Supplementary Information

Synthesis, spectroscopical studies, DFT, ADME, molecular docking analysis, antimalarial, antimicrobial activities of some *E*-imines and XRD structure of (*E*)-*N*-(2-bromobenzylidene)-2-(trifluoromethyl)benzenamine

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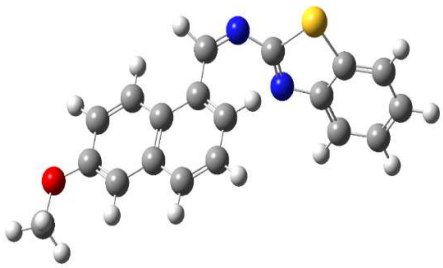
Received 26 September 2025; accepted (revised) 4 November 2025

DFT structure of imines-Optimized Structure (1-16)



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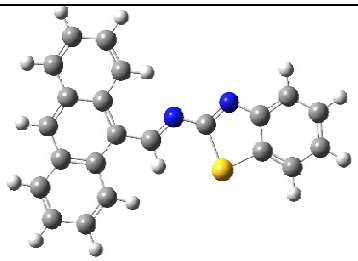

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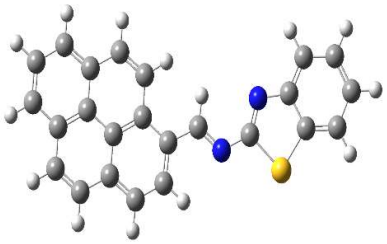

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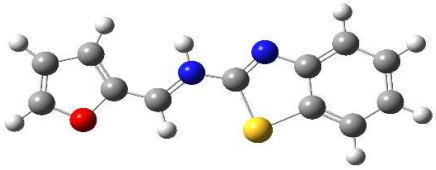

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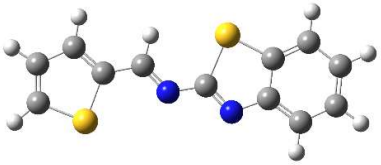

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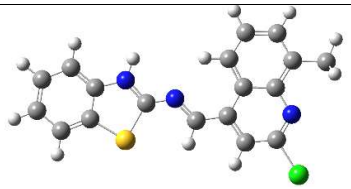

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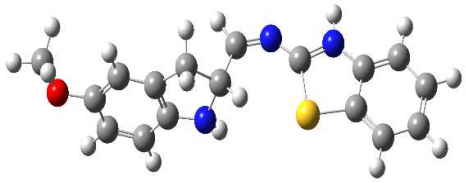

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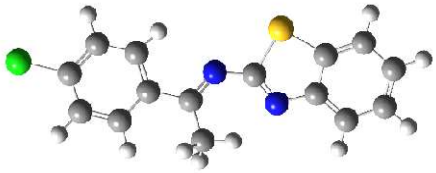

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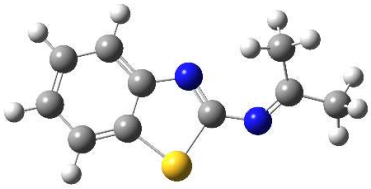

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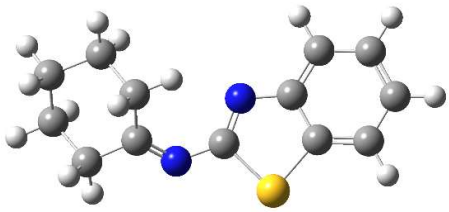

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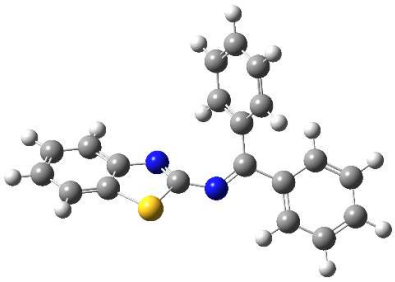

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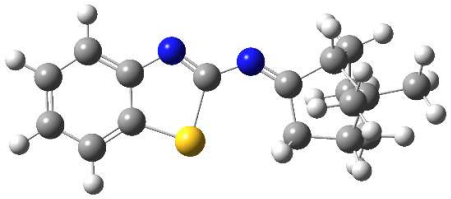

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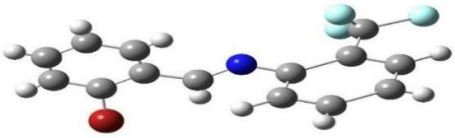

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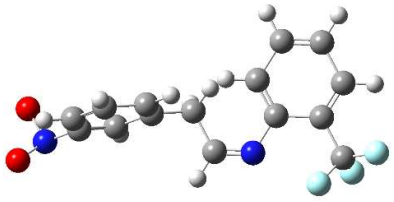

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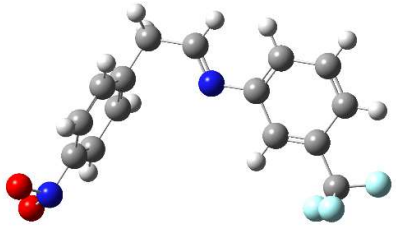

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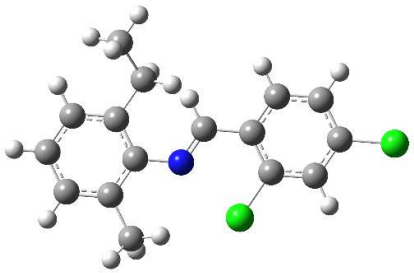

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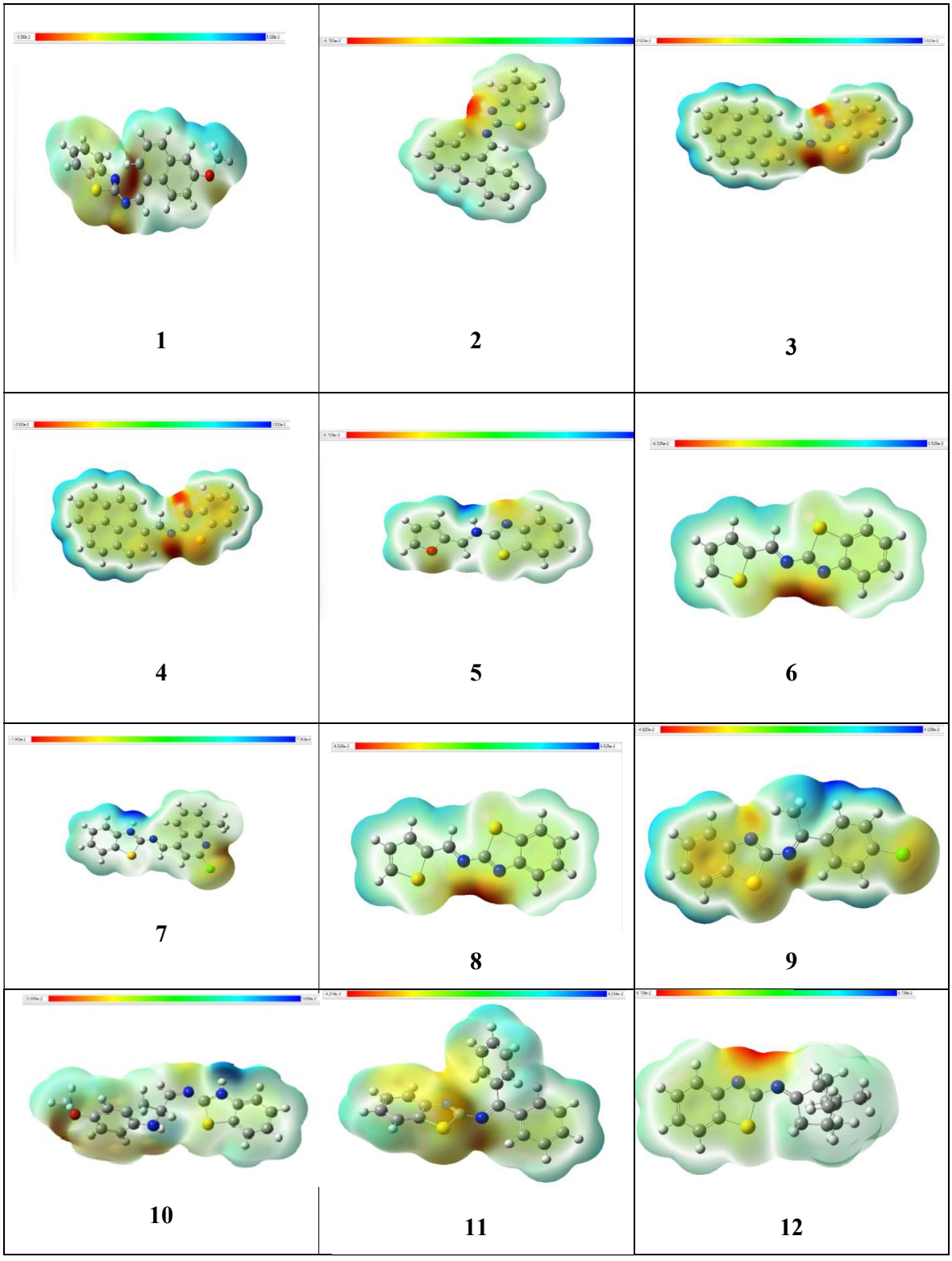
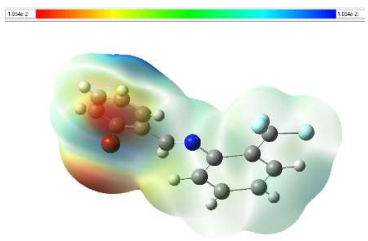
Molecular ESP evaluation of Schiff bases (1-16)





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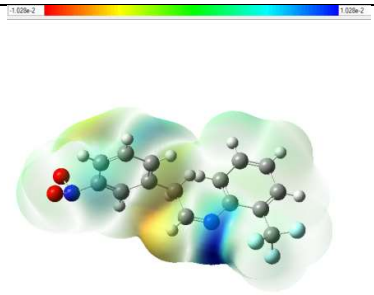

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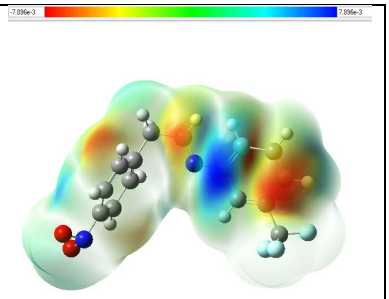

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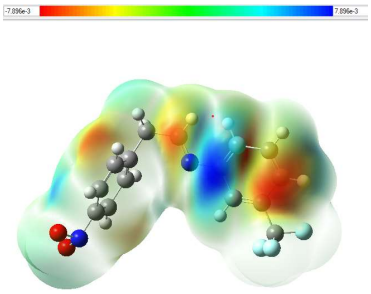

