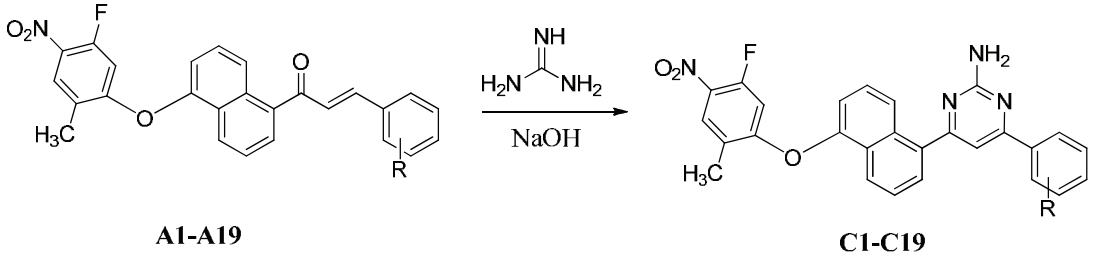
CHAPTER – V

SYNTHESIS AND CHARACTERIZATION OF PYRIMIDINES

CONTENTS

5.1 REACTION SCHEME

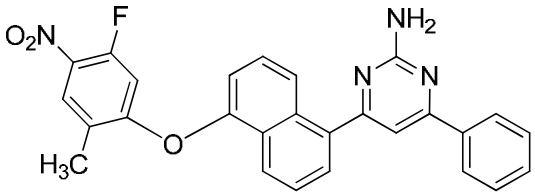
Pyrimidines **C1-C19** were planned to prepare by reaction between chalcones **A1-A19** and Guanidine in the presence of ethanol and 40% NaOH (**Scheme 5.1)**.



Scheme 5.1 Synthesis of Pyrimidines C1-C19

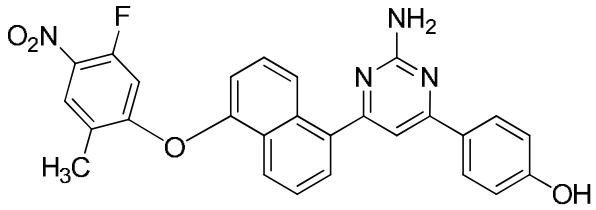
5.2 STRUCTURE OF COMPOUNDS C1 TO C19

Compound C1:



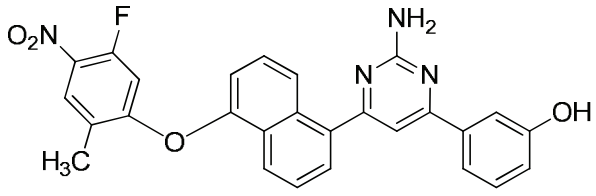
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-phenylpyrimidin-2-amine

Compound C2:



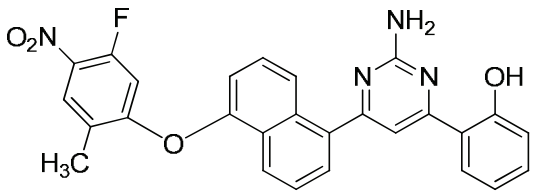
4-(2-amino-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-4-yl)phenol

Compound C3:



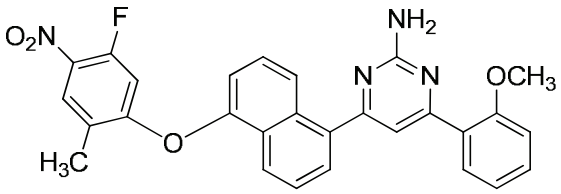
3-(2-amino-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-4-yl)phenol

Compound C4:



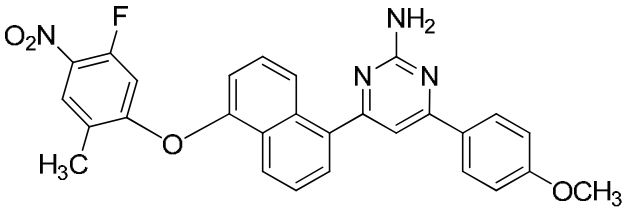
2-(2-amino-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-4-yl)phenol

Compound C5:



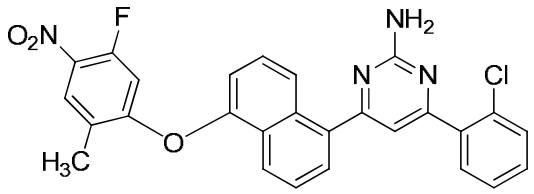
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-methoxyphenyl)pyrimidin-2-amine

Compound C6:



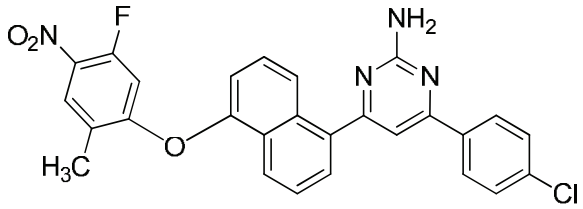
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-methoxyphenyl)pyrimidin-2-amine

Compound C7:



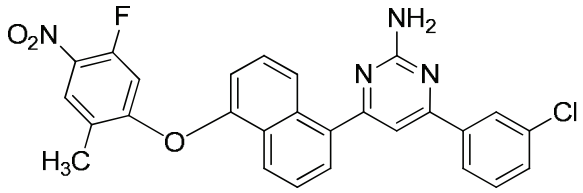
4-(2-chlorophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

Compound C8:



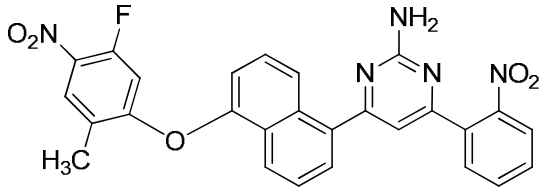
4-(4-chlorophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

Compound C9:



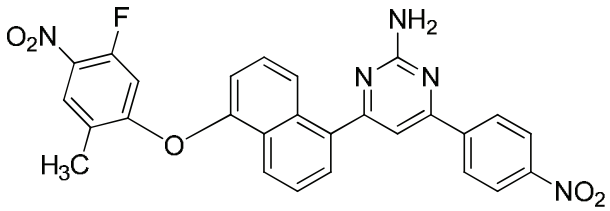
4-(3-chlorophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

Compound C10:



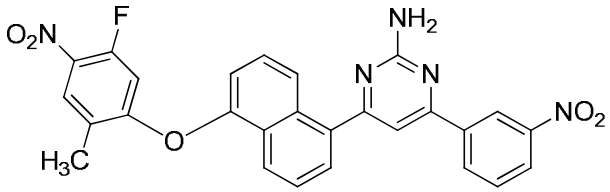
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-nitrophenyl)pyrimidin-2-amine

