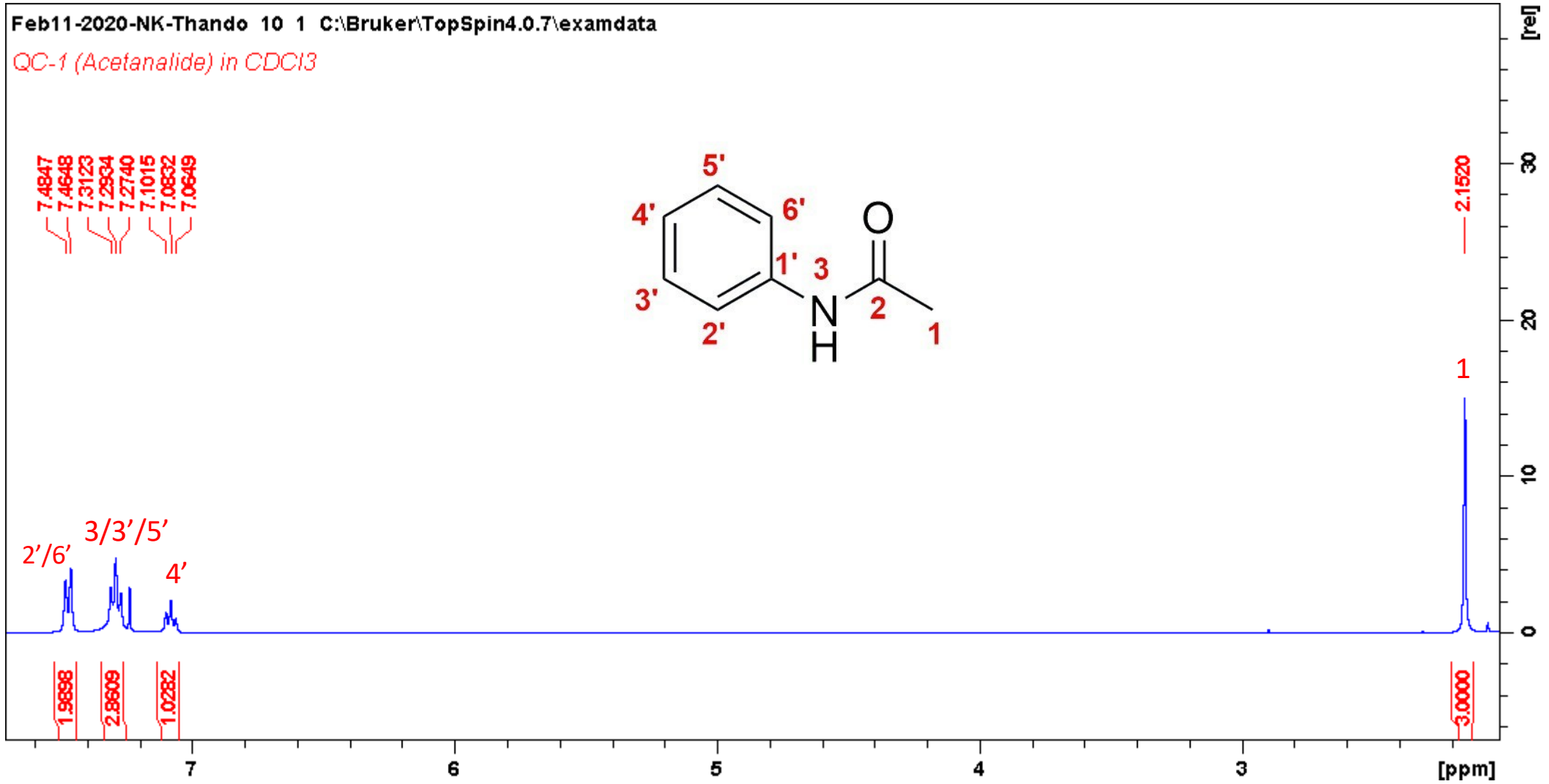
# Supplementary Material

# Synthesis, characterization and biological evaluation of 1-(1*H*-1,2,3- triazol-4-yl)methyl)-1-pyrazolo[3,4-*b*]quinoline derivatives

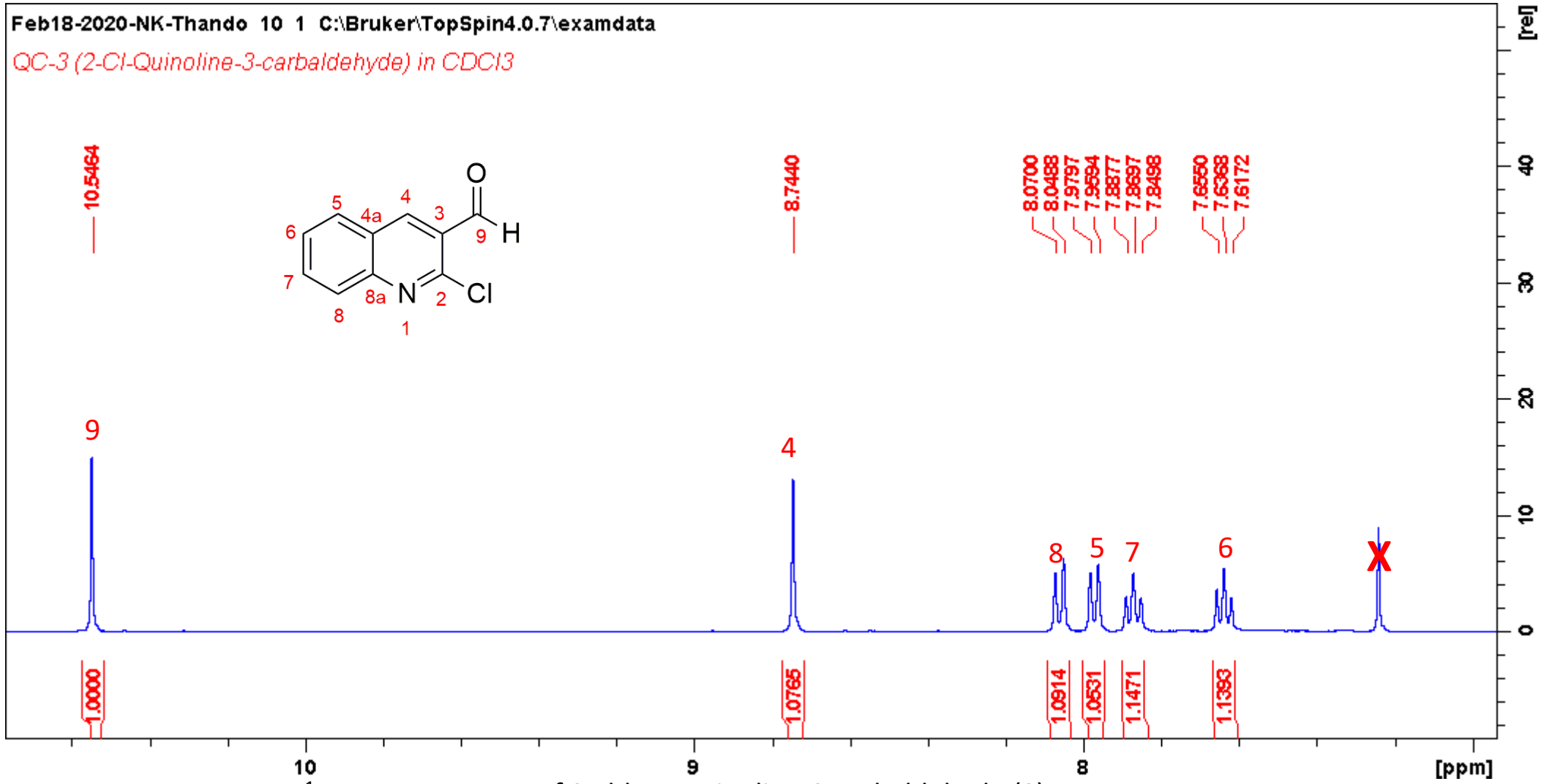
**Thandokazi A. Ntshele,[a] Sibusiso Senzani,[b] Nirasha Nundkumar, Kolawole Olofinsan,[c] Shahidul Islam,[c] Moganavelli Singh,[c] Sithabile Mokoena,[d] Rajshekhar Karpoormath,[d] and Neil A. Koorbanally*[a]**

*[a]School of Chemistry and Physics, [b]School of Laboratory Medicine and Medical Sciences, [c]School of Life Sciences, [d]School of Health Sciences, University of KwaZulu-Natal, Private Bag X54001, Durban, 4000, South Africa*
*Email: Koorbanally@ukzn.ac.za*

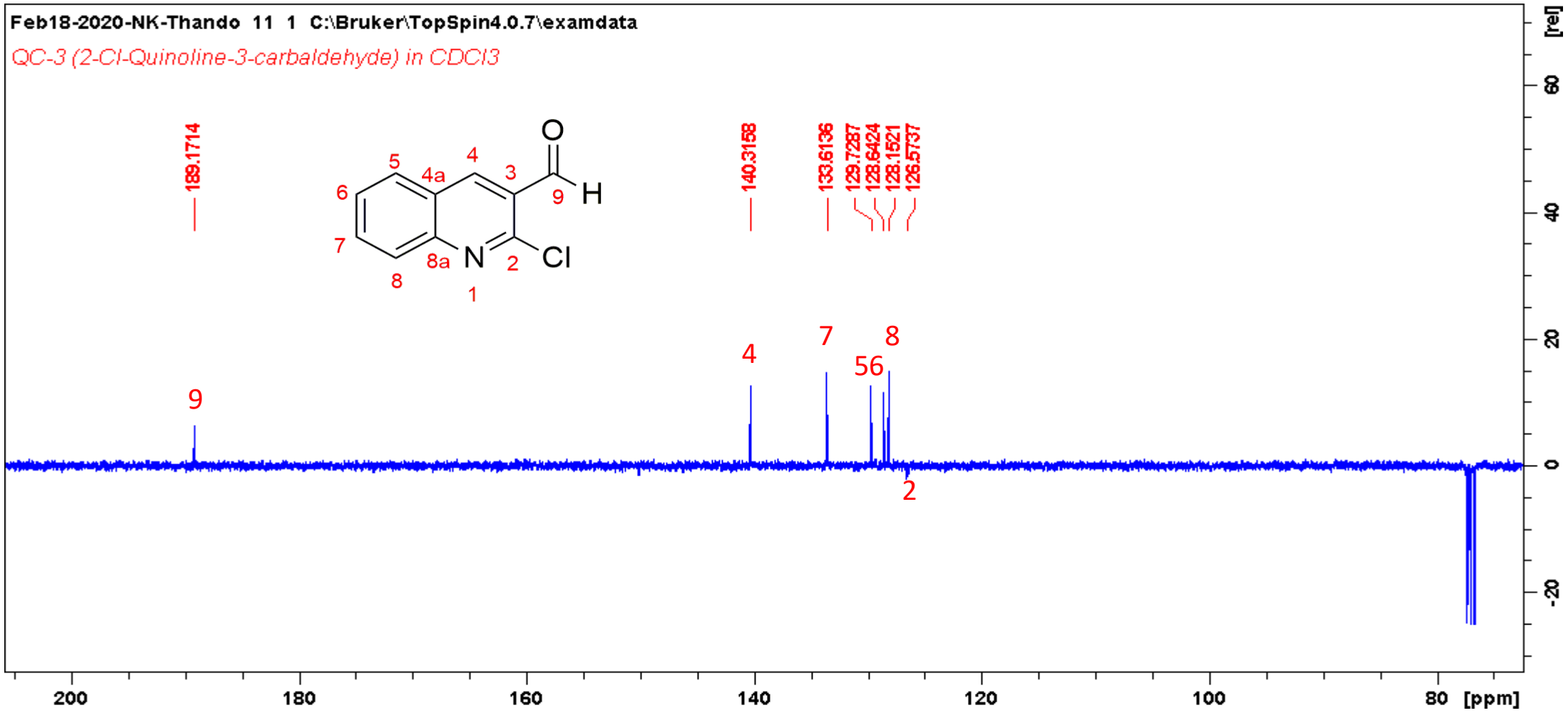
## Table of Contents



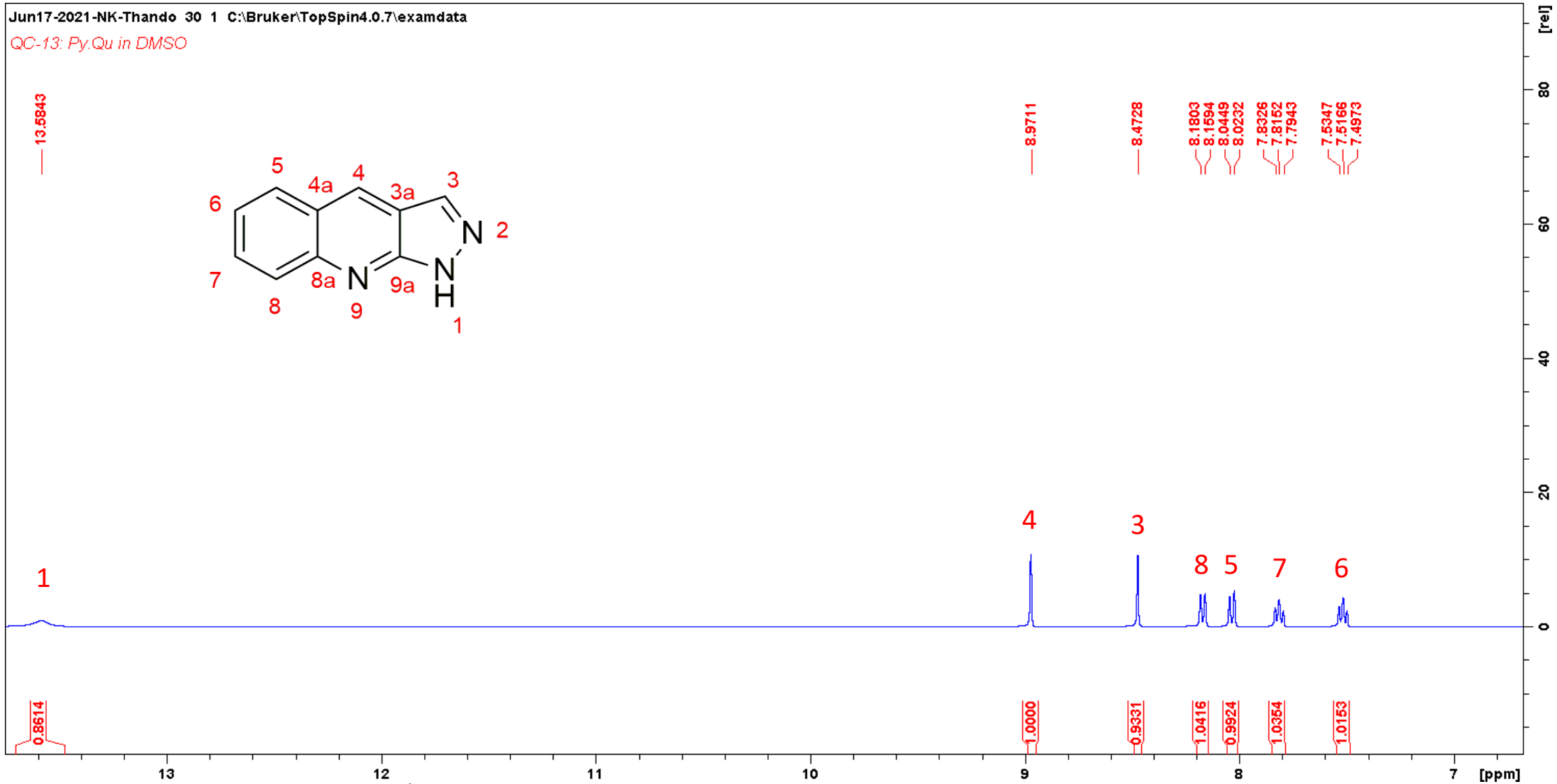

$^{1}$H NMR spectrum of acetanilide (**1**)



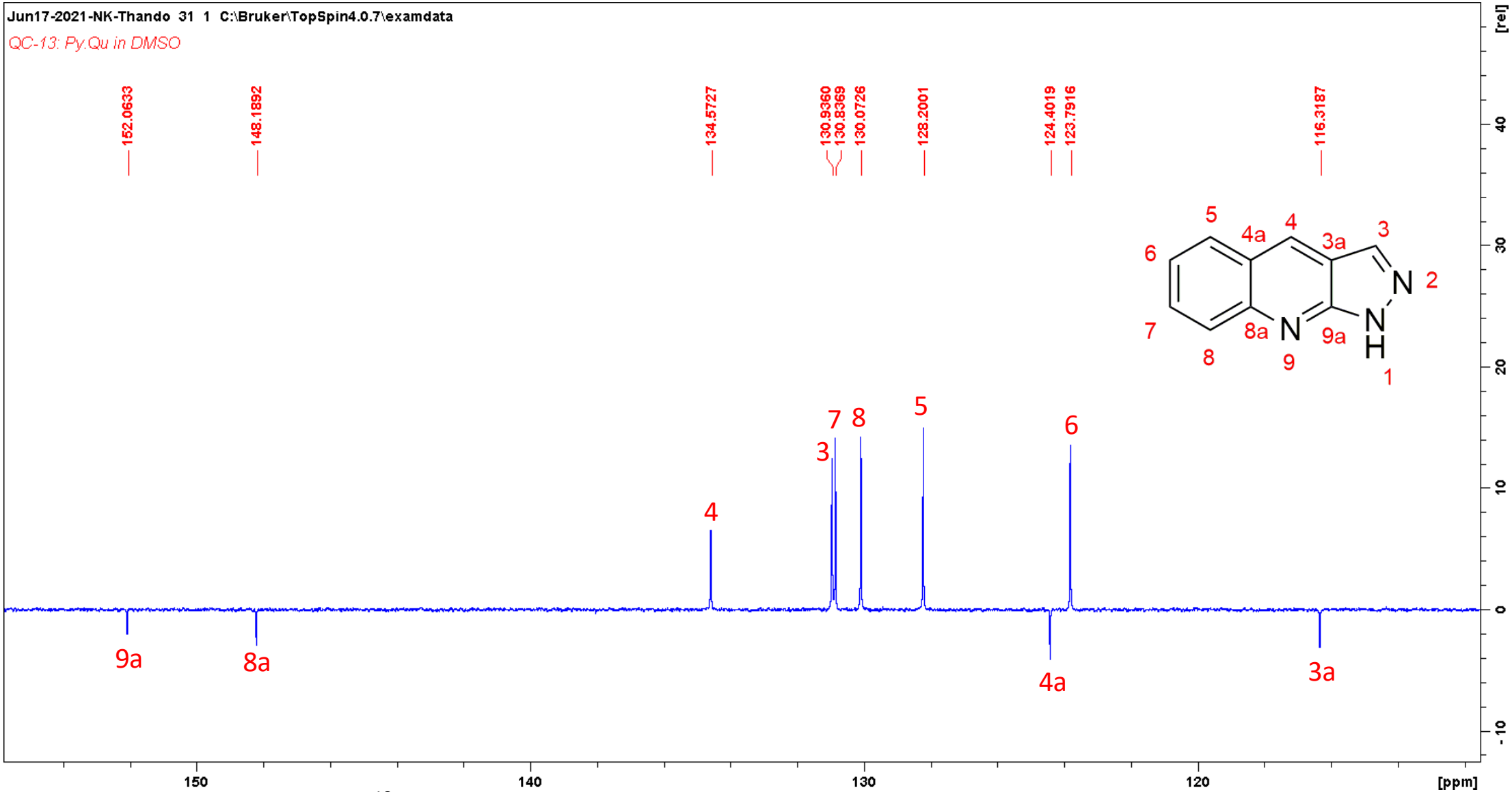

$^{1}$H NMR spectrum of 2-chloro-quinoline-3-carbaldehyde (**2**)



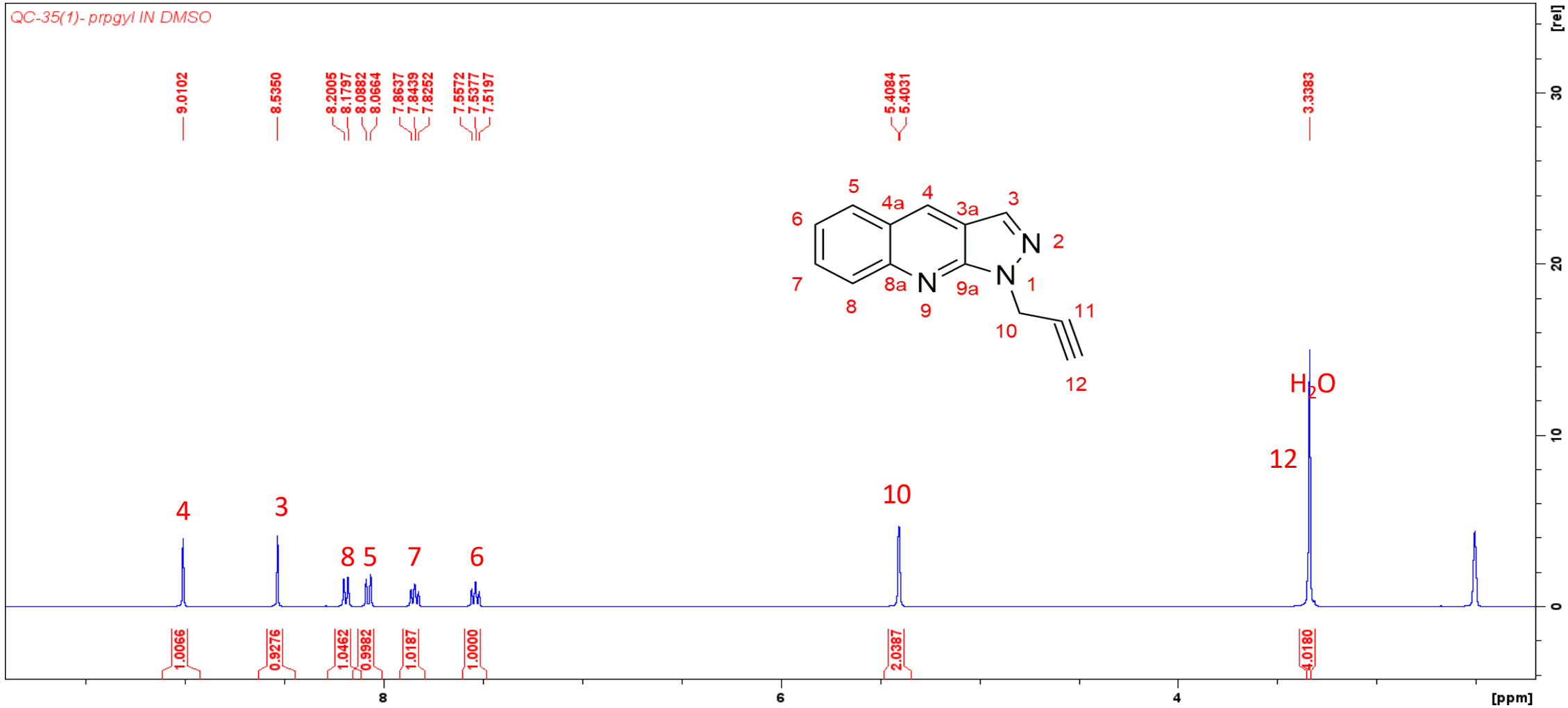

$^{13}$C NMR spectrum of 2-chloro-quinoline-3-carbaldehyde (**2**)



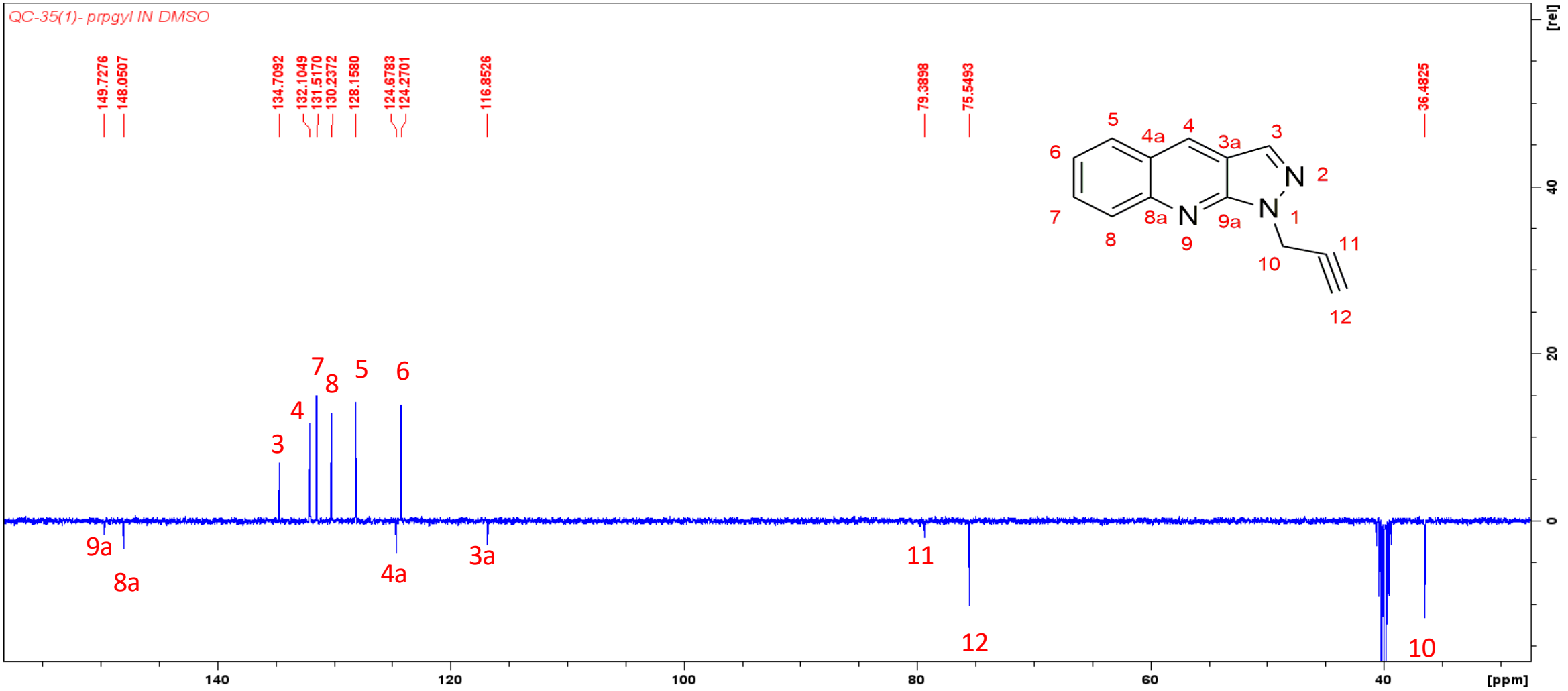

$^{1}$H NMR spectrum of 1*H*-pyrazolo[3,4-b]quinoline (**3**)



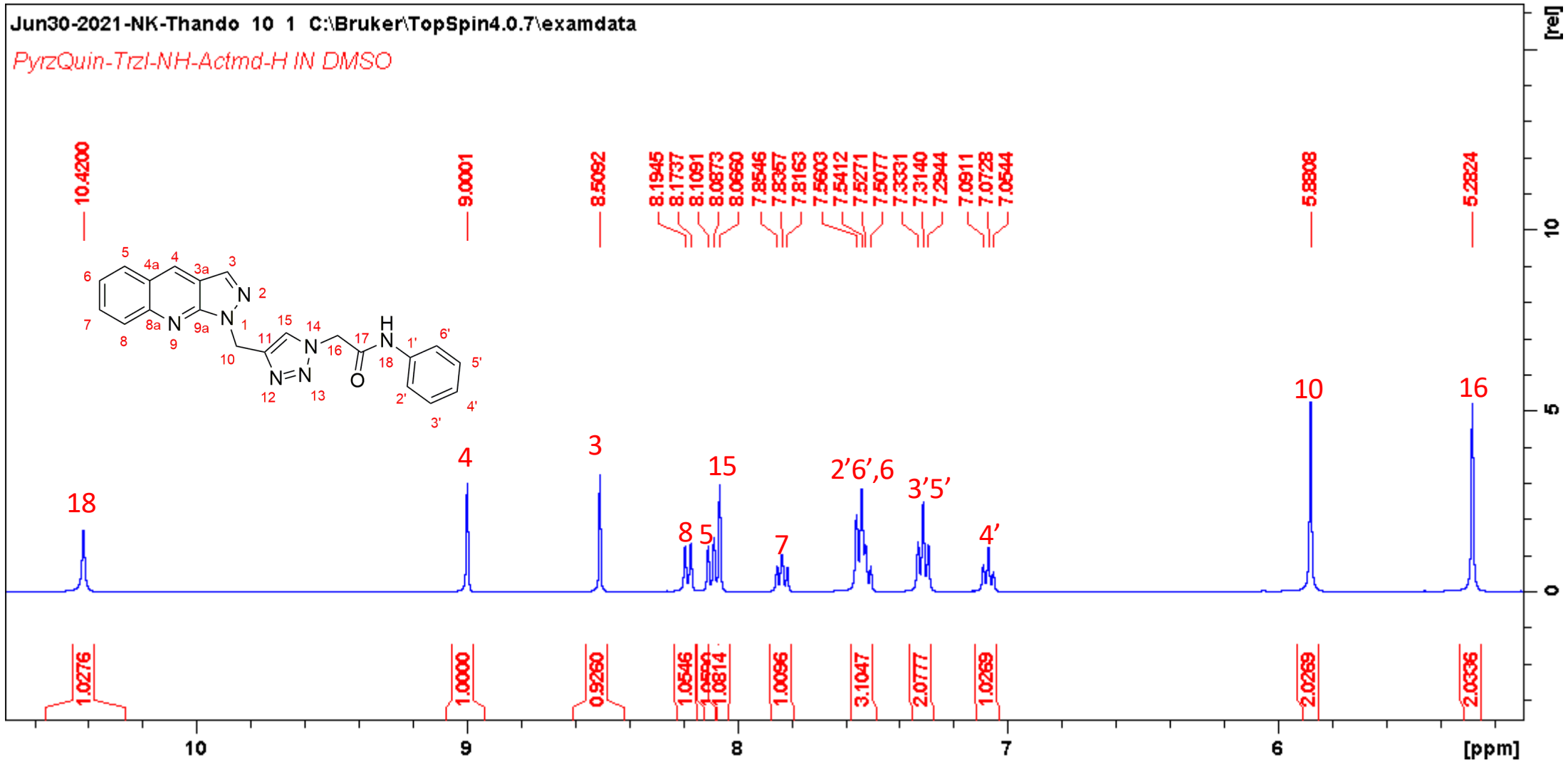

$^{13}$C NMR spectrum of 1*H*-pyrazolo[3,4-b]quinoline (**3**)



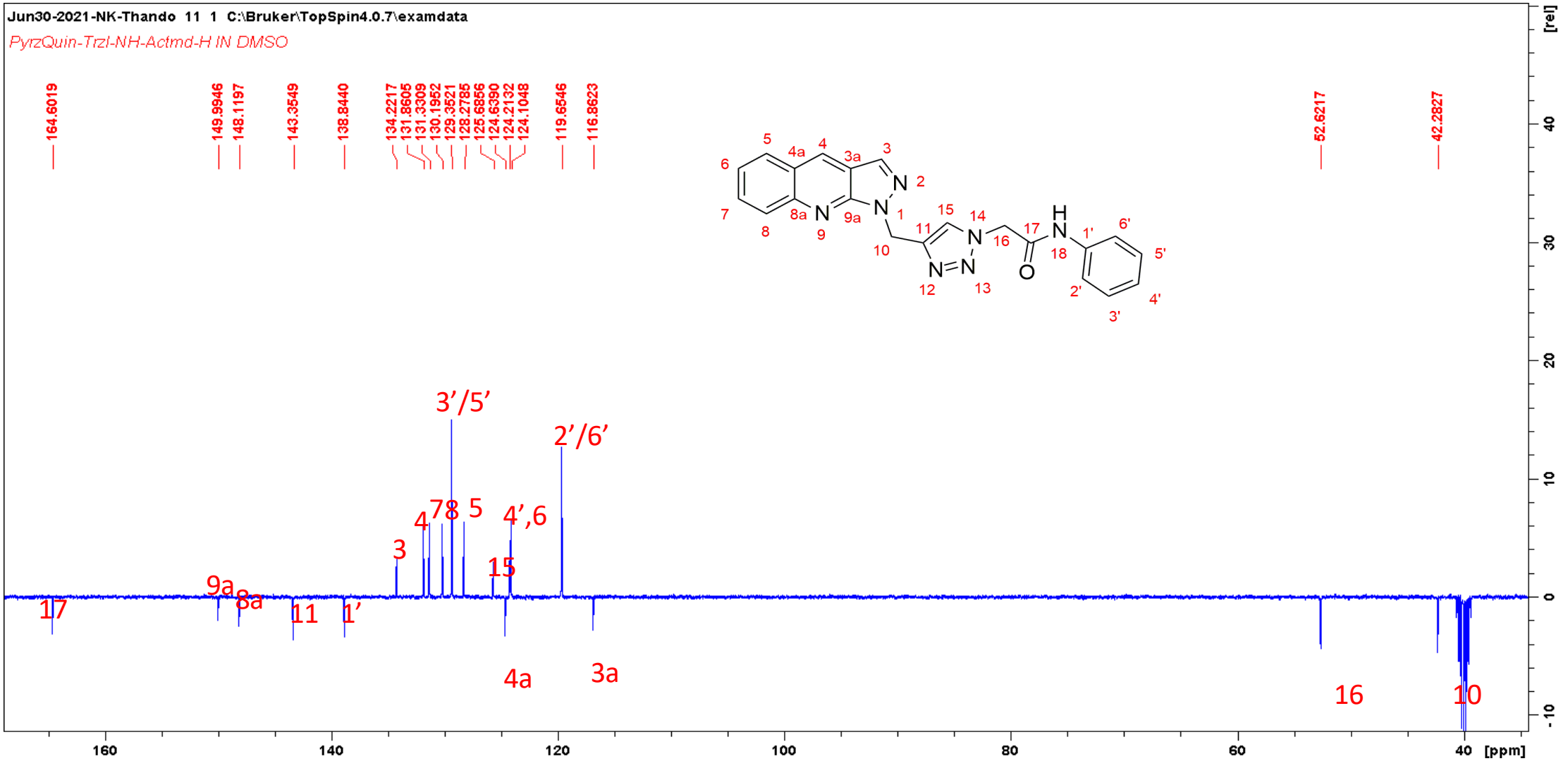

$^{1}$H NMR spectrum of 1-(prop-2-yn-1-yl)-1*H*-pyrazolo[3,4-b]quinoline (**4**)




$^{13}$C NMR spectrum of 1-(prop-2-yn-1-yl)-1*H*-pyrazolo[3,4-b]quinoline (**4**)




$^{1}$H NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-phenylacetamide (**9a**)



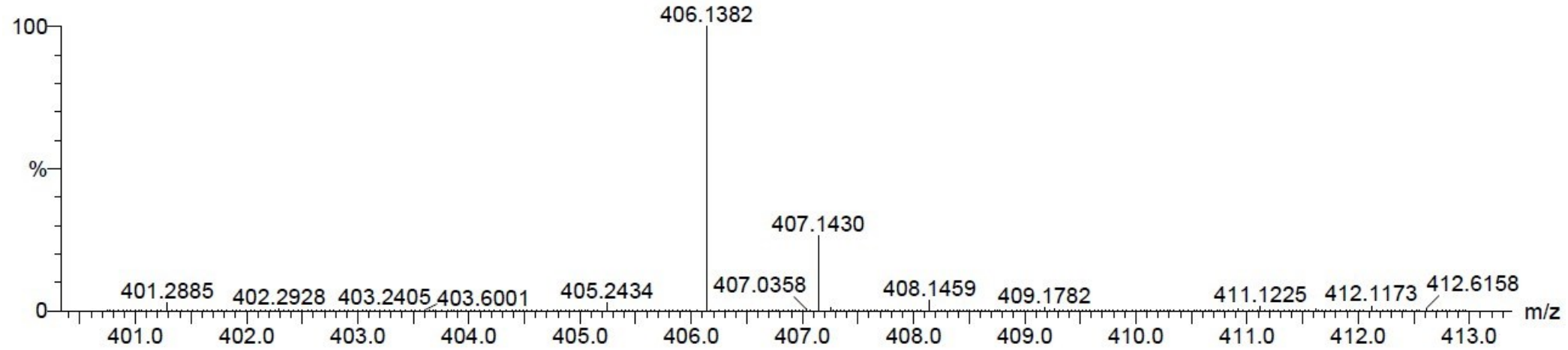

$^{13}$C NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-phenylacetamide (**9a**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-1 Na: 1-1