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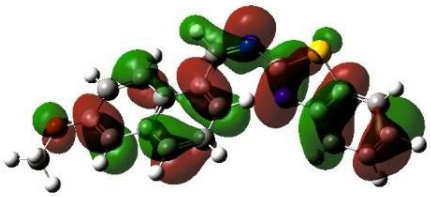
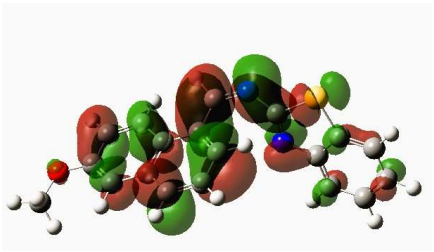
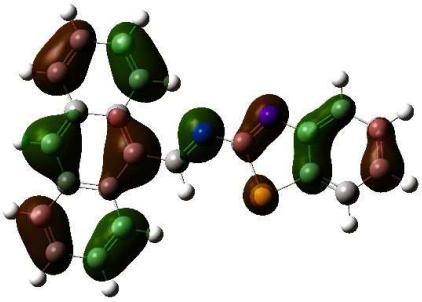
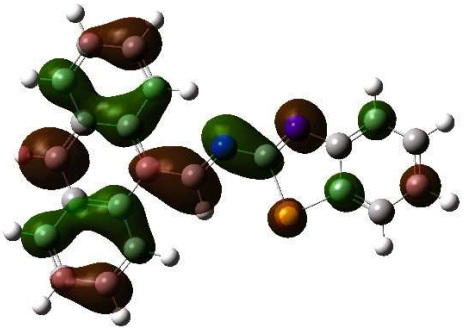
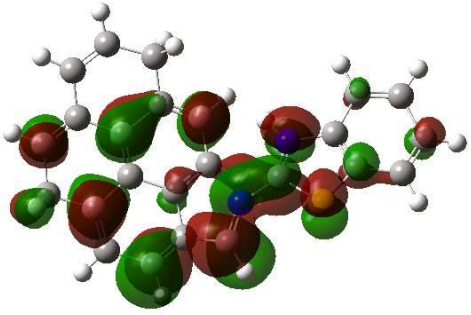
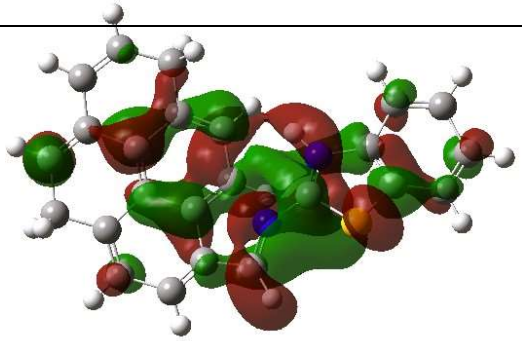
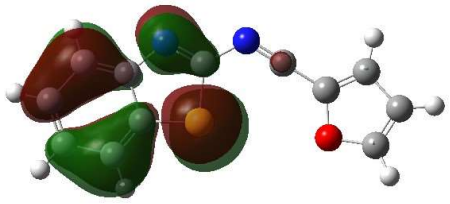
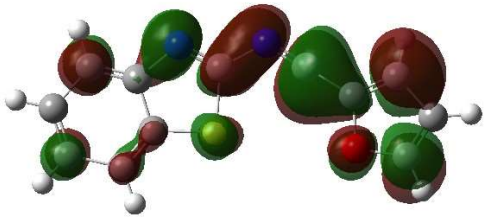
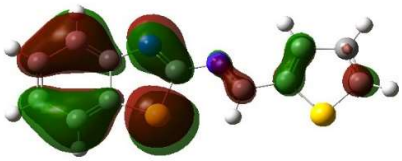
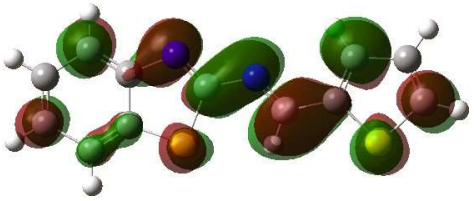
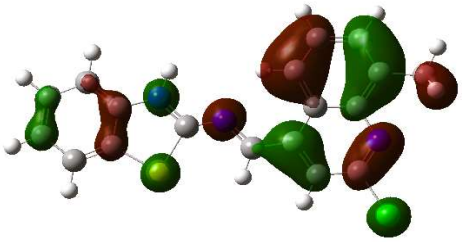
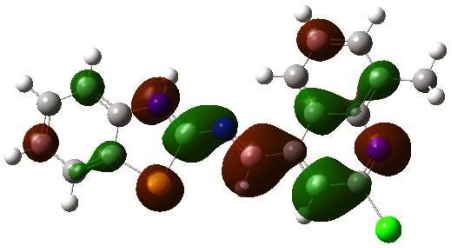
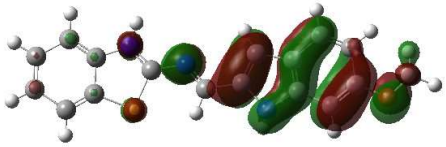
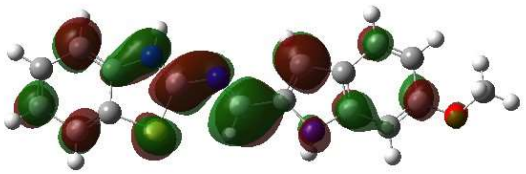
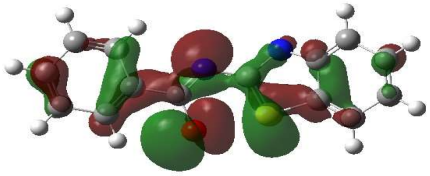
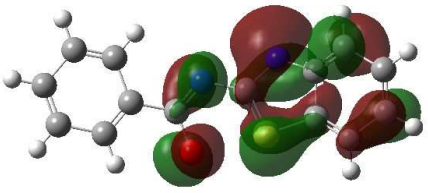
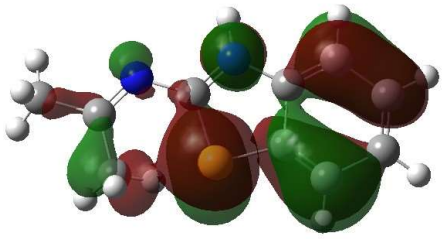
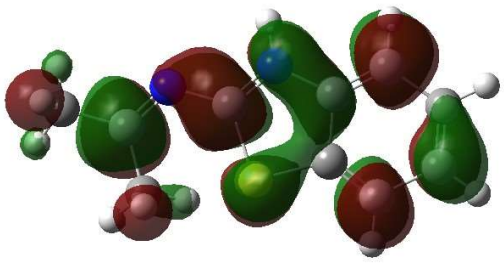
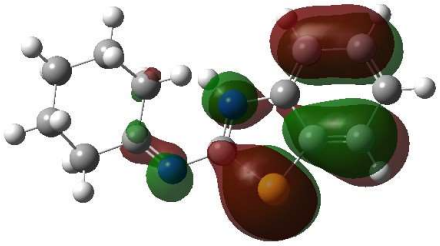
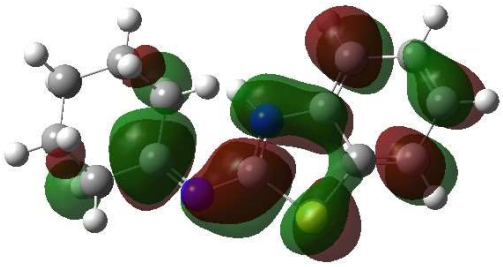
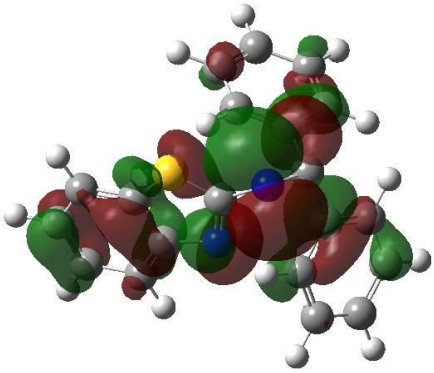
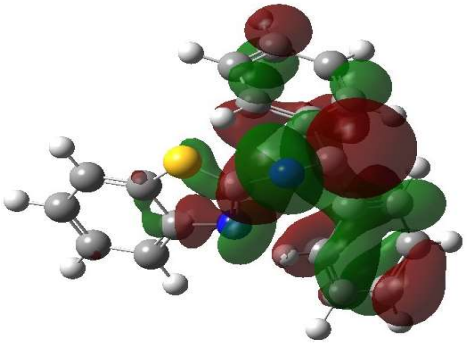
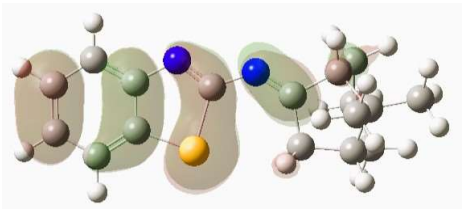
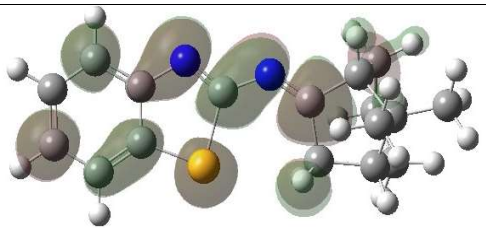
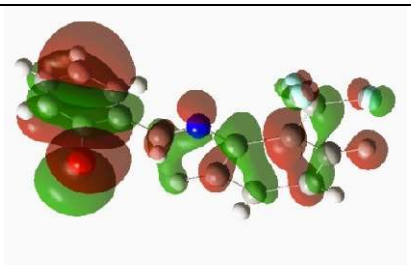
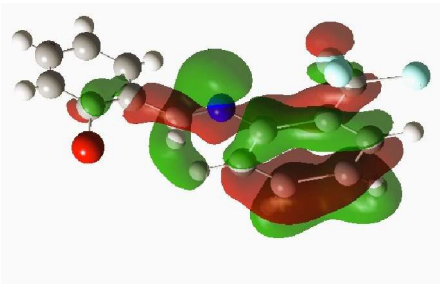
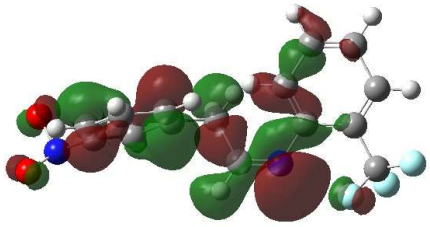
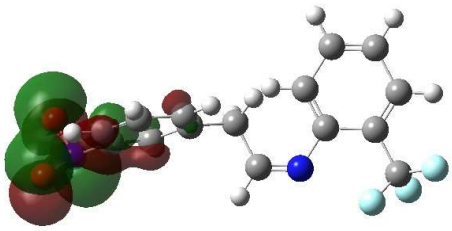
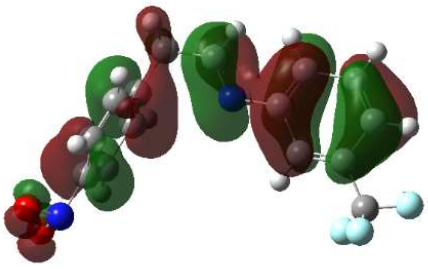
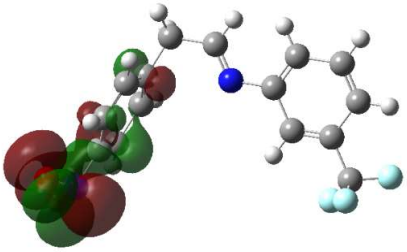
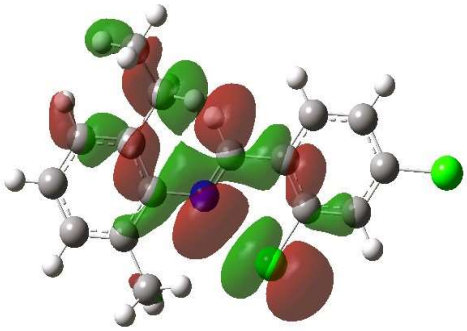
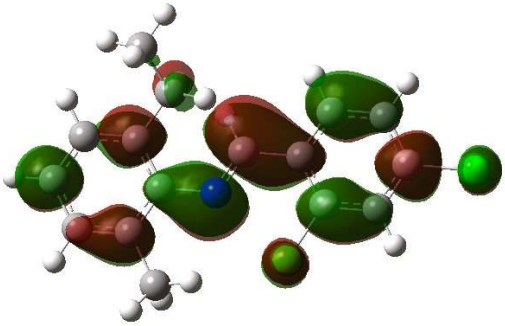
The HOMO and LUMO of the Schiff bases (1-16)

