

Synthesis, structure, and antiviral properties of novel 2-adamantyl-5-aryl-2*H*-tetrazoles

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SUPPLEMENTARY INFORMATION

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1. ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra

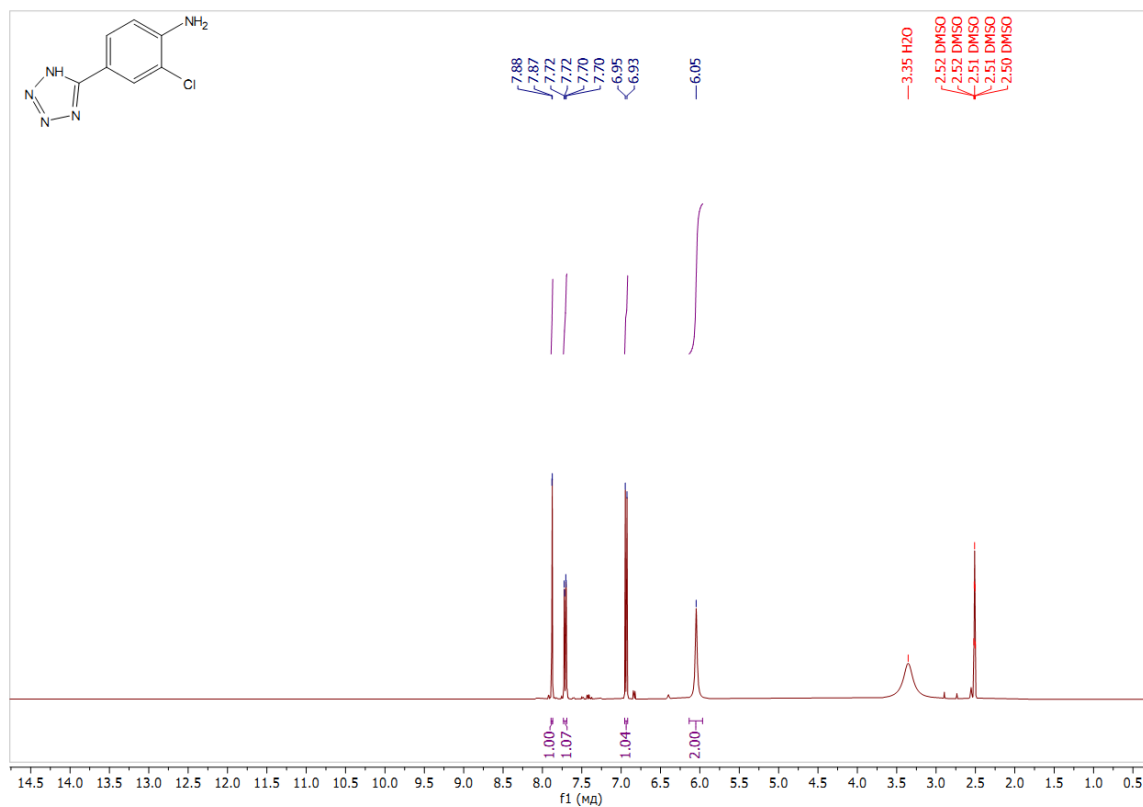


Fig. S1. ^1H spectra of **2e**

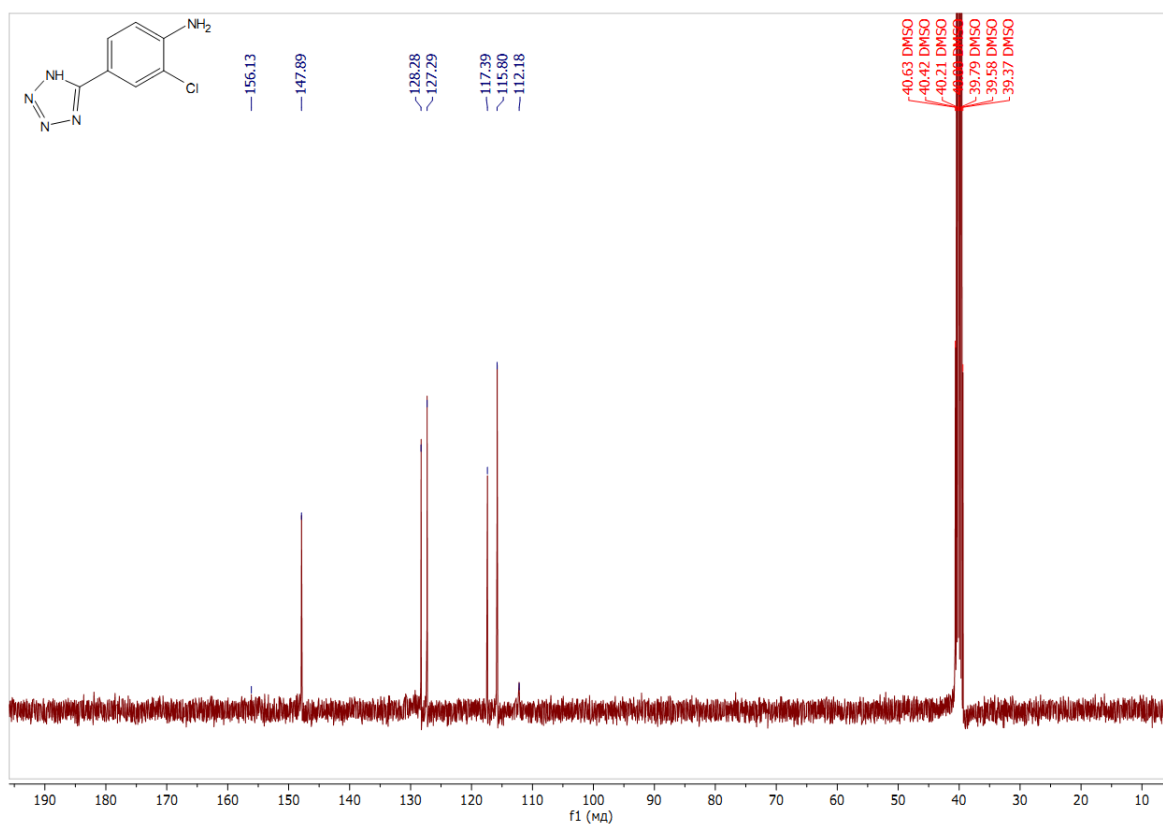