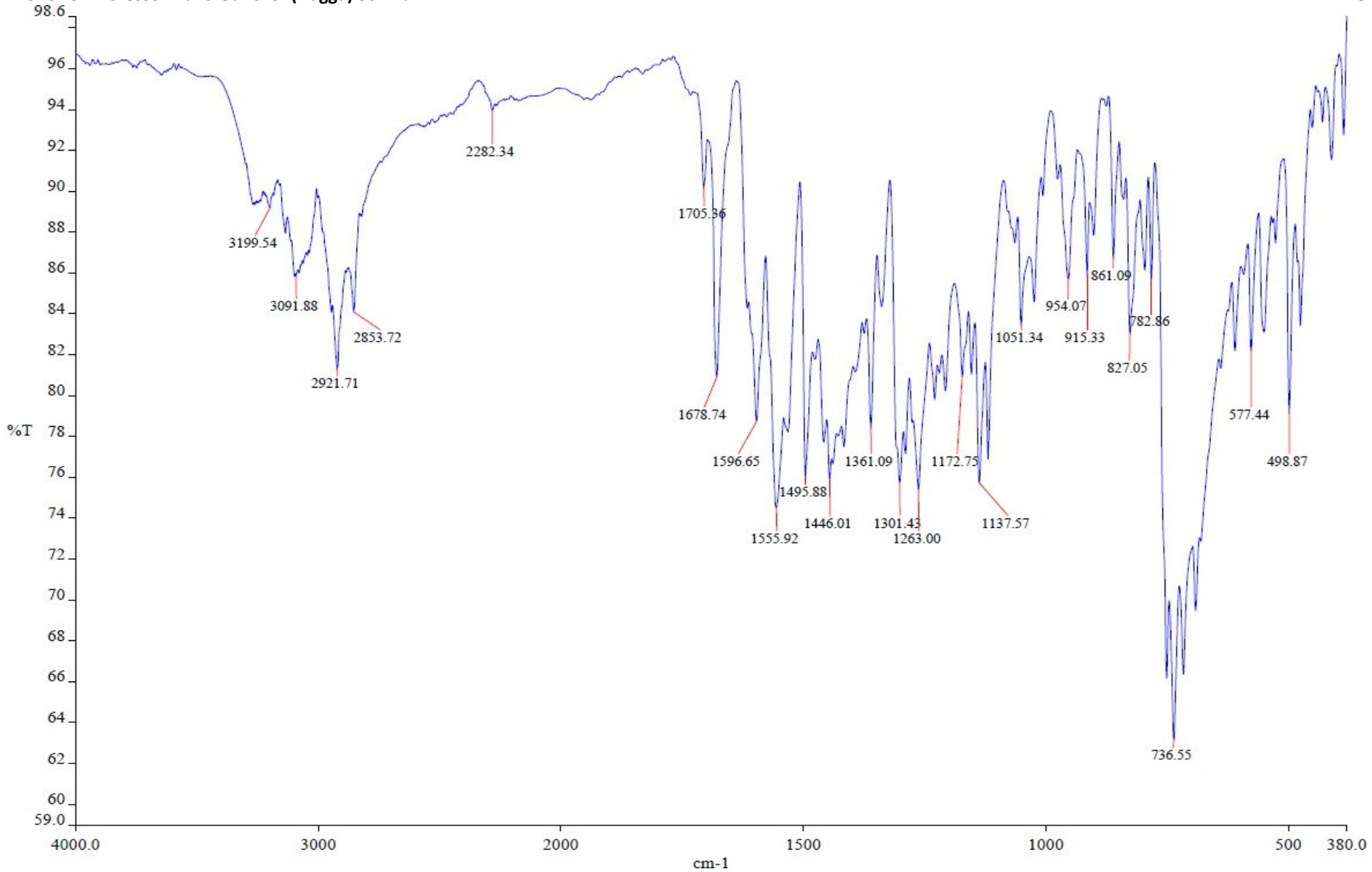
PyQuTriAc-H 4 (0.102) Cm (1:61)

TOF MS ES+
1.36e+005

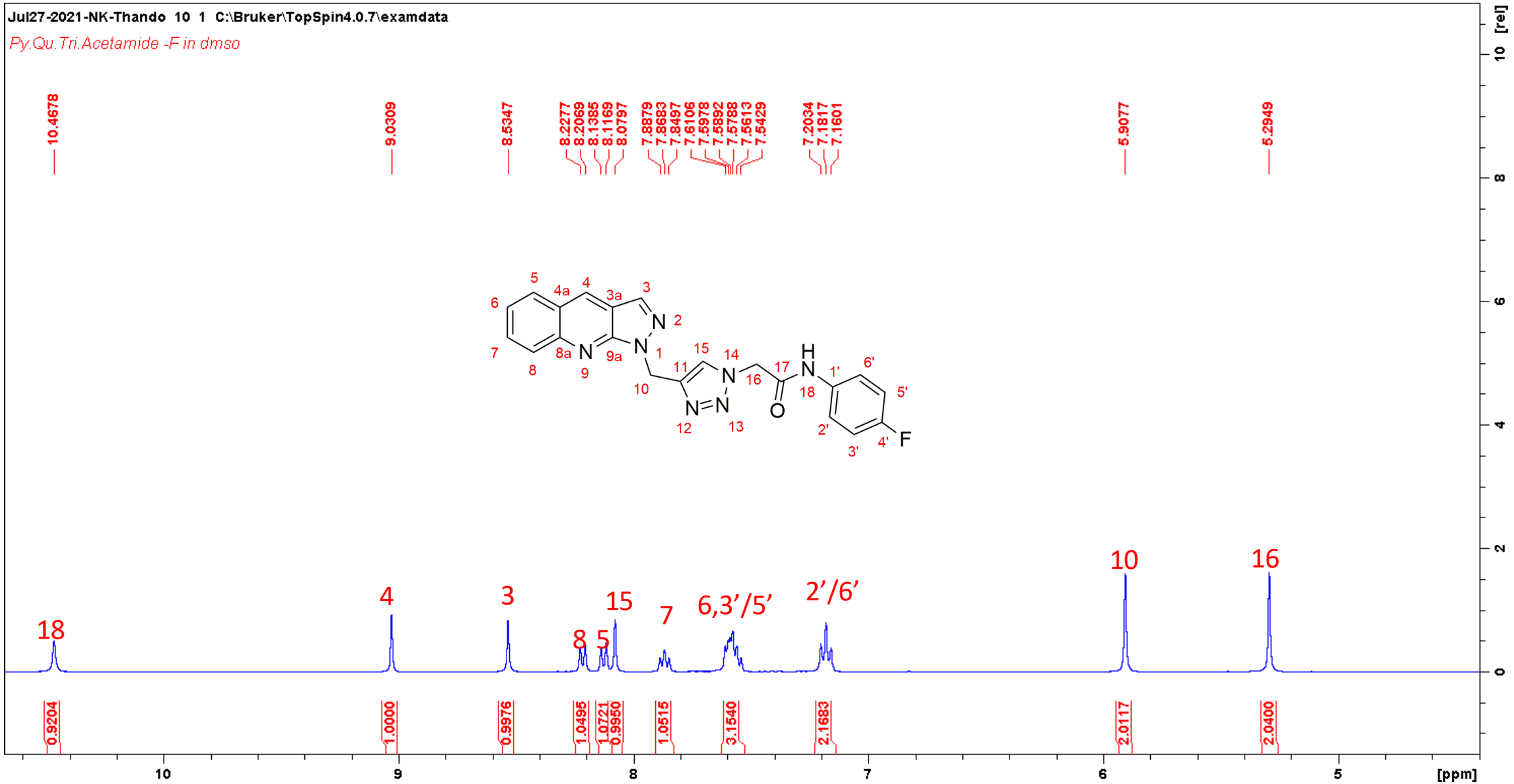



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 406.1382 | 406.1392 | -1.0 | -2.5 | 16.5 | 441.3 | 0.0 | C21 H17 N7 O Na |

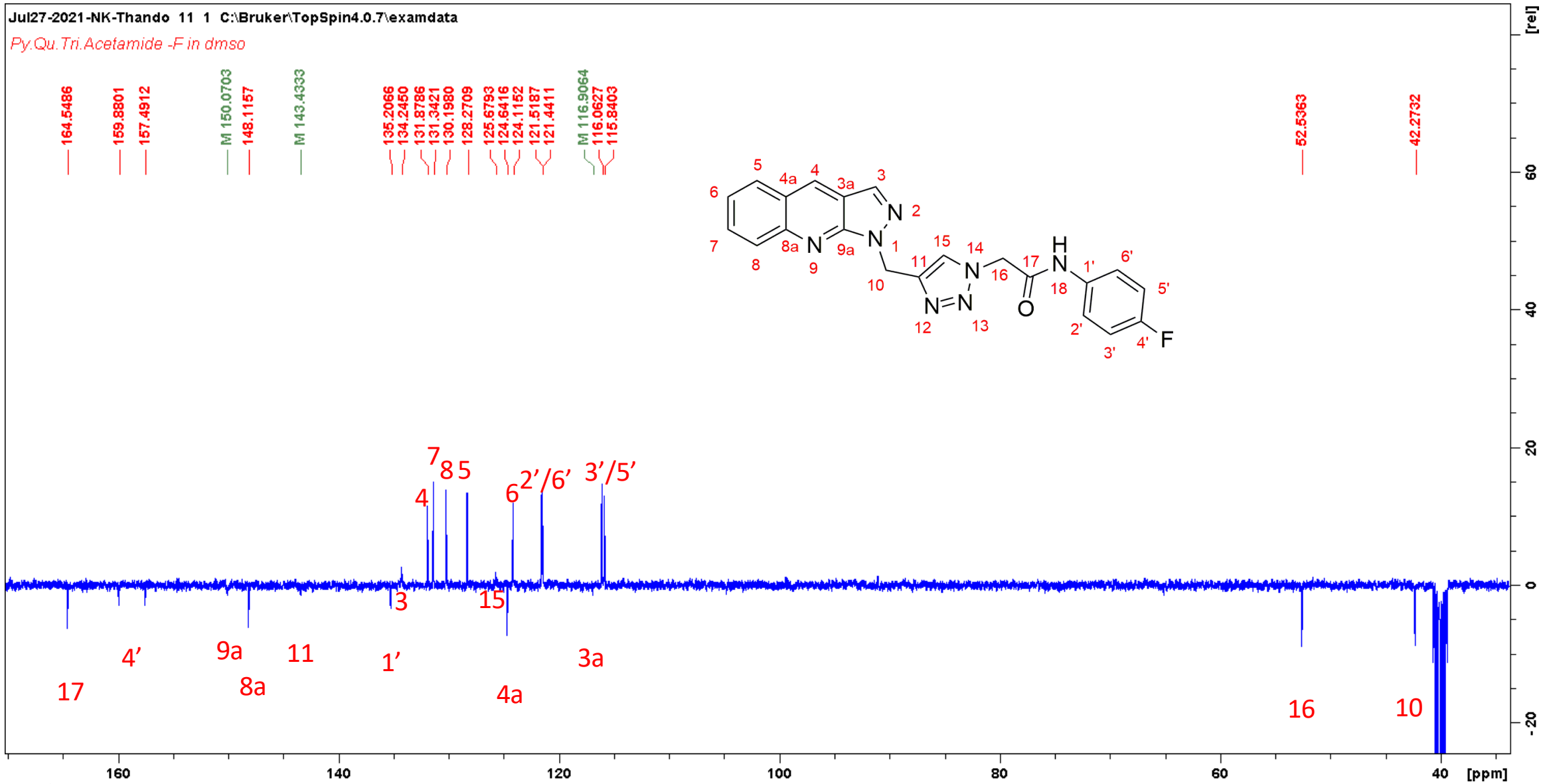
HRMS spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-phenylacetamide (**9a**)




FTIR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-phenylacetamide (**9a**)




$^{1}$H NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-fluorophenyl)acetamide (**9b**)



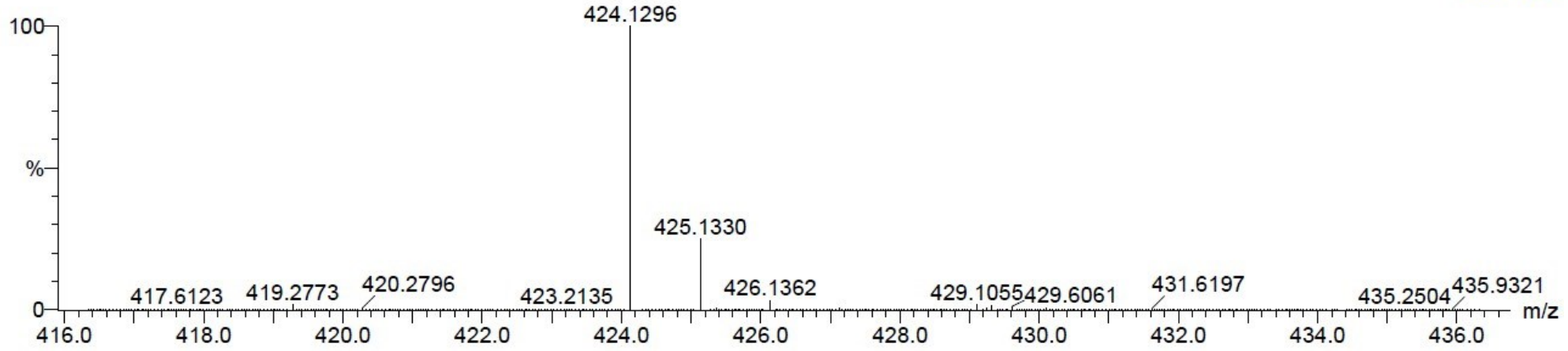

$^{13}$C NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-fluorophenyl)acetamide (**9b**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-1 Na: 1-1 F: 1-1

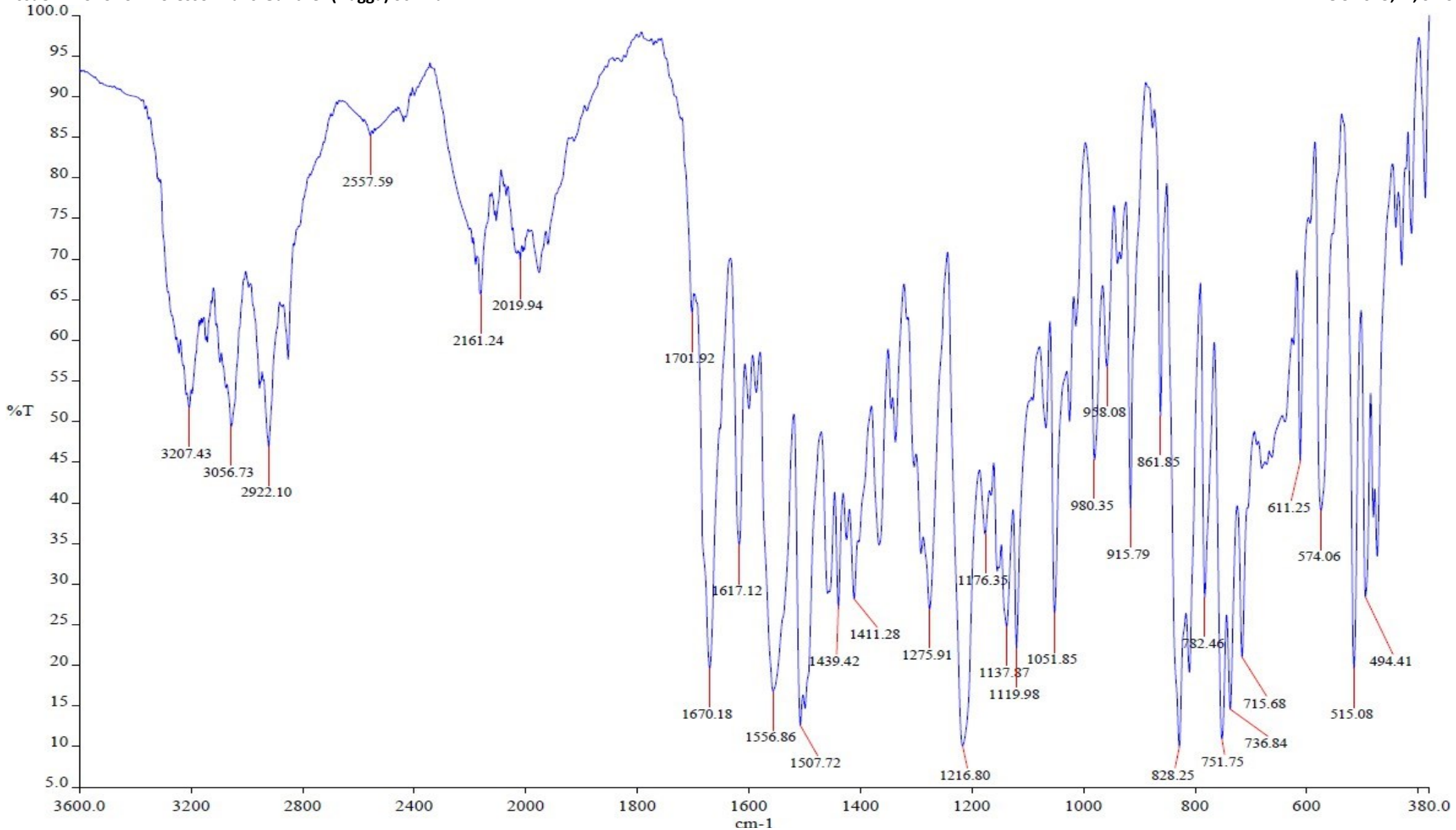
PyQuTriAc-F 14 (0.439) Cm (1:61)

TOF MS ES+
2.68e+005

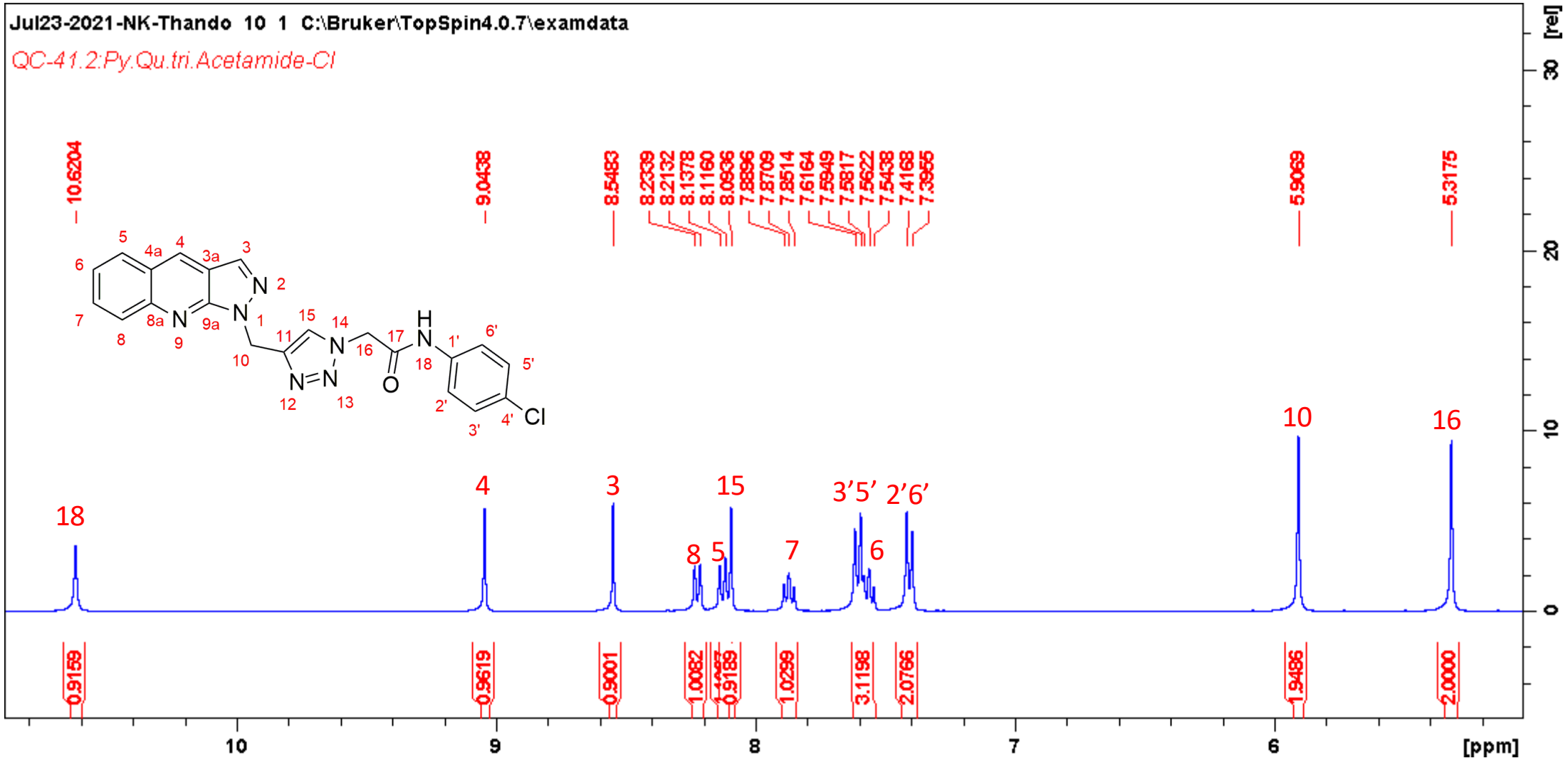



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 424.1296 | 424.1298 | -0.2 | -0.5 | 16.5 | 444.8 | 0.0 | C21 H16 N7 O Na F |

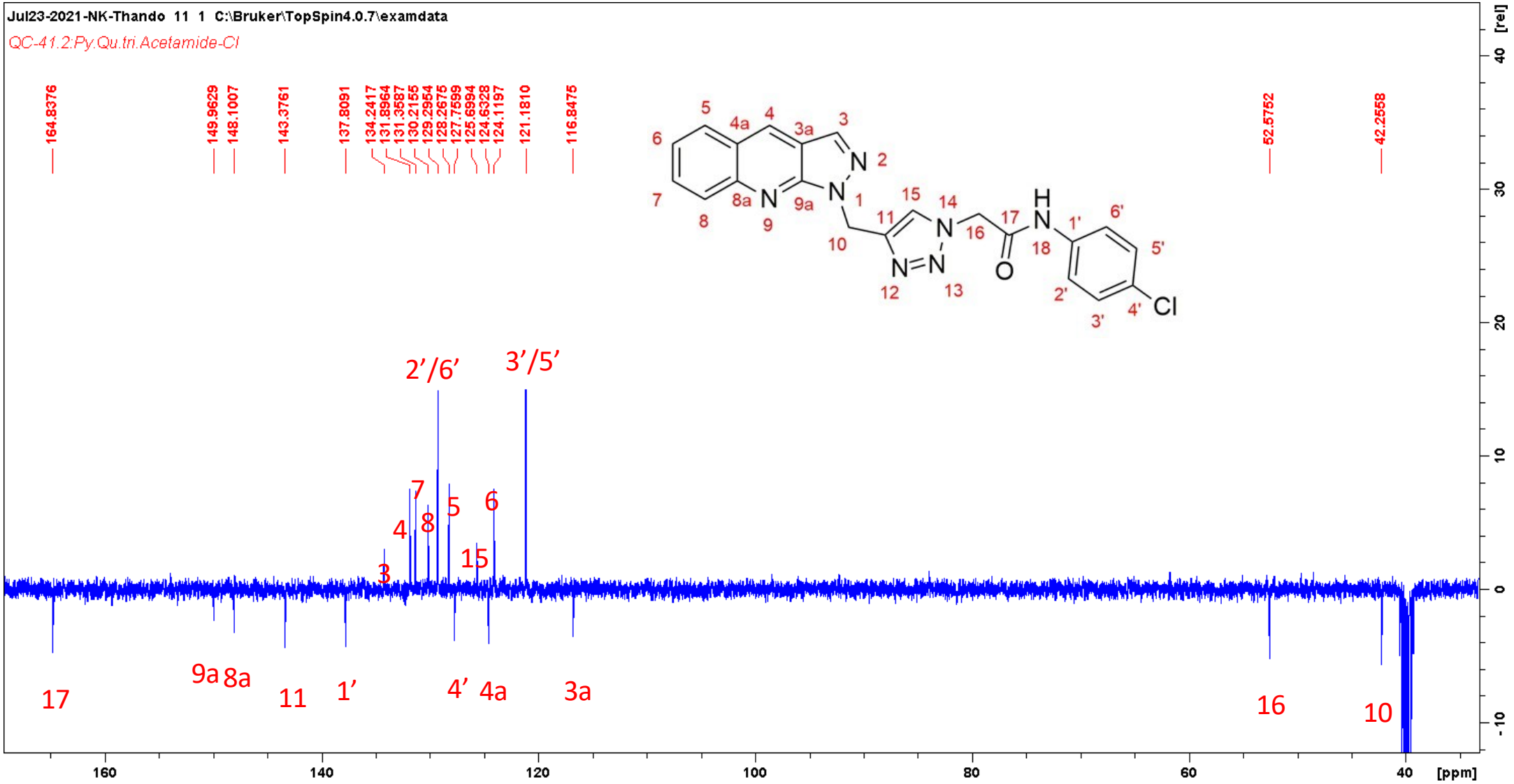
HRMS spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-fluorophenyl)acetamide (**9b**)




FTIR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-fluorophenyl)acetamide (**9b**)




$^{1}$H NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-chlorophenyl)acetamide (**9c**)



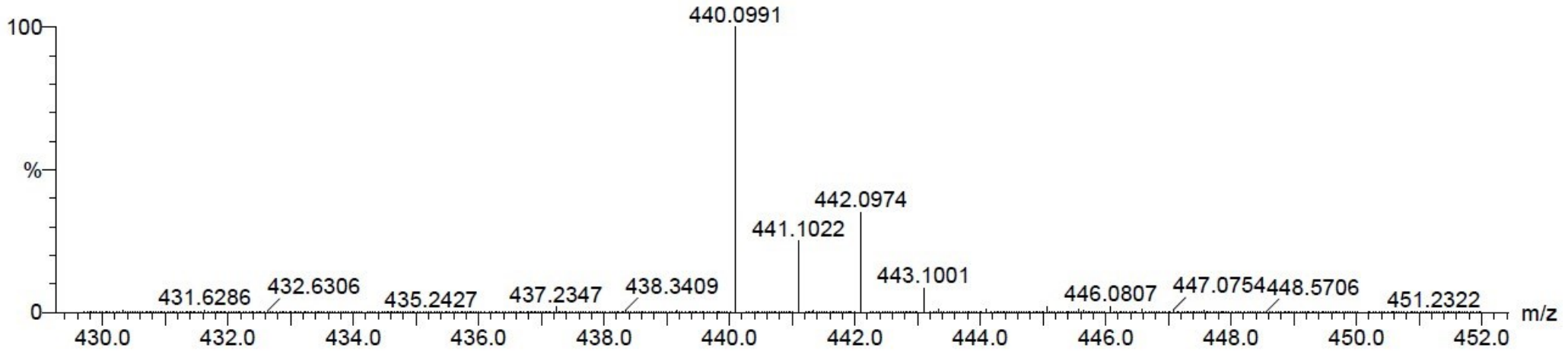

$^{13}$C NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-fluorophenyl)acetamide (**9c**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-1 Na: 1-1 Cl: 0-1

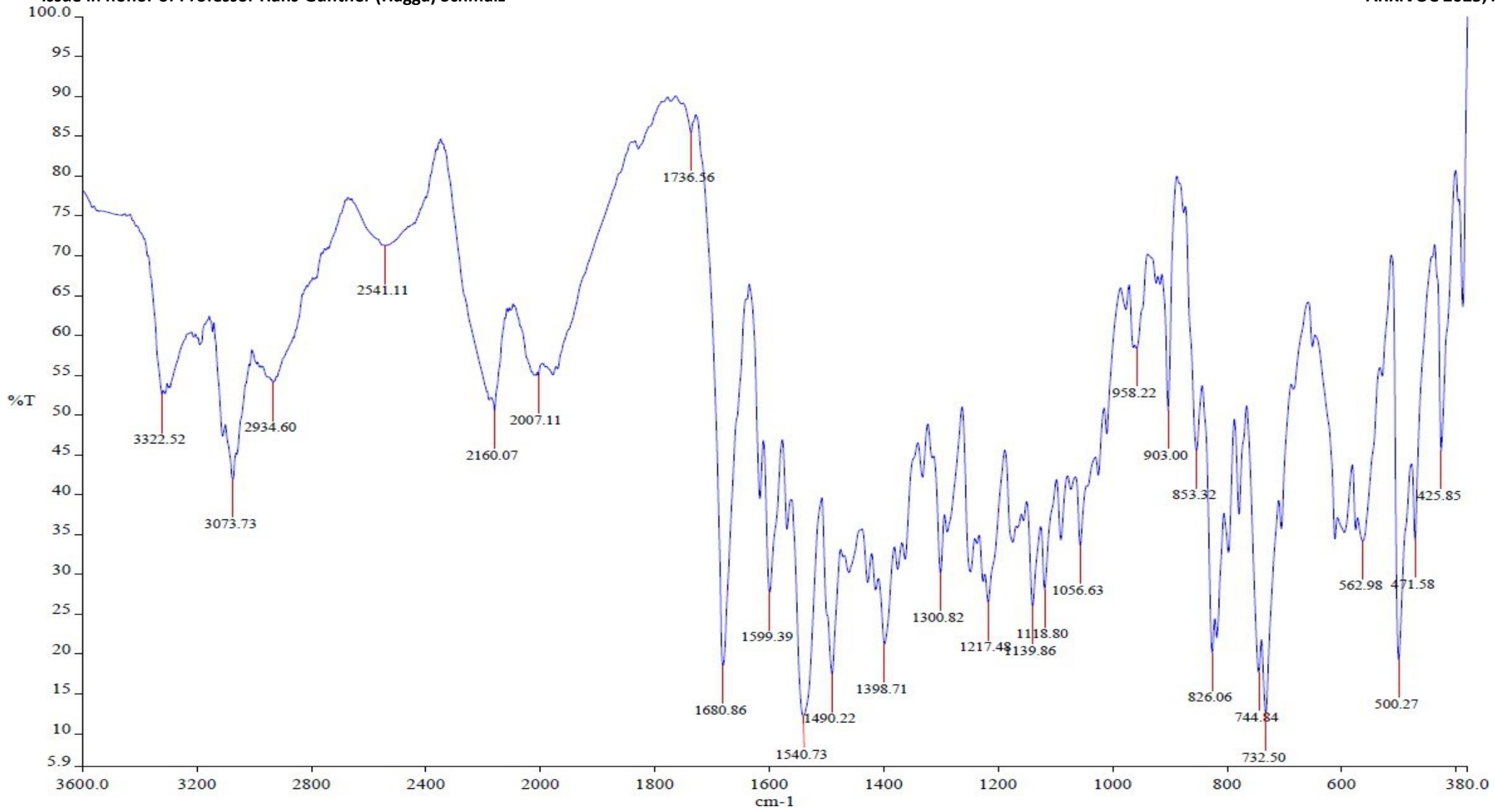
PyQuTriAc-Cl 43 (1.417) Cm (1:61)

TOF MS ES+
1.52e+005

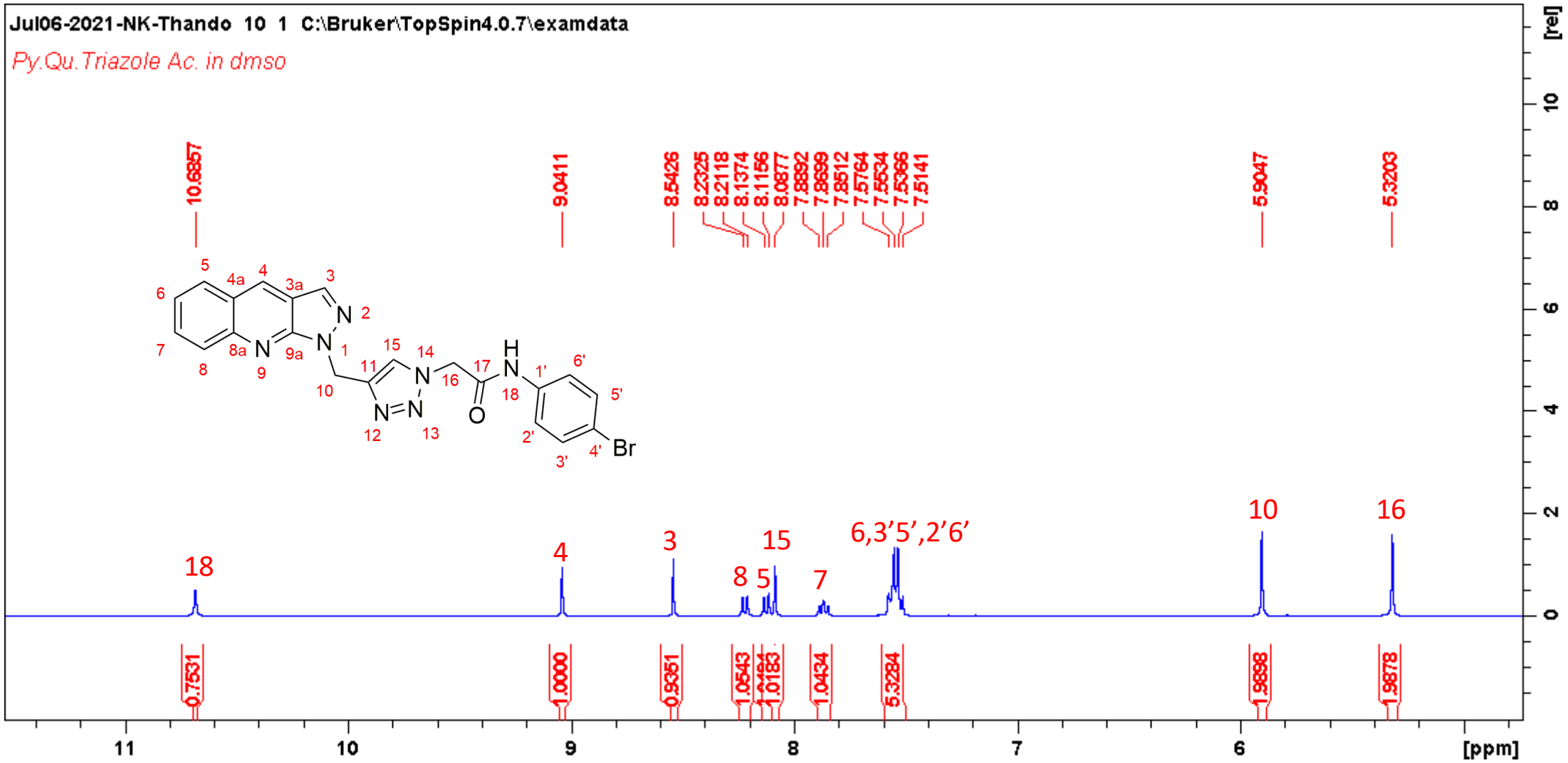



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 440.0991 | 440.1003 | -1.2 | -2.7 | 16.5 | 432.3 | 0.0 | C21 H16 N7 O Na Cl |

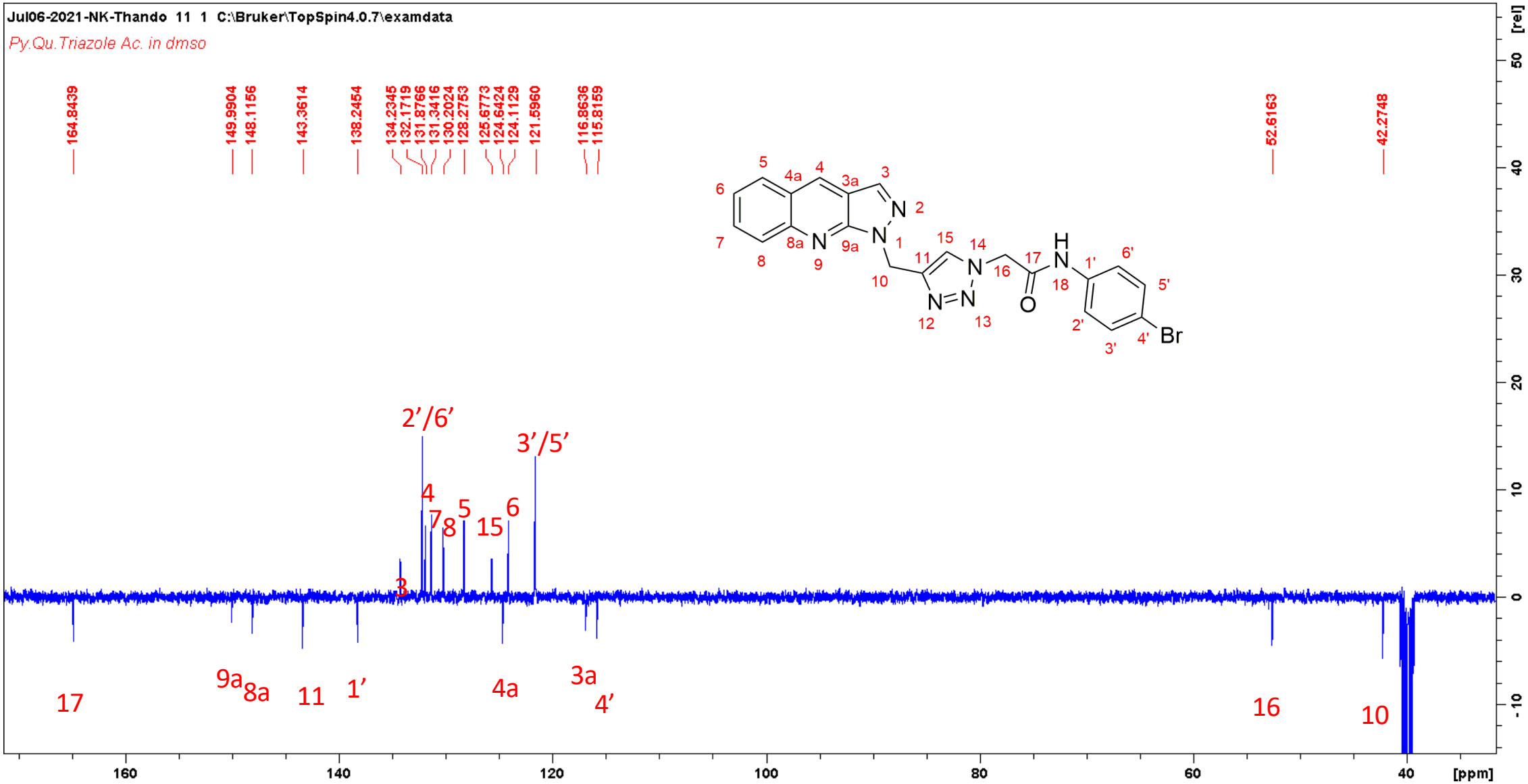
HRMS spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-chlorophenyl)acetamide (**9c**)