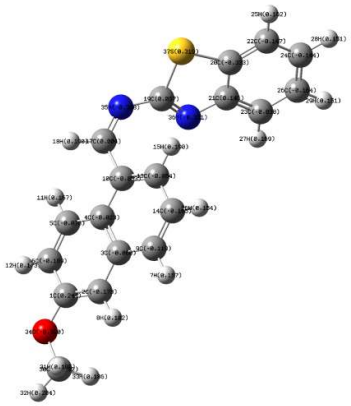
Entry	Homo	Energy gap	Lumo
1	 **-6.068**	**ΔG= 3.68 eV**	 **-2.367**
2	 **-5.714**	**ΔG= 2.76 eV**	 **-2.966**
3	 **-5.741**	**ΔG= 2.96 eV**	 **-2.775**

4	 **-6.149**	**ΔG= 3.77 eV**	 **-2.394**
5	 **-6.503**	**ΔG= 3.89 eV**	 **-2.612**
6	 **-6.286**	**ΔG= 3.19 eV**	 **-3.102**
7	 **-4.789**	**ΔG= 2.69 eV**	 **-2.095**
8	 **-6.394**	**ΔG= 3.80 eV**	 **2.585**

9	 **-6.340**	**ΔG= 4.51eV**	 **-1.823**
10	 **-6.231**	**ΔG= 4.52 eV**	 **-1.714**
11	 **4.520**	**ΔG= 3.81 eV**	 **-2.258**
12	 **-6.449**	**ΔG= 4.40 eV**	 **-2.014**

13	 **-4.843**	**ΔG=1.45 eV**	 **1.453**
14	 **-7.047**	**ΔG= 2.12 eV**	 **-4.925**
15	 **-7.292**	**ΔG= 2.66 eV**	 **-4.626**
16	 **-5.905**	**ΔG= 0.14 eV**	 **-1.932**

MULLIKEN CHARGES OF Imines 1-16



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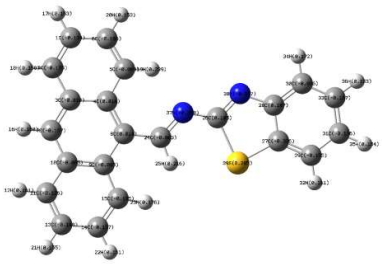

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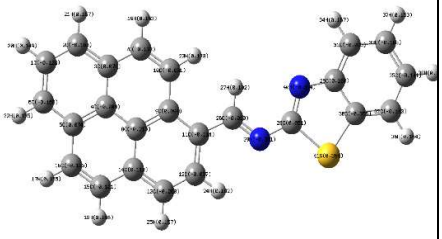

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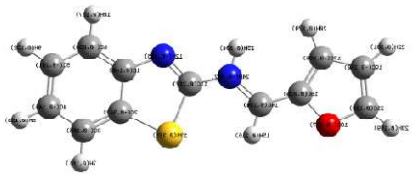

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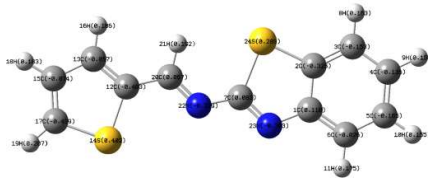

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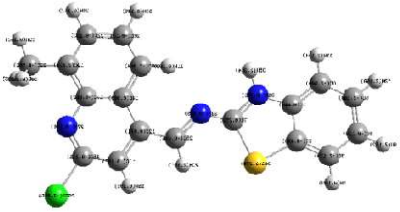

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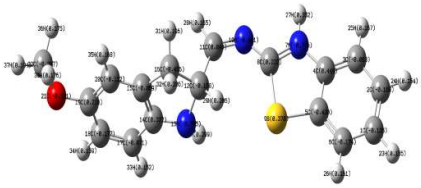

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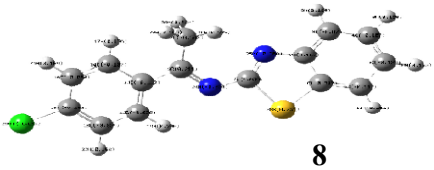

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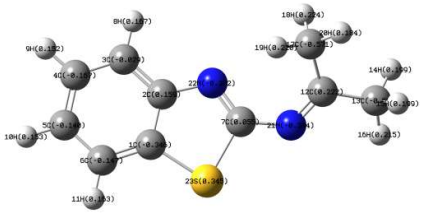

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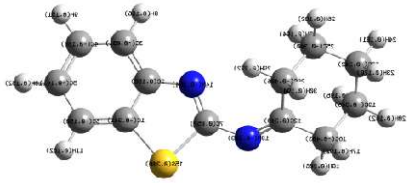

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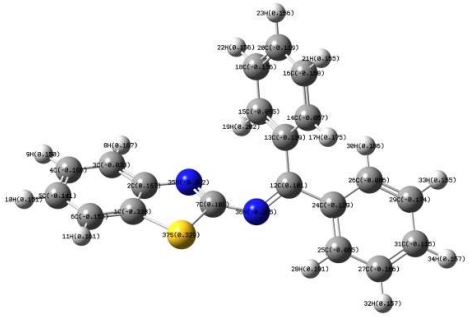

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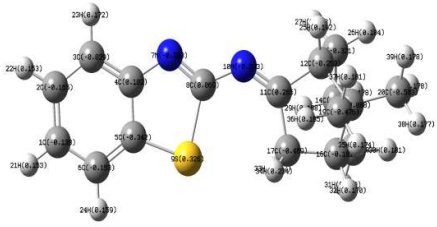

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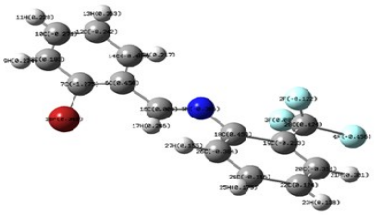

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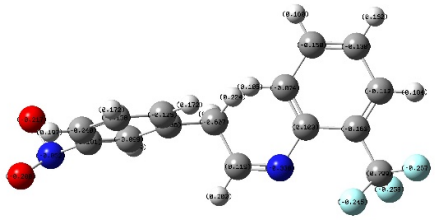

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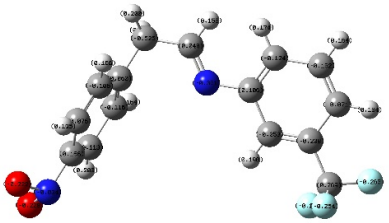

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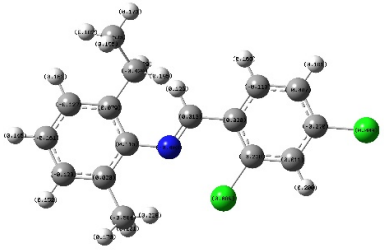
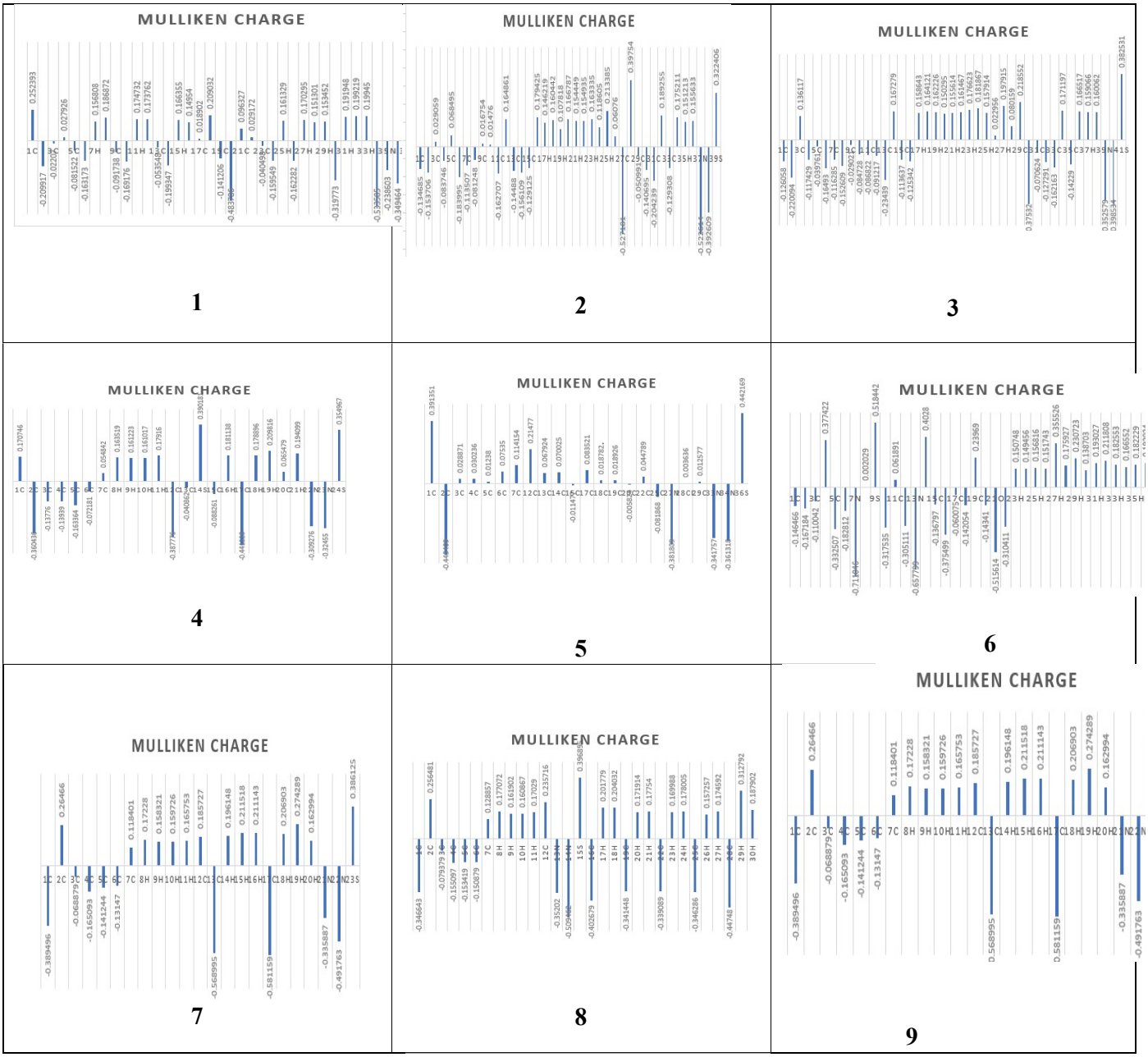
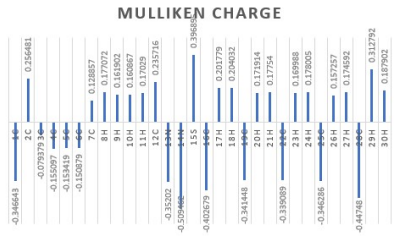


16

Mulliken charges of imines (1-16)





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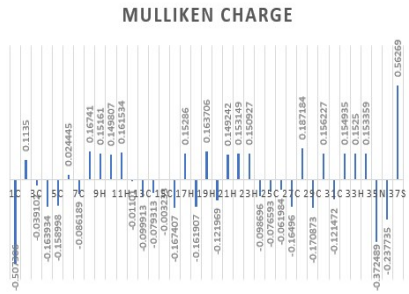

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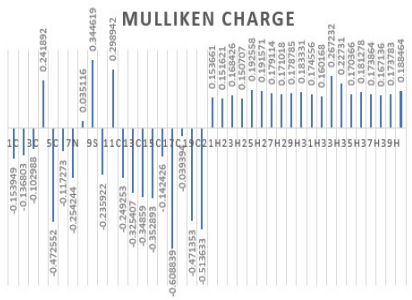

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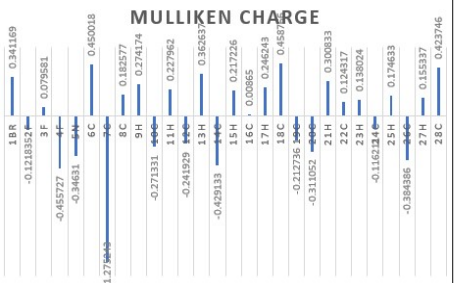

