1

Figure 9A2
Figure 9A3

Figure 9A4
**Synthesis and Characterization of s-Triazine and Imidazole Heterocycles**

**4.2.32 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(2-nitrobenzylidene)-1-(3,4,5-trimethylphenyl)-1H-imidazol-5(4H)-one - {9B}**

The compound the molecular formula is C$_{25}$H$_{20}$ClN$_3$O$_3$ and the molecular weight is: 445.89

**Assignment of $^1$H NMR Chemical shifts to different - protons (Figure-9B1)**

The $^1$H NMR signals were observed at 2.02ppm (s, 6H, - Me), 2.29ppm (s, 3H, - Me), 6.92-8.71ppm (m, 11H, Ar-CH and - C= CH)

**Assignment of $^{13}$C NMR Chemical shifts (6 ppm) to different carbons (Figure-9B2)**

The $^{13}$C NMR signals were observed at 18.09, 21.21, 122.0, 124.79, 127.12, 128.63, 129.06, 129.52, 129.89, 129.98, 130.09, 132.74, 133.94, 135.87, 138.68, 139.75, 140.85, 149.92, 161.80 and 169.71

**Assignment of the IR spectra (Figure-9B3)**

Characteristics peaks are observed at 2922 (-CH stretch, aromatic), 1725 (>C=O stretch, cyclic ring), 1640 (>C=N stretch, imidazole ring), 1521 (>C=C<, aromatic), 750 (-C-Cl), 1429 (>C=C, Stretch, cyclic ring), 1560 (-NO$_2$), 1451 ( N=O stretch), 750 (-C-Cl).

**HSQC NMR (Figure-9B4)**: The compound 9b HSQC NMR showed $^1$H NMR singlet at 2.02 ppm for the m- Me group (6H)protons attached to N- phenyl ring and related to peak at 18.09ppm in $^{13}$C NMR, singlet at 2.29ppm for the p- Me group protons attached to 2-phenyl ring and related to peak at 21.21ppm in $^{13}$C NMR, multiplet of ten protons and singlet for one proton - C=CH was observed at 6.92-8.71 ppm indication the presence of phenyl protons and related to peak at 122 to 169.71 ppm in $^{13}$C NMR.

The compound elemental analysis demonstrates the result as Carbon showed 67.36 % and the nitrogen showed 9.42 %

The melting point of the compound is 181-185 °C. Yield: 73 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9B1

Figure 9B2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9B3

Figure 9B4
The compound the molecular formula is $C_{25}H_{20}Cl_2N_2O$ and the molecular weight is: 435.34

Assignment of $^1$H NMR Chemical shifts to different - protons (Figure-9C1)
The $^1$H NMR signals were observed at 1.99ppm (s, 6H, - Me), 2.27ppm (s, 3H, - Me), 6.91-9.0ppm (m, 11H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts ($\delta$ ppm) to different carbons (Figure-9C2)
The $^{13}$C NMR signals were observed at 18.07,21.20, 123.93, 127.05, 127.44, 128.99, 129.41, 129.84, 129.93, 131.20, 132.23, 133.73, 135.92, 136.80, 139.42, 139.59 and 170.22

Assignment of the IR spectra (Figure-9C3)
Characteristics peaks are observed at 2924 (-CH stretch, aromatic), 1727 (>C=O stretch, cyclic ring), 1639 (>C=N stretch, imidazole ring), 1518 (>C=C< , aromatic), 1312 (- C - O stretching), 812 (-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-9C4)
The mass spectra display the molecular ion peaks at 434 (M$^+$), 399.1, 364.1, 281, 256, 221.1, 178, 150, 123, 116, 91, 65, 39
The compound 9b GCMS fragmentation as 2-(4-chlorophenyl)-4-(2-chlorobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 435.34, N-benzyldyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 68.99 % and the nitrogen showed 6.46 %
The melting point of the compound is 195-200 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9C1

Figure 9C2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9C3

Figure 9C4
4.2.34 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(4-chlorobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one-{9D}

The compound the molecular formula is C_{25}H_{20}Cl_2N_2O and the molecular weight is: 435.34

Assignment of \(^1\)H NMR Chemical shifts to different protons (Figure-9D1)

The \(^1\)H NMR signals were observed at 1.97 ppm (s, 6H, -Me), 2.27 ppm (s, 3H, -Me), 6.91-8.15 ppm (m, 11H, Ar-CH and -C=CH)

Assignment of \(^{13}\)C NMR Chemical shifts (δ ppm) to different carbons (Figure-9D2):
The \(^{13}\)C NMR signals were observed at 18.07, 18.32, 21.21, 127.44, 127.62, 129.01, 129.16, 129.34, 129.85, 130.22, 132.86, 133.73, 135.89, 136.59, 138.24, 138.62, 139.62, 159.75 and 170.34