Fig. S2. $^{13}\text{C}\{\text{H}\}$ spectra of **2e**

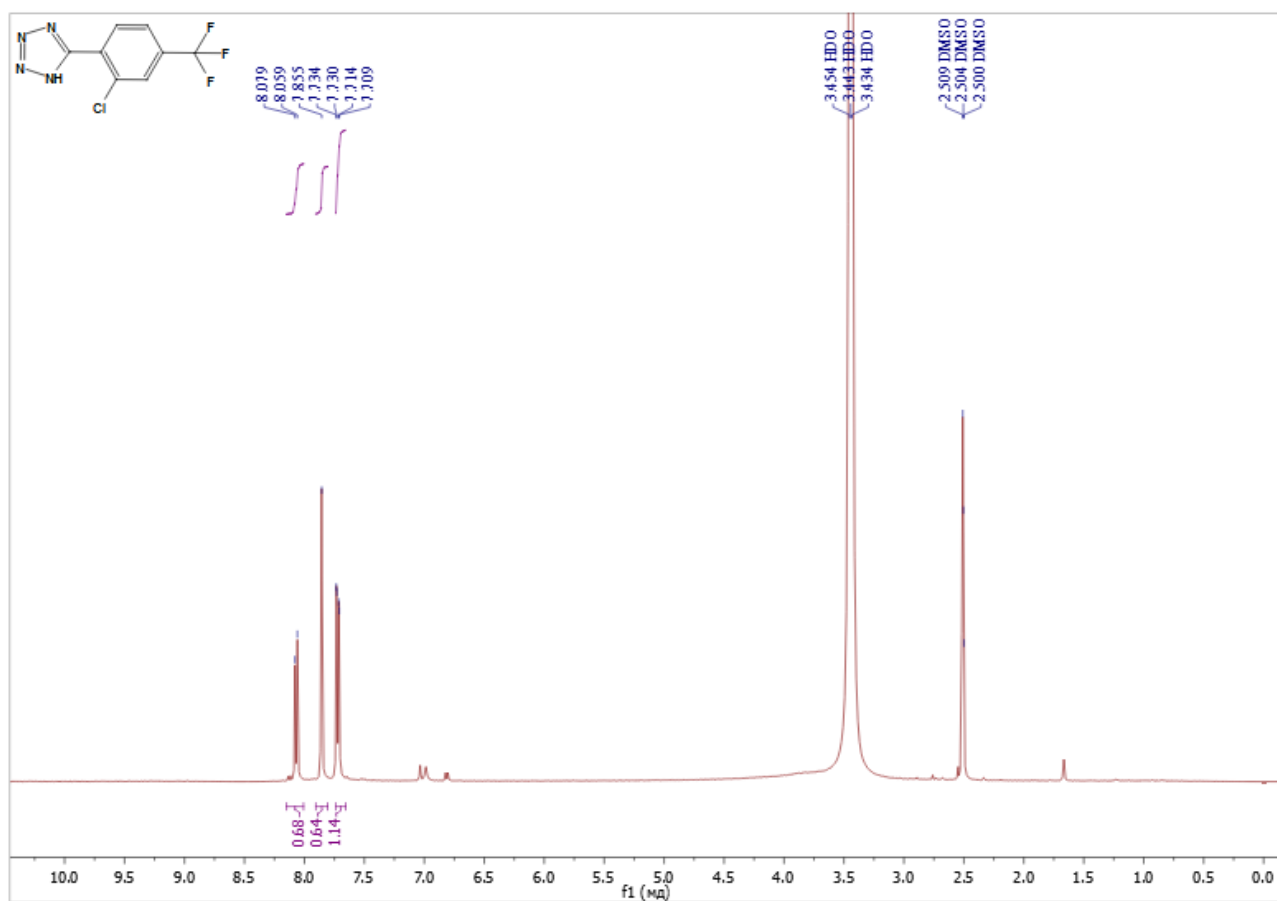


Fig. S3. ¹H spectra of **2f**

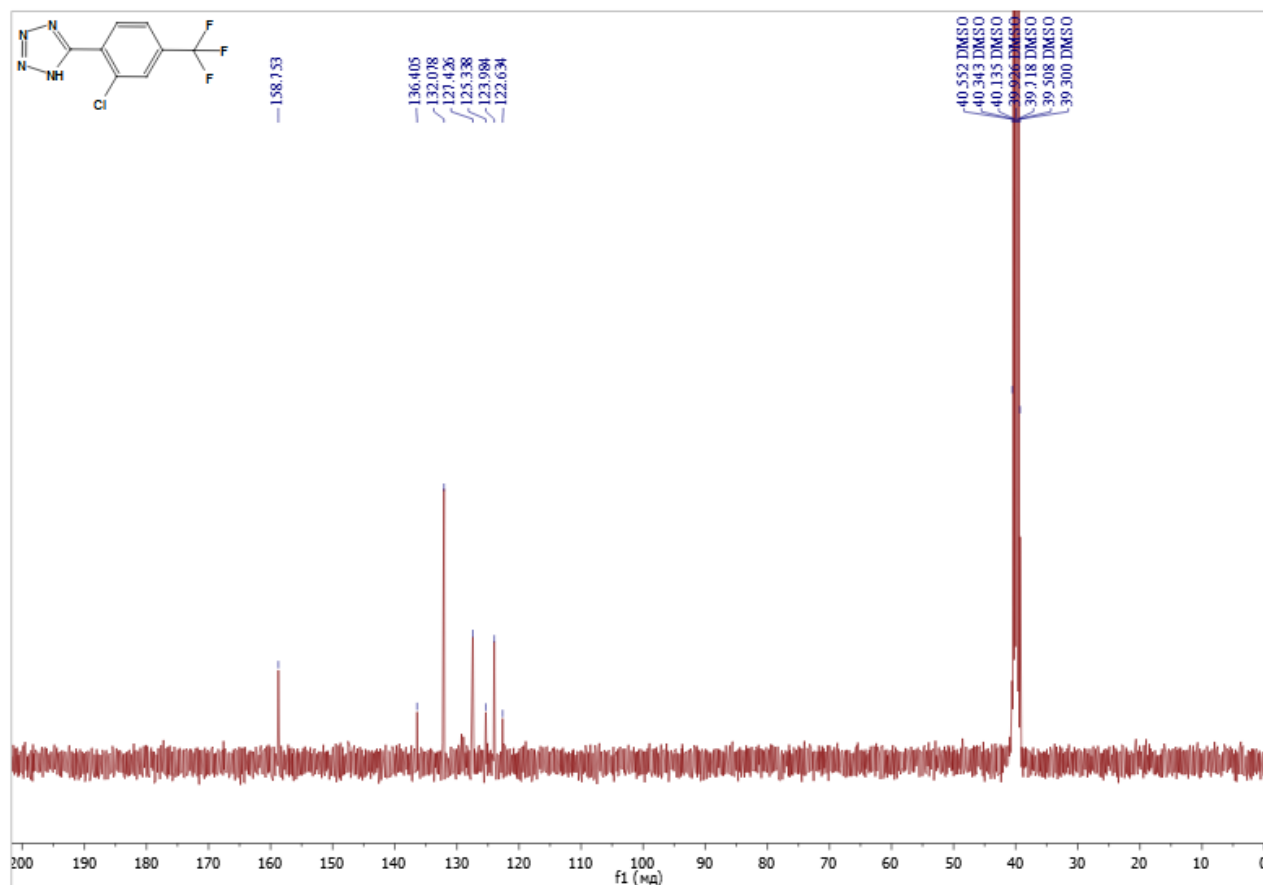


Fig. S4. ¹³C{H} spectra of **2f**