FTIR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-chlorophenyl)acetamide (**9c**)




$^{1}$H NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-bromophenyl)acetamide (**9d**)



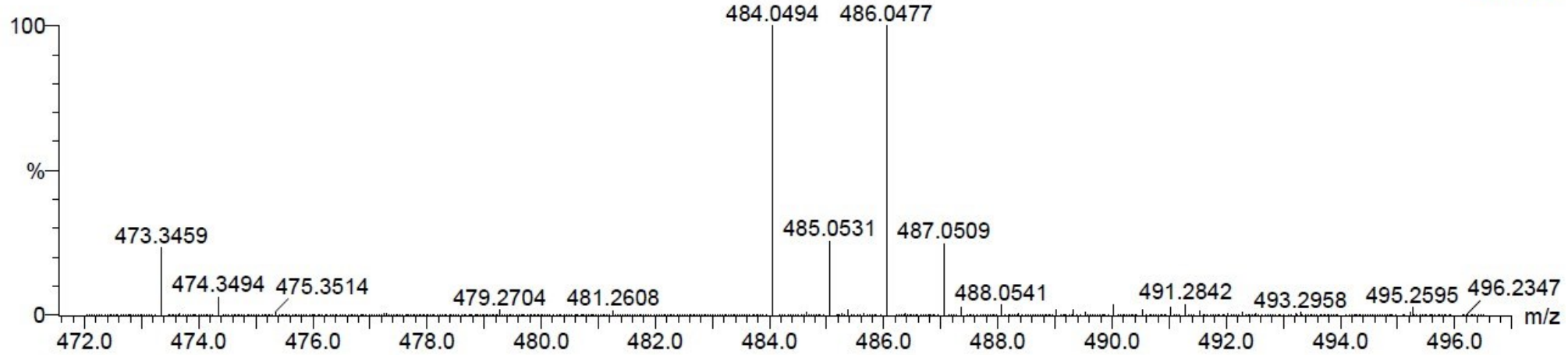

$^{13}$C NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-bromophenyl)acetamide (**9d**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-1 Na: 1-1 Br: 0-1

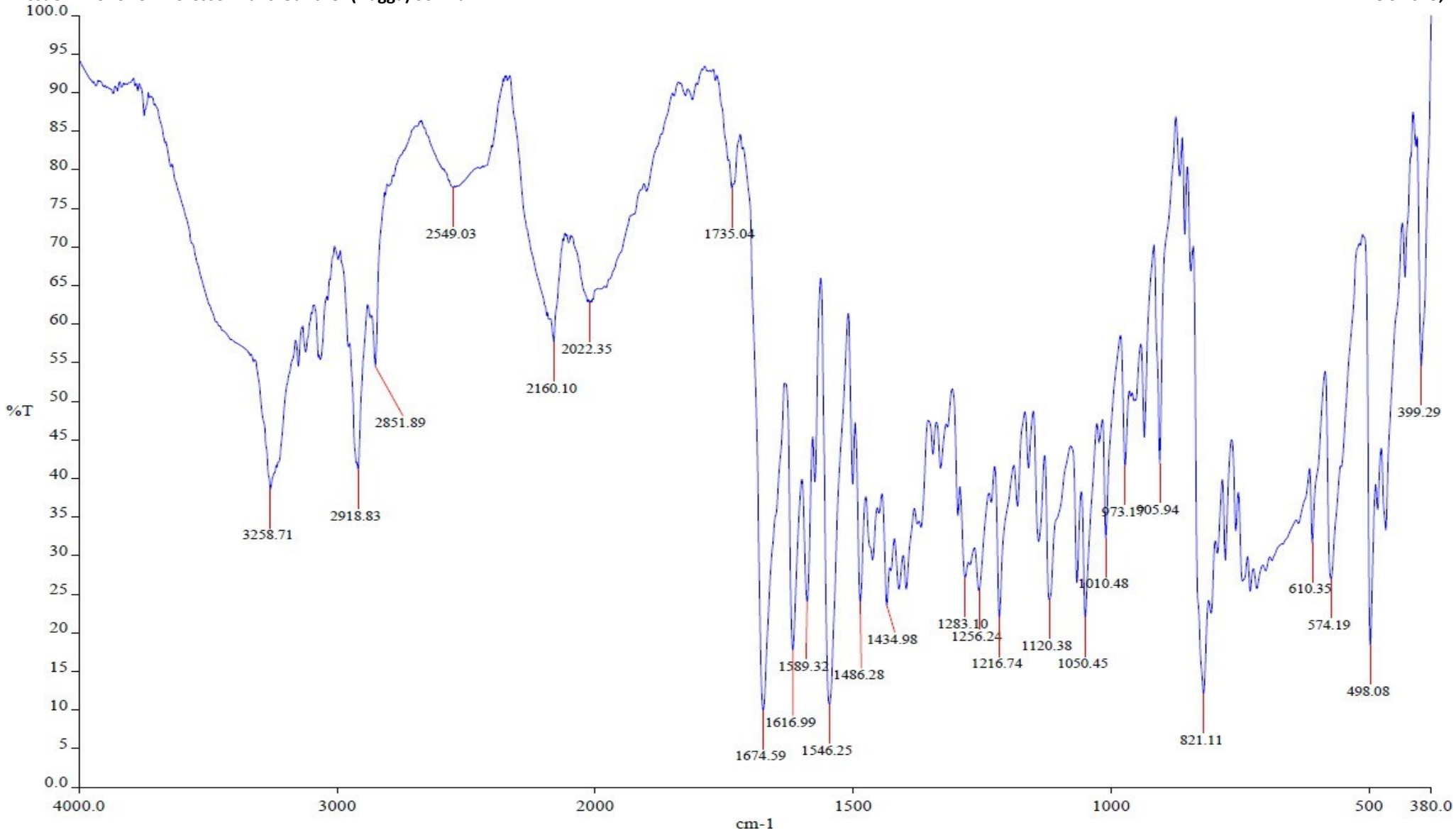
PyQuTriAc-Br 19 (0.607) Cm (1:61)

TOF MS ES+
1.40e+005

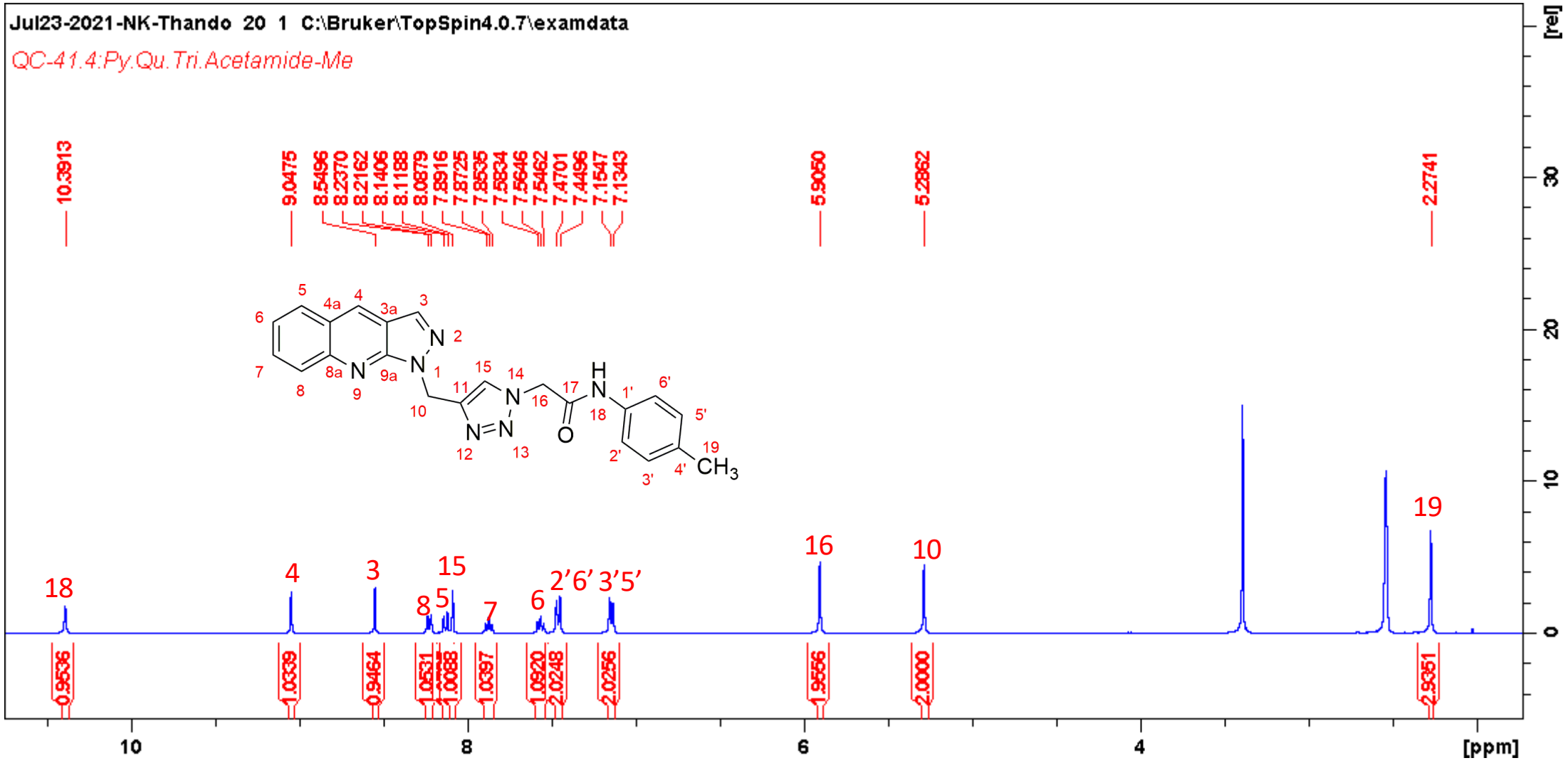



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 484.0494 | 484.0497 | -0.3 | -0.6 | 16.5 | 392.0 | 0.0 | C21 H16 N7 O Na Br |

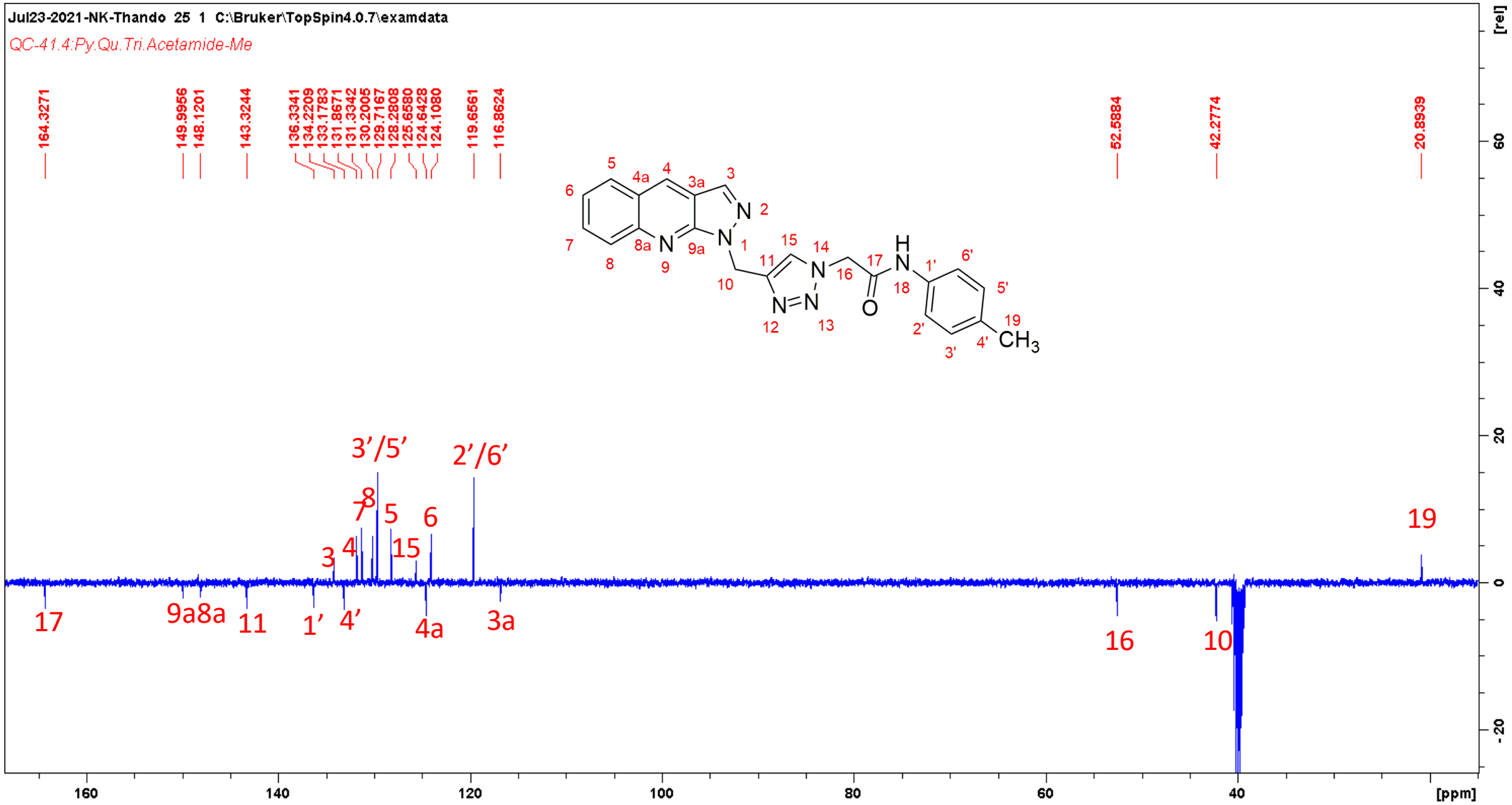
HRMS spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-bromophenyl)acetamide (**9d**)




FTIR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-bromophenyl)acetamide (**9d**)




$^{1}$H NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methylphenyl)acetamide (**9e**)



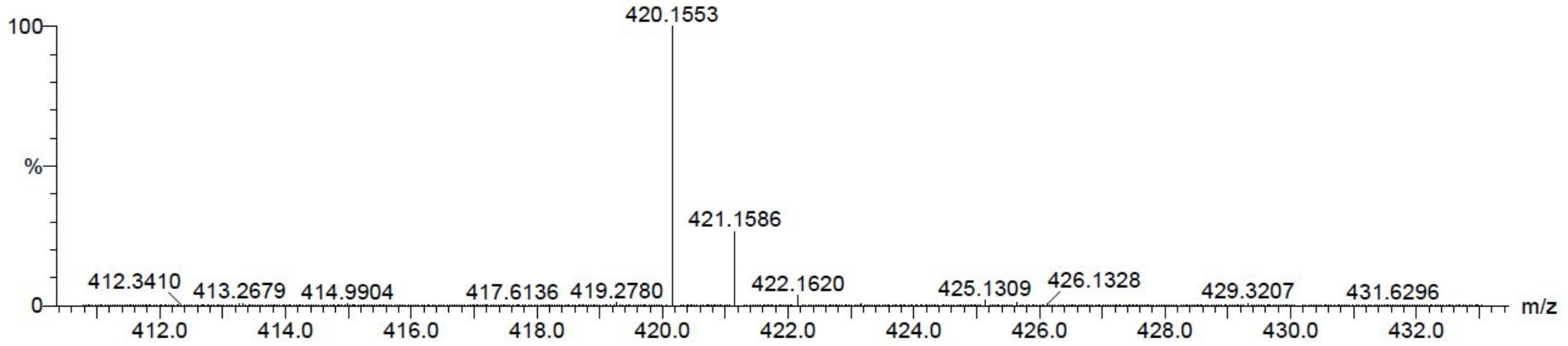

$^{13}$C NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methylphenyl)acetamide (**9e**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-1 Na: 1-1

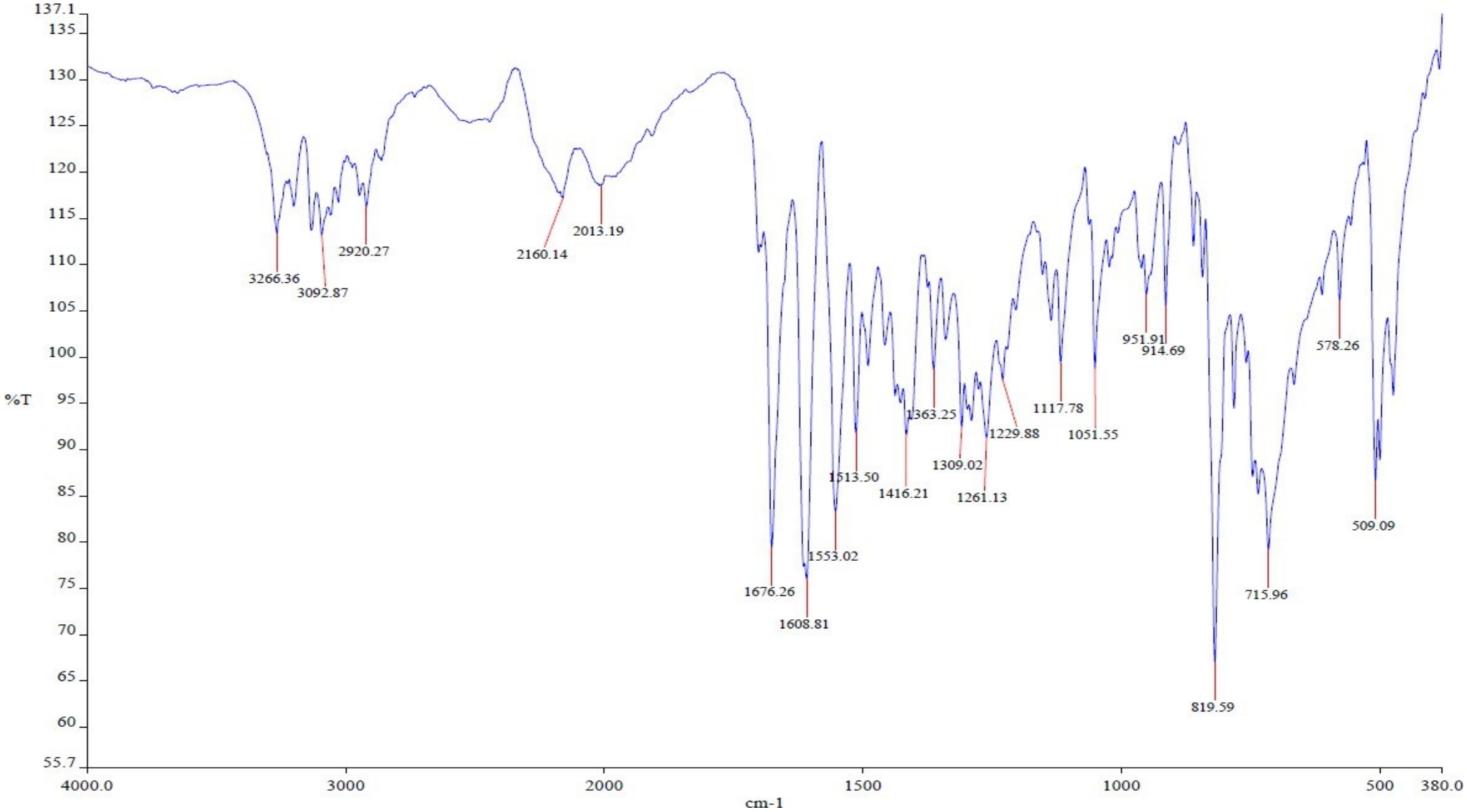
PyQuTriAc-CH3 2 (0.034) Cm (1:61)

TOF MS ES+
2.49e+005

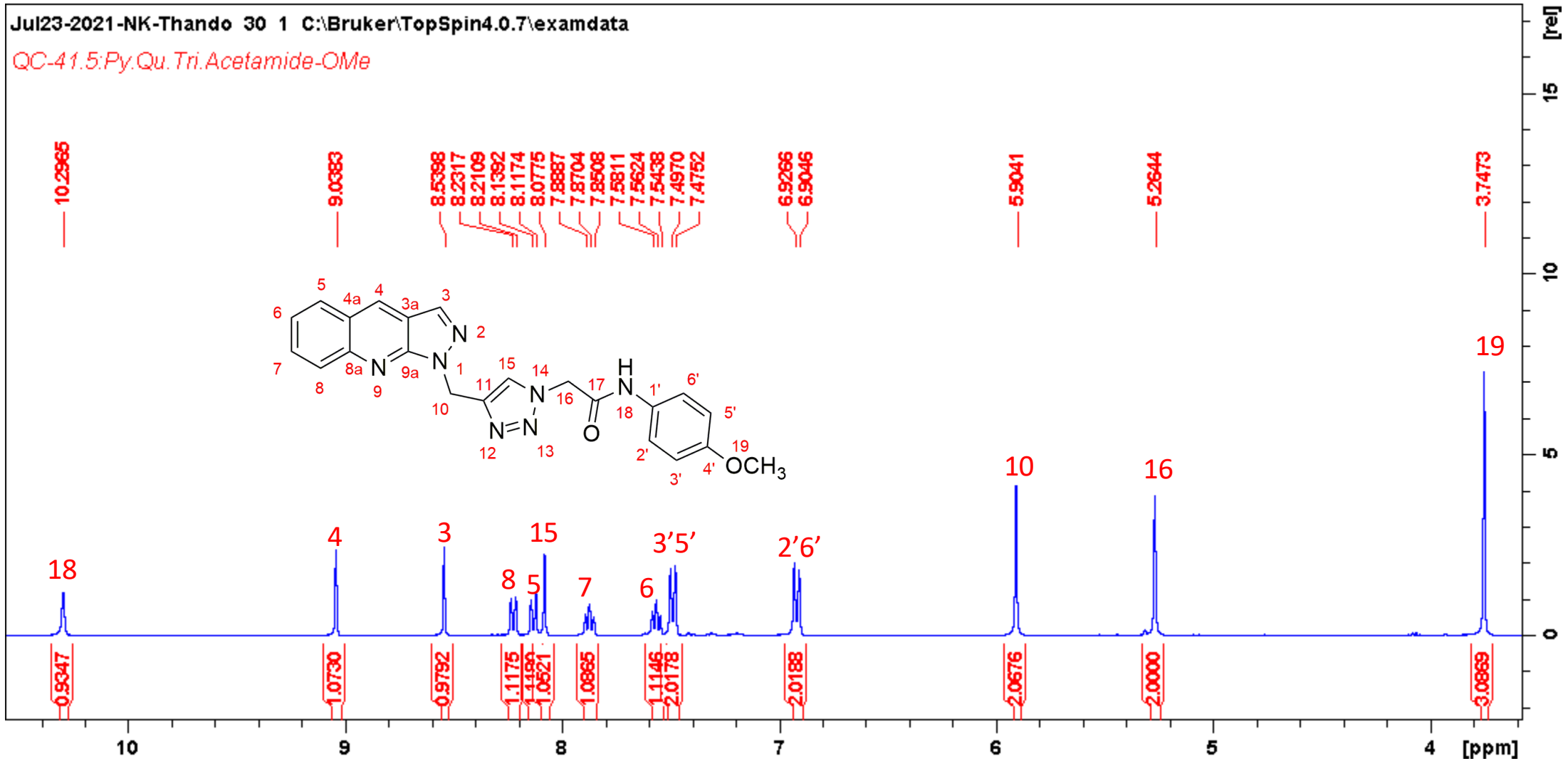



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 420.1553 | 420.1549 | 0.4 | 1.0 | 16.5 | 473.8 | 0.0 | C22 H19 N7 O Na |

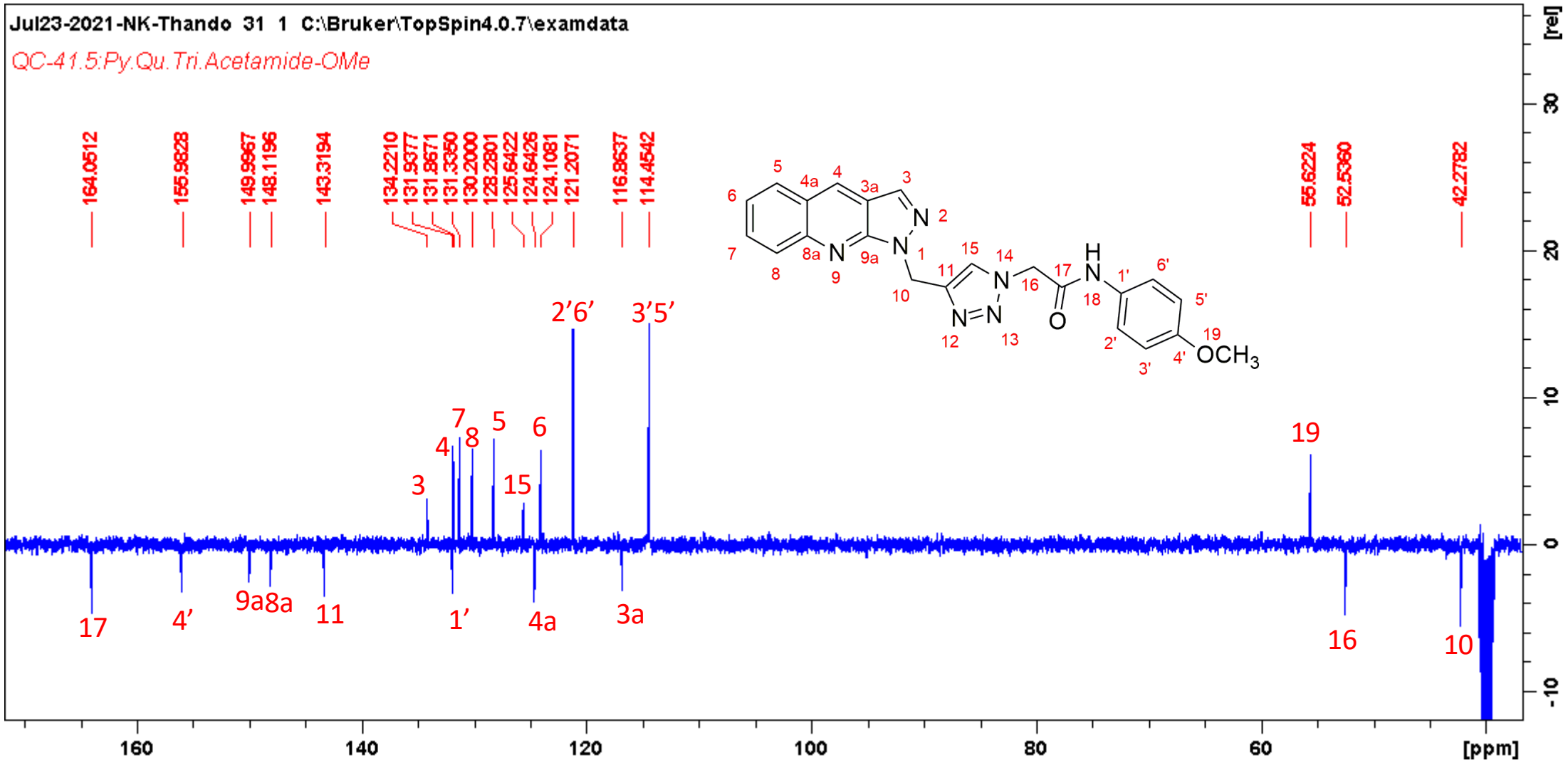
HRMS spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methylphenyl)acetamide (**9e**)




FTIR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methylphenyl)acetamide (**9e**)




$^{1}$H NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)acetamide (**9f**)



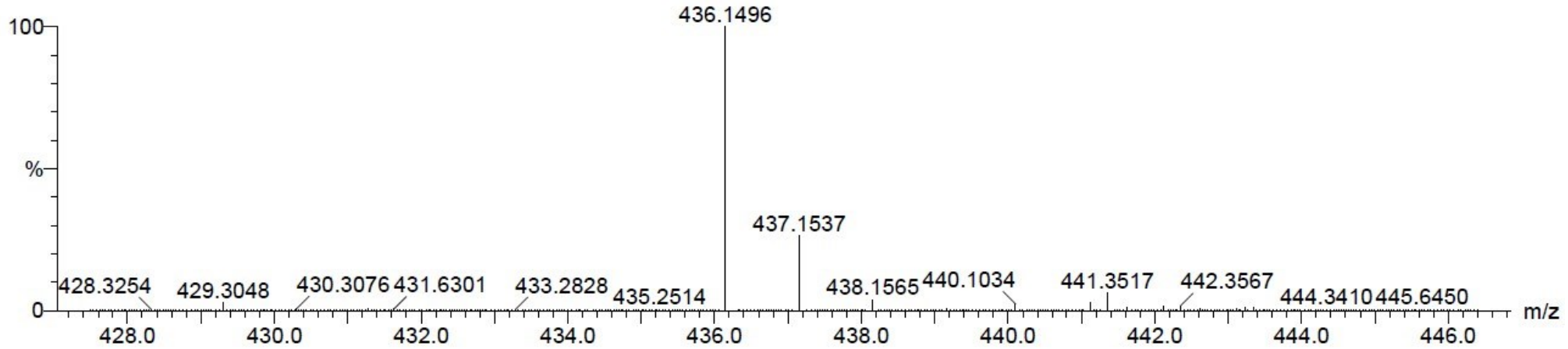

$^{13}$C NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)acetamide (**9f**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-2 Na: 1-1

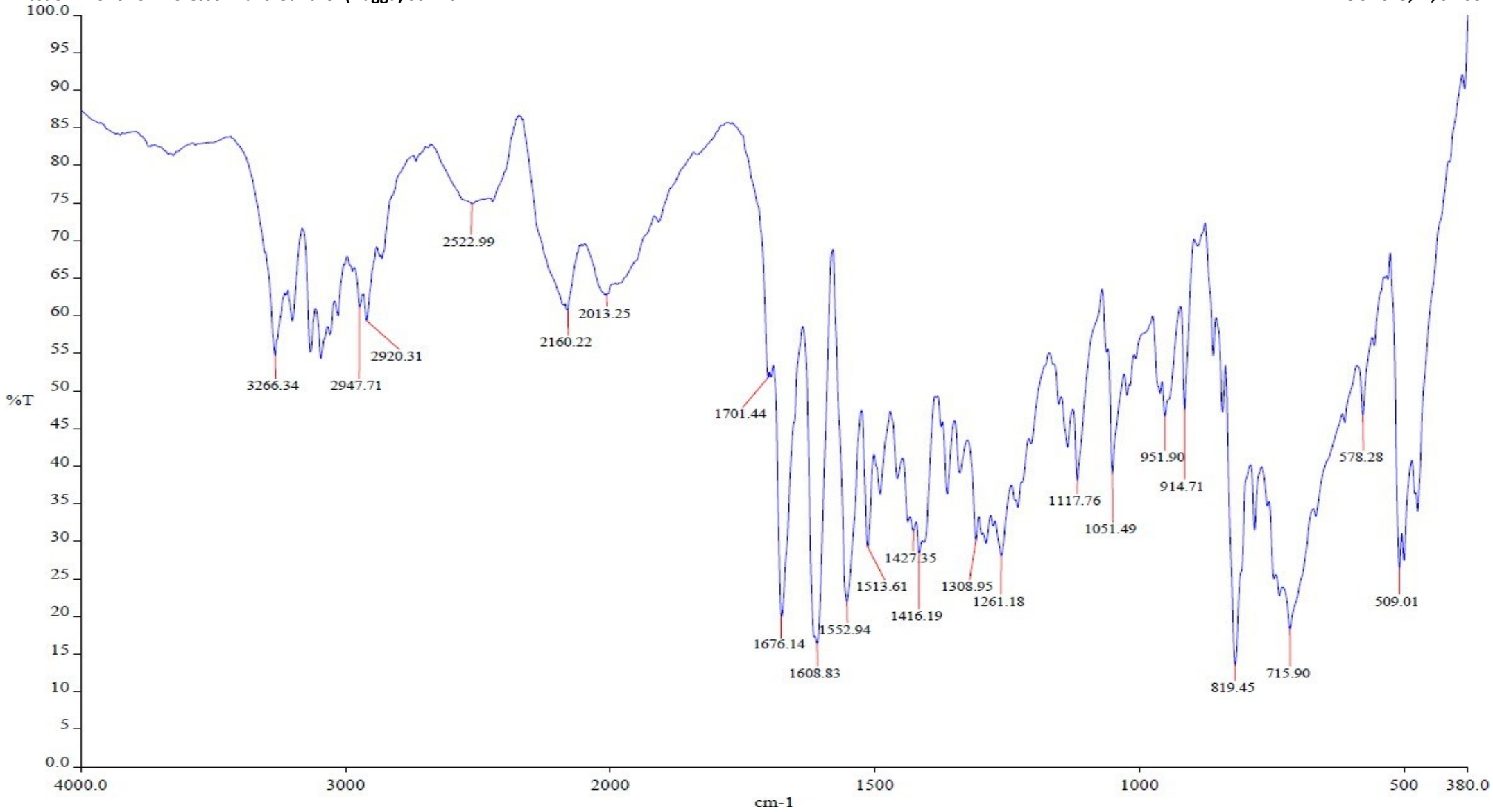
PyQuTriAc-OCH3 24 (0.776) Cm (1:61)

TOF MS ES+
1.80e+005

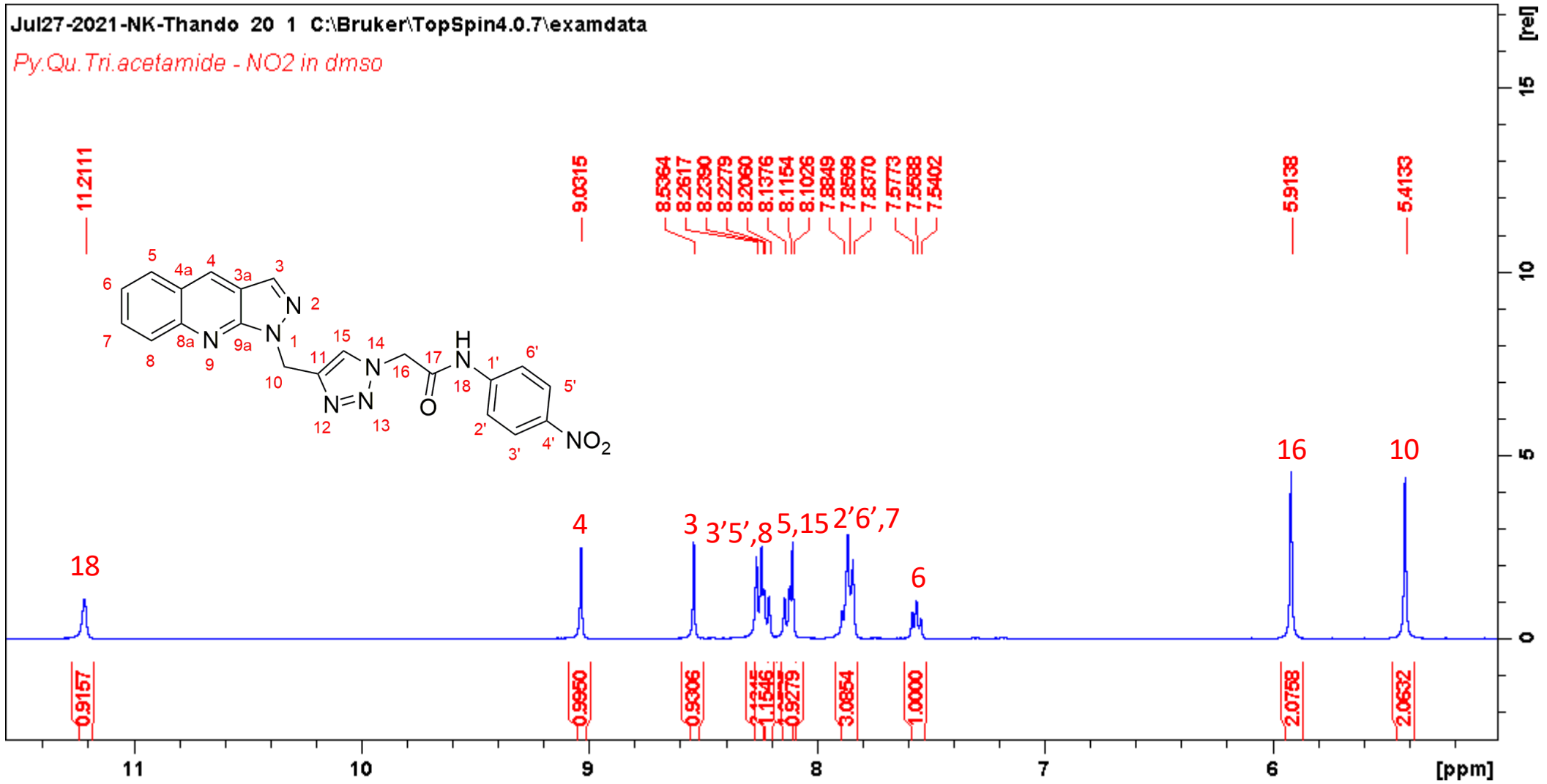



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 436.1496 | 436.1498 | -0.2 | -0.5 | 16.5 | 436.2 | 0.0 | C22 H19 N7 O2 Na |