Compound C11:



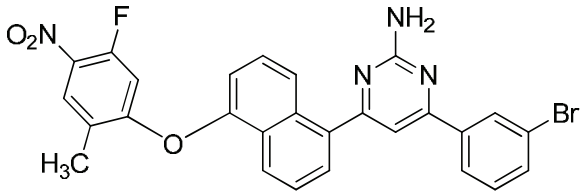
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-nitrophenyl)pyrimidin-2-amine

Compound C12:



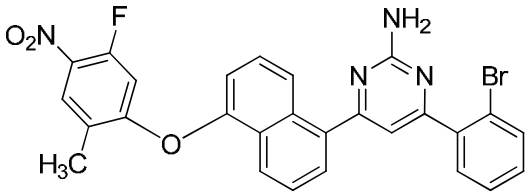
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3-nitrophenyl)pyrimidin-2-amine

Compound C13:



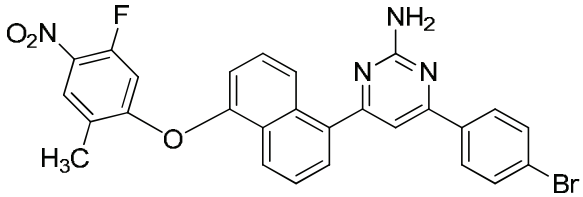
4-(3-bromophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

Compound C14:



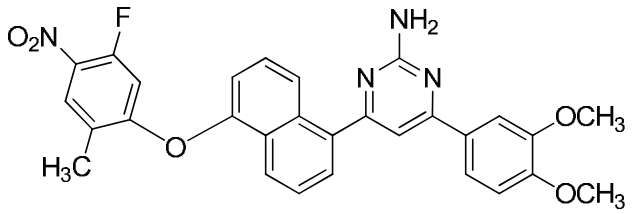
4-(2-bromophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

Compound C15:



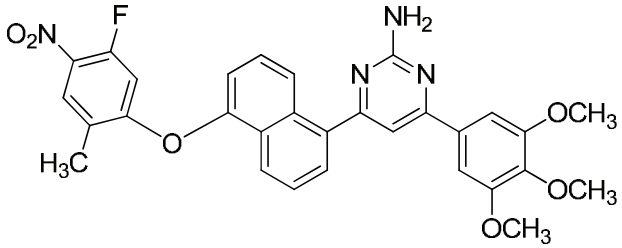
4-(4-bromophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

Compound C16:



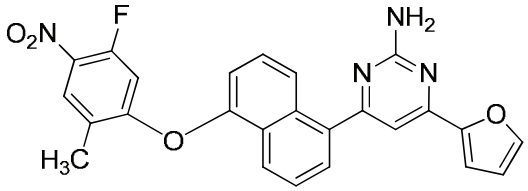
4-(3,4-dimethoxyphenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

Compound C17:



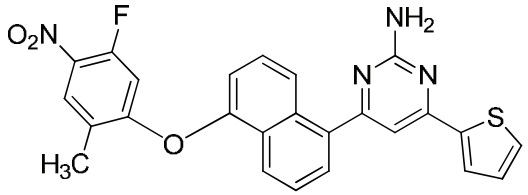
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3,4,5-trimethoxyphenyl)pyrimidin-2-amine

Compound C18:



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(furan-2-yl)pyrimidin-2-amine

Compound C19:



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(thiophen-2-yl)pyrimidin-2-amine

5.3 EXPERIMENTAL

5.3.1 Chemicals and Reagents

All chemicals used were of laboratory reagent grade and used without further purification**.** NaOH, Guanidine and ethanol were used as received from Merck, Mumbai, India.

5.3.2 General Experimental procedure

5.3.2.1 Synthesis of Pyrimidine biosynthesis C1

Chalcone **A1** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine,40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C1**.

5.3.2.2 Synthesis of Pyrimidine C2

Chalcone **A2** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine,40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C2**.

5.3.2.3 Synthesis of Pyrimidine C3

Chalcone **A3** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine,40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C3**.

5.3.2.4 Synthesis of Pyrimidine C4

Chalcone **A4** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C4**.

5.3.2.5 Synthesis of Pyrimidine C5

Chalcone **A5** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C5**.

5.3.2.6 Synthesis of Pyrimidine C6

Chalcone **A6** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C6**.

5.3.2.7 Synthesis of Pyrimidine C7

Chalcone **A7** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C7**.

5.3.2.8 Synthesis of Pyrimidine C8

Chalcone **A8** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C8**.

5.3.2.9 Synthesis of Pyrimidine C9

Chalcone **A9** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C9**.

5.3.2.10 Synthesis of Pyrimidine C10

Chalcone **A10** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for

1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C10**.

5.3.2.11 Synthesis of Pyrimidine C11

Chalcone **A11** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C11**.

5.3.2.12 Synthesis of Pyrimidine C12

Chalcone **A12** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C12**.

5.3.2.13 Synthesis of Pyrimidine C13

Chalcone **A13** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C13**.

5.3.2.14 Synthesis of Pyrimidine C14

Chalcone **A14** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C14**.

5.3.2.15 Synthesis of Pyrimidine C15

Chalcone **A15** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C15**.

5.3.2.16 Synthesis of Pyrimidine C16

Chalcone **A16** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C16**.

5.3.2.17 Synthesis of Pyrimidine C17

Chalcone **A17** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C17**.

5.3.2.18 Synthesis of Pyrimidine C18

Chalcone **A18** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C18**.

5.3.2.19 Synthesis of Pyrimidine C19

Chalcone **A19** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Guanidine, 40 ml ethanol and 40 ml 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is called **C19**.

5.4 CHARACTERSTICS DATA SHOWING SYNTHESIS OF PYRIMIDINE C1-C19.

Table 5.1 Synthesis of Pyrimidine C1-C19

Sr. No.	Compounds	R	Reaction Time (hr)	% Yield[b]
1	**C1**	-H	4	80
2	**C2**	4-OH	4	75
3	**C3**	3-OH	4	83
4	**C4**	2-OH	4	83
5	**C5**	2- OCH_3	4.5	82
6	**C6**	4-OCH_3	4.5	78
7	**C7**	2-Cl	3.5	72
8	**C8**	4-Cl	3.5	72
9	**C9**	3-Cl	3.5	68
10	**C10**	2-NO_2	3.5	75
11	**C11**	4-NO_2	3.5	68
12	**C12**	3-NO_2	3.5	67
13	**C13**	3-Br	4	80
14	**C14**	2- Br	4	72
15	**C15**	4- Br	4	82
16	**C16**	3, 4-$(OCH_3)_2$	4.5	80
17	**C17**	3,4,5-$(OCH_3)_3$	4.5	75
18	**C18**	2-furfuryl[c]	3.5	78
19	**C19**	2-Thineyl[c]	3.5	72

[a]Reaction is monitored by TLC, [b]Isolated yield and [c]Names of aldehyde groups

5.5 RESULTS AND DISCUSSION

Table 5.1 shows the data for various condensation products of reaction between various chalcones andguanidine. It clearly indicates that the compounds bearing electron withdrawing groups are synthesized in shorter reaction time as compared to compounds bearing electron donating group. Compounds **C7-C15** bearing electron withdrawing groups were synthesized in **3.5 to 4h** as compared to compounds bearing electron donating group. Compounds **C5, C6, C16** and **C17 which have** electron donating groups were synthesized in **4.5 h**.