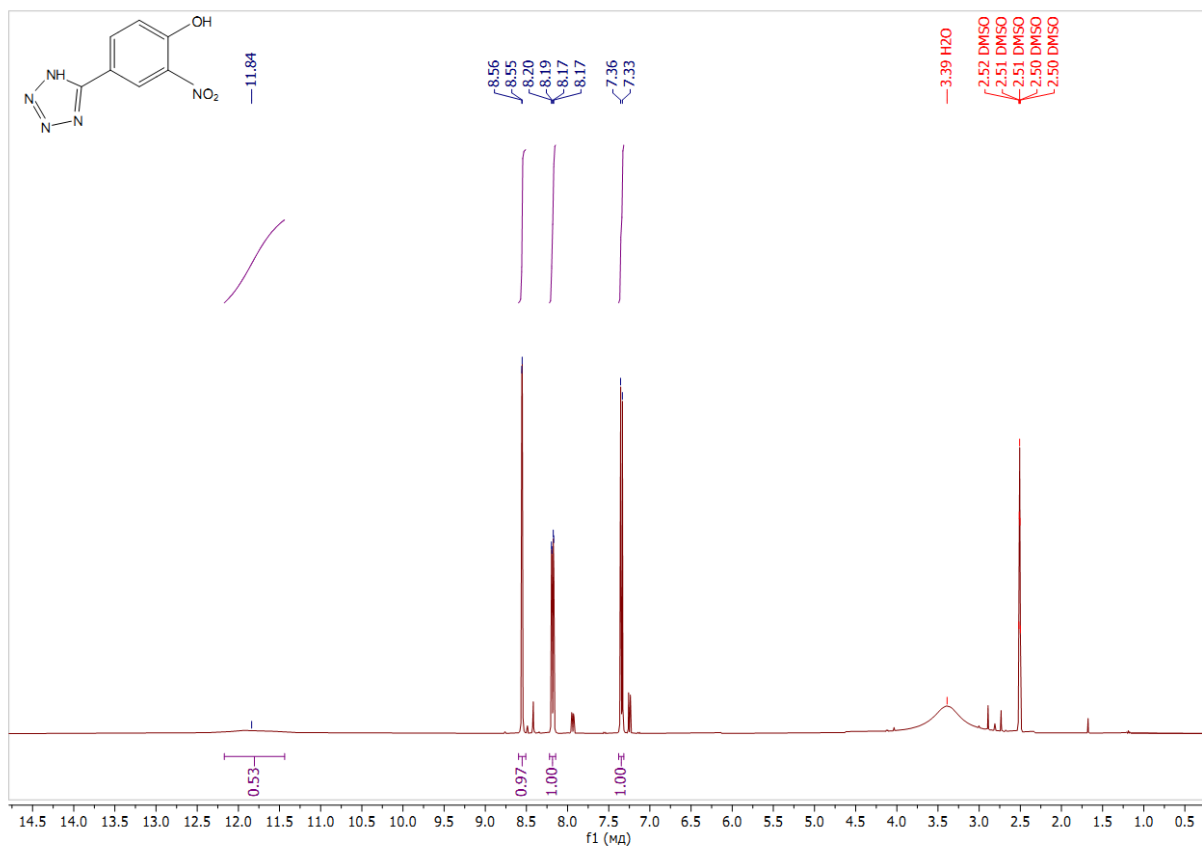


Fig. S5. ^1H spectra of **2g**

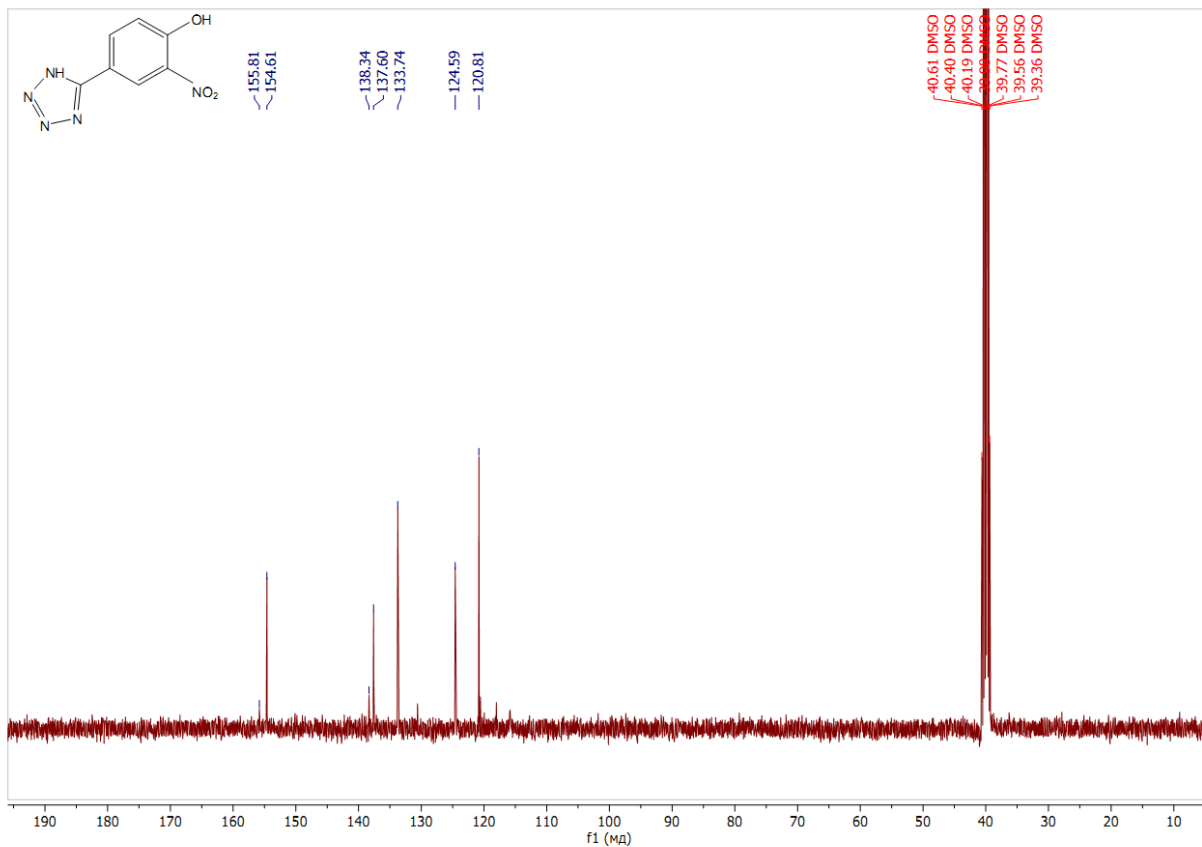


Fig. S6. $^{13}\text{C}\{\text{H}\}$ spectra of **2g**

