

Supplementary Information

Quinazoline fused 1,2,4-triazoles: PIDA-mediated synthesis, characterization, anti-breast cancer agents, ABTS radical scavenging efficacy, molecular docking, and DFT studies

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ABSTRACT: The present work demonstrates the PIDA-mediated mild synthesis of 3-aryl-5-phenyl-[1,2,4] triazolo[4,3-c]quinazolines **5a-5n** through an intramolecular oxidative-cyclization of twelve electronically dissimilar and newly prepared (*E*)-4-(2-benzylidenehydrazineyl)-2-phenyl-quinazolines **4a-4n** as key precursors. Structural confirmation of quinazoline-hydrazone and triazole has been established based on ¹H & ¹³C-NMR, IR, and HRMS data. Antiproliferative activity examination led to the identification of 5-phenyl-3-(2,3,4-trimethoxyphenyl)-[1,2,4] triazolo[4,3-c]quinazoline (**5g**) and 3-(2,3-dichlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c] quinazoline (**5j**), as most active (less than and comparable to standard), which exhibits cytotoxicity with IC₅₀ value of 1.14 mM and 1.39 mM respectively against MCF-7 cell line. **5g** and **5j** also shows significant potential against MDA-MB231 cell line with IC₅₀ of 2.79 mM and 1.95 mM respectively. Additionally, molecular modeling studies have been conducted to support the results and to study the binding interaction of the compound **5g** and **5j** with VEGFR-2 kinase enzyme (PDB ID:3U6J). Furthermore, systematically screening of **5a-5n** for ABTS radical scavenging activity, displays that 3-(4-

fluorophenyl)-5-phenyl-[1,2,4]triazolo [4,3-c] quinazoline **5h**, has highest antioxidant efficacy, with $IC_{50} = 11.2 \pm 0.14 \mu\text{g/ml}$. The antioxidant efficacy of **5a-5n** was also supported by DFT studies.

Remarks

“The standard compound, being a purified compound and highly active substance, was assessed using a lower concentration range (0 to 50 $\mu\text{g/ml}$). In contrast, the sample’s potency remains unbound; therefore, a broader concentration range (0 to 1000 $\mu\text{g/ml}$) was employed for the sample analysis.”

Calculations

$$\% \text{ RSA} = ((\text{Abs Control} - \text{Abs Sample}) / \text{Abs Control}) \times 100$$

RSA = Radical Scavenging Activity

Abs Control = Absorbance of control

Abs Sample = Absorbance of sample.

Starting precursor characterization data

Characterization data for (E)-4-(2-benzylidenehydrazinyl)-2-phenylquinazoline derivatives 4a-4n.

(E)-4-(2-(2-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4a)

Brown solid; Yield 70%; m.p. 138-140°C; $R_f = 0.43$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{22}H_{18}N_4$: 339.1559, found: 359.1606.

(E)-4-(2-(4-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4c).

Yellow solid; Yield 78%; $R_f = 0.35$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{22}H_{18}N_4$: 339.1559, found: 339.1800.

(E)-4-(2-(4-Isopropylbenzylidene)hydrazinyl)-2-phenylquinazoline (4d).

Pale yellow solid; Yield 90%; m.p. 108-112°C; $R_f = 0.62$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{24}H_{22}N_4$: 367.1859, found: 367.1918.

(E)-4-((2-(2-Phenylquinazolin-4-yl)hydrazono)methyl)phenol (4e).

Mustard solid; Yield 88%; $R_f = 0.56$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{21}H_{16}N_4O$: 341.1359, found: 341.1390.

(E)-4-(2-(4-Methoxybenzylidene)hydrazinyl)-2-phenylquinazoline (4f).

Pale yellow solid; Yield 74%; $R_f = 0.45$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{22}H_{18}N_4O$: 355.1559, found: 355.1765.

(E)-4-(2-(4-Fluorobenzylidene)hydrazinyl)-2-phenylquinazoline (4h).

Pale yellow solid; Yield 76%; $R_f = 0.48$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{21}H_{15}N_4F$: 343.1359, found: 343.1592.

(E)-4-(2-(4-Chlorobenzylidene)hydrazinyl)-2-phenylquinazoline (4i).

Yellow solid; Yield 85%; m.p. 178-182°C; $R_f = 0.30$ (ethyl acetate/n-hexane, 2:8); ^{13}C -NMR (100 MHz, DMSO- d_6 , 25°C, TMS): $\delta_c = 149.72$, 148.08, 146.53, 141.29, 134.46, 133.02, 132.42, 131.82, 130.45, 129.75, 128.53, 128.29, 127.94, 127.89, 127.37, 123.14, 116.58; HRMS m/z $[M+H]^+/[M+H+2]$ calcd for $C_{21}H_{15}ClN_4$: 359.1059/361.1059, found: 359.1083/361.1024.

(E)-4-(2-(2,3-Dichlorobenzylidene)hydrazinyl)-2-phenylquinazoline (4j).

Pale yellow solid; Yield 85%; m.p. 176-180°C; $R_f = 0.28$ (ethyl acetate/n-hexane, 2:8).

(E)-4-(2-(Naphthalen-1-ylmethylene)hydrazinyl)-2-phenylquinazoline (4k).

Yellow solid; Yield 92%; m.p. 204-206°C; $R_f = 0.72$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{25}H_{18}N_4$: 375.1559, found: 375.1604.

(E)-4-(2-(3-Nitrobenzylidene)hydrazinyl)-2-phenylquinazoline (4m).

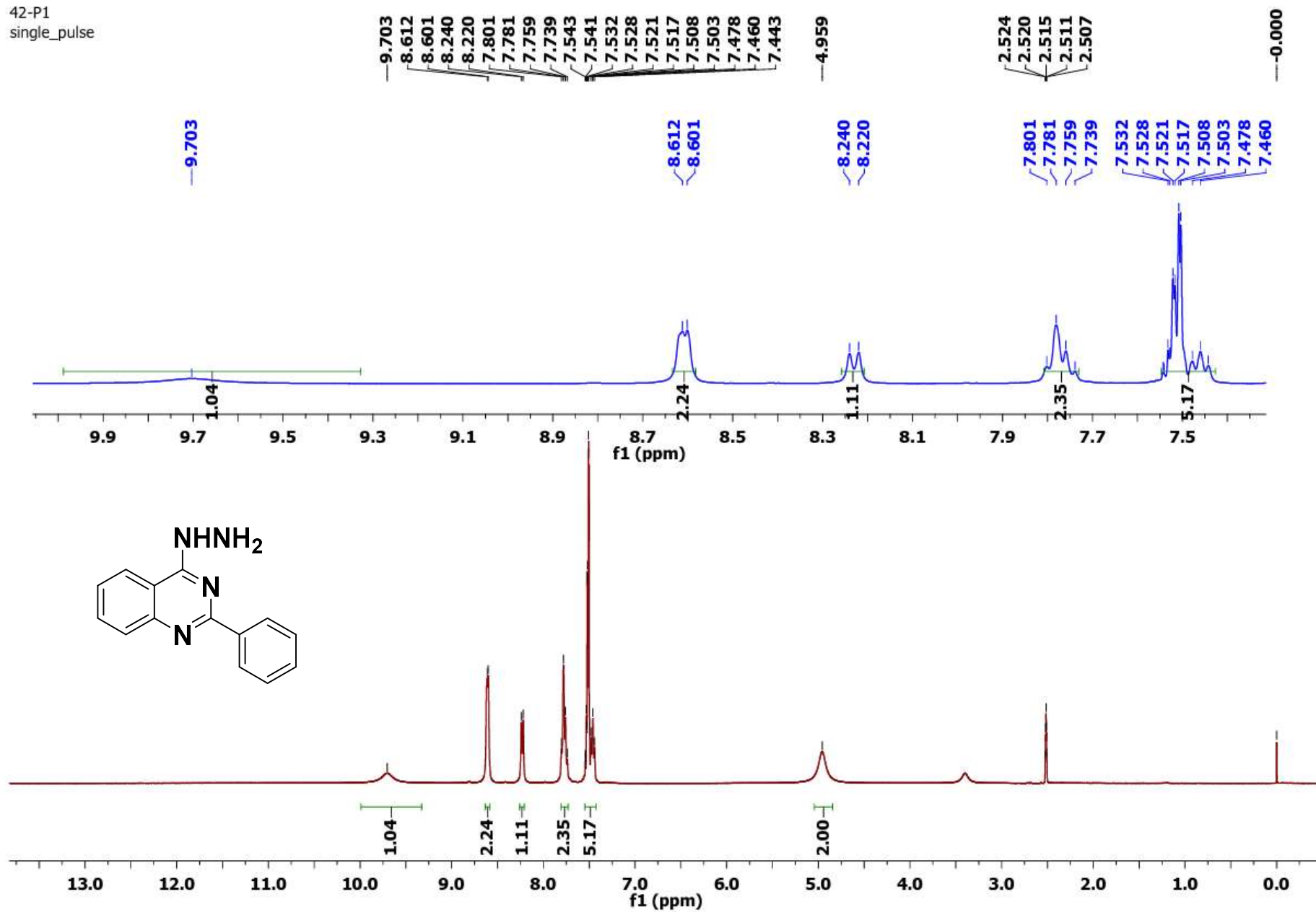
Yellow solid; Yield 95%; $R_f = 0.43$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{21}H_{15}N_5O_2$: 370.1259, found: 370.1298.

(E)-4-(2-(4-Nitrobenzylidene)hydrazinyl)-2-phenylquinazoline (4n).

Orange solid; Yield 95%; $R_f = 0.71$ (ethyl acetate/n-hexane, 2:8); HRMS m/z $[M+H]^+$ calcd for $C_{21}H_{15}N_5O_2$: 370.1259, found: 370.1300.

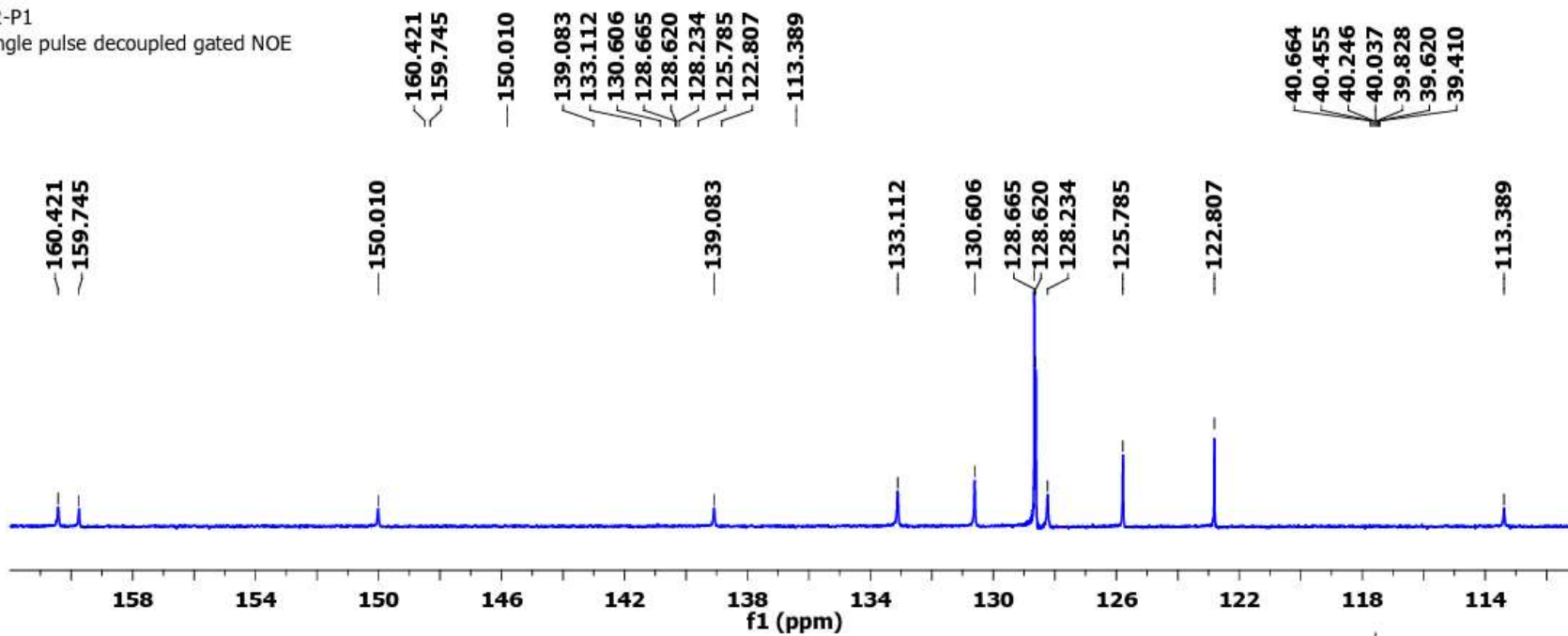
¹H-NMR SPECTRA: 4-Hydrazinyl-2-phenylquinazoline

42-P1
single_pulse



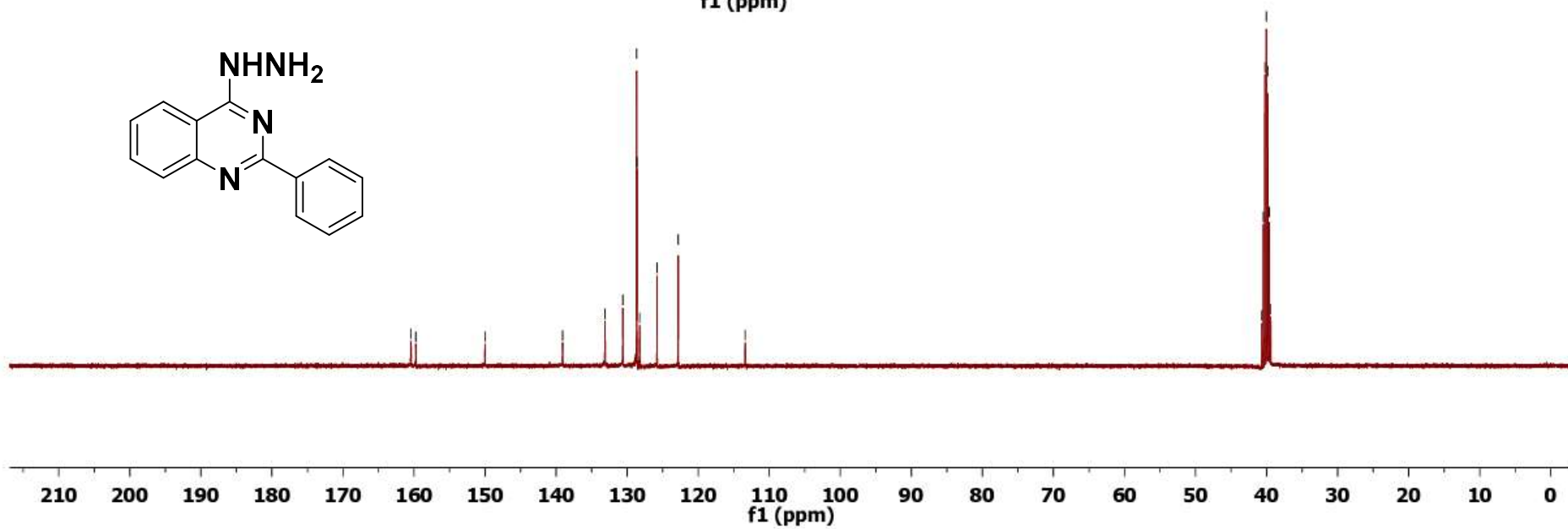
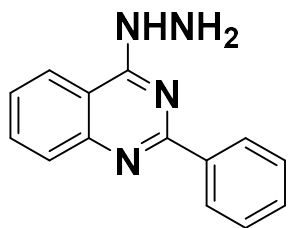
¹³C-NMR SPECTRA: 4-Hydrazinyl-2-phenylquinazoline

42-P1
single pulse decoupled gated NOE



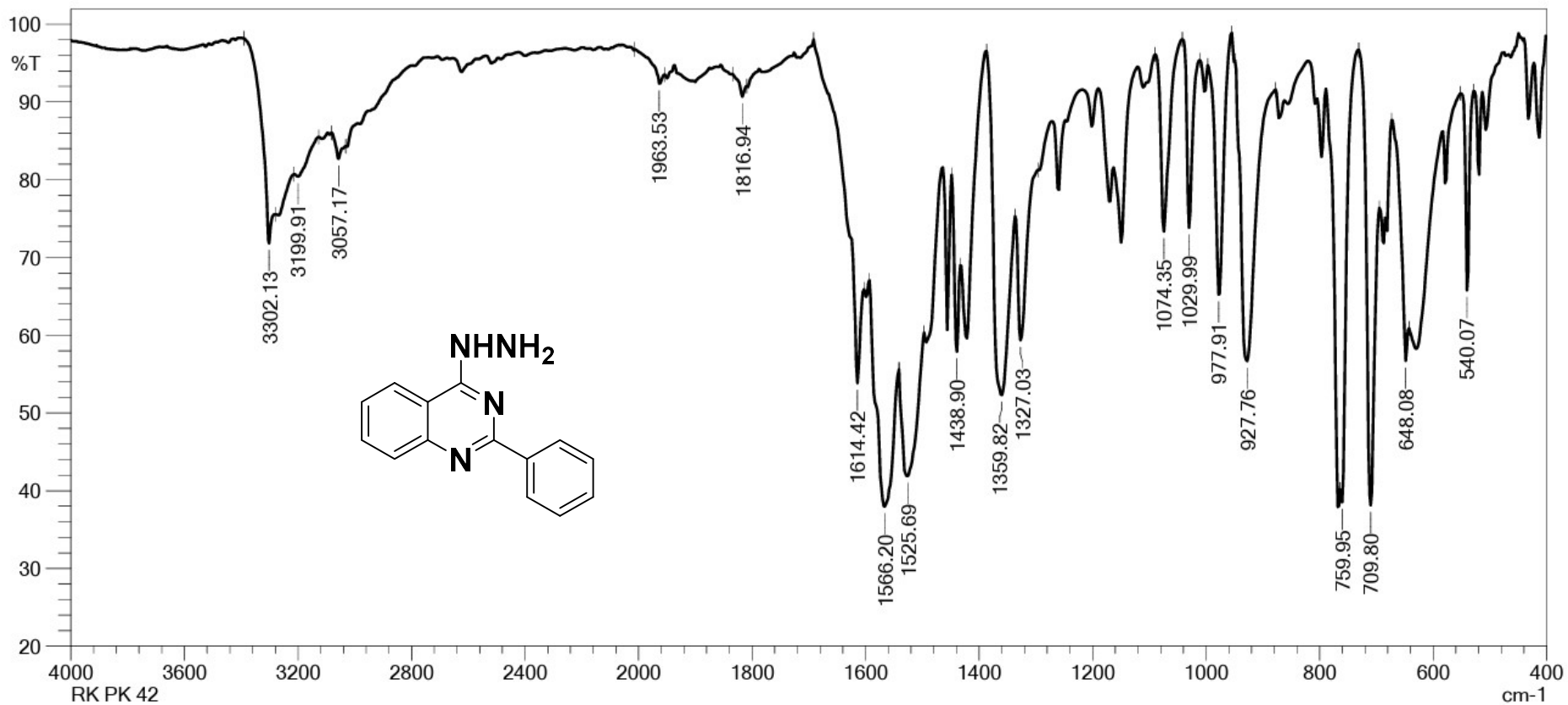
160.421
159.745
150.010
139.083
133.112
130.606
128.665
128.620
128.234
125.785
122.807
113.389

40.664
40.455
40.246
40.037
39.828
39.620
39.410



IR SPECTRA: 4-Hydrazinyl-2-phenylquinazoline

SHIMADZU



HRMS SPECTRA: (E)-4-(2-(2-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4a).

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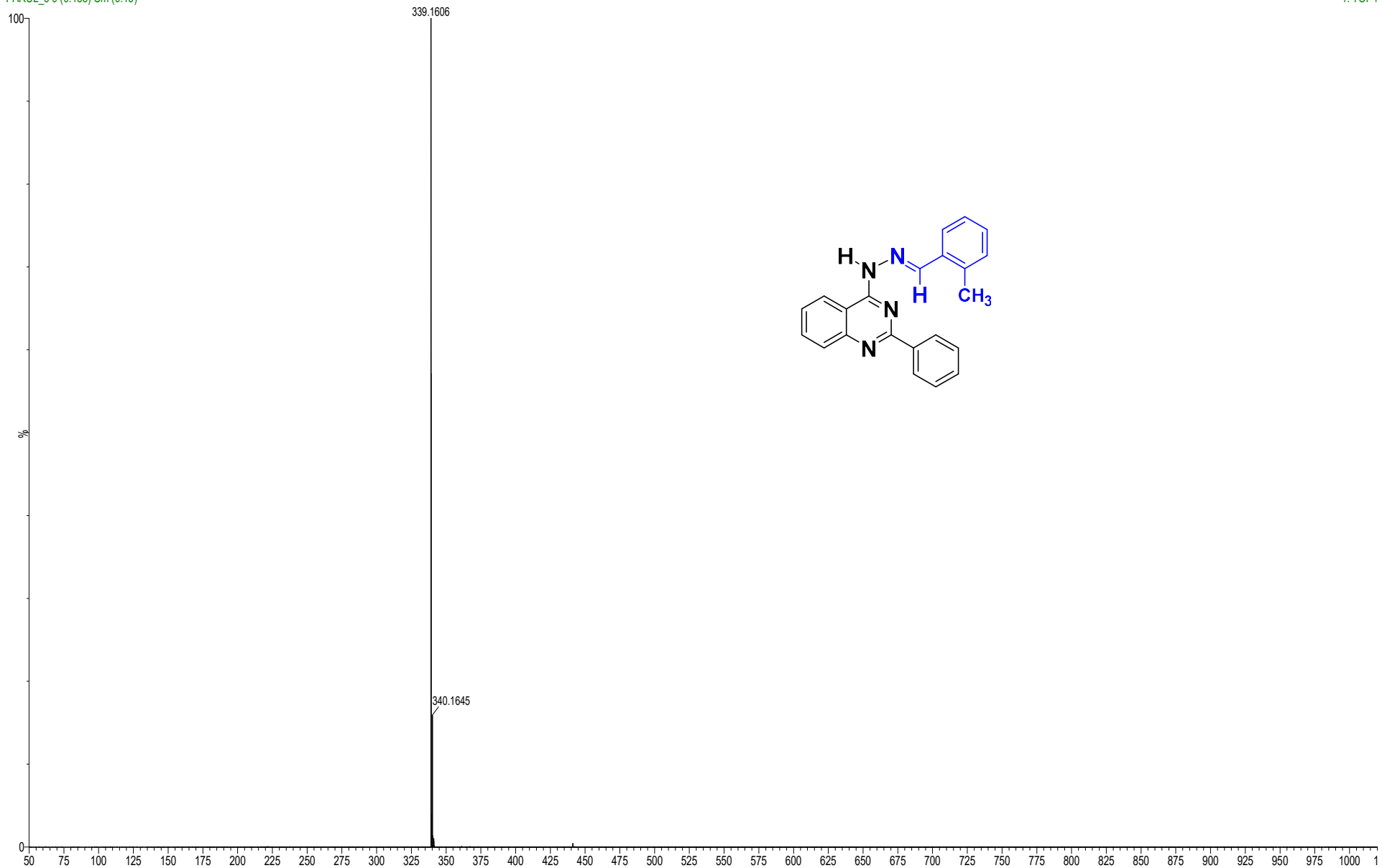
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14-M:

1:

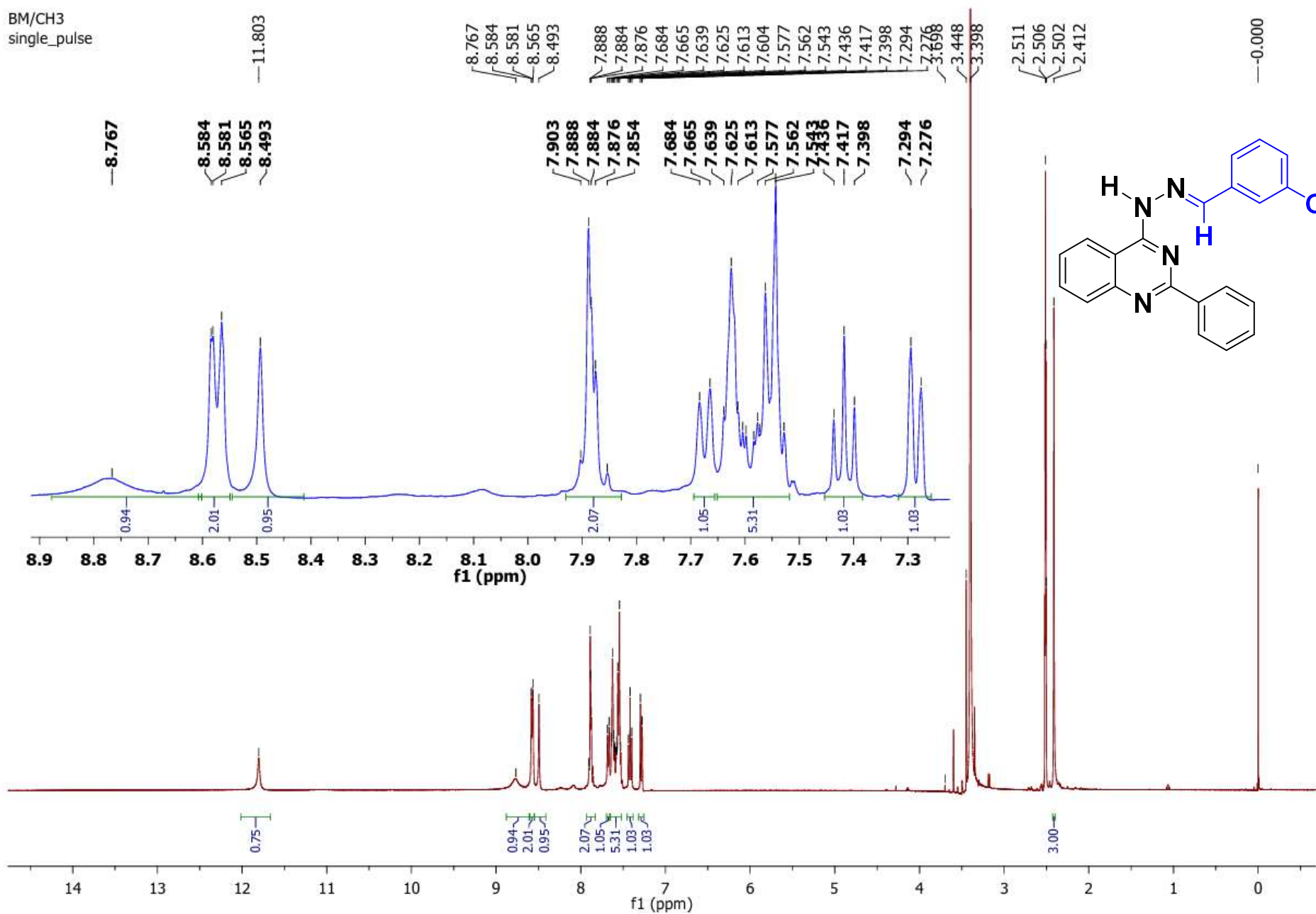
1: TOF

PARUL_3 9 (0.188) Cm (9:13)



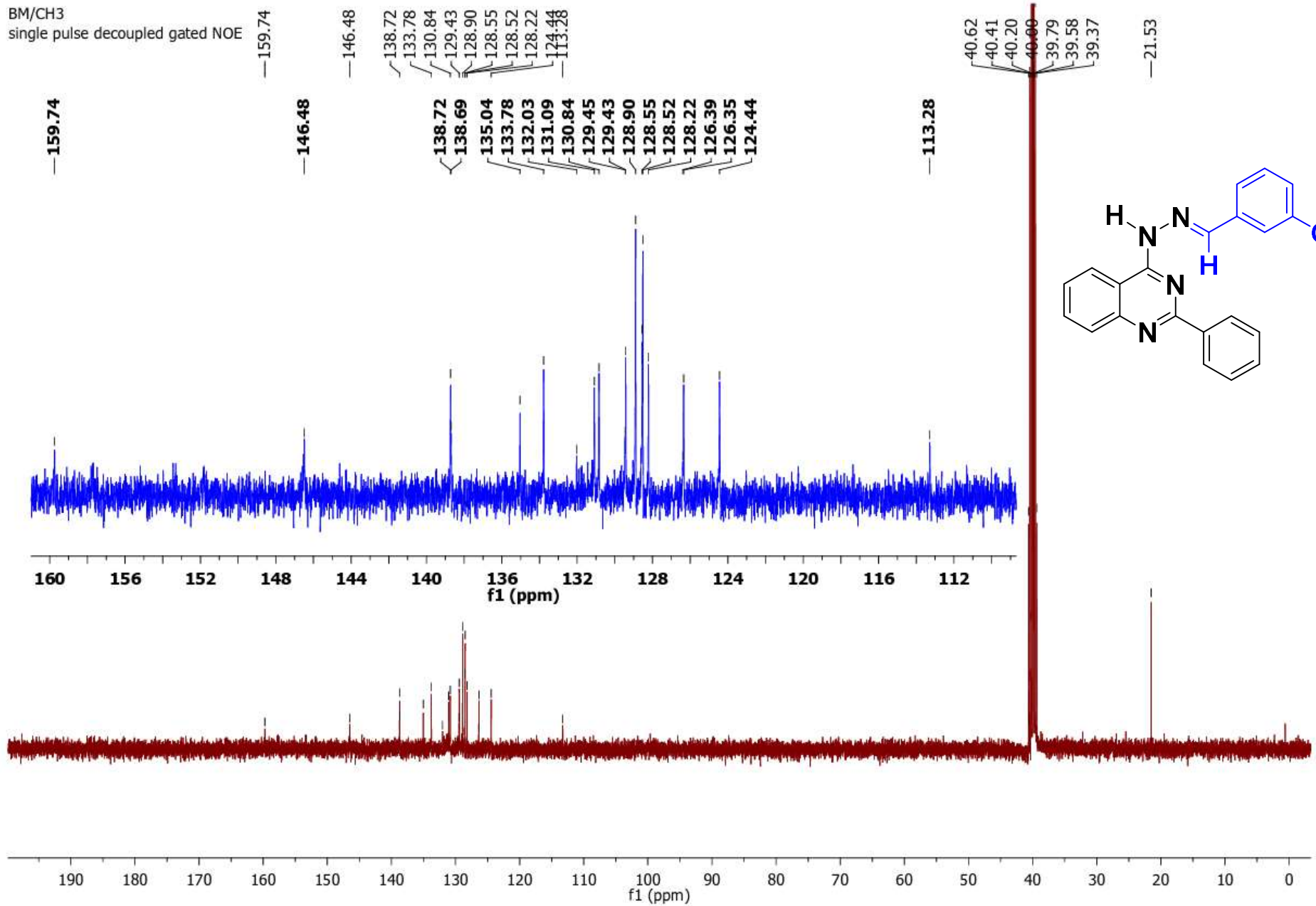
¹H-NMR SPECTRA: (E)-4-(2-(3-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4b).

BM/CH3
single_pulse

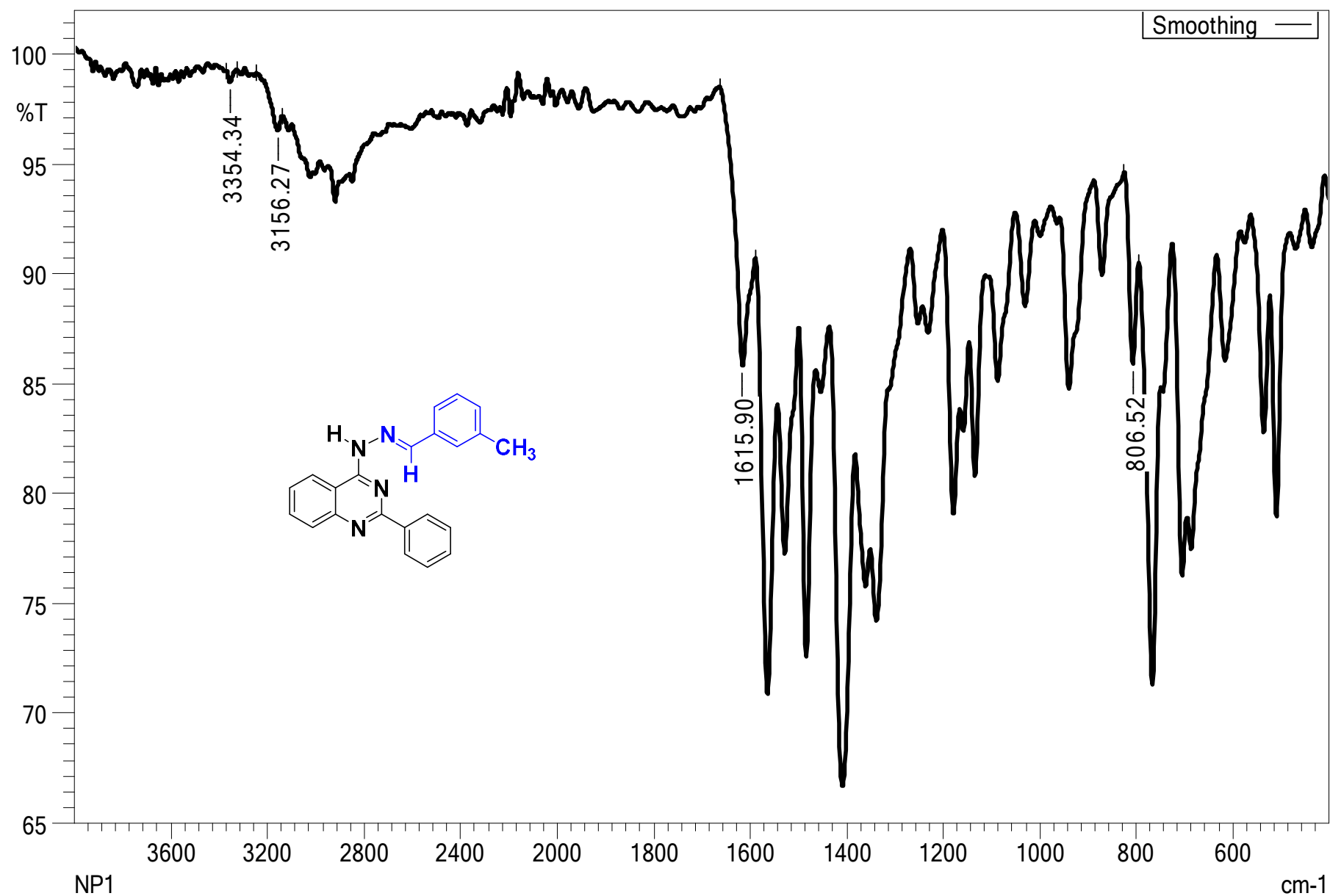


¹H-NMR SPECTRA: (E)-4-(2-(3-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4b).

BM/CH3
single pulse decoupled gated NOE



IR SPECTRA: (E)-4-(2-(3-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4b).



HRMS SPECTRA: (E)-4-(2-(3-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4b).

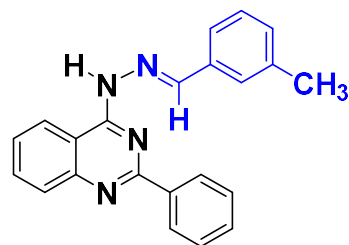
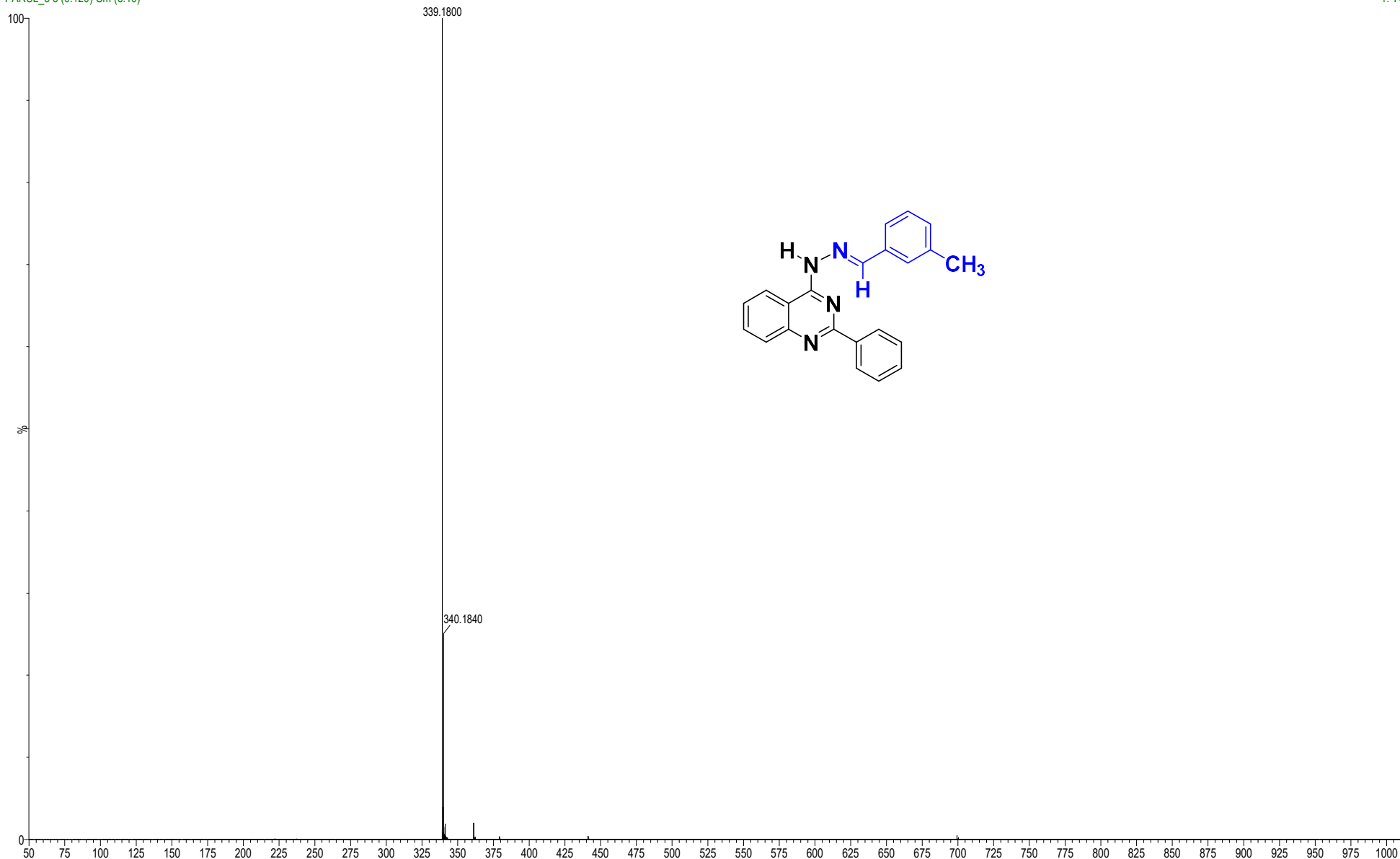
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SYNAPT-XS#DBA064

14

PARUL_5 5 (0.120) Cm (5:10)

1: T



HRMS SPECTRA: (E)-4-(2-(4-Methylbenzylidene)hydrazinyl)-2-phenylquinazoline (4c).

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SYNAPT-XS#DBA064

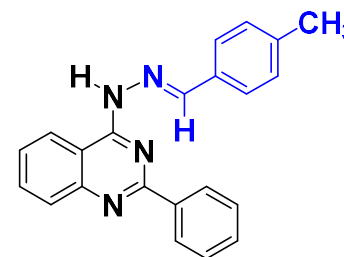
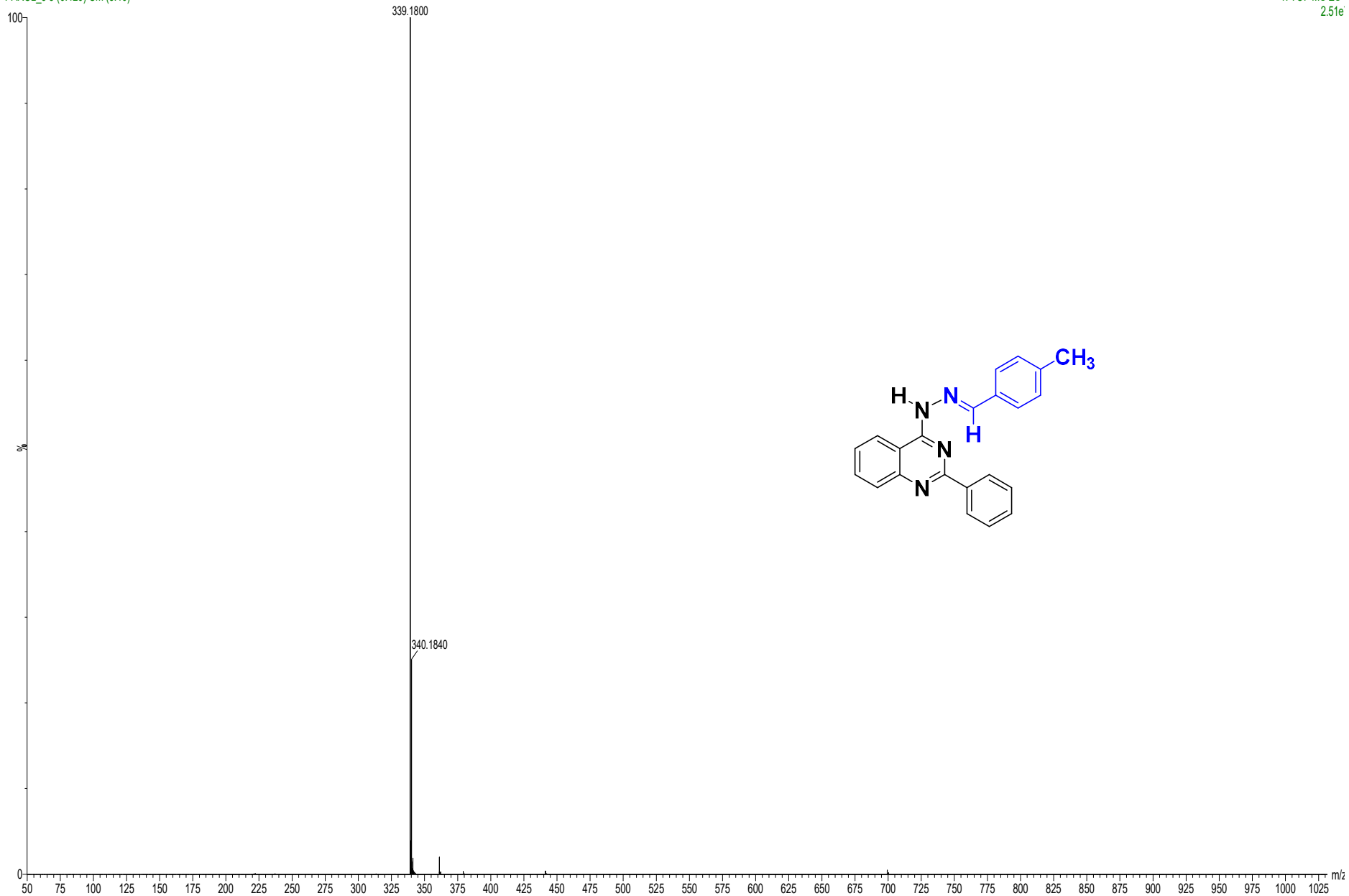
14-Mar-202

12:58:11

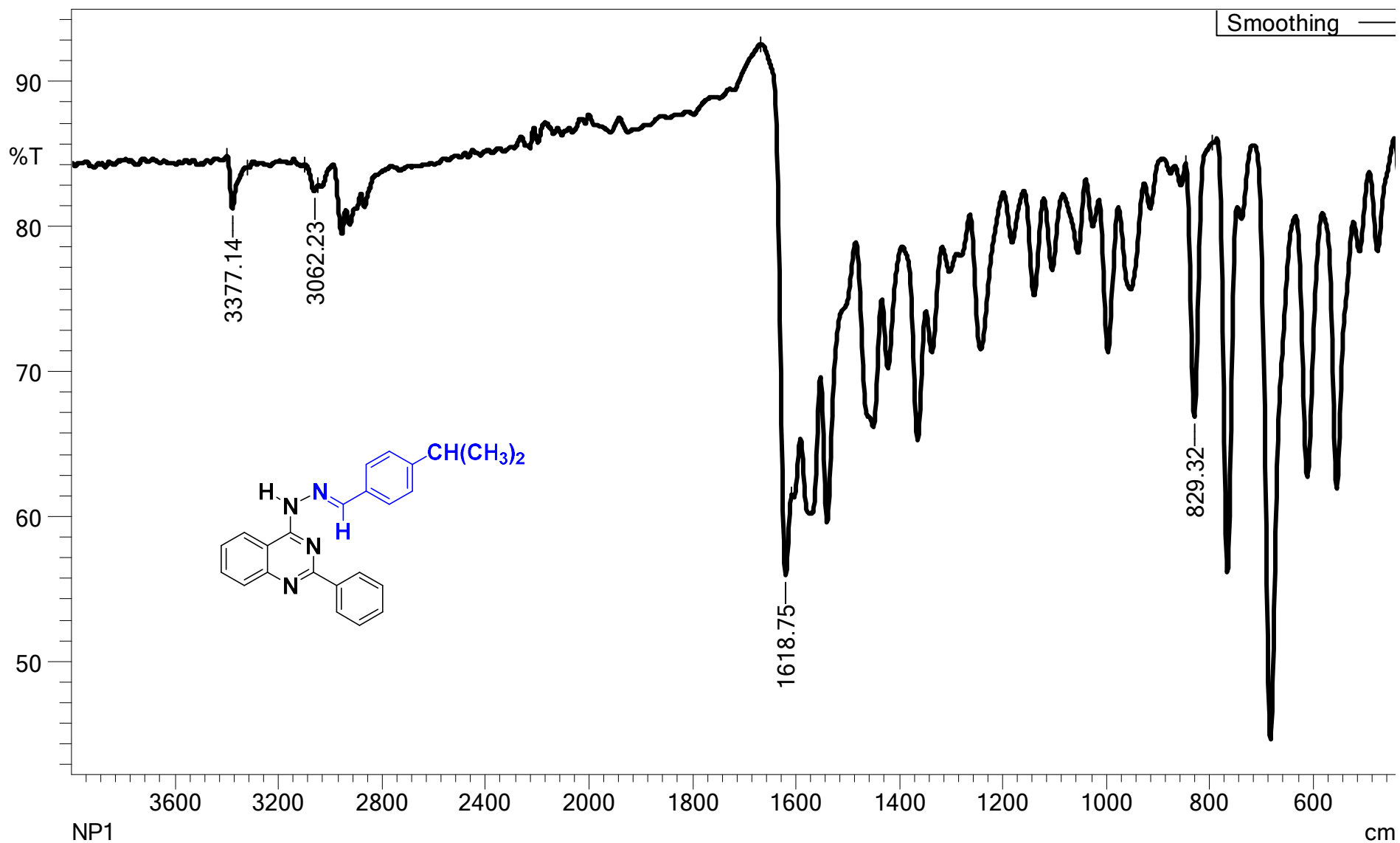
1: TOF MS ES+

2.51e

PARUL_5 5 (0.120) Cm (5.10)



IR SPECTRA: (E)-4-(2-(4-Isopropylbenzylidene)hydrazinyl)-2-phenylquinazoline (4d).