5.6 PHYSICAL DATA OF SYNTHESIZED DERIVATIVES

Table 5.2 Physical data of compounds C1 to C19

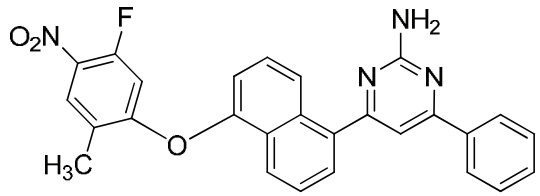
Comp.	R	Molecular Formula	Mol. Wt. (g/m)	% Yield	M.P. °C	% Carbon		% Hydrogen		% Nitrogen	
						Found	Calcd.	Found	Calcd.	Found	Calcd.
C1	-H	$C_{27}H_{19}FN_4O_3$	466.1	80	236	69.60	69.52	4.15	4.11	12.07	12.01
C2	4-OH	$C_{27}H_{19}FN_4O_4$	482.4	75	252	67.25	67.22	3.92	3.97	11.65	11.61
C3	3-OH	$C_{27}H_{19}FN_4O_4$	482.4	83	246	67.28	67.22	3.90	3.97	11.64	11.61
C4	2-OH	$C_{27}H_{19}FN_4O_4$	482.4	83	258	67.24	67.22	3.91	3.97	11.67	11.61
C5	2- OCH_3	$C_{28}H_{21}FN_4O_4$	496.4	82	244	67.70	67.74	4.20	4.26	11.20	11.28
C6	4-OCH_3	$C_{28}H_{21}FN_4O_4$	496.4	78	232	67.72	67.74	4.21	4.26	11.21	11.28
C7	2-Cl	$C_{27}H_{18}FClN_4O_3$	500.9	72	235	64.70	64.74	3.58	3.62	11.14	11.19
C8	4-Cl	$C_{27}H_{18}FClN_4O_3$	500.9	72	245	64.71	64.74	3.56	3.62	11.13	11.19
C9	3-Cl	$C_{27}H_{18}FClN_4O_3$	500.9	68	258	64.69	64.74	3.57	3.62	11.12	11.19
C10	2-NO_2	$C_{27}H_{18}FN_5O_5$	511.4	75	242	63.35	63.40	3.50	3.55	13.60	13.69

C11	4-NO_2	$C_{27}H_{18}FN_5O_5$	511.4	68	255	63.36	63.40	3.51	3.55	13.62	13.69
C12	3-NO_2	$C_{27}H_{18}FN_5O_5$	511.4	67	248	63.33	63.40	3.52	3.55	13.61	13.69
C13	3-Br	$C_{27}H_{18}FBrN_4O_3$	445.3	80	252	59.40	59.46	3.30	3.33	10.25	10.27
C14	2- Br	$C_{27}H_{18}FBrN_4O_3$	445.3	72	252	59.41	59.46	3.31	3.33	10.21	10.27
C15	4- Br	$C_{27}H_{18}FBrN_4O_3$	445.3	82	256	59.42	59.46	3.36	3.33	10.29	10.27
C16	3, 4-$(OCH_3)_2$	$C_{29}H_{23}FN_4O_5$	526.5	80	245	66.10	66.15	4.30	4.40	10.60	10.64
C17	3,4,5-$(OCH_3)_3$	$C_{30}H_{25}FN_4O_6$	556.5	75	257	64.70	64.74	4.45	4.53	10.11	10.07
C18	2-furfuryl	$C_{25}H_{17}FN_4O_4$	456.4	78	248	65.85	65.79	3.80	3.75	12.20	12.28
C19	2-Thineyl	$C_{25}H_{17}FSN_4O_3$	472.4	72	262	63.45	63.55	3.58	3.63	11.80	11.86

5.7 SPECTROSCOPIC CHARACTERIZATION OF COMPOUNDS C1-C19

For characterization,**compound C1** was taken as the model compound from the series and it was characterized by various spectroscopic methods such as ^{1}H NMR, ^{13}C NMR, MASS and IR spectroscopy. Its structures was decided by these spectroscopic techniques. (As shown in Fig. 5.1 to Fig. 5.4).

Compound C1



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-phenylpyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.6 ppm. All 13 aromatic protons appeared in aromatic region between δ 6.8 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.5 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Signal due to carbon of methine groups were found at δ 62.2 ppm. All aromatic carbons give signals at 129.4, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 and 160.2 δ ppm.

IR Spectroscopy (KBr)

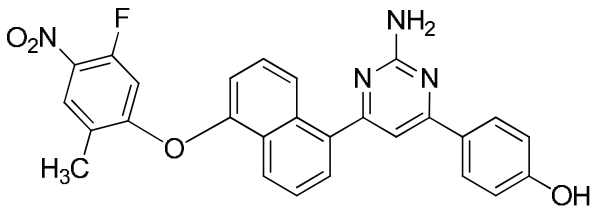
Infrared spectra recorded in KBr reveals that absorption at 3311 and 3415 cm^{-1} indicates the N-H stretching. The band at 3120 cm^{-1} shows aromatic C-H stretching. Bands at 2950 cm^{-1} indicates aliphatic C-H stretching of the methyl group. Bands at 1612, 1592 and 1569 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1}

indicates the N=O stretching. Absorption at 744 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations,.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 466.1, which indicates the molecular weight of the compound.

Compound C2



4-(2-amino-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-4-yl)phenol

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.4 ppm in downfield region. Singlet due to one –OH proton appeared at δ 2.7 ppm. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.8 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.3 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Signal due to carbon of methine groups were found at δ 62.2 ppm. All aromatic carbons give signals at 128.9, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 and 160.2 δ ppm.