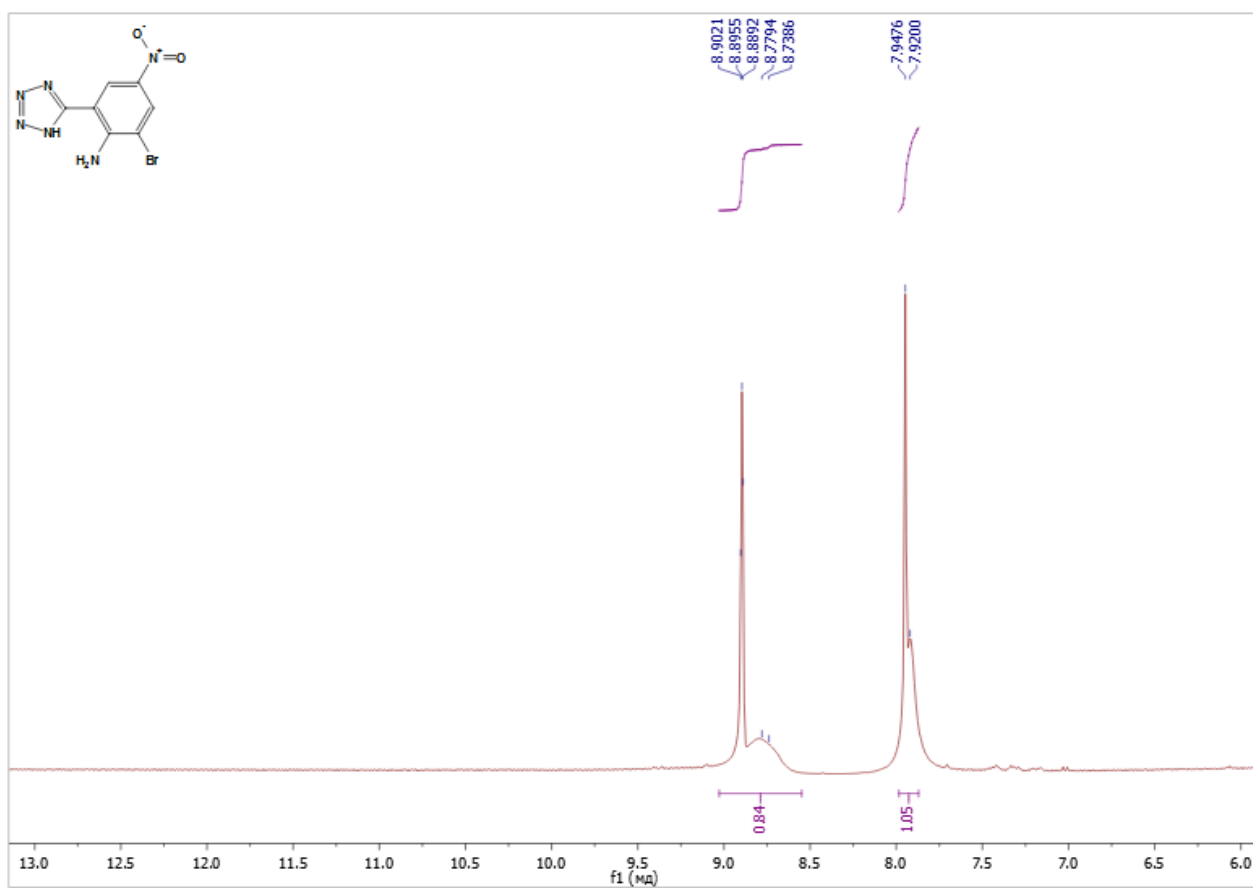


Fig. S7. ^1H spectra of **2i**

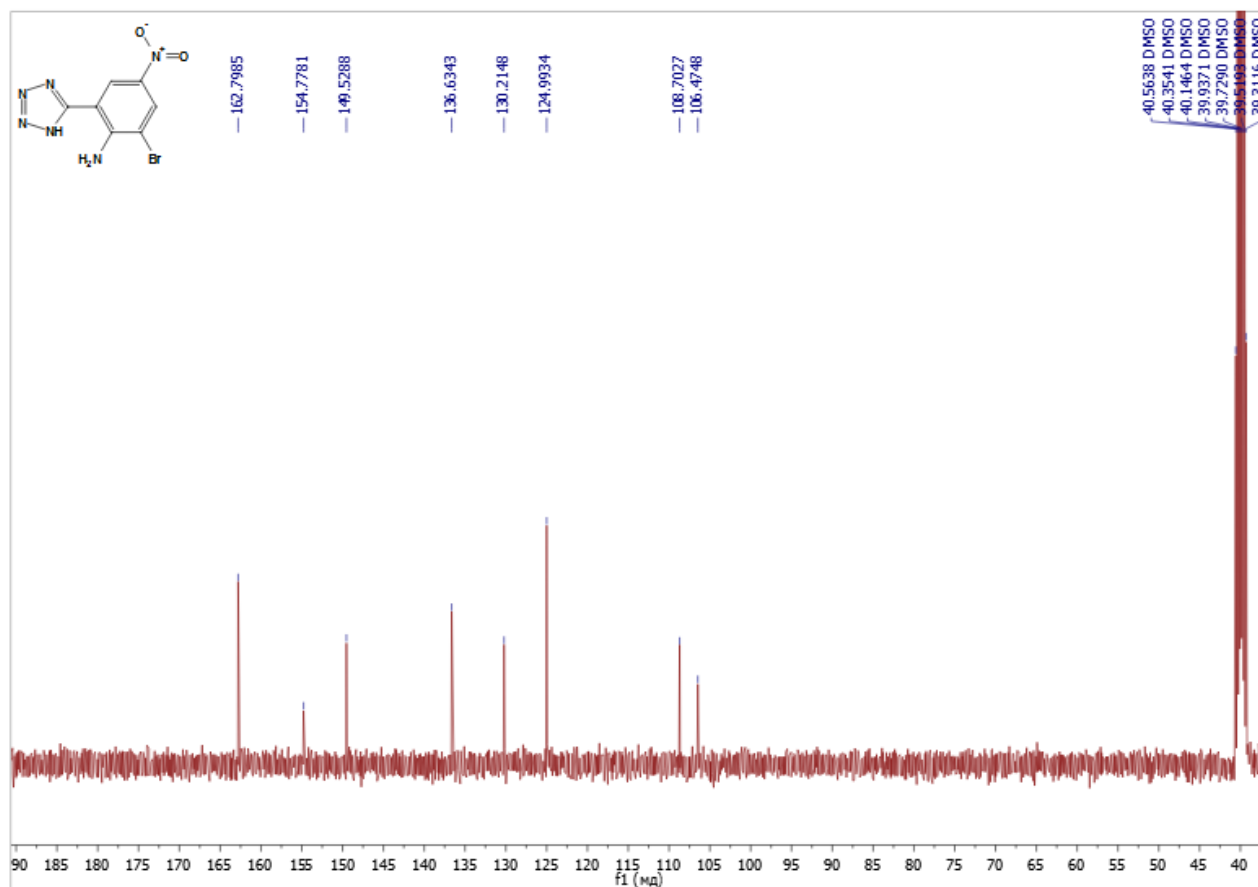


Fig. S8. $^{13}\text{C}\{^1\text{H}\}$ spectra of **2i**

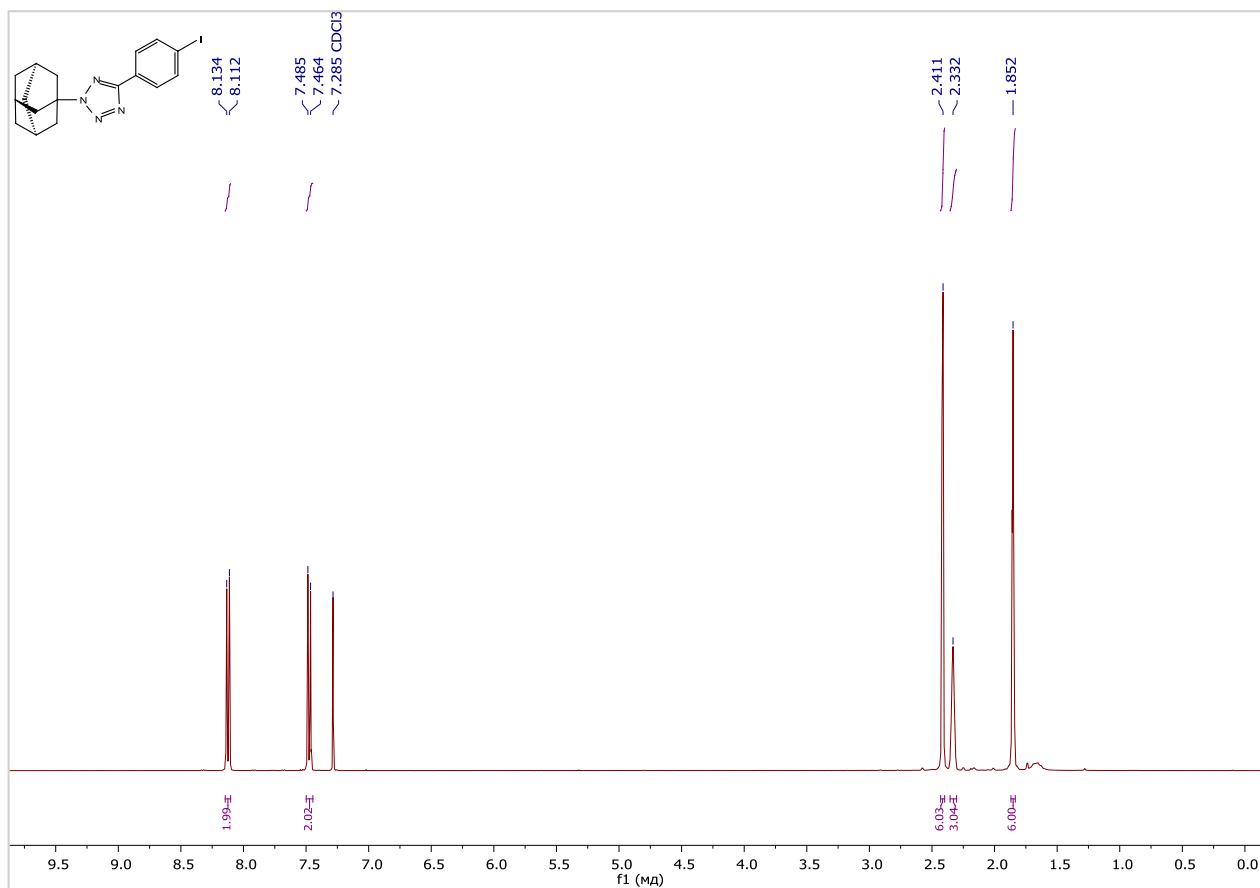