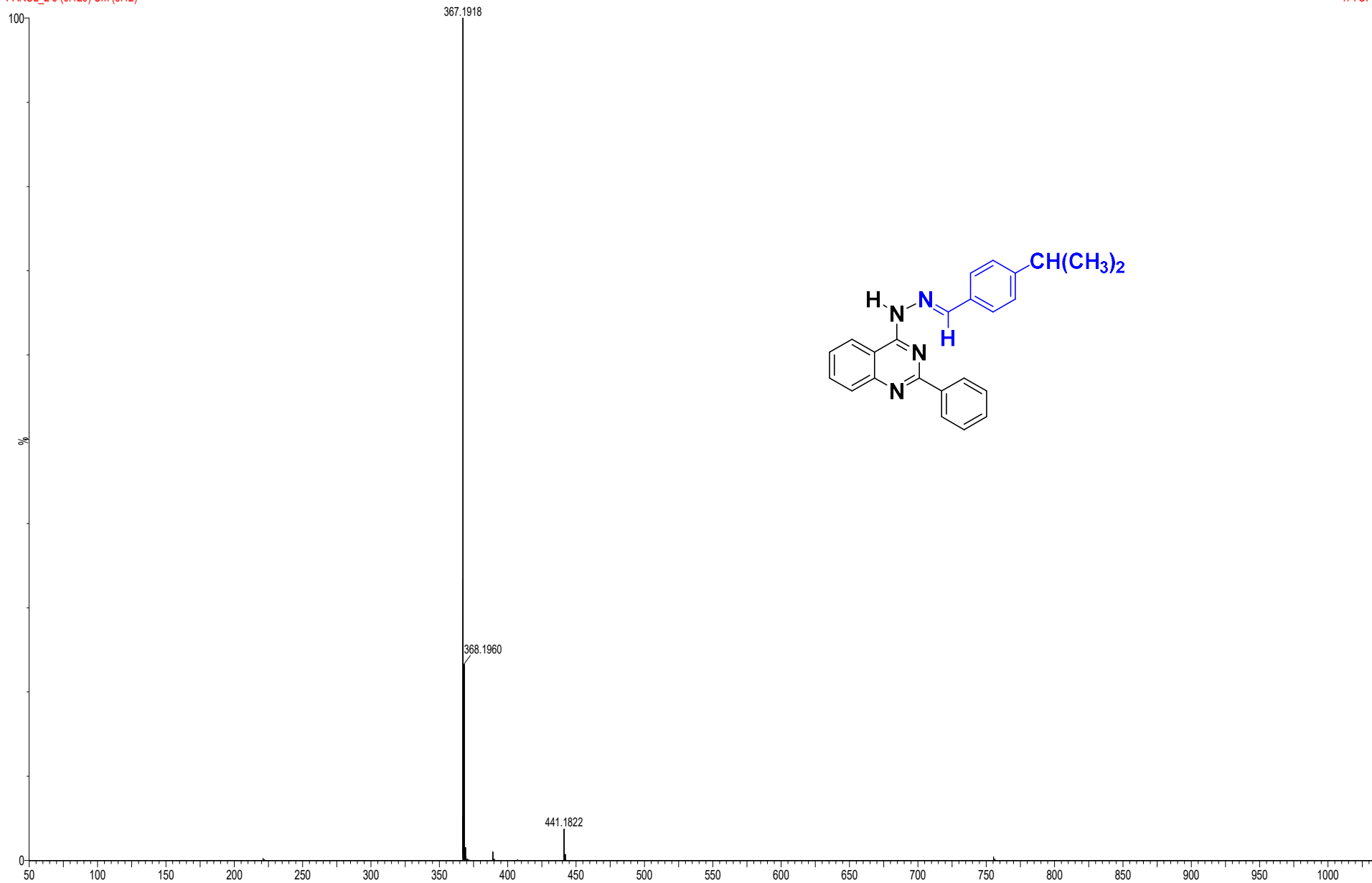
HRMS SPECTRA: (E)-4-(2-(4-Isopropylbenzylidene)hydrazinyl)-2-phenylquinazoline (4d).

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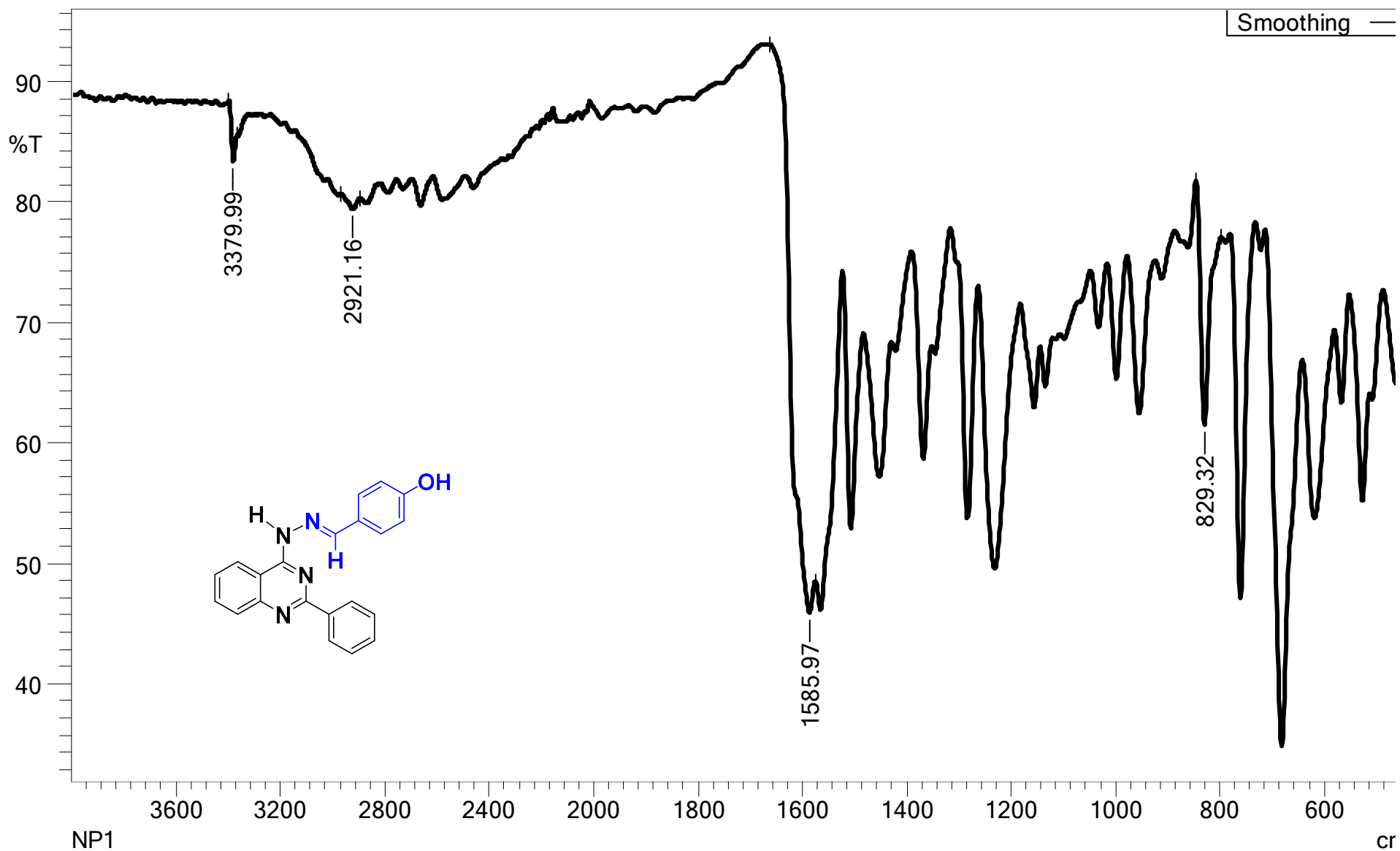
SYNAPT-XS#DBA064

14-M:
1:
1: TOF I

PARUL_2.5 (0.120) Cm (3:12)



IR SPECTRA: (E)-4-((2-(2-Phenylquinazolin-4-yl)hydrazono)methyl)phenol (4e).



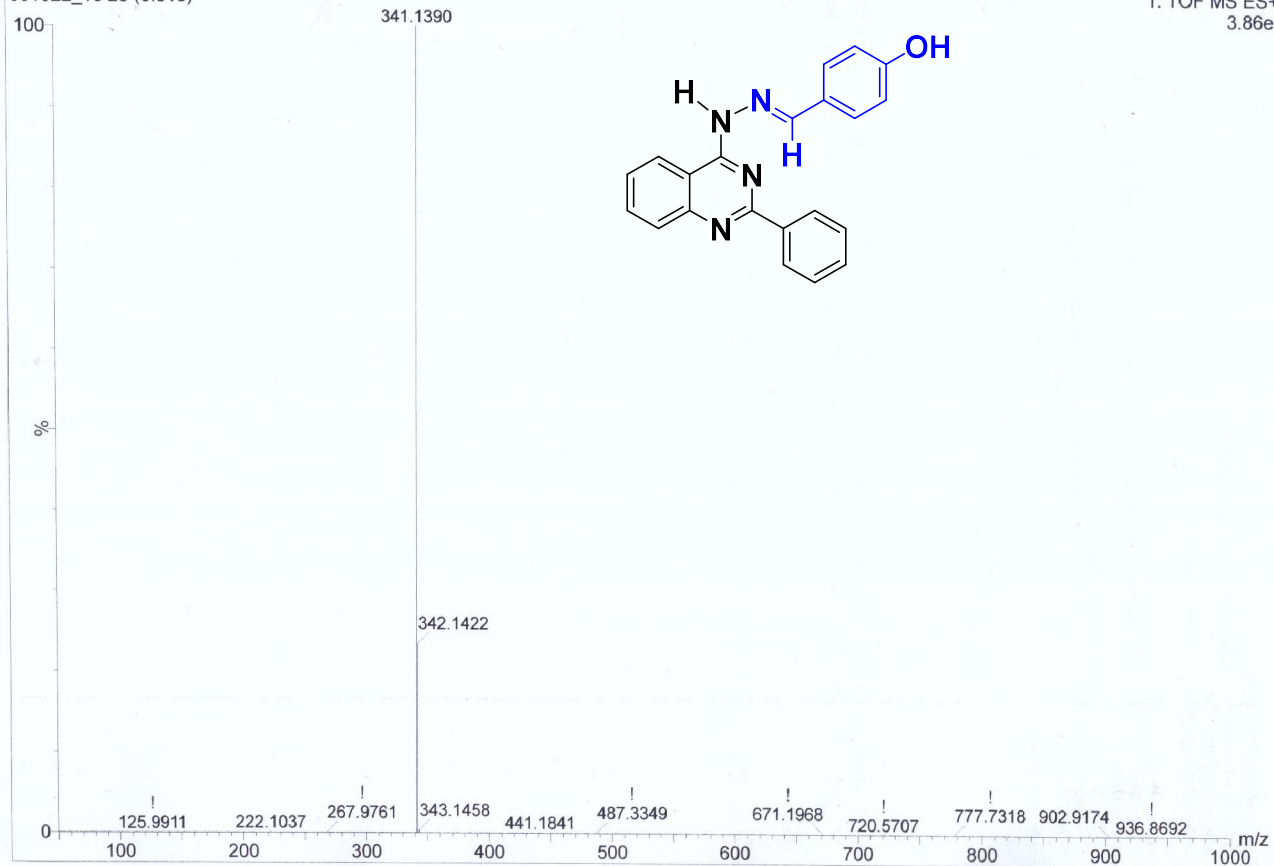
HRMS SPECTRA: (E)-4-((2-(2-Phenylquinazolin-4-yl)hydrazono)methyl)phenol (4e).

XEVO -G2XSQTOF#TFC2176
POSITIVE ION MODE
SS 1
061022_16 25 (0.519)

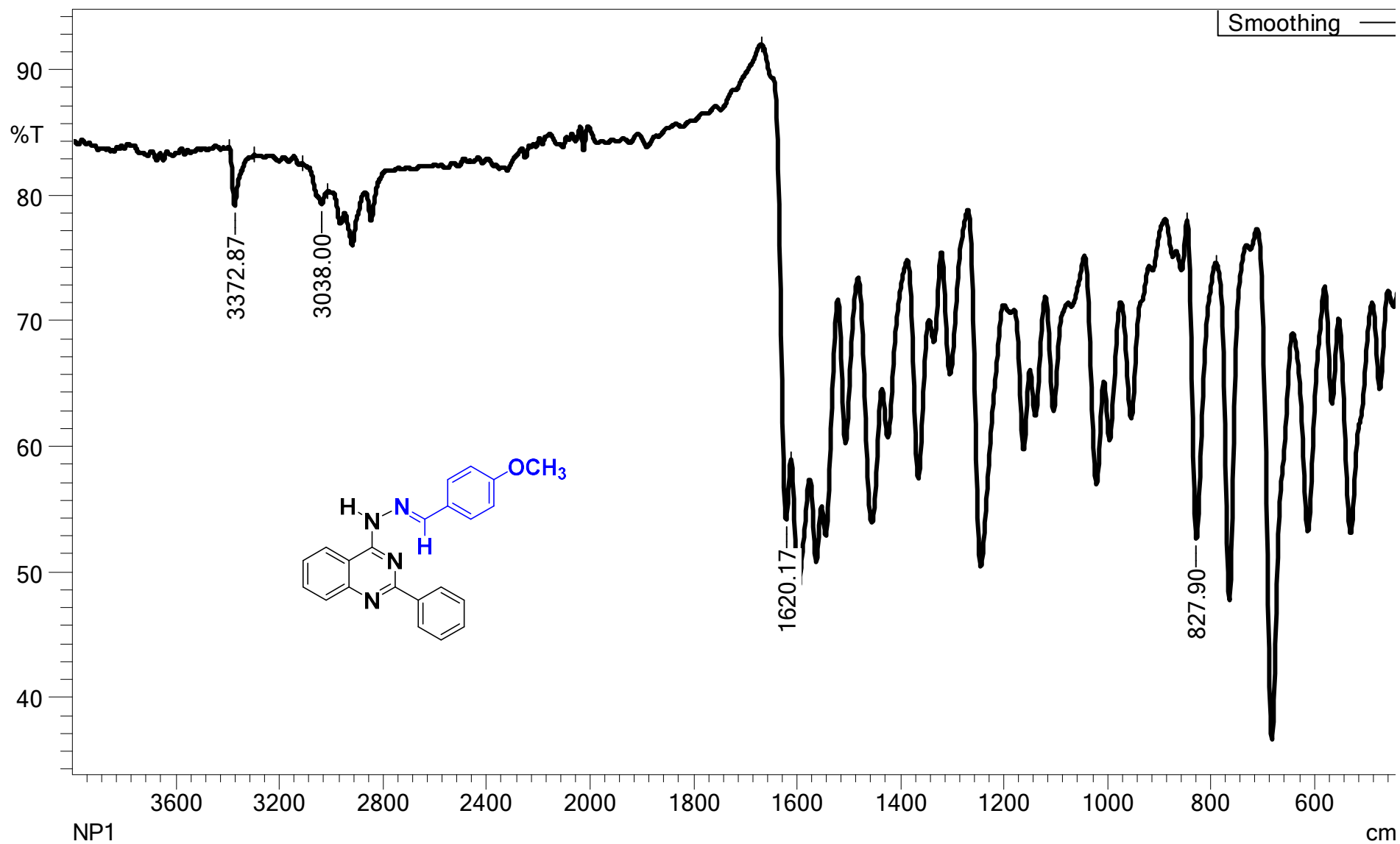
Capillary V 3, Cone V 40, Desolvation Gas 800
ESI

06-Oct-2022

1: TOF MS ES+
3.86e6



IR SPECTRA: (E)-4-(2-(4-Methoxybenzylidene)hydrazinyl)-2-phenylquinazoline (4n).



HRMS SPECTRA: (E)-4-(2-(4-Methoxybenzylidene)hydrazinyl)-2-phenylquinazoline (4f).

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SYNAPT-XS#DBA064

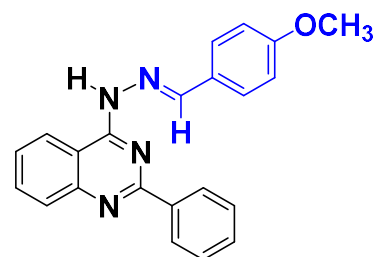
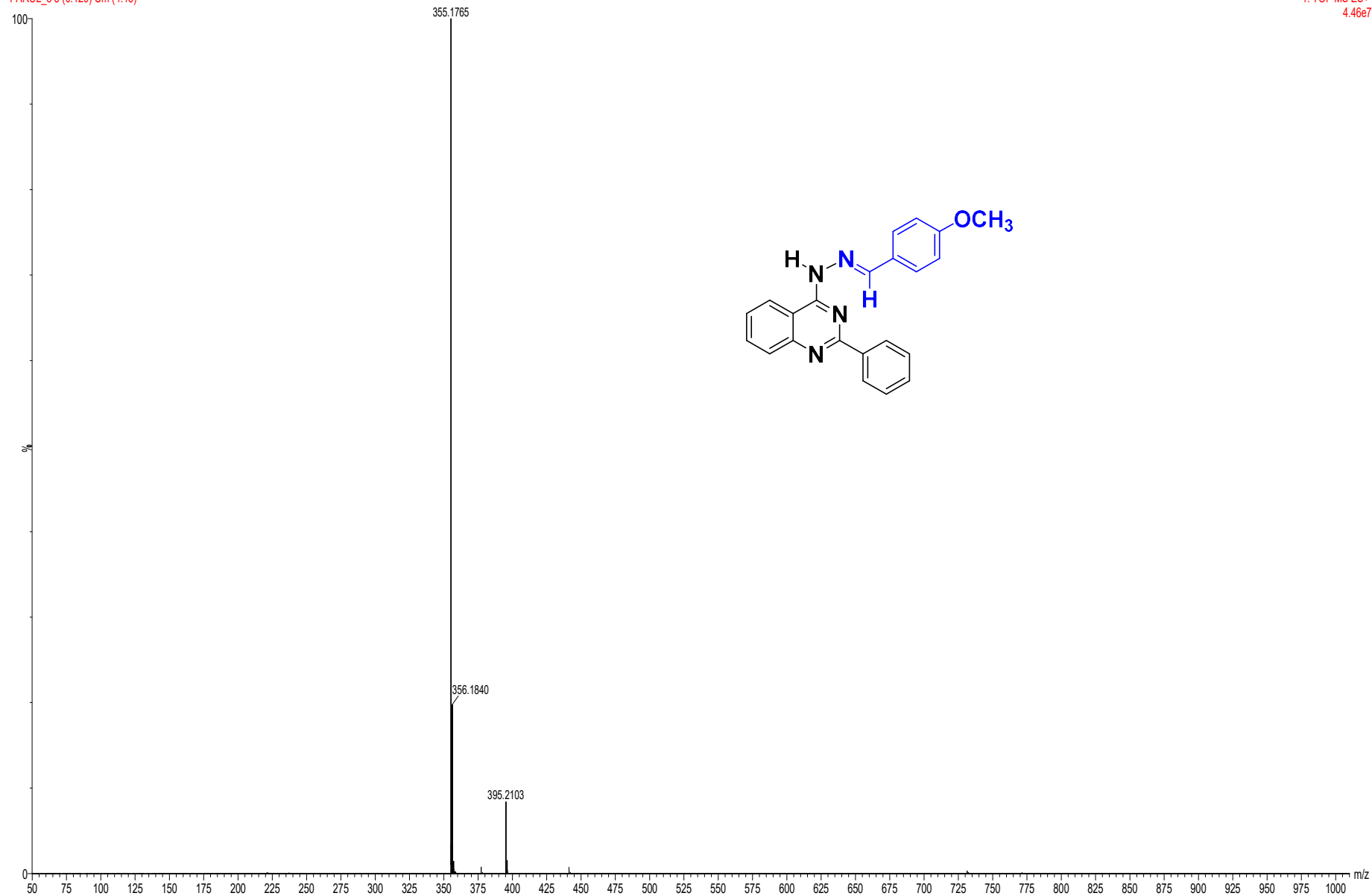
14-Mar-2023

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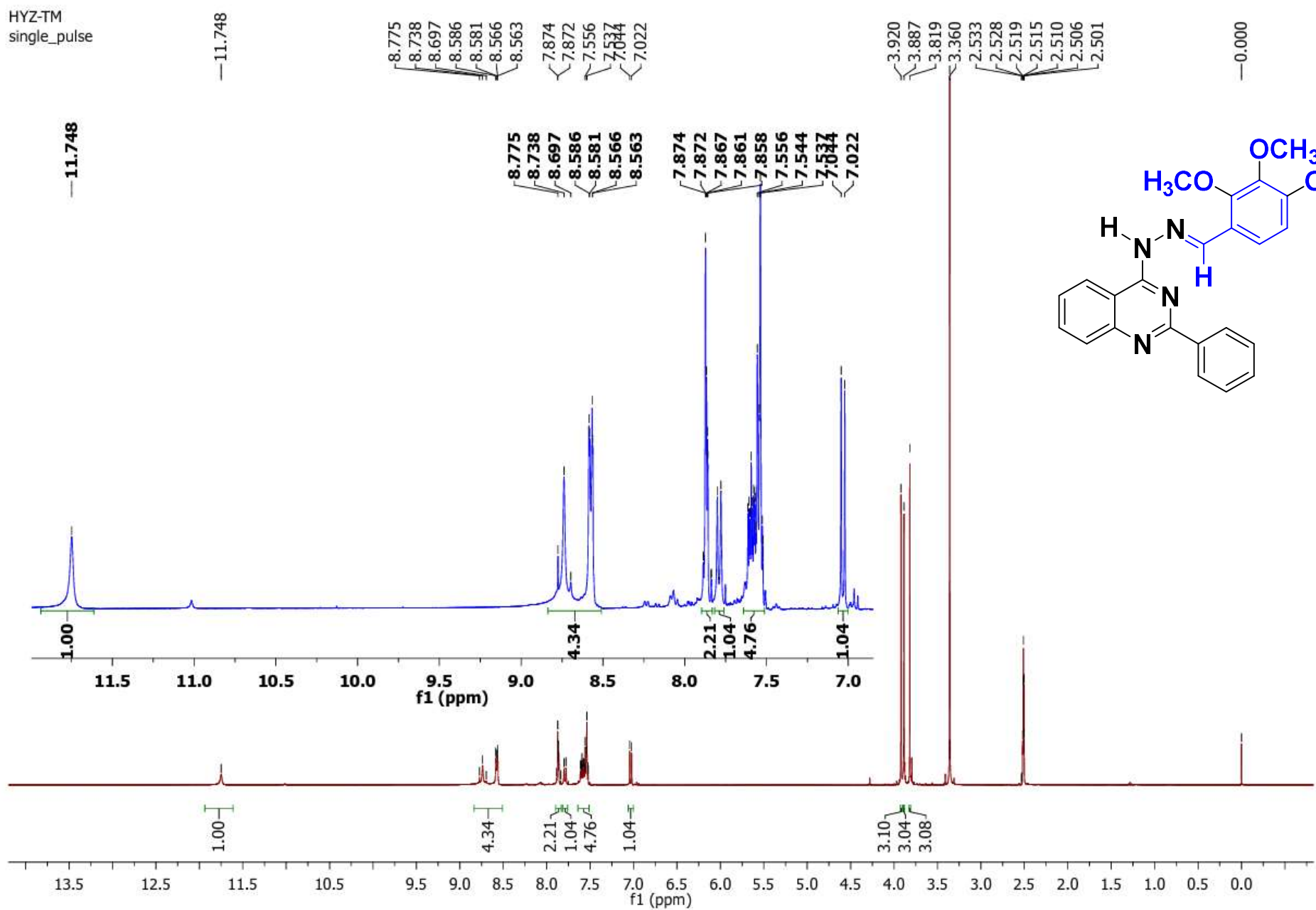
1: TOF MS ES+

4.46e7

PARUL_8.5 (0.120) Cm (4:15)



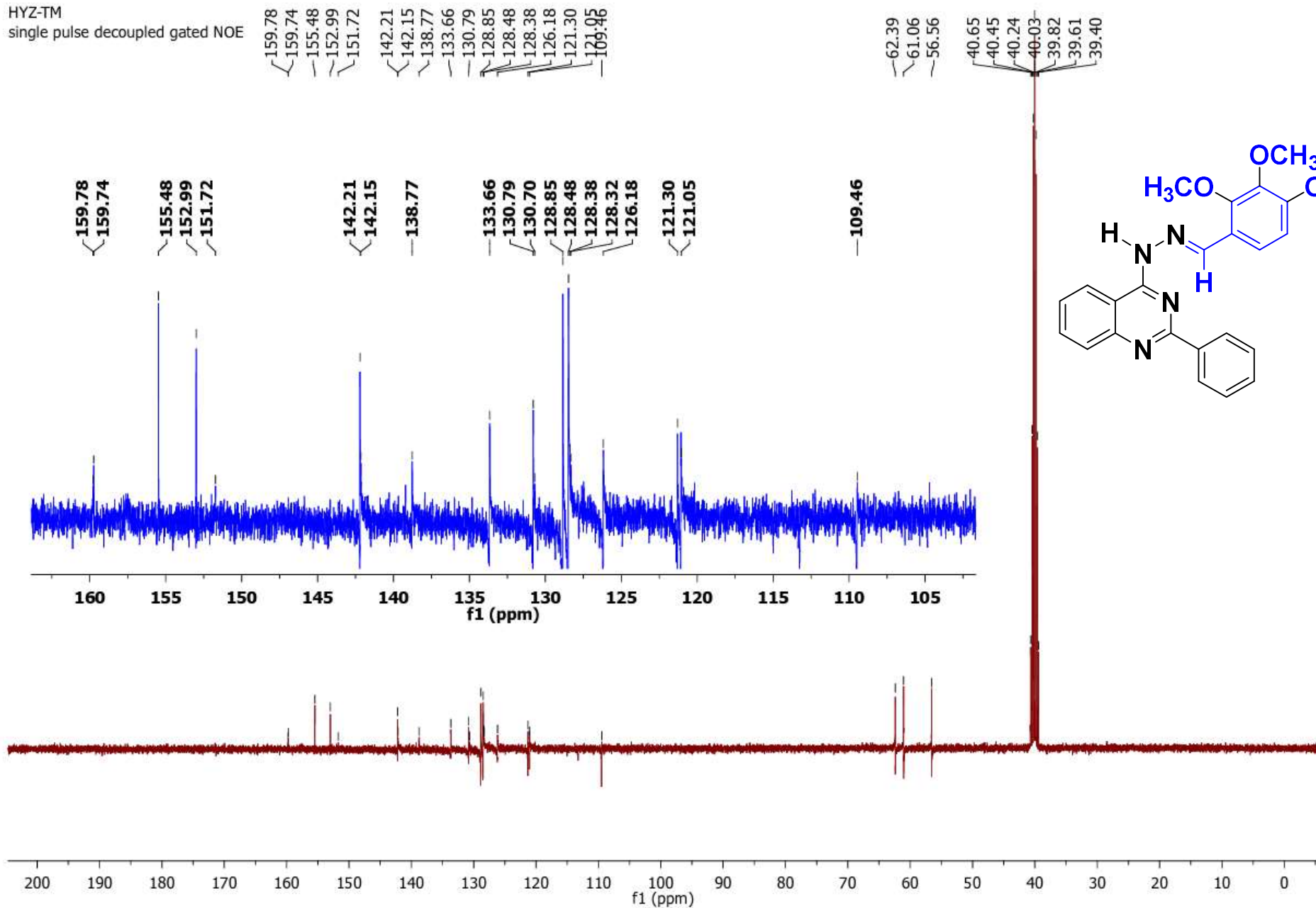
¹H-NMR SPECTRA: (E)-2-Phenyl-4-(2-(2,3,4-trimethoxybenzylidene)hydrazinyl)quinazoline (4g).



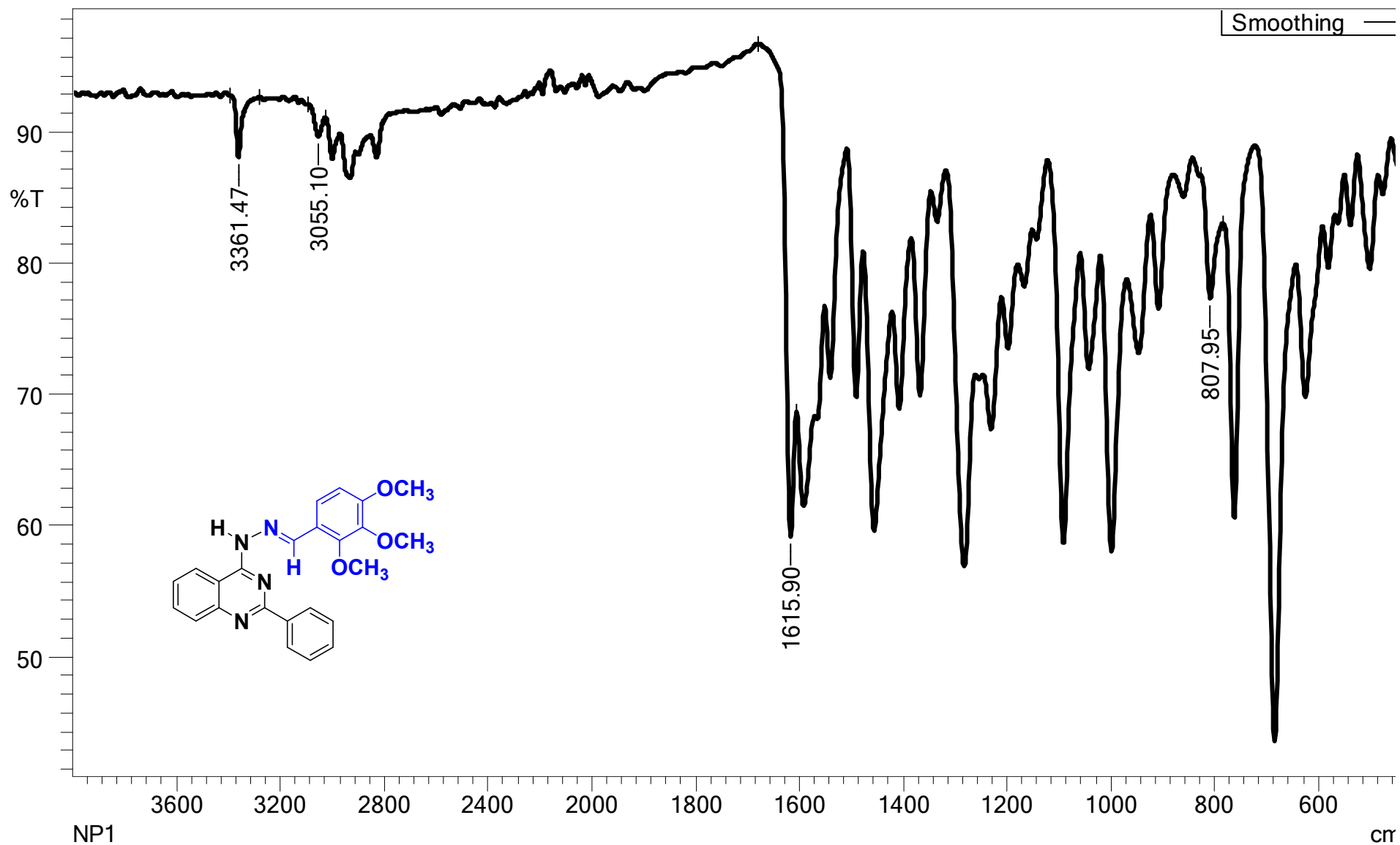
¹³C-NMR SPECTRA: (E)-2-Phenyl-4-(2-(2,3,4-trimethoxybenzylidene)hydrazinyl)quinazoline (4g).

HYZ-TM

single pulse decoupled gated NOE



IR SPECTRA: (E)-4-(2-(2,3,4-Trimethoxybenzylidene)hydrazinyl)-2-phenylquinazoline (4g).



HRMS SPECTRA: (E)-4-(2-(2,3,4-Trimethoxybenzylidene)hydrazinyl)-2-phenylquinazoline (4g).

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SYNAPT-XS#DBA064

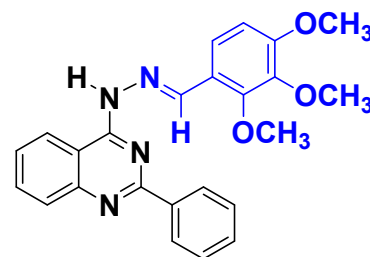
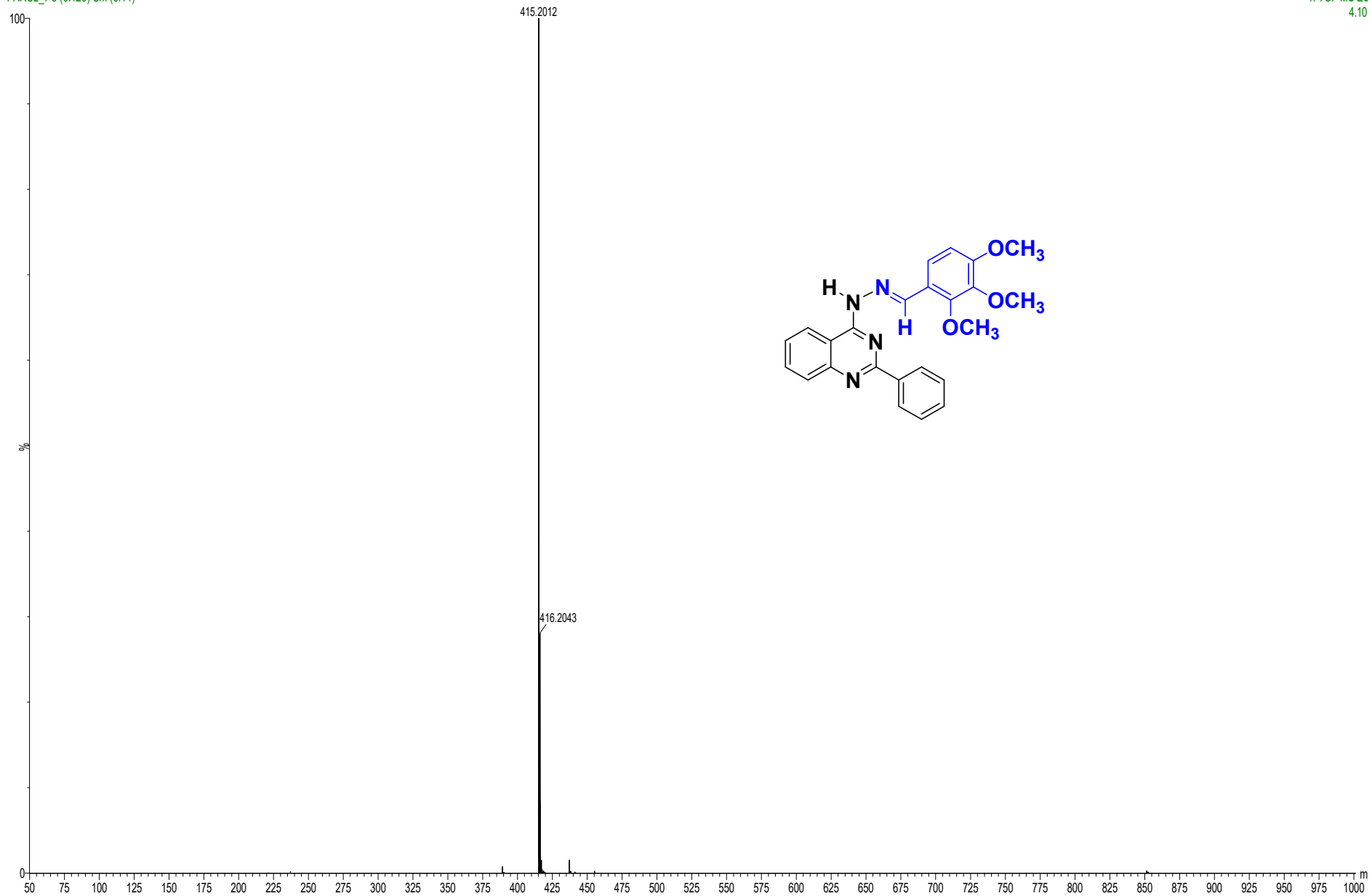
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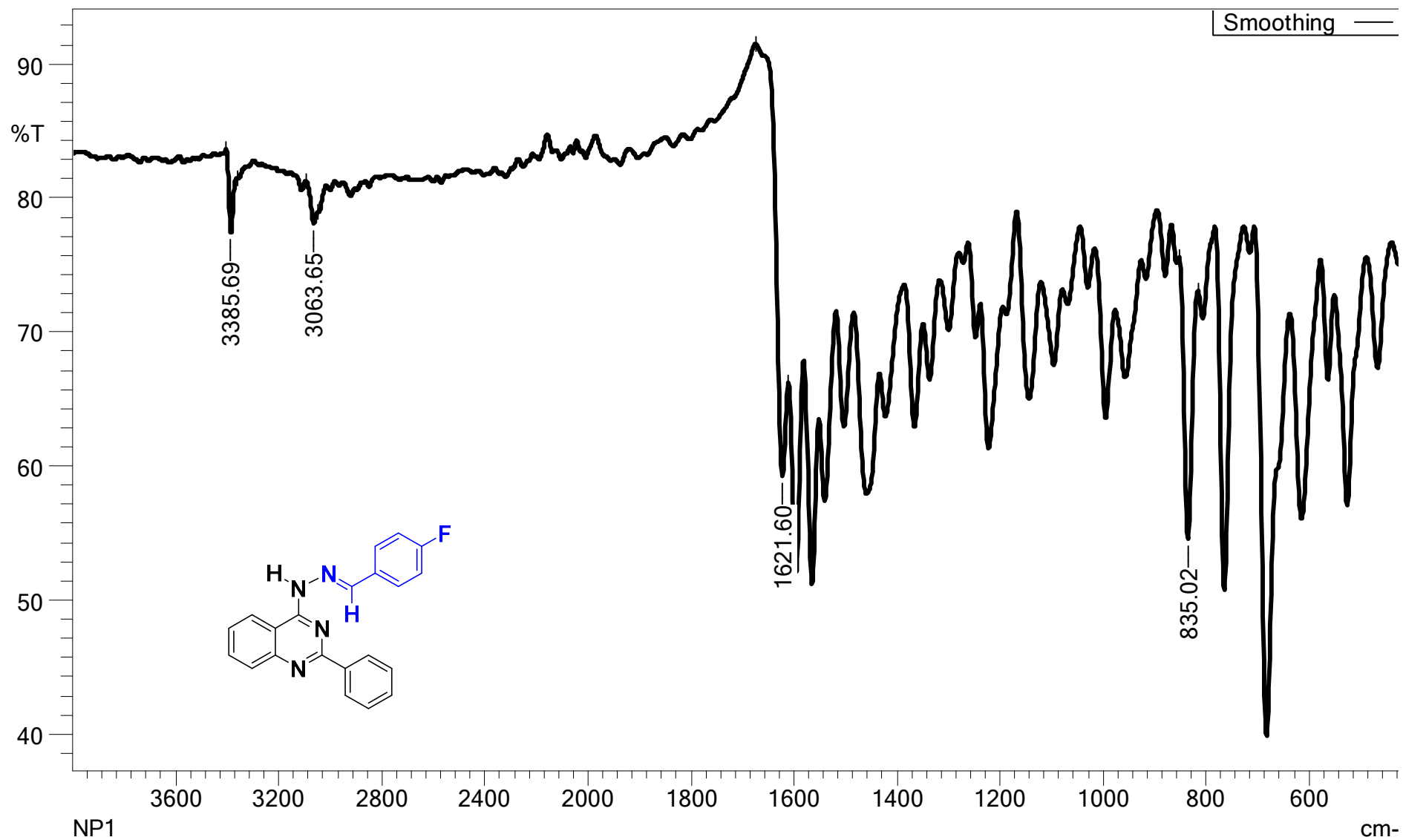
1: TOF MS ES

4.10

PARUL_7.5 (0.120) Cm (5:14)



IR SPECTRA: (E)-4-(2-(4-Fluorobenzylidene)hydrazinyl)-2-phenylquinazoline (4h).



HRMS SPECTRA: (E)-4-(2-(4-Fluorobenzylidene)hydrazinyl)-2-phenylquinazoline (4h).