IR Spectroscopy (KBr)

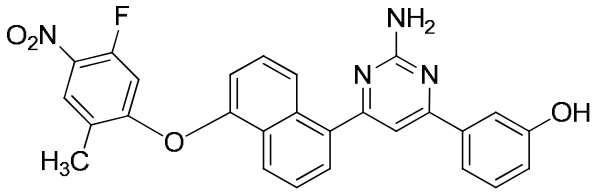
Infrared spectra recorded in KBr reveals that absorption 3415 cm^{-1} indicates the O-H stretching and the band at 3360 and 3310 cm^{-1} shows the N-H stretching. Bands at 3120 cm^{-1} indicates the aromatic C-H stretching. Bands at 2950 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1592 and 1569 cm^{-1} indicates the

C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 745 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations,.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 482.4, which indicates the molecular weight of the compound.

Compound C3



3-(2-amino-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-4-yl)phenol

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.4 ppm in downfield region. Singlet due to one –OH proton appeared at δ 2.7 ppm. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.6 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Signal due to carbon of methine groups were found at δ 62.1 ppm. All aromatic carbons give signals at 129.4, 130.4, 140.2, 146.6, 151.7, 153.6, 155.1 and 160.2 δ ppm.

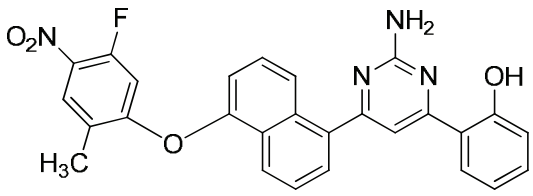
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption 3415 cm^{-1} indicates the O-H stretching and the band at 3360 indicates the N-H stretching. Bands at 3120 cm^{-1} indicates the aromatic C-H stretching. Bands at 2951 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1611, 1592 and 1569 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 746 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations,.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 482.4, which indicates the molecular weight of the compound.

Compound C4



2-(2-amino-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-4-yl)phenol

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. Singlet due to one –OH proton appeared at δ 2.6 ppm. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH_2 proton comes at δ 4.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Signal due to carbon of methine groups were found at δ 61.1 ppm. All aromatic carbons give signals at 129.9, 130.4, 131.6, 146.6, 151.7, 154.7, 156.1 and 161.2 δ ppm.

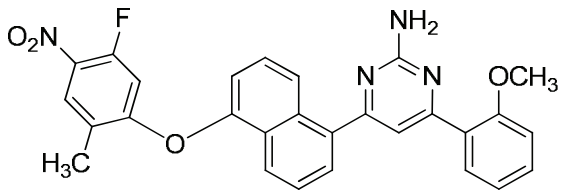
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption 3420 cm^{-1} indicates the O-H stretching and the bands at 3360 and 3310 cm^{-1} indicates the N-H stretching. Bands at 3120 cm^{-1} indicates the aromatic C-H stretching. Bands at 2952 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1611, 1590 and 1565 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 750 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations,.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 482.4, which indicates the molecular weight of the compound.

Compound C5



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-methoxyphenyl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. Singlet due to –OCH_3 proton appeared at δ 3.4 ppm. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH_2 proton comes at δ 4.5 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Signal due to –OCH_3 group is appeared at 39.0 δ ppm. Signal due to carbon of methine groups were found at δ 61.1 ppm. All aromatic carbons give signals at 127.9, 129.4, 131.6, 140.2, 151.7, 154.7, 156.1 and 161.2 δ ppm.

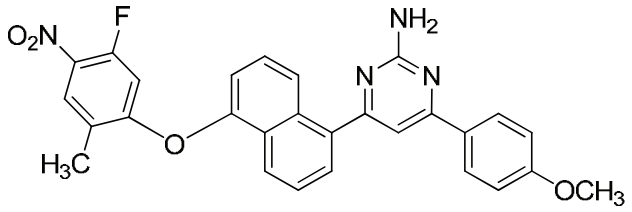
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3312 and 3310 cm^{-1} indicates the N-H stretching, respectively. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Value at 2951 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1612, 1590 and 1568 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 745 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations,.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 496.4, which indicates the molecular weight of the compound.

Compound C6



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-methoxyphenyl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. Singlet due to –OCH_3 proton appeared at δ 3.4 ppm. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.4 to 8.4 ppm. Singlet due to NH_2 proton comes at δ 4.6 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.1 δ ppm. Signal due to –OCH_3 group is appeared at 39.0 δ ppm. Signal due to carbon of methine groups were found at δ 61.1 ppm. All aromatic carbons give signals at 127.9, 129.4, 131.6, 140.2, 146.6, 152.7, 157.1 and 160.2 δ ppm.

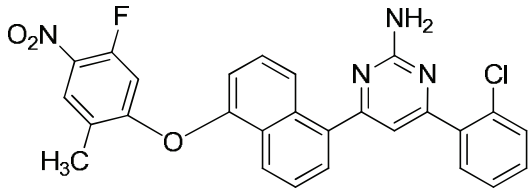
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3410 and 3316 cm^{-1} indicates the N-H stretching, respectively. The band at 3132 cm^{-1} indicates the aromatic C-H stretching. Value at 2971 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1612, 1590 and 1568 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 740 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 496.4, which indicates the molecular weight of the compound.

Compound C7



4-(2-chlorophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 33.0 δ ppm. Signal due to carbon of methine groups were found at δ 62.2 ppm. All aromatic carbons give signals at 129.4, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 and 160.2 δ ppm.

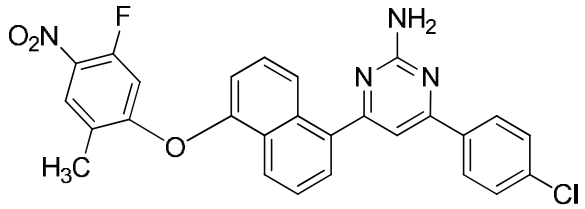
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3350 and 3311 cm^{-1} indicates the N-H stretching, respectively. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Value at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1592 and 1567 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 744 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 500.9, which indicates the molecular weight of the compound.

Compound C8



4-(4-chlorophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.5 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 31.5 δ ppm. Signal due to carbon of methine groups were found at δ 61.2 ppm. All aromatic carbons give signals at 128.5, 130.2, 140.2, 146.6, 151.9, 153.6, 155.1 and 160.2 δ ppm.

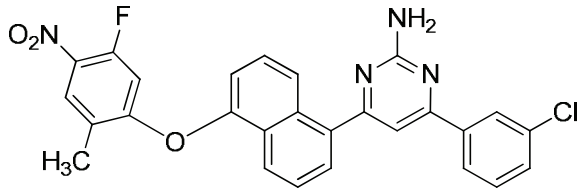
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3410 and 3370 cm^{-1} indicates the N-H stretching, respectively. The band at 3121 cm^{-1} indicates the aromatic C-H stretching. Value at 2980 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1595 and 1567 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 746 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 500.9, which indicates the molecular weight of the compound.