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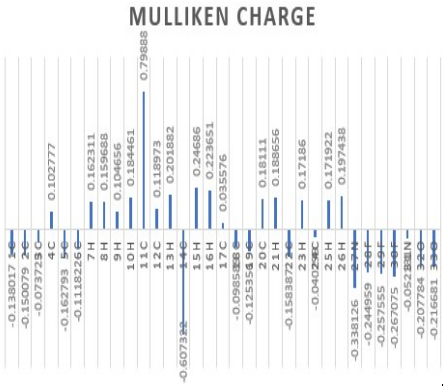

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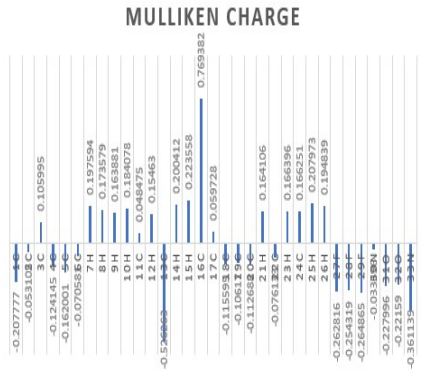

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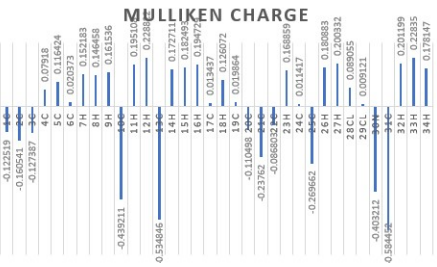
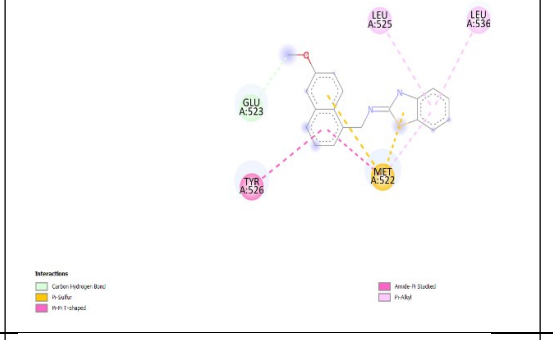
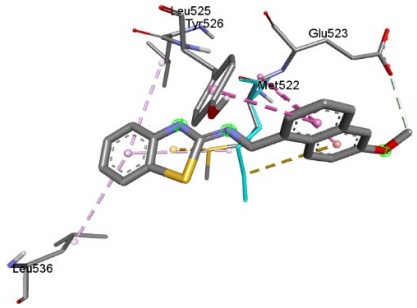
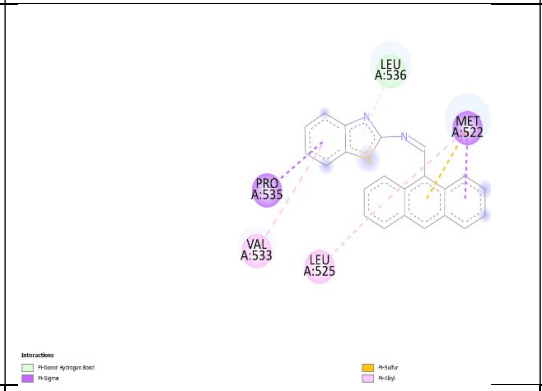
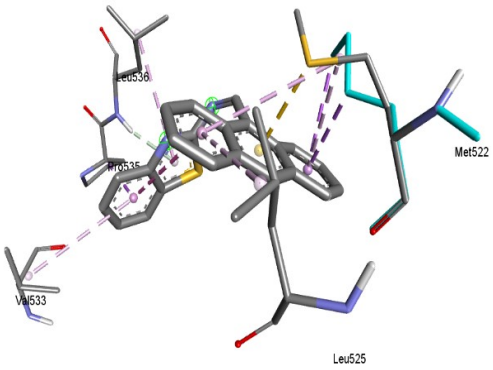
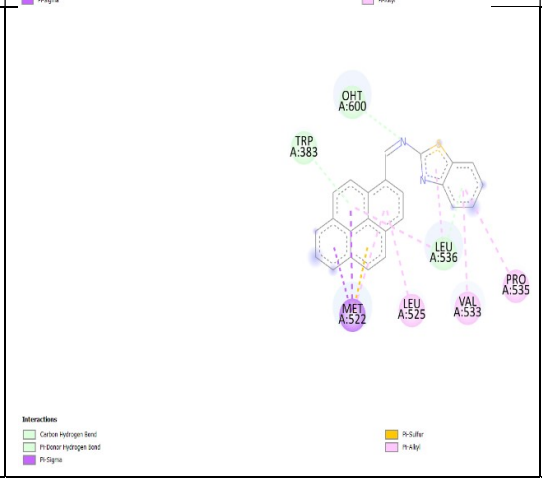
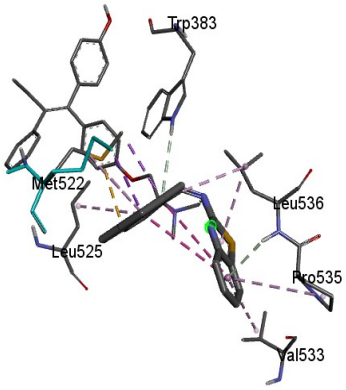
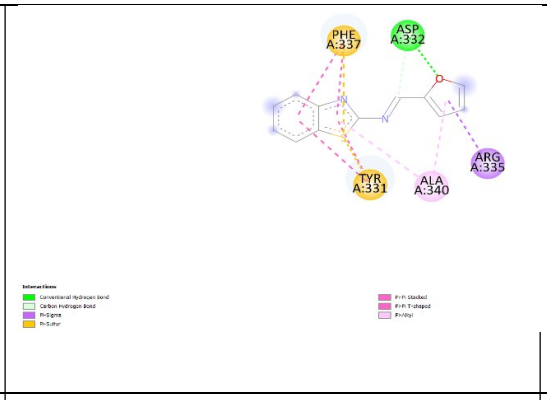
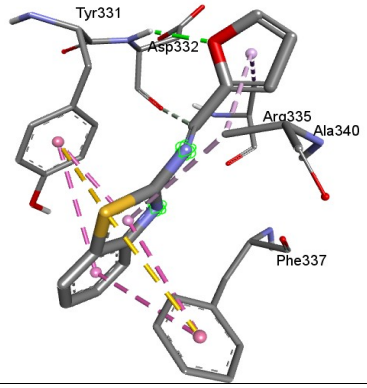
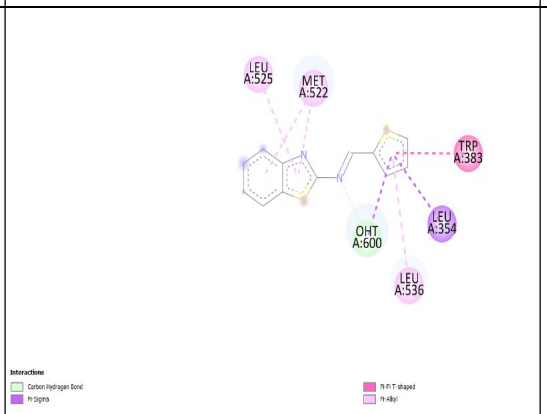
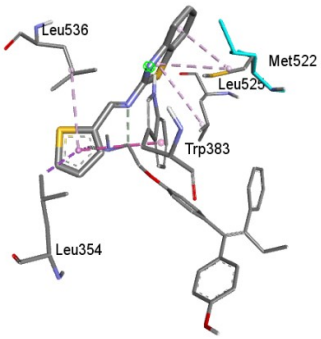
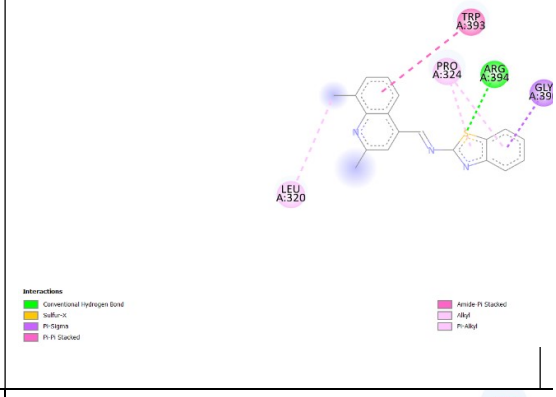
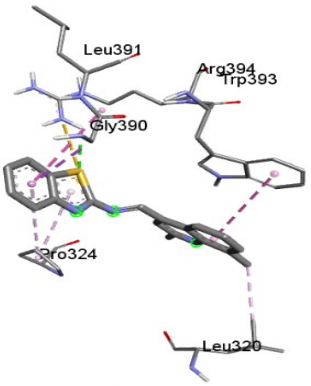
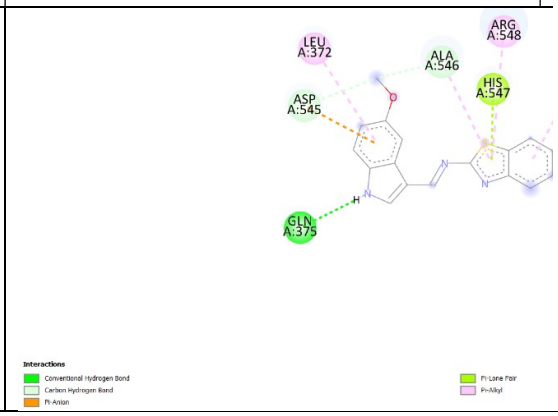
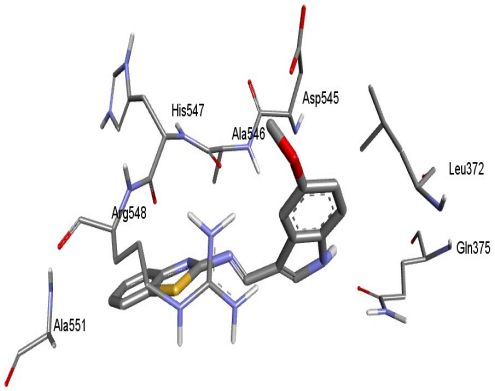
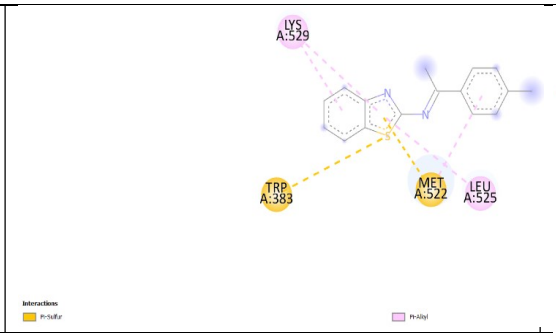
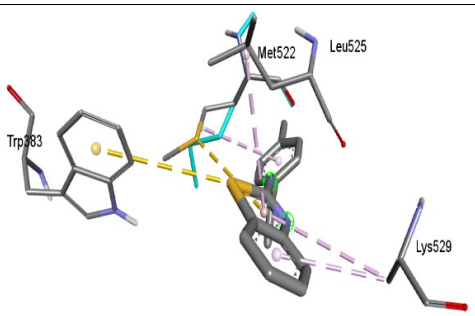
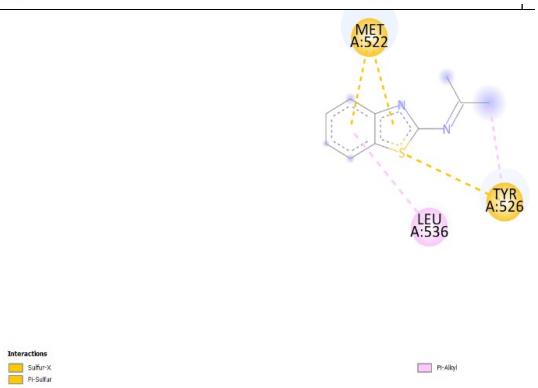
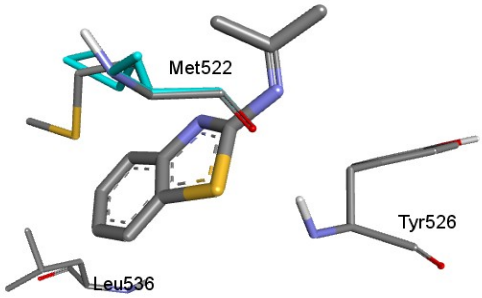
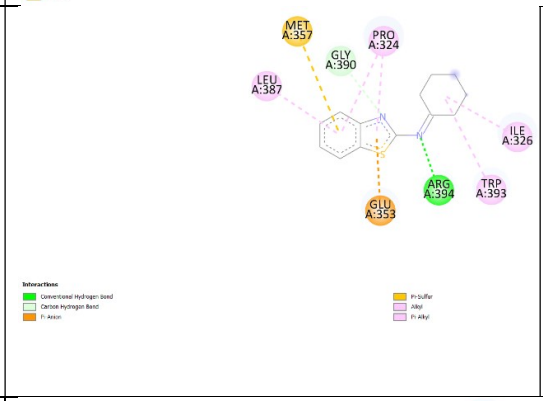
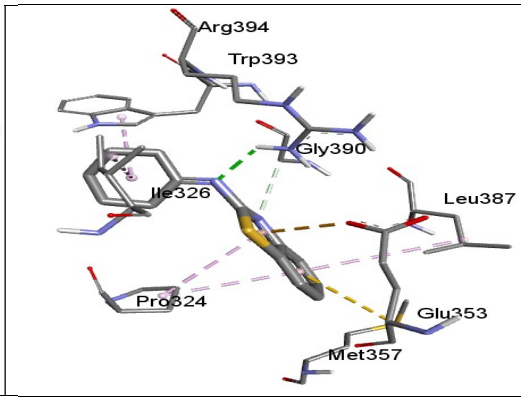
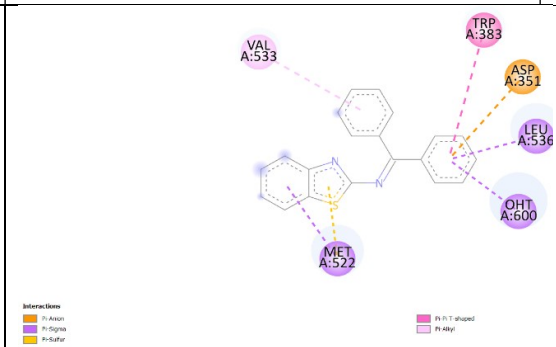
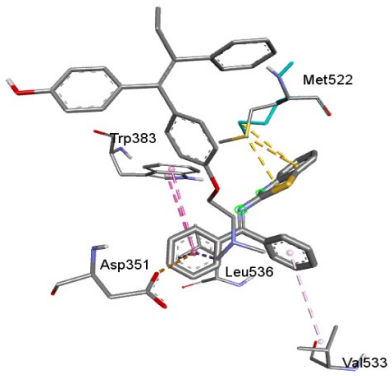