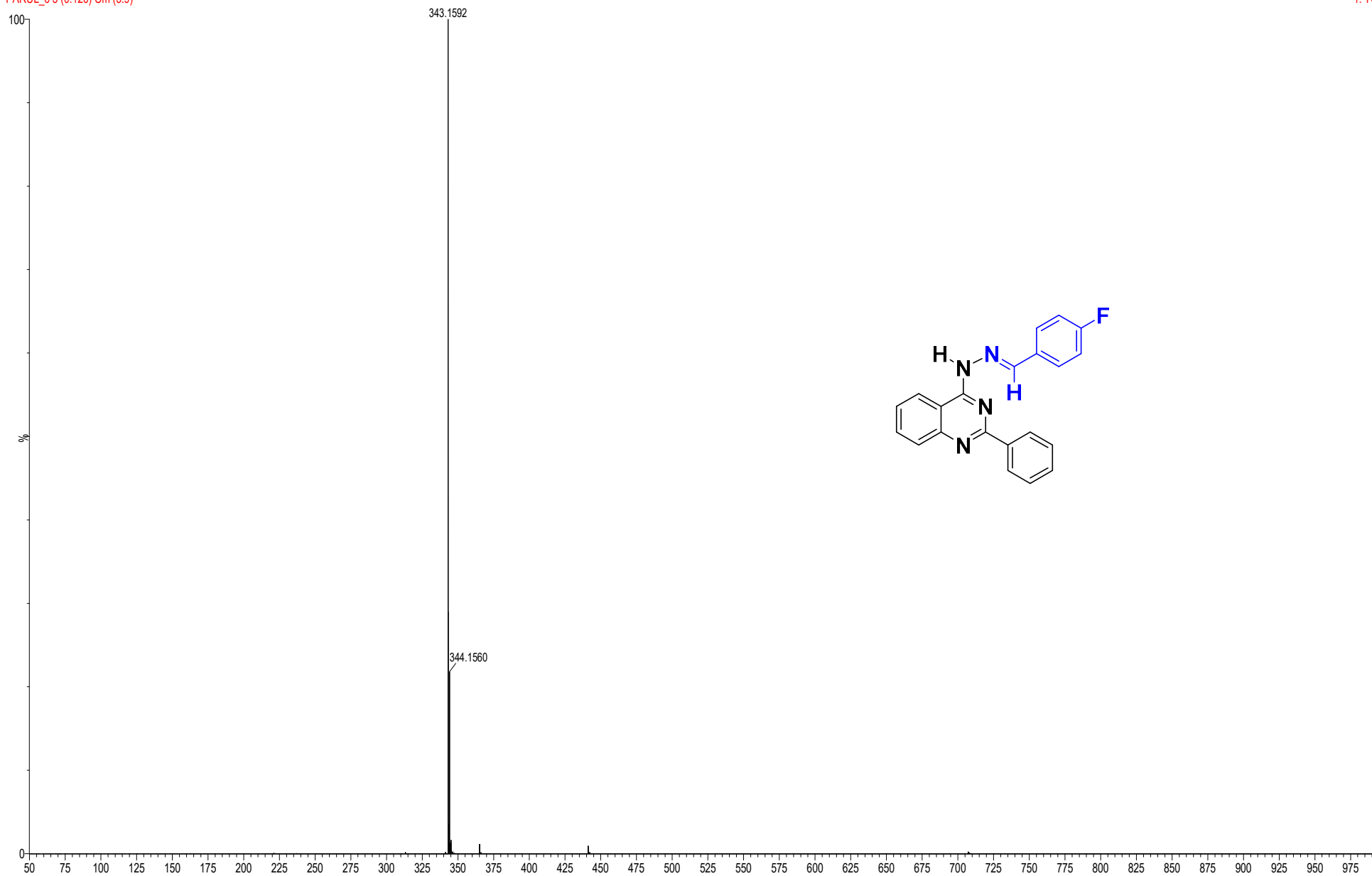
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SYNAPT-XS#DBA064

14-

PARUL_6 5 (0.120) Cm (3:9)

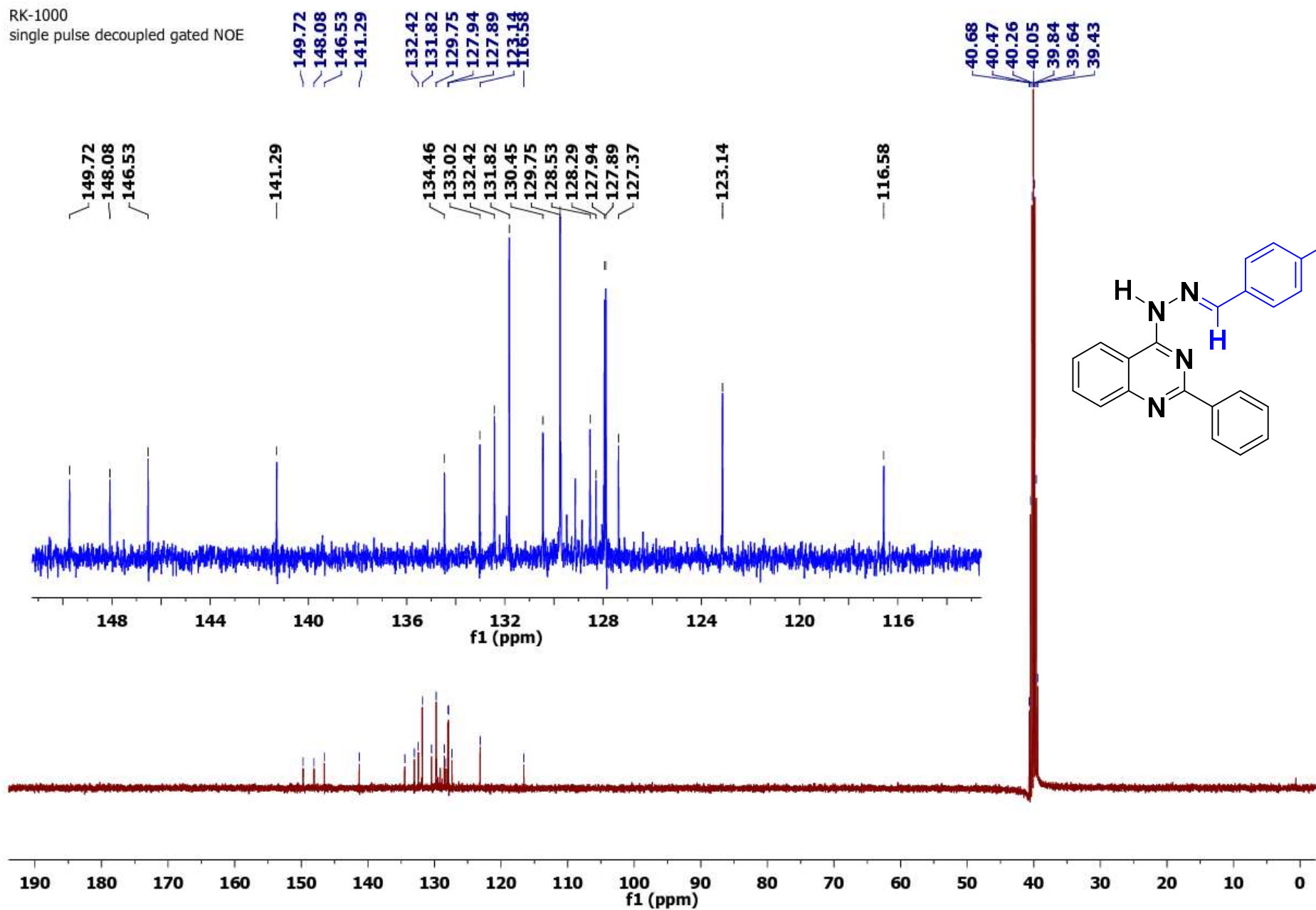
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¹³C-NMR SPECTRA: 4-(2-(4-Chlorobenzylidene)hydrazinyl)-2-phenylquinazoline (4i).

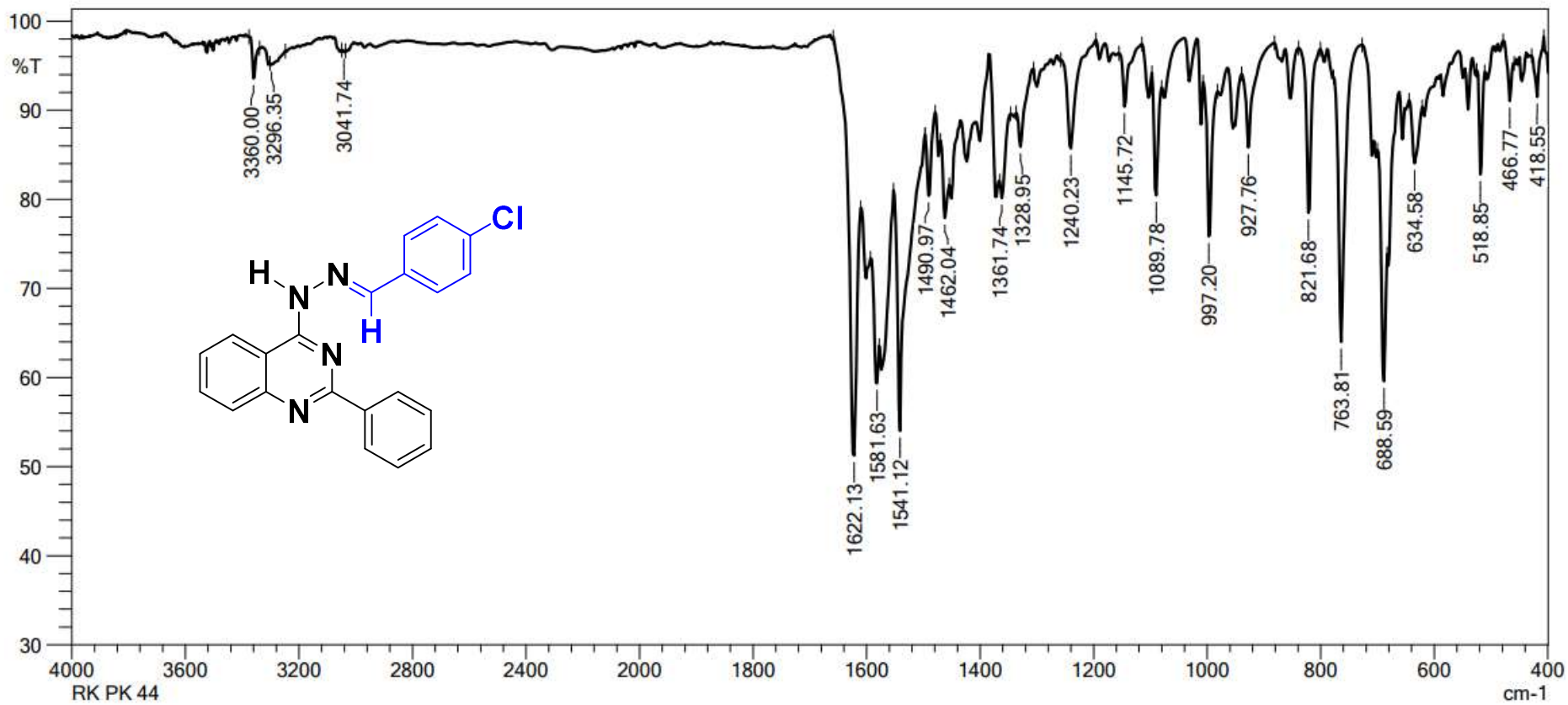
RK-1000

single pulse decoupled gated NOE



IR SPECTRA: (E)-4-(2-(4-Chlorobenzylidene)hydrazinyl)-2-phenylquinazoline (4i).

SHIMADZU



HRMS SPECTRA: (E)-4-(2-(4-Chlorobenzylidene)hydrazinyl)-2-phenylquinazoline (4i).

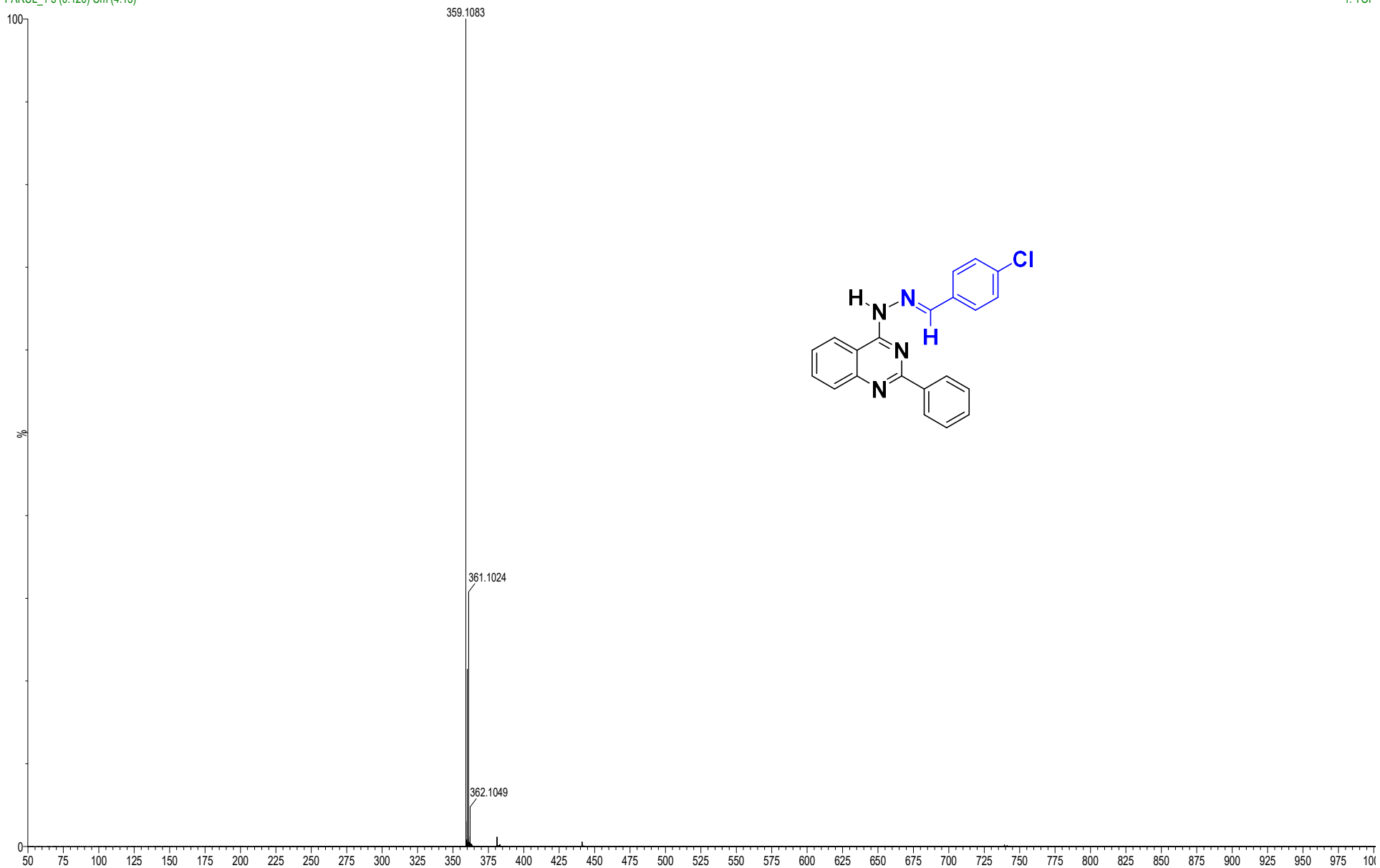
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SYNAPT-XS#DBA064

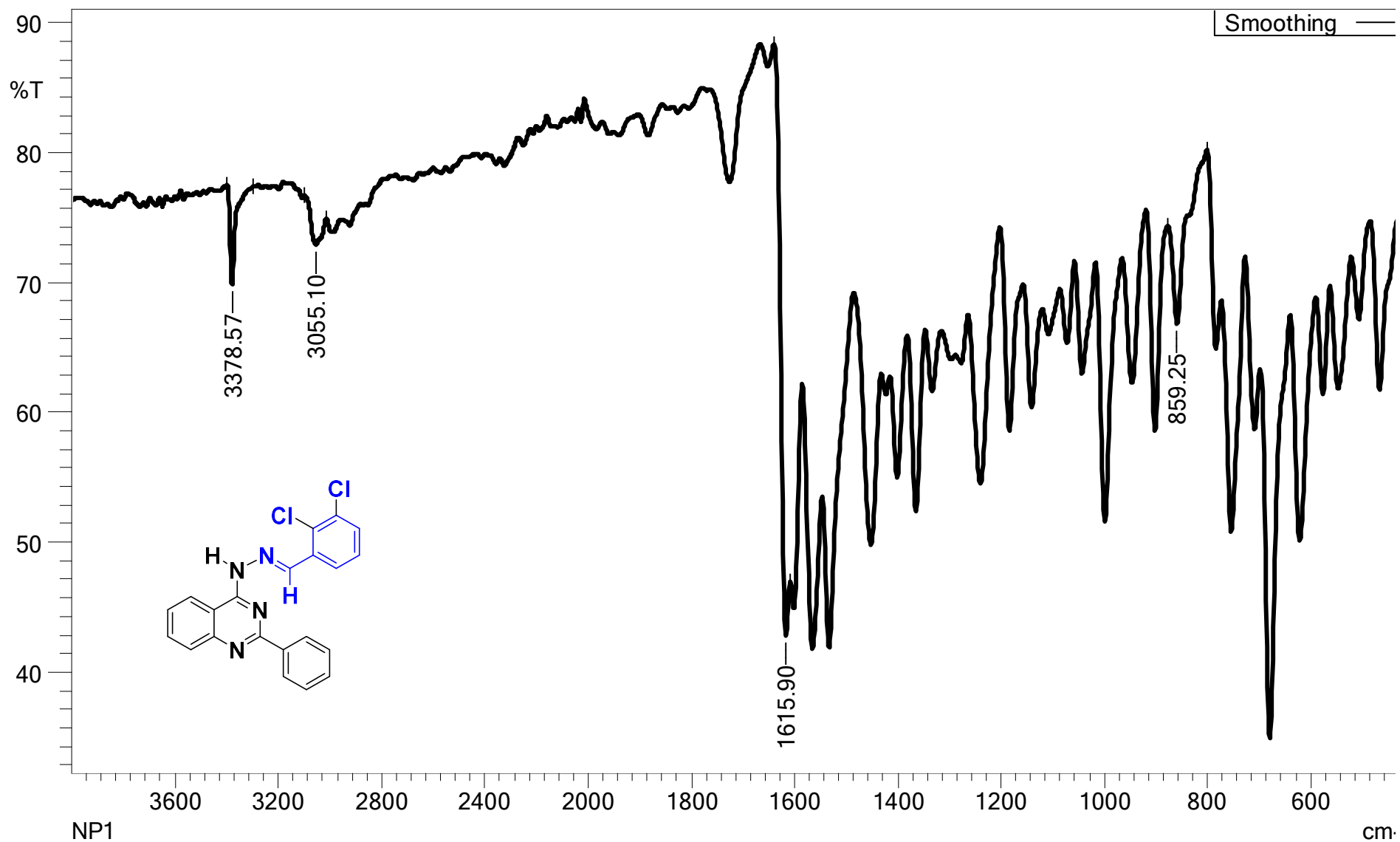
14-M

PARUL_1 5 (0.120) Cm (4:13)

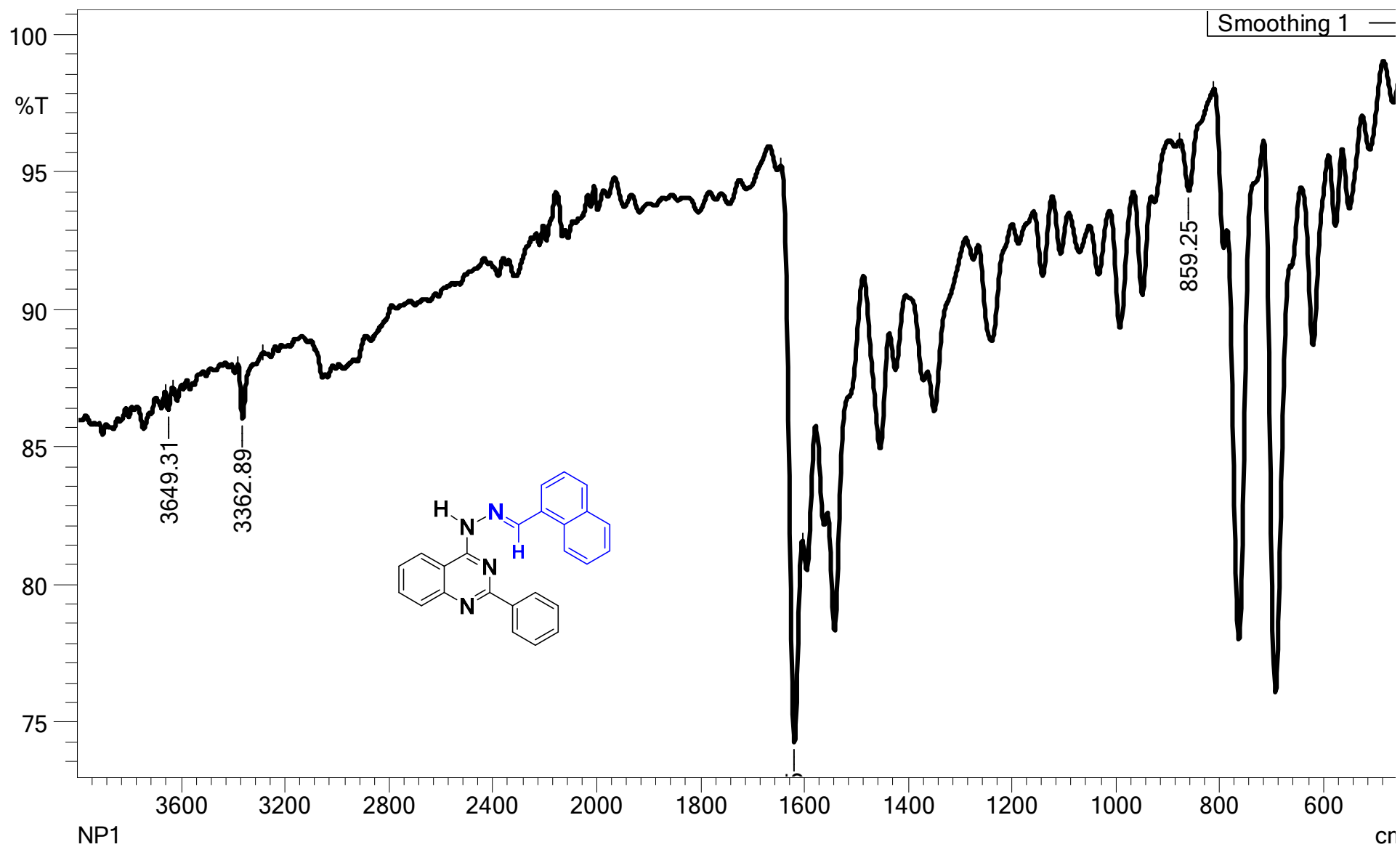
1: TOF



IR SPECTRA: (E)-4-(2-(2,3-Dichlorobenzylidene)hydrazinyl)-2-phenylquinazoline (4j).



IR SPECTRA: (E)-4-(2-(Naphthalen-1-ylmethylene)hydrazinyl)-2-phenylquinazoline (4k).



HRMS SPECTRA: (E)-4-(2-(Naphthalen-1-ylmethylene)hydrazinyl)-2-phenylquinazoline (4k).

XEVO -G2XSQTOF#TFC2176

POSITIVE ION MODE

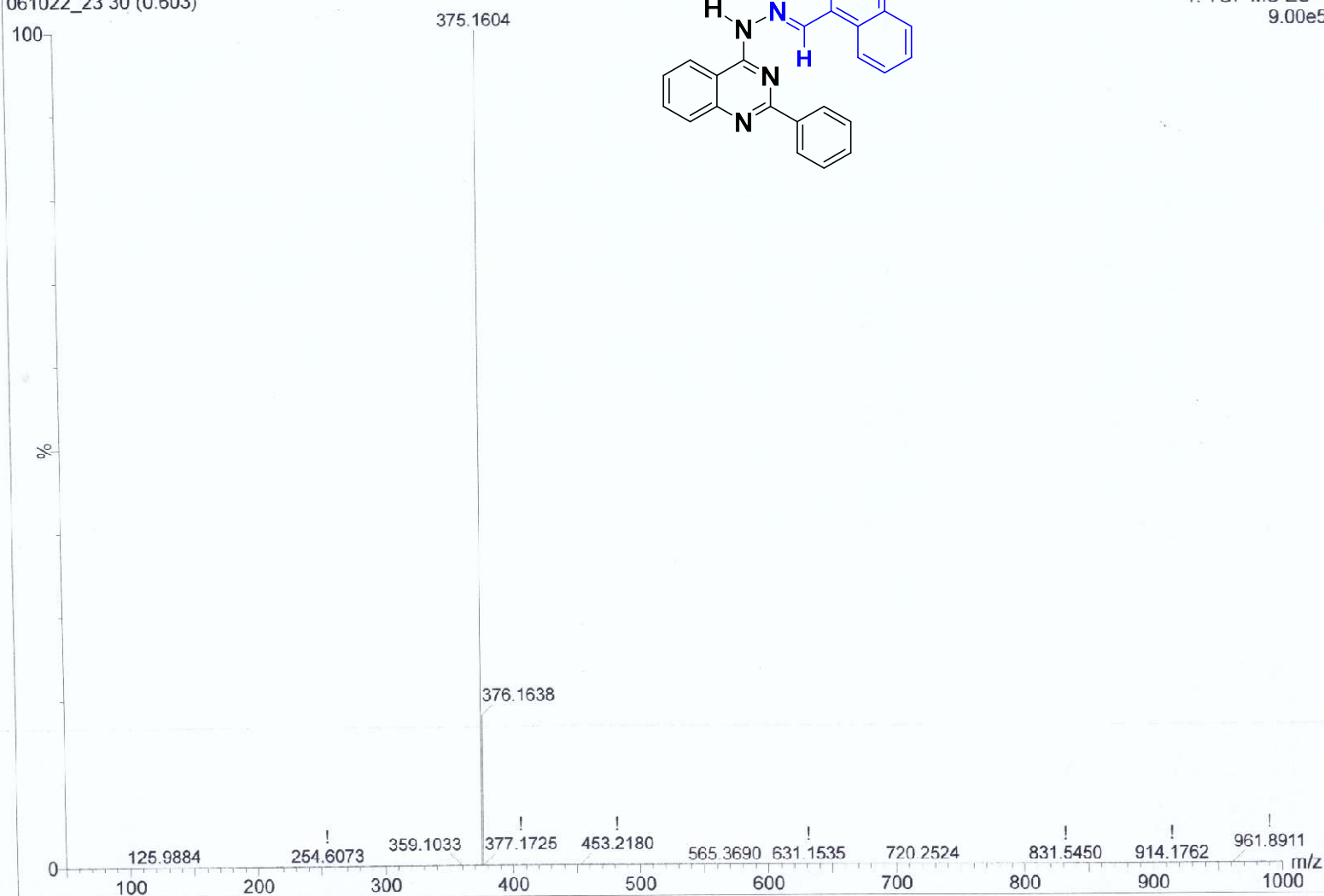
SS 8

061022_23 30 (0.603)

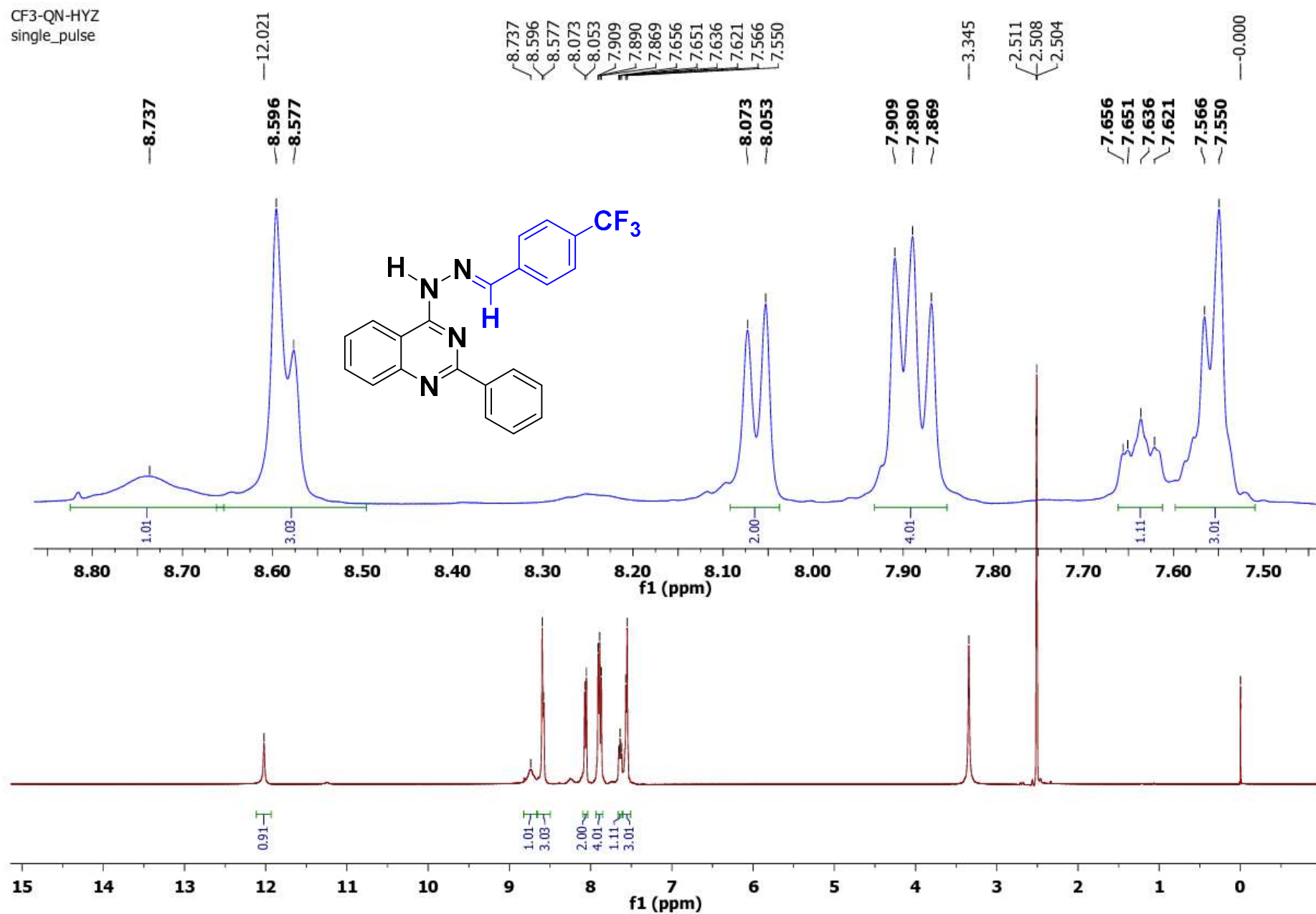
Capillary V 3, Cone V 40, Desolvation Gas 800
ESI

06-Oct-2022

1: TOF MS ES+
9.00e5

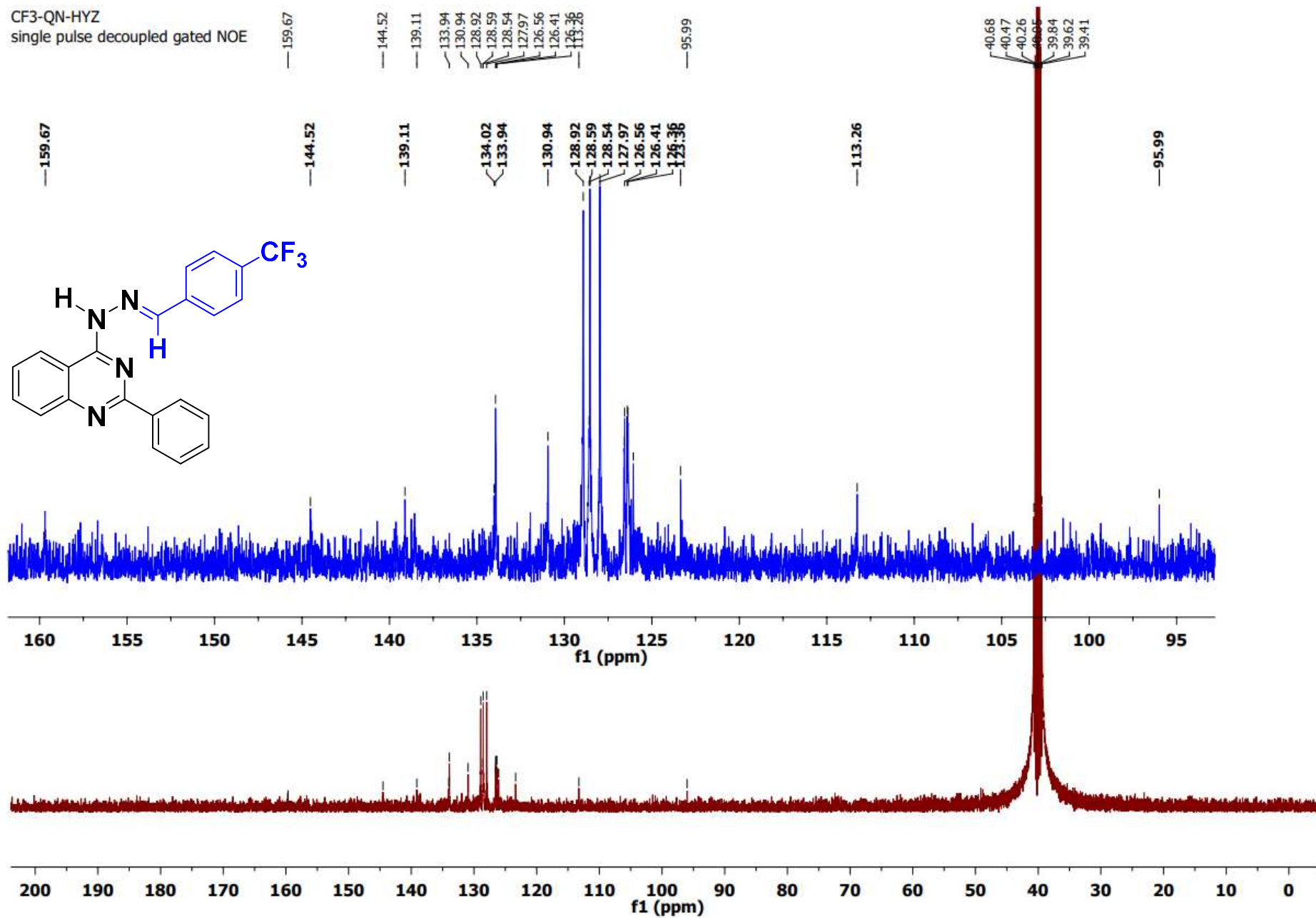


¹H-NMR SPECTRA: (E)-2-phenyl-4-(2-(4-(trifluoromethyl)benzylidene)hydrazinyl)quinazoline (4I).

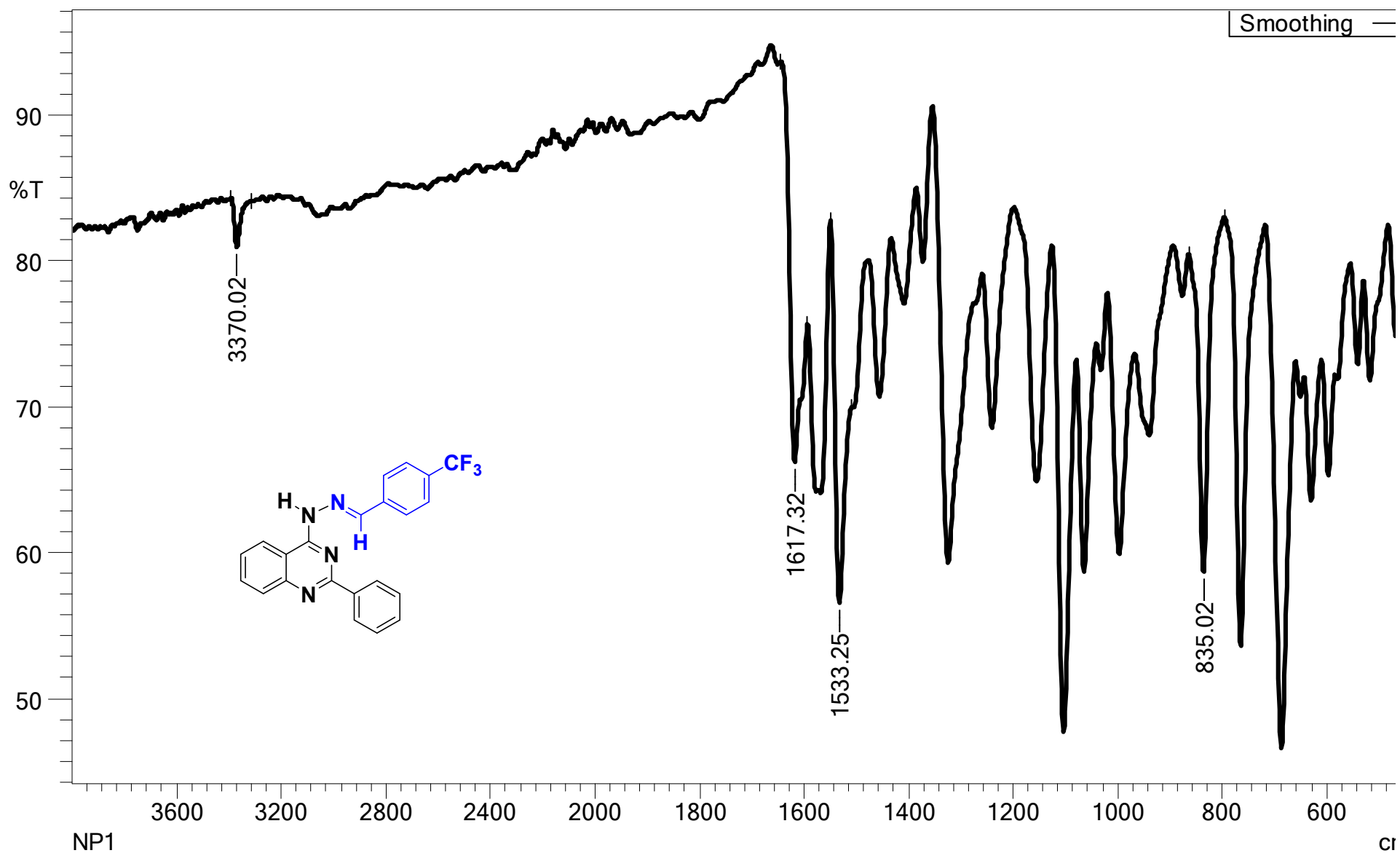


¹³C-NMR SPECTRA: (E)-2-phenyl-4-(2-(4-(trifluoromethyl)benzylidene)hydrazinyl)quinazoline (4I).

CF3-QN-HYZ
single pulse decoupled gated NOE



IR SPECTRA: (E)-2-Phenyl-4-(2-(4-(trifluoromethyl)benzylidene)hydrazinyl)quinazoline (4I).



HRMS SPECTRA: (E)-2-Phenyl-4-(2-(4-(trifluoromethyl)benzylidene)hydrazinyl)quinazoline (4I).

XEVO -G2XSQTOF#TFC2176
POSITIVE ION MODE
SS 2

061022_17 26 (0.535)

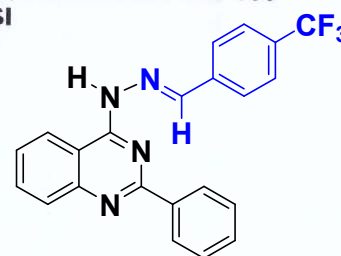
Capillary V 3, Cone V 40, Desolvation Gas 800
ESI

06-Oct-2022

1: TOF MS ES+
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100

393.1322



%

394.1353

0

125.9863

168.9842

272.6638

393.0568

395.1399

494.2313

615.9993

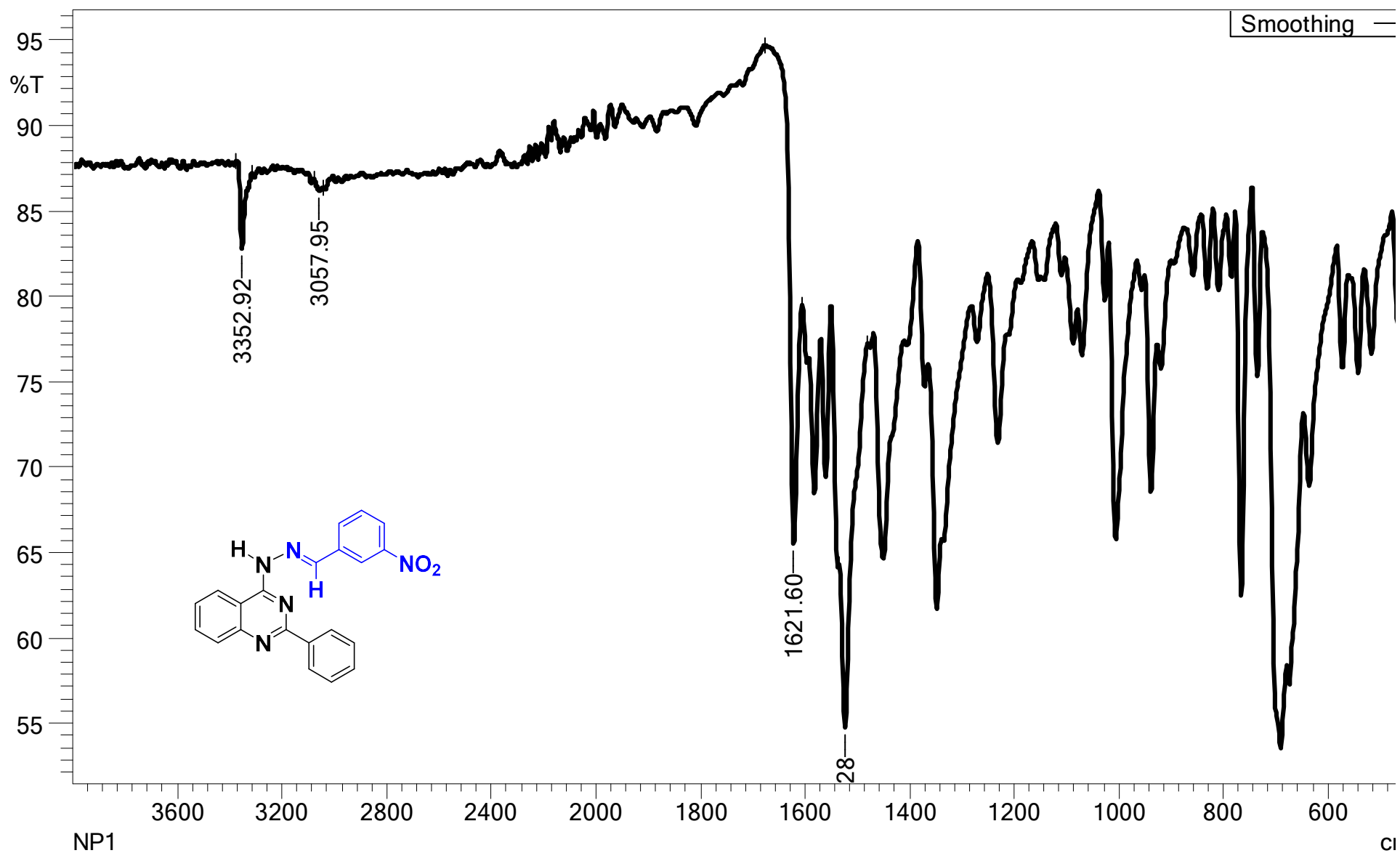
732.9033

831.4384

930.9108

981.0486

IR SPECTRA: (E)-4-(2-(3-Nitrobenzylidene)hydrazinyl)-2-phenylquinazoline (4m).



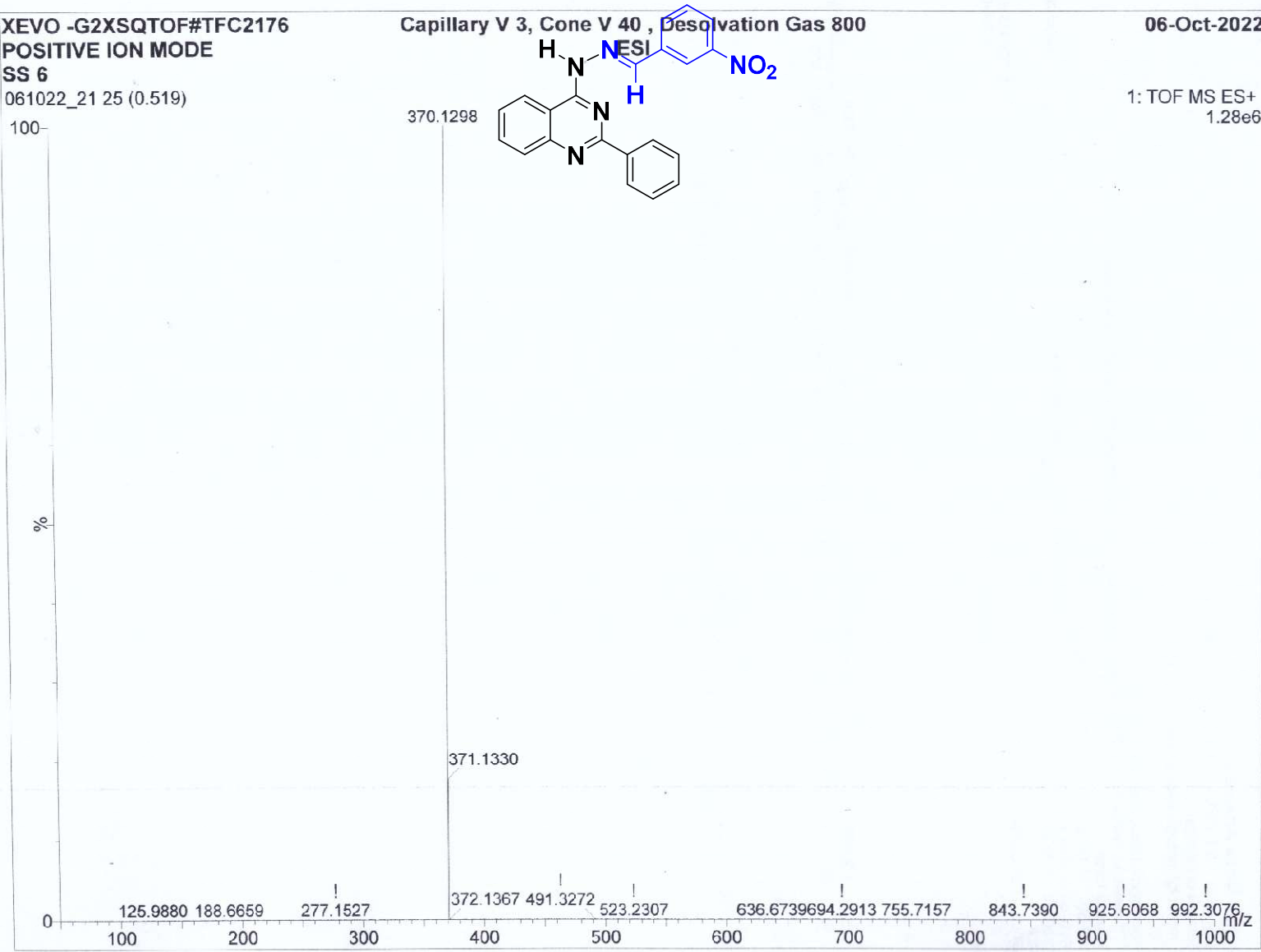
HRMS SPECTRA: (E)-4-(2-(3-Nitrobenzylidene)hydrazinyl)-2-phenylquinazoline (4m).