Compound C9



4-(3-chlorophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.6 ppm in downfield region. One vinylic group give singlet at δ 5.5 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.4 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.1 δ ppm. Signal due to carbon of methine groups were found at δ 62.2 ppm. All aromatic carbons give signals at 129.4, 132.6, 140.2, 146.6, 151.9, 152.6, 155.1 and 160.2 δ ppm.

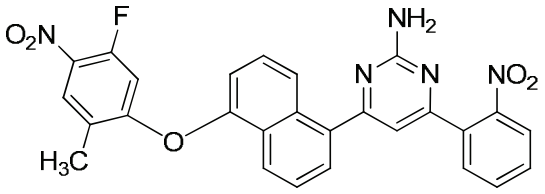
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3370 and 3320 cm^{-1} indicates the N-H stretching, respectively. The band at 3121 cm^{-1} indicates the aromatic C-H stretching. Value at 2985 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1609, 1595 and 1567 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 746 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 500.9, which indicates the molecular weight of the compound.

Compound C10



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-nitrophenyl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 31.2 δ ppm. Signal due to carbon of methine groups were found at δ 62.2 ppm. All aromatic carbons give signals at 128.4, 131.6, 140.2, 146.6, 155.8, 153.6, 155.2 and 160.1 δ ppm.

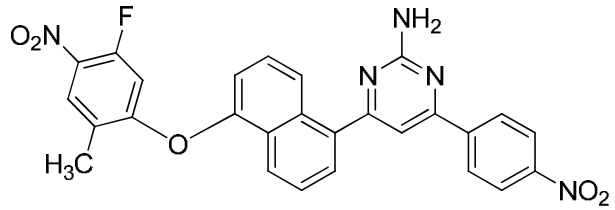
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3340 and 3315 cm^{-1} indicates the N-H stretching, respectively. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Value at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1592 and 1567 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 740 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 511.4, which indicates the molecular weight of the compound.

Compound C11



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-nitrophenyl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.5 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 31.2 δ ppm. Signal due to carbon of methine groups were found at δ 61.2 ppm. All aromatic carbons give signals at 129.4, 131.6, 140.2, 146.6, 151.9, 153.6, 155.1 and 160.2 δ ppm.

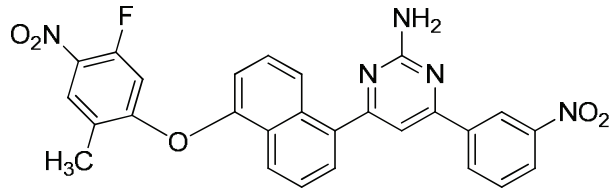
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3350 and 3310 cm^{-1} indicates the N-H stretching. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Value at 2982 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1591 and 1567 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 742 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 511.4, which indicates the molecular weight of the compound.

Compound C12



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3-nitrophenyl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.4 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.6 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 31.4 δ ppm. Signal due to carbon of methine groups were found at δ 61.2 ppm. All aromatic carbons give signals at 126.4, 131.6, 141.2, 146.6, 151.8, 153.6, 154.1 and 160.2 δ ppm.

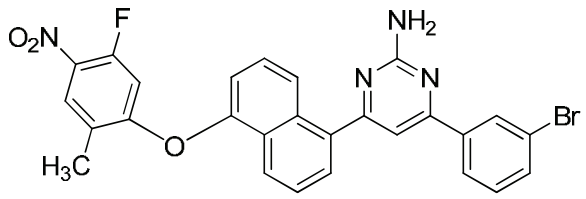
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3411 and 3350 cm^{-1} indicates the N-H stretching. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Value at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1592 and 1567 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 744 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 511.4, which indicates the molecular weight of the compound.

Compound C13



4-(3-bromophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.6 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 31.1 δ ppm. Signal due to carbon of methine groups were found at δ 62.2 ppm. All aromatic carbons give signals at 129.4, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 and 160.2 δ ppm.

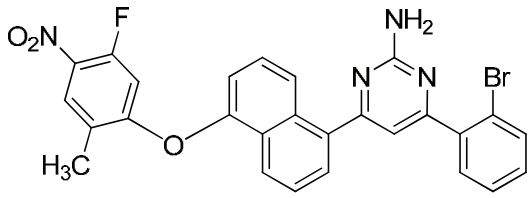
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3350 and 3316 cm^{-1} indicates the N-H stretching. The band at 3121 cm^{-1} indicates the aromatic C-H stretching. Value at 2930 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1591 and 1565 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 740 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 445.3, which indicates the molecular weight of the compound.

Compound C14



4-(2-bromophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.5 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Signal due to carbon of methine groups were found at δ 61.2 ppm. All aromatic carbons give signals at 129.4, 131.6, 140.2, 146.6, 151.9, 153.6, 155.1 and 160.2 δ ppm.

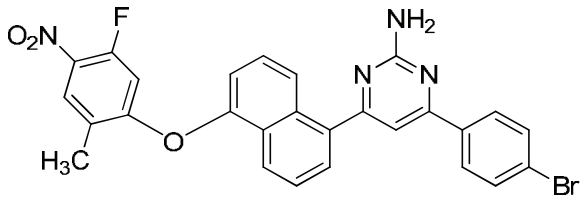
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3360 and 3310 cm^{-1} indicates the N-H stretching. The band at 3123 cm^{-1} indicates the aromatic C-H stretching. Value at 2930 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1593 and 1560 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 750 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 445.3, which indicates the molecular weight of the compound.

Compound C15



4-(4-bromophenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.4 ppm in downfield region. One vinylic group give singlet at δ 5.6 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH_2 proton comes at δ 4.4 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.1 δ ppm. Signal due to carbon of methine groups were found at δ 62.2 ppm. All aromatic carbons give signals at 128.9, 130.3, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 and 161.2 δ ppm.

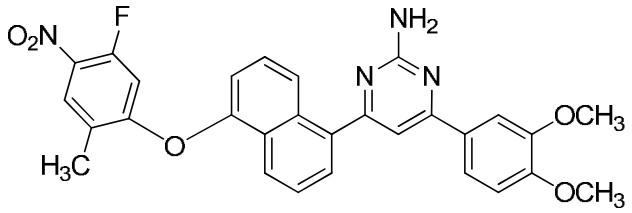
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3340 and 3310 cm^{-1} indicates the N-H stretching. The band at 3105 cm^{-1} indicates the aromatic C-H stretching. Value at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1610, 1590 and 1550 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 750 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 445.3, which indicates the molecular weight of the compound.