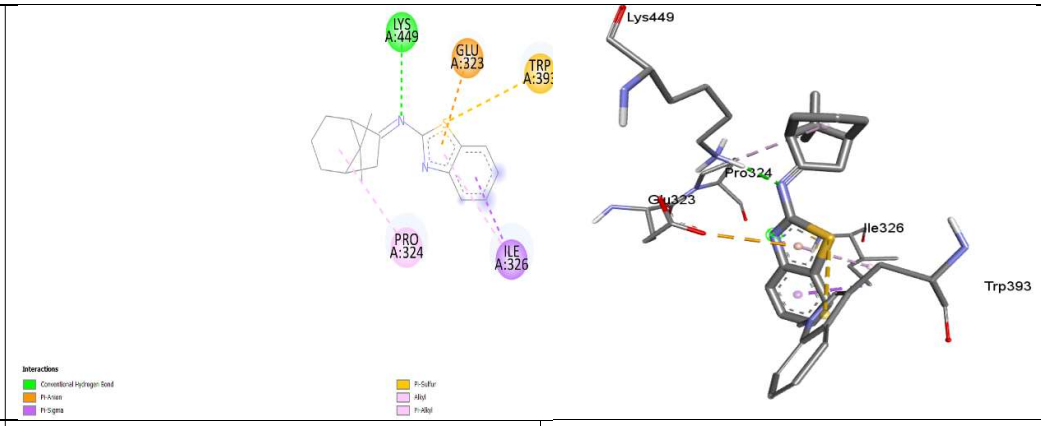
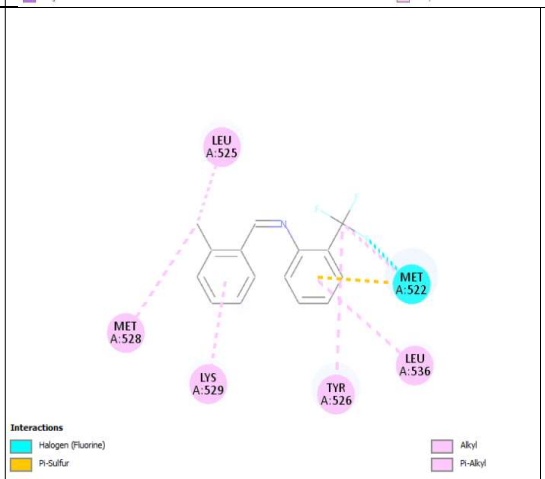
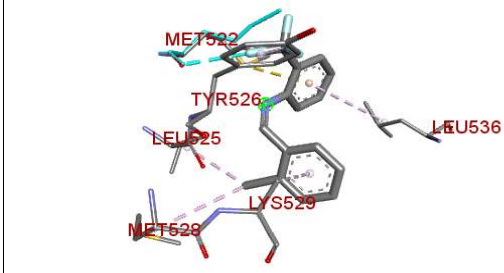
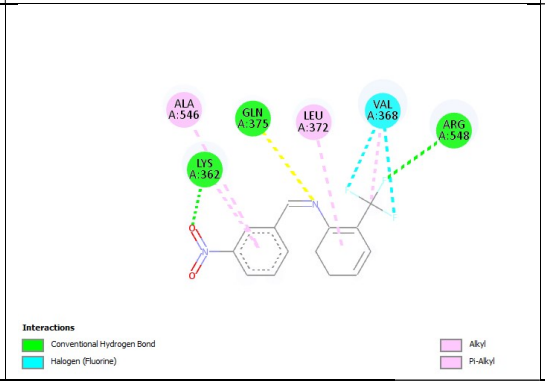
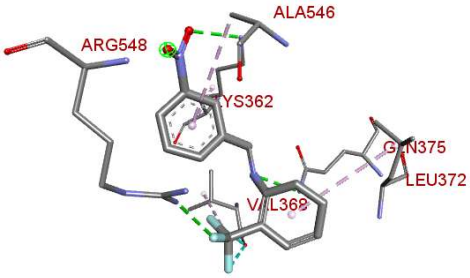
16

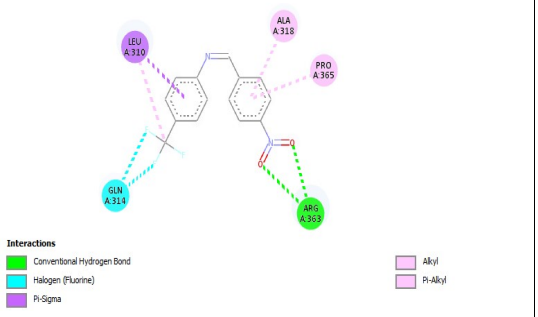
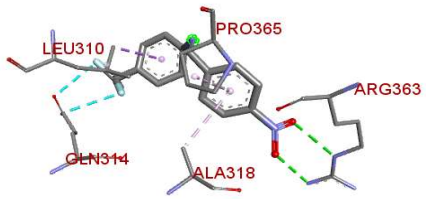
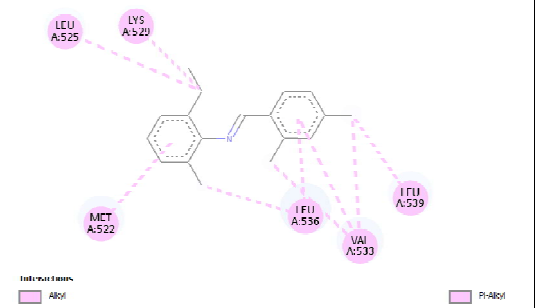
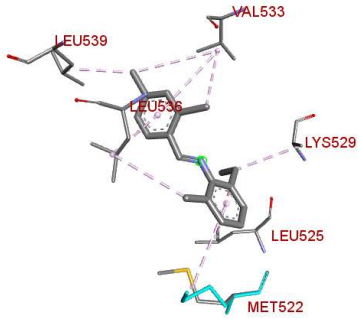
The Molecular Docking 2D and 3D structure of imines (1-16)

Entry	2D	3D
1		
2		
3		

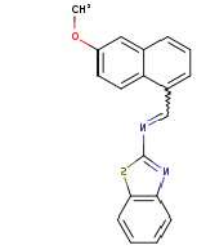
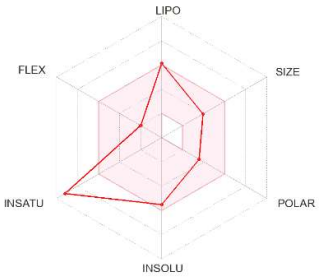
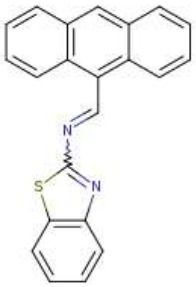
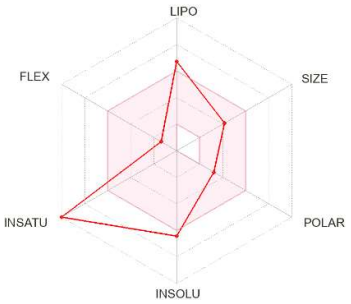
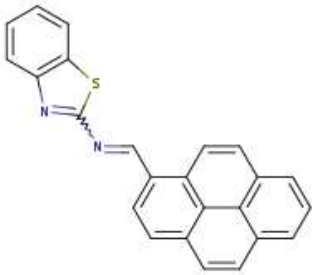
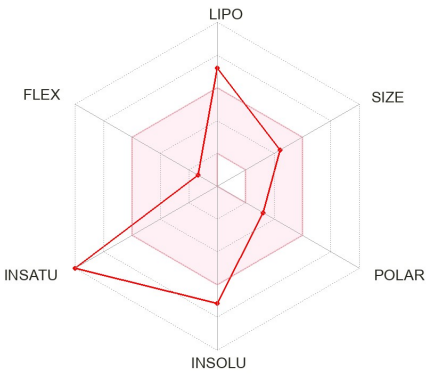
4	 PHE A:337 ASP A:332 ARG A:335 TYR A:331 ALA A:340	 Tyr331 Asp332 Arg335 Ala340 Phe337
5	 LEU A:525 MET A:522 TRP A:383 LEU A:354 OHT A:600 LEU A:536	 Leu536 Met522 Leu525 Trp383 Leu354
6	 TRP A:393 PRO A:324 ARG A:394 LEU A:320	 Leu391 Arg394 Trp393 Gly390 Pro324 Leu320
7	 ARG A:548 LEU A:372 ALA A:546 HIS A:547 ASP A:545 GLN A:375	 His547 Asp545 Ala546 Leu372 Arg548 Gln375 Ala551