Fig. S9. ¹H spectra of **3a**

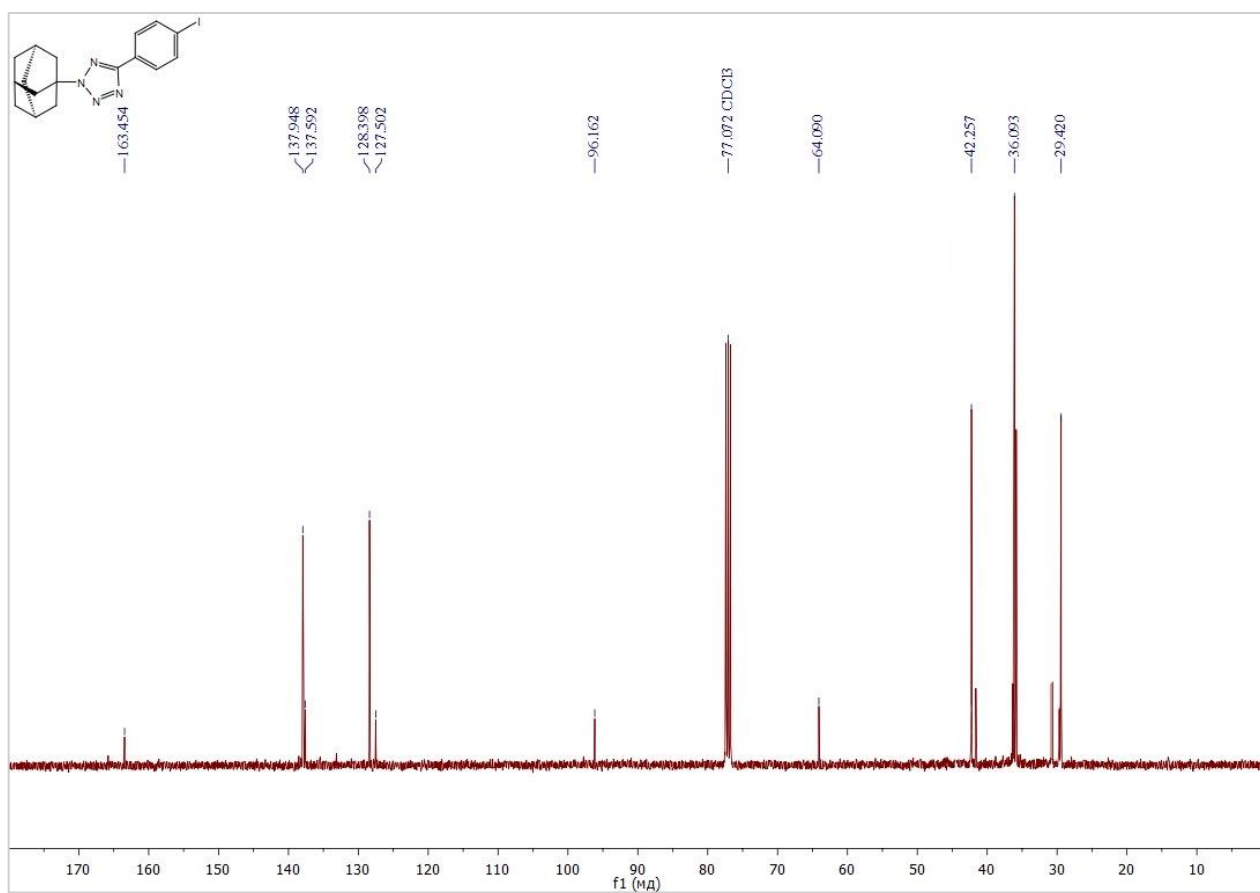


Fig. S10. ¹³C{¹H} spectra of **3a**

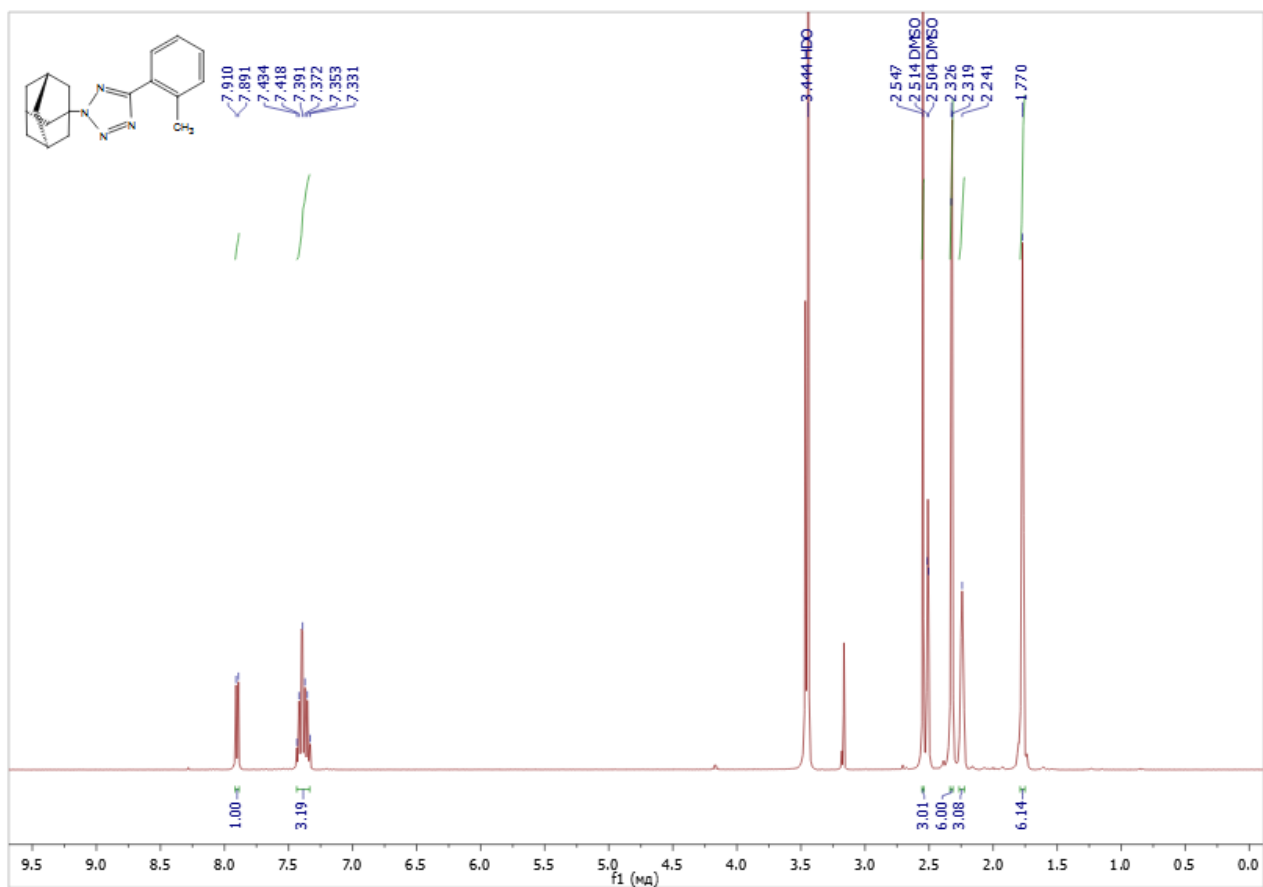


Fig. S11. ¹H spectra of **3b**