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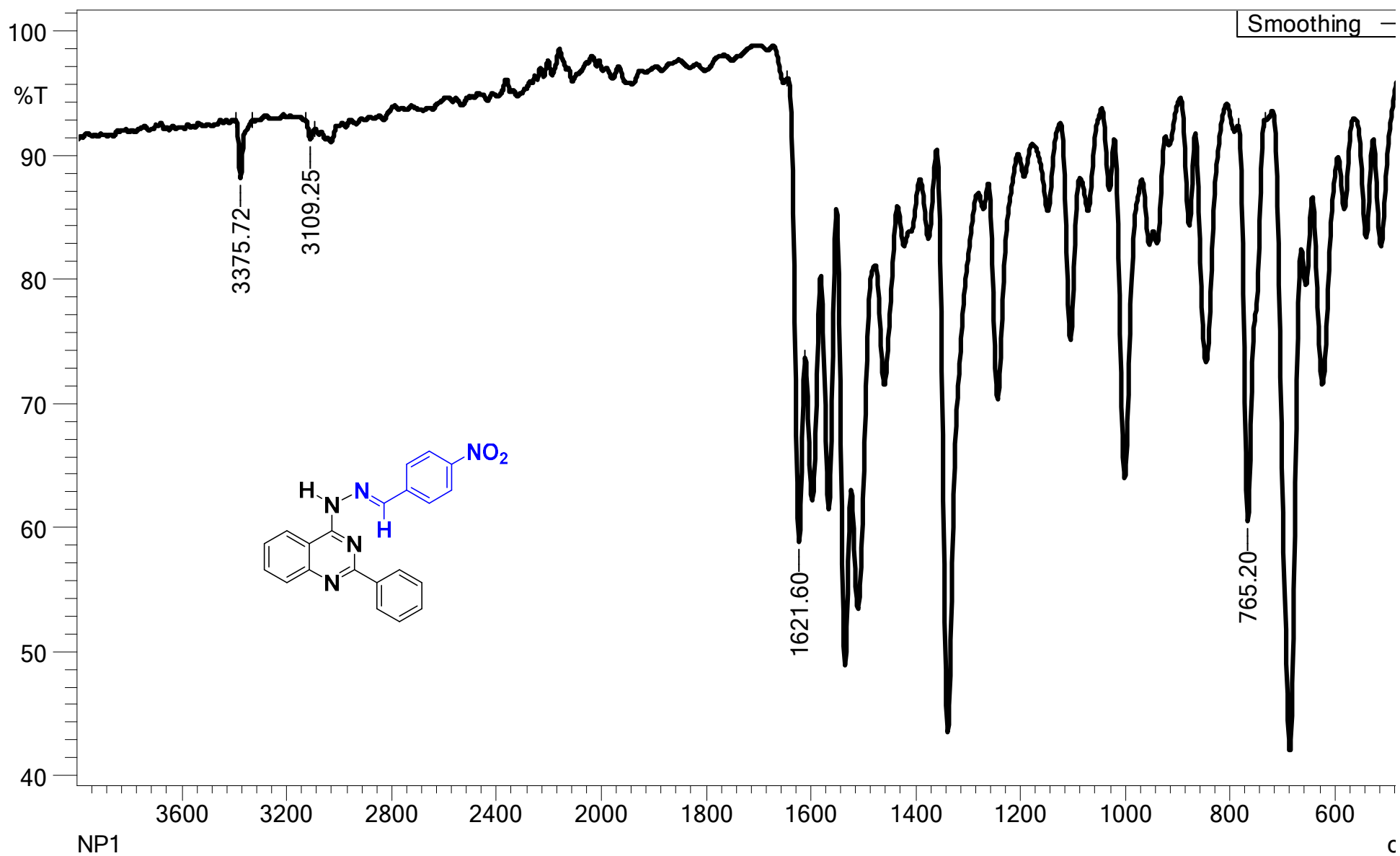
Capillary V 3, Cone V 40, Desolvation Gas 800

06-Oct-2022

1: TOF MS ES+
1.28e6



IR SPECTRA: (E)-4-(2-(4-Nitrobenzylidene)hydrazinyl)-2-phenylquinazoline (4n).



HRMS SPECTRA: (E)-4-(2-(4-Nitrobenzylidene)hydrazinyl)-2-phenylquinazoline (4n).

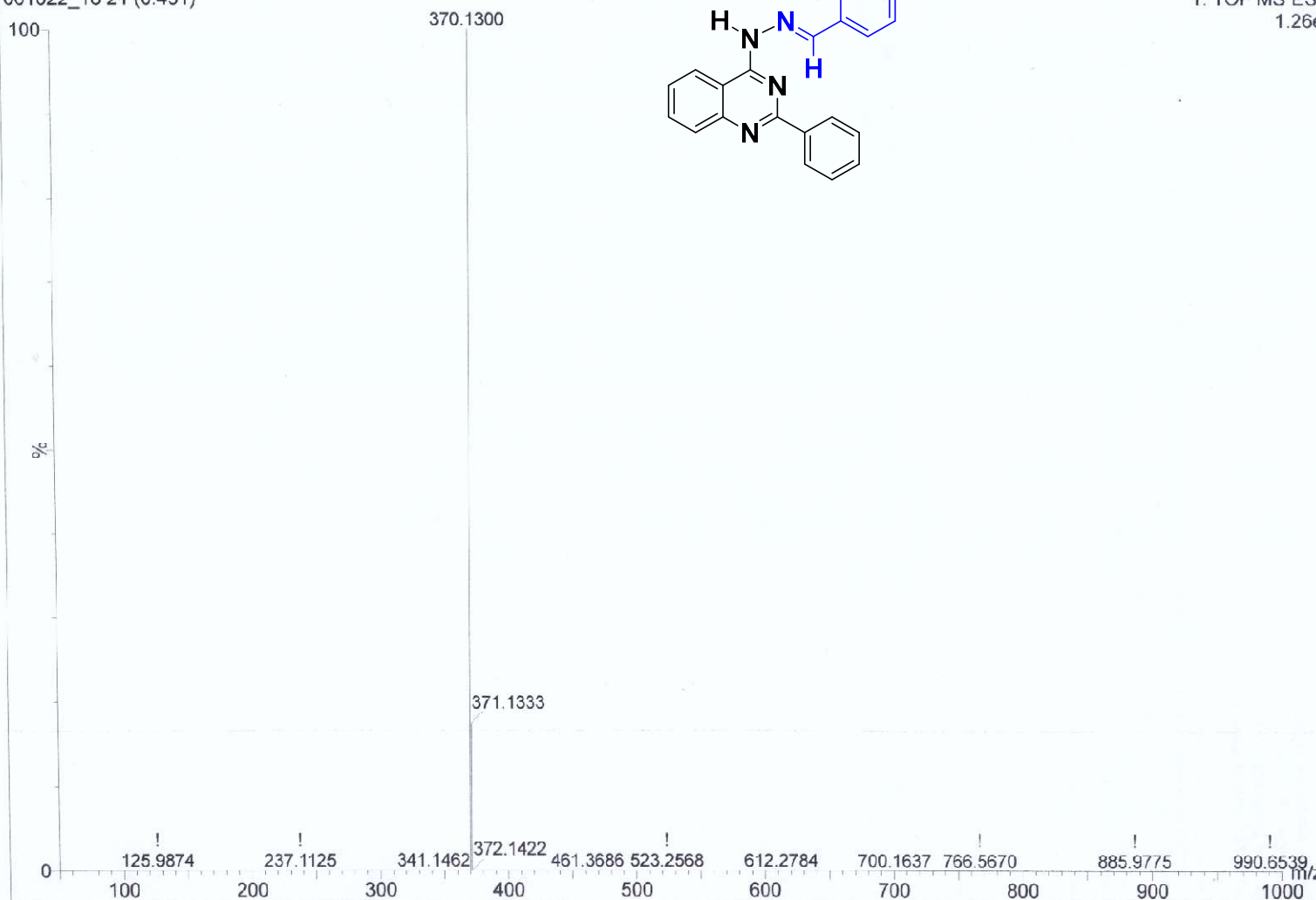
XEVO -G2XSQTOF#TFC2176
POSITIVE ION MODE
SS 3

061022_18 21 (0.431)

Capillary V 3, Cone V 40 , Desolvation Gas 800
ESI

06-Oct-2022

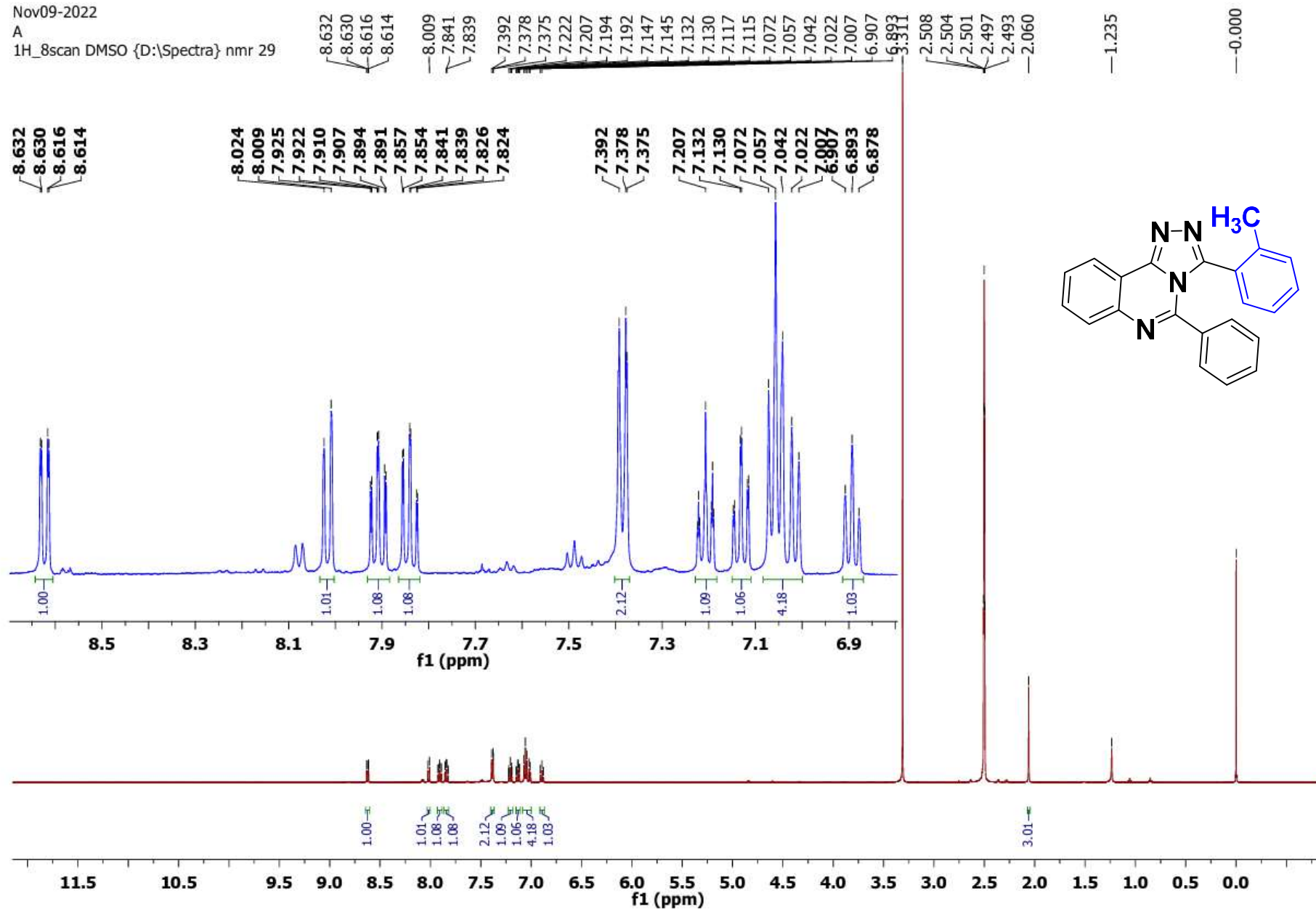
1: TOF MS ES+
1.26e6



¹H-NMR SPECTRA: 3-(2-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5a).

Nov09-2022

A
1H_8scan DMSO {D:\Spectra} nmr 29

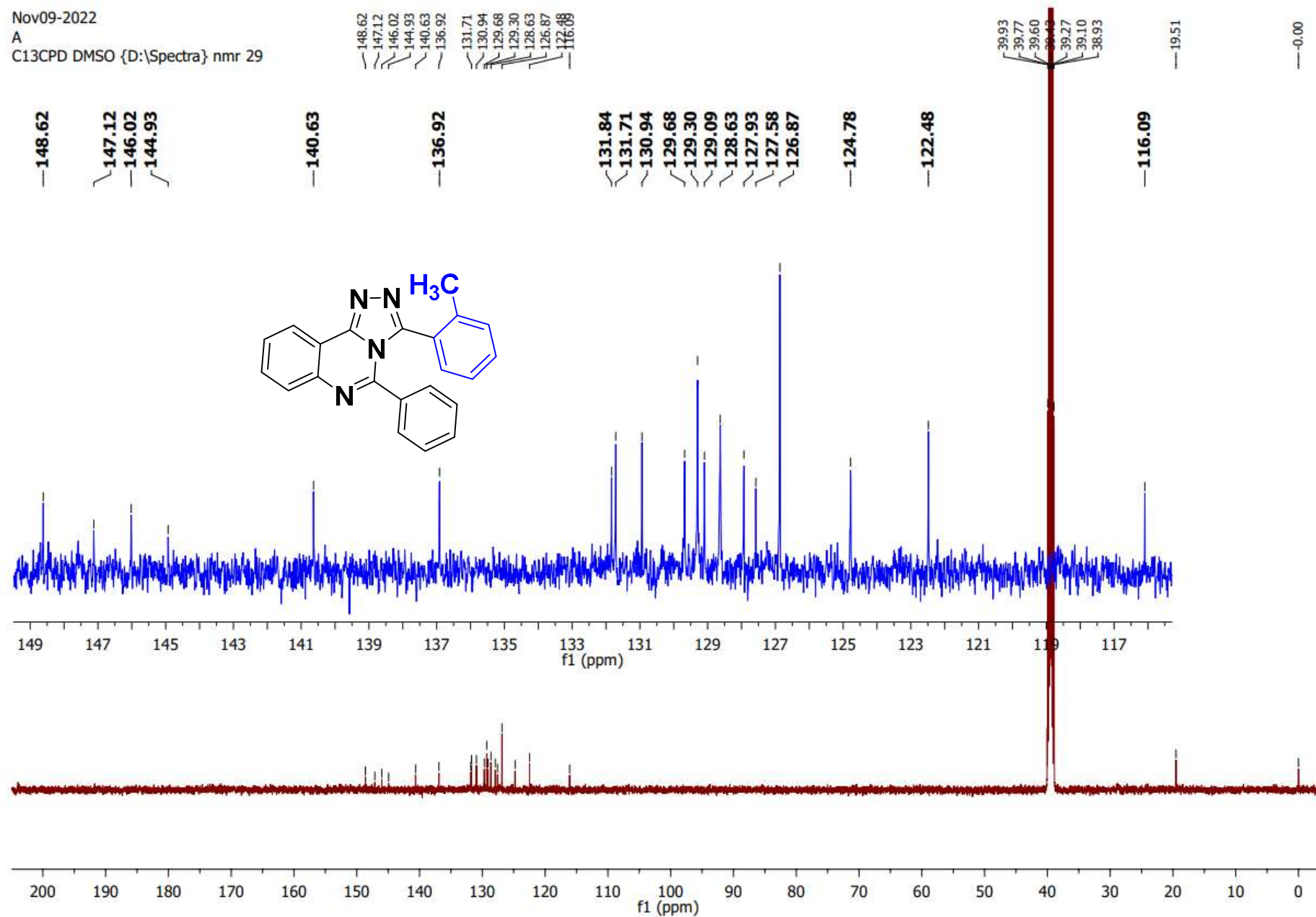


¹³C-NMR SPECTRA: 3-(2-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5a).

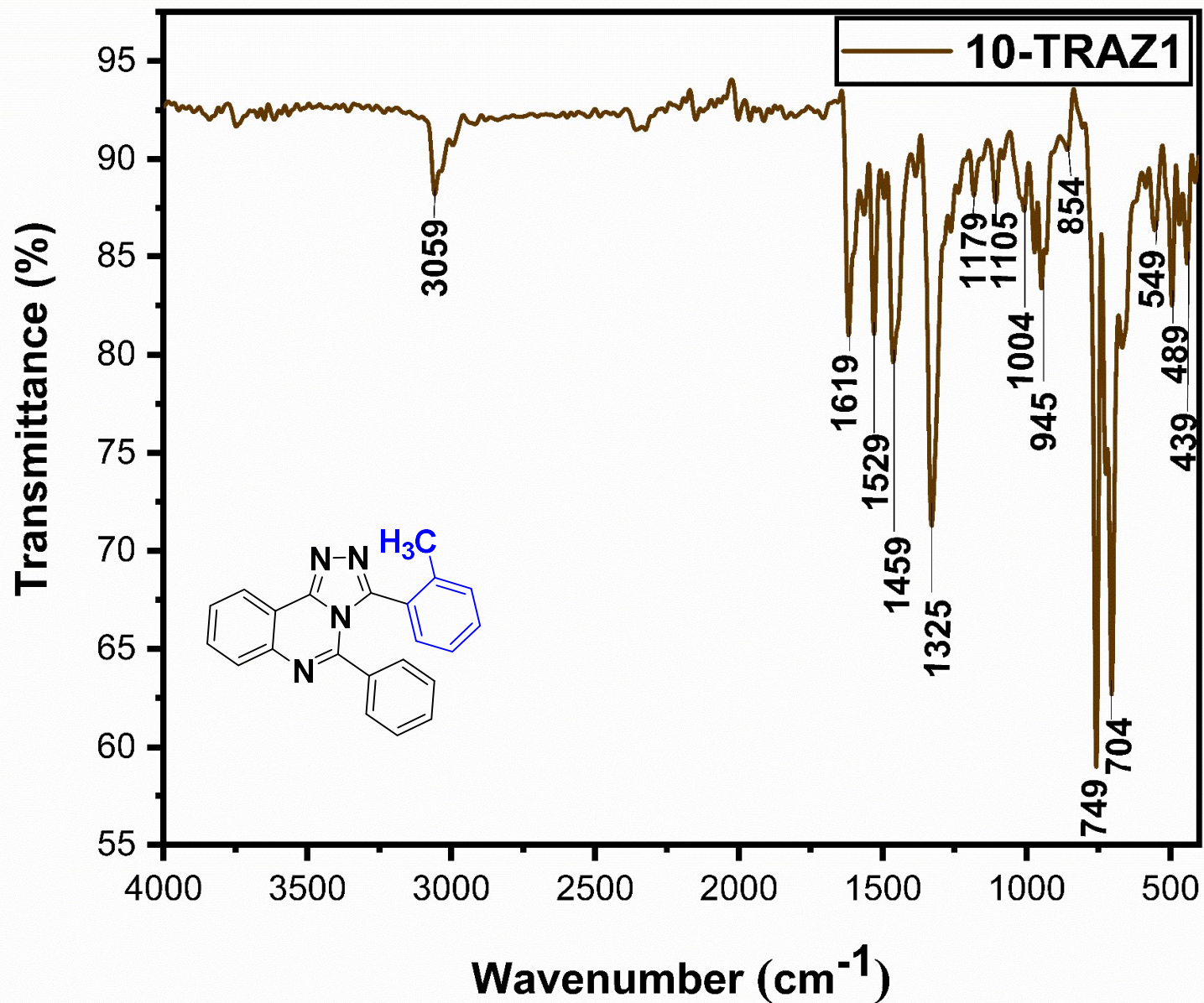
Nov09-2022

A

C13CPD DMSO {D:\Spectra} nmr 29



IR SPECTRA: 3-(2-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5a).



HRMS SPECTRA: 3-(2-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5a).

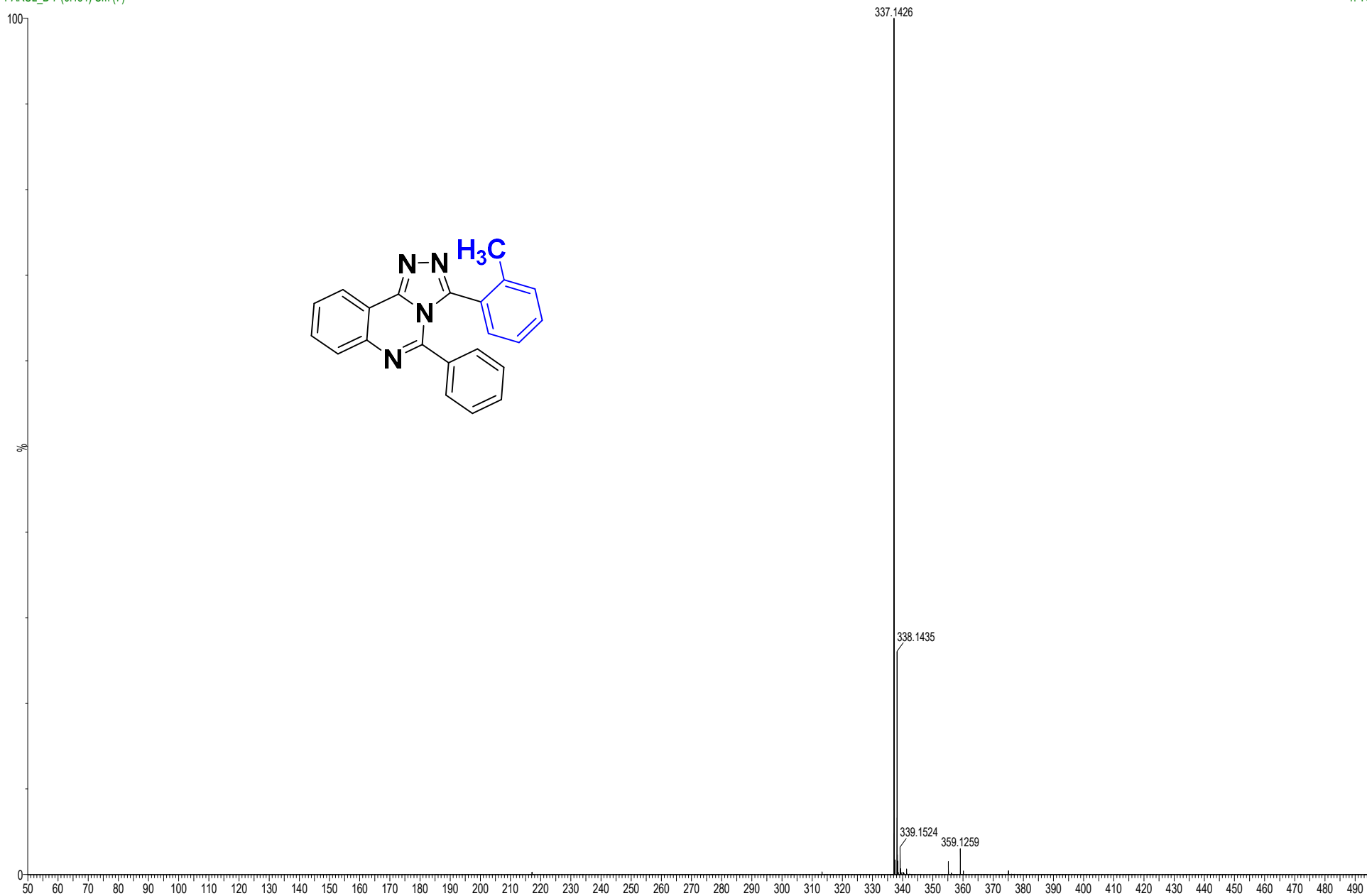
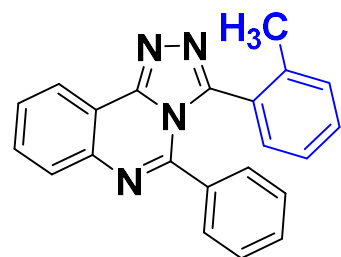
SAIF,PANJAB UNIVERSITY,CHANDIGARH

SYNAPT-XS#DBA064

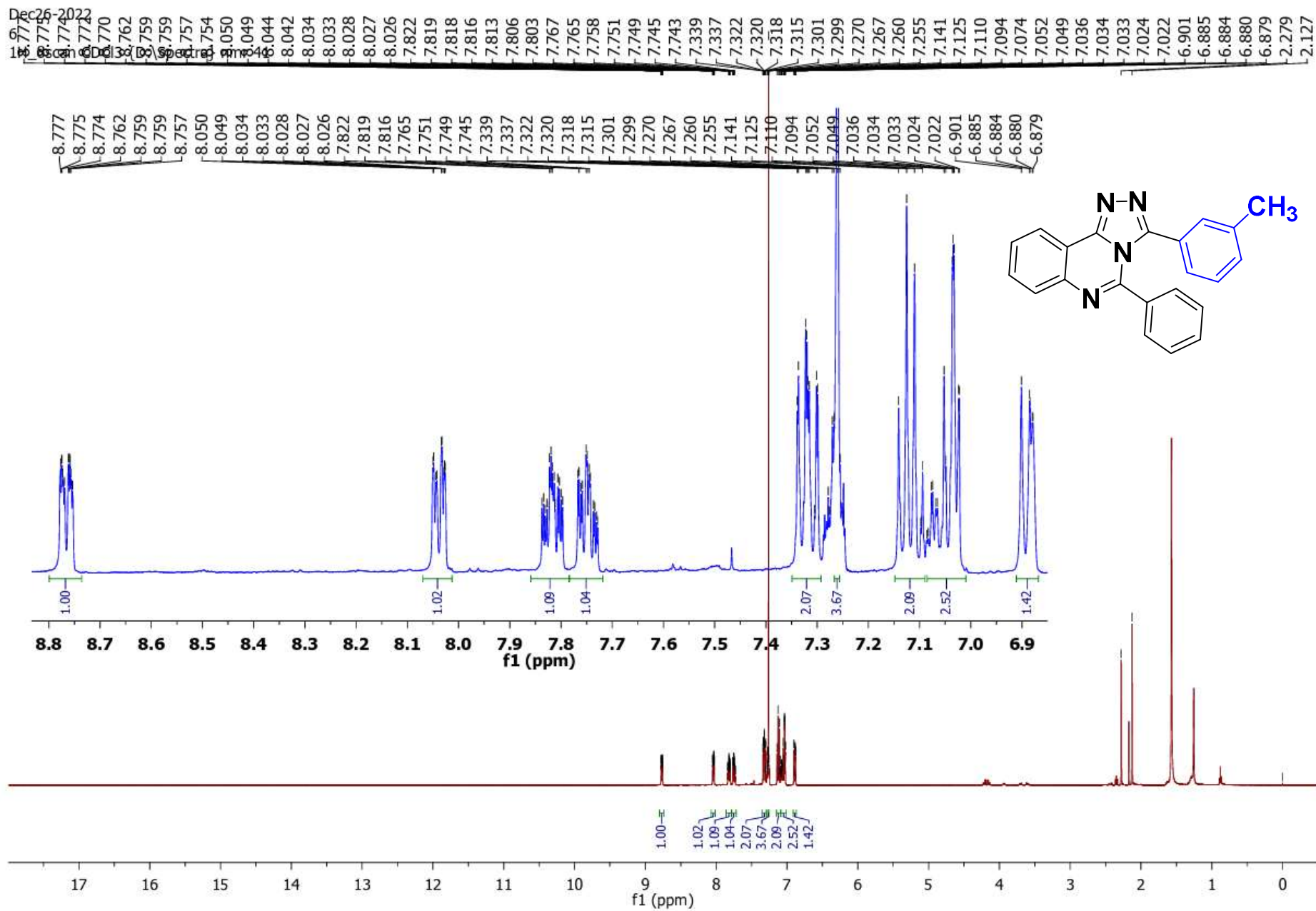
27-

PARUL_D 7 (0.154) Cm (7)

1: TO



¹H-NMR SPECTRA: 3-(3-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5b).

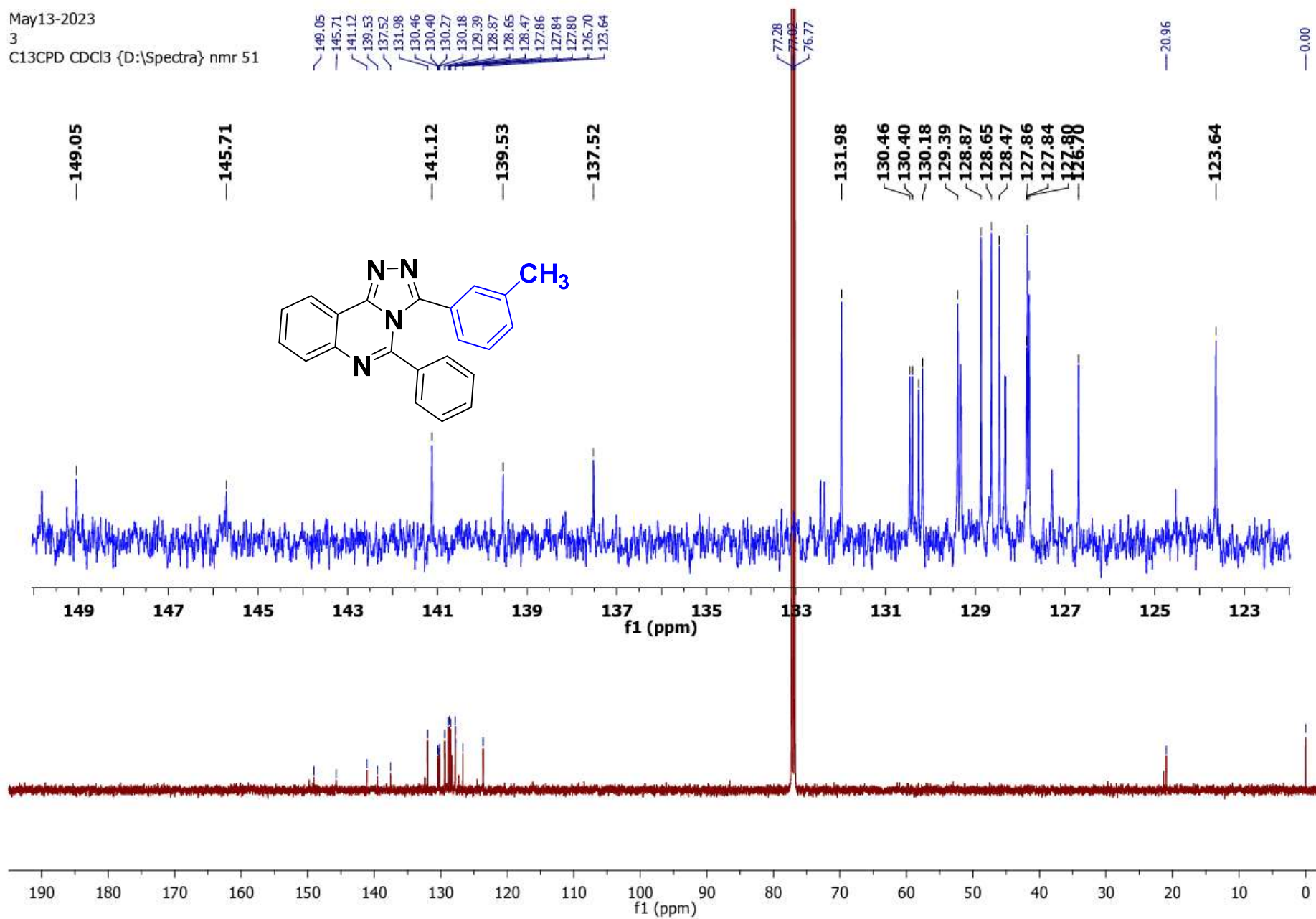


¹³C-NMR SPECTRA: 3-(3-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5b).

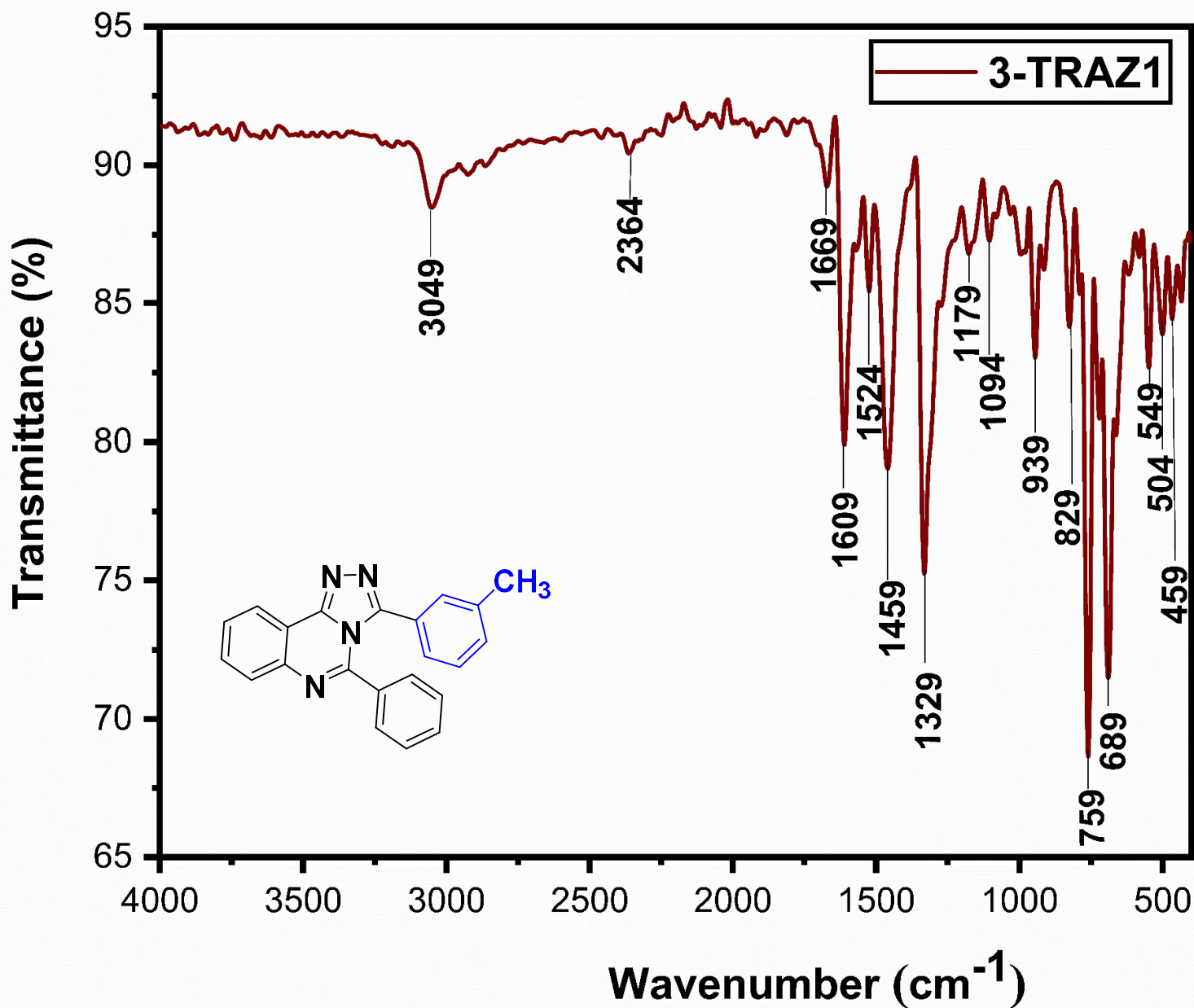
May13-2023

3

C13CPD CDCl3 {D:\Spectra} nmr 51



¹³C-NMR SPECTRA: 3-(3-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5b).



HRMS SPECTRA: 3-(3-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5b).

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SYNAPT-XS#DBA064

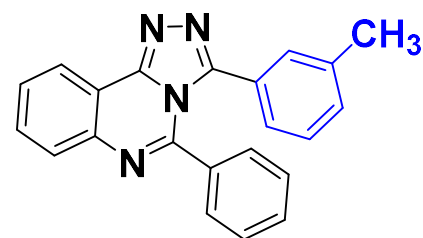
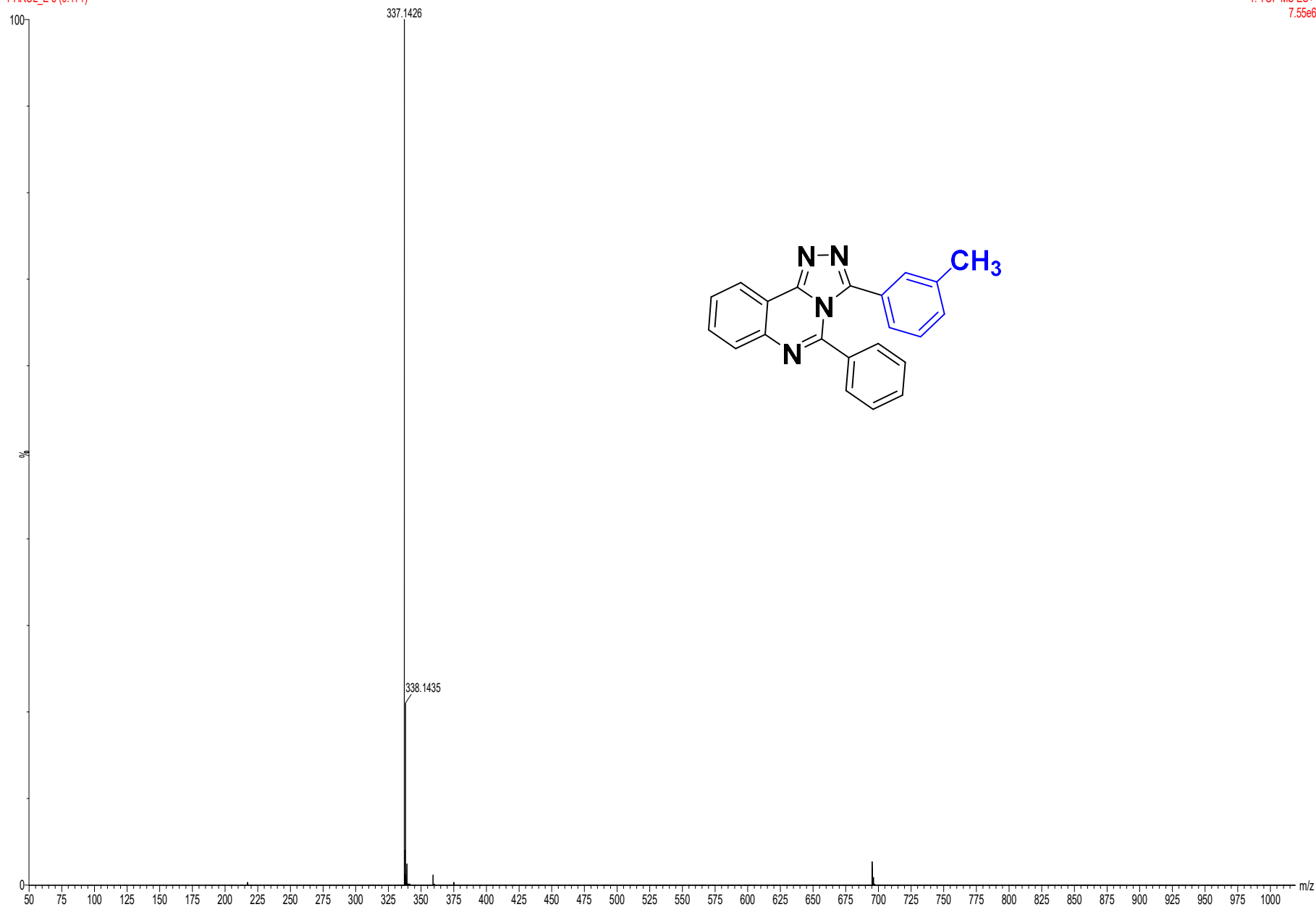
27-Feb-2023

11:04:59

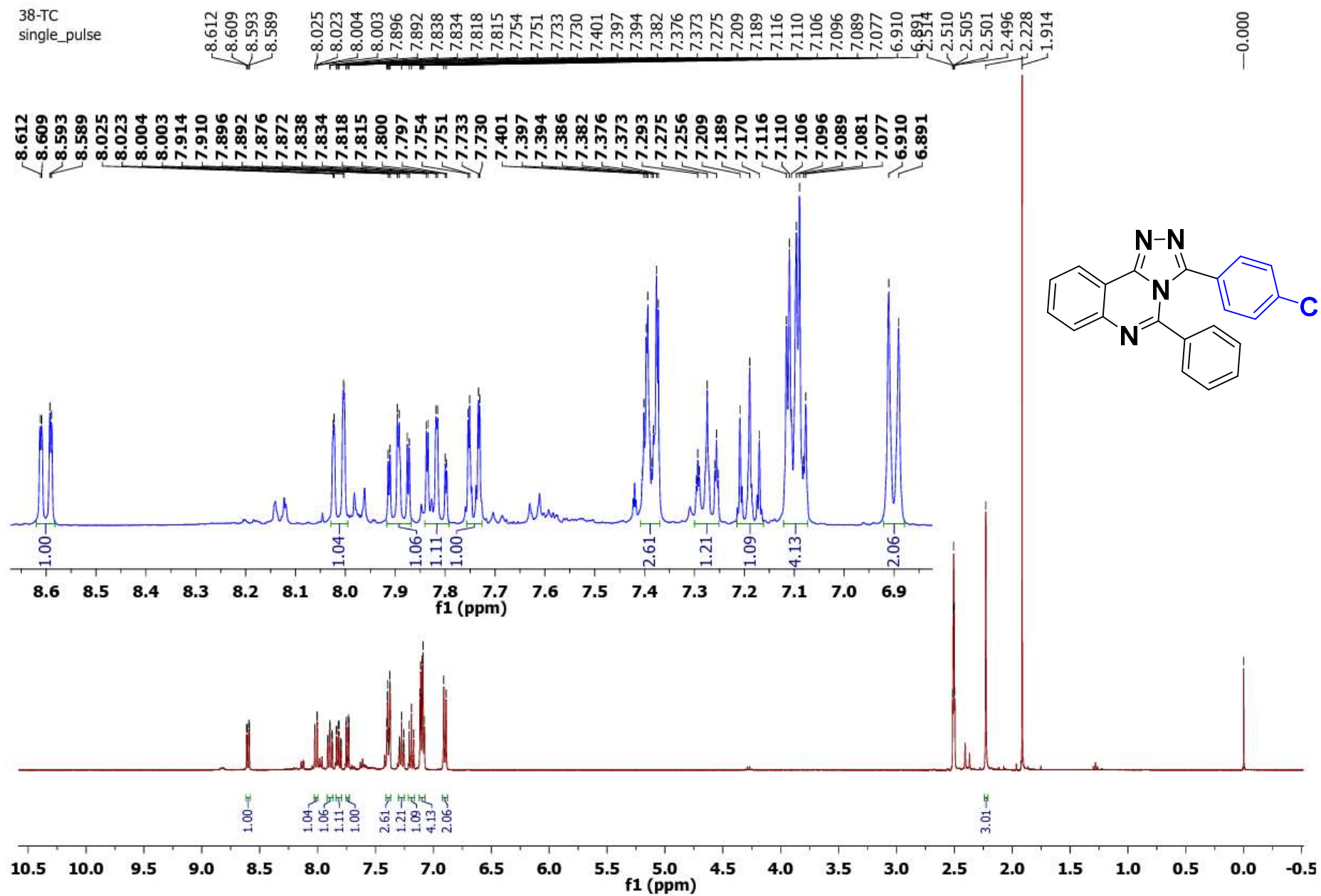
1: TOF MS ES+

7.55e6

PARUL_E 8 (0.171)

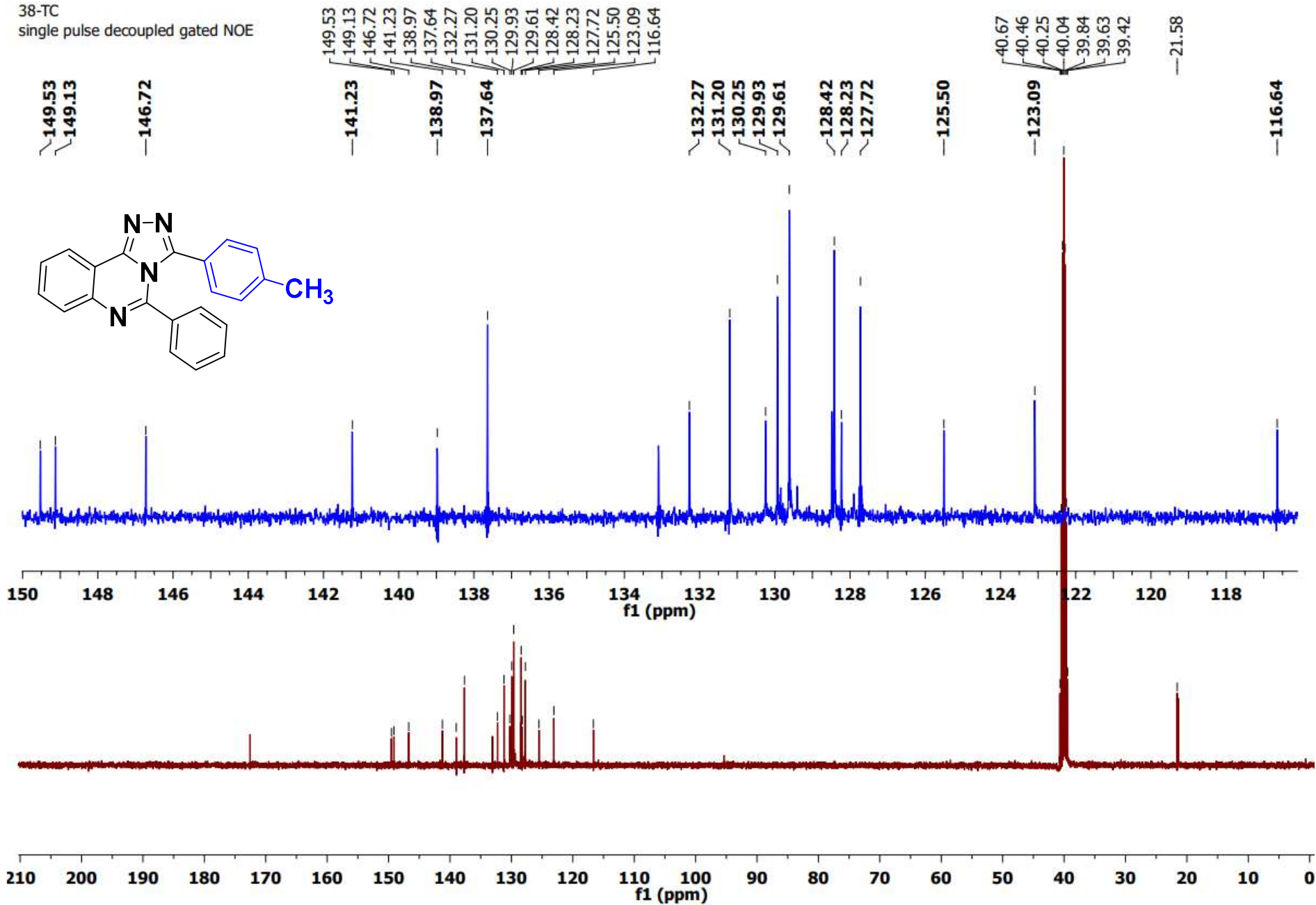


¹H-NMR SPECTRA: 3-(4-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5c).