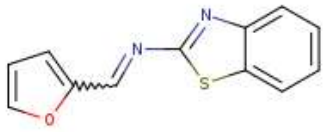
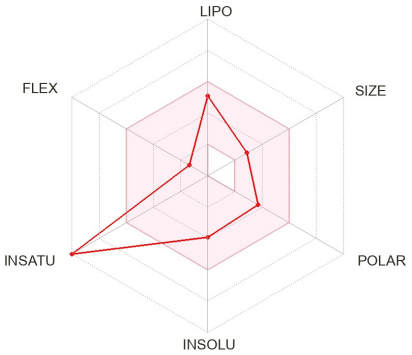
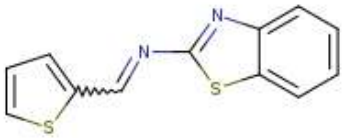
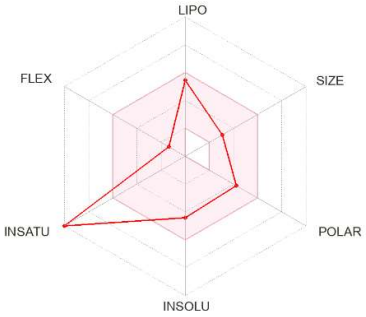
8	 LYS A:529 TRP A:383 MET A:522 LEU A:525 Interactions Pi-Sulfur Pi-Alkyl	 Met522 Leu525 Trp383 Lys529
9	 MET A:522 TYR A:526 LEU A:536 Interactions Sulfur-X Pi-Sulfur Pi-Alkyl	 Met522 Tyr526 Leu536
10	 MET A:357 GLY A:390 PRO A:324 LEU A:387 ILE A:326 ARG A:394 TRP A:393 GLU A:353 Interactions Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Anion Pi-Sulfur Alkyl Pi-Alkyl	 Arg394 Trp393 Gly390 Ile326 Leu387 Pro324 Glu353 Met357
11	 TRP A:383 VAL A:533 ASP A:351 LEU A:536 OHT A:600 MET A:522 Interactions Pi-Anion Pi-Sigma Pi-Sulfur Pi-Pi T-shaped Pi-Alkyl	 Met522 Trp383 Asp351 Leu536 Val533

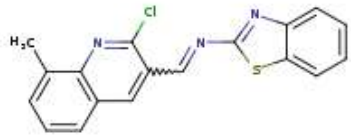
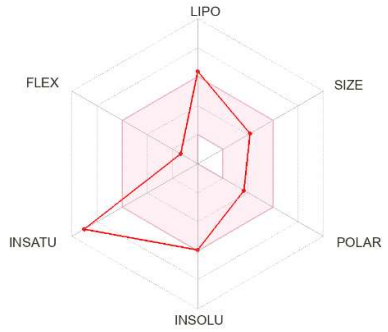
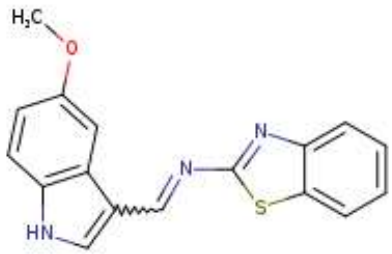
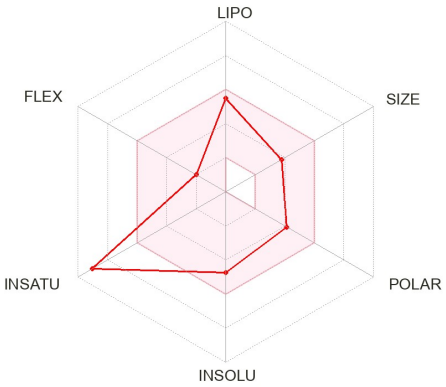
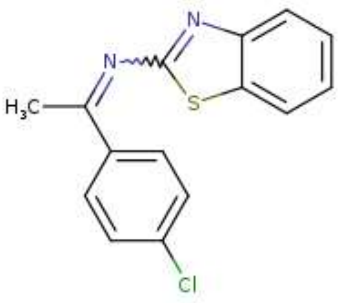
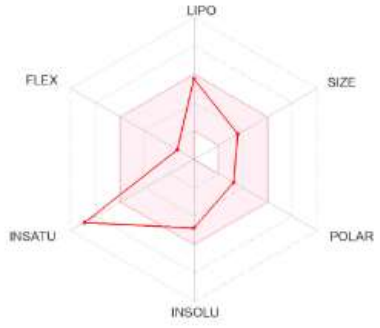
12	 LYS A:449 GLU A:323 TRP A:39 PRO A:324 ILE A:326 Interactions Conventional Hydrogen Bond Pi-Anion Pi-Sigma Pi-Sulfur Alkyl Pi-Alkyl Lys449 Pro324 Glu323 Ile326 Trp393	
13	 LEU A:525 MET A:522 MET A:528 LYS A:529 TYR A:526 LEU A:536 Interactions Halogen (Fluorine) Pi-Sulfur Alkyl Pi-Alkyl	 MET522 TYR526 LEU525 LEU536 LYS529 MET528
14	 ALA A:546 GLN A:375 LEU A:372 VAL A:368 ARG A:548 LYS A:362 Interactions Conventional Hydrogen Bond Halogen (Fluorine) Alkyl Pi-Alkyl	 ALA546 ARG548 LYS362 GLN375 LEU372 VAL368

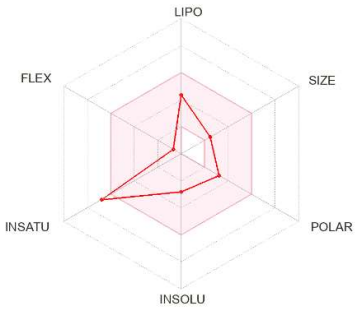
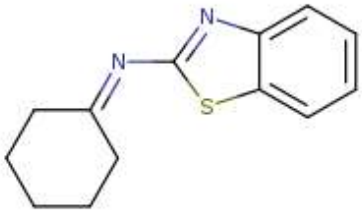
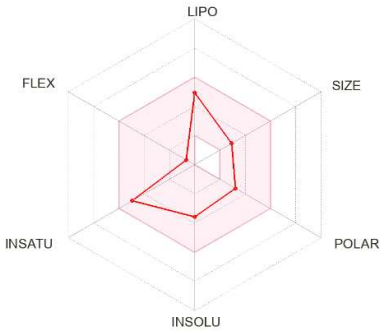
15	 LEU A:310 ALA A:318 PRO A:365 GLN A:314 ARG A:363 Interactions Conventional Hydrogen Bond Halogen (Fluorine) Pi-Sigma Alkyl Pi-Alkyl	 PRO365 LEU310 ARG363 GLN314 ALA318
16	 LEU A:525 LYS A:529 MET A:522 LEU A:536 LEU A:539 VAL A:533 Alkyl Pi-Alkyl	 VAL533 LEU539 LEU536 LYS529 LEU525 MET522

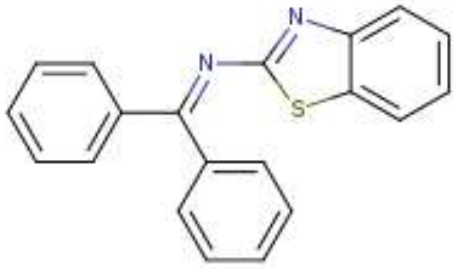
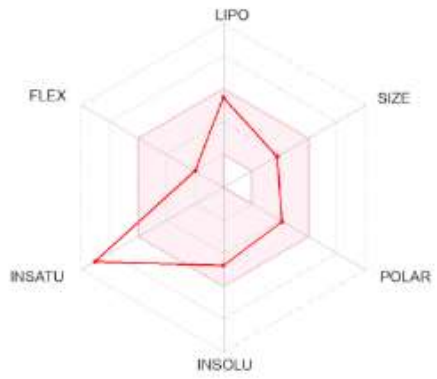
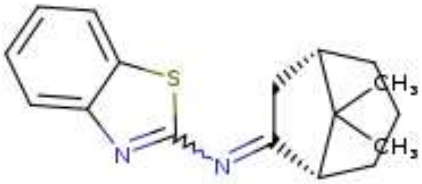
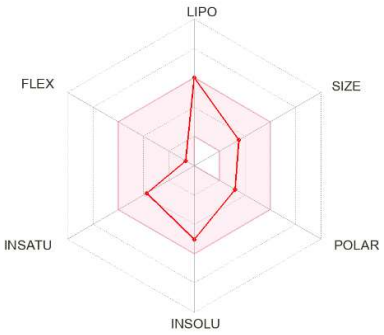
ADME study-Bioavailability Radar for compound (1 to 16)

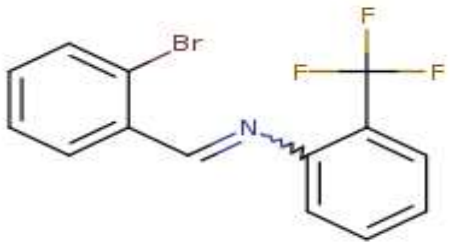
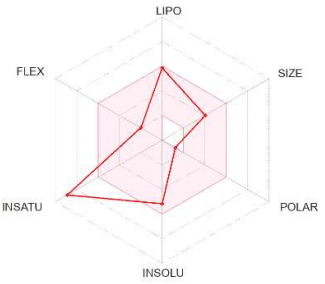
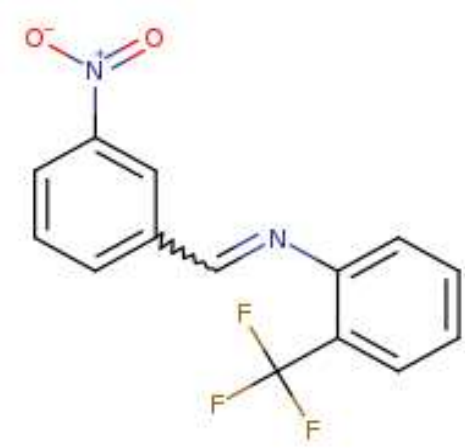
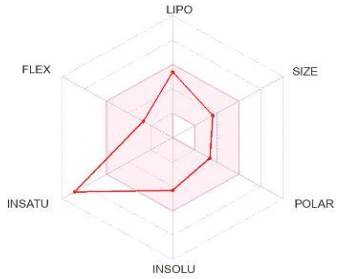
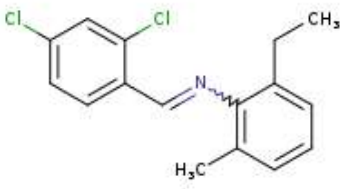
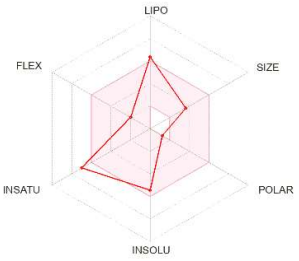
Entry	Compound	Radar
1	 COC1=CC=C2C(C=NC3=NC4=C(S3)C=CC=C4)=CC=CC2=C1	
2	 S1C2=C(C=CC=C2)N=C1\N=C\C1=C2C=CC=CC2=CC2=C1C=CC=C2	
3		

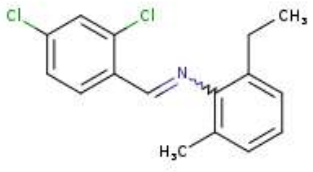
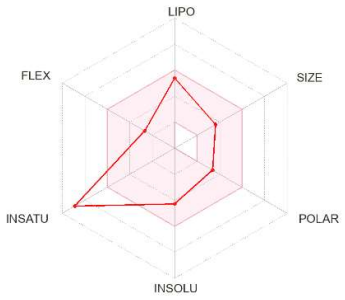
	S1C2=C(C=CC=C2)N=C1\N=C/C1=CC=C2C=CC3=CC=CC4=C3C2=C1C=C4	
4	 **O1C=CC=C1\C=N/C1=NC2=CC=CC=C2S1**	
5	 **S1C=CC=C1C=NC1=NC2=CC=CC=C2S1**	