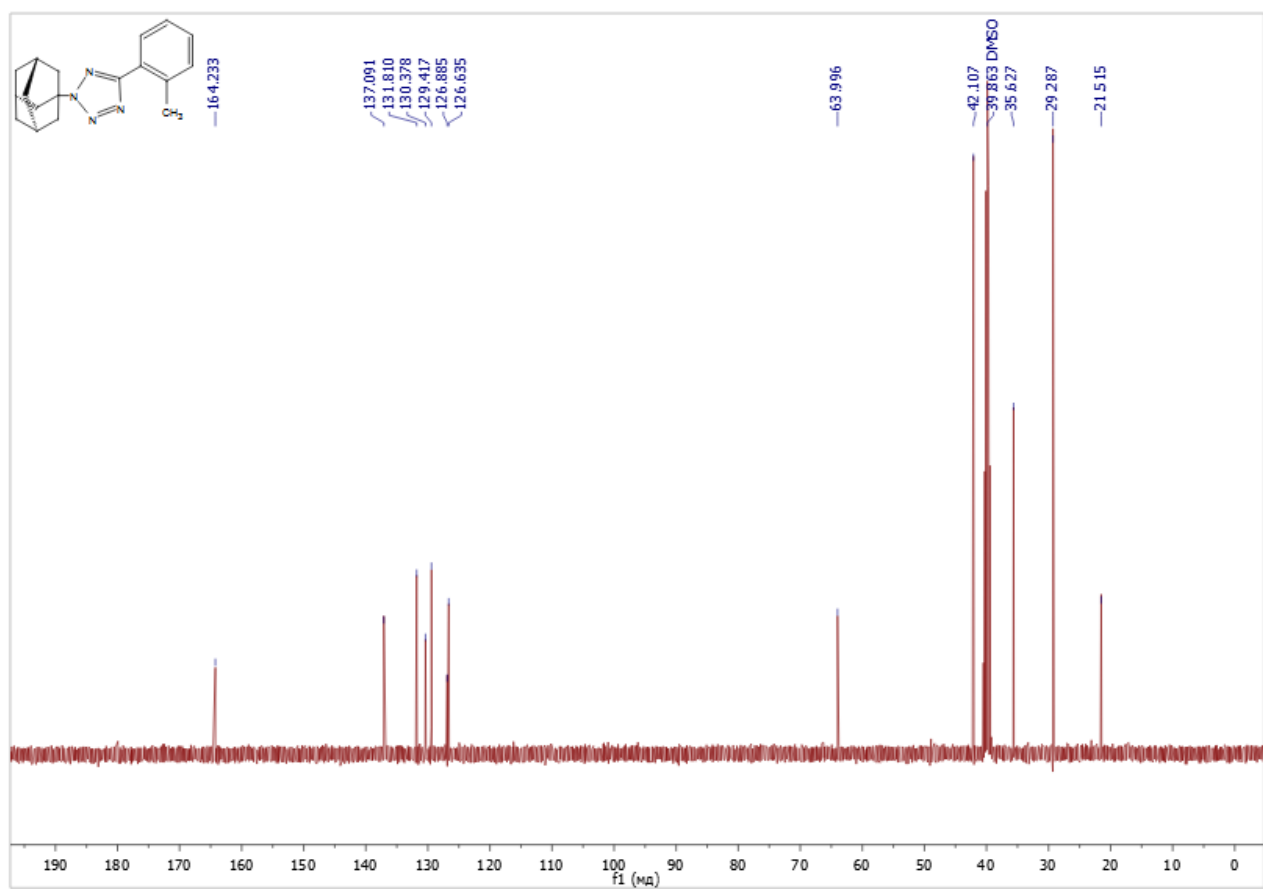


Fig. S12. ¹³C{¹H} spectra of **3b**

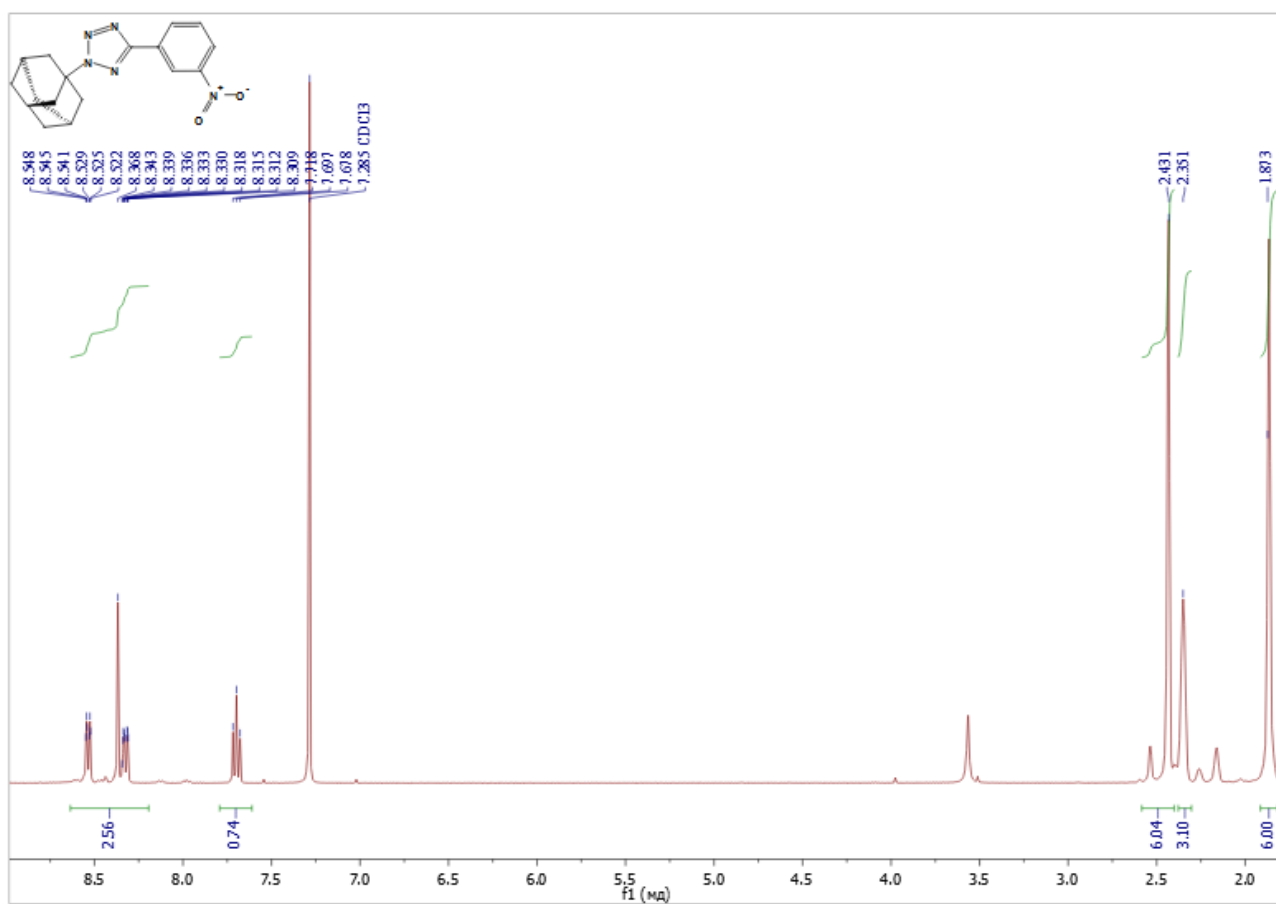


Fig. S13. ¹H spectra of **3c**

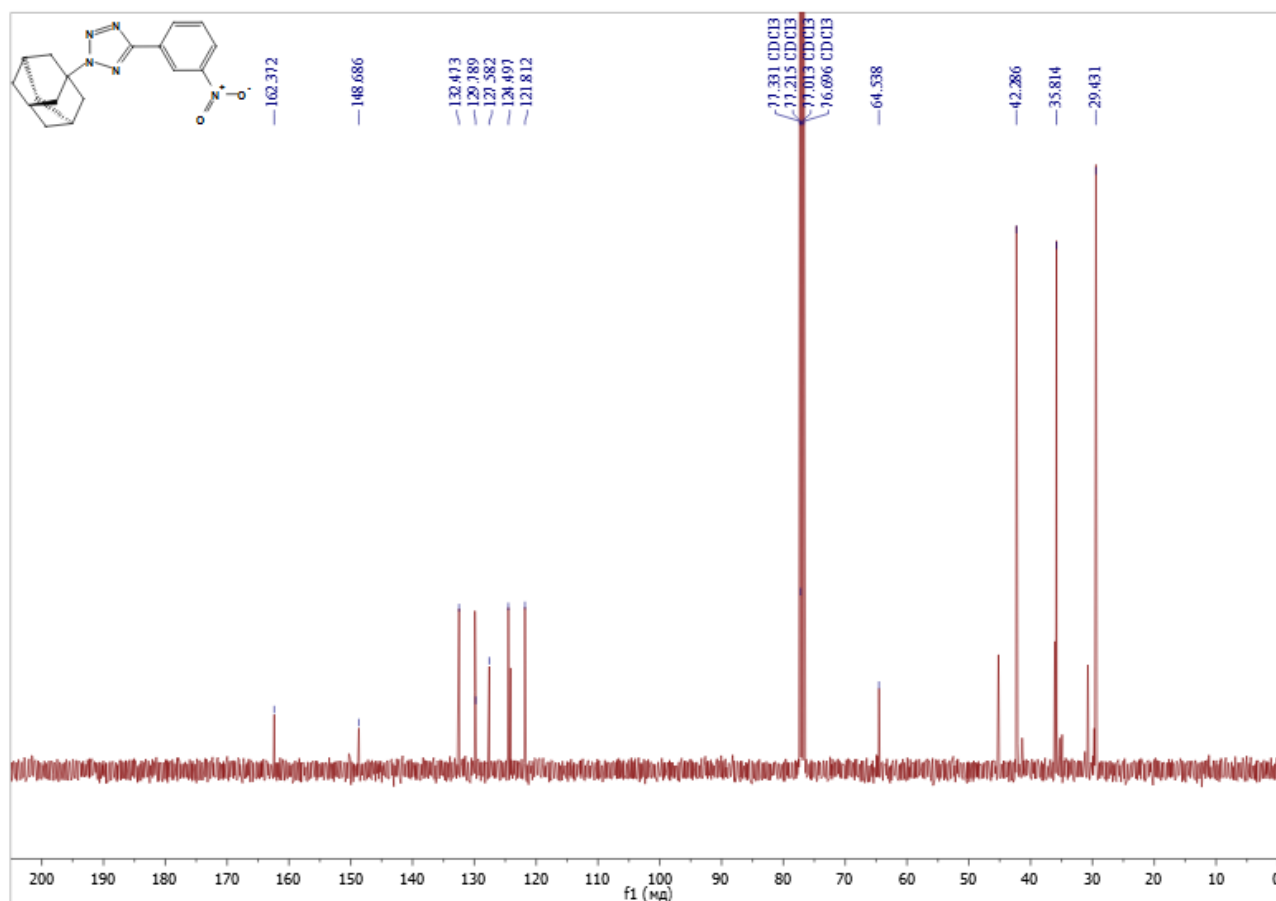