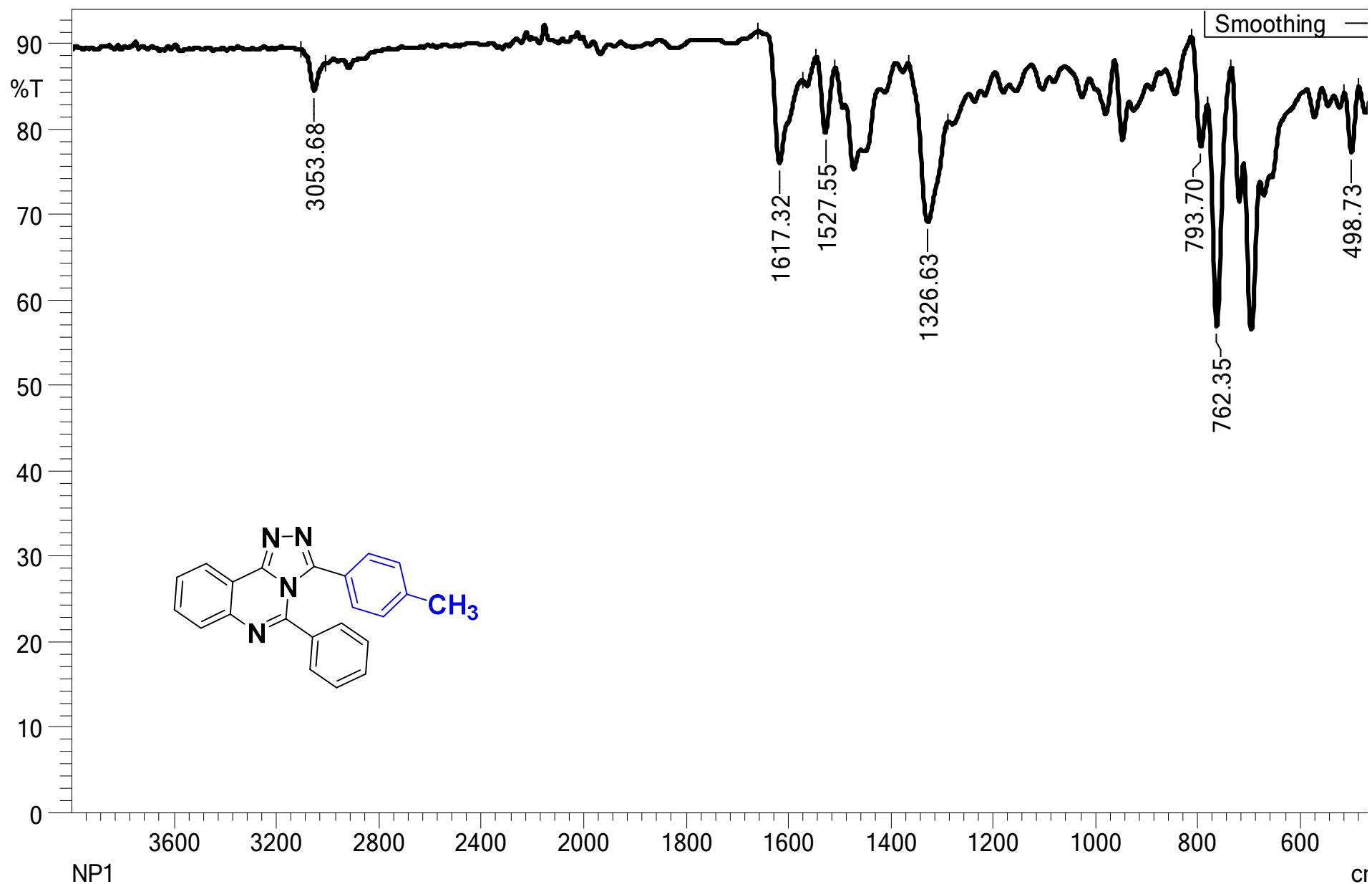


¹³C-NMR SPECTRA: 3-(4-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5c).

38-TC
single pulse decoupled gated NOE



IR SPECTRA: 3-(4-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5c).



HRMS SPECTRA: 3-(4-Methylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5c).

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SYNAPT-XS#DBA064

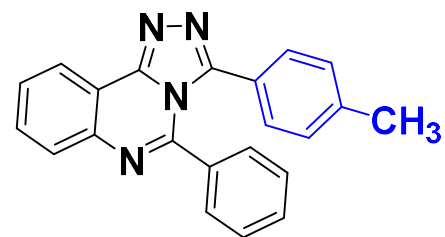
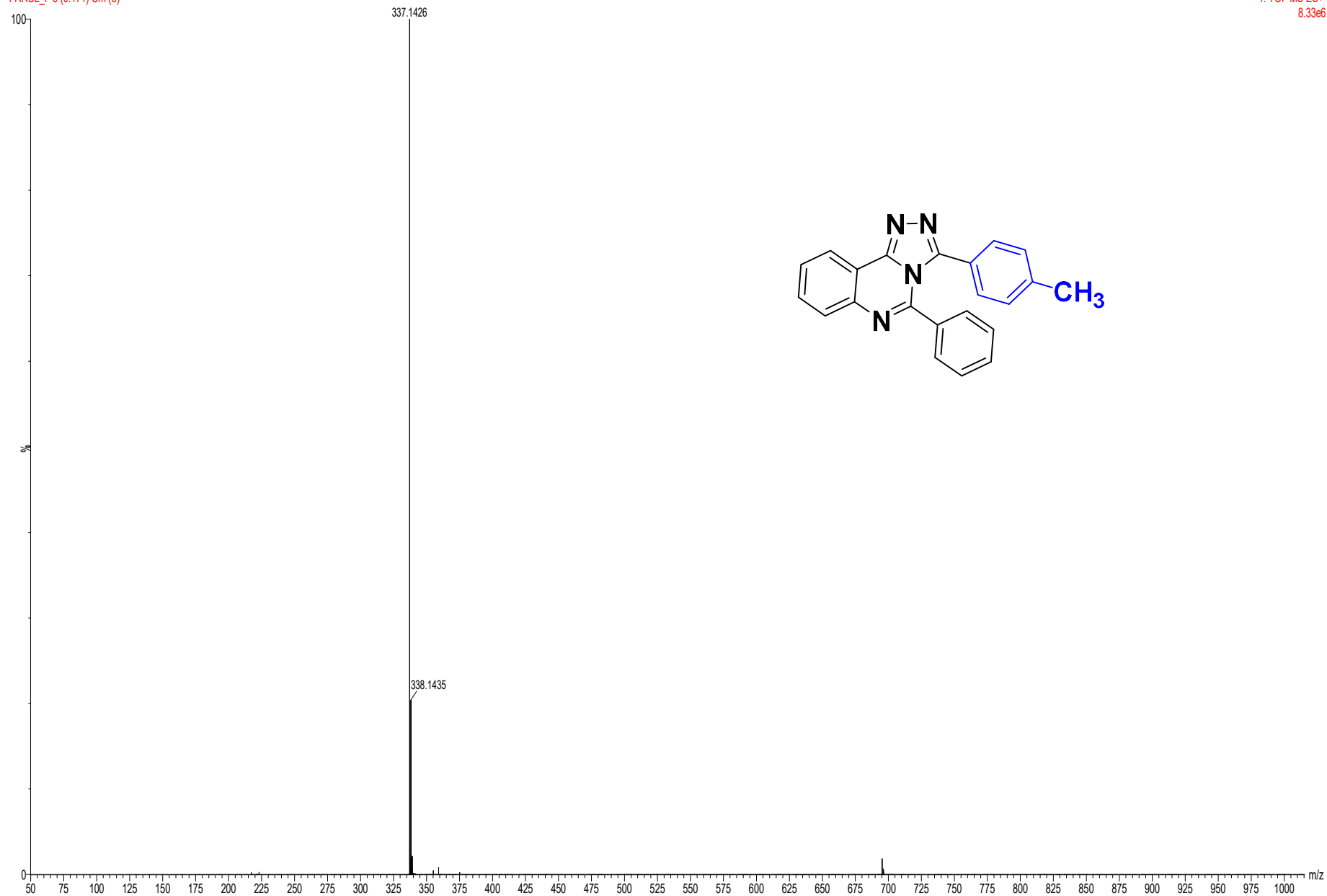
27-Feb-2023

11:07:41

1: TOF MS ES+

8.33e6

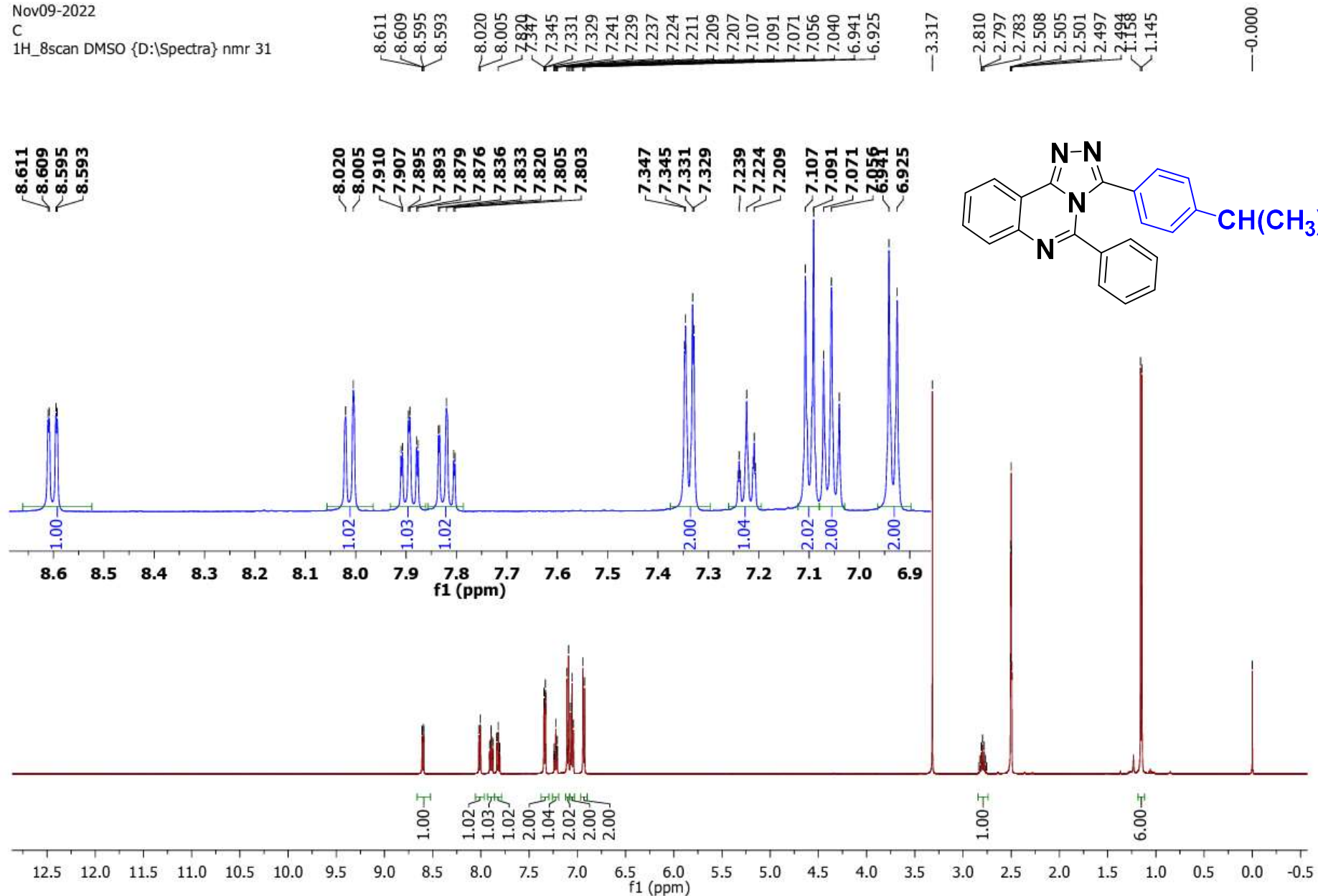
PARUL_F 8 (0.171) Cm (8)



¹H-NMR SPECTRA: 3-(4-Isopropylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5d).

Nov09-2022

C
1H_8scan DMSO {D:\Spectra} nmr 31

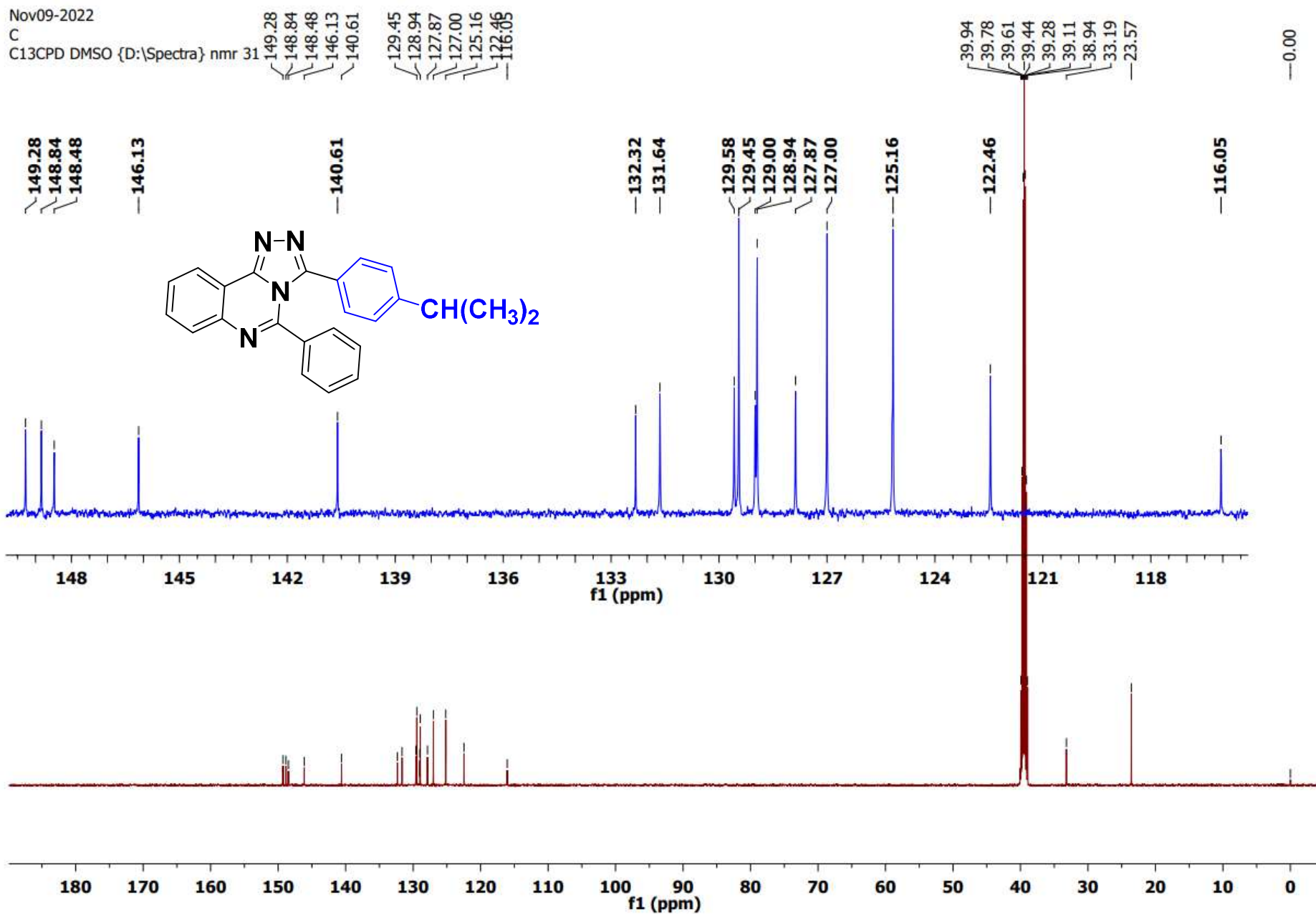


¹³C-NMR SPECTRA: 3-(4-Isopropylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5d).

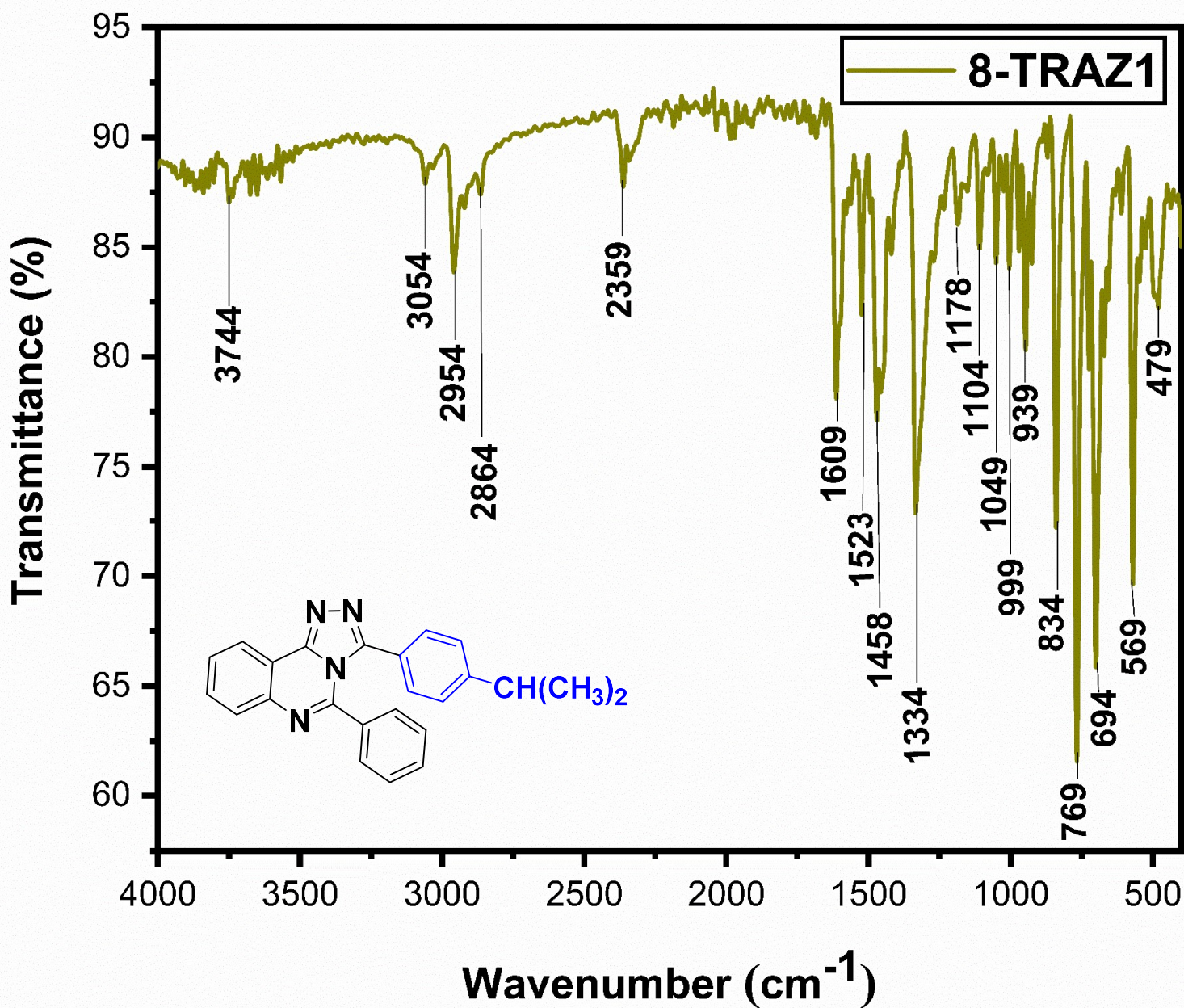
Nov09-2022

C

C13CPD DMSO {D:\Spectra} nmr 31



IR SPECTRA: 3-(4-Isopropylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5d).



HRMS SPECTRA: 3-(4-Isopropylphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5d).

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SYNAPT-XS#DBA064

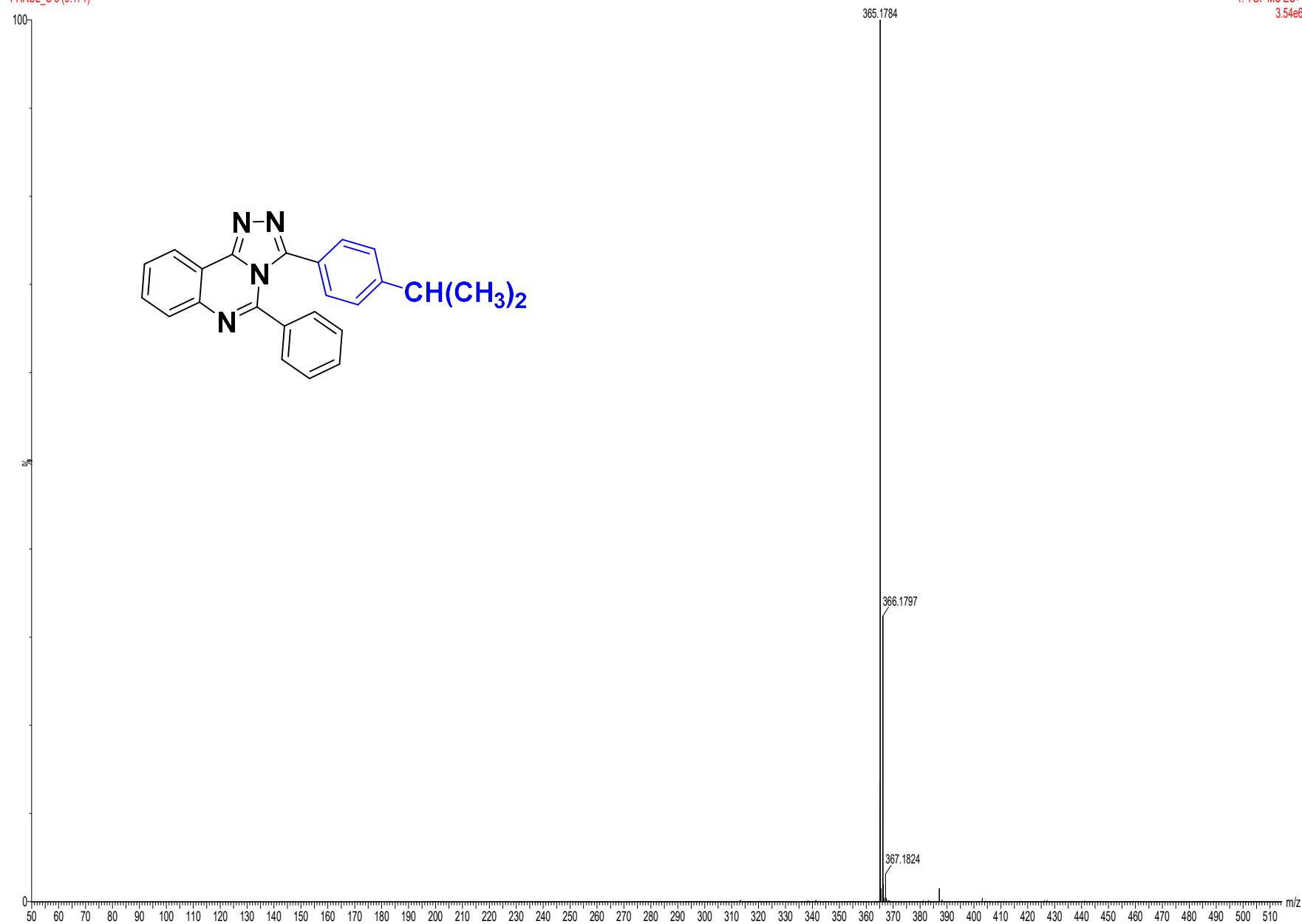
27-Feb-2023

10:59:42

1: TOF MS ES+

3.54e6

PARUL_C 8 (0.171)

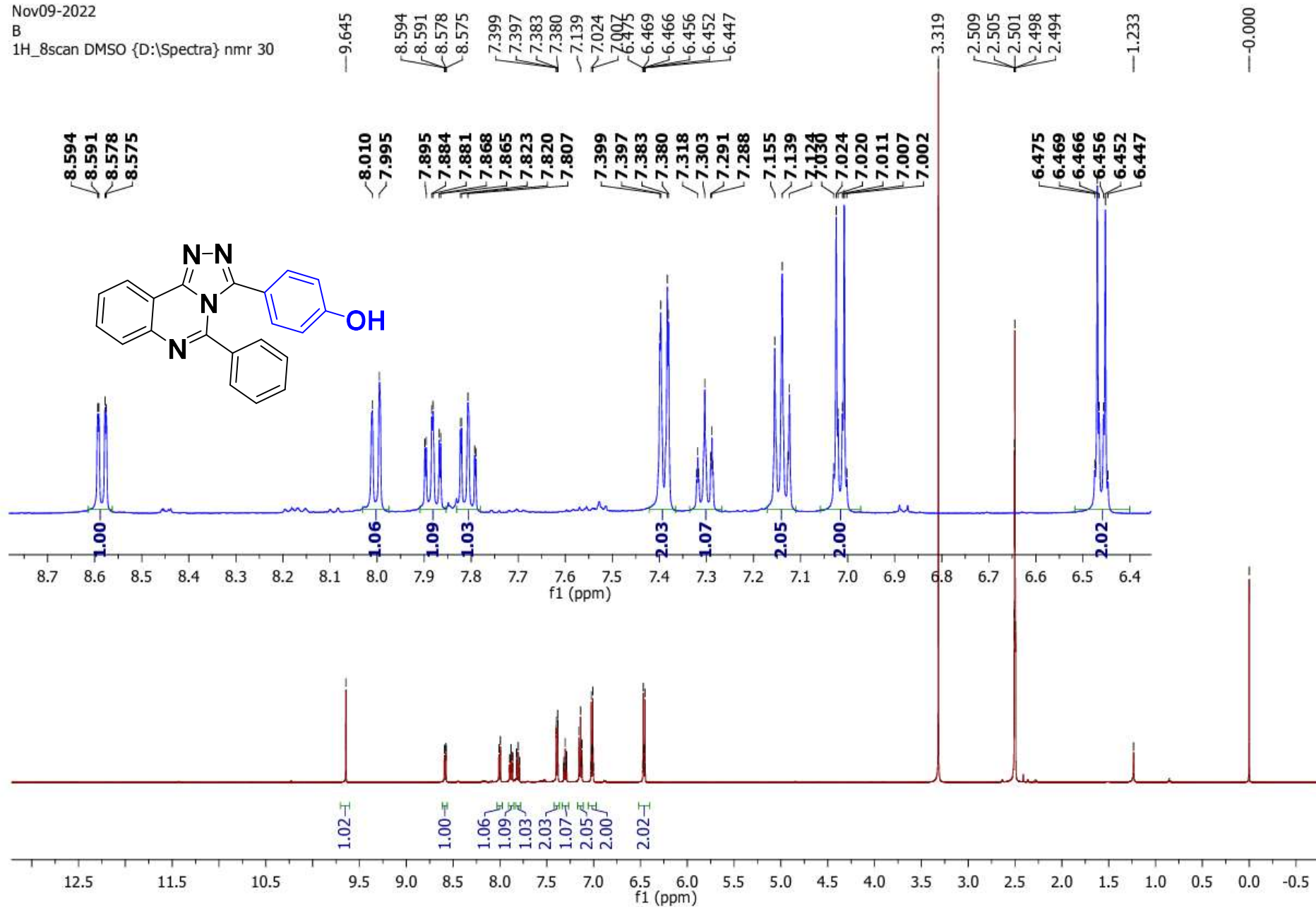


¹H-NMR SPECTRA: 4-(5-Phenyl-[1,2,4]triazolo[4,3-c]quinazolin-3-yl)phenol (5e).

Nov09-2022

B

1H_8scan DMSO {D:\Spectra} nmr 30

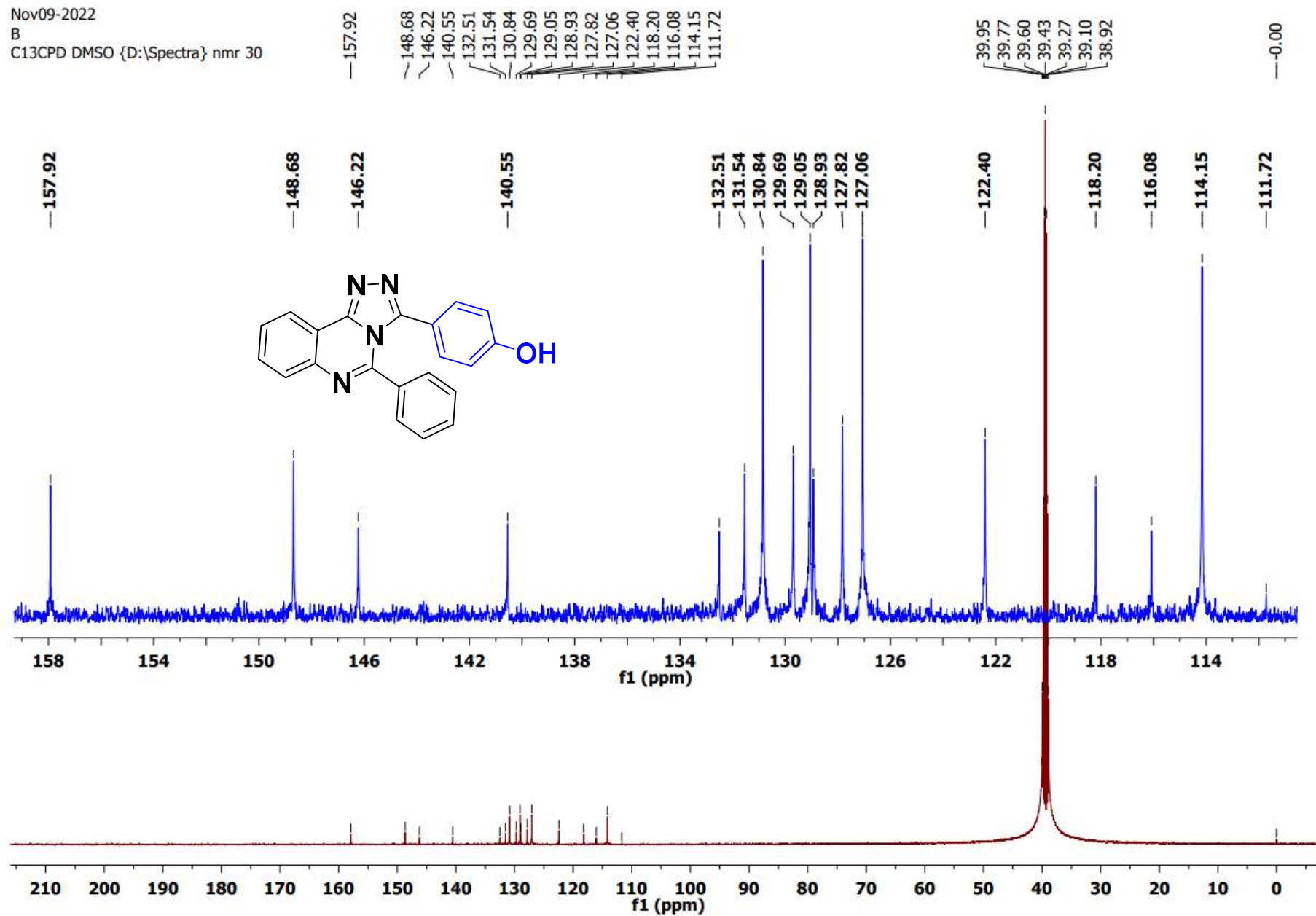


¹³C-NMR SPECTRA: 4-(5-Phenyl-[1,2,4]triazolo[4,3-c]quinazolin-3-yl)phenol (5e).

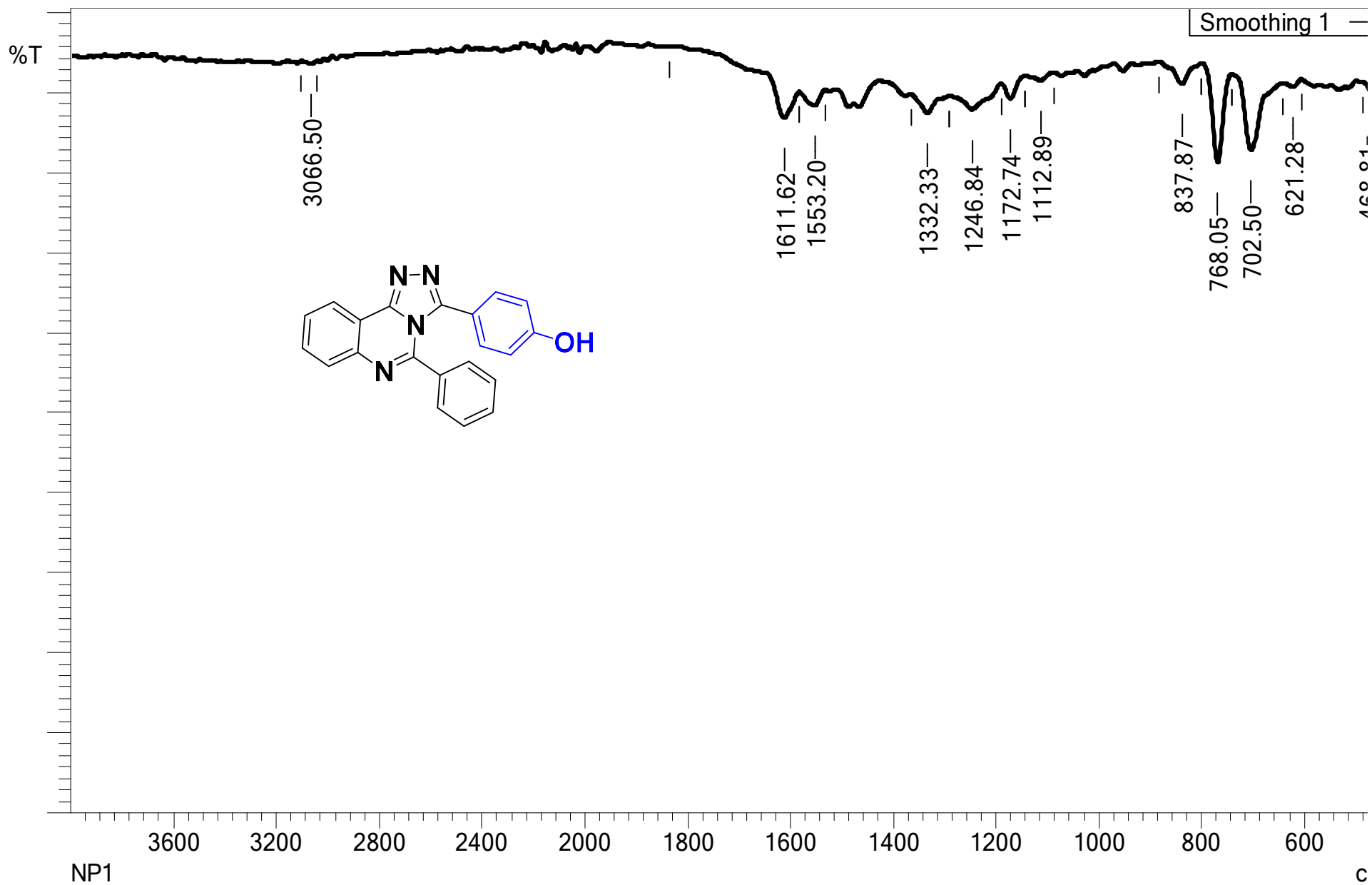
Nov09-2022

B

C13CPD DMSO {D:\Spectra} nmr 30



IR SPECTRA: 4-(5-Phenyl-[1,2,4]triazolo[4,3-c]quinazolin-3-yl)phenol (5e).



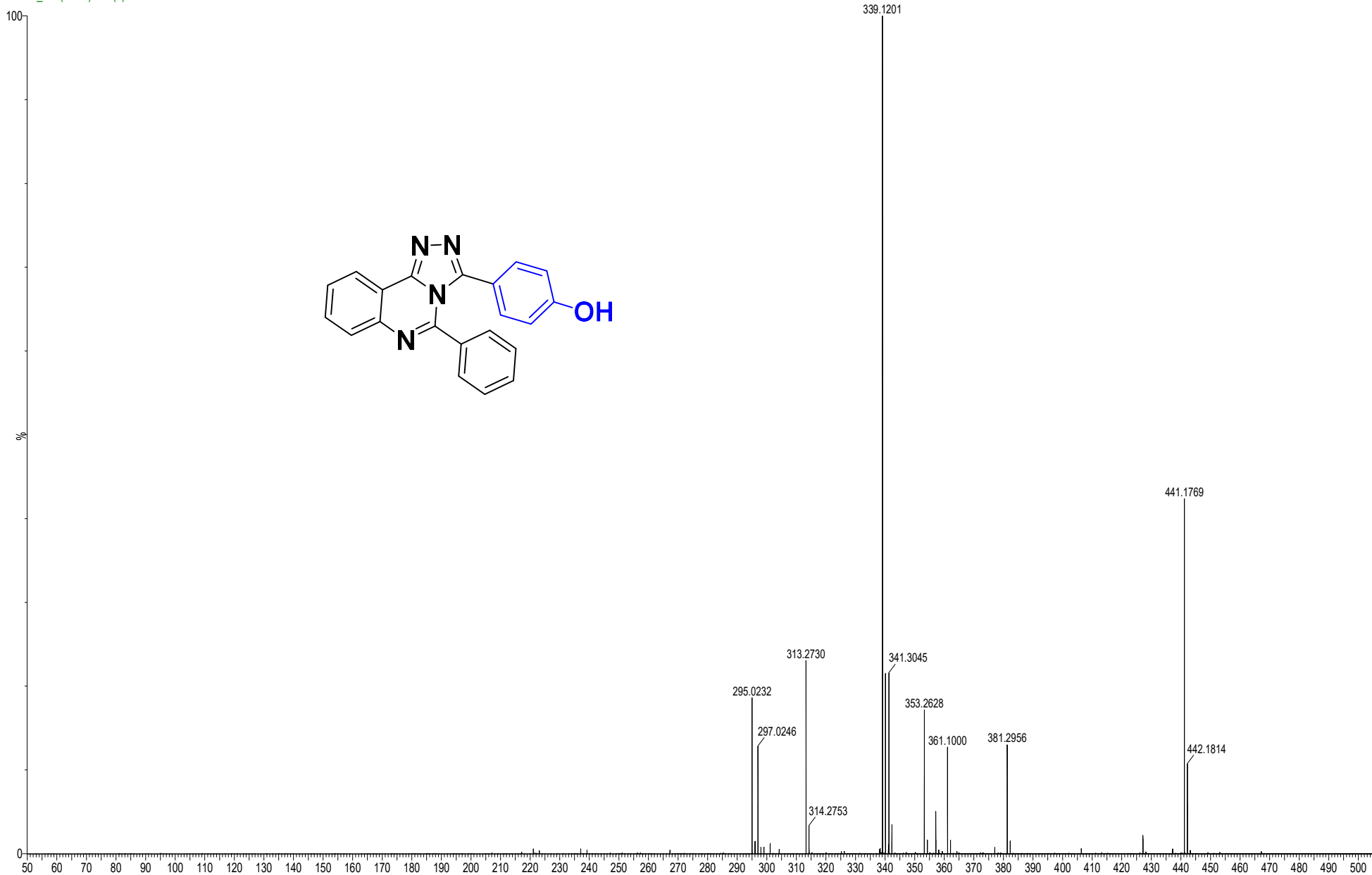
HRMS SPECTRA: 4-(5-Phenyl-[1,2,4]triazolo[4,3-c]quinazolin-3-yl)phenol (5e).

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SYNAPT-XS#DBA064

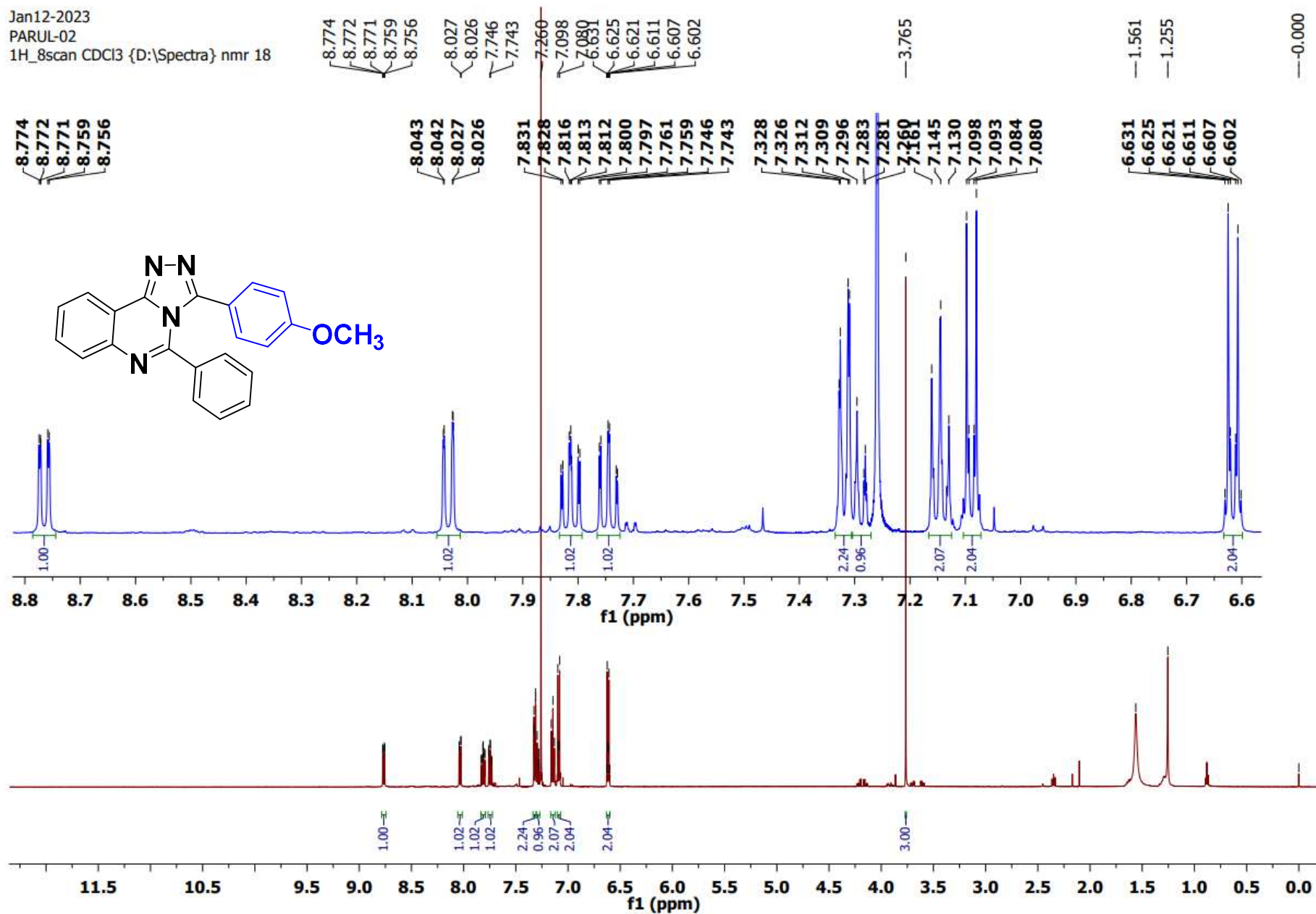
PARUL_B 5 (0.120) Cm (5)

1:



¹H-NMR SPECTRA: 3-(4-Methoxyphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5f).