6	 **CC1=CC=CC2=C1N=C(Cl)C(\C=N\C1=NC3=CC=CC=C3S1)=C2**	
7	 **COC1=CC2=C(NC=C2C=NC2=NC3=CC=CC=C3S2)C=C1**	
8		

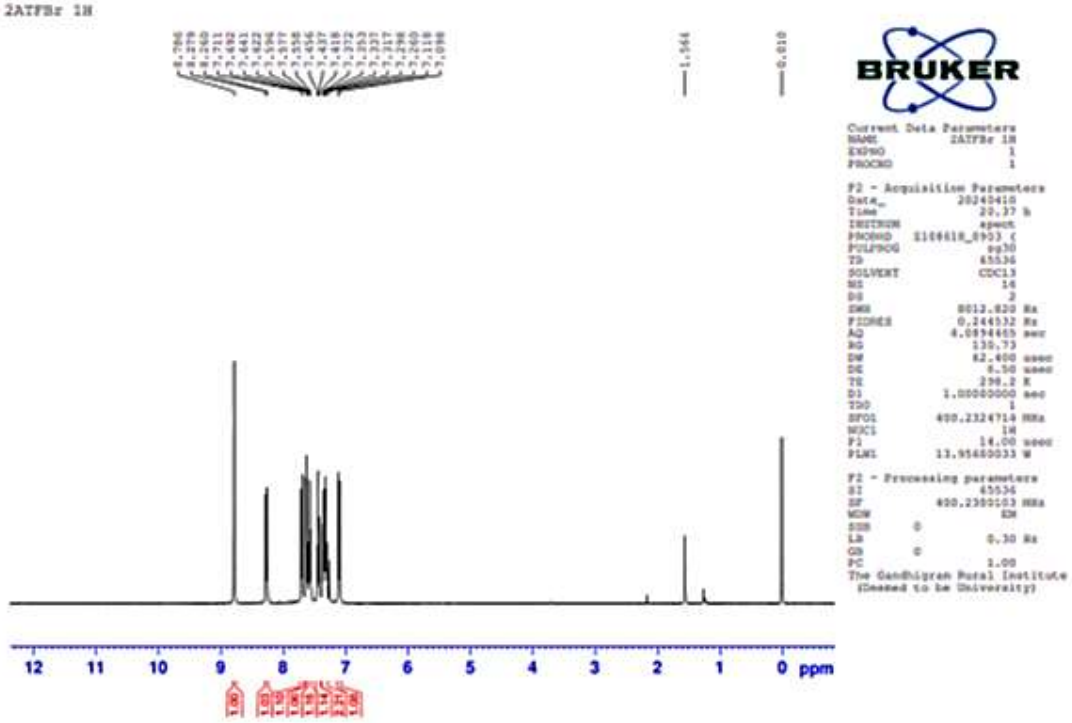
	C\C(=N/C1=NC2=CC=CC=C2S1)C1=CC=C(Cl)C=C1	
9	 **CC(C)=NC1=NC2=CC=CC=C2S1**	
10	 **C1CCC(CC1)=NC1=NC2=CC=CC=C2S1**	

11	 **S1C(N=C(C2=CC=CC=C2)C2=CC=CC=C2)=NC2=CC=CC=C12**	
12	 **CC1(C)[COOH]2CC(=NC3=NC4=CC=CC=C4S3)[COH]1CCC2**	

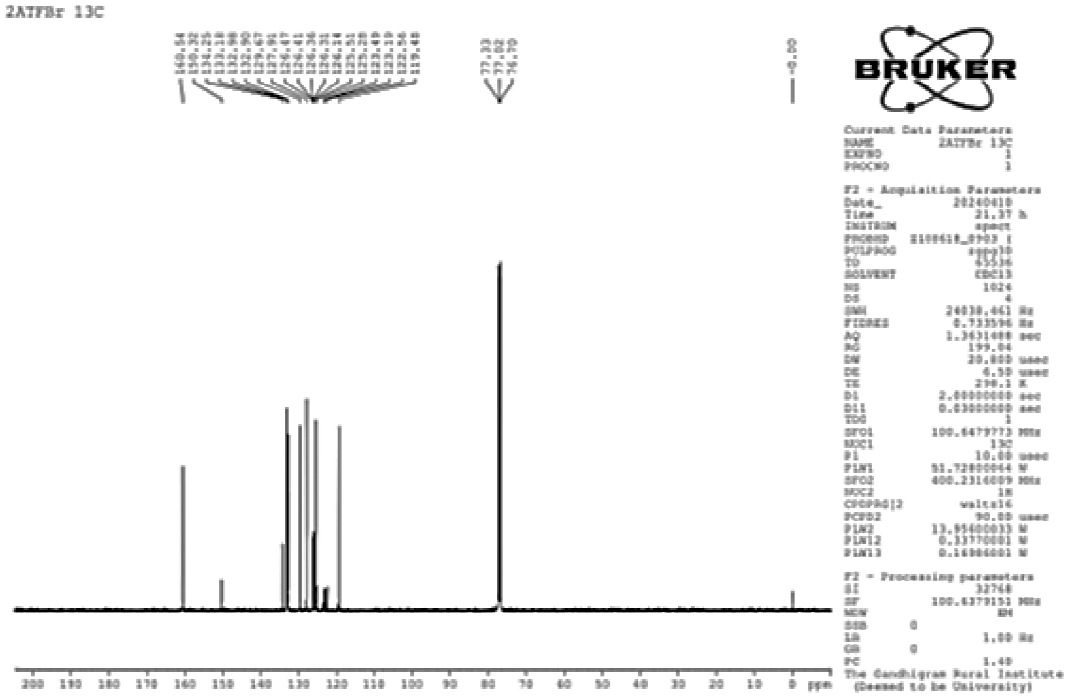
13	 **FC(F)(F)C1=CC=CC=C1\N=C/C1=CC=CC=C1Br**	
14	 **[O][N+](=O)C1=CC(\C=N/C2=CC=CC=C2C(F)(F)F)=CC=C1**	
15		

	CCC1=CC=CC(C)=C1\N=C/C1=CC=C(Cl)C=C1Cl	
16	  **CCC1=CC=CC(C)=C1\N=C/C1=CC=C(Cl)C=C1Cl**	

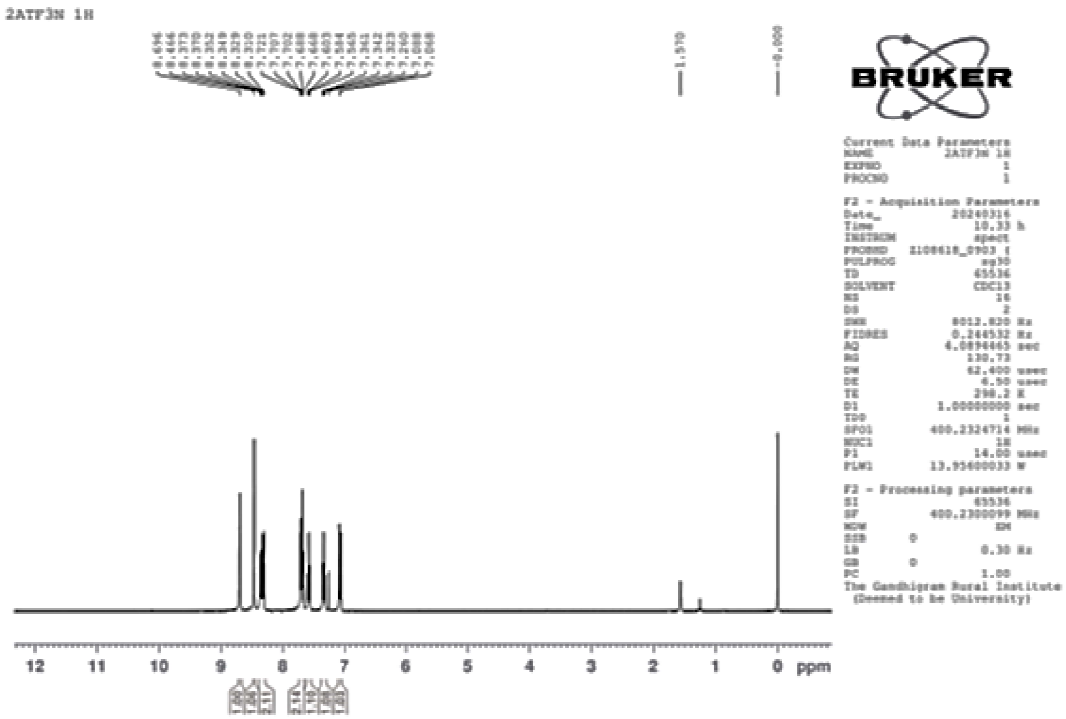
NMR Spectra of *E*-imine compounds (13-16)



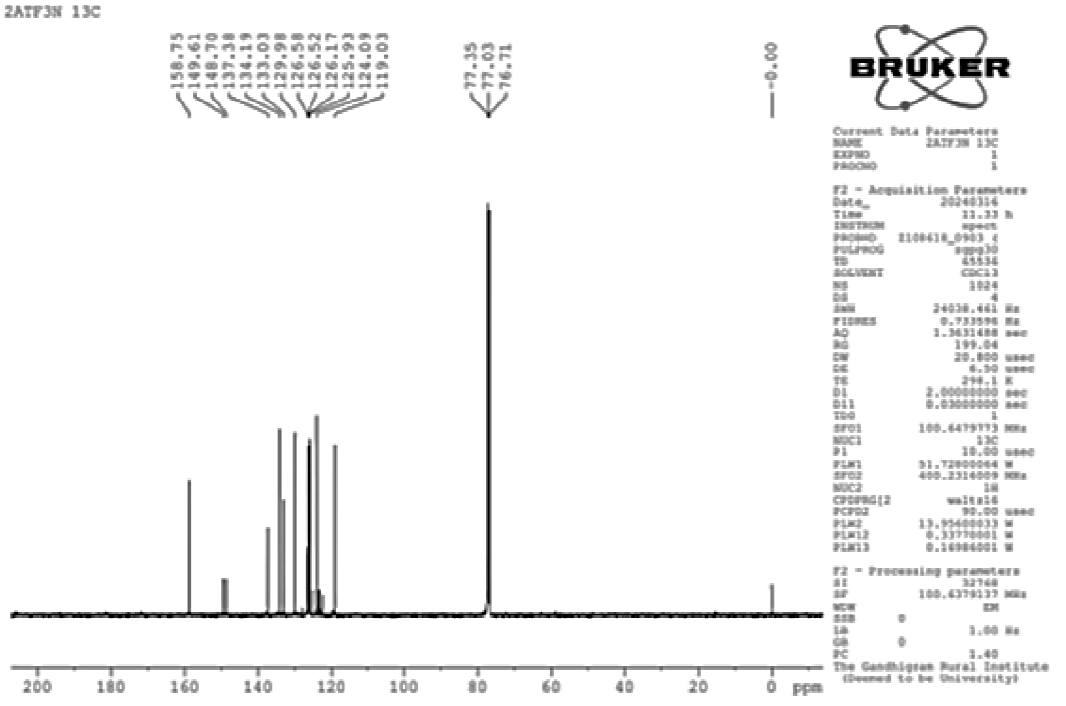
^{1}H NMR spectrum of (E)-N-(2-bromobenzylidene)-2-(trifluoromethyl)aniline (13)