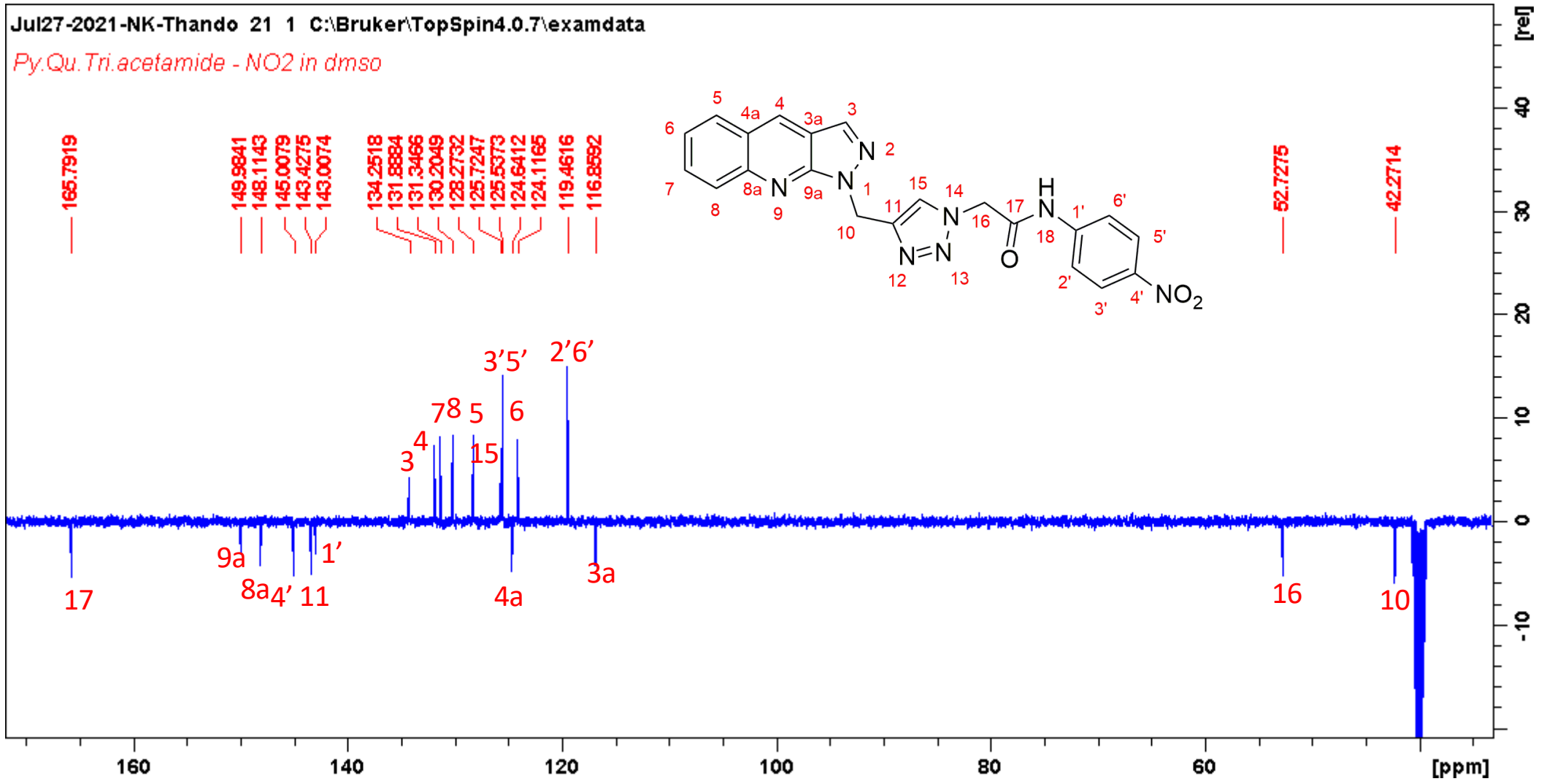
HRMS spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)acetamide (**9f**)




FTIR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)acetamide (**9f**)




$^{1}$H NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-nitrophenyl)acetamide (**9g**)



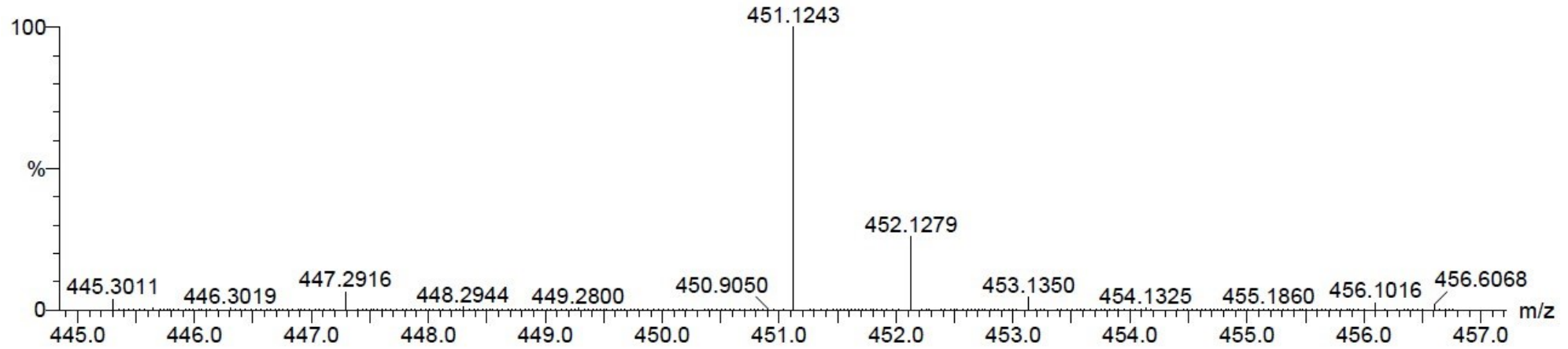

$^{13}$C NMR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-nitrophenyl)acetamide (**9g**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 1-1

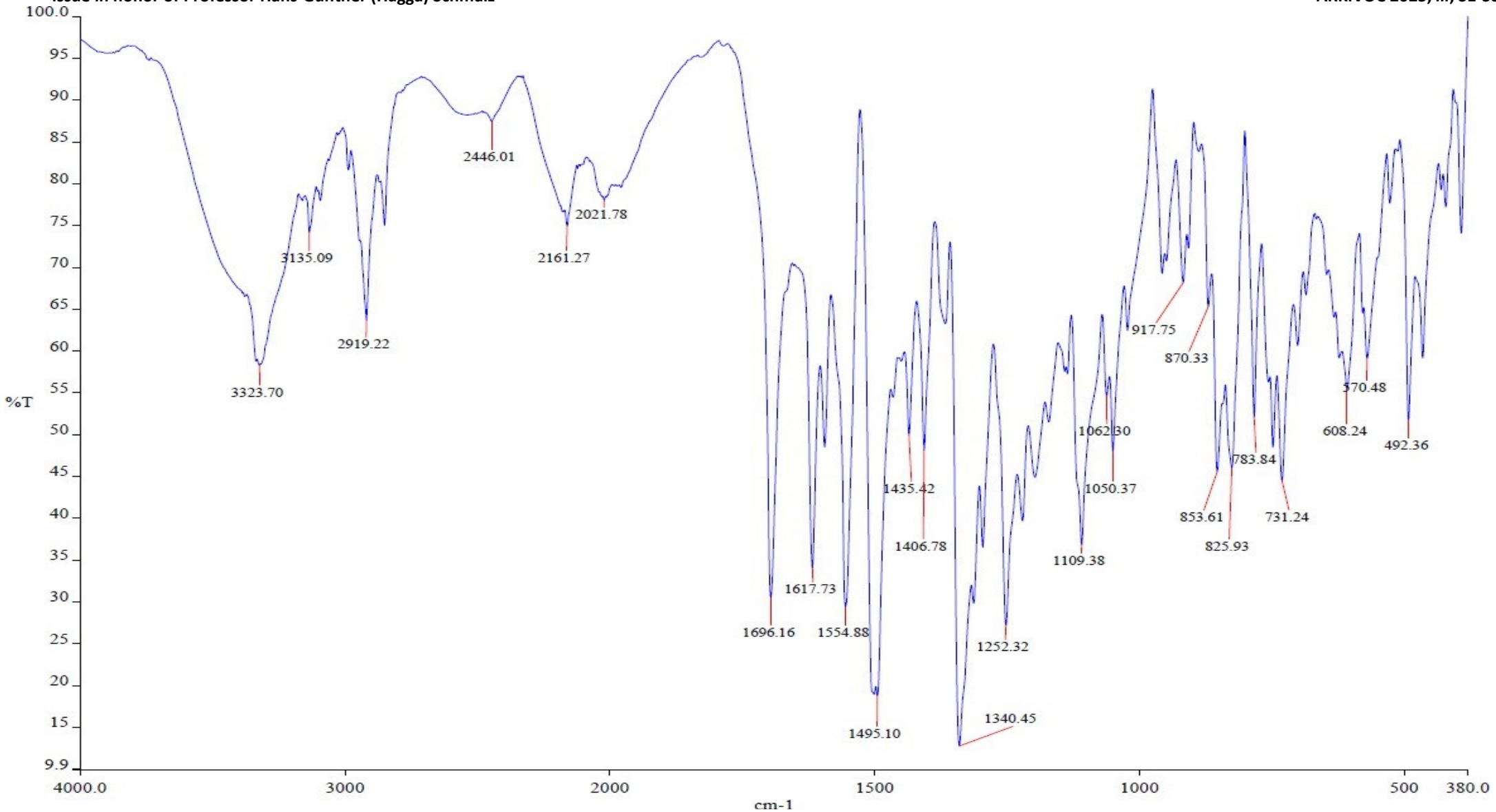
PyQuTriAc-NO2 54 (1.788) Cm (1:61)

TOF MS ES+
1.77e+005

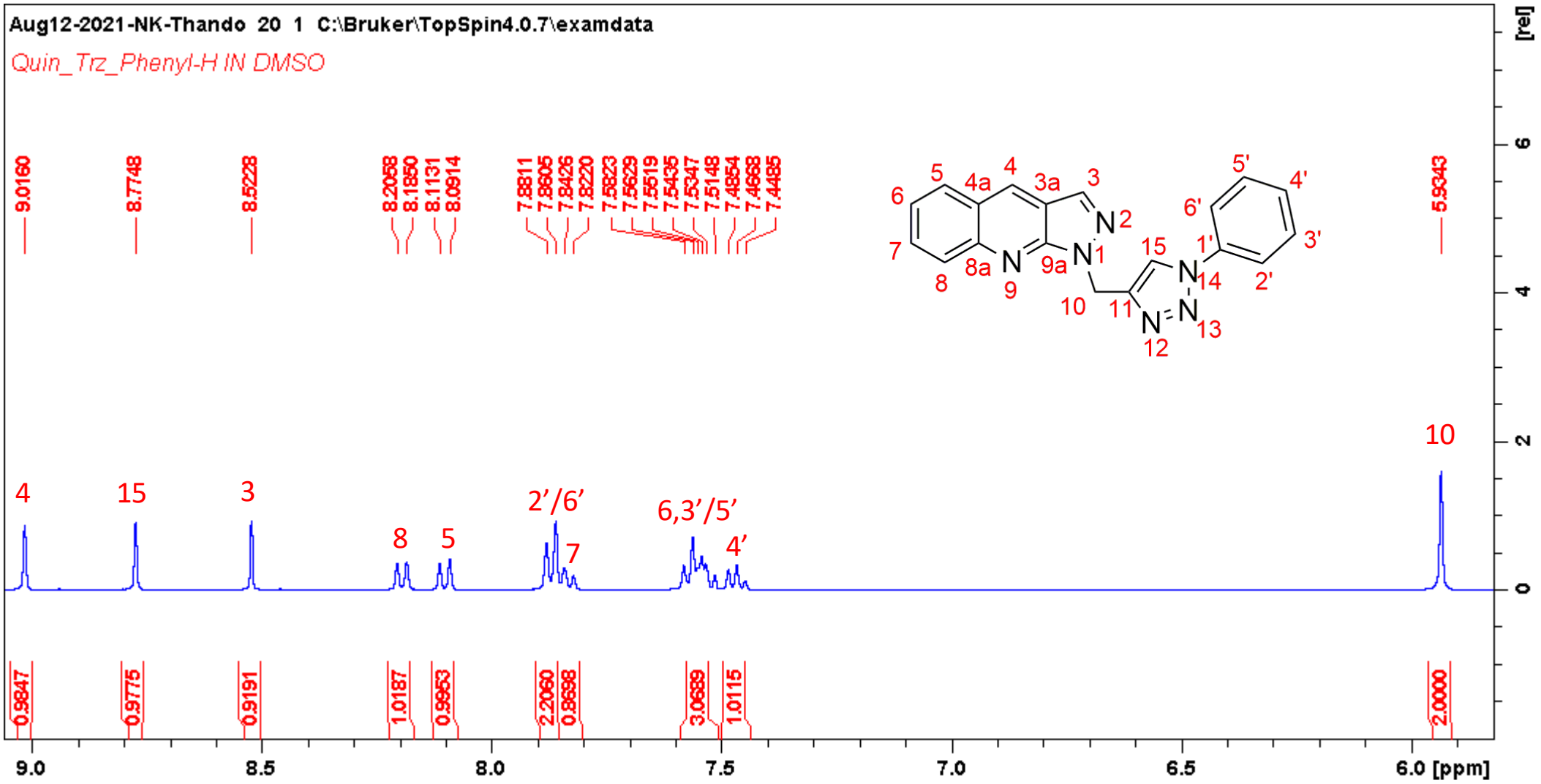



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 451.1243 | 451.1243 | 0.0 | 0.0 | 17.5 | 413.5 | 0.0 | C21 H16 N8 O3 Na |

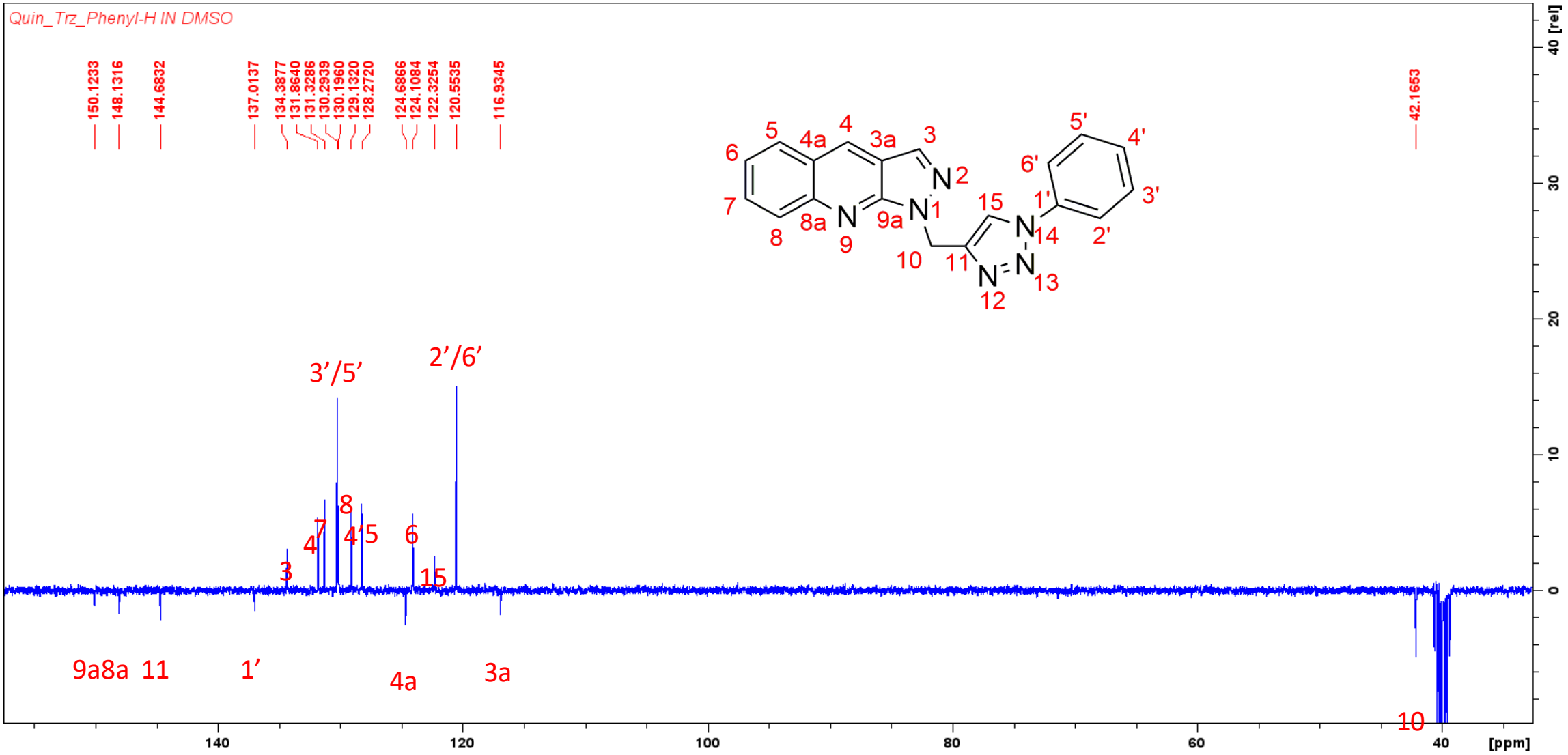
HRMS spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-nitrophenyl)acetamide (**9g**)




FTIR spectrum of 2-(4-((1*H*-pyrazolo[3,4-b]quinolin-1-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-nitrophenyl)acetamide (**9g**)




$^{1}$H NMR spectrum of 1-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10a**)



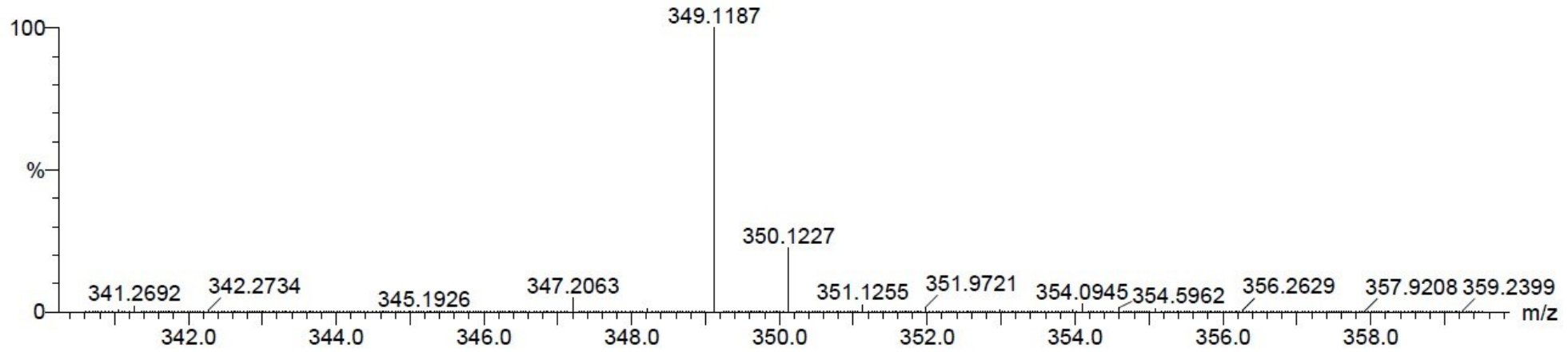

$^{13}$C NMR spectrum of 1-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10a**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 Na: 1-1

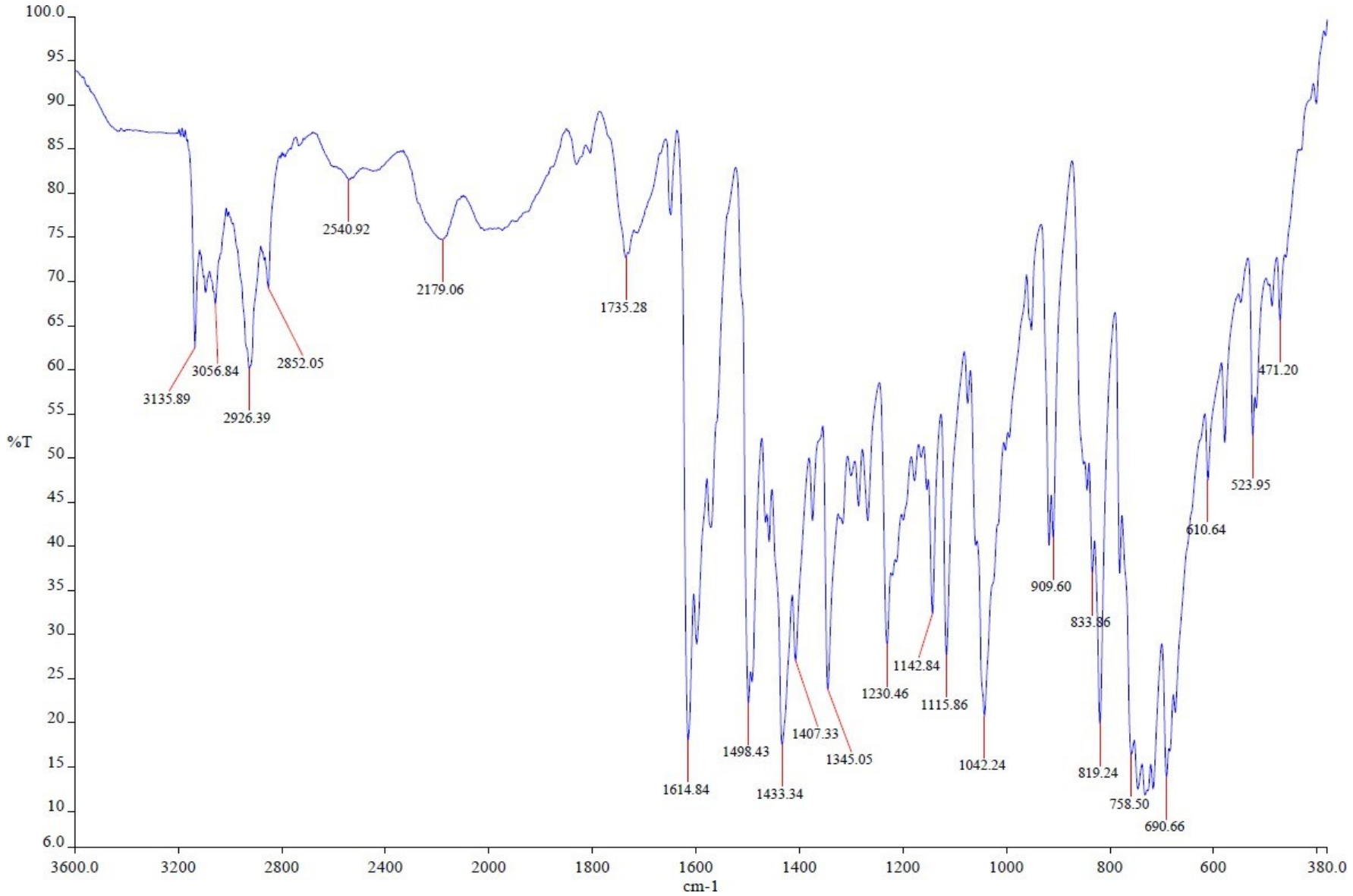
PyQuiTriPh-H 33 (1.079) Cm (1:61)

TOF MS ES+
4.68e+005

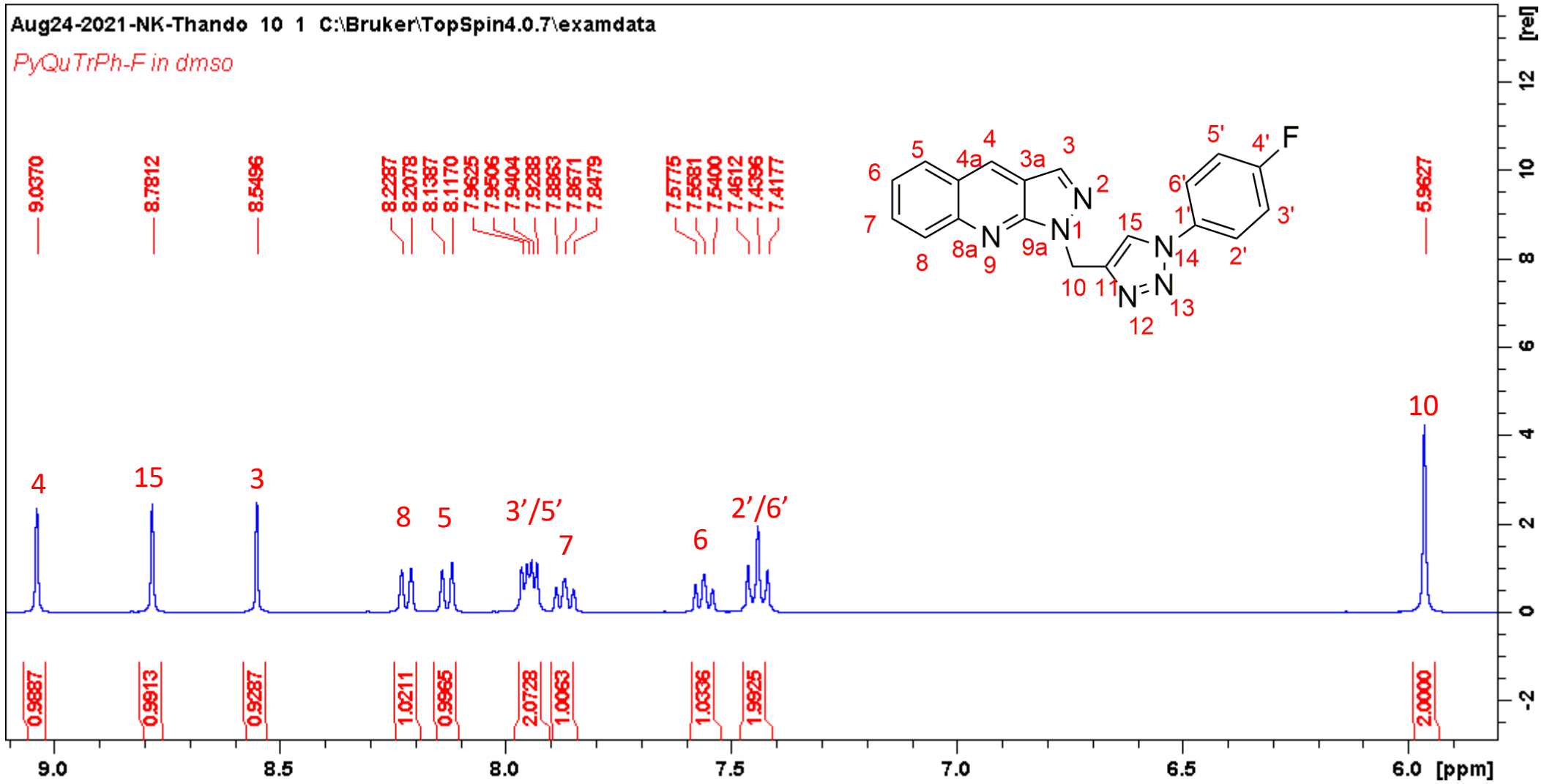



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 349.1187 | 349.1178 | 0.9 | 2.6 | 15.5 | 534.5 | 0.0 | C19 H14 N6 Na |

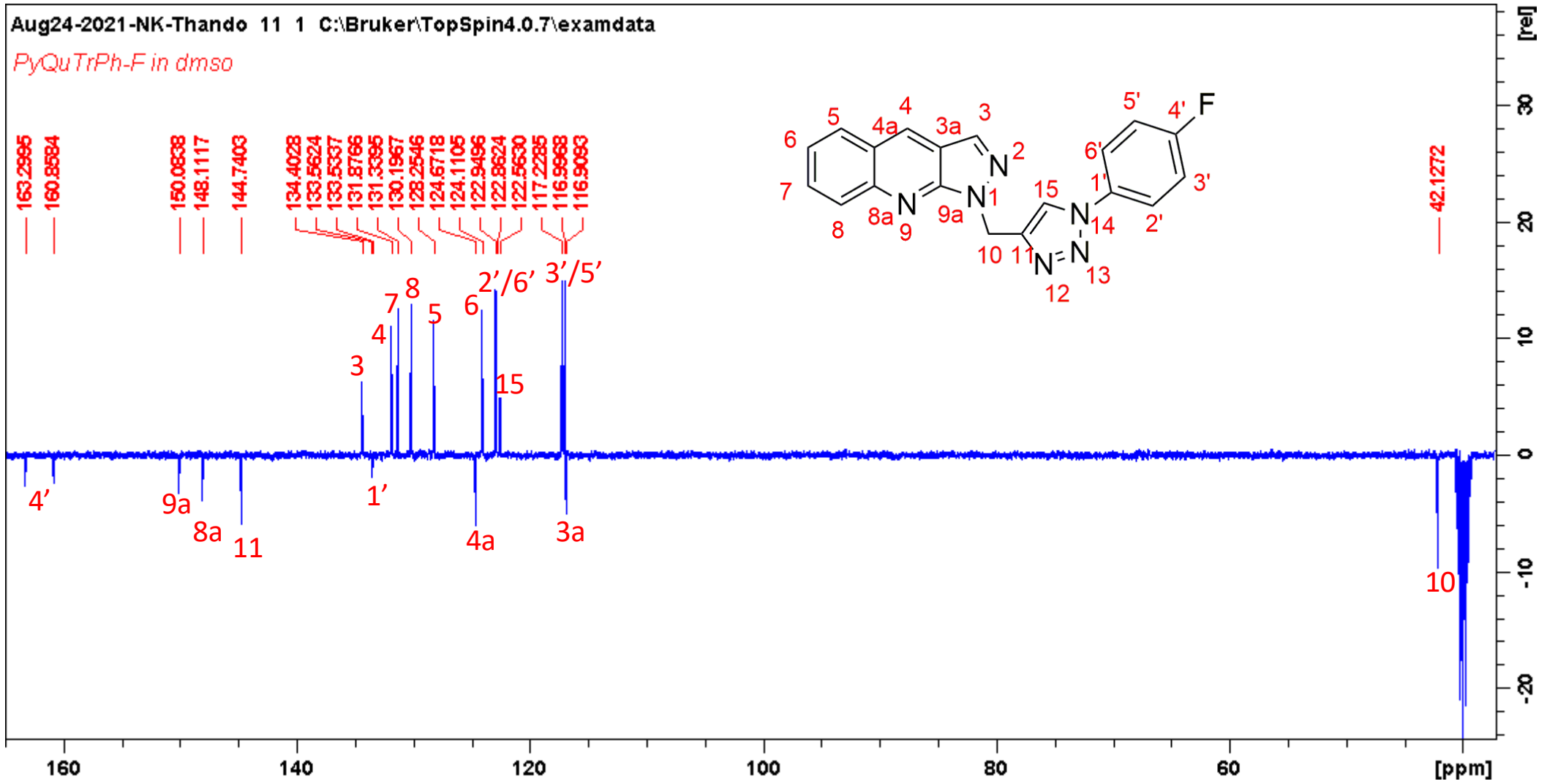
HRMS spectrum of 1-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10a**)




FTIR spectrum of 1-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10a**)




$^{1}$H NMR spectrum of 1-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10b**)



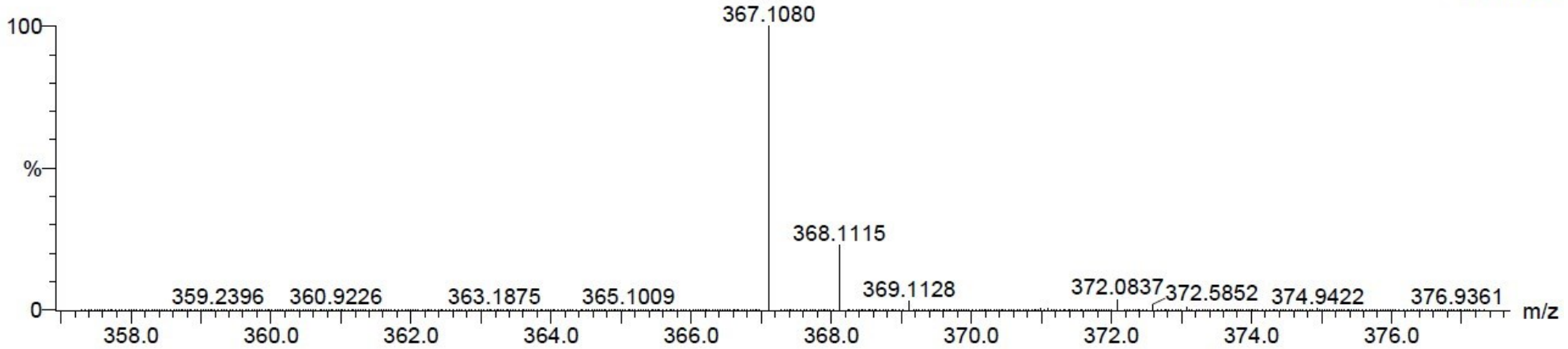

$^{13}$C NMR spectrum of 1-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10b**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 Na: 1-1 F: 1-1

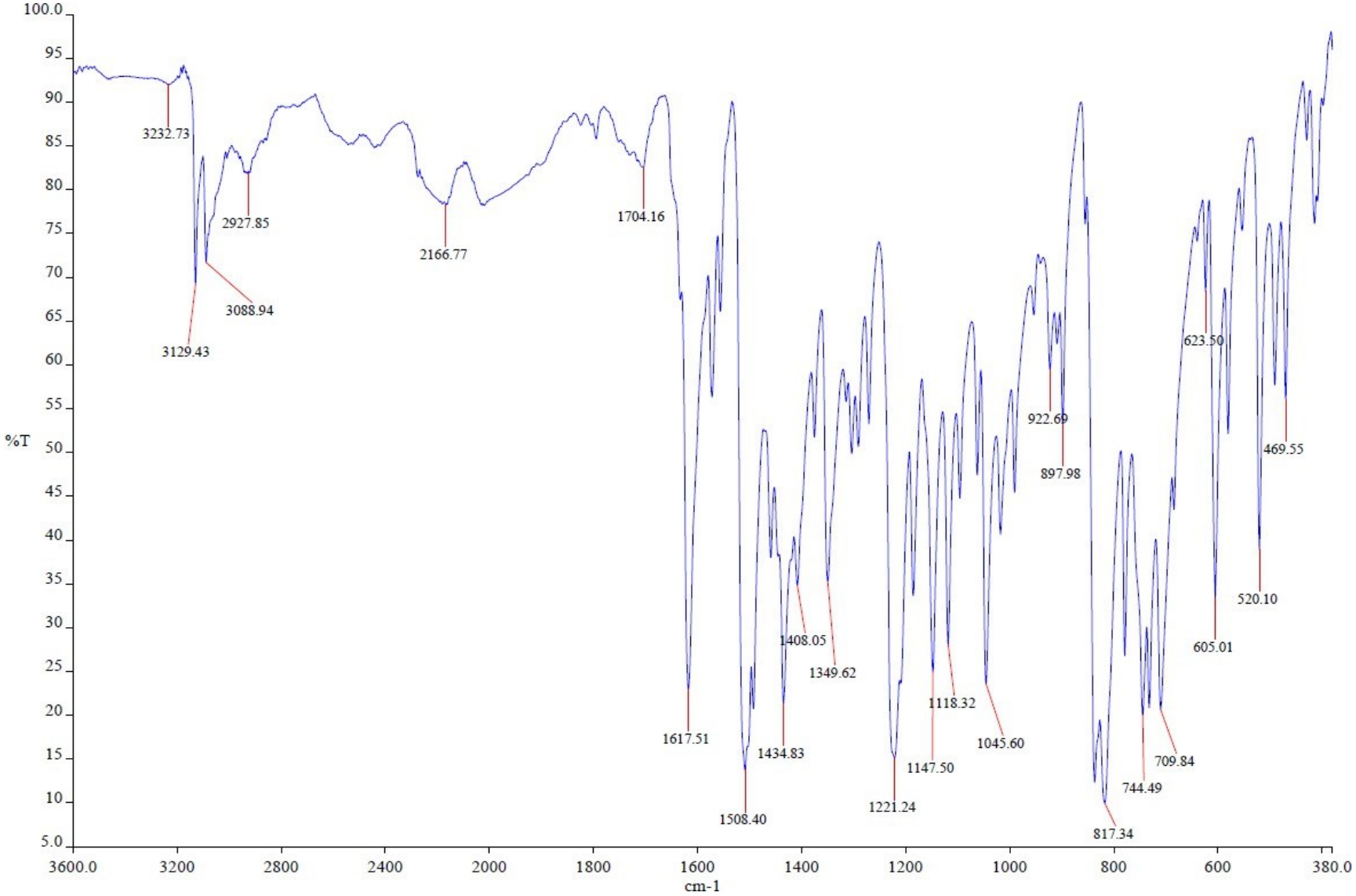
PyQuiTriPh-F 15 (0.473) Cm (1:61)