Jan12-2023
 PARUL-02
 1H_8scan CDCl3 {D:\Spectra} nmr 18

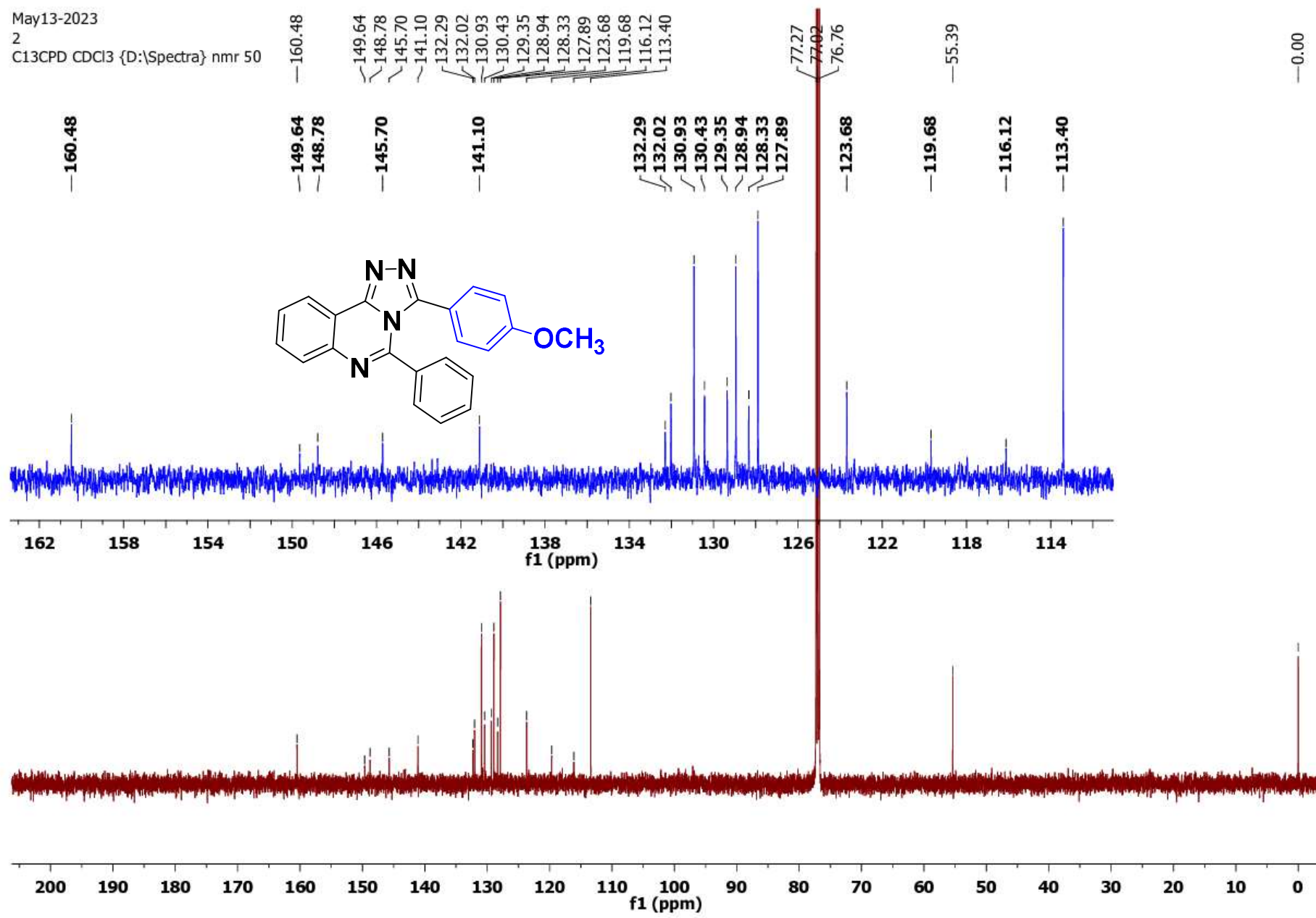


¹³C-NMR SPECTRA: 3-(4-Methoxyphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5f).

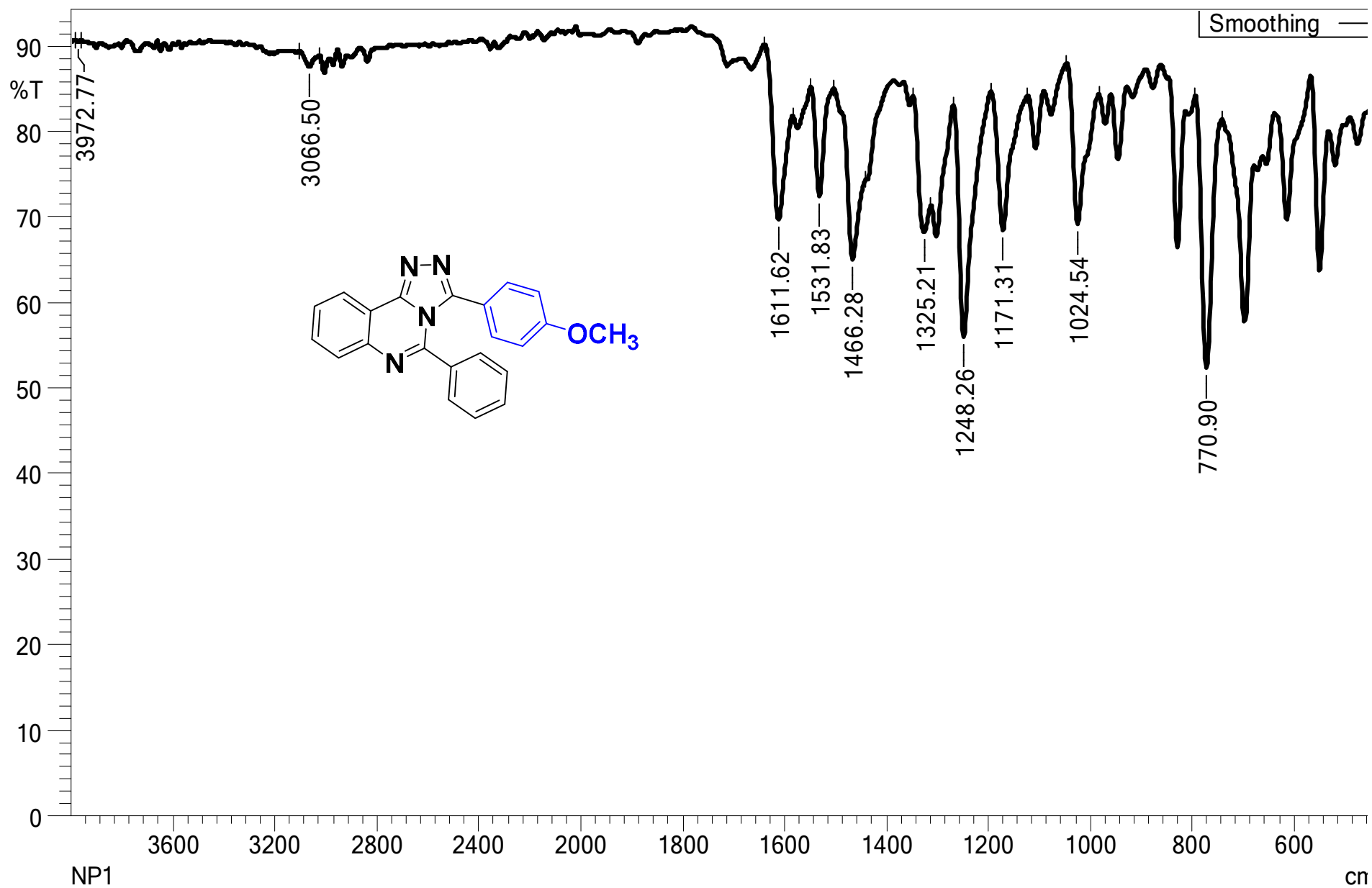
May13-2023

2

C13CPD CDCl3 {D:\Spectra} nmr 50



IR SPECTRA: 3-(4-Methoxyphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5f).



HRMS SPECTRA: 3-(4-Methoxyphenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5f).

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SYNAPT-XS#DBA064

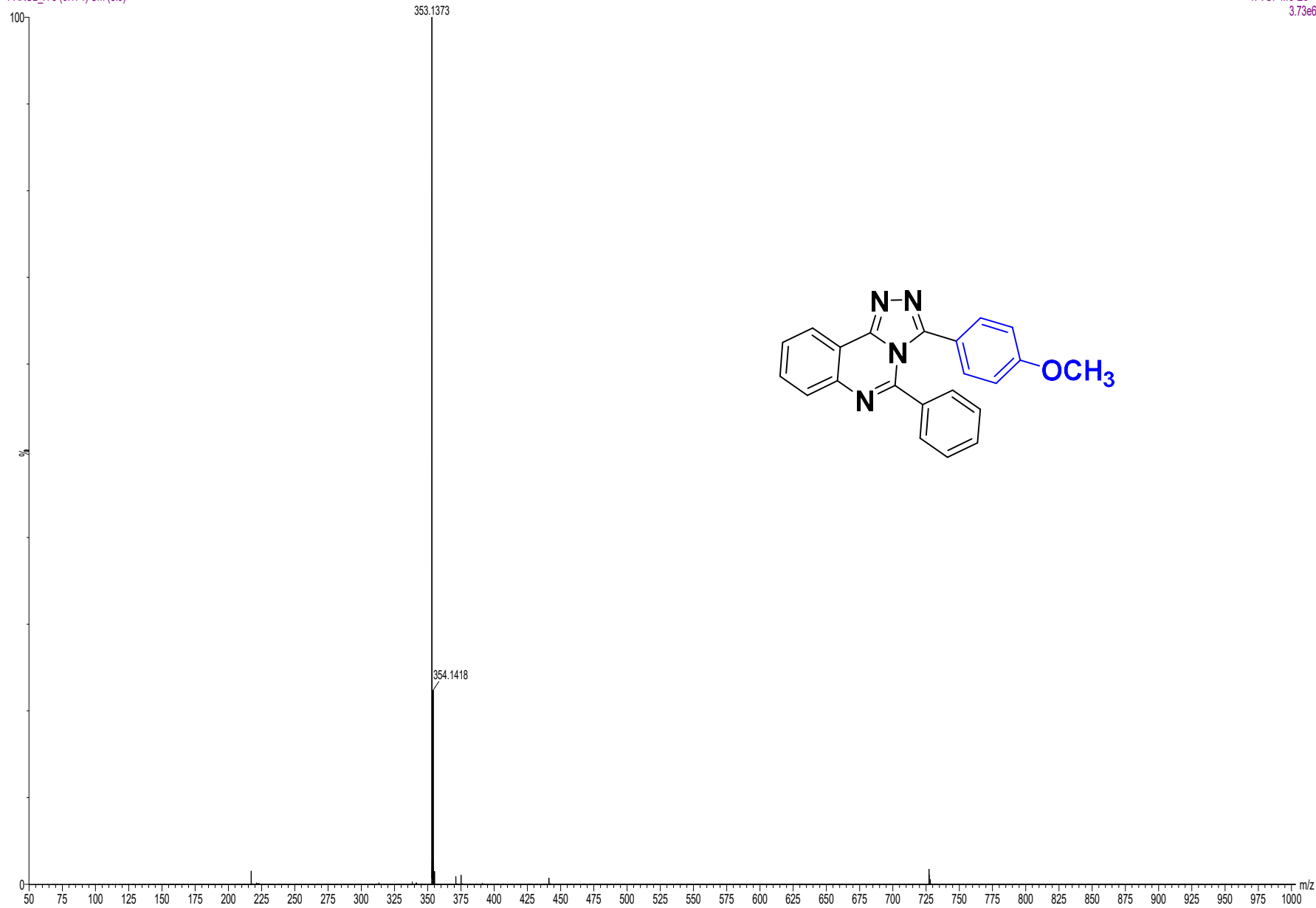
27-Feb-2023

11:13:07

1: TOF MS ES+

3.73e6

PARUL_H 8 (0.171) Cm (8:9)

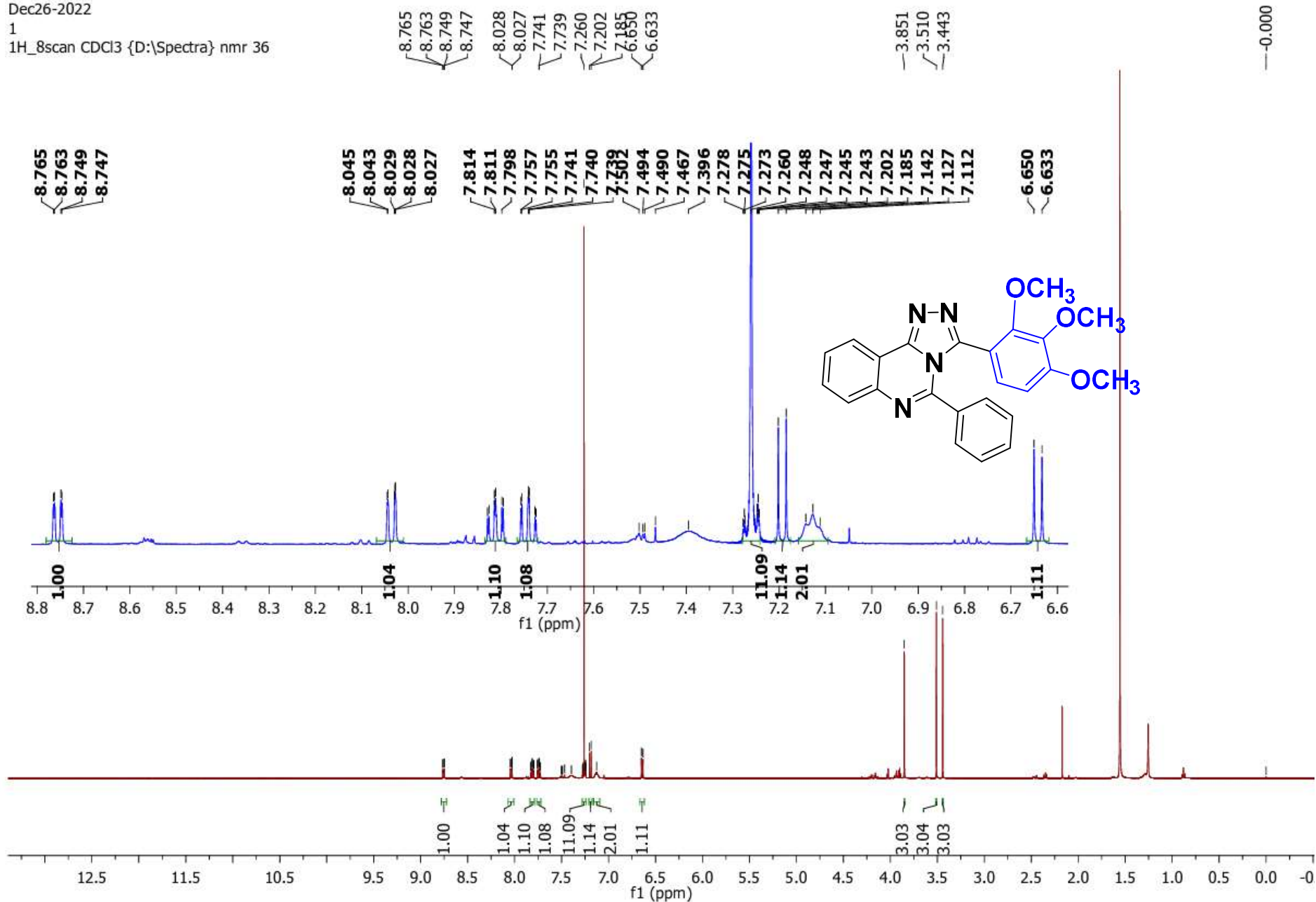


¹H-NMR SPECTRA: 5-Phenyl-3-(2,3,4-trimethoxyphenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5g).

Dec26-2022

1

1H_8scan CDCl3 {D:\Spectra} nmr 36

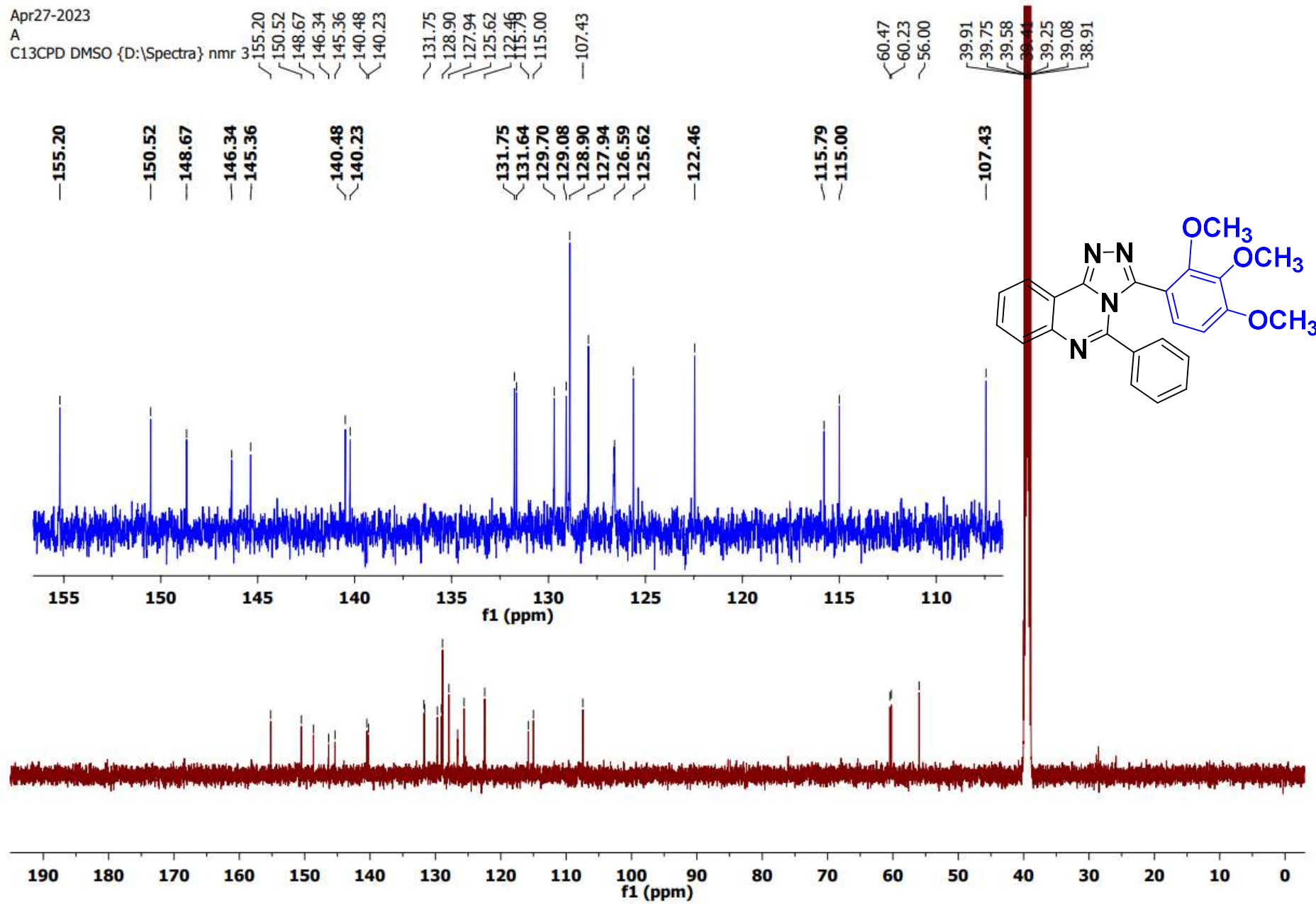


¹³C-NMR SPECTRA: 5-Phenyl-3-(2,3,4-trimethoxyphenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5g).

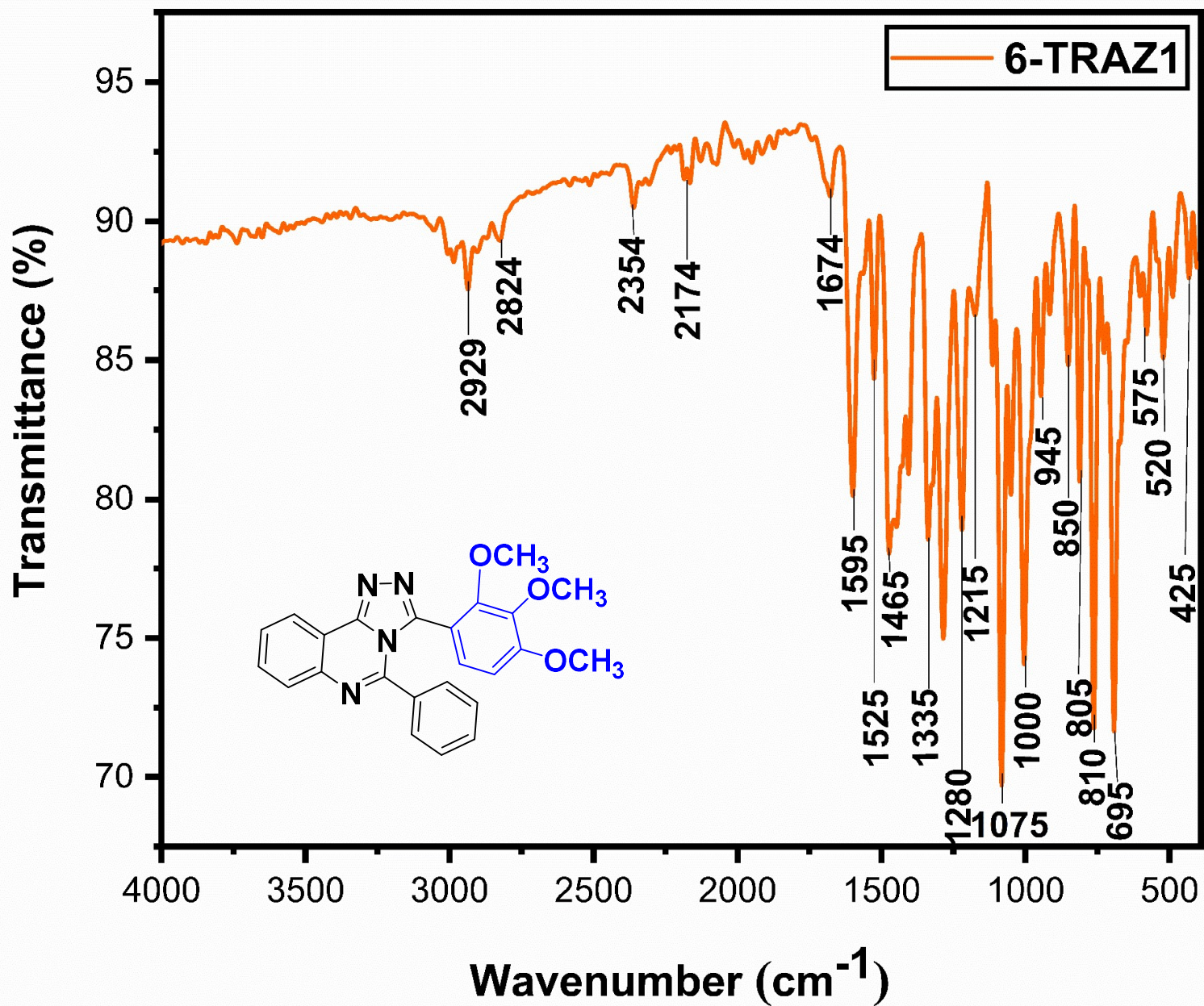
Apr27-2023

A

C13CPD DMSO {D:\Spectra} nmr 3



¹³C-NMR SPECTRA: 5-Phenyl-3-(2,3,4-trimethoxyphenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5g).



HRMS SPECTRA: 5-Phenyl-3-(2,3,4-trimethoxyphenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5g).

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SYNAPT-XS#DBA064

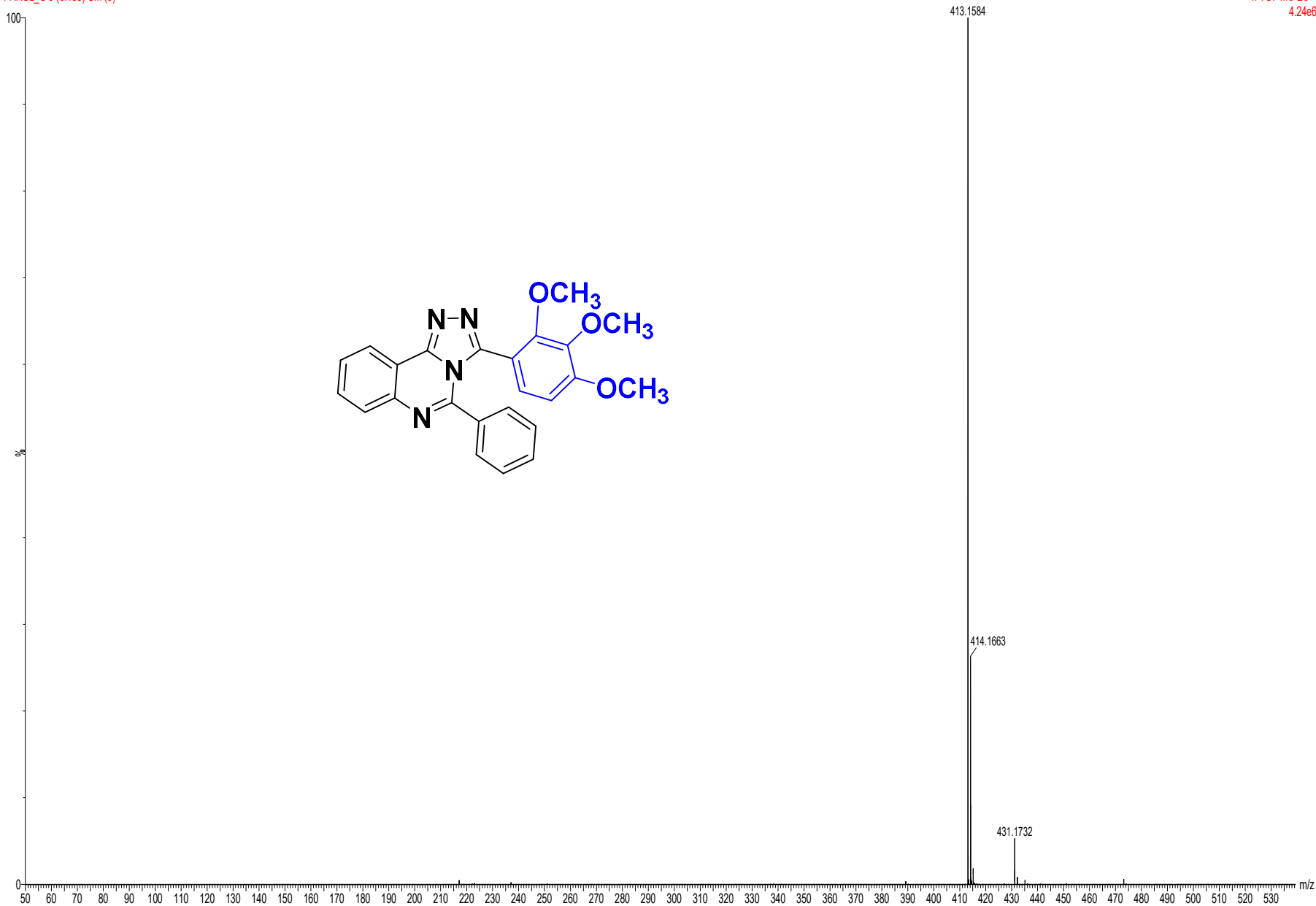
27-Feb-2023

11:10:26

1: TOF MS ES+

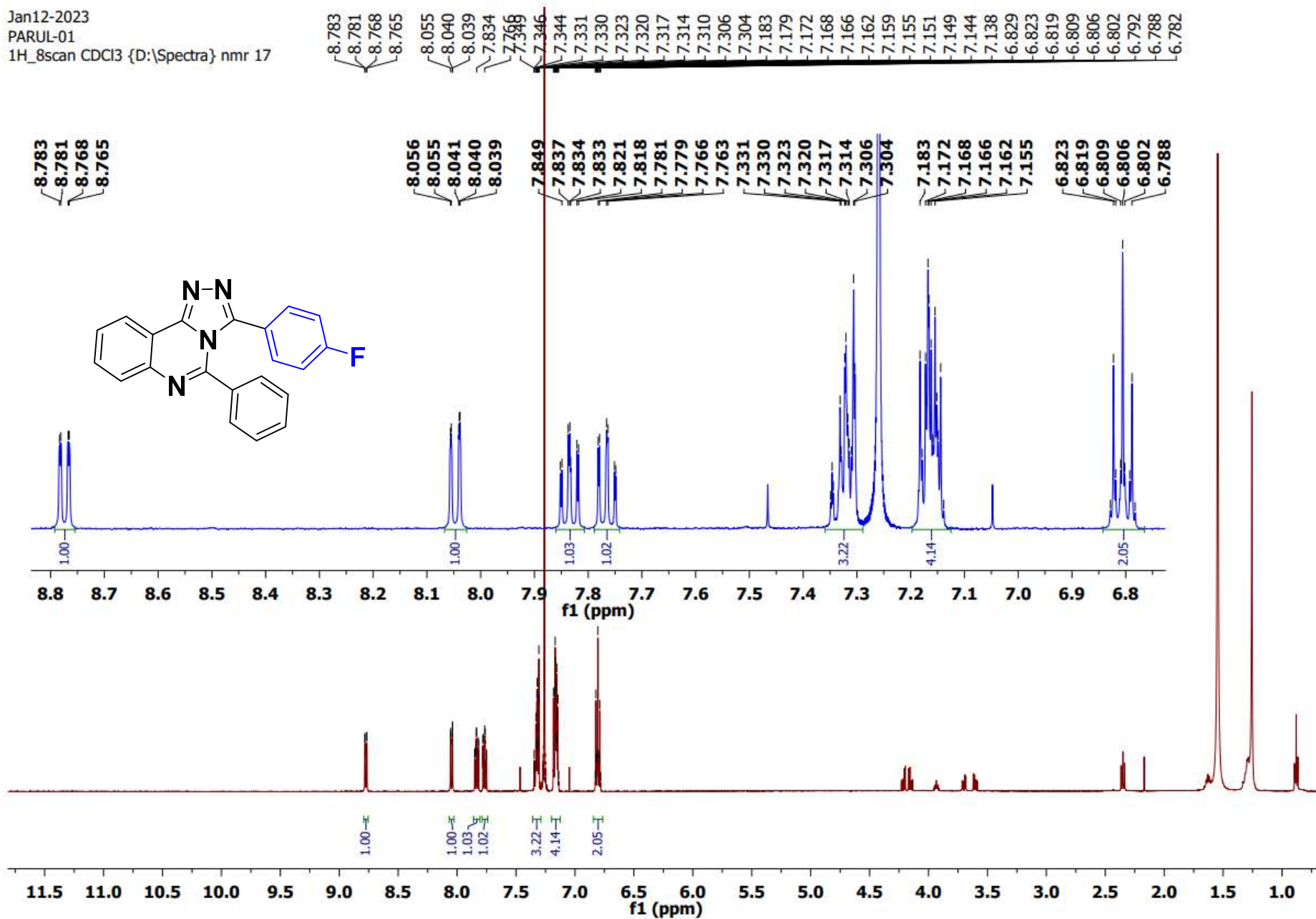
4.24e6

PARUL_G 9 (0.188) Cm (9)

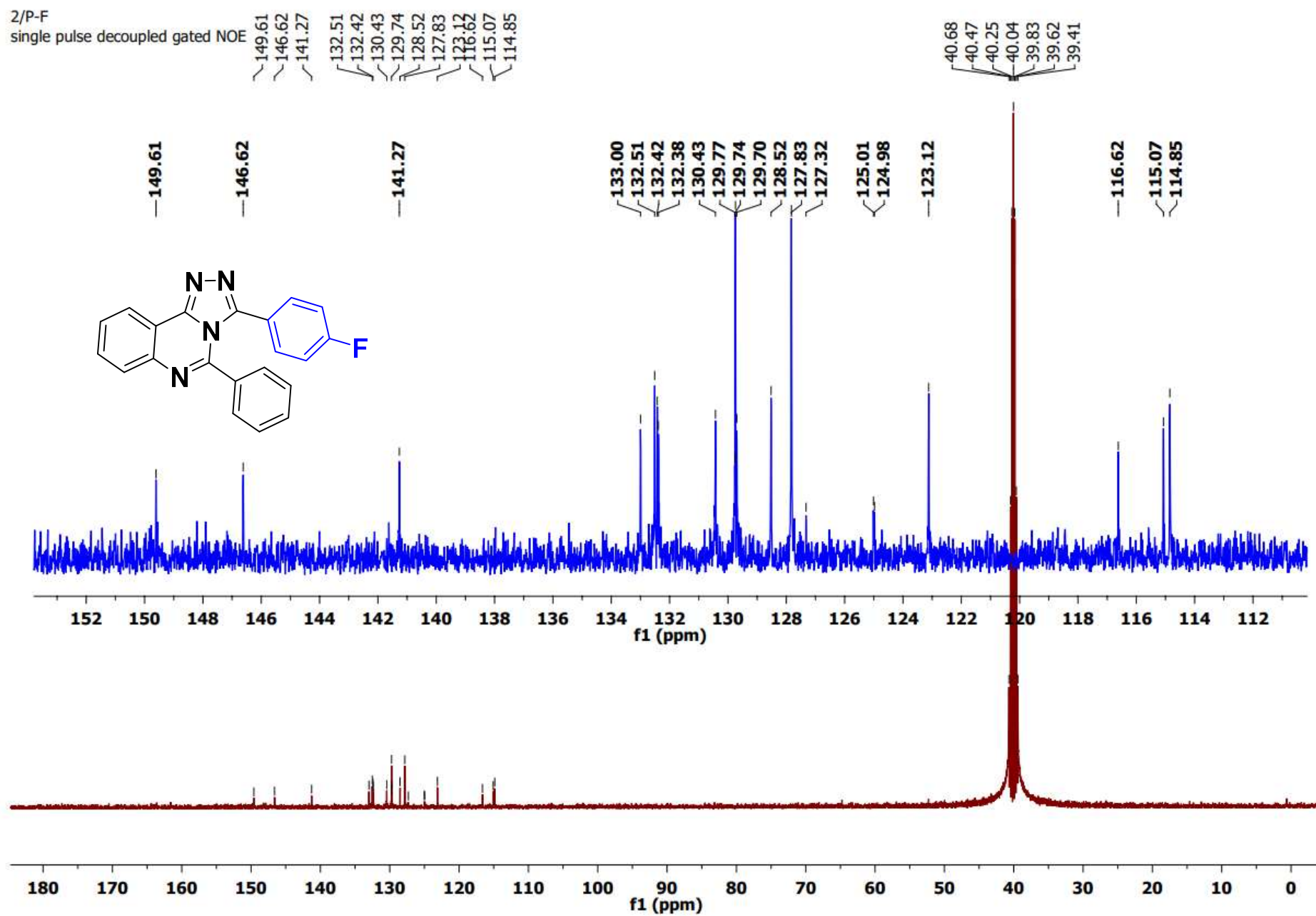


¹H-NMR SPECTRA: 3-(4-Fluorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5h).

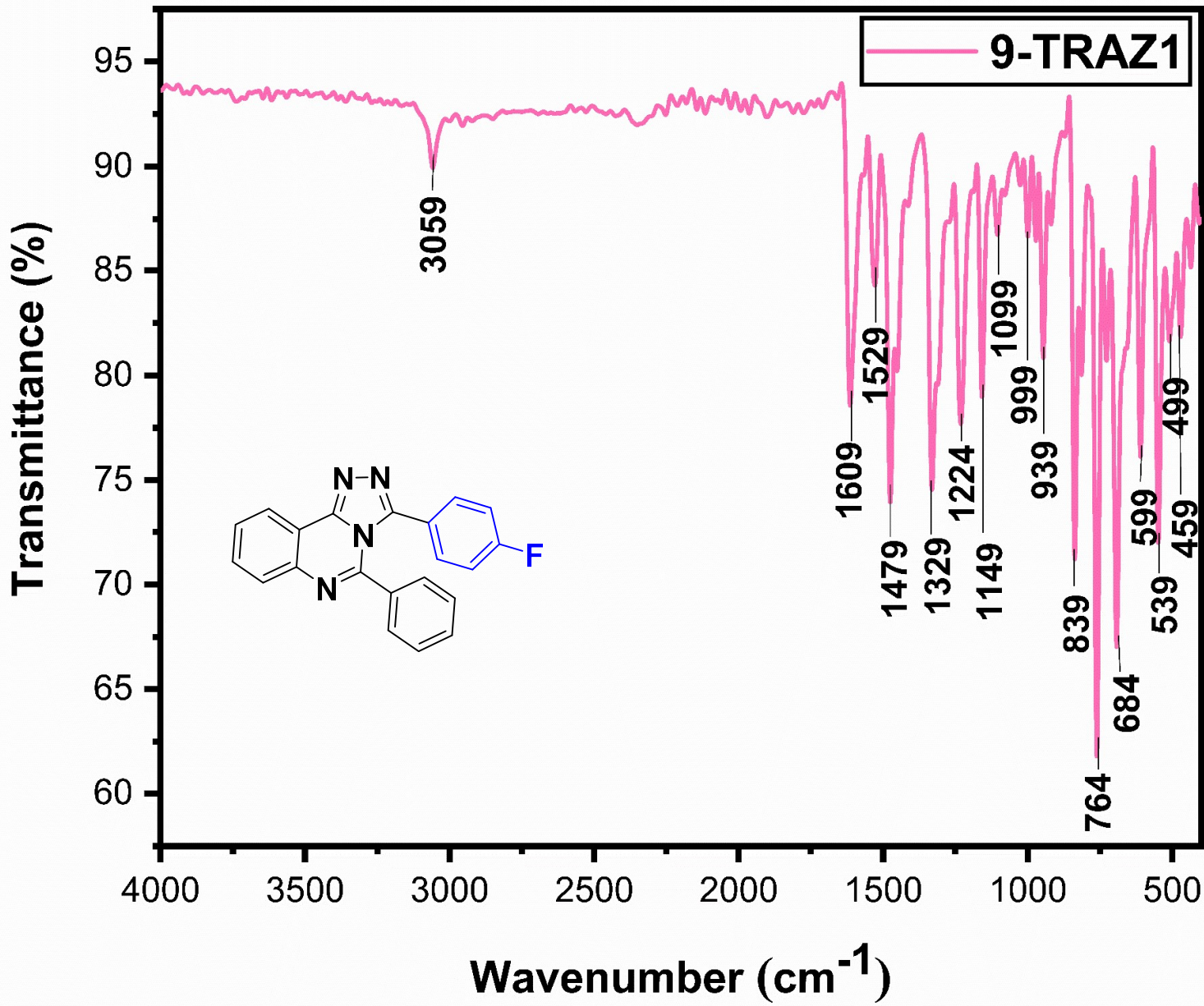
Jan12-2023
PARUL-01
1H_8scan CDCl3 {D:\Spectra} nmr 17



¹³C-NMR SPECTRA: 3-(4-Fluorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5h).



IR SPECTRA: 3-(4-Fluorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5h).



HRMS SPECTRA: 3-(4-Fluorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5h).

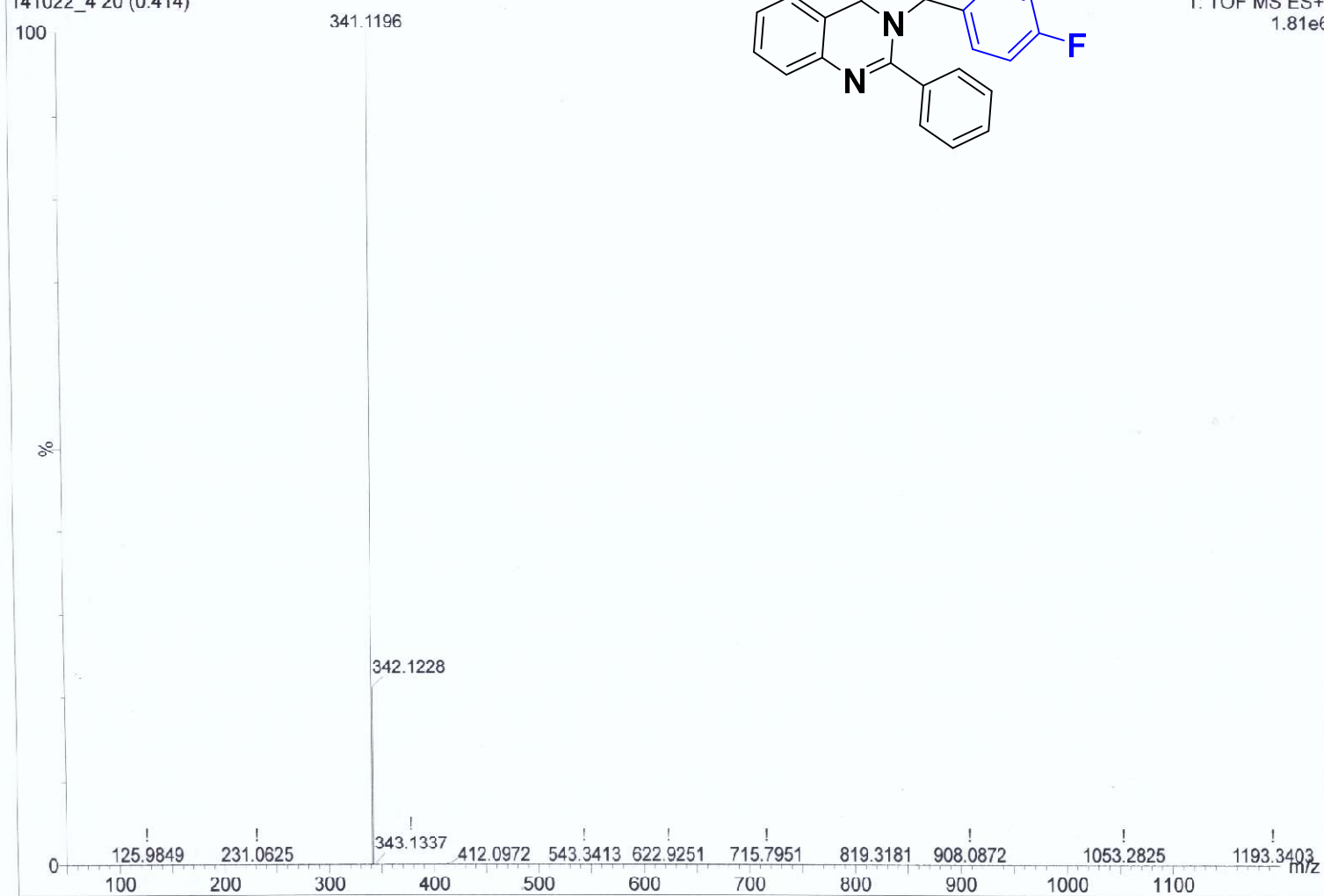
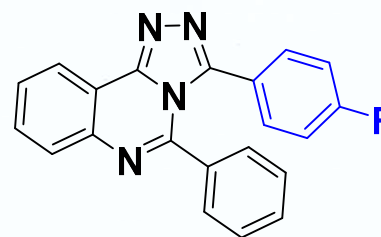
XEVO -G2XSQTOF#TFC2176
POSITIVE ION MODE
SS 12

Capillary V 3, Cone V 40, Desolvation Gas 800
ESI

14-Oct-2022

141022_4 20 (0.414)

1: TOF MS ES+
1.81e6

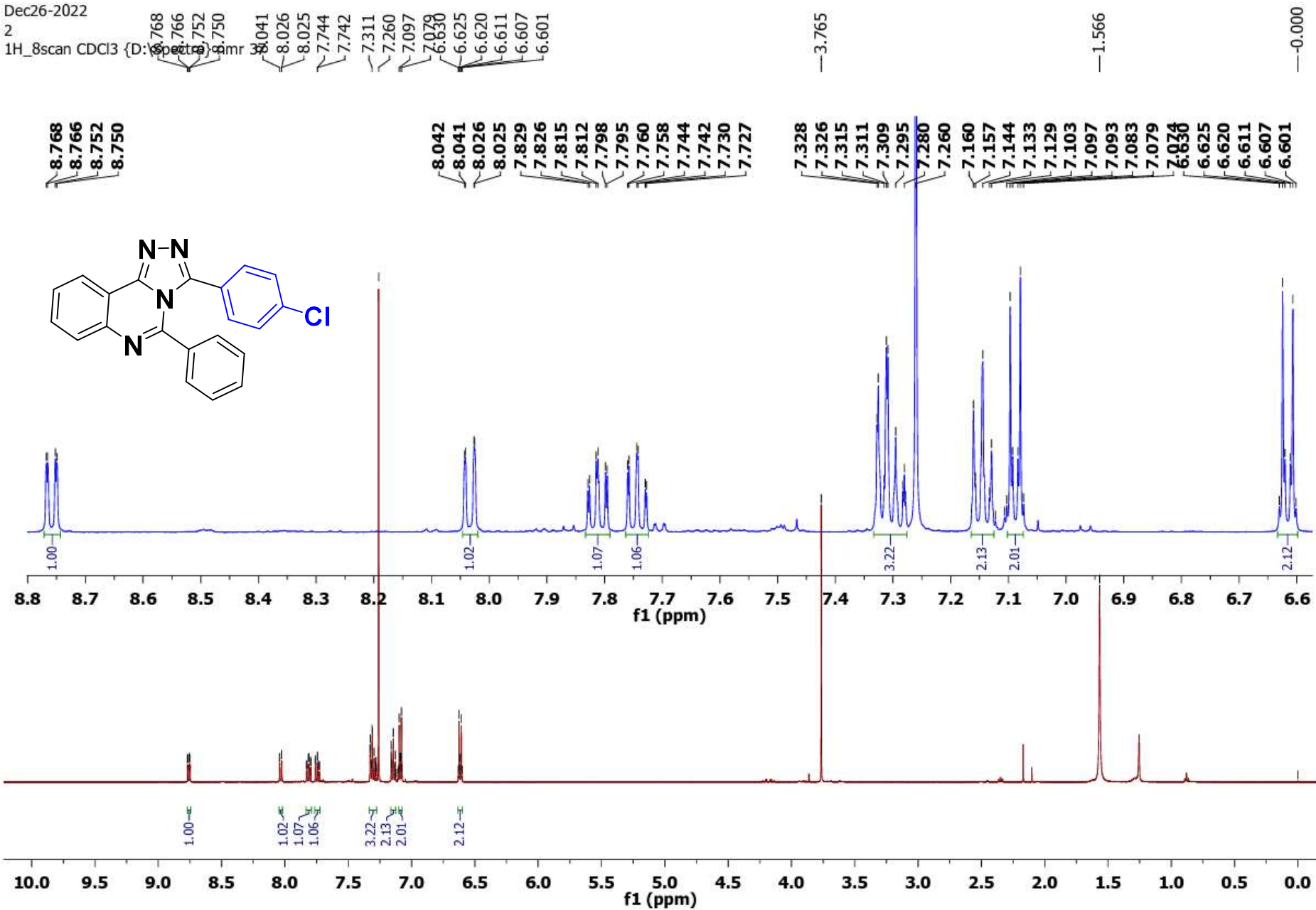


¹H-NMR SPECTRA: 3-(4-Chlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5i).