Assignment of the IR spectra (Figure-9D3):
Characteristics peaks are observed at 2914 (-CH stretch, aromatic), 1738 (>C=O stretch, cyclic ring), 1649 >C=N stretch, imidazole ring), 1538 (>C=C<, aromatic), 1298 (-C - O stretching), 639 (-C-Cl), 1420 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-9D4)
The mass spectra display the molecular ion peaks at 434.1(M^+), 399.1, 355.1, 282, 256.1, 221.1, 178, 150, 139, 116, 91.1, 65, 41.1

The compound 9d GCMS fragmentation as 2-(4-chlorophenyl)-4-(4-chlorobenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 435.34, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 68.99 % and the nitrogen showed 6.46 %
The melting point of the compound is 183-185 °C. Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
Synthesis and Characterization of 1,3,5-Triazine and Imidazole Heterocycles
4.2.35 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(4-methoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one- {9E}

The compound the molecular formula is C_{26}H_{23}ClN_{2}O_{2} and The molecular weight is: 430.92

Assignment of $^{1}$H NMR Chemical shifts to different - protons (Figure-9E1)

The $^{1}$H NMR signals were observed at 1.96ppm (s, 6H, - Me), 2.2ppm (s, 3H, - Me), 3.81ppm (s, 3H, -OMe), 6.90-8.20 ppm (m, 11H, Ar-CH and - C= CH)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure-9E2)

The $^{13}$C NMR signals were observed at 18.09, 21.21, 55.45, 114.49, 127.34, 127.83, 128.90, 129.18, 129.550, 129.78, 130.50, 134.70, 135.96, 136.56, 137.69, 139.41, 158.02, 161.74 and 170.47

Assignment of the IR spectra (Figure-9E3)

Characteristics peaks are observed at 2930 (-CH stretch, aromatic), 1727 (>C=O stretch, cyclic ring),1638 (>C=N stretch, imidazole ring), 1529 (>C=C< , aromatic), 1397 (-C-O stretching), 758(-C-Cl)

Proposed fragmentation pattern (GCMS) (Figure-9E4)

The mass spectra display the molecular ion peaks at 430.1(M$^{+}$), 380.1, 281, 256.1, 221.1, 174.1, 150, 138.9, 116, 91, 65, 39

The compound 9e GCMS fragmentation as 2-(4-chlorophenyl)-4-(4-methoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW:

430.92, N-benzyldyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as

Carbon showed 72.49 % and the nitrogen showed 5.53 %

The melting point of the compound is 166-170 °C. Yield: 68 %
Figure 9E3

Figure 9E4
SYNTHESIS AND CHARACTERIZATION OF S-TRIAZINE AND IMIDAZOLE HETEROCYCLES

4.2.36 CHARACTERIZATION OF 2-(4-CHLOROPHENYL)-4-(3,4-DIMETHOXYBENZYLIDENE)-1-(3,4,5-TRIMETHYLPHENYL)-4H-IMIDAZOL-5-ONE {9F}

The compound the molecular formula is C_{27}H_{25}ClN_{2}O_{3} and the molecular weight is: 460.95

Assignment of 1H NMR Chemical shifts to different - protons (Figure-9F1)
The 1H NMR signals were observed at 1.98 ppm (s, 6H, -Me), 2.27 ppm (s, 3H, -Me), 3.90 ppm (s, 3H, -OMe), 3.94 ppm (s, 3H, -OMe), 6.87-8.25 ppm (m, 10H, Ar-CH and -C=CH)

Assignment of 13C NMR Chemical shifts (δ ppm) to different carbons (Figure-9F2): The 13C NMR signals were observed at 18.07, 21.20, 55.86, 56.0, 110.92, 114.28, 127.28, 127.72, 127.84, 128.95, 129.0, 129.61, 129.79, 130.48, 135.95, 136.64, 137.74, 139.45, 149.10, 151.59, 157.94 and 170.39

Assignment of the IR spectra (Figure-9F3): Characteristics peaks are observed at 2880 (-CH stretch, aromatic), 1730 (>C=O stretch, cyclic ring), 1658 (>C=N stretch, imidazole ring), 1519 (>C=C<, aromatic), 1343 (-C - O stretching), 776 (-C=Cl), 1402 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-9F4)
The mass spectra display the molecular ion peaks at 460.1 (M^+), 447, 256, 204, 176.1, 139, 91, 66.1, 41. The compound 9f GCMS fragmentation as 2-(4-chlorophenyl)-4-(3,4-dimethoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 460.95, N-benzyldiyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 70.39 % and the nitrogen showed 6.12 %
The melting point of the compound is 210-214 °C. Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9F1

Figure 9F2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9F3

Figure 9F4
The compound the molecular formula is C_{26}H_{23}ClN_{2}O_{2} and the molecular weight is: 430.92

**Assignment of \(^{1}\)H NMR Chemical shifts (δ ppm) to different protons (Figure-9G1)**

The \(^{1}\)H NMR signals were observed at 1.97ppm (s, 6H, -Me), 2.26ppm (s, 3H, -Me), 3.83ppm (s, 3H, -OMe), 6.87-8.93 ppm (m, 11H, Ar-CH and -C=CH)