TOF MS ES+
3.24e+005

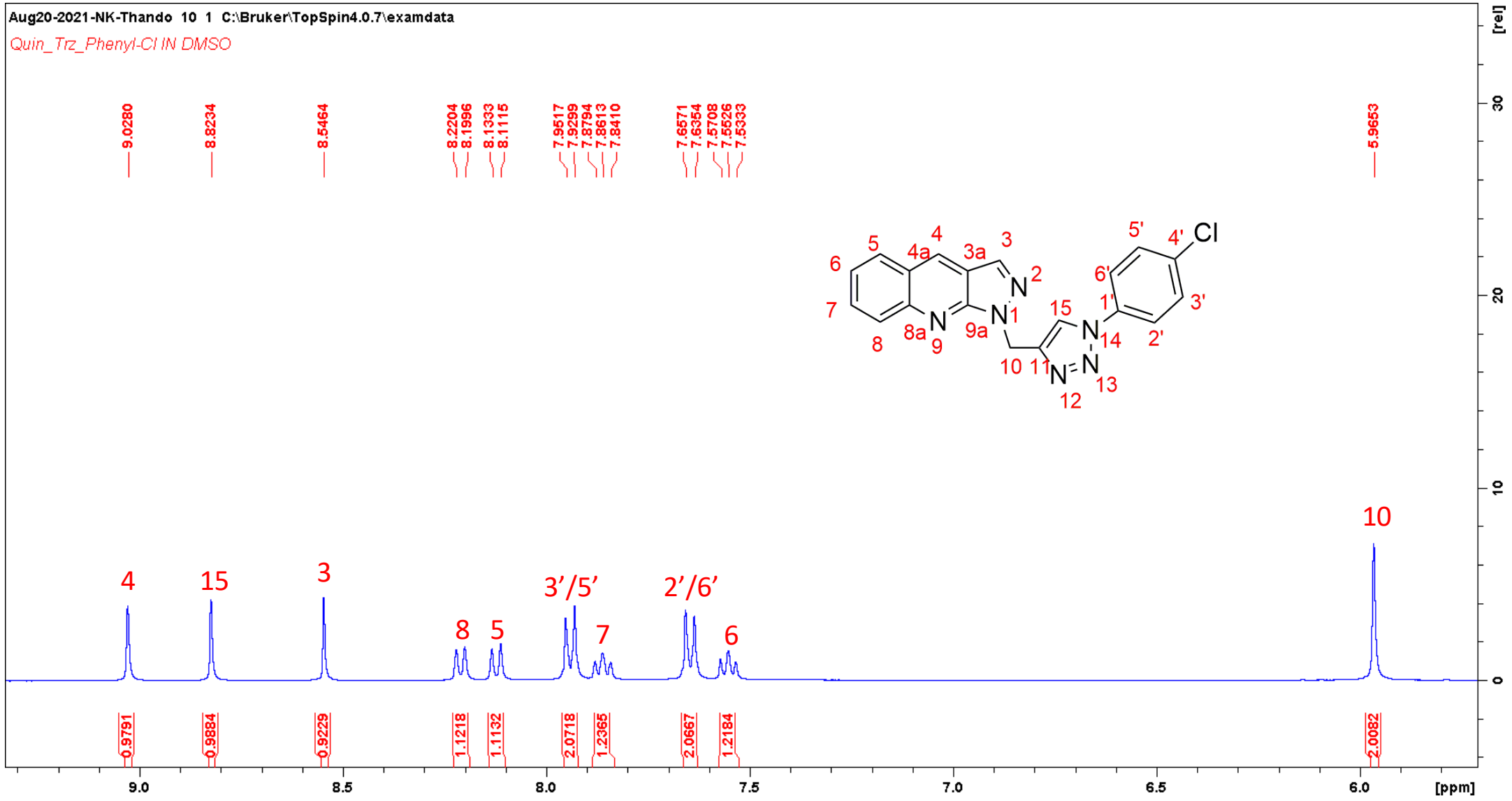



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 367.1080 | 367.1083 | -0.3 | -0.8 | 15.5 | 491.1 | 0.0 | C19 H13 N6 Na F |

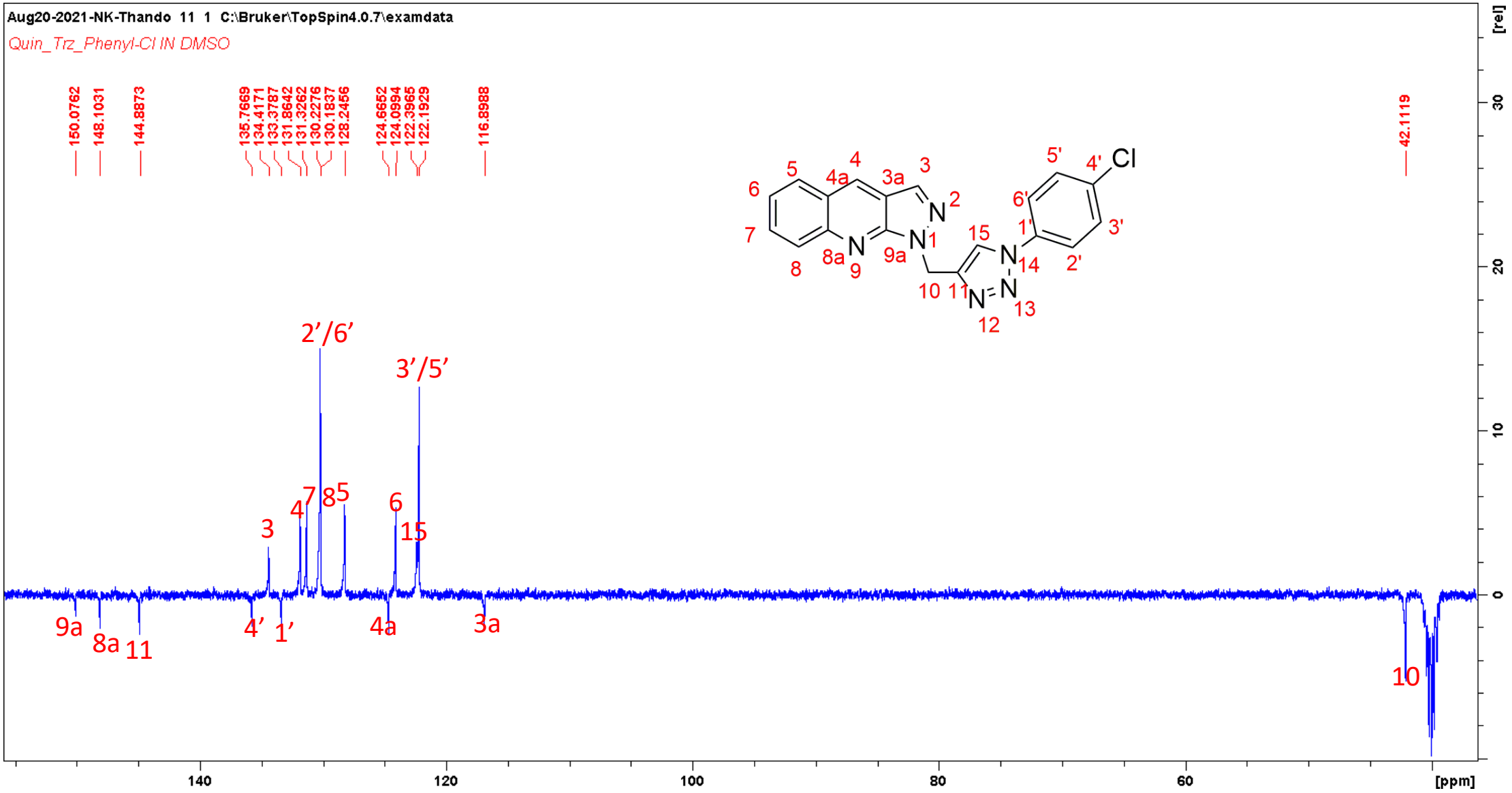
HRMS spectrum of 1-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10b**)




FTIR spectrum of 1-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10b**)




$^{1}$H NMR spectrum of 1-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10c**)




$^{13}$C NMR spectrum of 1-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10c**)

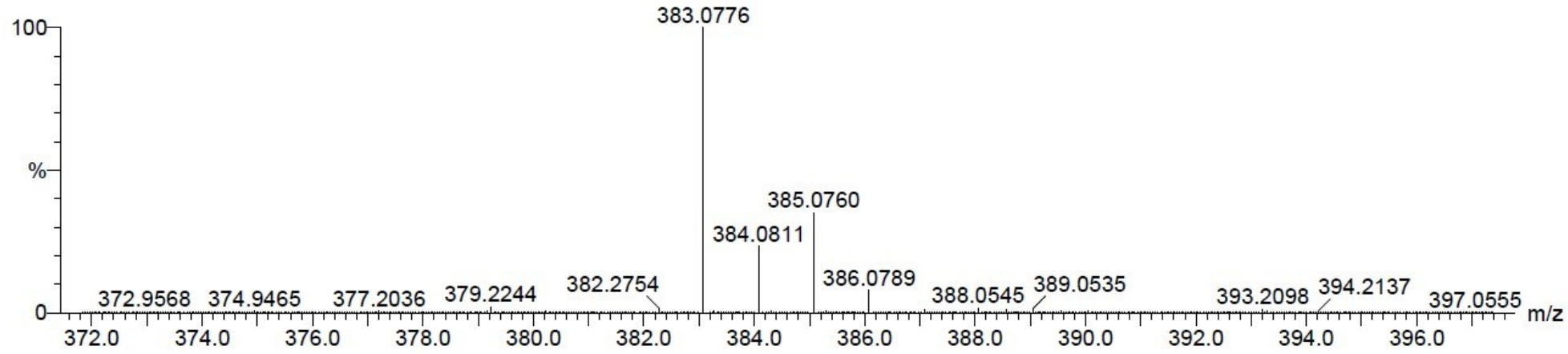
## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 Na: 1-1 Cl: 0-1

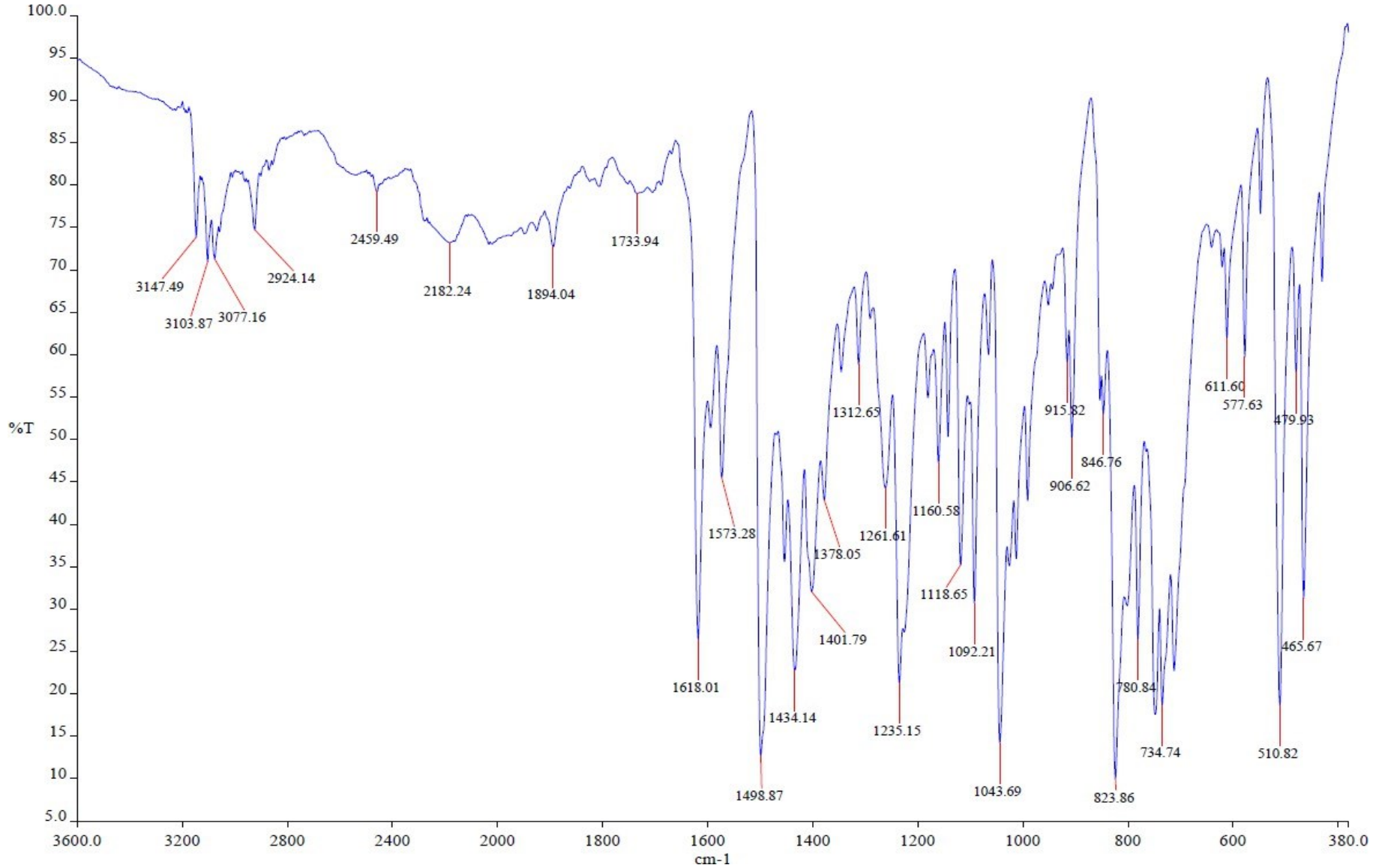
PyQuiTriPh-Cl 15 (0.472) Cm (1:61)

TOF MS ES+
1.10e+005

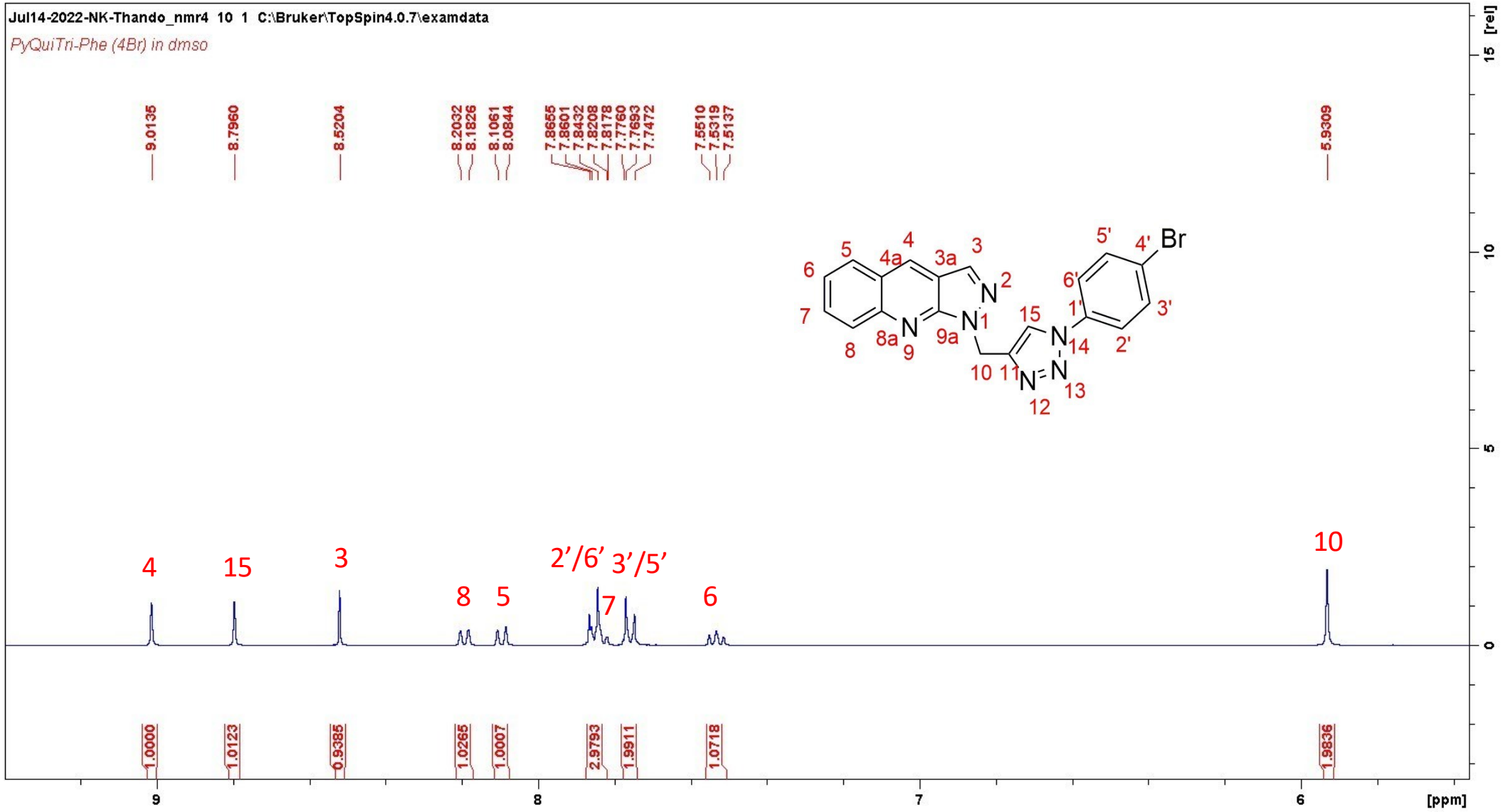



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 383.0776 | 383.0788 | -1.2 | -3.1 | 15.5 | 411.0 | 0.0 | C19 H13 N6 Na Cl |

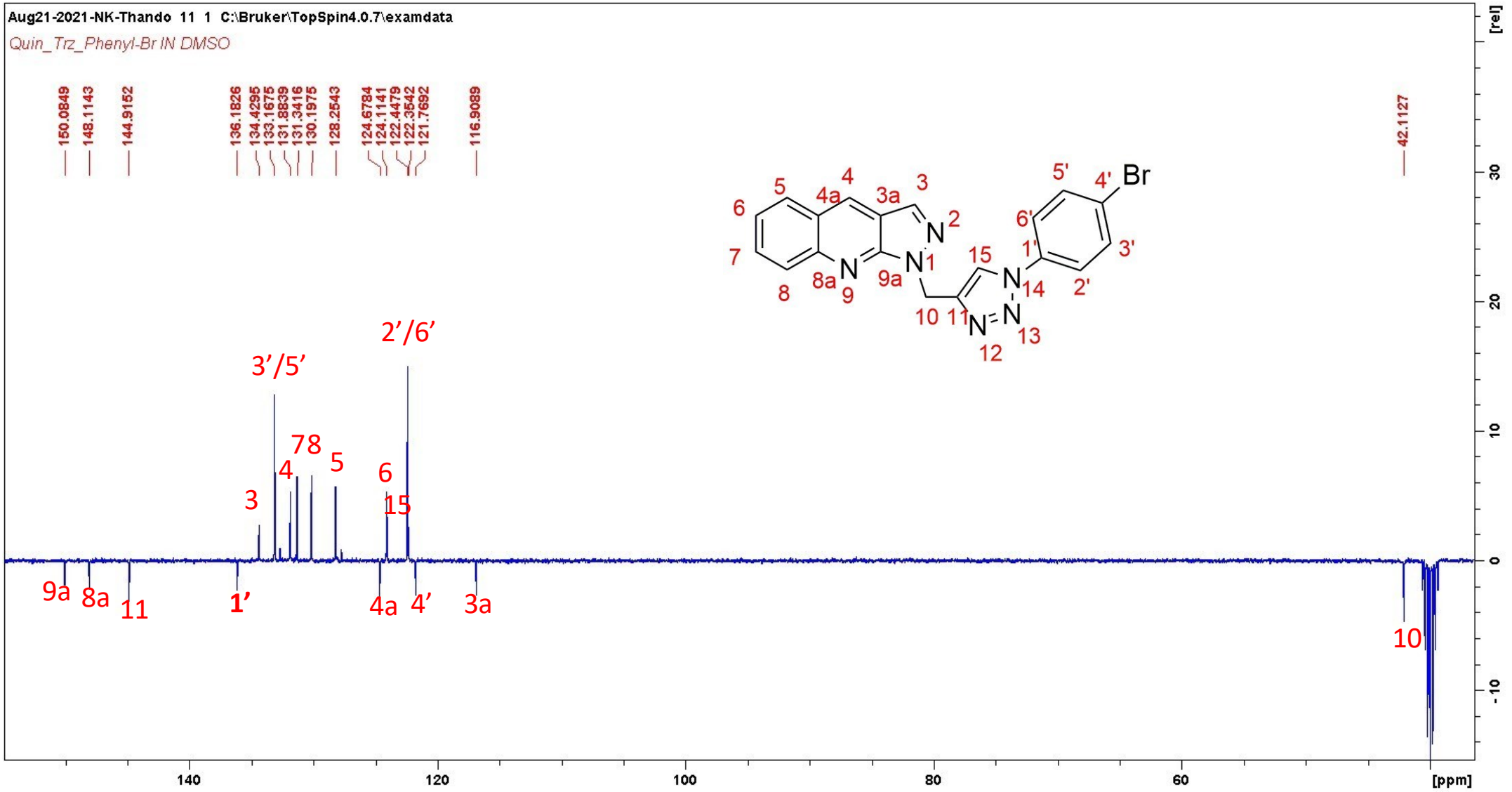
HRMS spectrum of 1-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10c**)




FTIR spectrum of 1-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10c**)




$^{1}$H NMR spectrum of 1-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10d**)



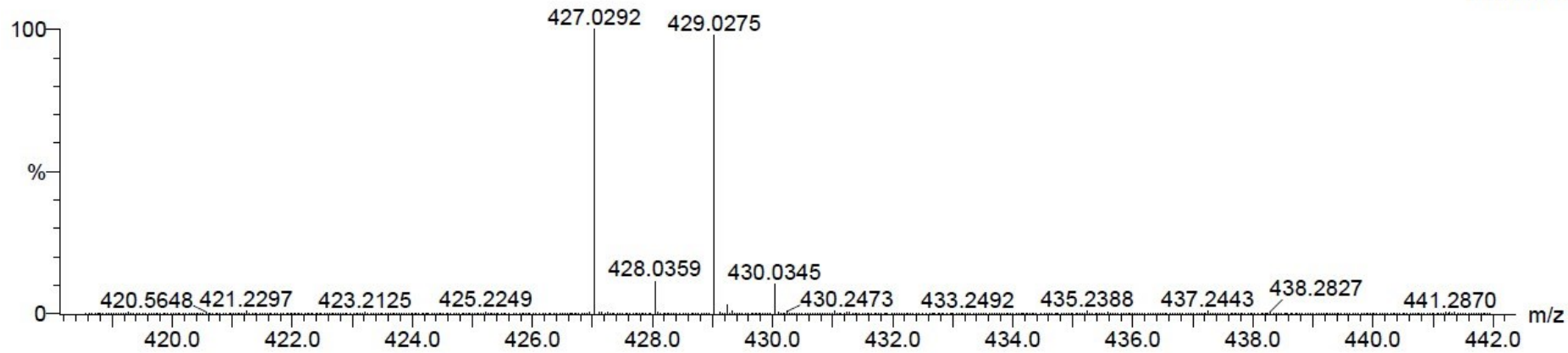

$^{13}$C NMR spectrum of 1-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10d**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 Na: 0-1 Br: 0-1

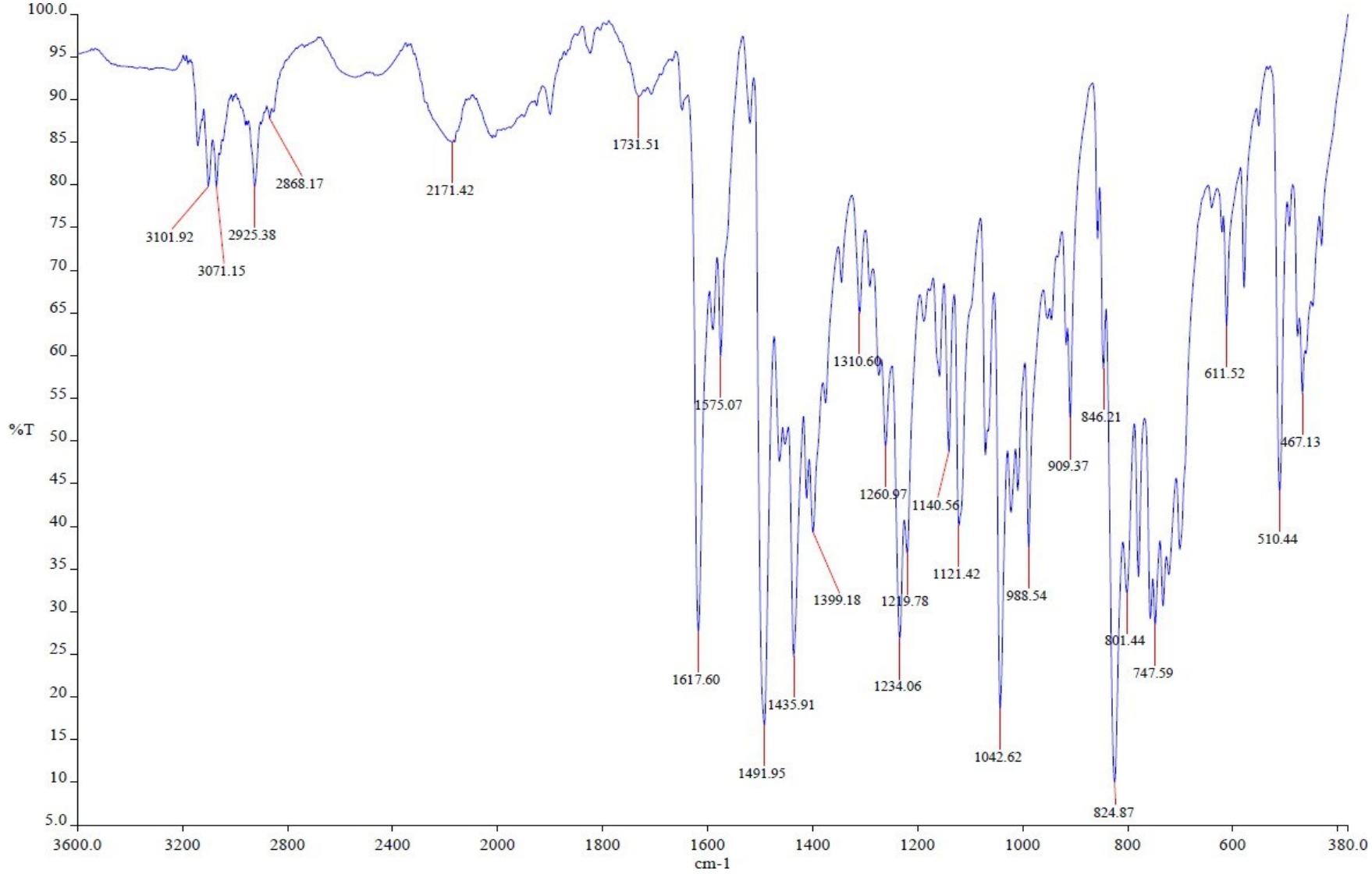
PyQuiTriPh-Br 56 (1.932) Cm (1:58)

TOF MS ES+
1.67e+004

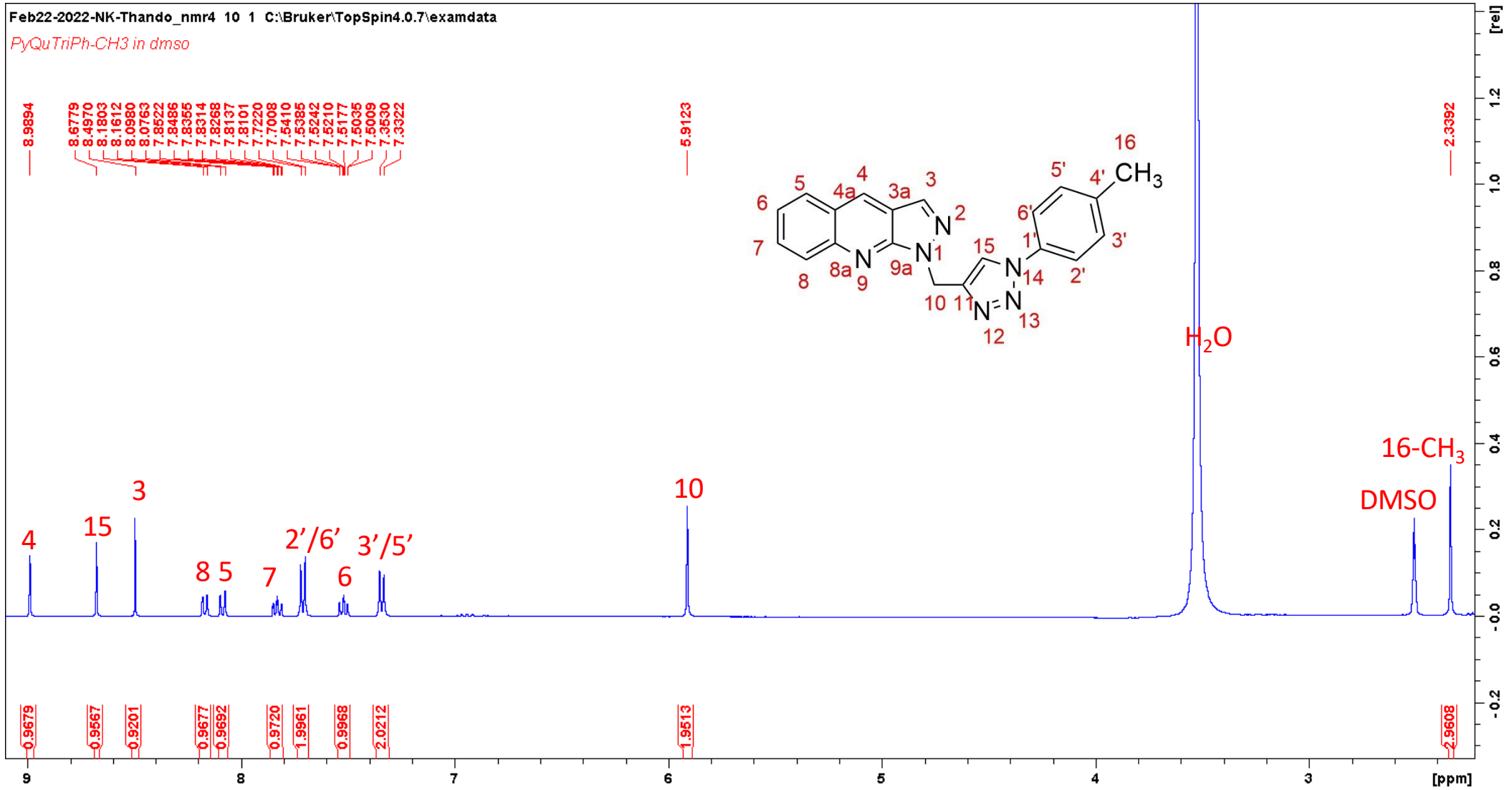



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 427.0292 | 427.0283 | 0.9 | 2.1 | 15.5 | 302.1 | 0.0 | C19 H13 N6 Na Br |

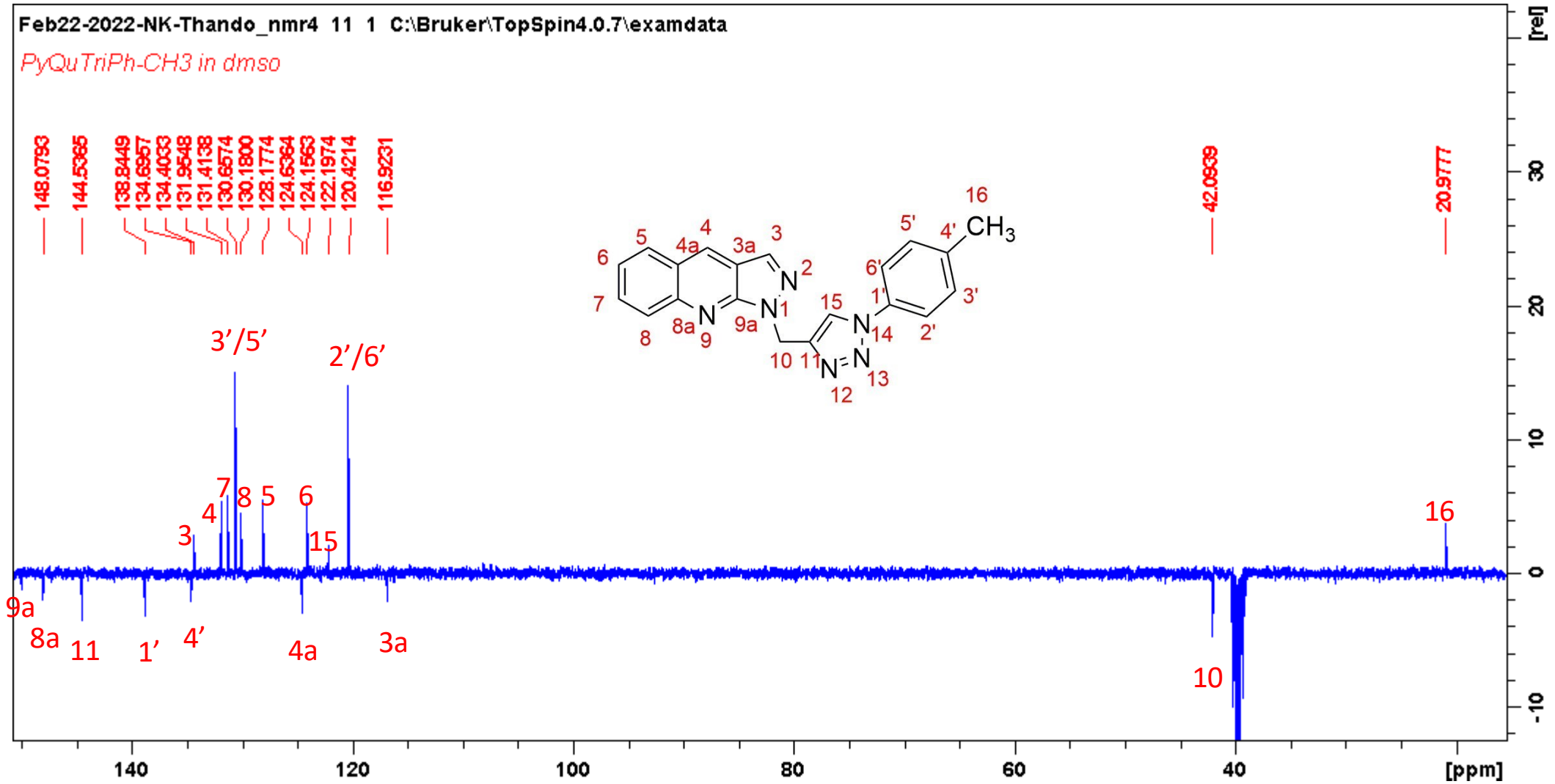
HRMS spectrum of 1-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10d**)




FTIR spectrum of 1-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10d**)




$^{1}$H NMR spectrum of 1-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10e**)



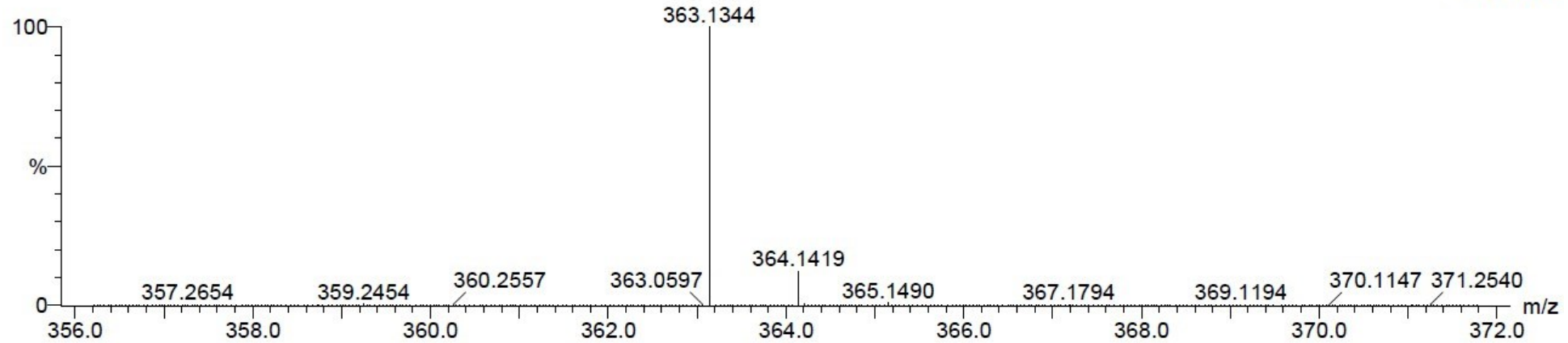

$^{13}$C NMR spectrum of 1-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10e**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 15-20 N: 5-10 Na: 0-1 Br: 0-1