Dec26-2022

2

1H_8scan CDCl3 (DMSO-d₆)

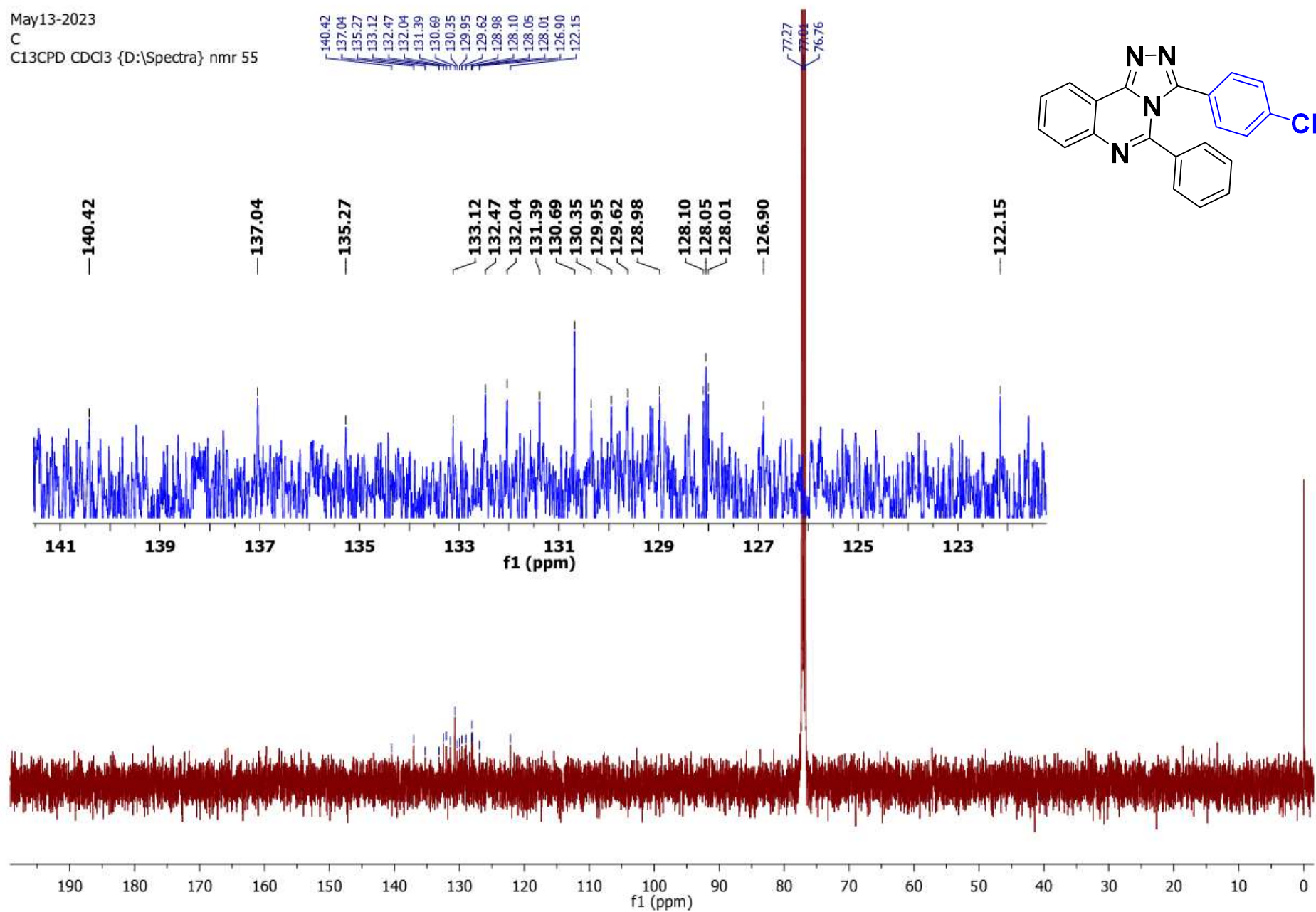


¹³C-NMR SPECTRA: 3-(4-Chlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5i).

May13-2023

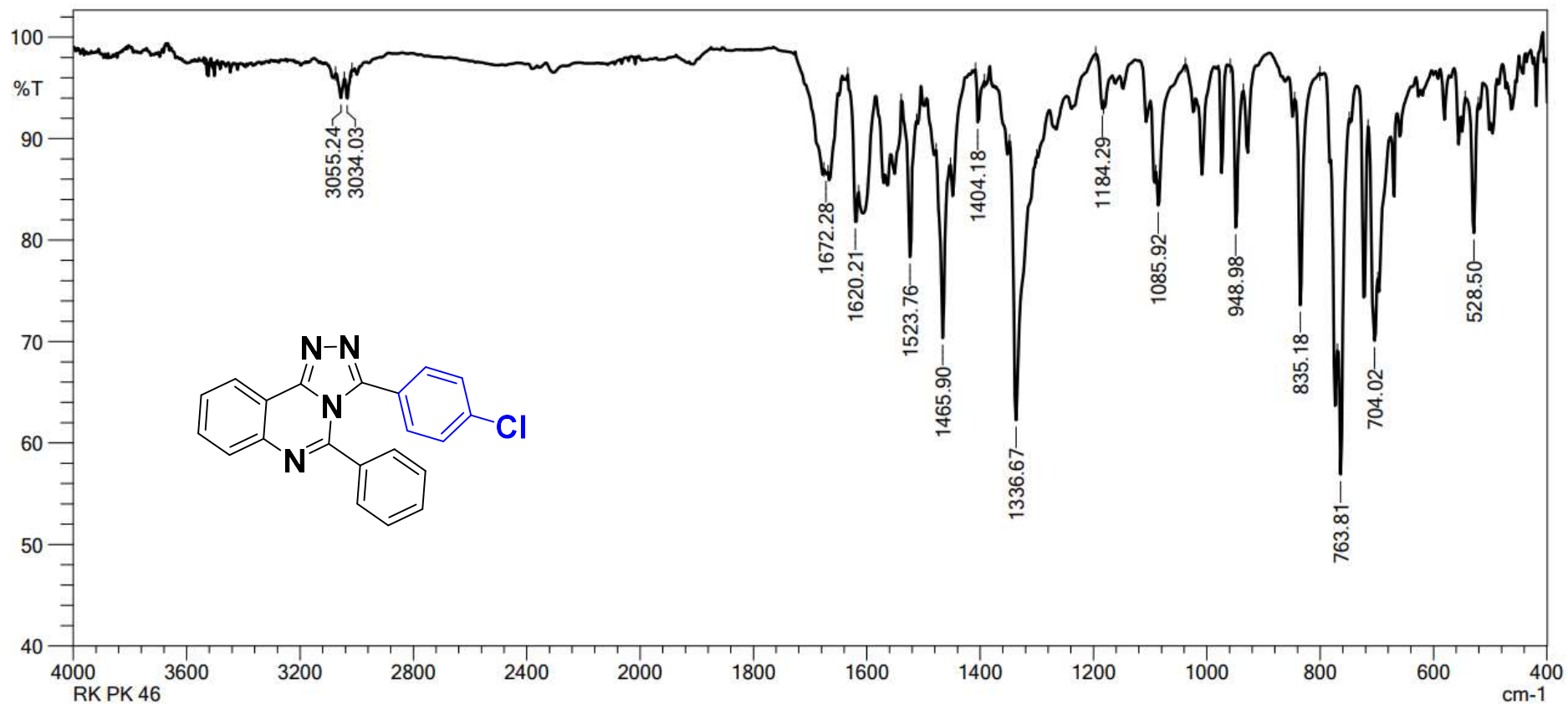
C

C13CPD CDCl3 {D:\Spectra} nmr 55



IR SPECTRA: 3-(4-Chlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5i).

SHIMADZU



HRMS SPECTRA: 3-(4-Chlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5i).

XEVO -G2XSQTOF#TFC2176

Capillary V 3, Cone V 40 , Desolvation Gas 800
ESI

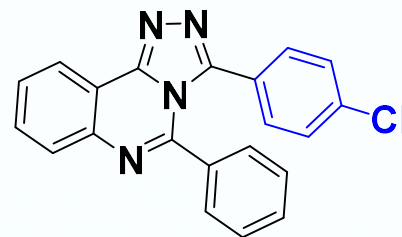
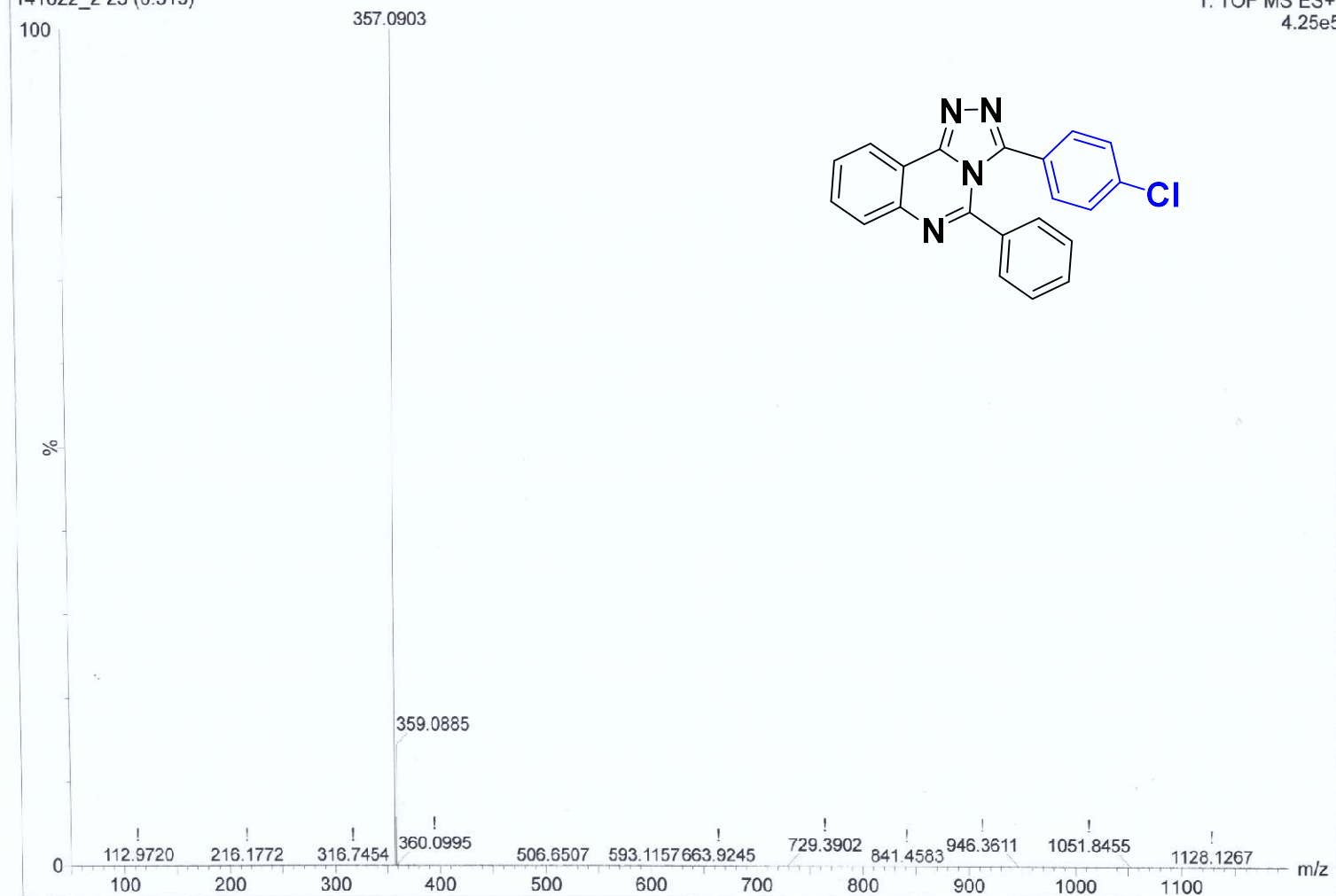
14-Oct-2022

POSITIVE ION MODE

SS 10

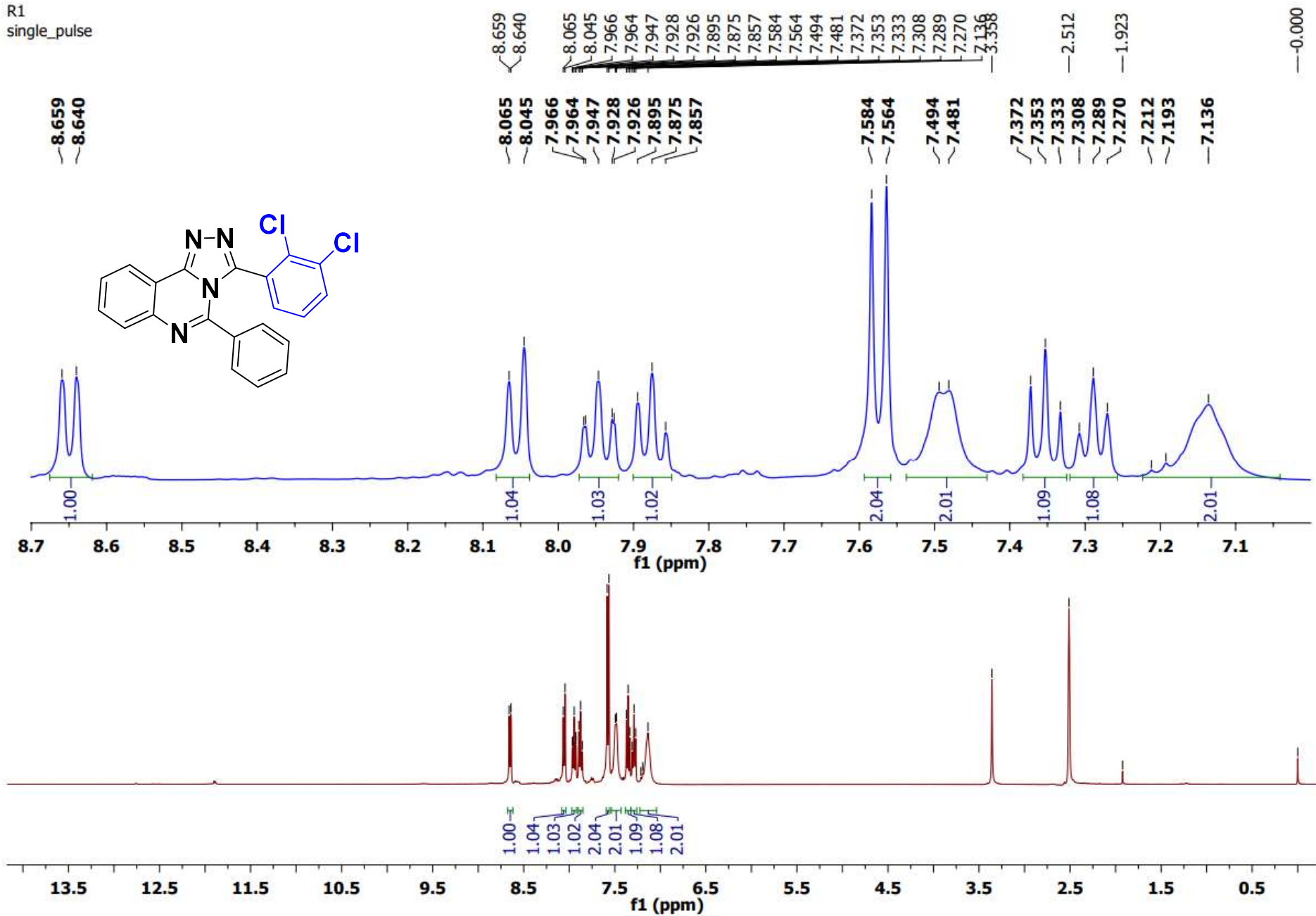
141022_2 25 (0.519)

1: TOF MS ES+
4.25e5



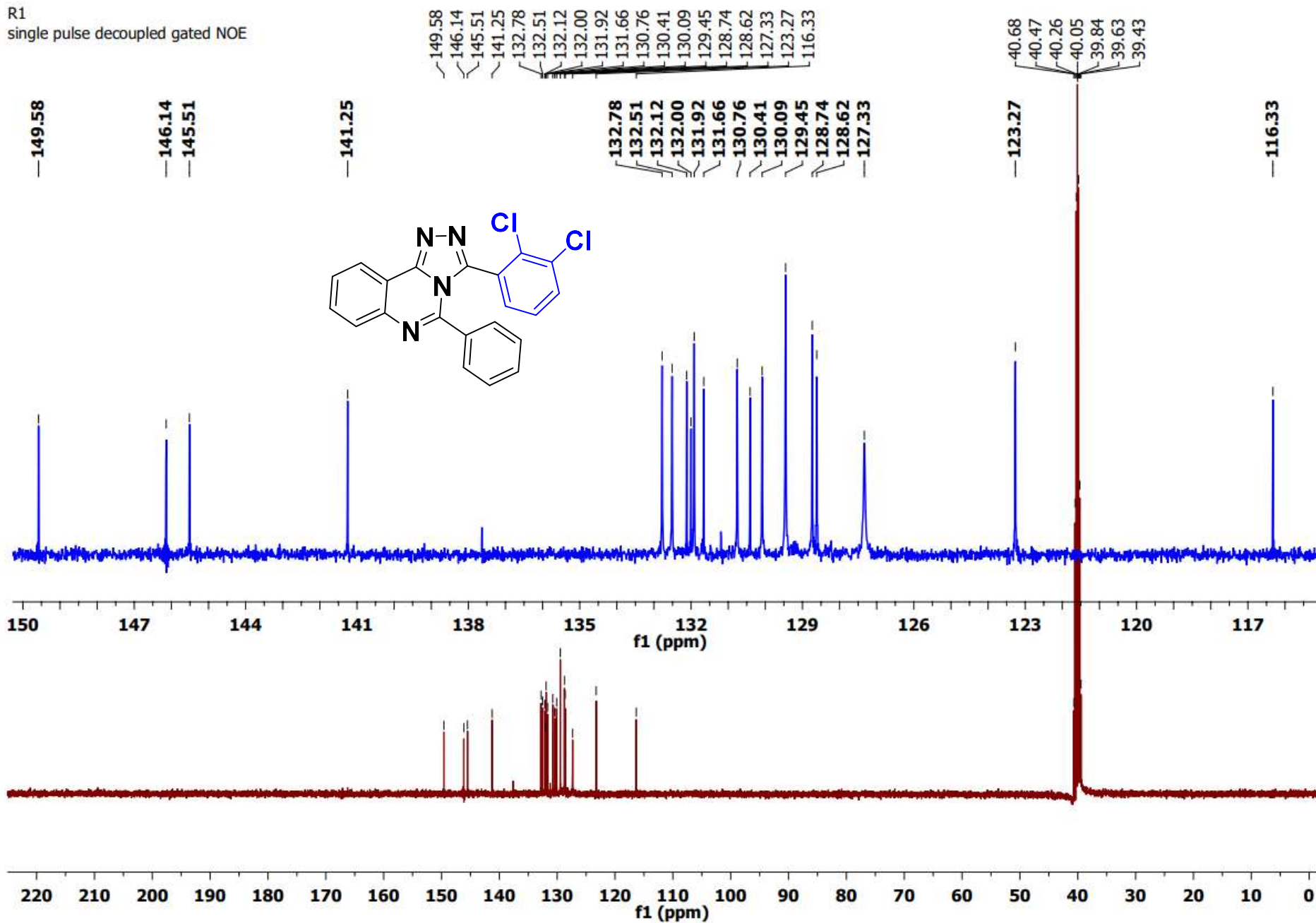
¹H-NMR SPECTRA: 3-(2,3-Dichlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5j).

R1
single_pulse

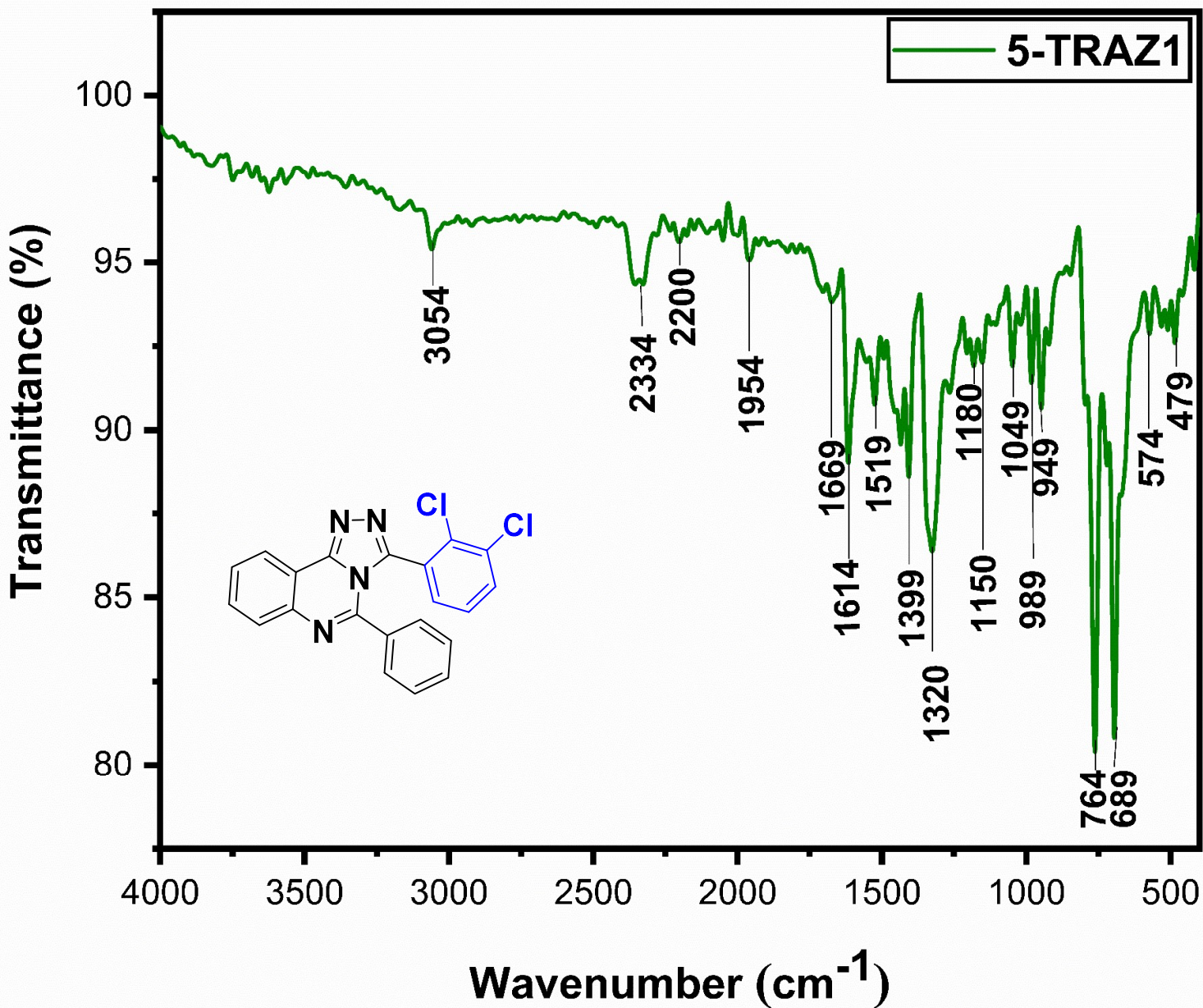


¹³C-NMR SPECTRA: 3-(2,3-Dichlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5j).

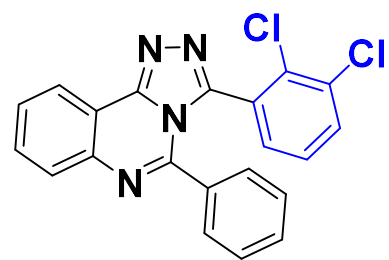
R1
single pulse decoupled gated NOE



IR SPECTRA: 3-(2,3-Dichlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5j).



HRMS SPECTRA: 3-(2,3-Dichlorophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5j).



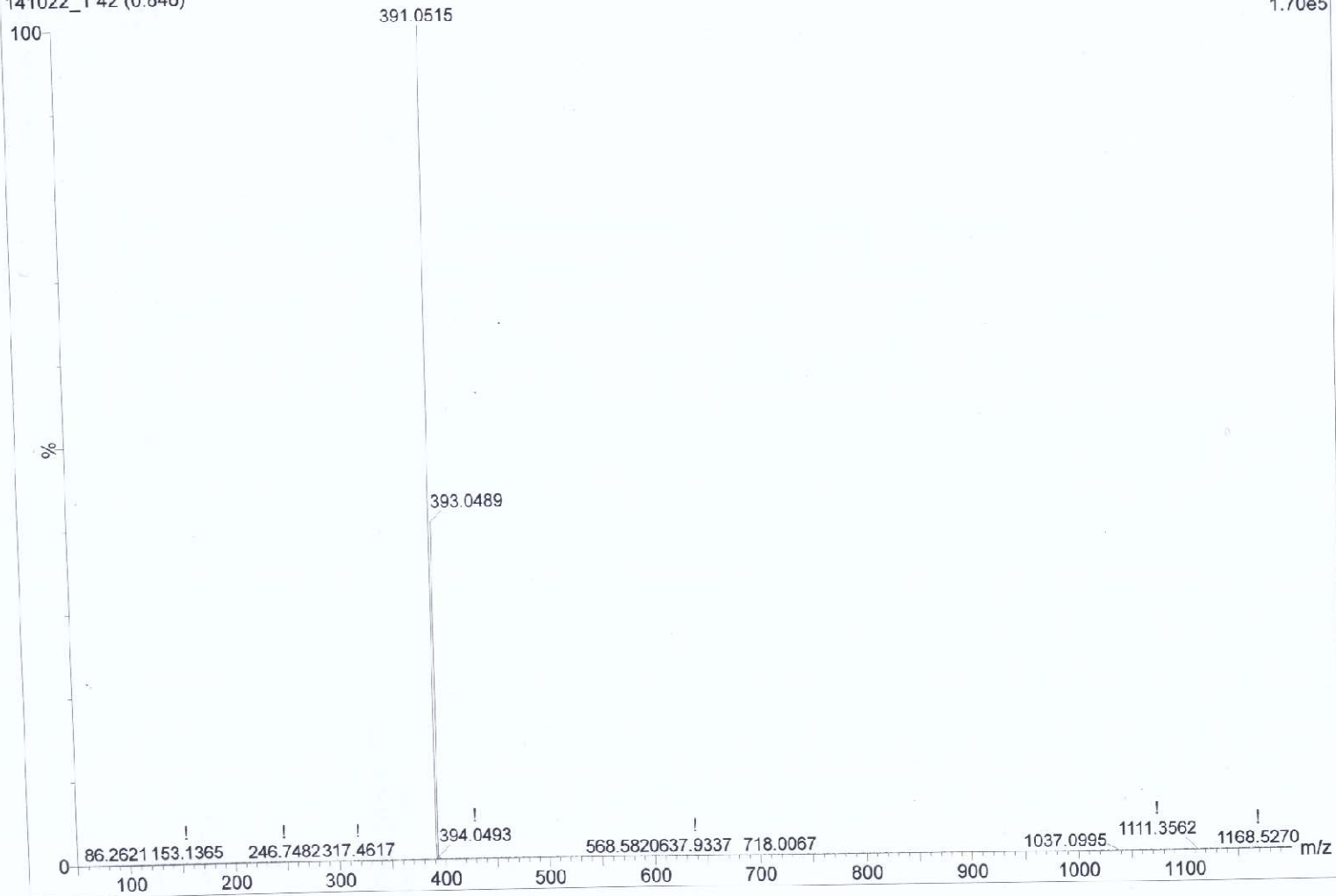
XEVO -G2XSQTOF#TFC2176
POSITIVE ION MODE
SS 9

Capillary V 3, Cone V 40, Desolvation Gas 800
ESI

14-Oct-2022

1: TOF MS ES+
1.70e5

141022_1 42 (0.846)

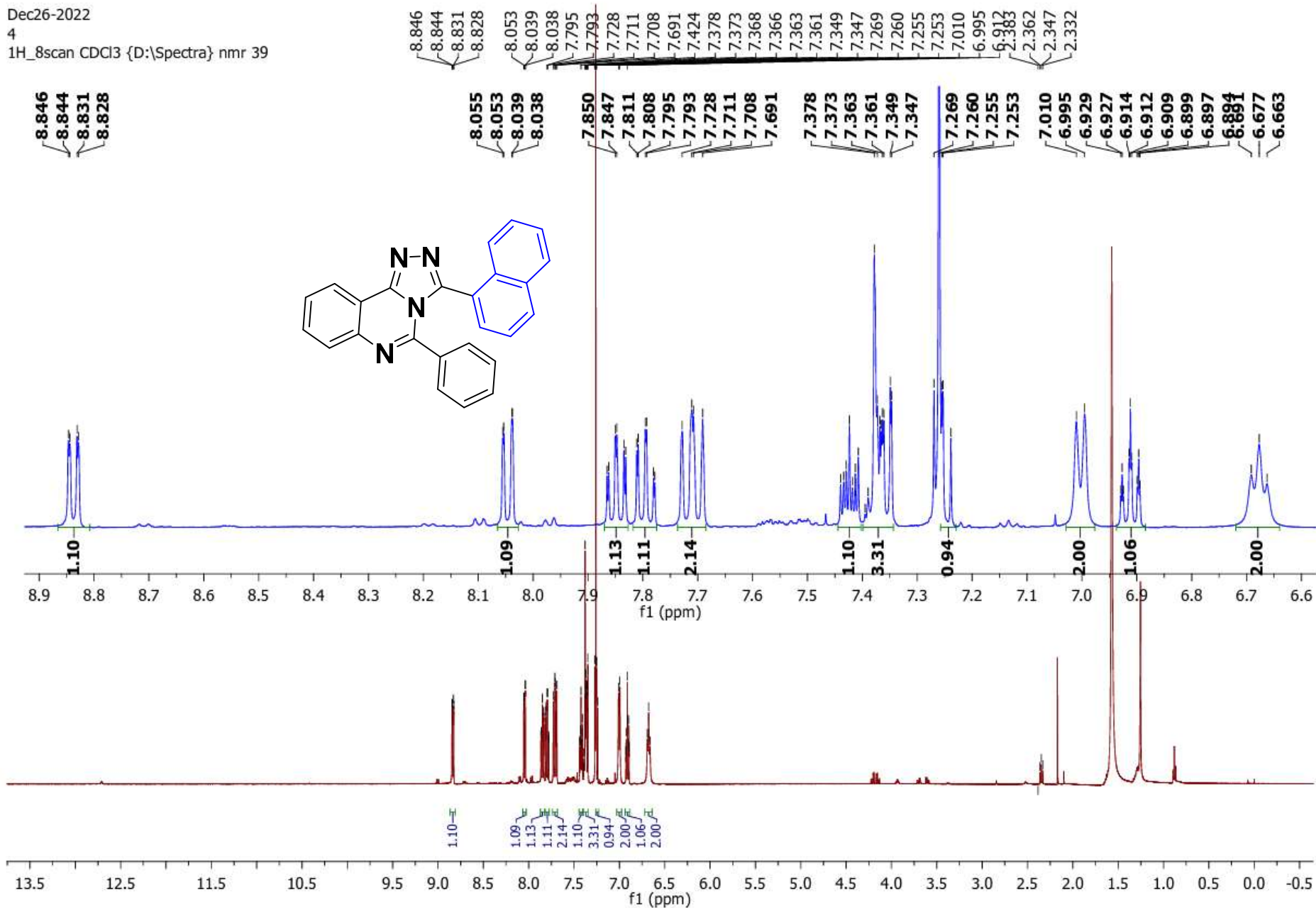


¹H-NMR SPECTRA: 3-(Naphthalen-1-yl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5k).

Dec26-2022

4

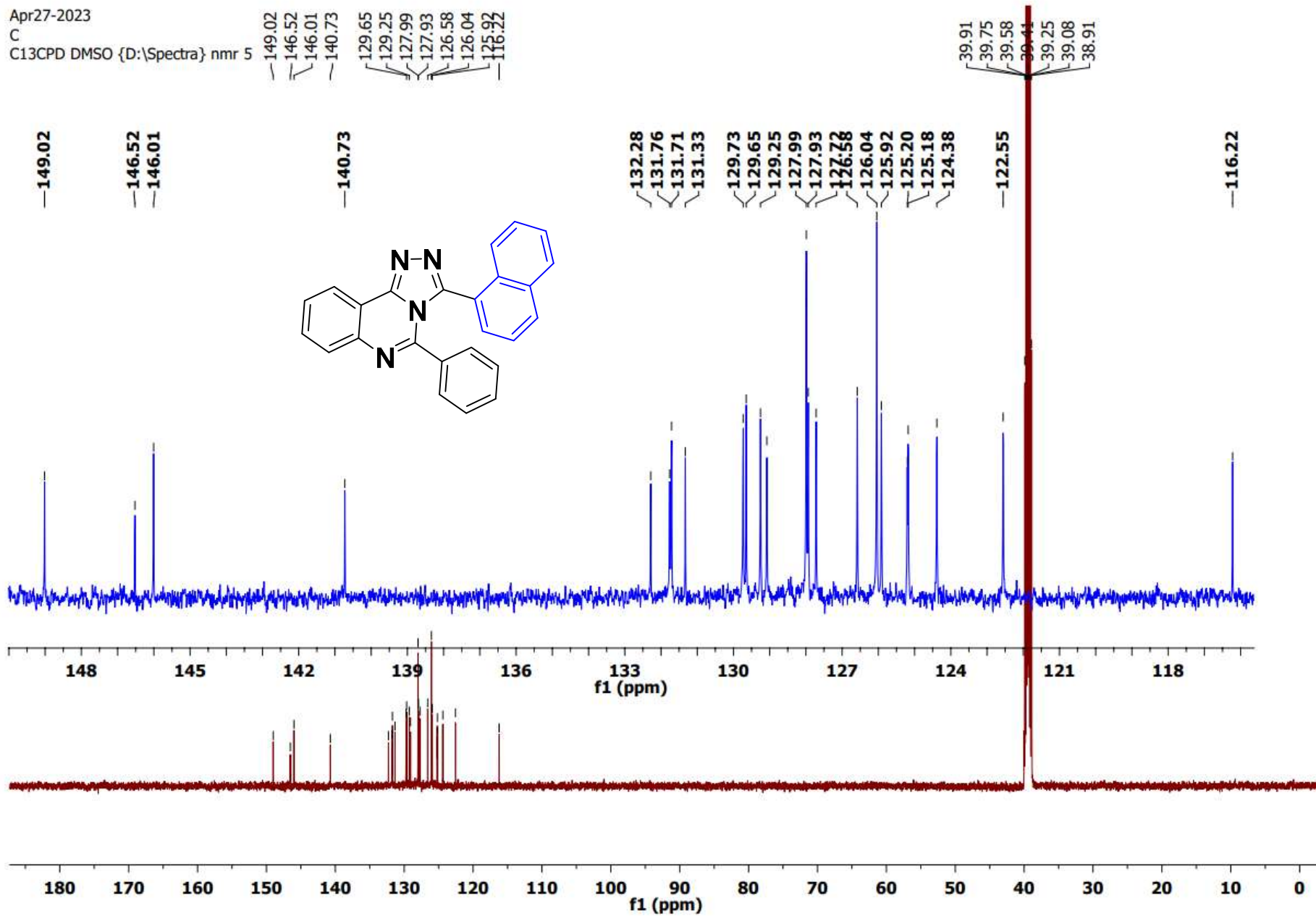
1H_8scan CDCl3 {D:\Spectra} nmr 39



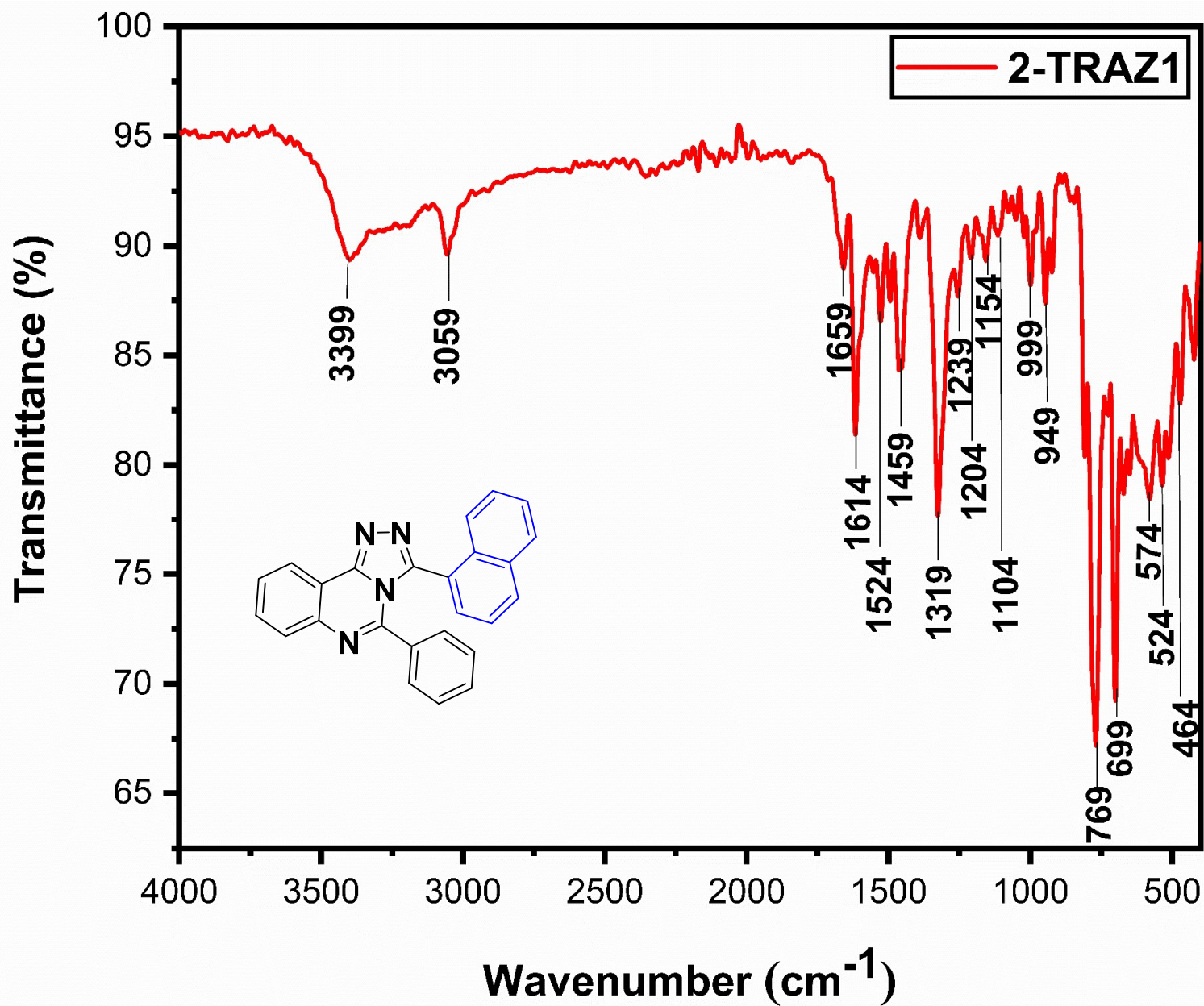
¹³C-NMR SPECTRA: 3-(Naphthalen-1-yl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5k).

Apr27-2023

C
C13CPD DMSO {D:\Spectra} nmr 5



IR SPECTRA: 3-(Naphthalen-1-yl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5k).



HRMS SPECTRA: 3-(Naphthalen-1-yl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5k).