**Assignment of \(^{13}\)C NMR Chemical shifts (δ ppm) to different carbons (Figure-9G2)**: The \(^{13}\)C NMR signals were observed at 18.08, 21.21, 55.62, 110.72, 120.98, 123.39, 123.41, 127.81, 128.89, 129.27, 129.77, 130.52, 132.29, 133.28, 135.99, 137.78, 137.80, 139.38, 158.71, 159.52 and 170.43

**Assignment of the IR spectra (Figure-9G3)**: Characteristics peaks are observed at 2930 (-CH stretch, aromatic), 1729 (>C=O stretch, cyclic ring), 1653 (>C=N stretch, imidazole ring), 1515 (>C=C, Stretch, cyclic ring), 1491 (>C=C, Stretch, cyclic ring)

**Proposed fragmentation pattern (GCMS) (Figure-9G4)**: The mass spectra display the molecular ion peaks at 430.1 (M\(^{+}\)), 399.1, 337, 282, 256, 221, 174.1, 146, 138.9, 119, 91, 65, 39. The compound 9g GCMS fragmentation as 2-(4-chlorophenyl)-4-(2-methoxybenzylidene)-1-(3,4,5-trimethylphenyl)-4H-imidazol-5-one MW: 430.92, N-benzylidyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylum, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 72.52 % and the nitrogen showed 6.52 %

The melting point of the compound is 228-232 °C. Yield: 73 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9G1

Figure 9G2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9G3

Figure 9G4
4.2.38 CHARACTERIZATION OF 2-(4-chlorophenyl)-4-(4- Mebenzylidene)-1-(3,4,5-trimethylphenyl)-1H-imidazol-5(4H)-one - {9H}

The compound the molecular formula is C_{26}H_{23}ClN_{2}O and the molecular weight is: 414.92

Assignment of {\textsuperscript}{1}H NMR Chemical shifts to different - protons (Figure-9H1)
The {\textsuperscript}{1}H NMR signals were observed at 1.97ppm (s, 6H, - Me), 2.29ppm (s, 3H, - Me), 2.38ppm (s, 3H, - Me), 6.91-8.11 ppm (m, 11H, Ar-CH and - C= CH)

Assignment of {\textsuperscript}{13}C NMR Chemical shifts (δ ppm) to different carbons (Figure-9H2):
The {\textsuperscript}{13}C NMR signals were observed at 18.07, 21.20, 21.81, 127.74, 128.91, 129.27, 129.65, 129.70, 129.79, 130.44, 131.67, 132.72, 135.96, 137.66, 137.86, 139.46, 141.35, 158.71 and 170.51

Assignment of the IR spectra (Figure-9H3): Characteristics peaks are observed at 2924 (-CH stretch, aromatic), 1728 (>C=O stretch, cyclic ring), 1635 (>C=N stretch, imidazole ring), 1498 (>C=C<, aromatic), 1348 ( - C - O stretching), 639 (-C-Cl), 1409 (>C=C, Stretch, cyclic ring), 1483 (- Me group )

Proposed fragmentation pattern (GCMS) (Figure-9H4)
The mass spectra display the molecular ion peaks at 414.2 (M\textsuperscript{+}), 364.1, 295, 256.1, 221.1, 178, 138.9, 119, 91, 66, 41. The compound 9h GCMS fragmentation as 2-(4-chlorophenyl)-4-(4- Mebenzylidene)-1-(3,4,5-trimethylphenyl)-1H-imidazol-5(4H)-one MW: 414.92, N-benzyldyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as Carbon showed 75.29 % and the nitrogen showed 6.77 %
The melting point of the compound is 191-195 °C. Yield: 72 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9H1

Figure 9H2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9H3

Figure 9H4
4.2.39 CHARACTERIZATION OF 2-(4-chlorophenyl)- 4-(3-bromobenzylidene)-1-(3,4,5-trimethylphenyl)-1H-imidazol-5(4H)-one - {9I}

The compound the molecular formula is C_{25}H_{20}BrClN_{2}O and the molecular weight is: 479.79

Assignment of \textsuperscript{1}H NMR Chemical shifts to different - protons (Figure-9I1)
The \textsuperscript{1}H NMR signals were observed at 1.96ppm (s, 6H, - Me), 2.26ppm (s, 3H, - Me), 6.91-8.47ppm (m, 11H, Ar-CH and - C= CH)

Assignment of \textsuperscript{13}C NMR Chemical shifts (δ ppm) to different carbons (Figure-9I2): The \textsuperscript{13}C NMR signals were observed at 18.05, 21.21, 122.88, 127.07, 127.33, 129.05, 129.41, 129.86, 130.20, 130.25, 131.07, 133.19, 134.98, 135.89, 136.34, 138.39, 139.21, 139.66, 160.23 and 170.29

Assignment of the IR spectra (Figure-9I3)
Characteristics peaks are observed at 2969 (-CH stretch, aromatic), 1719 (>C=O stretch, cyclic ring), 1635 (>C=N stretch, imidazole ring), 1512 (>C=C< , aromatic), 1366 (- C - O stretching), 810 (-C-Cl), 1409 (>C=C, Stretch, cyclic ring), 669 (C-Br stretch, aromatic)