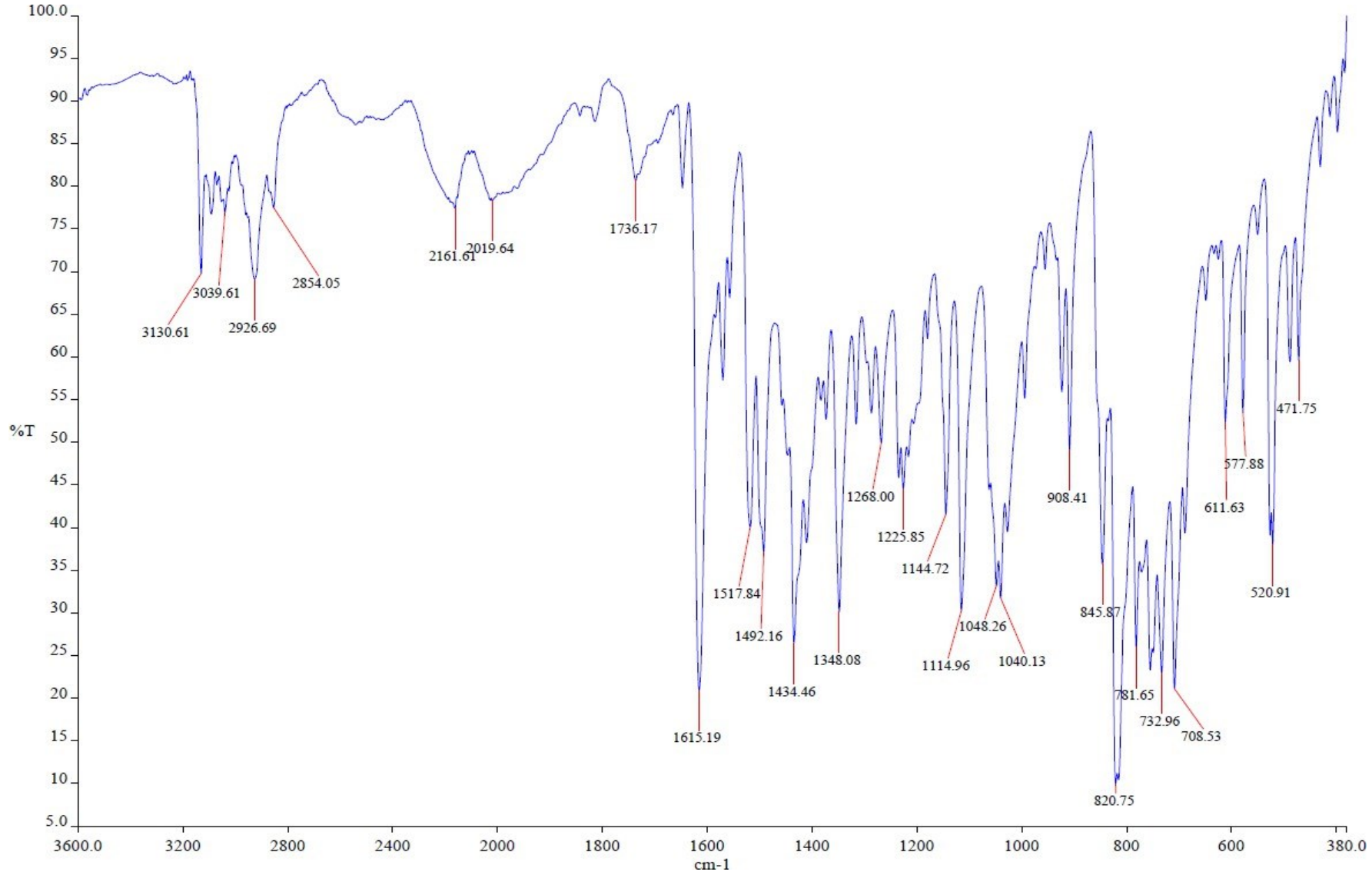
PyQuiTriPh-CH3 29 (0.983) Cm (1:58)

TOF MS ES+
3.76e+004

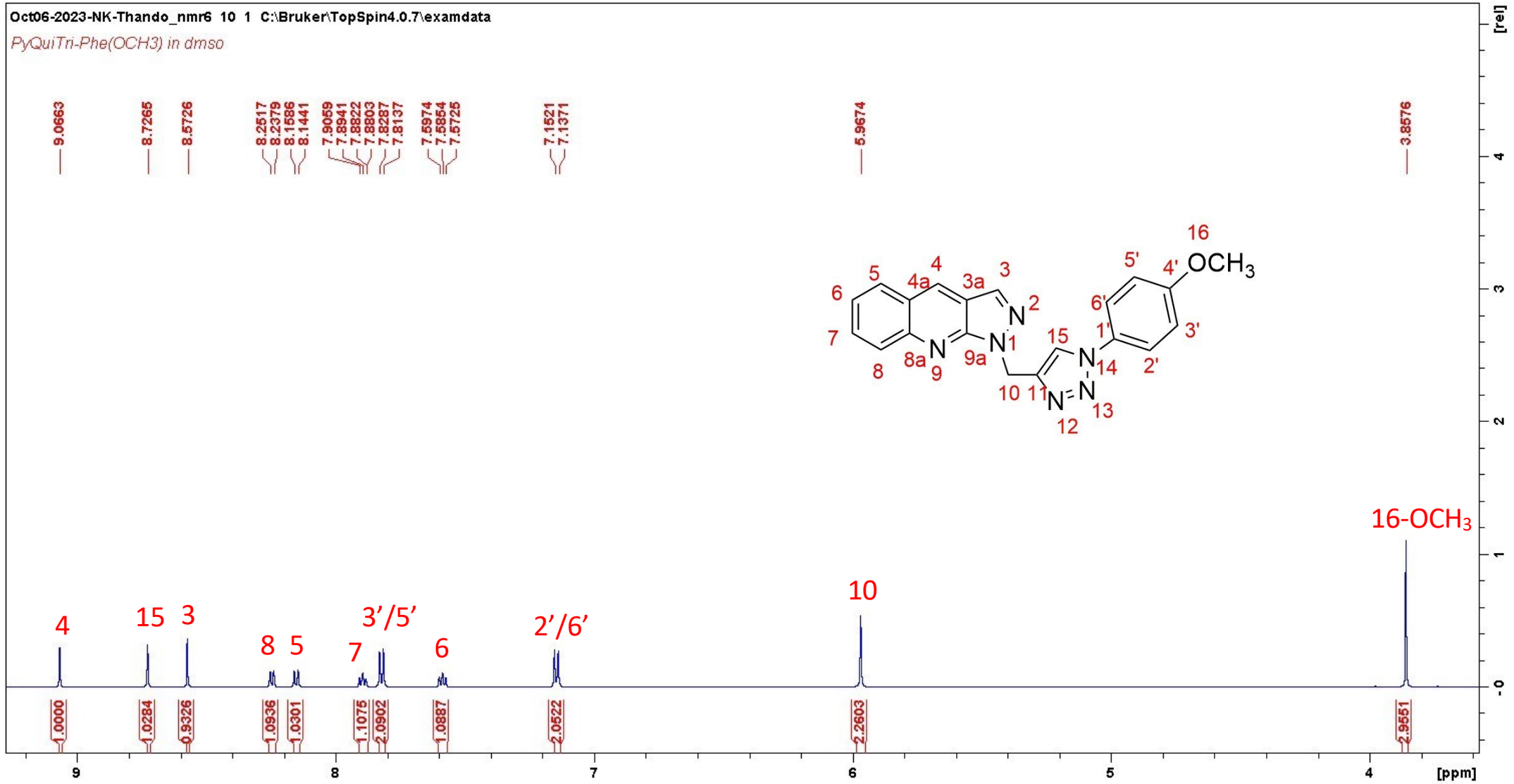



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 363.1344 | 363.1334 | 1.0 | 2.8 | 15.5 | 250.5 | 0.0 | C20 H16 N6 Na |

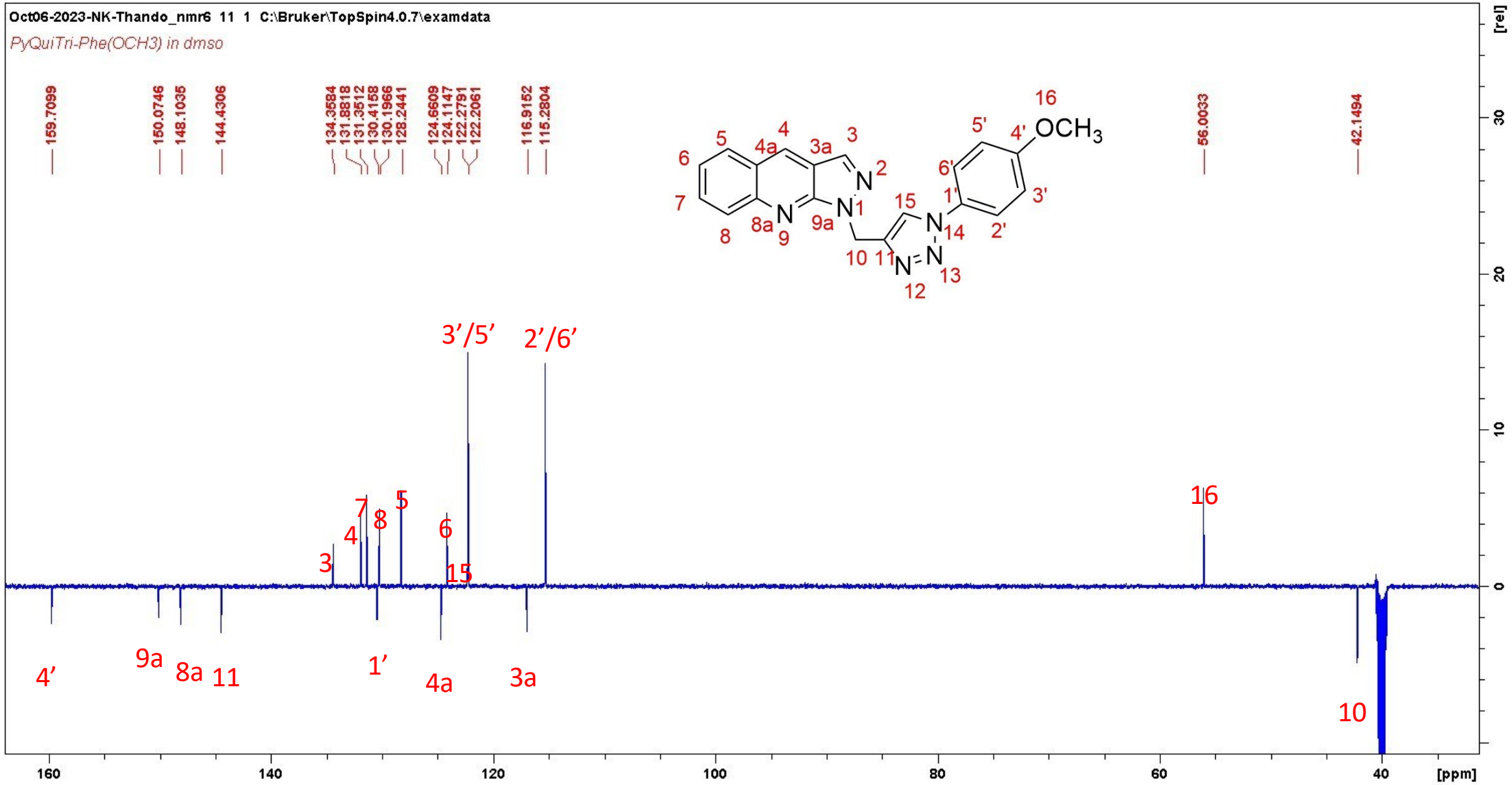
HRMS spectrum of 1-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10e**)




FTIR spectrum of 1-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10e**)




$^{1}$H NMR spectrum of 1-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10f**)



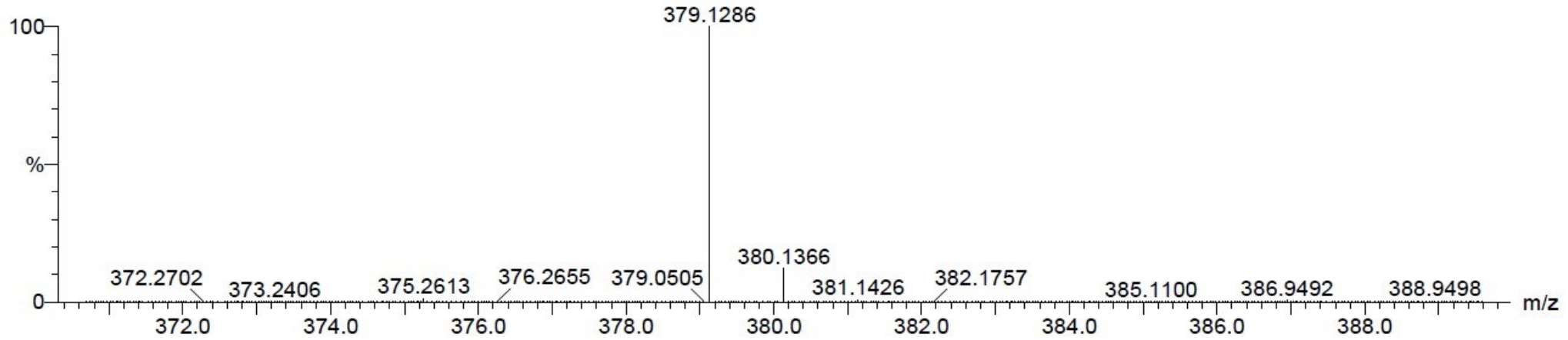

$^{13}$C NMR spectrum of 1-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10f**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 15-20 N: 5-10 O: 0-5 Na: 1-1

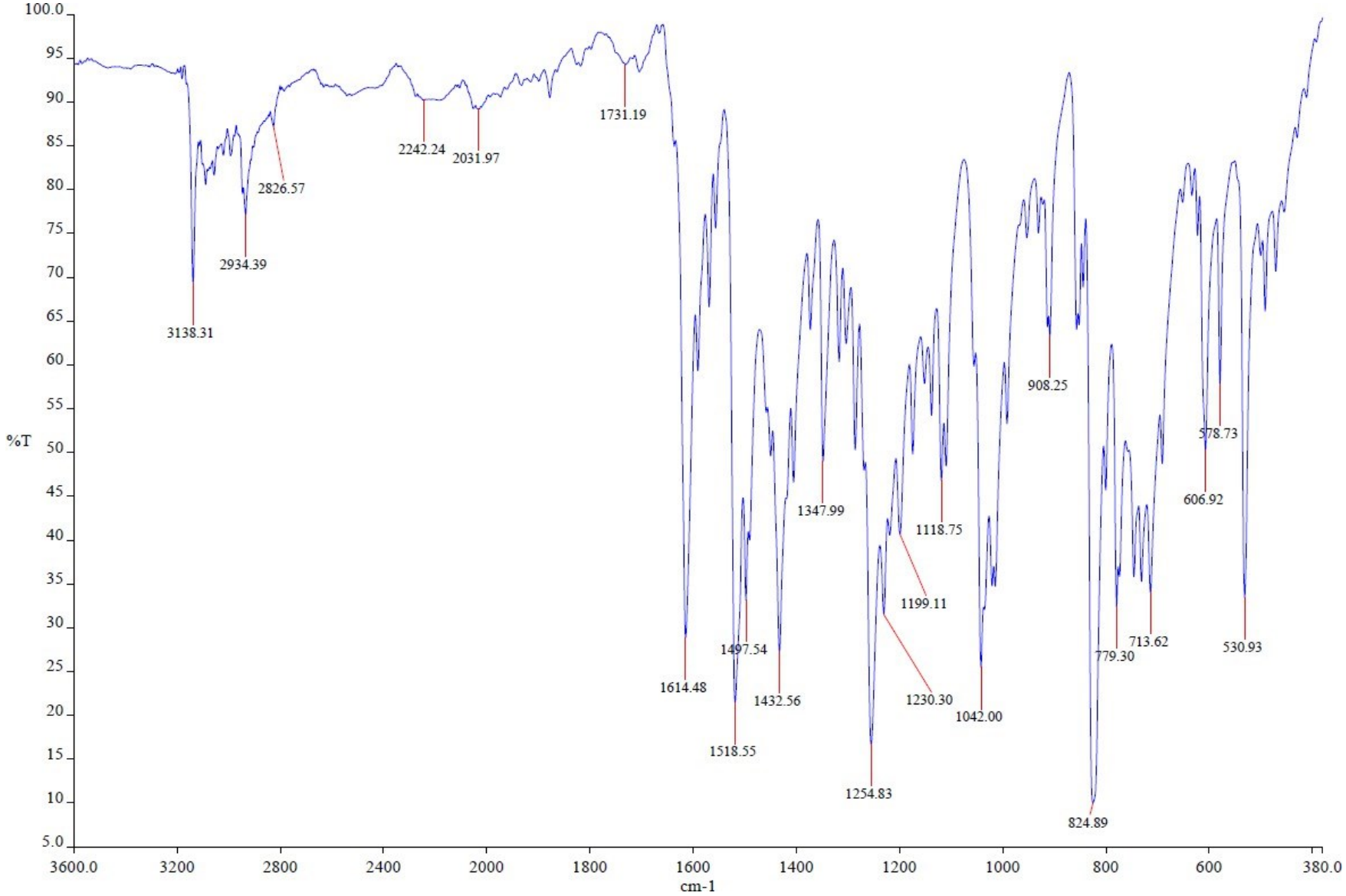
PyQuiTriPh-OCH3 11 (0.351) Cm (1:58)

TOF MS ES+
4.30e+004

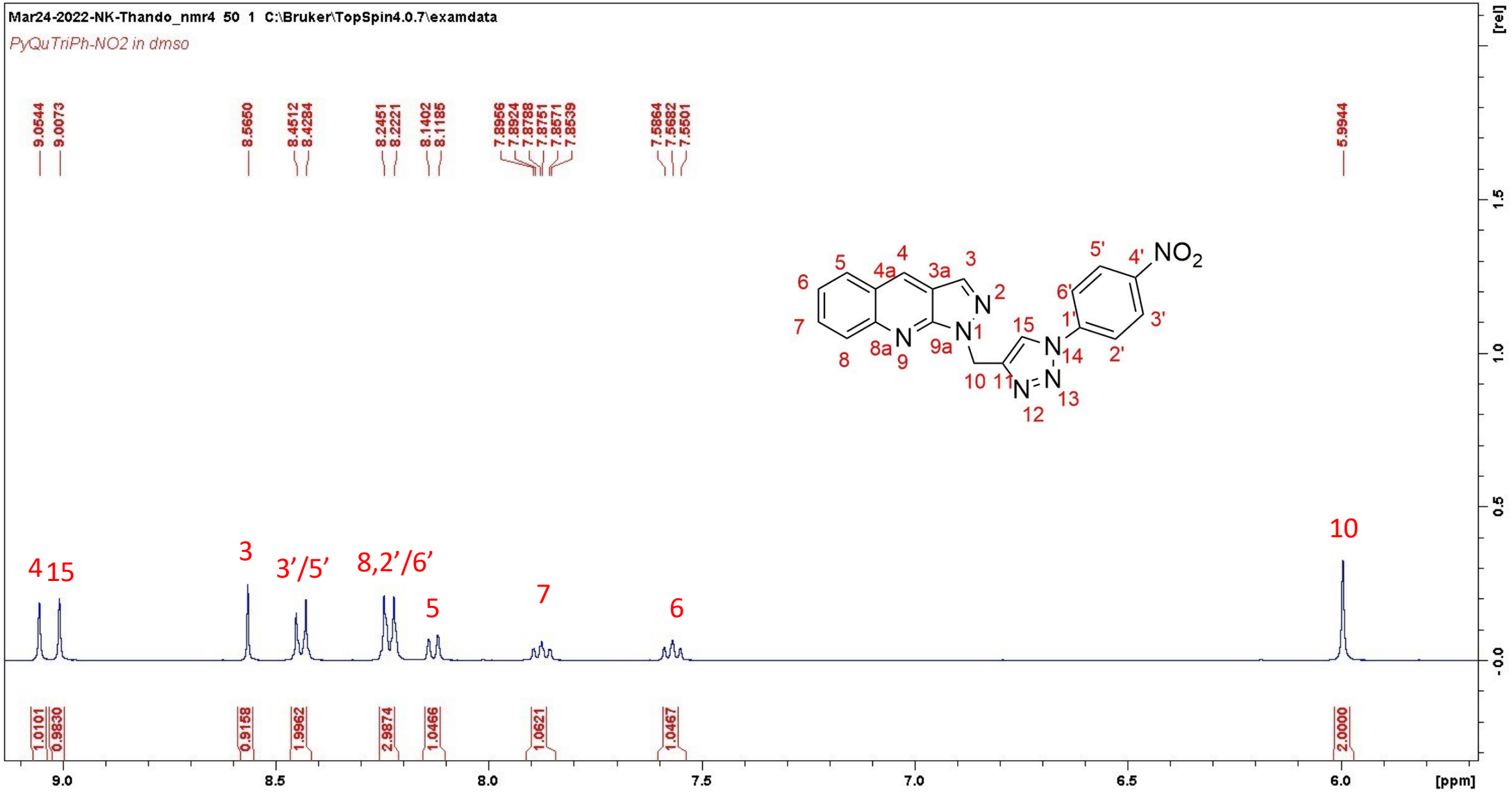



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 379.1286 | 379.1283 | 0.3 | 0.8 | 15.5 | 237.5 | 0.0 | C20 H16 N6 O Na |

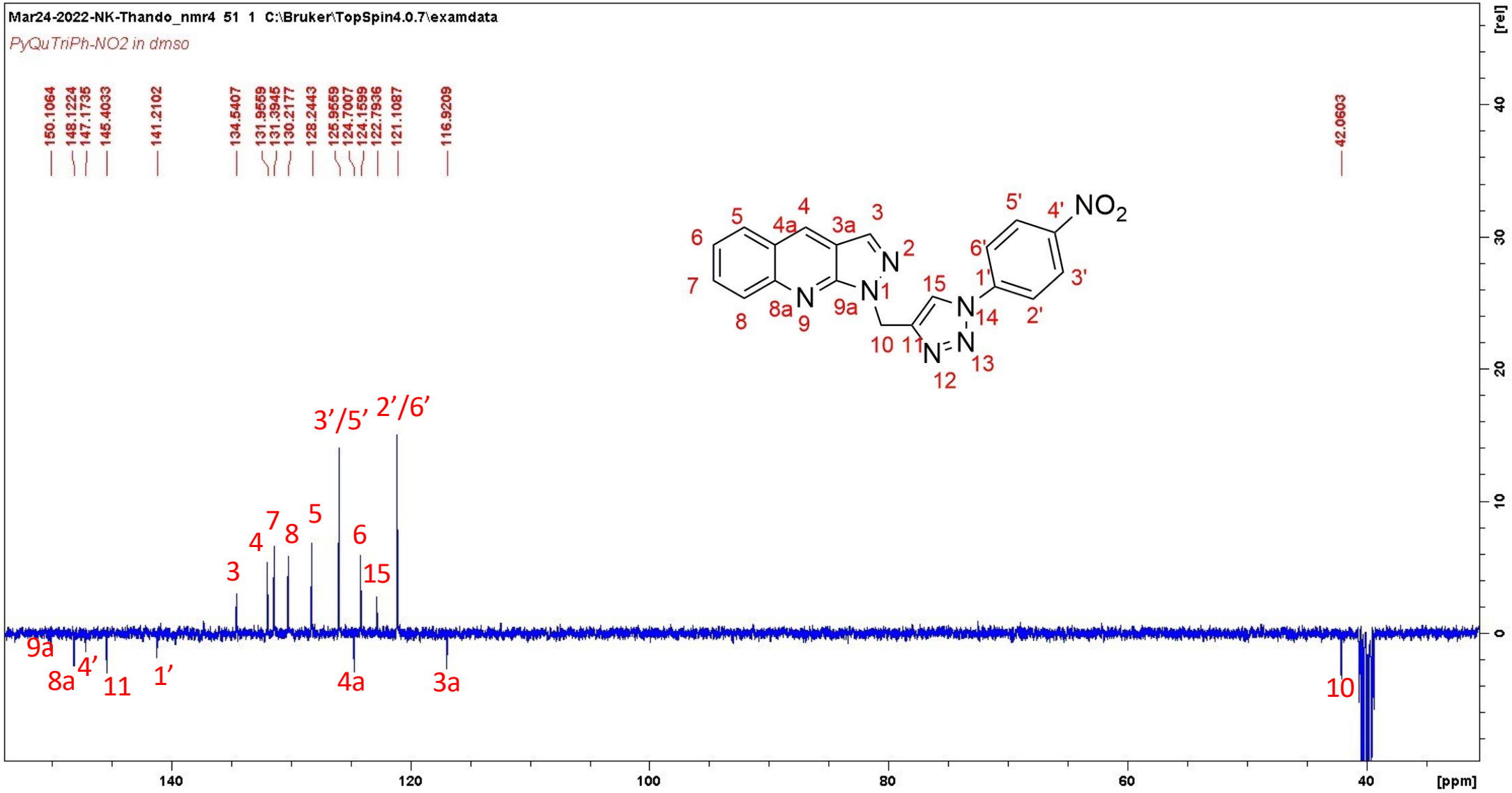
HRMS spectrum of 1-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10f**)




FTIR spectrum of 1-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10f**)




$^{1}$H NMR spectrum of 1-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10g**)



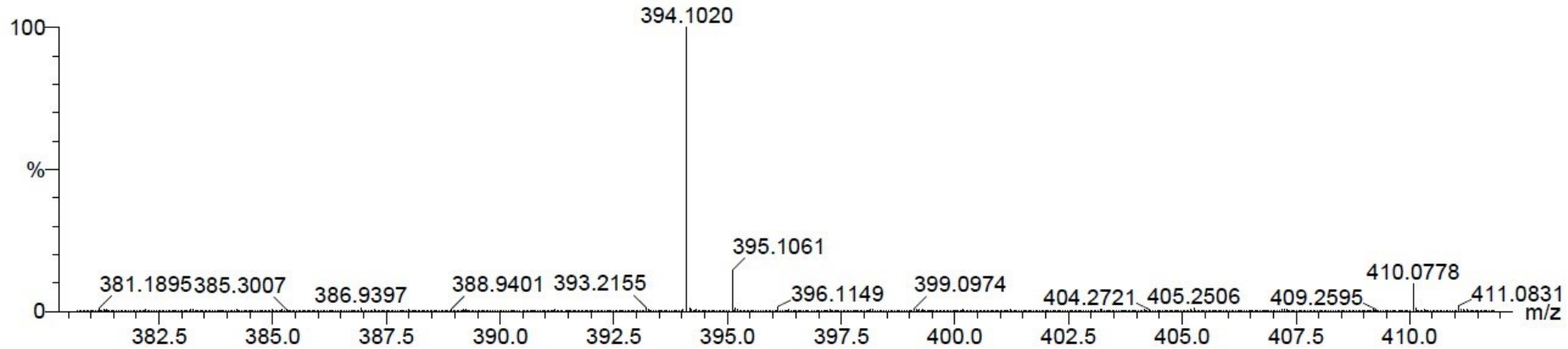

$^{13}$C NMR spectrum of 1-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10g**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 O: 0-5 Na: 1-1

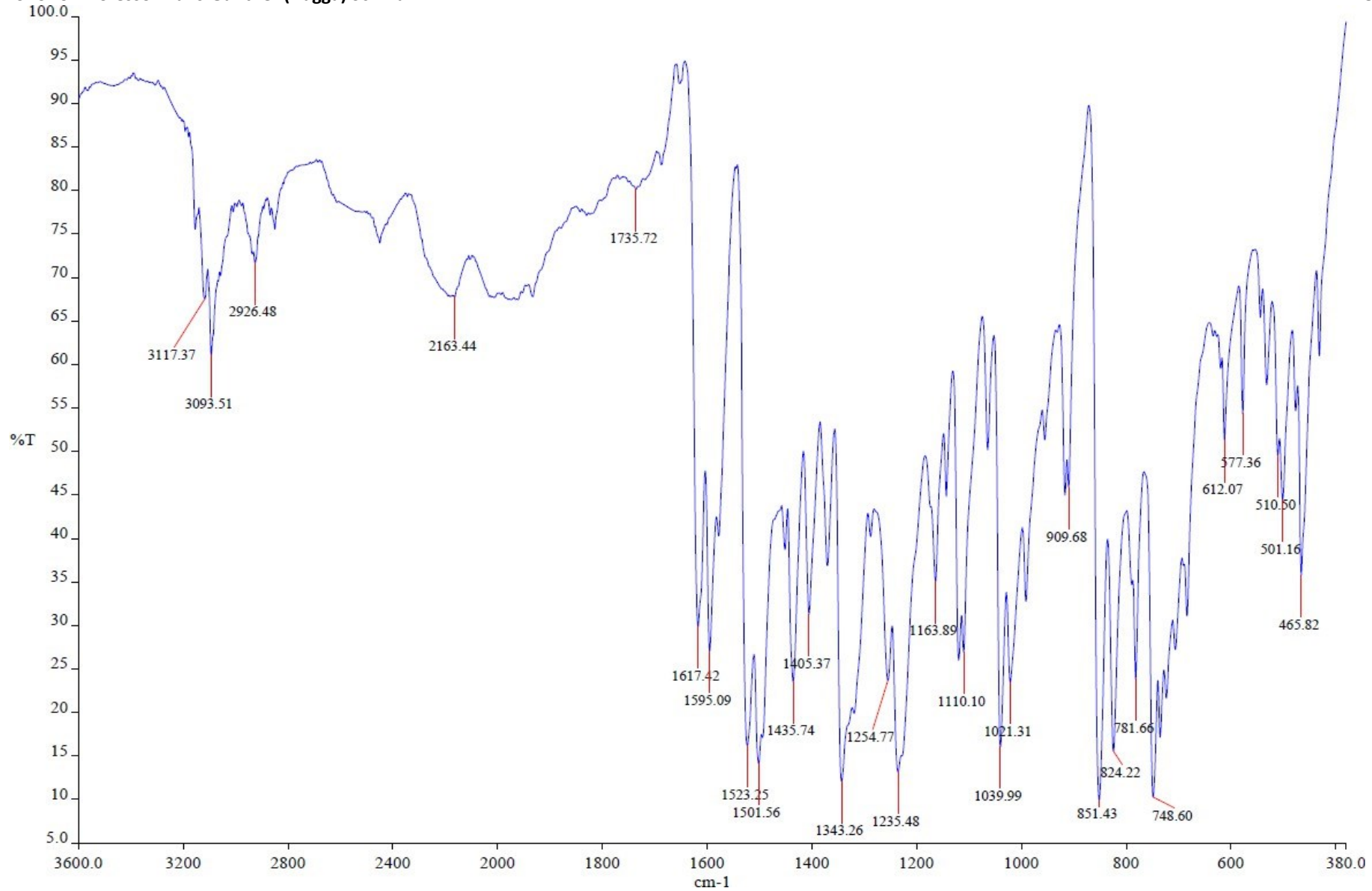
PyQuiTriPh-NO2 8 (0.236) Cm (1:61)

TOF MS ES+
1.43e+004

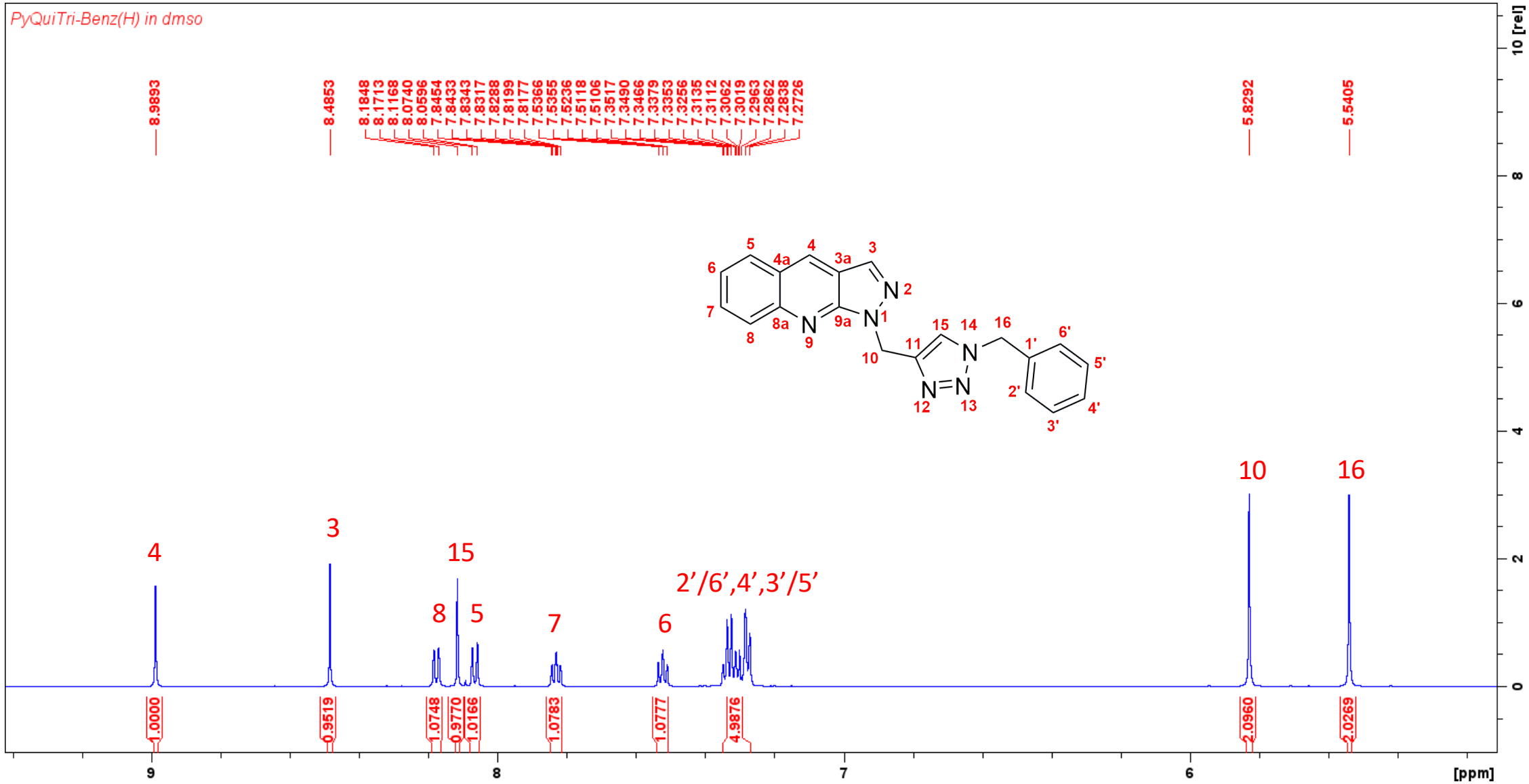



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 394.1020 | 394.1028 | -0.8 | -2.0 | 16.5 | 355.6 | 0.0 | C19 H13 N7 O2 Na |