Compound C16



4-(3,4-dimethoxyphenyl)-6-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. Singlet due to two –OCH_3 protons appeared at δ 3.5 ppm. One vinylic group give singlet at δ 5.6 ppm. All 11 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH_2 proton comes at δ 4.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 31.2 δ ppm. Singlet due to two –OCH_3 protons appeared at 39.0 and 40.1 δ ppm. Signal due to carbon of methine groups were found at δ 61.1 ppm. All aromatic carbons give signals at 127.9, 131.6, 140.2, 146.6, 152.7, 154.7, 157.1 and 160.2 δ ppm.

IR Spectroscopy (KBr)

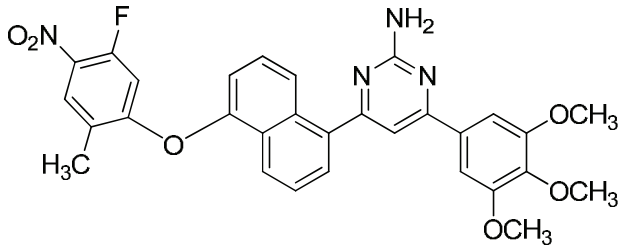
Infrared spectra recorded in KBr reveals that absorption at 3320 and 3315 cm^{-1} indicates the N-H stretching. The band at 3130 cm^{-1} indicates the aromatic C-H stretching. Value at 2970 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1612, 1592 and 1592 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1}

indicates the N=O stretching. Absorption at 741 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 526.5, which indicates the molecular weight of the compound.

Compound C17



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3,4,5-trimethoxyphenyl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. Singlet due to three $–OCH_3$ protons appeared at δ 3.4 ppm. One vinylic group give singlet at δ 5.6 ppm. All 10 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH_2 proton comes at δ 4.5 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Singlet due to two $–OCH_3$ protons appeared at 39.0 and 40.1 δ ppm. Signal due to carbon of methine groups were found at δ 61.1 ppm. All aromatic carbons give signals at 127.9, 131.6, 140.2, 146.6, 152.7, 154.7, 157.1 and 160.2 δ ppm.

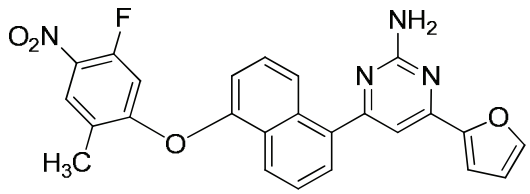
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3410 and 3312 cm^{-1} indicates the N-H stretching. The band at 3130 cm^{-1} indicates the aromatic C-H stretching. Value at 2972 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1612, 1590 and 1565 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 740 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 526.5, which indicates the molecular weight of the compound.

Compound C18



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(furan-2-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.8 ppm. All 11 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH_2 proton comes at δ 4.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 31.2 δ ppm. Signal due to carbon of methine groups were found at δ 62.1 ppm. All aromatic carbons give signals at 128.9, 131.4, 131.6, 142.2, 146.6, 153.7, 154.7, 157.1 and 161.3 δ ppm.

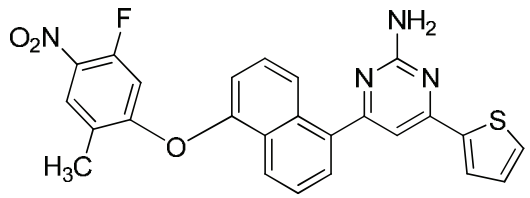
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3350 and 3315 cm^{-1} indicates the N-H stretching. The band at 3130 cm^{-1} indicates the aromatic C-H stretching. Value at 2929 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1613, 1590 and 1560 cm^{-1} indicates the C=C stretching and band at 1480 cm^{-1} indicates the N=O stretching. Absorption at 745 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 456.4, which indicates the molecular weight of the compound.

Compound C19



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(thiophen-2-yl)pyrimidin-2-amine

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. One vinylic group give singlet at δ 5.6 ppm. All 11 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH_2 proton comes at δ 4.3 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.0 δ ppm. Singlet due to two $–OCH_3$ protons appeared at 39.0 and 40.1 δ ppm. Signal due to carbon of methine groups were found at δ 61.1 ppm. All aromatic carbons give signals at 129.4, 131.4, 131.6, 142.2, 146.6, 152.7, 154.7, 157.1 and 161.2 δ ppm.

IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3350 and 3315 cm^{-1} indicates the N-H stretching. The band at 3130 cm^{-1} indicates the aromatic C-H stretching. Value at 2973 cm^{-1} shows aliphatic C-H stretching of the methyl group. Value at 1612, 1590 and 1565 cm^{-1} indicates the C=C stretching and band at 1480cm^{-1} indicates the N=O stretching. Absorption at 745 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the mass spectrum of the given compound, molecular ion peak was found at M+ 472.4, which indicates the molecular weight of the compound.