Proposed fragmentation pattern (GCMS) (Figure-9I4)
The mass spectra display the molecular ion peaks at 480.1(M\textsuperscript{+}), 399.1, 282, 256.1, 221.1, 194, 167, 138, 119, 91.1, 66, 41.1

The compound 9i GCMS fragmentation as 2-(4-chlorophenyl)- 4-(3-bromobenzylidene)-1-(3,4,5-trimethylphenyl)-1H-imidazol-5(4H)-one MW: 479.79, N-benzyldiyne-2- phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethyiun, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04 , prop-2-yn-1-ylium MW: 39.02

The compound elemental analysis demonstrates the result as
Carbon showed 62.62 % and the nitrogen showed 5.86 %
The melting point of the compound is 176-180 °C. Yield: 73 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9I1

Figure 9I2
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9I3

Figure 9I4
The compound the molecular formula is $C_{28}H_{27}ClN_2O_4$ and the molecular weight is: 490.97

Assignment of $^1H$ NMR Chemical shifts to different - protons (Figure-9J1)
The $^1H$ NMR signals were observed at 1.98ppm (s, 6H, -Me), 2.27ppm ( s, 3H, -Me), 3.88ppm ( s, 3H, -OMe), 3.89ppm ( s, 6H, -OMe), 6.91-7.59 ppm(m, 9H, Ar-CH and - C= CH)

Assignment of $^{13}C$ NMR Chemical shifts (δ ppm) to different carbons (Figure-9J2)
The $^{13}C$ NMR signals were observed at 18.06, 21.20, 56.14, 61.09, 109.93, 127.69, 129.01, 129.03, 129.25,129.75, 129.83, 130.37, 135.92, 137.64, 137.99, 139.55, 140.69, 153.21, 158.78 and 170.37

Assignment of the IR spectra (Figure-9J3)
Characteristics peaks are observed at 2980 ( -CH stretch, aromatic), 1723 (>C=O stretch, cyclic ring), 1639 (>C=N stretch, oxazole ring), 1510 (>C=C<, aromatic), 1349 (- C - O stretching), 813 (-C-Cl), 1490 (>C=C, Stretch, cyclic ring)

Proposed fragmentation pattern (GCMS) (Figure-9J4)
The mass spectra display the molecular ion peaks at 490.1( M$^+$), 475, 281, 256, 240, 206.1, 173.1, 146, 119, 91, 65, 39. The compound 9i GCMS fragmentation as 2-(4-chlorophenyl)-4-(3,4,5-trimethoxybenzylidene)-1-(3,4,5-trimethylphenyl)-1H-imidazol-5(4H)-one MW: 490.97, N-benzyldiyne-2-phenylethenaminium MW: 206.10, 2-phenylethenaminium MW: 120.08, phenylmethylium, MW: 91.05, cyclopenta-2,4-dien-1-ylium MW: 65.04, prop-2-yn-1-ylium MW: 39.02
The compound elemental analysis demonstrates the result as
Carbon showed 68.53 % and the nitrogen showed 5.74 %
The melting point of the compound is 211-216 °C. Yield: 71 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 9J3

Figure 9J4
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.3. CHARACTERIZATION OF S-TRIAZINE COMPOUNDS.

4.3.1 CHARACTERIZATION OF N\textsuperscript{2}, N\textsuperscript{4}-bis(6-bromobenzo[d]thiazol-2-yl)-N\textsubscript{6}-phenyl-1,3,5-triazine-2,4,6-triamine -{Br1}

The compound the molecular formula is C\textsubscript{23}H\textsubscript{14}Br\textsubscript{2}N\textsubscript{8}S\textsubscript{2} and The molecular weight is:626.35

Assignment of \textsuperscript{1}H NMR Chemical shifts (δ ppm) to different protons (Figure Br\textsubscript{1}-\textsuperscript{1}H)

The \textsuperscript{1}H NMR (DMSO) signals were observed at 11.2ppm (s, 2H, -NH), 10.9ppm (s, 1H, -NH), 7 ppm to 9 ppm (m, 11H, Ar-H).

Assignment of \textsuperscript{13}C NMR Chemical shifts (δ ppm) to different carbons (Figure Br\textsubscript{1}-\textsuperscript{13}C)

The \textsuperscript{13}C NMR (DMSO) signals were observed at 30.9, 113.9, 116, 118, 120, 121, 123, 124, 125, 128, 129, 130, 132, 150and 168.89 ppm.

Assignment of the IR spectra (Figure Br\textsubscript{1}- IR)

Characteristics peaks are observed at 3500 (-NH stretch, sec. amine), 3083 (-C-H stretch, aromatic), 1048 (-C-N stretch, s-triazine), 1593 (-C=N stretch, s-triazine), 813 (-C-N, s-triazine), 658 (C-S-C, Stretch, thiazolo),1048 ( Ar-Br, stretch, bromide).