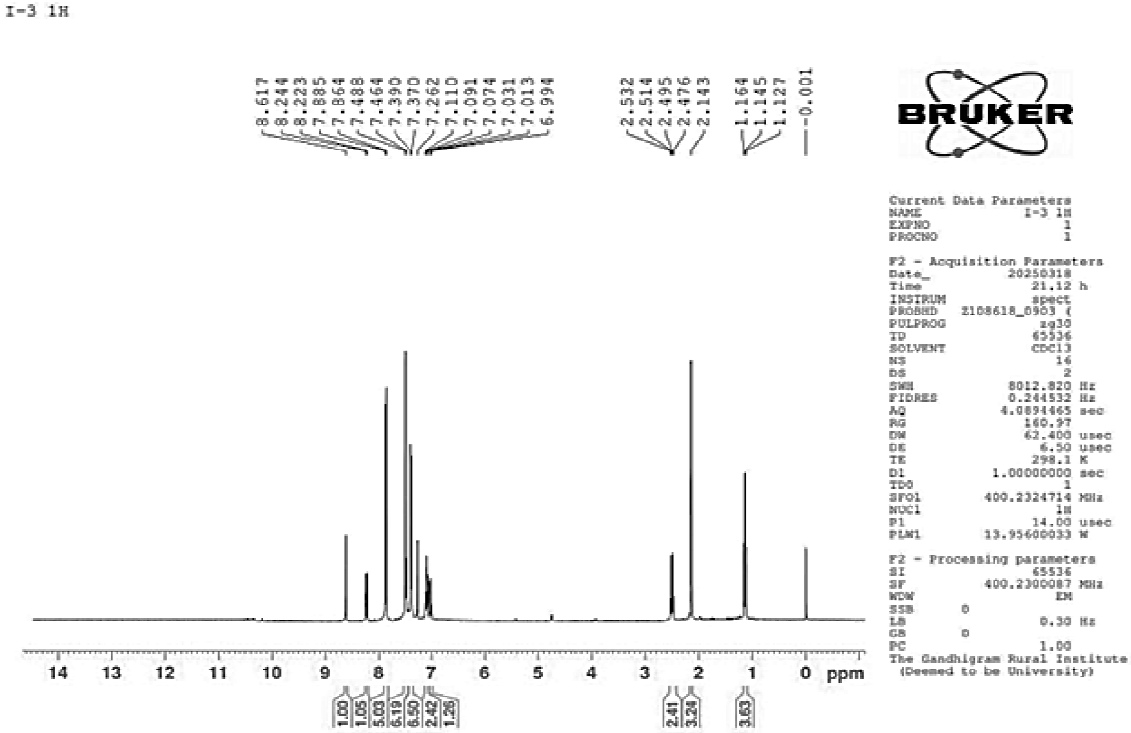
^{13}C NMR spectrum of (E)-N-(2-bromobenzylidene)-2-(trifluoromethyl)aniline (13)



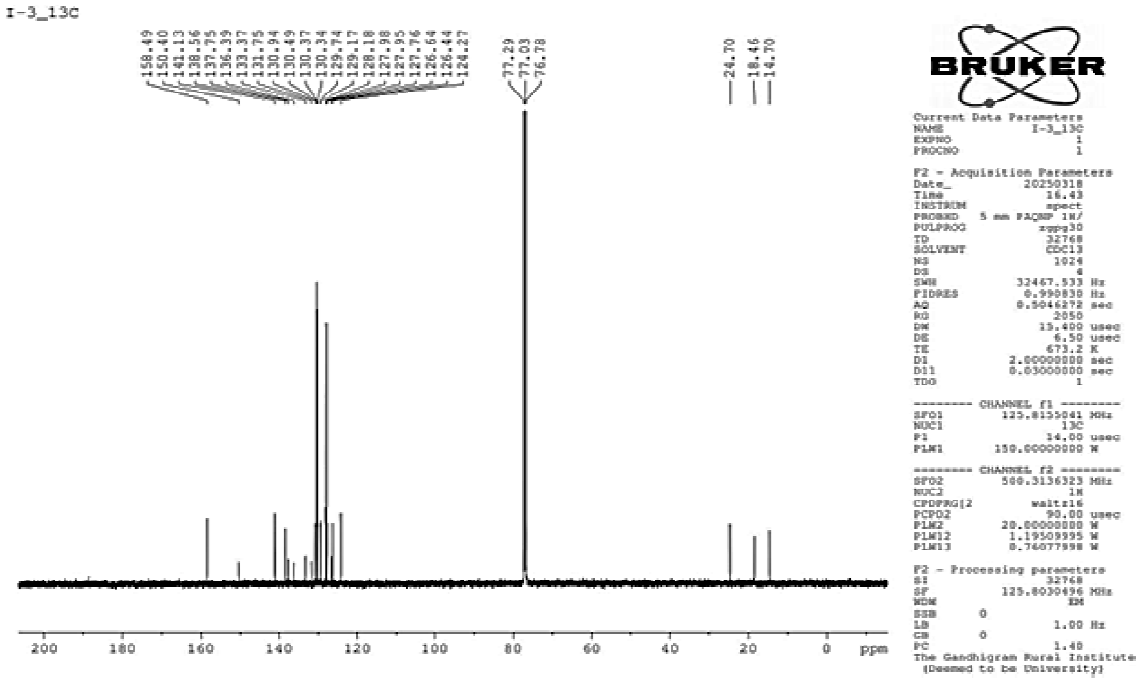
^{1}H NMR spectrum of (E)-N-(3-nitrobenzylidene)-2-(trifluoromethyl)aniline (14)



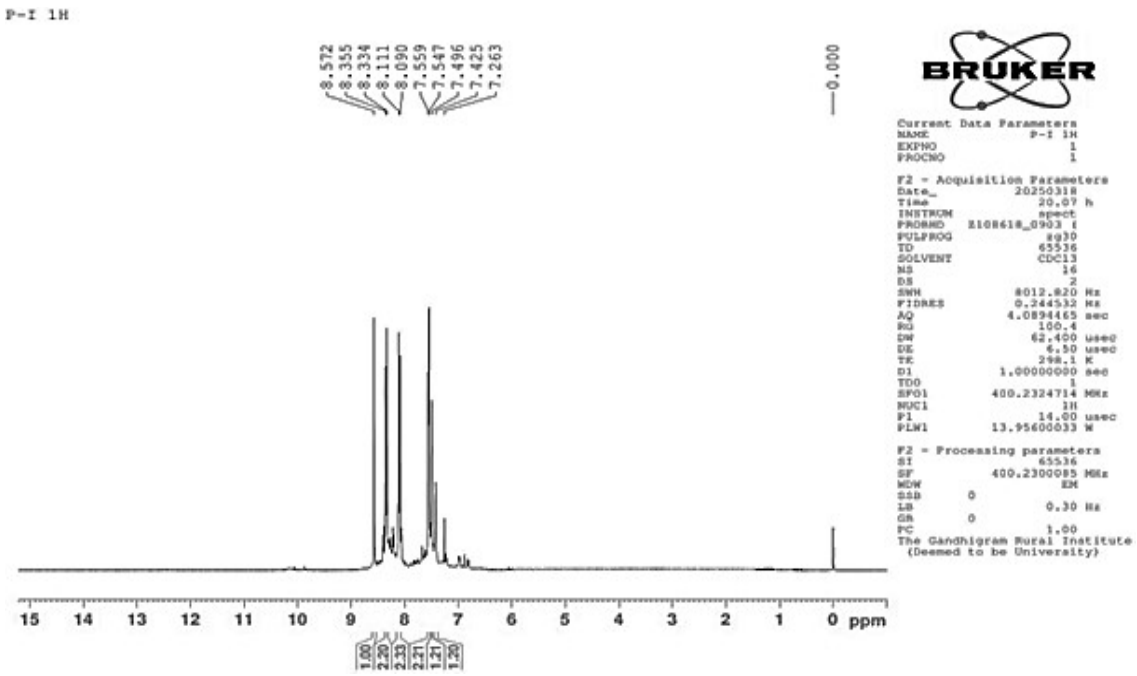
^{13}C NMR spectrum of (E)-N-(3-nitrobenzylidene)-2-(trifluoromethyl)aniline (14)



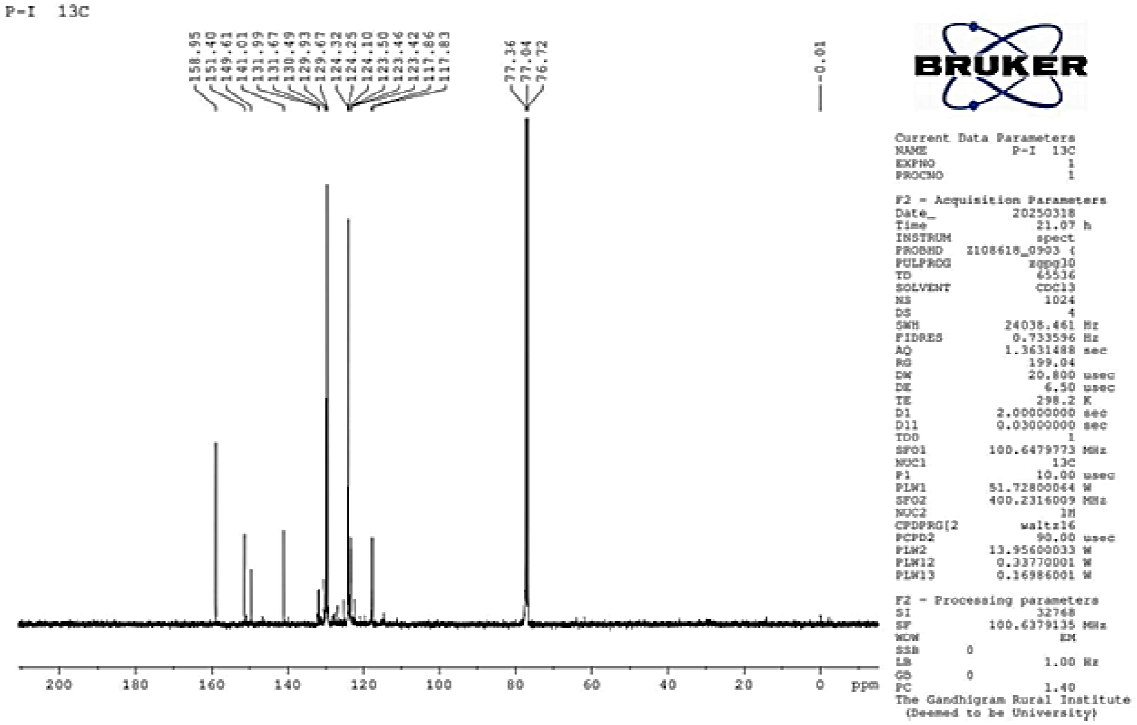
^{1}H NMR spectrum of (*E*)-*N*-(2,4-Dichlorobenzylidene)-2-ethyl-6-methylbenzenamine (15)



^{13}C NMR spectrum of (*E*)-*N*-(2,4-Dichlorobenzylidene)-2-ethyl-6-methylbenzenamine (15)



^{1}H NMR spectrum of (*E*)-*N*-(4-nitrobenzylidene)-3-(trifluoromethyl)benzenamine (16)



^{13}C NMR spectrum of (*E*)-*N*-(4-Nitrobenzylidene)-3-(trifluoromethyl)benzenamine (16)

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ATF2B_071124_0m_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ATF2B_071124_0m_a

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Bond precision:   C-C = 0.0052 A          Wavelength=0.71073

Cell:             a=10.0047(12)     b=7.9137(10)        c=16.739(2)
                  alpha=90          beta=102.161(4)     gamma=90
Temperature:      300 K

                 Calculated                Reported
Volume           1295.6(3)                 1295.6(3)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C14 H9 Br F3 N            C14 H9 Br F3 N
Sum formula      C14 H9 Br F3 N            C14 H9 Br F3 N
Mr               328.12                    328.13
Dx,g cm-3        1.682                     1.682
Z                4                         4
Mu (mm-1)        3.193                     3.193
F000             648.0                     648.0
F000'            647.23
h,k,lmax         13,10,22                  13,10,22
Nref             3224                      3208
Tmin,Tmax        0.480,0.629               0.552,0.746
Tmin'            0.444

Correction method= # Reported T Limits: Tmin=0.552 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 28.300

R(reflections)= 0.0488( 1888)                    wR2(reflections)=
                                                 0.1285( 3208)
S = 1.028                 Npar= 172
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         12 Report
                  3  0  0,  -2  0  2,  -2  1  2,  -1  1  2,   1  0  2,   1  1  2,
                  2  0  2,   2  1  2,  -2  0  4,   0  0  4,   1  0  4,   1  1  4,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          6 Note
                  3  0  0,   2  1  2,  -2  0  4,   0  0  4,   1  0  4,   1  1  4,
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Alert level G

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PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          4 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.755 Note
             Predicted wR2: Based on SigI**2  3.42 or SHELX Weight 12.50
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock ATF2B_071124_0m_a - ellipsoid plot