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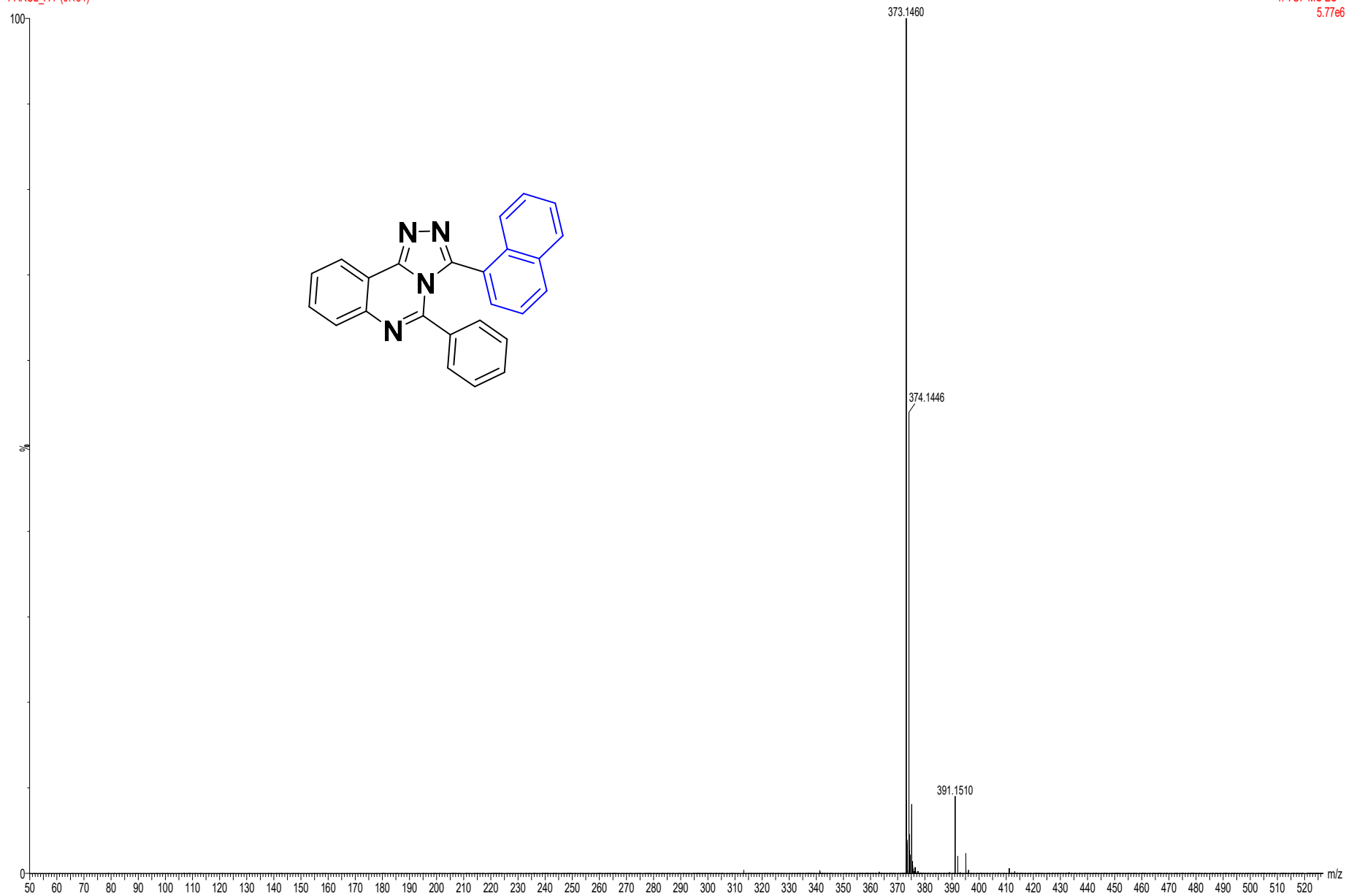
SYNAPT-XS#DBA064

27-Feb-2023

10:53:57

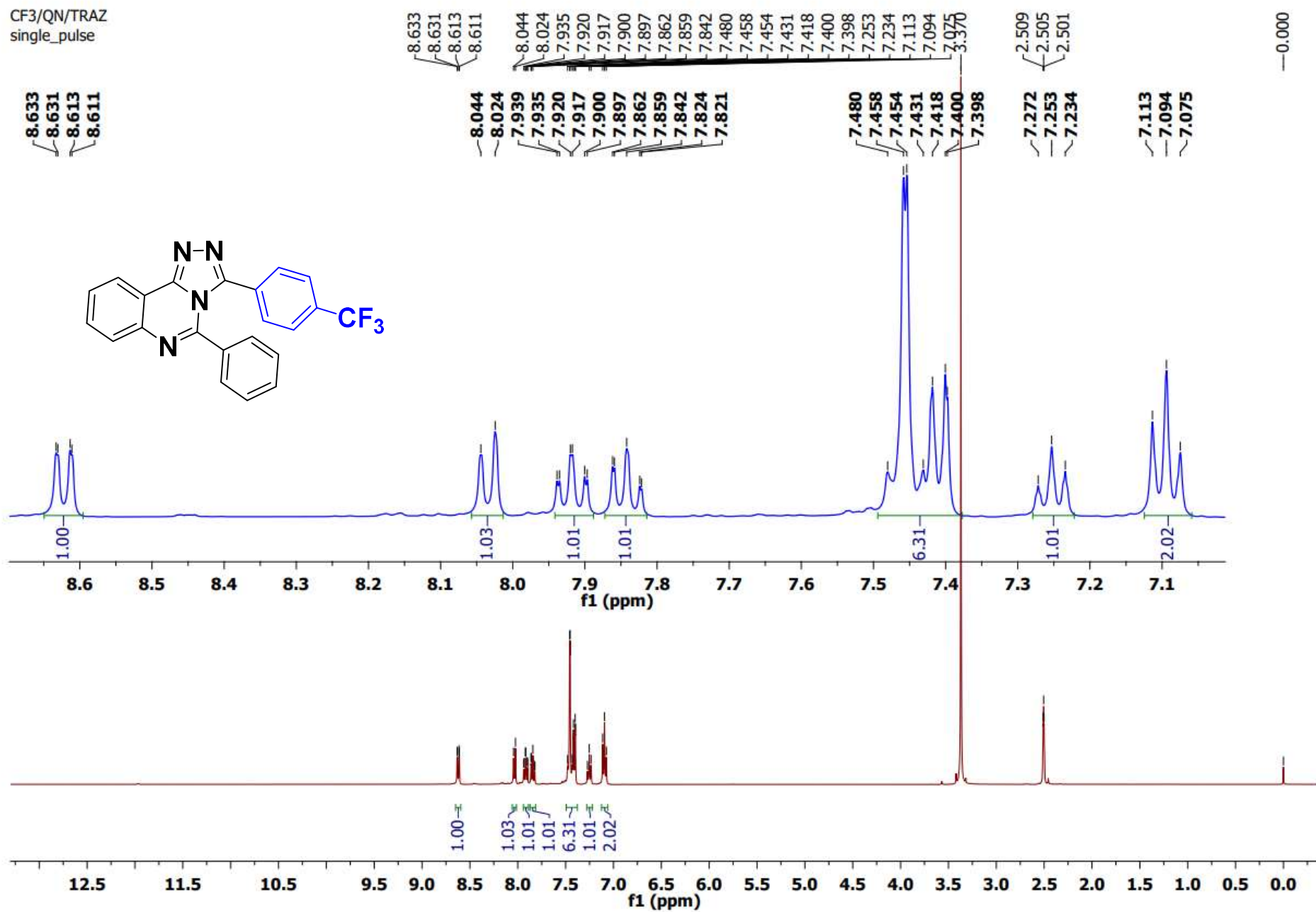
1: TOF MS ES+
5.77e6

PARUL_A 7 (0.154)



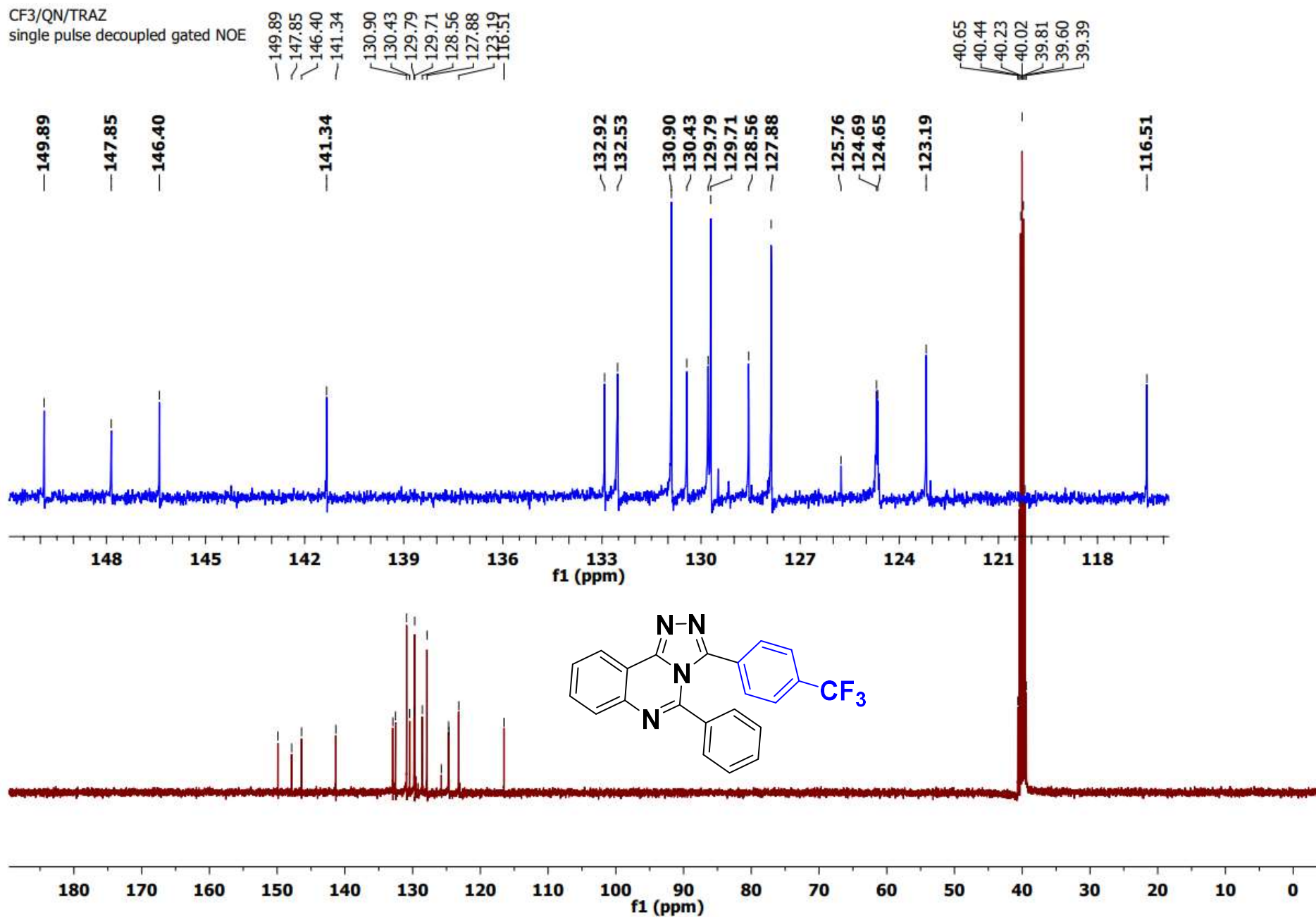
¹H-NMR SPECTRA: 5-Phenyl-3-(4-(trifluoromethyl)phenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5l).

CF3/QN/TRAZ
single_pulse

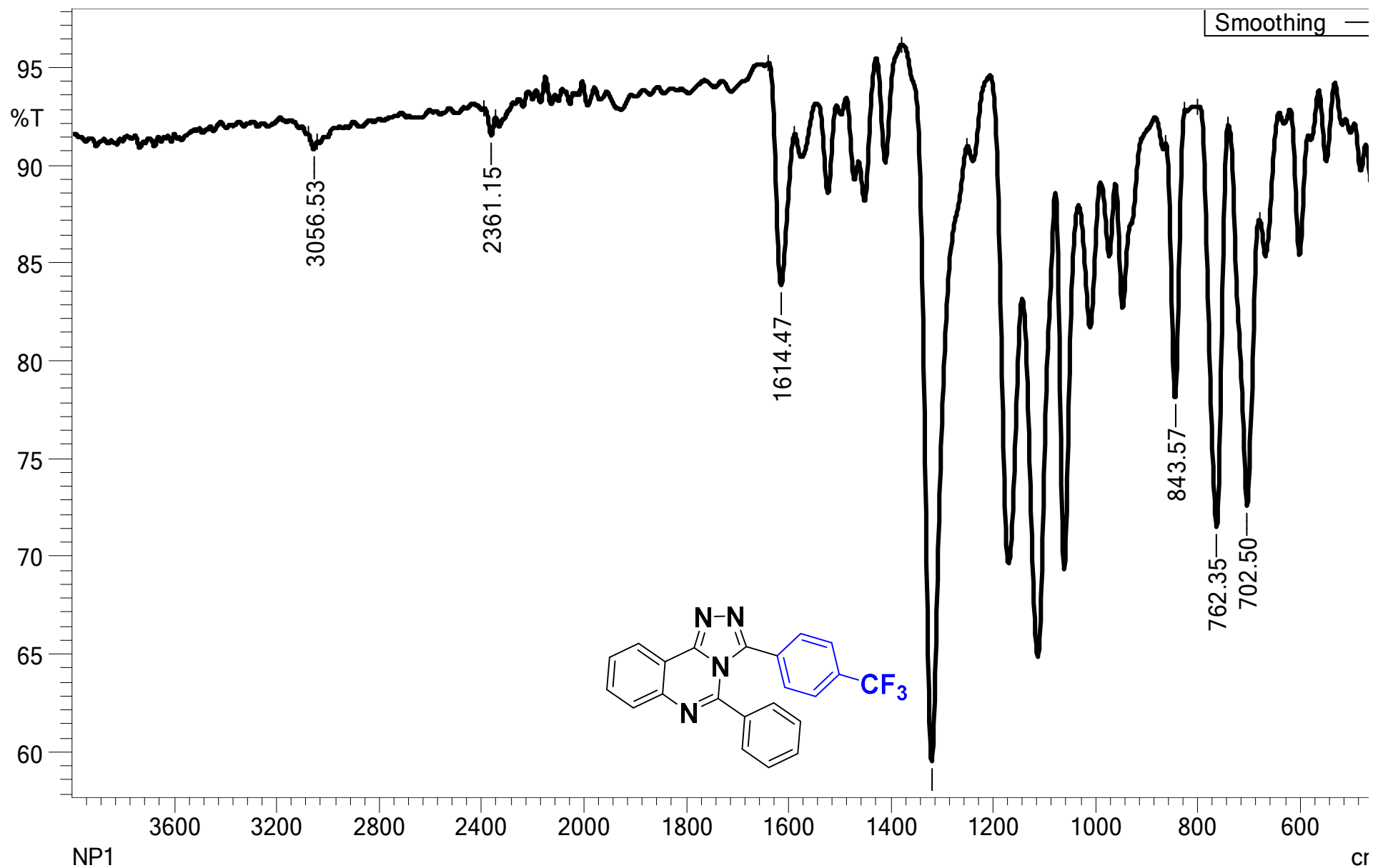


¹³C-NMR SPECTRA: 5-Phenyl-3-(4-(trifluoromethyl)phenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5I).

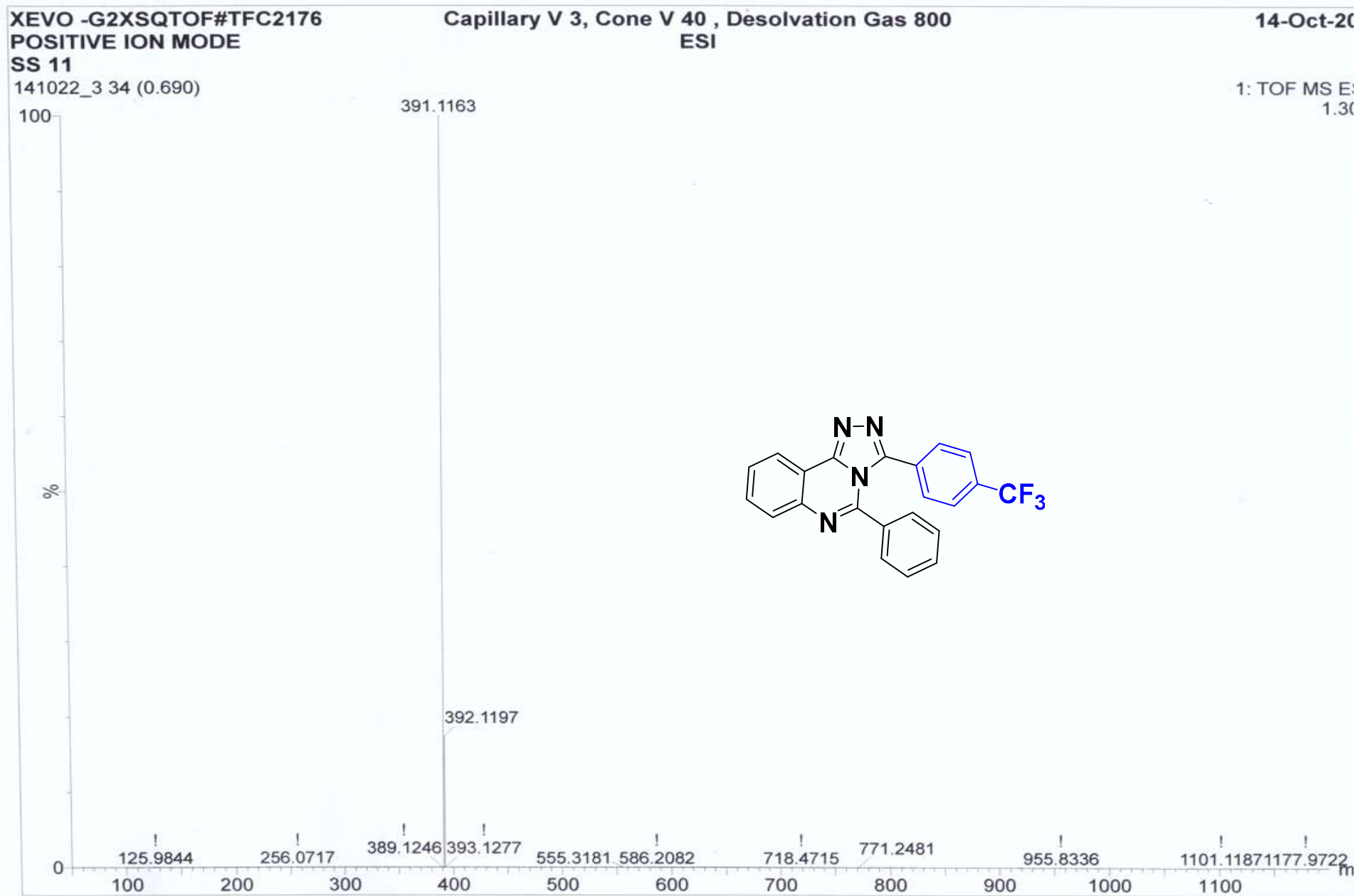
CF3/QN/TRAZ
single pulse decoupled gated NOE



IR SPECTRA: 5-Phenyl-3-(4-(trifluoromethyl)phenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5l).



¹³C-NMR SPECTRA: 5-Phenyl-3-(4-(trifluoromethyl)phenyl)-[1,2,4]triazolo[4,3-c]quinazoline (5l).

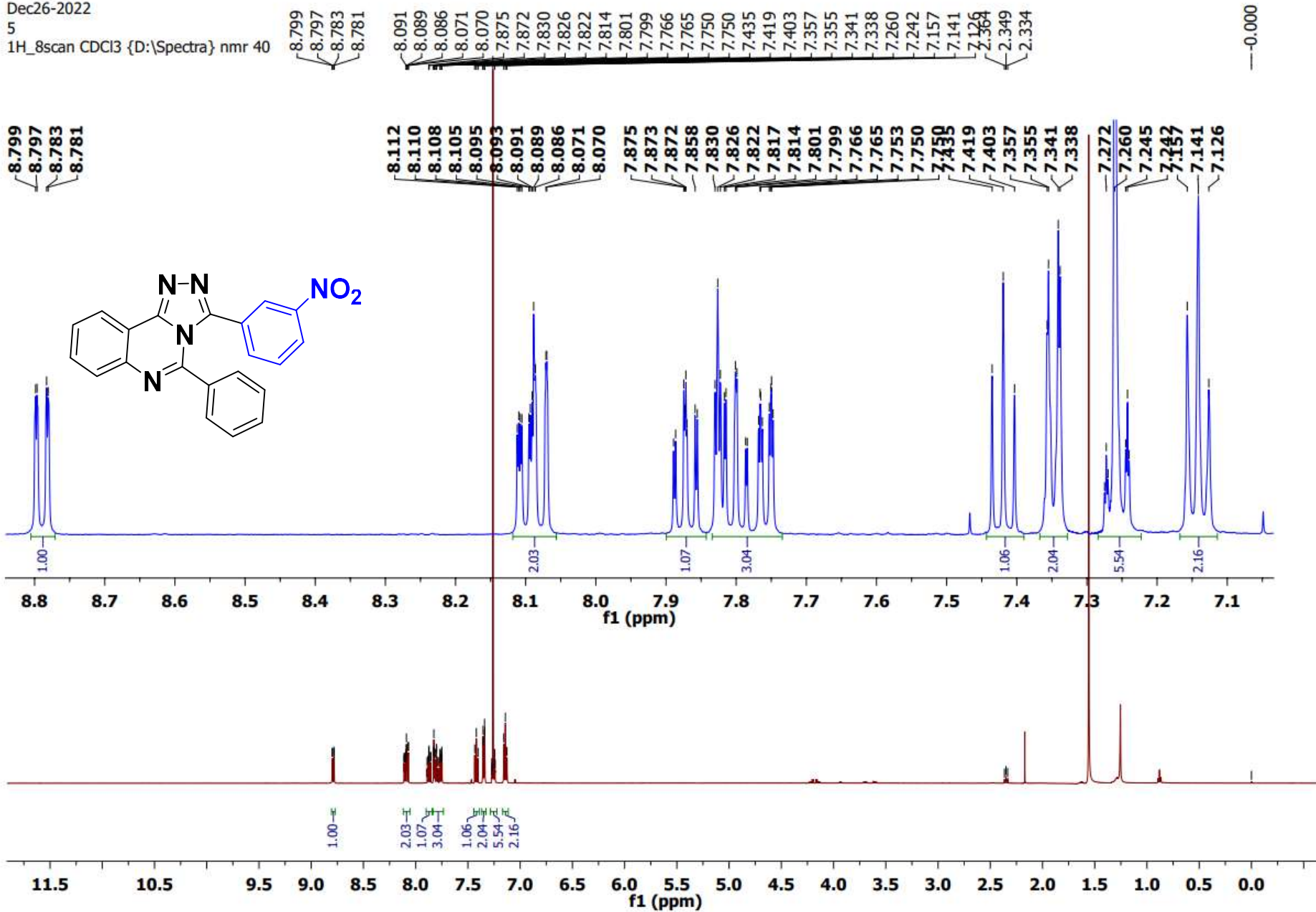


¹H-NMR SPECTRA: 3-(3-Nitrophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5m).

Dec26-2022

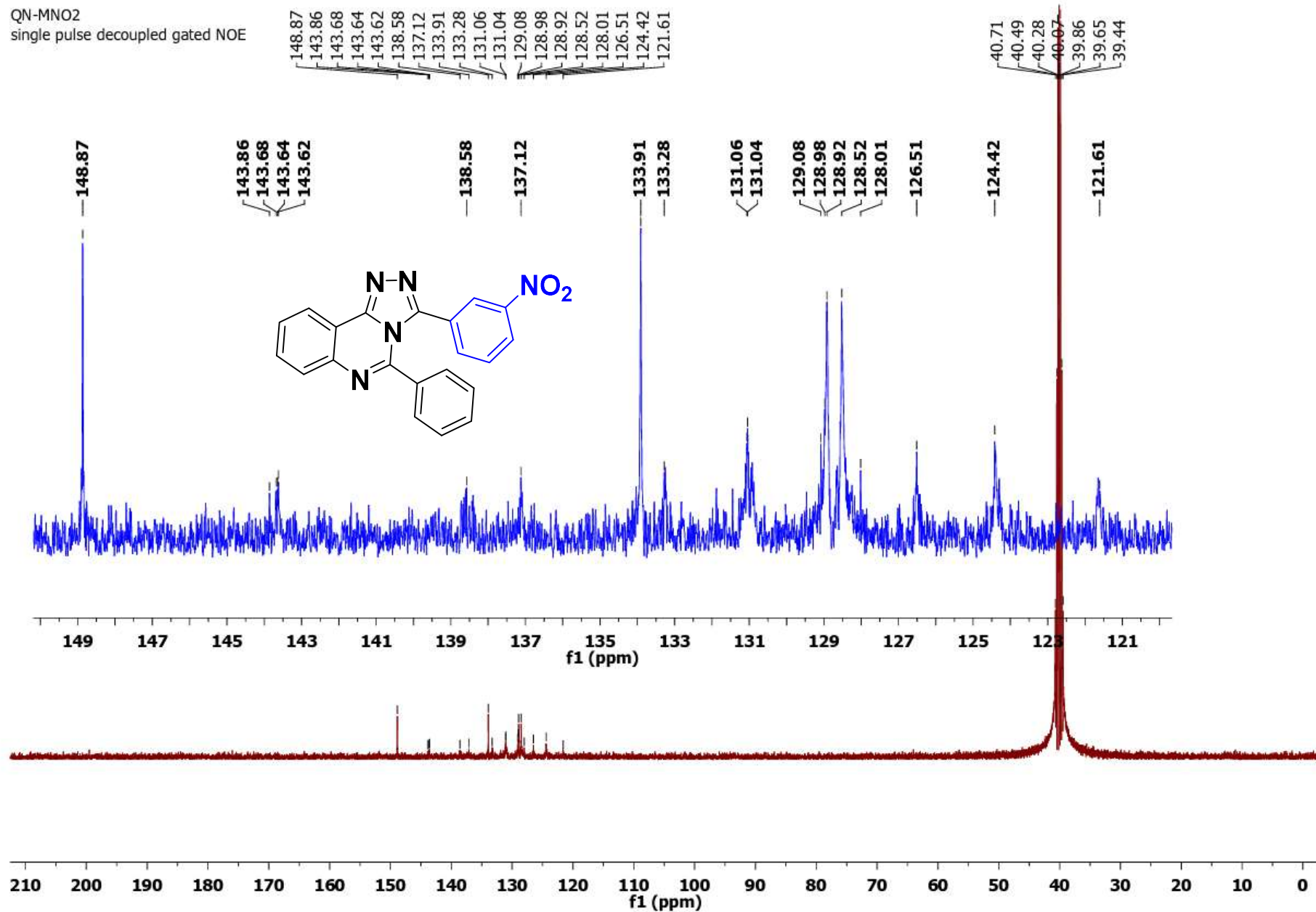
5

1H_8scan CDCl3 {D:\Spectra} nmr 40

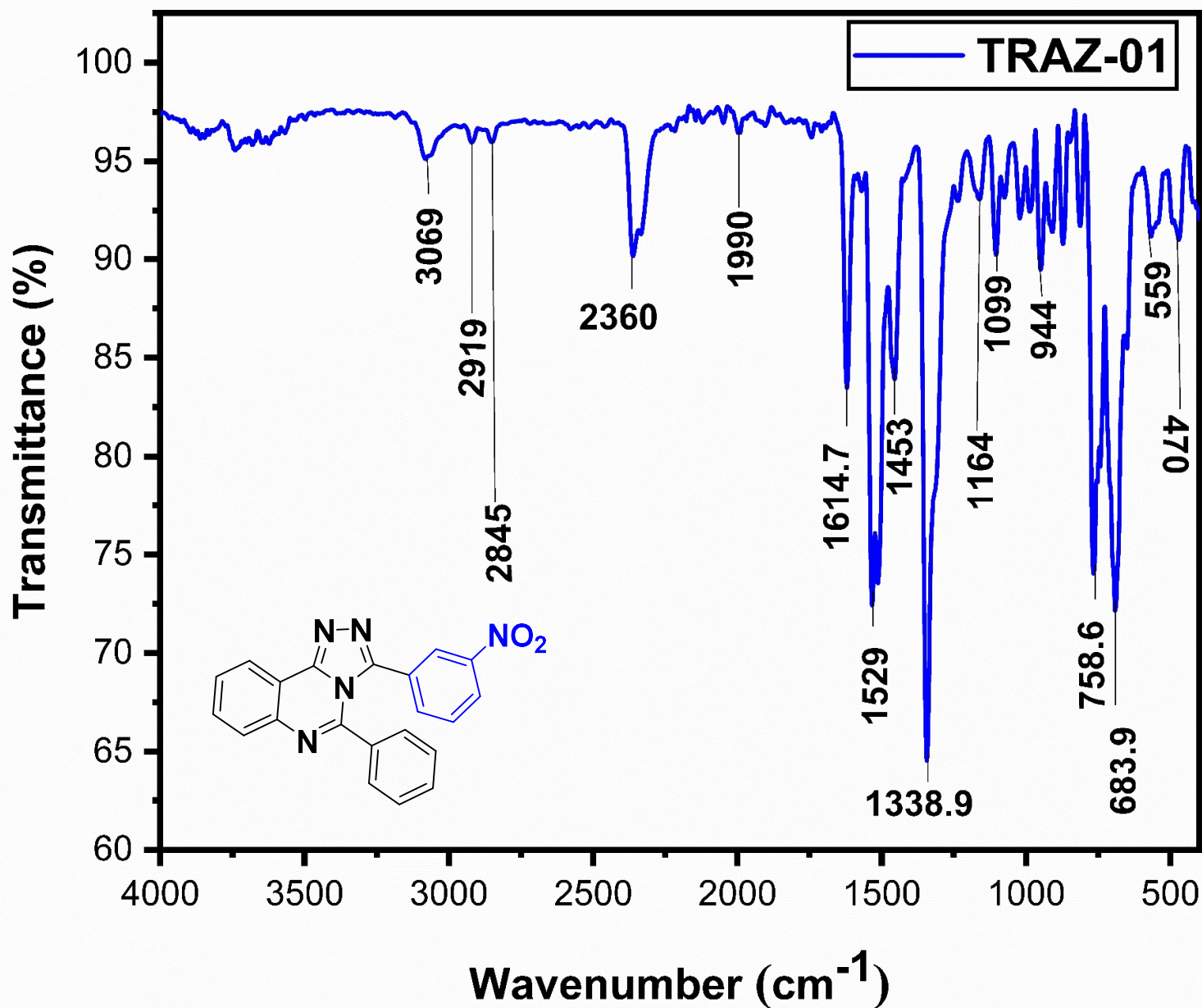


¹³C-NMR SPECTRA: 3-(3-Nitrophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5m).

QN-MNO2
single pulse decoupled gated NOE



IR SPECTRA: 3-(3-Nitrophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5m).



HRMS SPECTRA: 3-(3-Nitrophenyl)-5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5m).

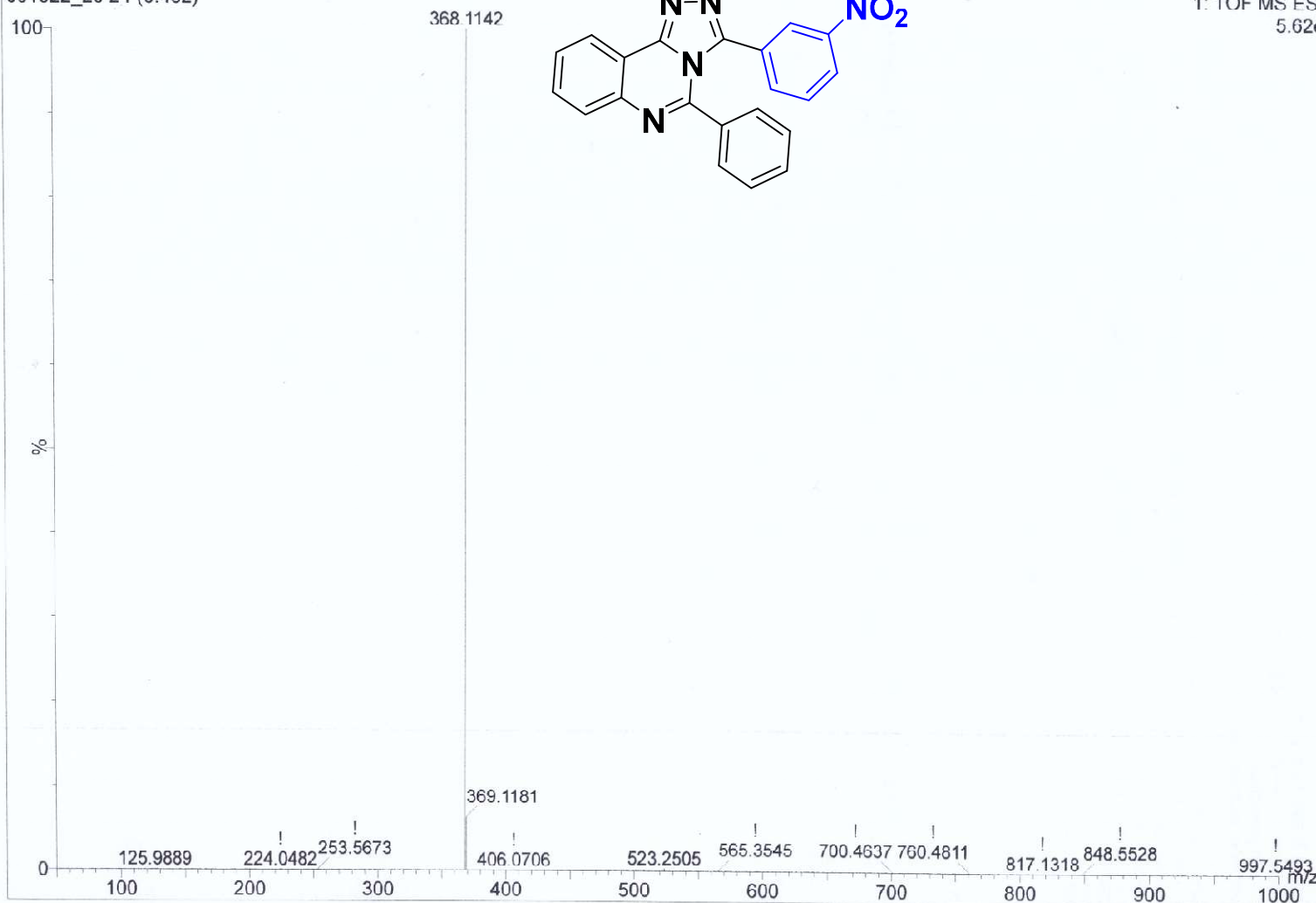
XEVO -G2XSQTOF#TFC2176
POSITIVE ION MODE
SS 5

061022_20 24 (0.482)

Capillary V 3, Cone V 40, Desolvation Gas 800
ESI

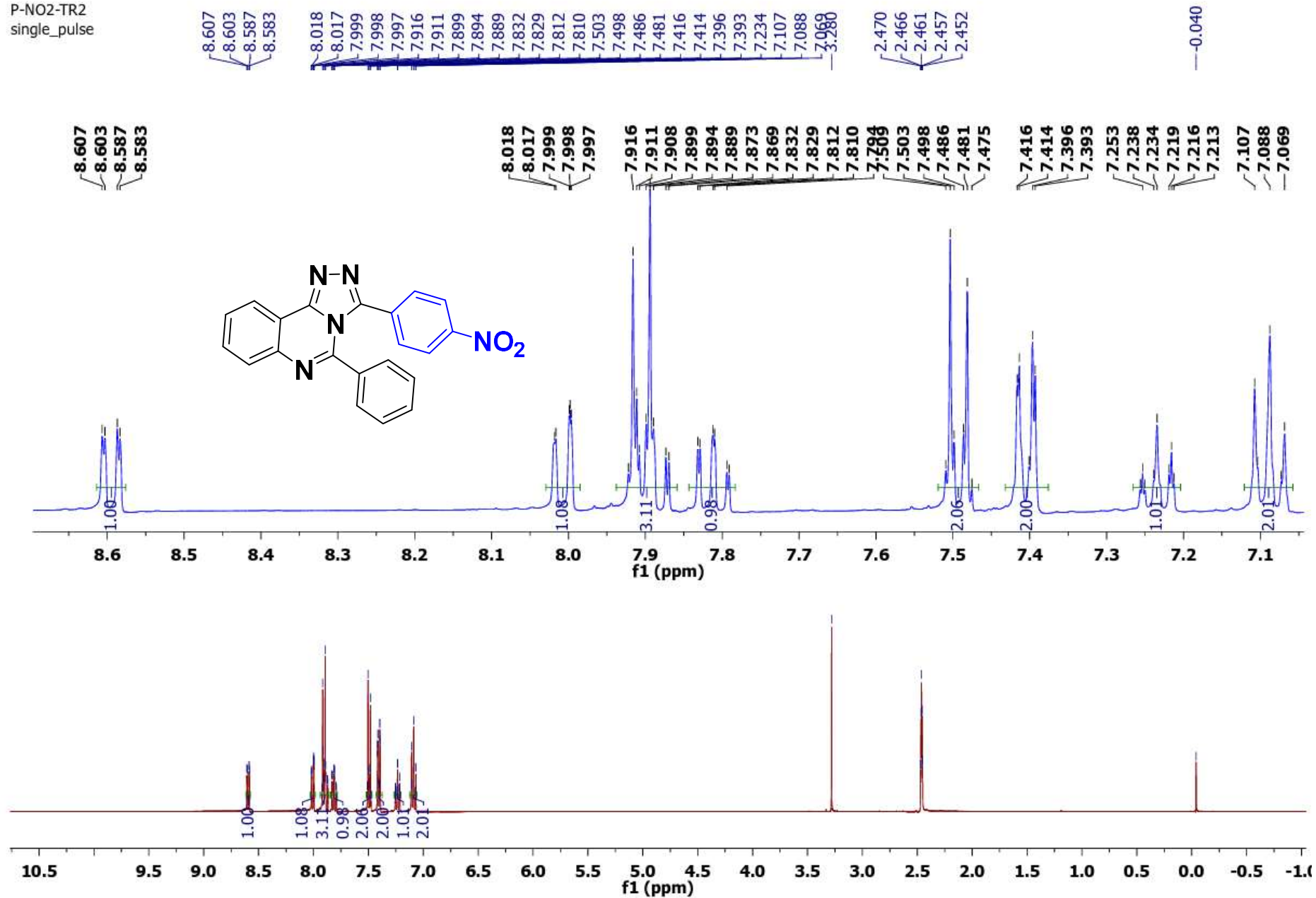
06-Oct-2022

1: TOF MS ES+
5.02e5



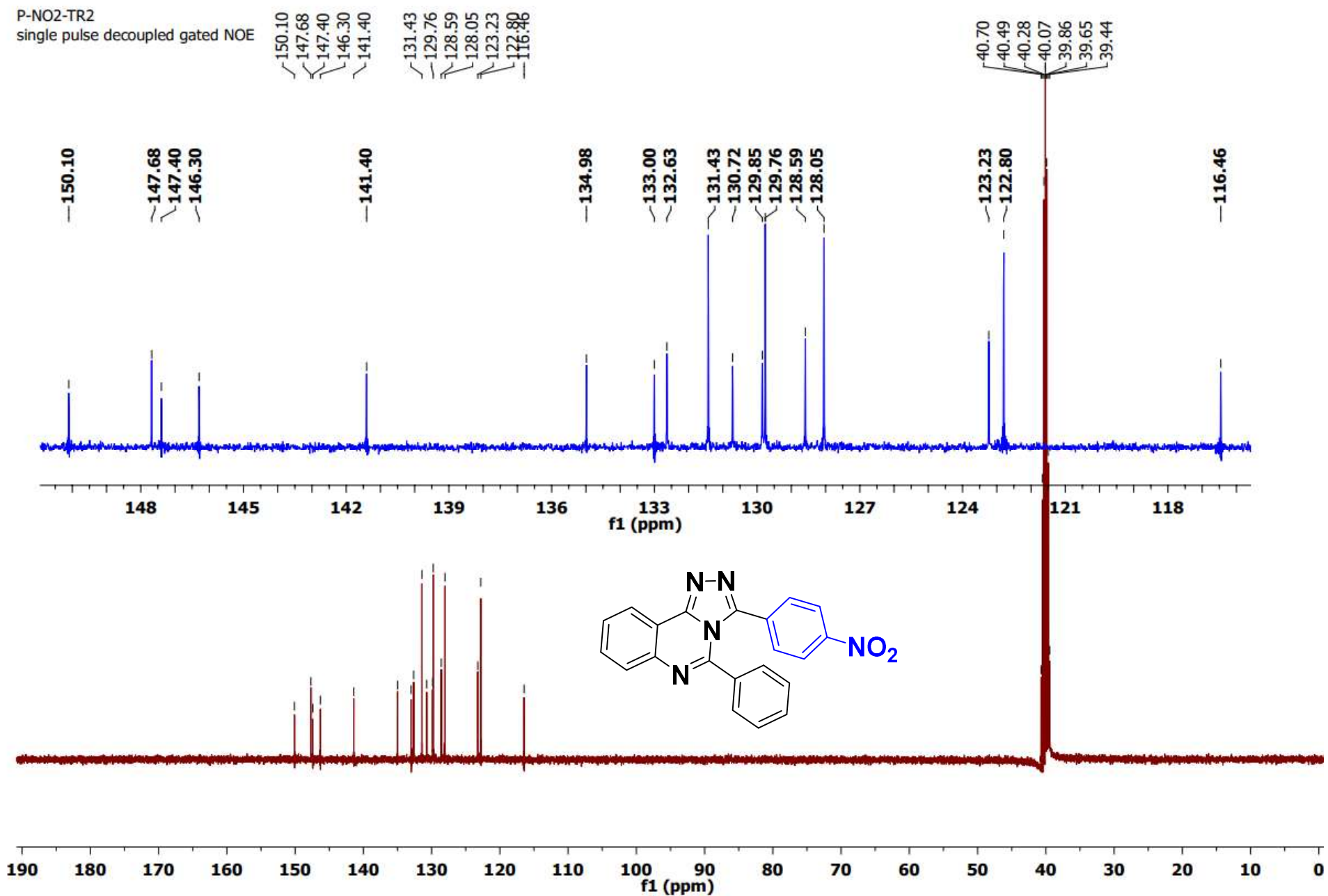
¹H-NMR SPECTRA: 3-(4-Nitrophenyl)- 5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5n).

P-NO2-TR2
single_pulse

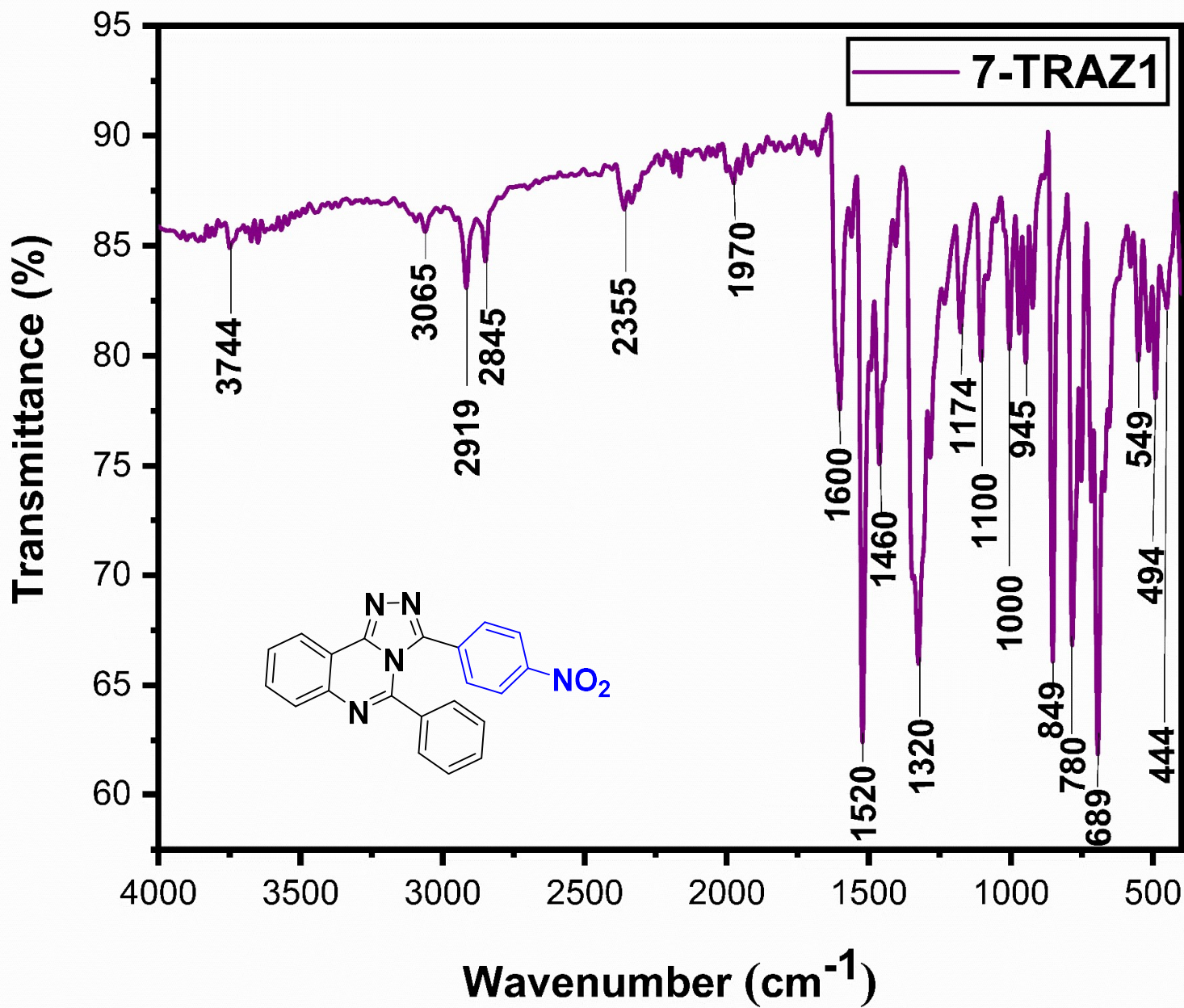


¹³C-NMR SPECTRA: 3-(4-Nitrophenyl)- 5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5n).

P-NO2-TR2
single pulse decoupled gated NOE



IR SPECTRA: 3-(4-Nitrophenyl)- 5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5n).



HRMS SPECTRA: 3-(4-Nitrophenyl)- 5-phenyl-[1,2,4]triazolo[4,3-c]quinazoline (5n).

XEVO -G2XSQTOF#TFC2176
POSITIVE ION MODE
SS 13

Capillary V 3, Cone V 40, Desolvation Gas 800
ESI

14-Oct-2022

141022_5 31 (0.620)

1: TOF MS ES+
7.82e5