The compound elemental analysis demonstrates the result as

Carbon showed 44.05 % and the nitrogen showed 17.85 %

The melting point of the compound is 225-230 °C. Yield: 68 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Br₁ -¹H

Figure Br₁ -¹³C
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure BR1 - IR

[IR spectra with wavenumbers and bands labeled]

[Diagram with molecular structure and labels]
4.3.2 CHARACTERIZATION OF N², N⁴-bis(6-bromobenzo[d]thiazol-2-yl)-N⁶-(3-chlorophenyl-1,3,5-triazine-2,4,6-triamine -{Br2}

The compound the molecular formula is C_{23}H_{13}Br_{2}ClN_{8}S_{2} and the molecular weight is: 660.79

Assignment of ¹H NMR Chemical shifts (δ ppm) to different protons (Figure Br₂-¹H)
The ¹H NMR (DMSO) signals were observed at 10.9 ppm (s, 2H, -NH), 12.1 ppm (s, 1H, -NH), 6.8 ppm to 8 ppm (m, 10H, Ar-H)

Assignment of ¹³C NMR Chemical shifts (δ ppm) to different carbons (Figure Br₂-¹³C)
The ¹³C NMR (DMSO) signals were observed at 30.89, 108, 112, 119, 120, 132, 124, 125, 128, 129, 130, 131, 133, 151, 167.8, 168.1 ppm

Assignment of the IR spectra (Figure Br₂- IR)
Characteristics peaks are observed at 3400 (-NH stretch, sec. amine), 3048 (-C-H stretch, aromatic), 1591 (-C=N stretch, s-triazine), 1179 (-C-N stretch, s-triazine), 1081 ( Ar-Br, stretch, bromide), 862 (-C-N, s-triazine), 658 (C-S-C, Stretch, thiazolo).

The compound elemental analysis demonstrates the result as
Carbon showed 41.60 % and the nitrogen showed 16.95 %

The melting point of the compound is 215-220 °C.
Yield: 56 %
Figure Br₂ -¹H

Figure Br₂ -¹³C
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Br2 - IR
4.3.3 CHARACTERIZATION OF N\textsuperscript{2}, N\textsuperscript{4}-bis(6-bromobenzo[d]thiazol-2-yl)-N\textsubscript{6}-(4-nitrophenyl)-1,3,5-triazine-2,4,6-triamine-{Br5}

The compound the molecular formula is \(C\textsubscript{23}H\textsubscript{13}Br\textsubscript{2}N\textsubscript{9}O\textsubscript{2}S\textsubscript{2}\) and the molecular weight is : 671.35

Assignment of \(^1\text{H} \text{NMR}\) Chemical shifts (\(\delta \text{ ppm}\)) to different protons (Figure Br5-\(^1\text{H}\))

The \(^1\text{H} \text{NMR}\) (DMSO) signals were observed at 10.9 ppm (s, 2H, -NH), 12.1 ppm (s, 1H, -NH), 6.8 ppm to 8 ppm (m, 10H, Ar-H)

Assignment of \(^{13}\text{C} \text{NMR}\) Chemical shifts (\(\delta \text{ ppm}\)) to different carbons (Figure Br5-\(^{13}\text{C}\))

The \(^{13}\text{C} \text{NMR}\) (DMSO) signals were observed at 112, 119, 123, 126, 128, 133, 136, 152, 156, 167.

Assignment of the IR spectra (Figure Br5- IR)

Characteristics peaks are observed at 3462 (-NH stretch, sec. amine), 3362 (-C-H stretch, aromatic), 1599 (-C=N stretch, s-triazine), 1113 (-C-N stretch, s-triazine), 1048 (Ar-Br, stretch, bromide), 841 (-C-N, s-triazine), 639 (C-S-C, Stretch, thiazolo), 1599, 1300 (-NO\textsubscript{2}, stretch ).

The compound elemental analysis demonstrates the result as

Carbon showed 41.11 % and the nitrogen showed 18.76 %

The melting point of the compound is 129-134 °C.
Synthesis and Characterization of $s$-Triazine and Imidazole Heterocycles

Yield: 67 %

Figure Br$_5$-$^1$H

Figure Br$_5$-$^{13}$C
Synthesis and Characterization of \( s \)-Triazine and Imidazole Heterocycles

**Figure Br 5-IR**

![IR Spectrum Diagram]

<table>
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<th>Wave Number cm(^{-1})</th>
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<tr>
<td>3362</td>
</tr>
<tr>
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<td>1970</td>
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</tr>
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<td>1113</td>
</tr>
<tr>
<td>641</td>
</tr>
<tr>
<td>633</td>
</tr>
</tbody>
</table>
4.3.4 CHARACTERIZATION OF \( \text{N}^2, \text{N}^4\)-bis(6-bromobenzo[d]thiazol-2-yl)-N6-(pyridin-4-yl)-1,3,5-triazine-2,4,6-triamine-{Br9}

The compound the molecular formula is \( \text{C}_{22}\text{H}_{13}\text{Br}_{2}\text{N}_{9}\text{S}_{2} \) and The molecular weight is: 627.34