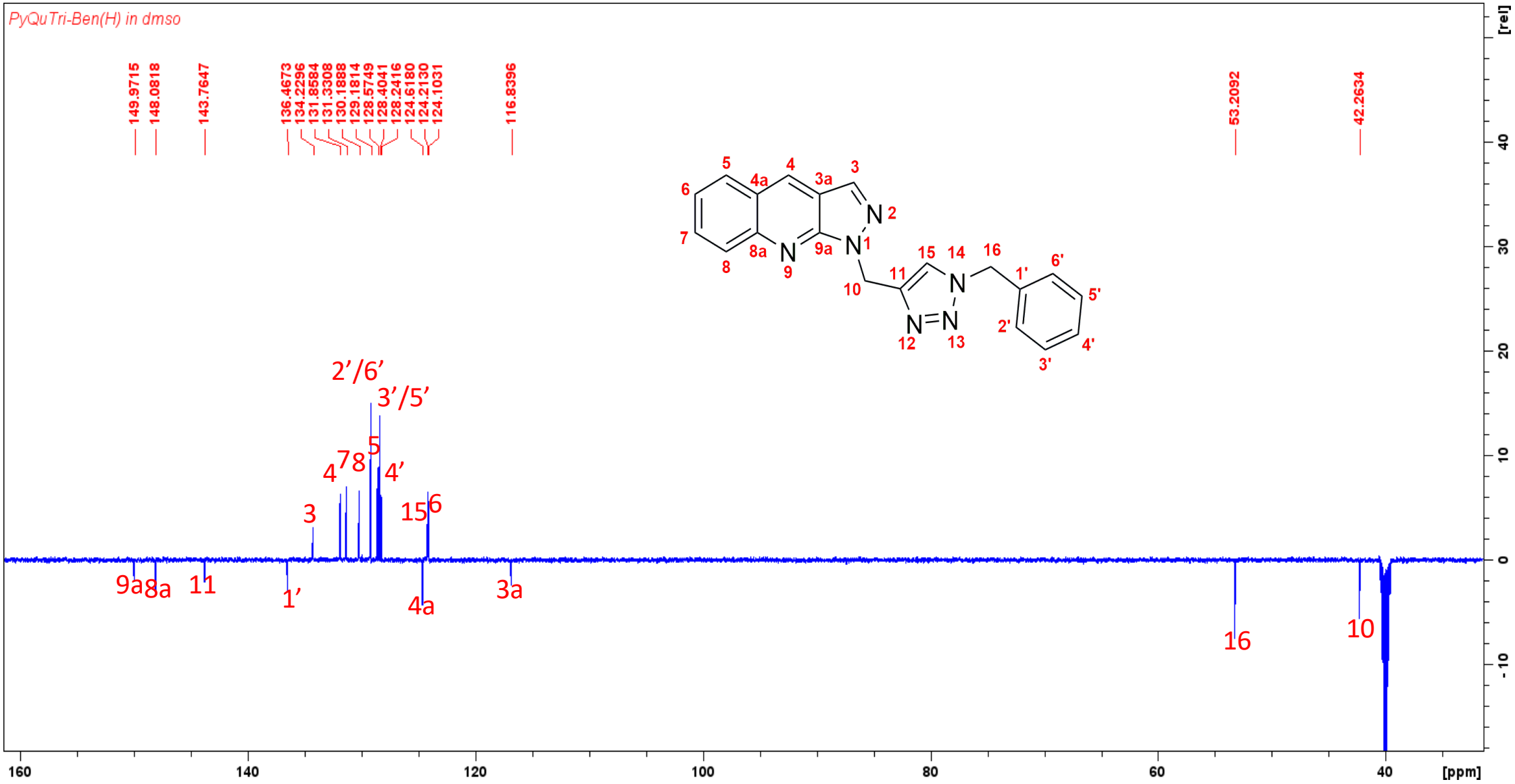
HRMS spectrum of 1-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10g**)



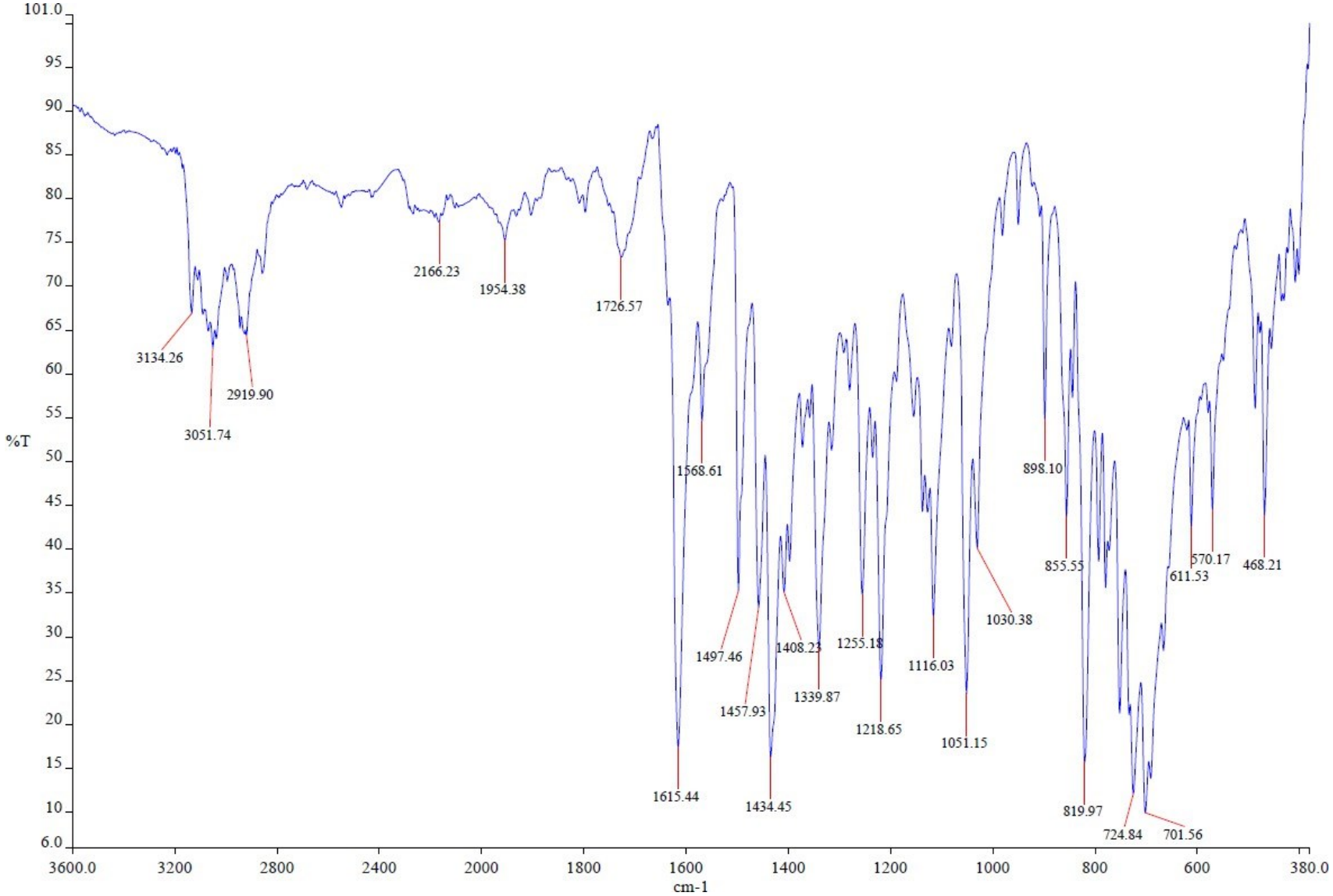

FTIR spectrum of 1-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**10g**)



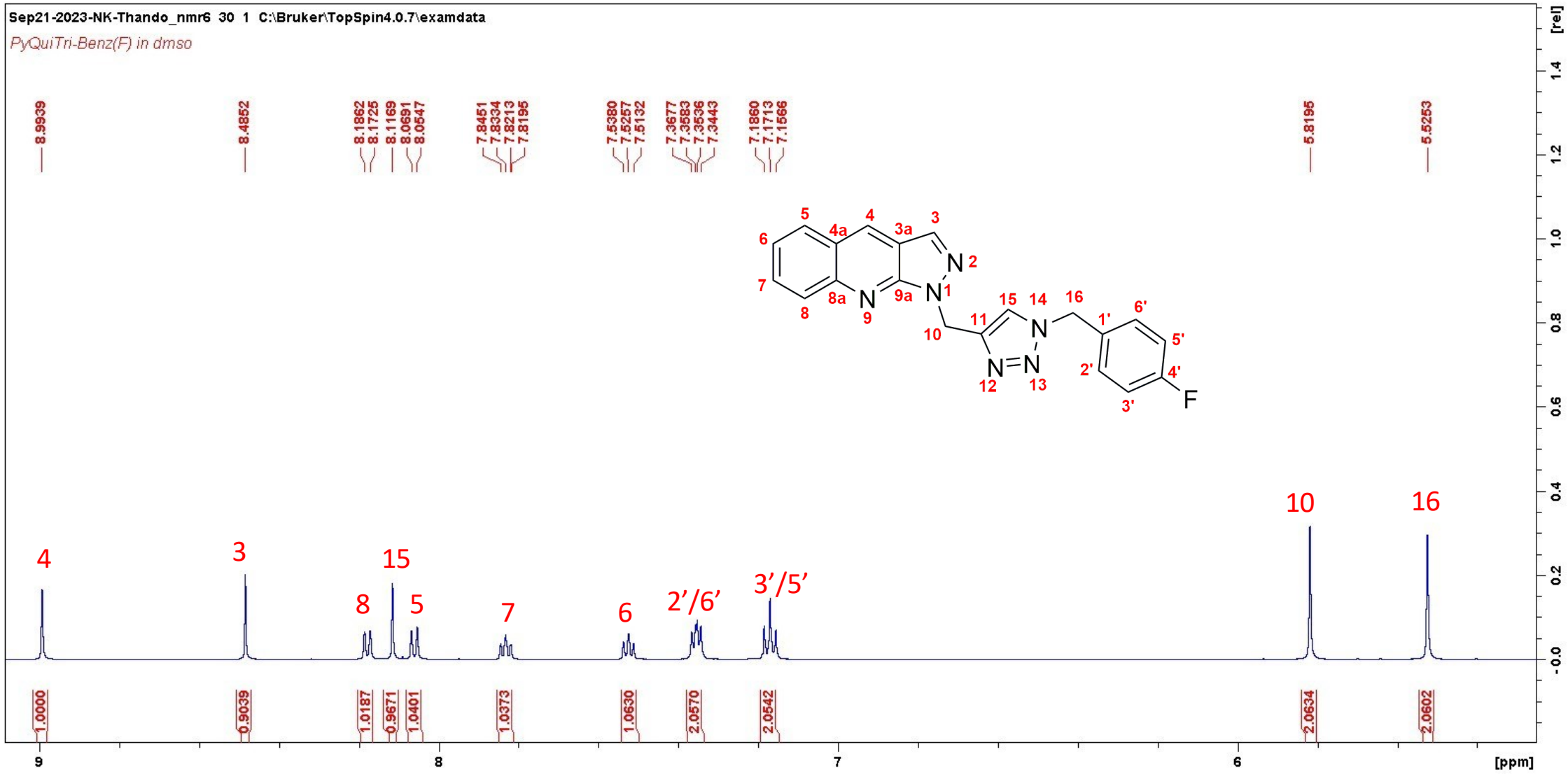

$^{1}$H NMR spectrum of 1-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11a**)



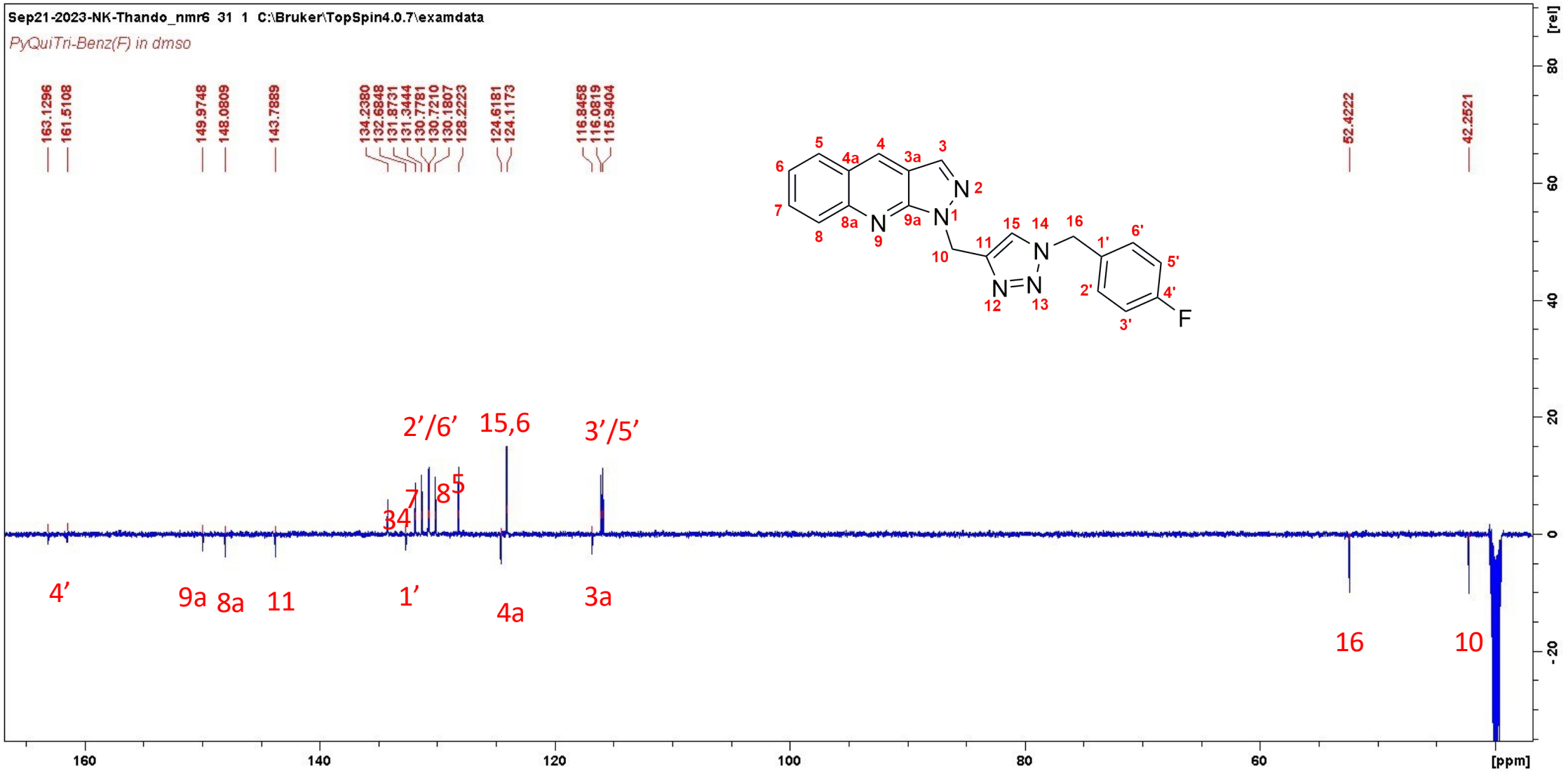

$^{13}$C NMR spectrum of 1-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11a**)




FTIR spectrum of 1-((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11a**)




$^{1}$H NMR spectrum of 1-((1-(4-fluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11b**)



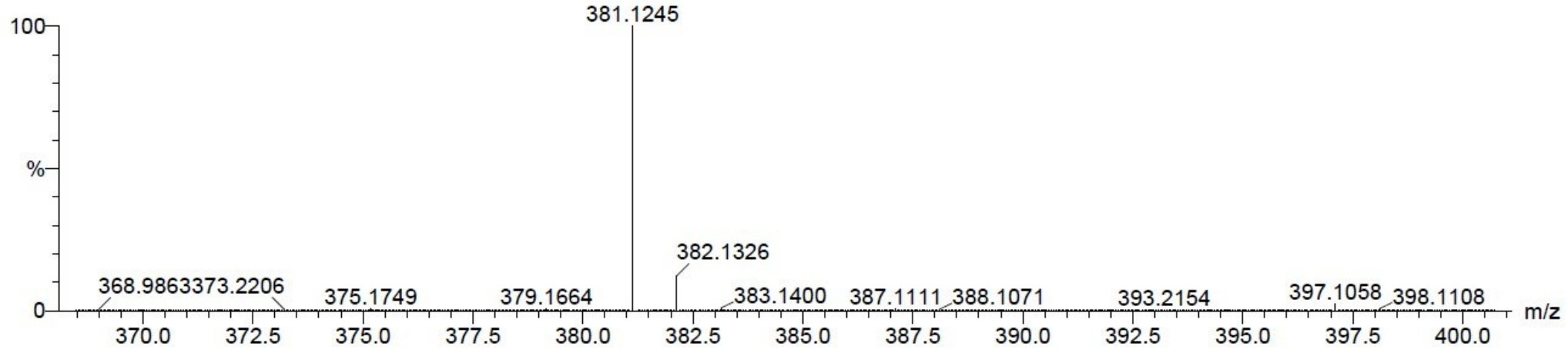

$^{13}$C NMR spectrum of 1-((1-(4-fluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11b**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 F: 1-1 Na: 1-1

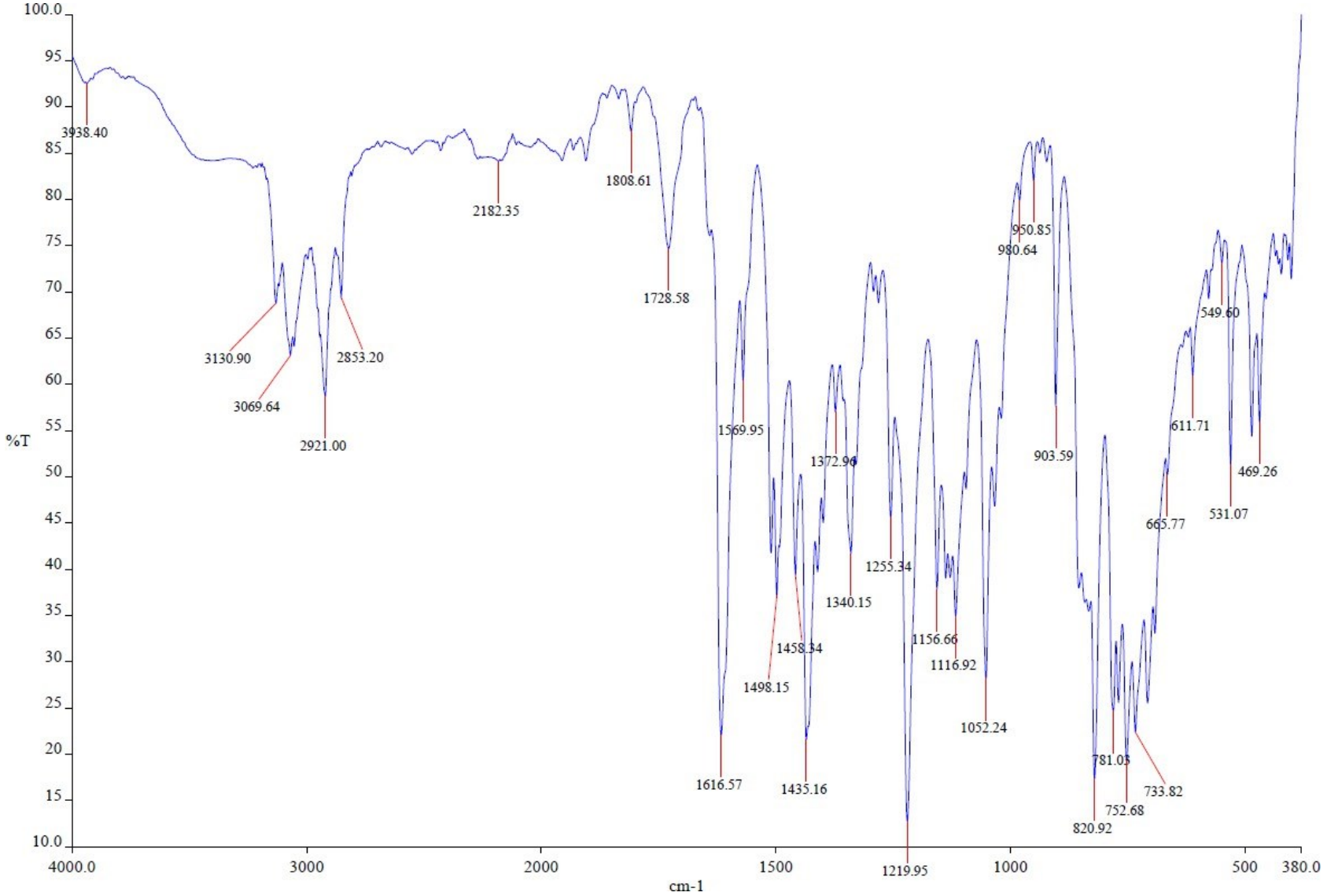
PyQuiTriBen-F 46 (1.518) Cm (1:61)

TOF MS ES+
1.39e+005

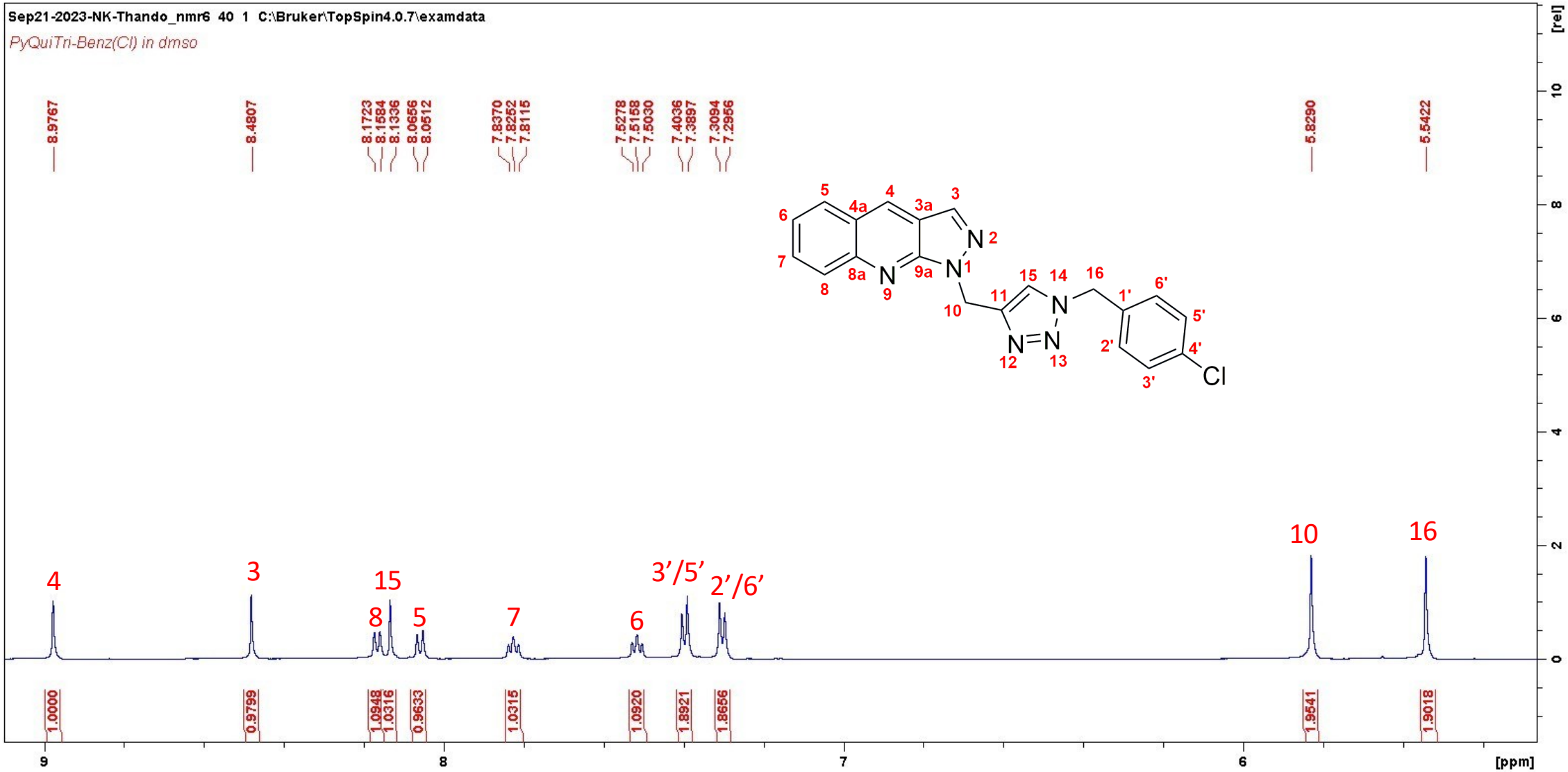



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 381.1245 | 381.1240 | 0.5 | 1.3 | 15.5 | 319.2 | 0.0 | C20 H15 N6 F Na |

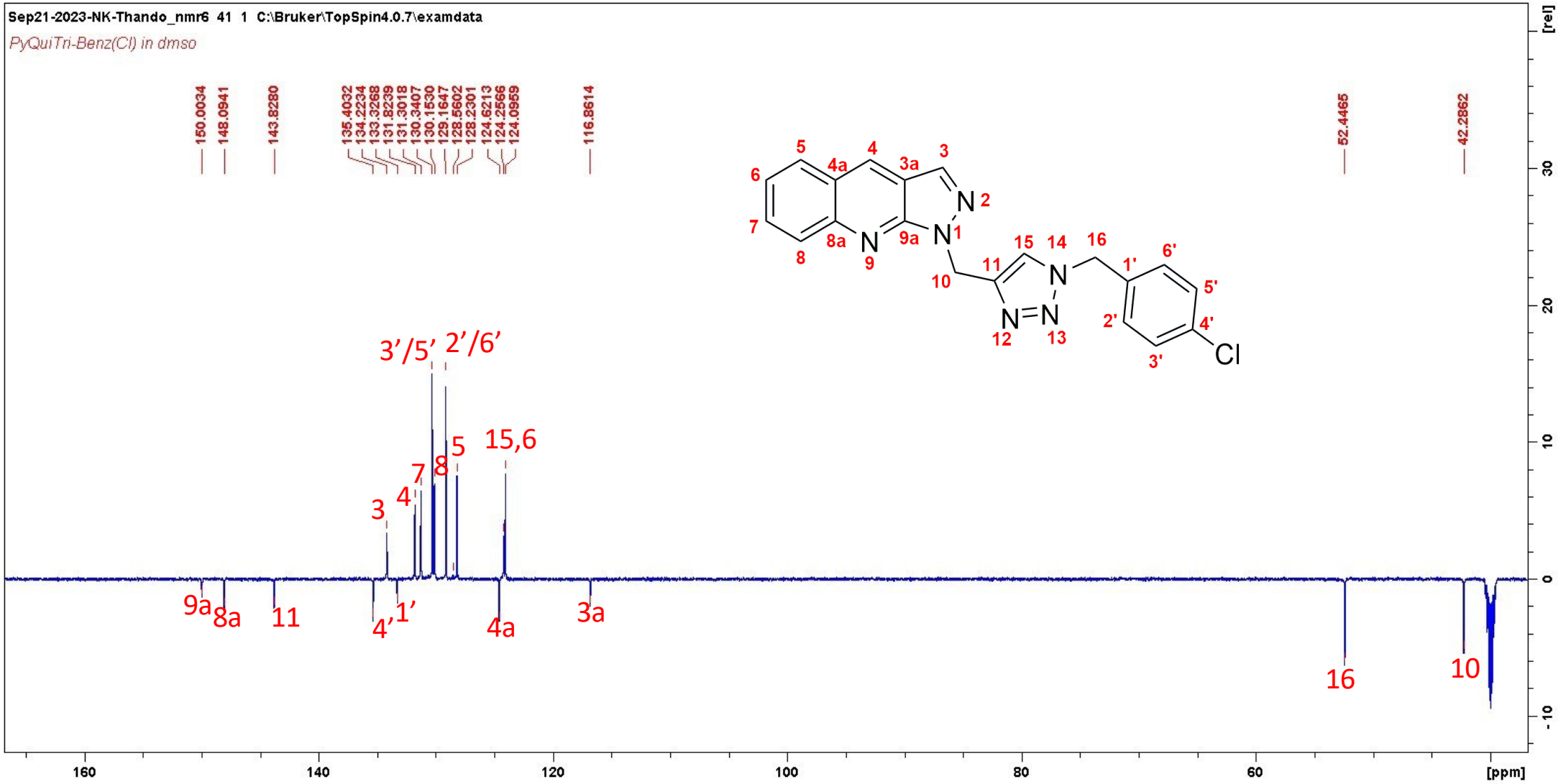
HRMS spectrum of 1-((1-(4-fluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11b**)




FTIR spectrum of 1-((1-(4-fluorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11b**)




$^{1}$H NMR spectrum of 1-((1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11c**)



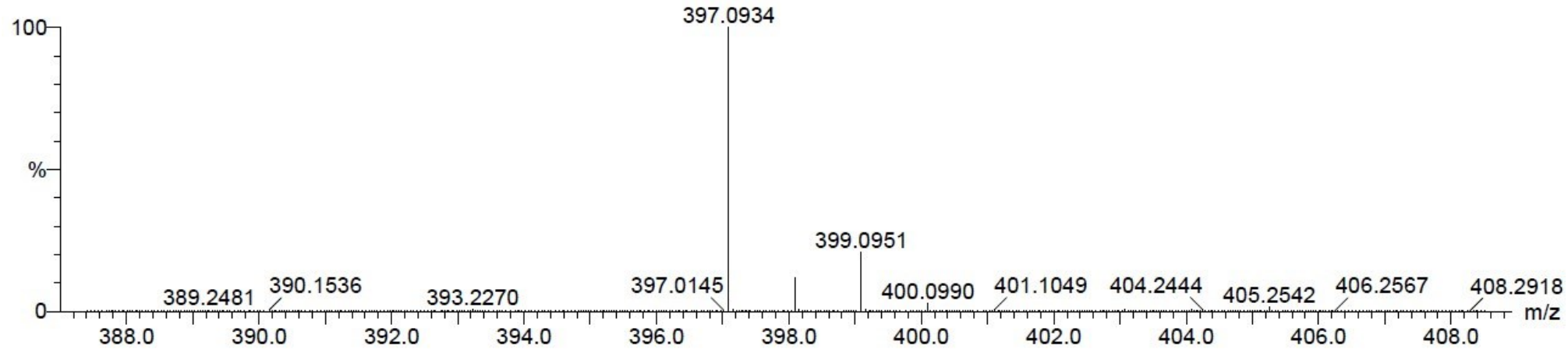

$^{13}$C NMR spectrum of 1-((1-(4-chorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11c**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 Na: 1-1 Cl: 0-1

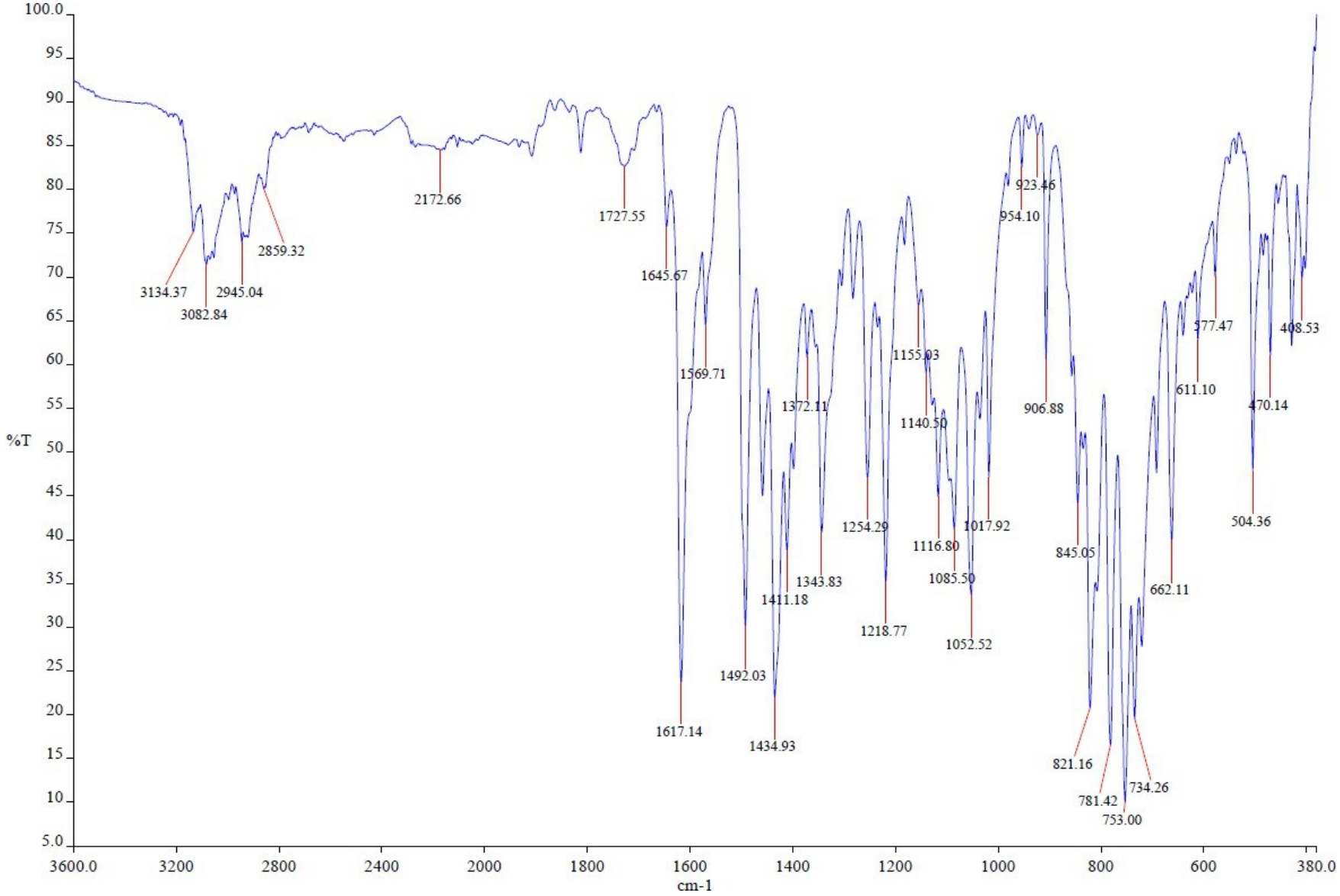
PyQuiTriBen-Cl 15 (0.472) Cm (1:58)

TOF MS ES+
2.29e+004

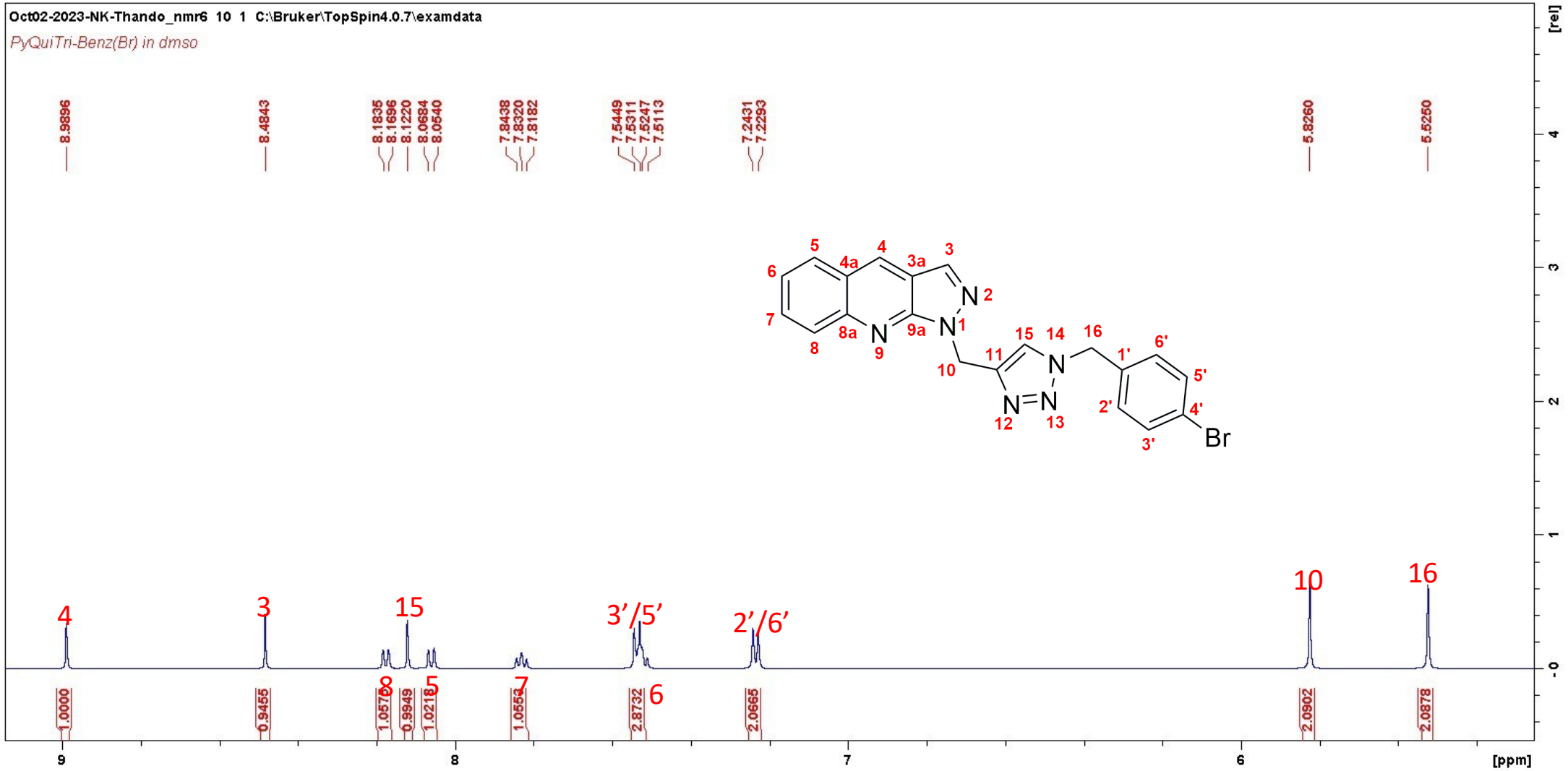



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 397.0934 | 397.0944 | -1.0 | -2.5 | 15.5 | 239.4 | 0.0 | C20 H15 N6 Na Cl |