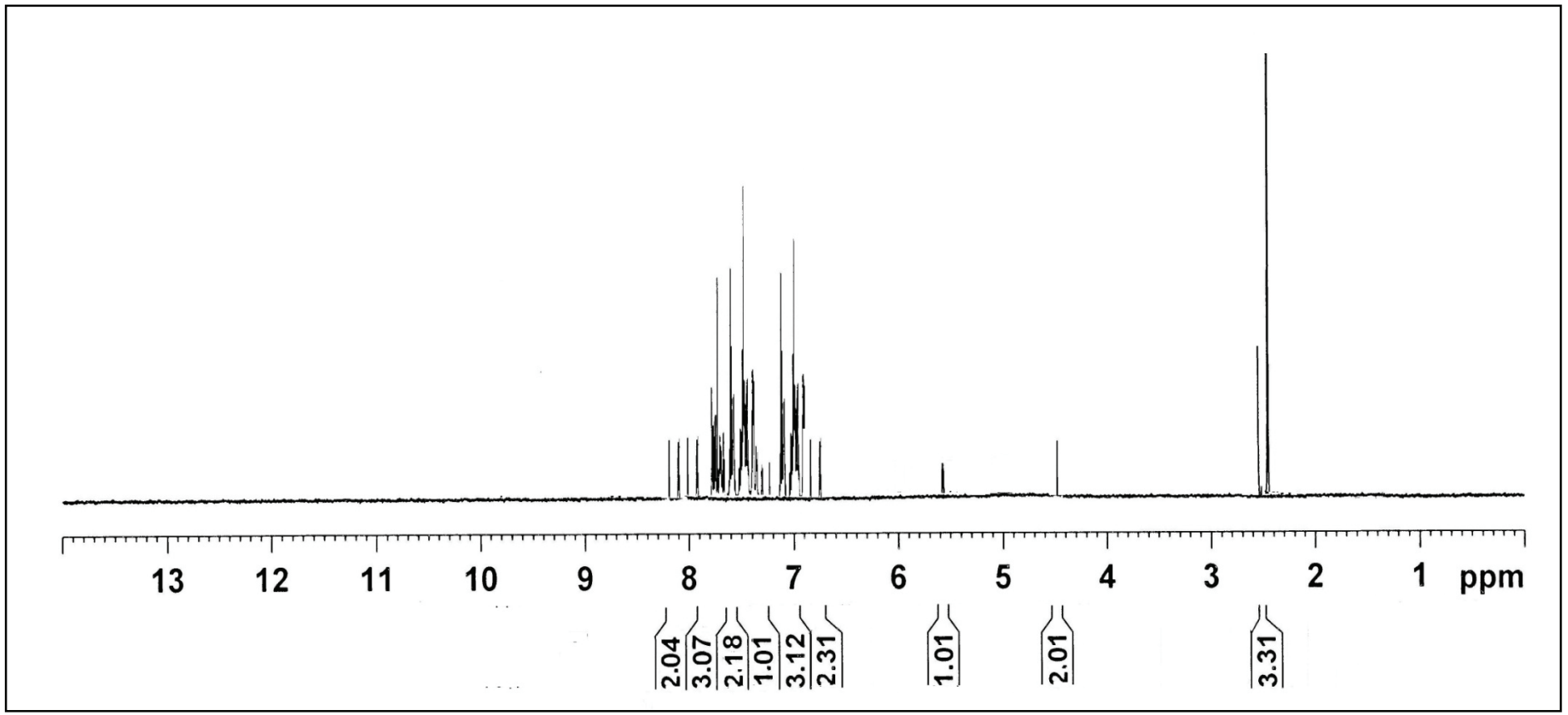


Fig. 5.1: ^{1}H NMR spectrum of C1

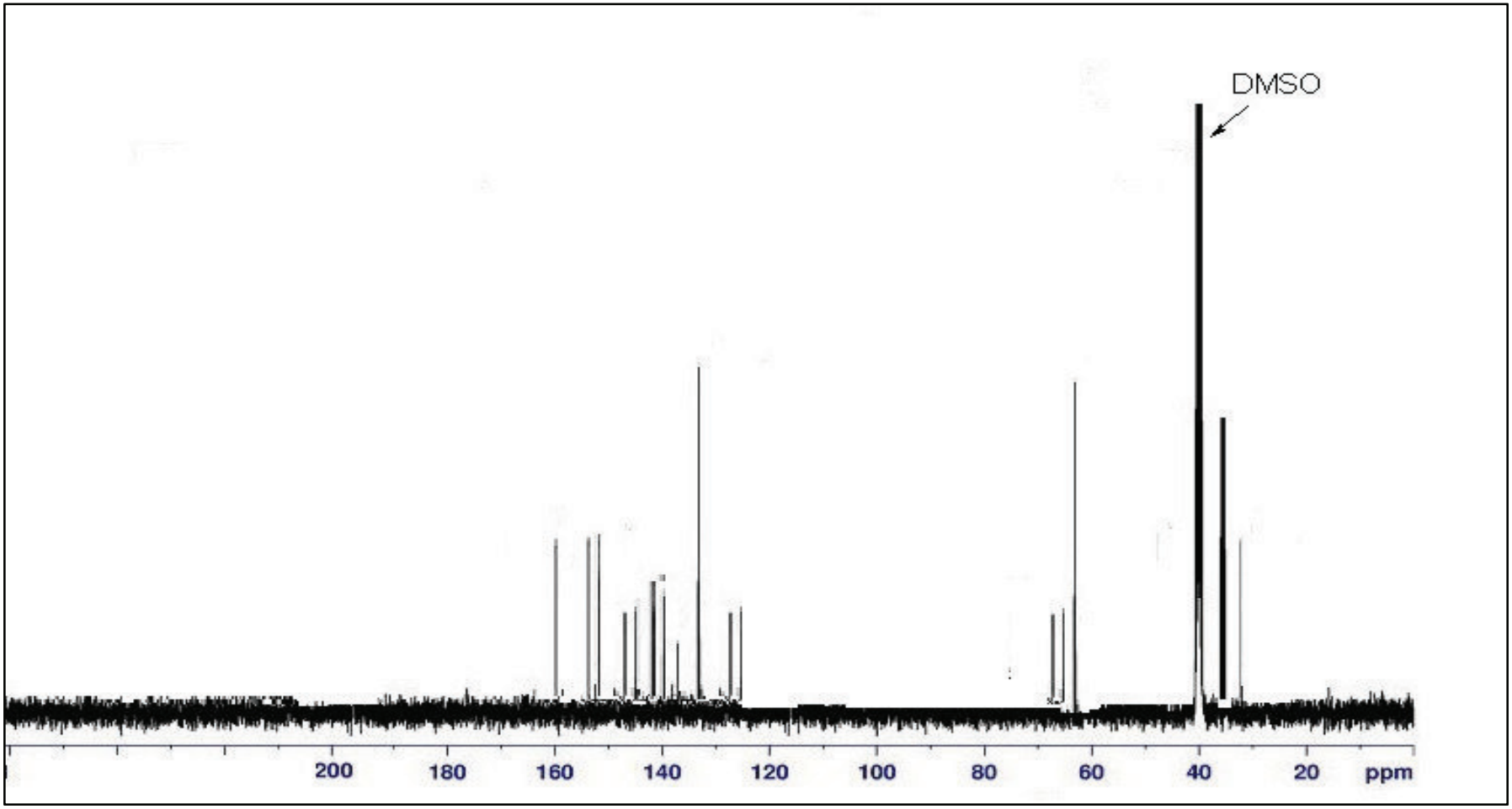


Fig. 5.2: ^{13}C NMR spectrum of C1