**Assignment of \(^1\text{H} \text{NMR Chemical shifts (δ ppm)} \) to different protons (Figure Br9-\(^1\text{H}\))**

The \(^1\text{H} \text{NMR (DMSO)} \) signals were observed at 11.2ppm (s, 2H, -NH), 10.9ppm (s, 1H, -NH), 7 ppm to 9 ppm (m, 10H, Ar-H)

**Assignment of \(^{13}\text{C} \text{NMR Chemical shifts (ppm)} \) to different carbons (Figure Br9-\(^{13}\text{C}\))**

The \(^{13}\text{C} \text{NMR (DMSO)} \) signals were observed at 30, 109, 116,118, 124, 125, 126, 129, 130, 131, 133, 136, 140, 150, 160, 168 ppm

**Assignment of the IR spectra (Figure Br9- \text{IR})**

Characteristics peaks are observed at 3400 (-NH stretch, sec. amine), 3210 (-C-H stretch, aromatic),1600 (-C=N stretch, s-triazine), 1150 (-C-N stretch, s-triazine), 1050 ( Ar-Br, stretch, bromide), 850 (-C-N, s-triazine), 650 (C-S-C, Stretch, thiazolo).

The compound elemental analysis demonstrates the result as Carbon showed 42.09 % and the nitrogen showed 20.06 %

The melting point of the compound is 225-230 °C.

Yield: 69 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Br₉-¹H

Figure Br₉-¹³C
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Br9-IR
4.3.5 CHARACTERIZATION OF $N^2, N^4$-bis(6-bromobenzo[d]thiazol-2-yl)-N6-(4-hydroxyphenyl)-1,3,5-triazine-2,4,6-triamine-{Br12}

The compound the molecular formula is $C_{23}H_{14}Br_2N_8OS_2$ and the molecular weight is 642.35.

**Assignment of $^1H$ NMR Chemical shifts (δ ppm) to different protons (Figure Br12-$^1H$)**

The $^1H$ NMR (DMSO) signals were observed at 11.2 ppm (s, 2H, -NH), 10.9 ppm (s, 1H, -NH), 6.5 ppm to 9 ppm (m, 11H, Ar-H).

**Assignment of $^{13}C$ NMR Chemical shifts (δ ppm) to different carbons (Figure Br12-$^{13}C$)**

The $^{13}C$ NMR (DMSO) signals were observed at 115, 116, 117, 119, 125, 129, 130, 131, 132, 133, 136, 146, 168 ppm.

**Assignment of the IR spectra (Figure Br12-IR)**

Characteristics peaks are observed at 3465 (-NH stretch, sec. amine), 3065 (-C-H stretch, aromatic), 1623 (-C=N stretch, s-triazine), 1167 (-C-N stretch, s-triazine), 1048 (Ar-Br stretch, bromide), 813 (-C-N, s-triazine), 660 (C-S-C, Stretch, thiazolo).

The compound elemental analysis demonstrates the result as Carbon showed 44.94 % and the nitrogen showed 17.42 %.

The melting point of the compound is 195-200 °C.

Yield: 60 %
Figure Br_{12}-IR
4.3.6 CHARACTERIZATION OF $N^2, N^4$-bis(6-chlorobenzo[d]thiazol-2-yl)-N6-phenyl-1,3,5-triazine-2,4,6-triamine - {Cl 1}

The compound the molecular formula is $C_{23}H_{14}Cl_2N_8S_2$ and The molecular weight is: 537.45

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure Cl$_1$-$^1$H)
The $^1$H NMR (DMSO) signals were observed at 11.2ppm (s, 2H, -NH), 10.9ppm (s, 1H, -NH), 6.5 ppm to 8 ppm (m, 11H, Ar-H)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure Cl$_1$-$^{13}$C)
The $^{13}$C NMR (DMSO) signals were observed at 30, 34, 07, 117, 118, 120, 121, 122, 123, 124, 126, 127, 128, 129, 130, 131, 137, 142, 150, 168

Assignment of the IR spectra (Figure Cl$_1$- IR)
Characteristics peaks are observed at 3300 (-NH stretch, sec. amine), 3060 (-C-H stretch, aromatic), 1518 (-C=N stretch, s-triazine), 1100 (-C-N stretch, s-triazine), 766 ( Ar-Cl, stretch), 811 (-C-N, s-triazine), 692 (C-S-C, Stretch, thiazolo).