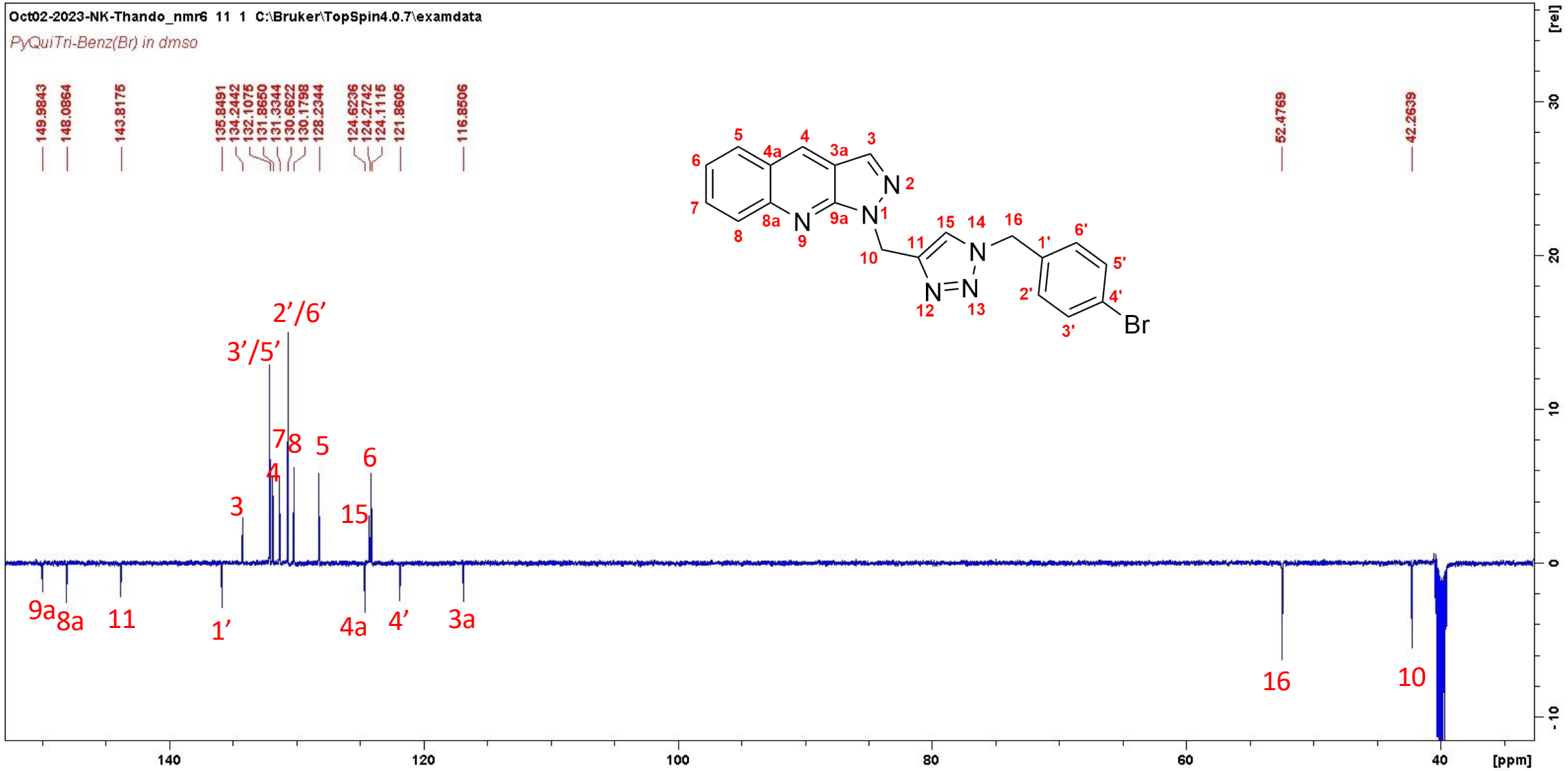
HRMS spectrum of 1-((1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11c**)




FTIR spectrum of 1-((1-(4-chlorobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11c**)




$^{1}$H NMR spectrum of 1-((1-(4-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11d**)



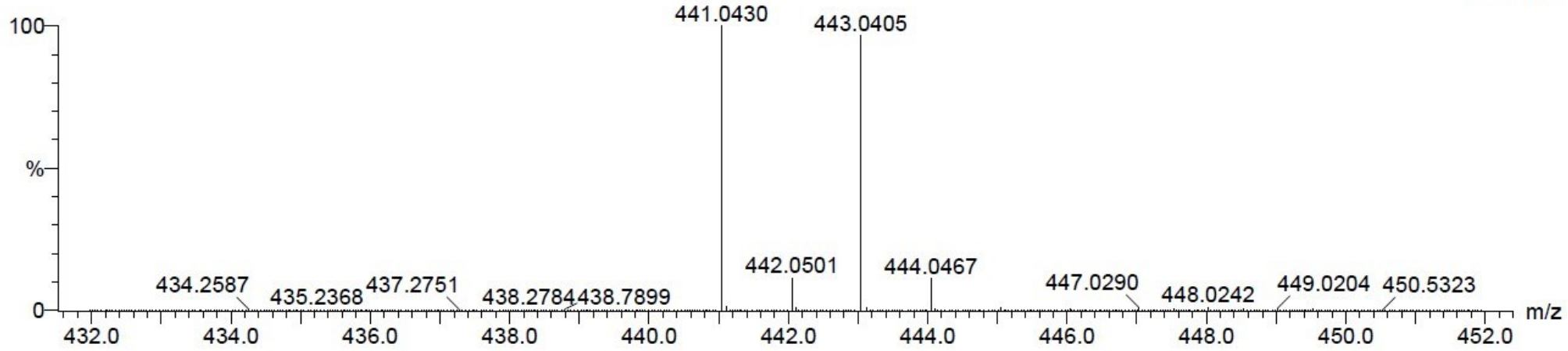

$^{13}$C NMR spectrum of 1-((1-(4-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11d**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 5-10 Na: 1-1 Br: 0-1

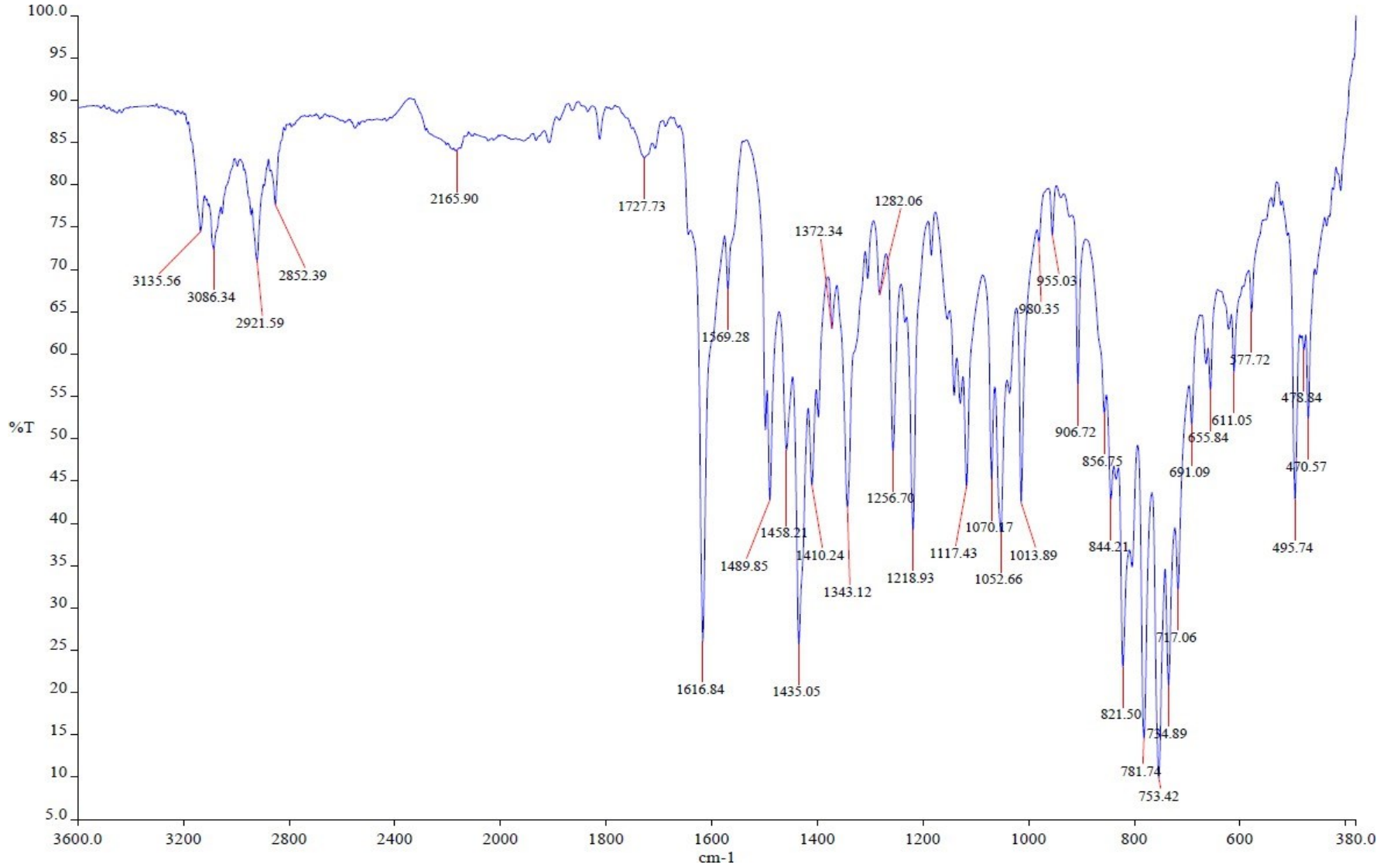
PyQuiTriBen-Br 47 (1.551) Cm (1:61)

TOF MS ES+
1.36e+004

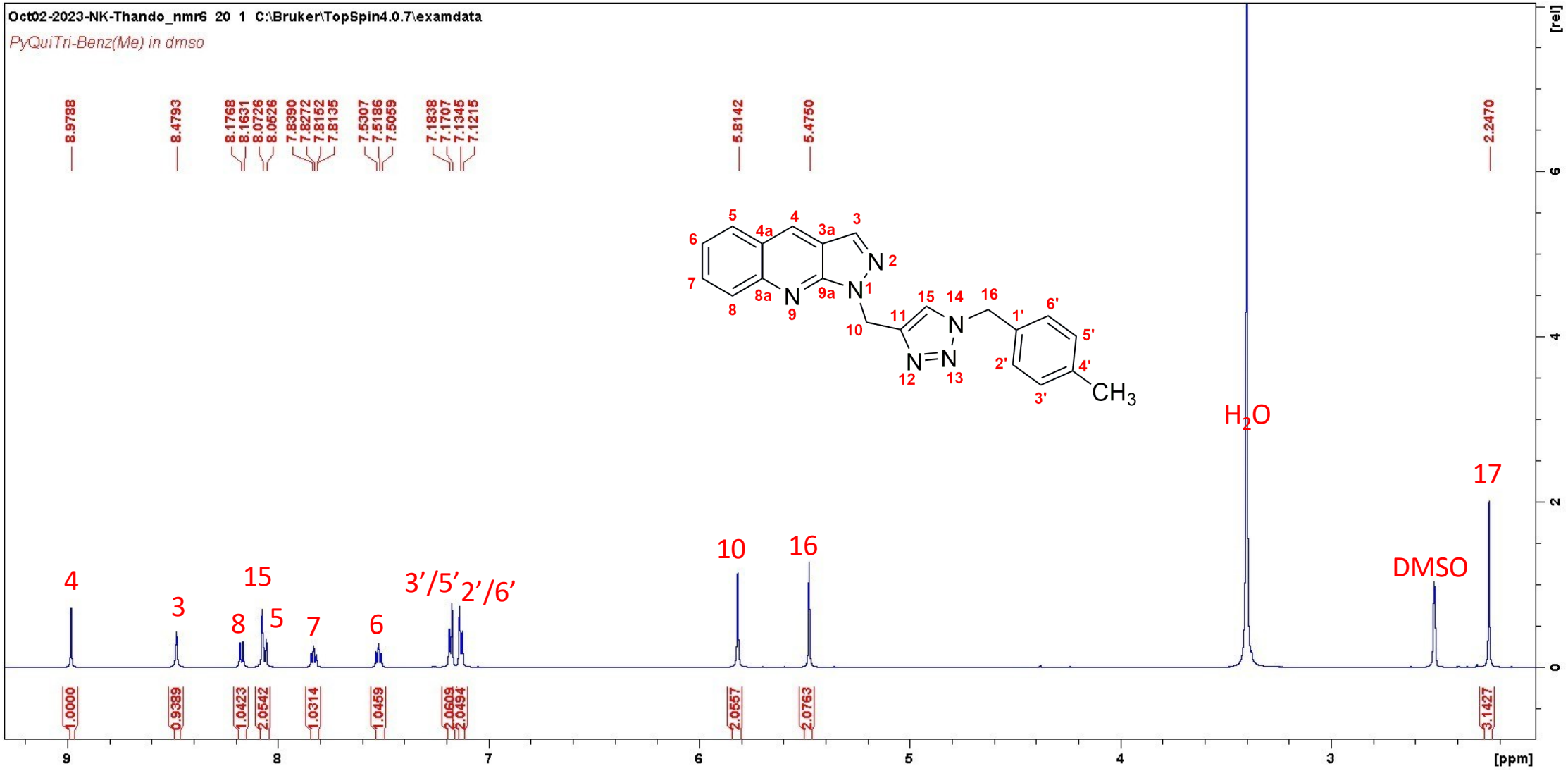



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 441.0430 | 441.0439 | -0.9 | -2.0 | 15.5 | 255.7 | 0.0 | C20 H15 N6 Na Br |

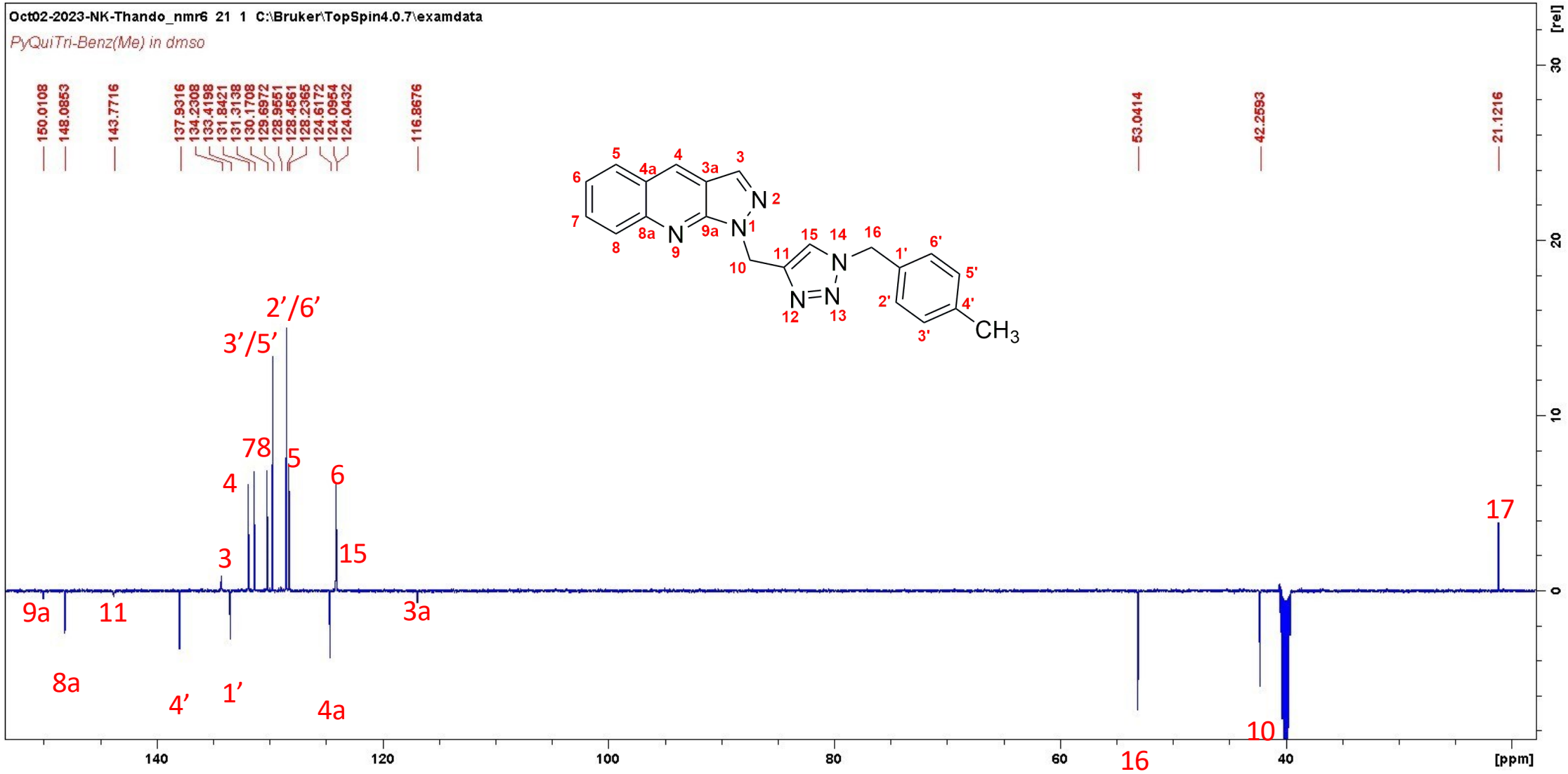
HRMS spectrum of 1-((1-(4-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11d**)




FTIR spectrum of 1-((1-(4-bromobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11d**)




$^{1}$H NMR spectrum of 1-((1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11e**)



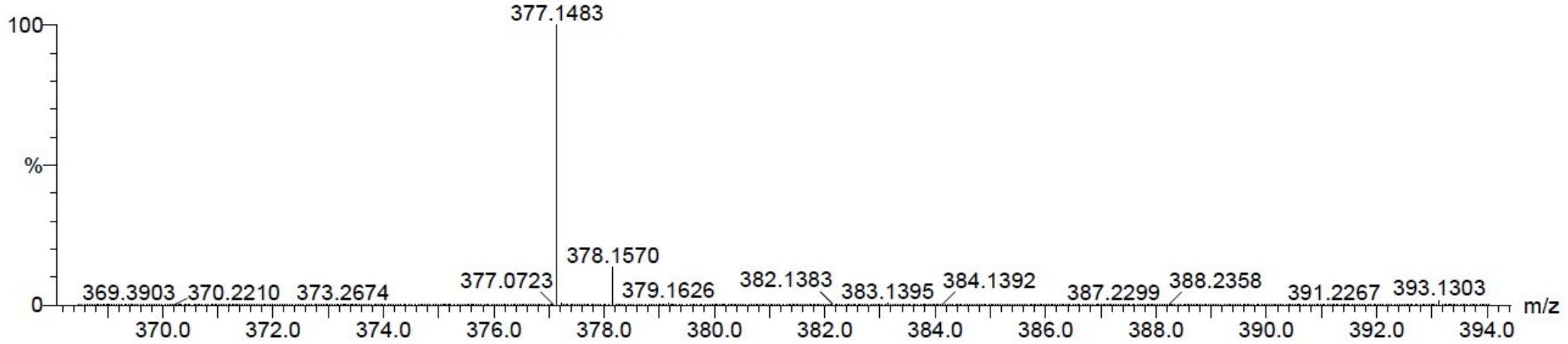

$^{13}$C NMR spectrum of 1-((1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11e**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 Na: 1-1

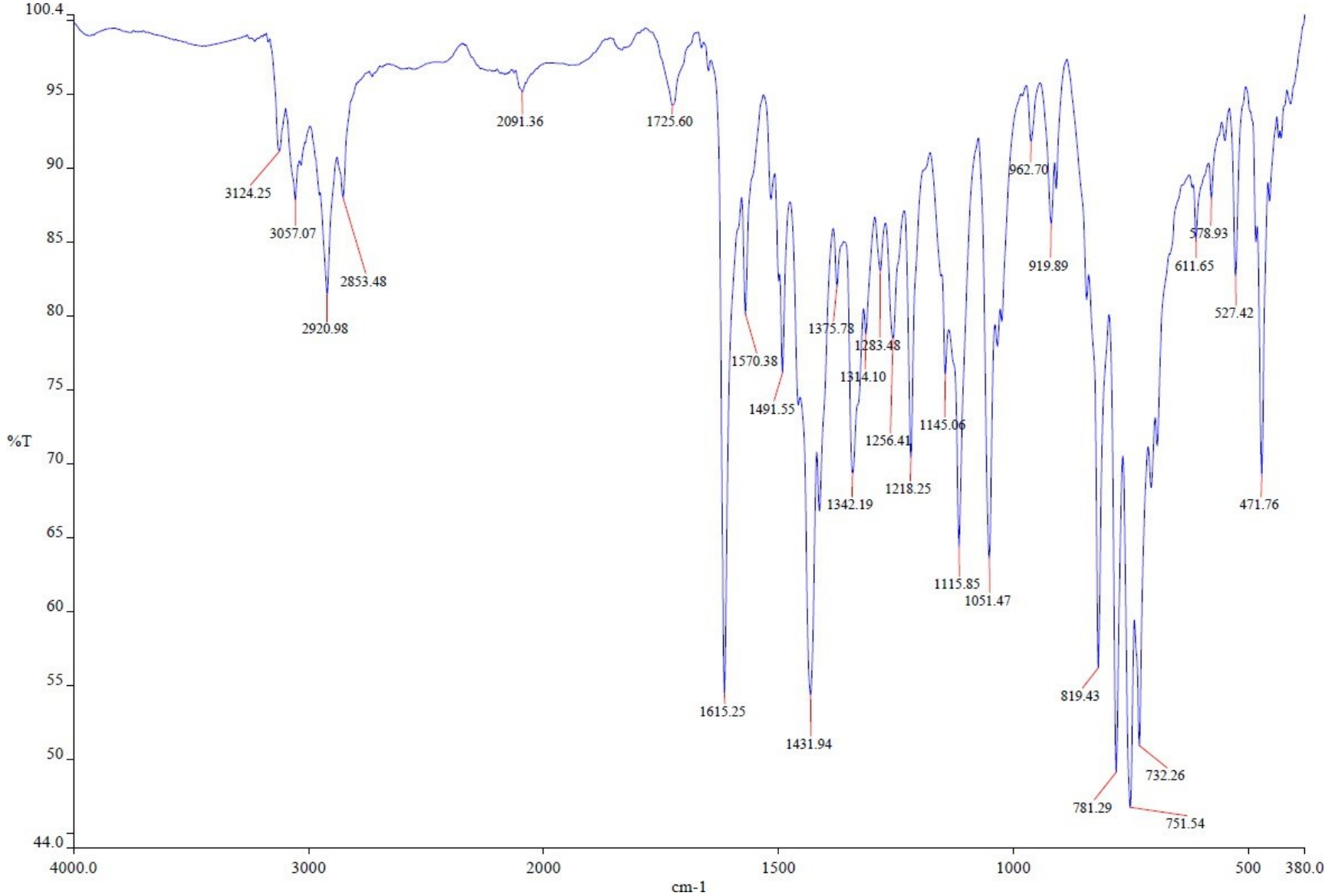
PyQuiTriBen-CH3 28 (0.911) Cm (1:61)

TOF MS ES+
6.84e+004

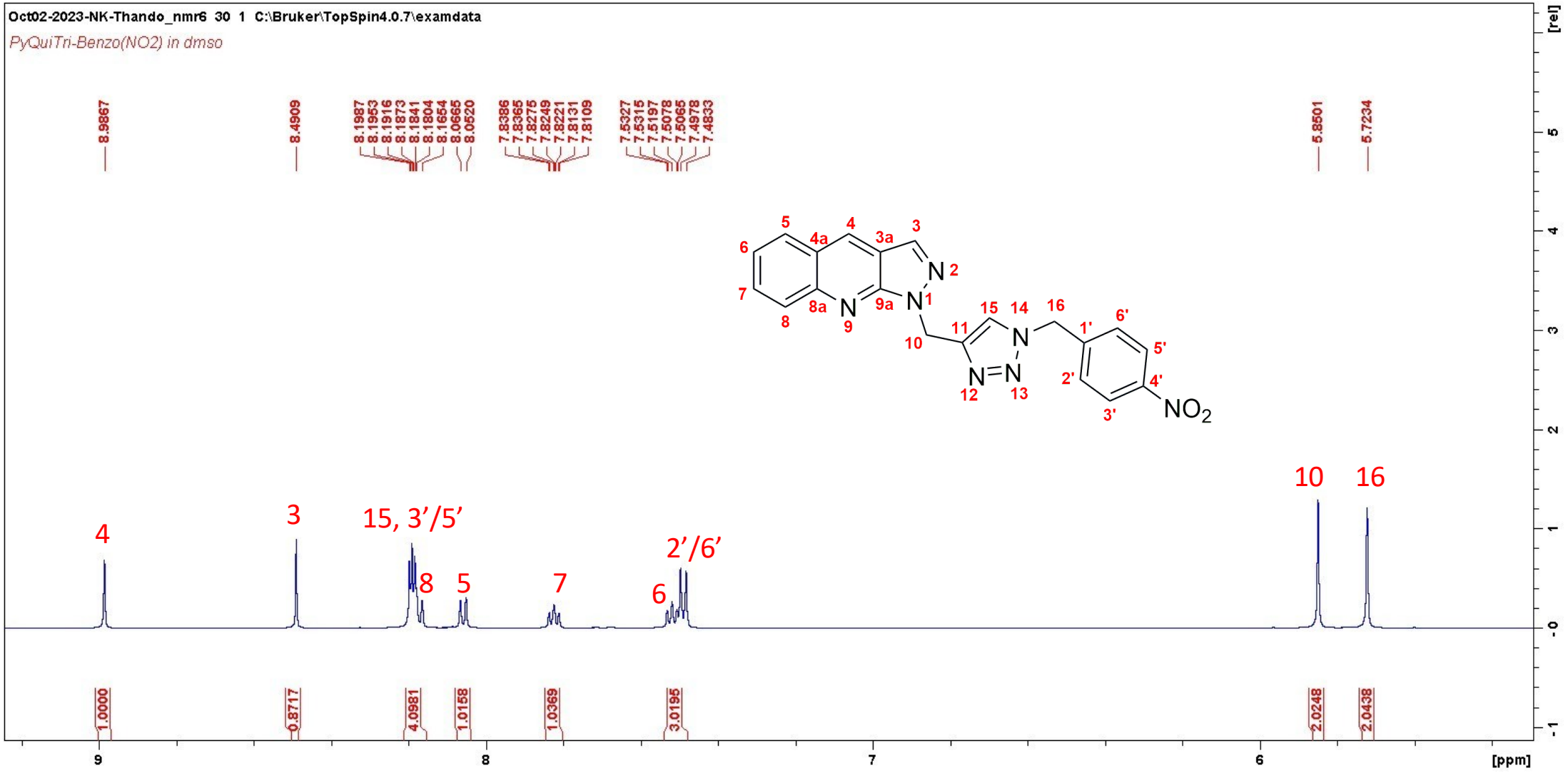



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 377.1483 | 377.1491 | -0.8 | -2.1 | 15.5 | 260.9 | 0.0 | C21 H18 N6 Na |

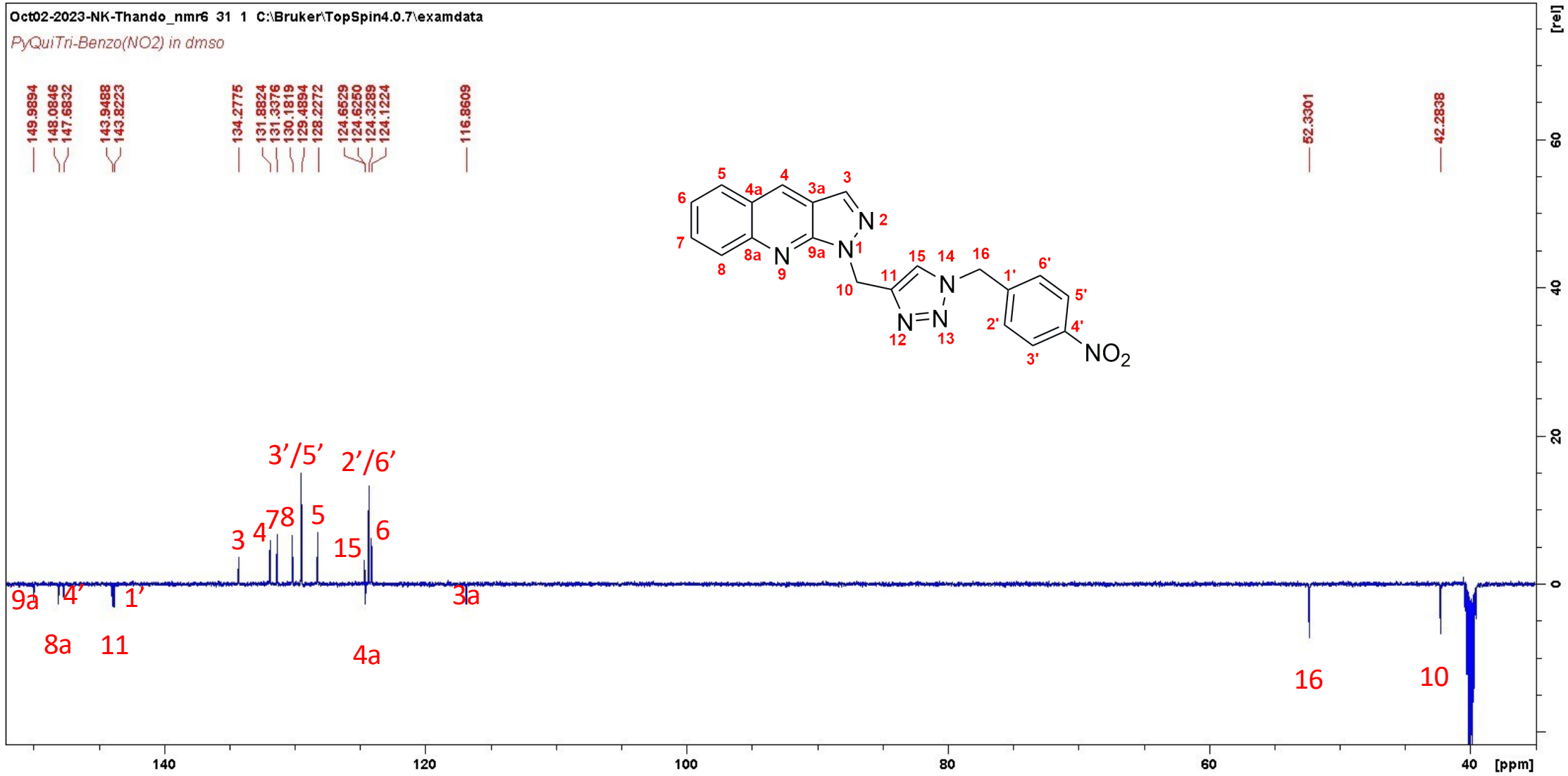
HRMS spectrum of 1-((1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11e**)




FTIR spectrum of 1-((1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11e**)




$^{1}$H NMR spectrum of 1-((1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11f**)



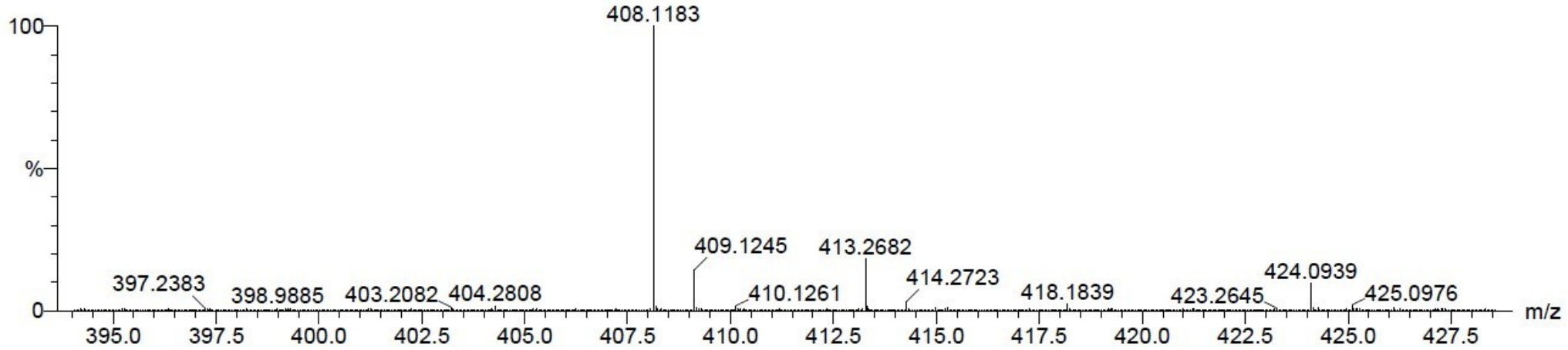

$^{13}$C NMR spectrum of 1-((1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11f**)

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 1-1

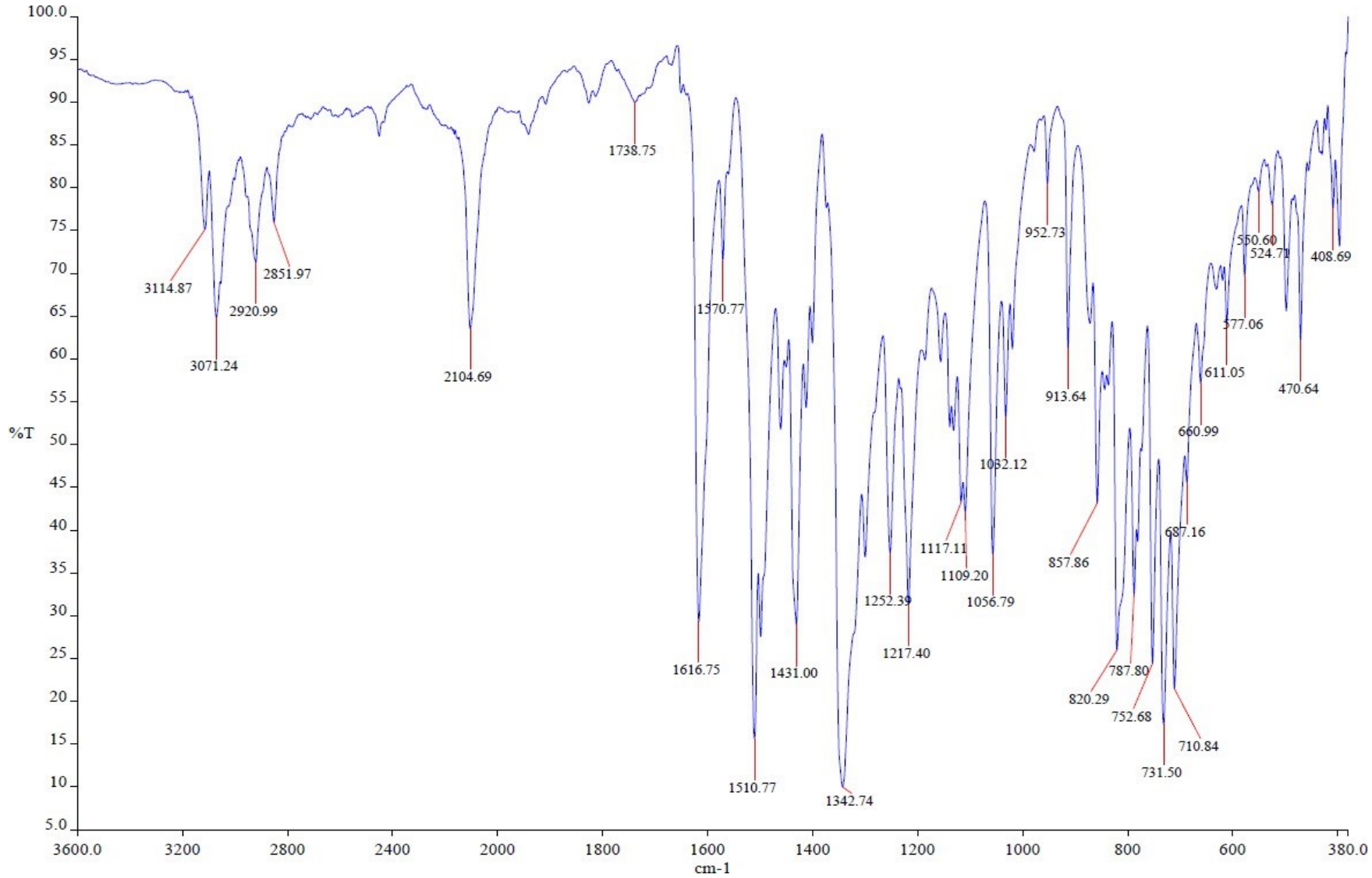
PyQuiTriBen-NO2 12 (0.371) Cm (1:61)

TOF MS ES+
1.20e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 500.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 408.1183 | 408.1185 | -0.2 | -0.5 | 16.5 | 304.3 | 0.0 | C20 H15 N7 O2 Na |

HRMS spectrum of 1-((1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11f**)




FTIR spectrum of 1-((1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrazolo[3,4-b]quinoline (**11f**)