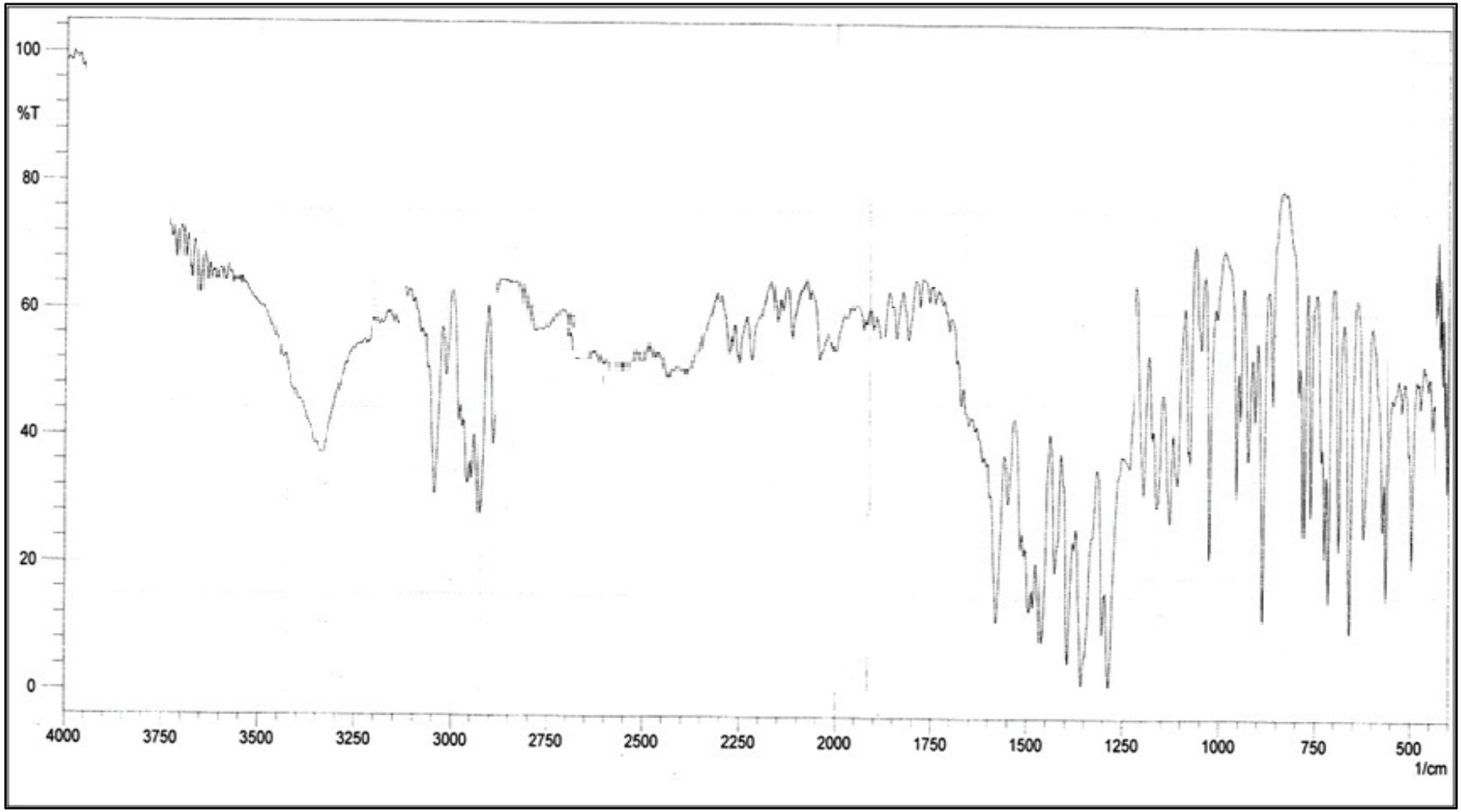


Fig. 5.3: IR spectrum of C1

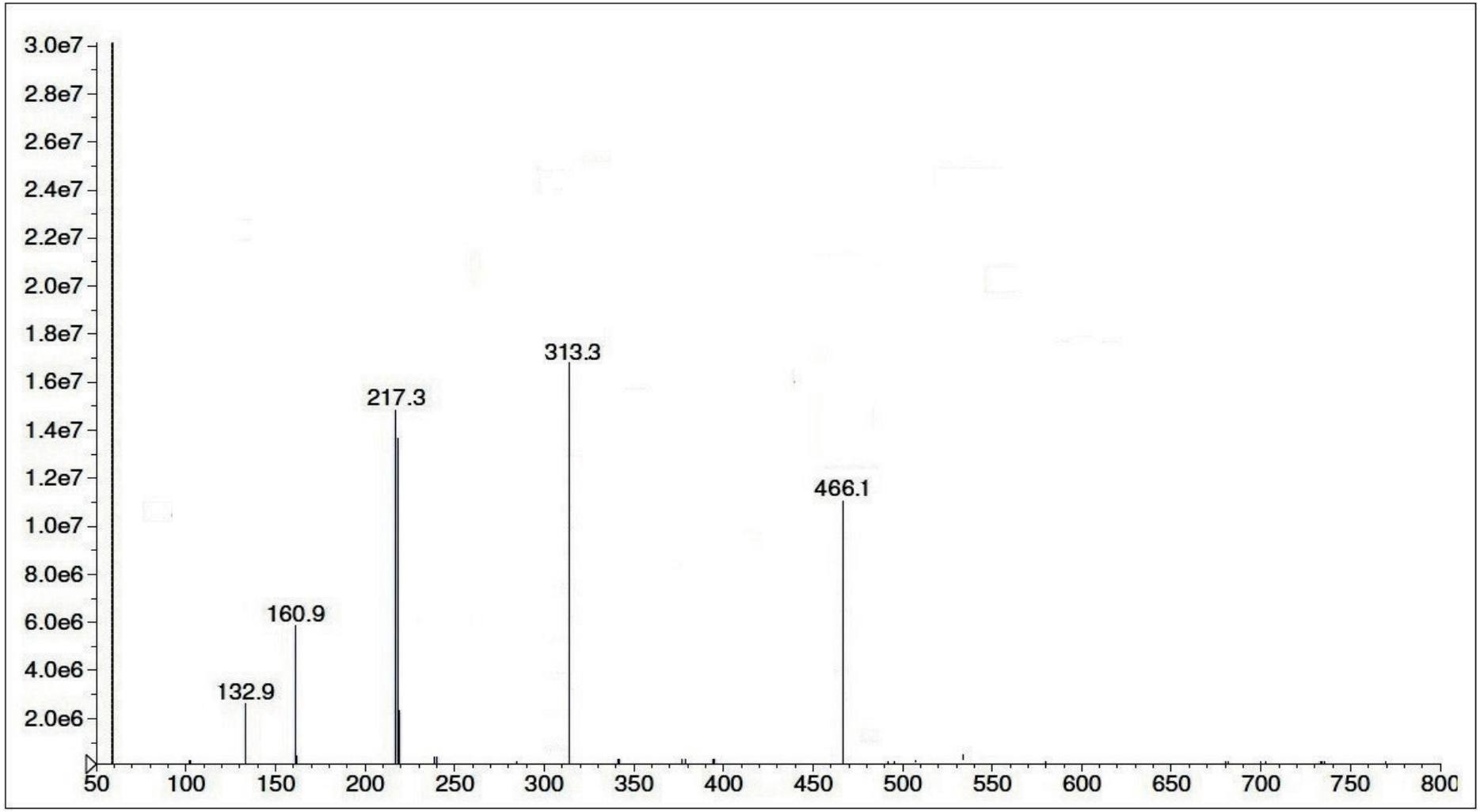


Fig. 5.4: Mass spectrum of C1

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