The compound elemental analysis demonstrates the result as
Carbon showed 51.15 % and the nitrogen showed 20.60 %
The melting point of the compound is 200-205 °C.
Yield: 64 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Cl-¹H

Figure Cl-¹³C
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Cl-IR
4.3.7 CHARACTERIZATION OF N², N⁴-bis(6-chlorobenzo[d]thiazol-2-yl)-N⁶-(4-chlorophenyl)-1,3,5-triazine-2,4,6-triamine - {Cl 3}

The compound the molecular formula is C₂₃H₁₃Cl₃N₈S₂ and The molecular weight is: 571.89

Assignment of ¹H NMR Chemical shifts (δ ppm) to different protons (Figure Cl₃-¹H)
The ¹H NMR (DMSO) signals were observed at 11.2ppm (s, 2H, -NH), 10.9ppm (s, 1H, -NH), 6.5 ppm to 8 ppm (m, 10H, Ar-H)

Assignment of ¹³C NMR Chemical shifts (δ ppm) to different carbons (Figure Cl₃-¹³C)
The ¹³C NMR (DMSO) signals were observed at 29, 30, 107, 115, 119, 120, 121, 122, 124, 126, 128, 129, 131, 133, 124, 150, 152, 156, 167, 168

Assignment of the IR spectra (Figure Cl₃-IR)
Characteristics peaks are observed at 3300 (-NH stretch, sec. amine), 3084 (-C-H stretch, aromatic), 1524 (-C=N stretch, s-triazine), 1100 (-C=N stretch, s-triazine), 767 (Ar-Cl, stretch), 812 (-C-N s-triazine), 659 (C-S-C, Stretch, thiazolo).

The compound elemental analysis demonstrates the result as
Carbon showed 48.12 % and the nitrogen showed 19.48 %

The melting point of the compound is 175-180 °C.

Yield: 58 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Cl$_3$-$^1$H

Figure Cl$_3$-$^{13}$C
Figure Cl3-IR
4.3.8 CHARACTERIZATION OF $N^2, N^4$-bis(6-chlorobenzo[d]thiazol-2-yl)-N6-(3-nitrophenyl)-1,3,5-triazine-2,4,6-triamine- {Cl 4}

![Chemical Structure](image)

The compound the molecular formula is $C_{23}H_{13}C_{12}N_{9}O_{2}S_{2}$ and the molecular weight is 582.44

Assignment of $^1H$ NMR Chemical shifts (δ ppm) to different protons (Figure Cl4-$^1H$)

The $^1H$ NMR (DMSO) signals were observed at 11.2ppm (s, 2H, -NH), 10.9ppm (s, 1H, -NH), 6.5 ppm to 8 ppm (m, 10H, Ar-H)

Assignment of $^{13}C$ NMR Chemical shifts (δ ppm) to different carbons (Figure Cl4-$^{13}C$)

The $^{13}C$ NMR (DMSO) signals were observed at 29, 30, 107, 110, 115, 118, 120, 121, 122, 125, 126, 127, 128, 130, 131, 132, 142, 148, 149, 150, 151, 167

Assignment of the IR spectra (Figure Cl4- IR)

Characteristics peaks are observed at 3300 (-NH stretch, sec. amine), 3060 (-C-H stretch, aromatic), 1518 (-C=N stretch, s-triazine), 1100 (-C-N stretch, s-triazine), 766 ( Ar-Cl, stretch), 811 (-C-N, s-triazine), 692 (C-S-C, Stretch, thiazolo),1524, 1350 ( -NO$_2$,stretch).

The compound elemental analysis demonstrates the result as

Carbon showed 47.41 % and the nitrogen showed 21.52 %

The melting point of the compound is 170-175 °C. Yield: 62 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Cl₄⁻¹H

Figure Cl₄⁻¹³C
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles
4.3.9 CHARACTERIZATION OF N$_2$, N$_4$-bis(6-chlorobenzo[d]thiazol-2-yl)-N6-(4-fluorophenyl)-1,3,5-triazine-2,4,6-triamine- {Cl 7}

![Chemical Structure]

The compound the molecular formula is C$_{23}$H$_{13}$Cl$_2$F$_3$N$_8$S$_2$ and the molecular weight is: 555.44

**Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure Cl$_7$-$^1$H)**

The $^1$H NMR (DMSO) signals were observed at 11.2 ppm (s, 2H, -NH), 10.9 ppm (s, 1H, -NH), 6.5 ppm to 8 ppm (m, 10H, Ar-H)

**Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure Cl$_7$-$^{13}$C)**

The $^{13}$C NMR (DMSO) signals were observed at 24, 107, 107, 115, 116, 120, 121, 122, 126, 127, 128, 131, 132, 150, 159, 168, 169

**Assignment of the IR spectra (Figure Cl$_7$- IR)**

Characteristics peaks are observed at 3397 (-NH stretch, sec. amine), 3065 (-C-H stretch, aromatic), 1506 (-C=N stretch, s-triazine), 1101 (-C=N stretch, s-triazine), 1268 (Ar-F, stretch), 811 (-C-N, s-triazine), 715 (C-S-C, Stretch, thiazolo).

The compound elemental analysis demonstrates the result as

Carbon showed 49.62 % and the nitrogen showed 20.09 %

The melting point of the compound is 200-205 °C.

Yield: 63 %
Synthesis and Characterization of 2-Triazine and Imidazole Heterocycles

Figure Cl\textsubscript{7}-\textsuperscript{1}H

Figure Cl\textsubscript{7}-\textsuperscript{13}C
Figure CI7-IR
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

4.3.10 CHARACTERIZATION OF N$_2$N$_4$-bis(6-chlorobenzo[d]thiazol-2-yl)-N6-(pyridin-4-yl)-1,3,5-triazine-2,4,6-triamine- {Cl 9}

The compound the molecular formula is C$_{22}$H$_{13}$Cl$_2$N$_9$S$_2$ and the molecular weight is: 538.43

Assignment of $^1$H NMR Chemical shifts (δ ppm) to different protons (Figure Cl$_9$-$^1$H)

The $^1$H NMR (DMSO) signals were observed at 11.2 ppm (s, 2H, -NH), 10.9 ppm (s, 1H, -NH), 6.5 ppm to 8 ppm (m, 10H, Ar-H)

Assignment of $^{13}$C NMR Chemical shifts (δ ppm) to different carbons (Figure Cl$_9$-$^{13}$C)

The $^{13}$C NMR (DMSO) signals were observed at 107, 108, 118, 121, 122, 125, 126, 127, 128, 131, 140, 142, 150, 167, 168

Assignment of the IR spectra (Figure Cl$_9$-IR)

Characteristics peaks are observed at 3300 (-NH stretch, sec. amine), 3061 (-C-H stretch, aromatic), 1522 (-C=N stretch, s-triazine), 1100 (-C-N stretch, s-triazine), 1140 (-C-N stretch, pyridine), 1050, 766 (Ar-Cl, stretch), 812 (-C-N, s-triazine), 659 (C=S=C, Stretch, thiazo).

The compound elemental analysis demonstrates the result as
Carbon showed 49.03 % and the nitrogen showed 23.31 %

The melting point of the compound is 235-240 °C.

Yield: 62 %
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Cl₉⁻¹H

Figure Cl₉⁻¹³C
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure Cl9-IR
4.4 CHARACTERIZATION OF 1,2,4-TRIAZINE COMPOUNDS.

4.4.1 CHARACTERIZATION OF 5-(3,4-dimethoxybenzylidene)-2-phenyl-3-(m-tolyl)-1,2-dihydro-1,2,4-triazin-6(5H)-one: {10f}

The compound the molecular formula is \( \text{C}_{25}\text{H}_{23}\text{N}_{3}\text{O}_{3} \) and the molecular weight is: 413.47

Assignment of \(^1\text{H} \) NMR Chemical shifts (\( \delta \) ppm) to different protons (Figure 10f-\(^1\text{H}\))

The \(^1\text{H} \) NMR (\( \text{CDCl}_3 \)) signals were observed at 1.99ppm (s, 6H, -OMe), 2.10ppm (s, 3H, -Me) 6.0-7.7 ppm (m,14 H, Ar-CH and -C=CH)

Assignment of \(^{13}\text{C} \) NMR Chemical shifts (\( \delta \) ppm) to different carbons (Figure10f-\(^{13}\text{C}\))

Peaks present at 19.5, 20.96, 112.24, 113.72, 121.52, 128.99, 146.87, 147.52, 170.26, and 176.92ppm

The compound elemental analysis demonstrates the result as

Carbon showed 72.58 % and the nitrogen showed 10.12 %

The melting point of the compound is 160-165 °C

Yield: 68%
Synthesis and Characterization of s-Triazine and Imidazole Heterocycles

Figure 10f - $^1$H NMR

Figure 10f - $^{13}$C NMR
4.4.2 CHARACTERIZATION OF 2-phenyl-3-(m-tolyl)-5-(3,4,5-trimethoxybenzylidene)-1,2-dihydro-1,2,4-triazin-6(5H)-one: \{10j\}

The compound the molecular formula is \( \text{C}_{26}\text{H}_{25}\text{N}_{3}\text{O}_{4} \) and the molecular weight is: 443.49

The compound elemental analysis demonstrates the result as
Carbon showed 70.38 % and the nitrogen showed 9.43 %
The melting point of the compound is 220-225 °C
Yield: 65 %

4.4.3 CHARACTERIZATION OF 3-(4-chlorophenyl)-5-(3,4-dimethoxybenzylidene)-2-phenyl-1,2-dihydro-1,2,4-triazin-6(5H)-one \{11f\}

The compound the molecular formula is \( \text{C}_{24}\text{H}_{20}\text{ClN}_{3}\text{O}_{3} \) and the molecular weight is: 433.89

The compound elemental analysis demonstrates the result as
Carbon showed 66.40 % and the nitrogen showed 9.64 %
The melting point of the compound is 225-230 °C. Yield: 62 %
4.4.4 CHARACTERIZATION OF 3-(4-chlorophenyl)-2-phenyl-5-(3,4,5-trimethoxybenzylidene)-1,2-dihydro-1,2,4-triazin-6(5H)-one {11f}

The compound the molecular formula is C_{25}H_{22}ClN_{3}O_{4} and the molecular weight is: 463.91

The compound elemental analysis demonstrates the result as
Carbon showed 64.52 % and the nitrogen showed 9.04 %
The melting point of the compound is 205-210 °C
Yield: 67 %