Fig. S14. ¹³C spectra of **3c**

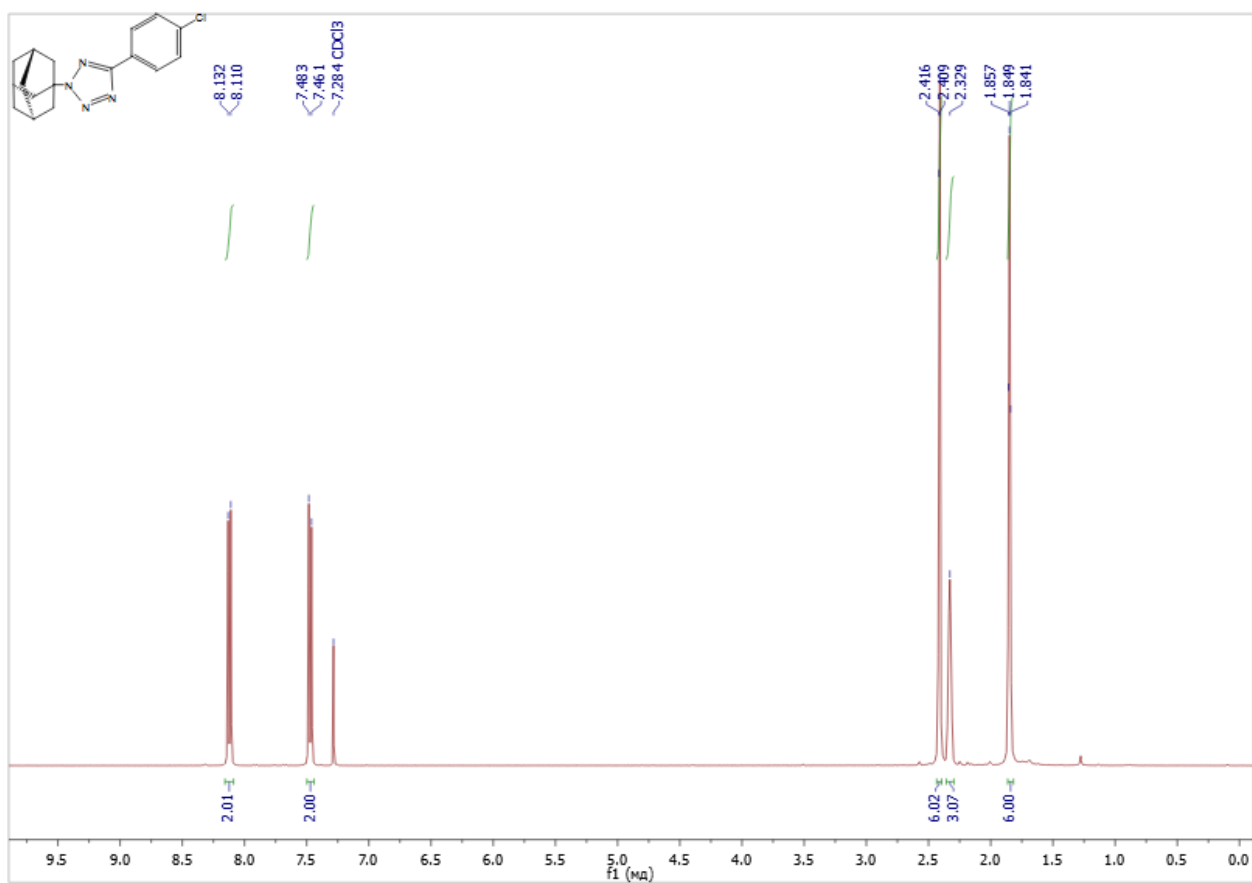


Fig. S15. ^1H spectra of **3d**

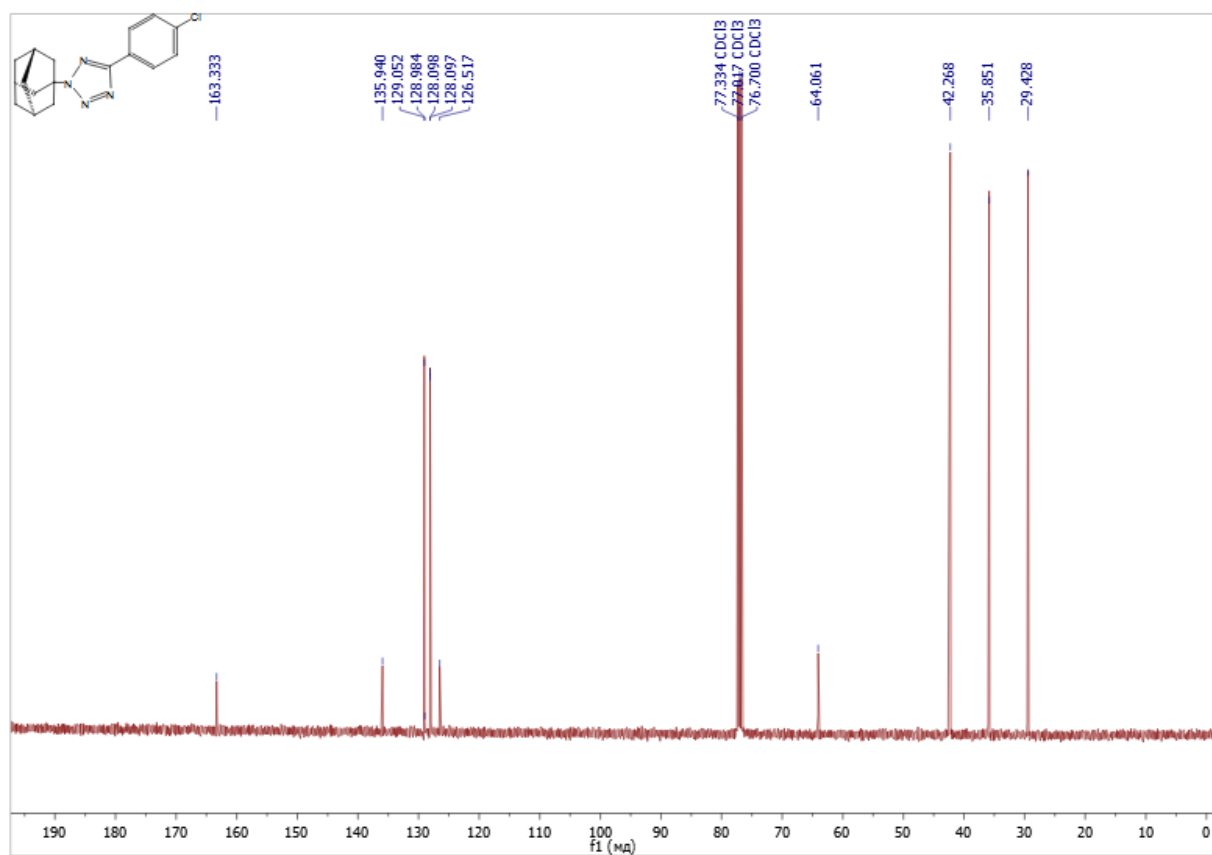


Fig. S16. $^{13}\text{C}\{^1\text{H}\}$ spectra of **3d**

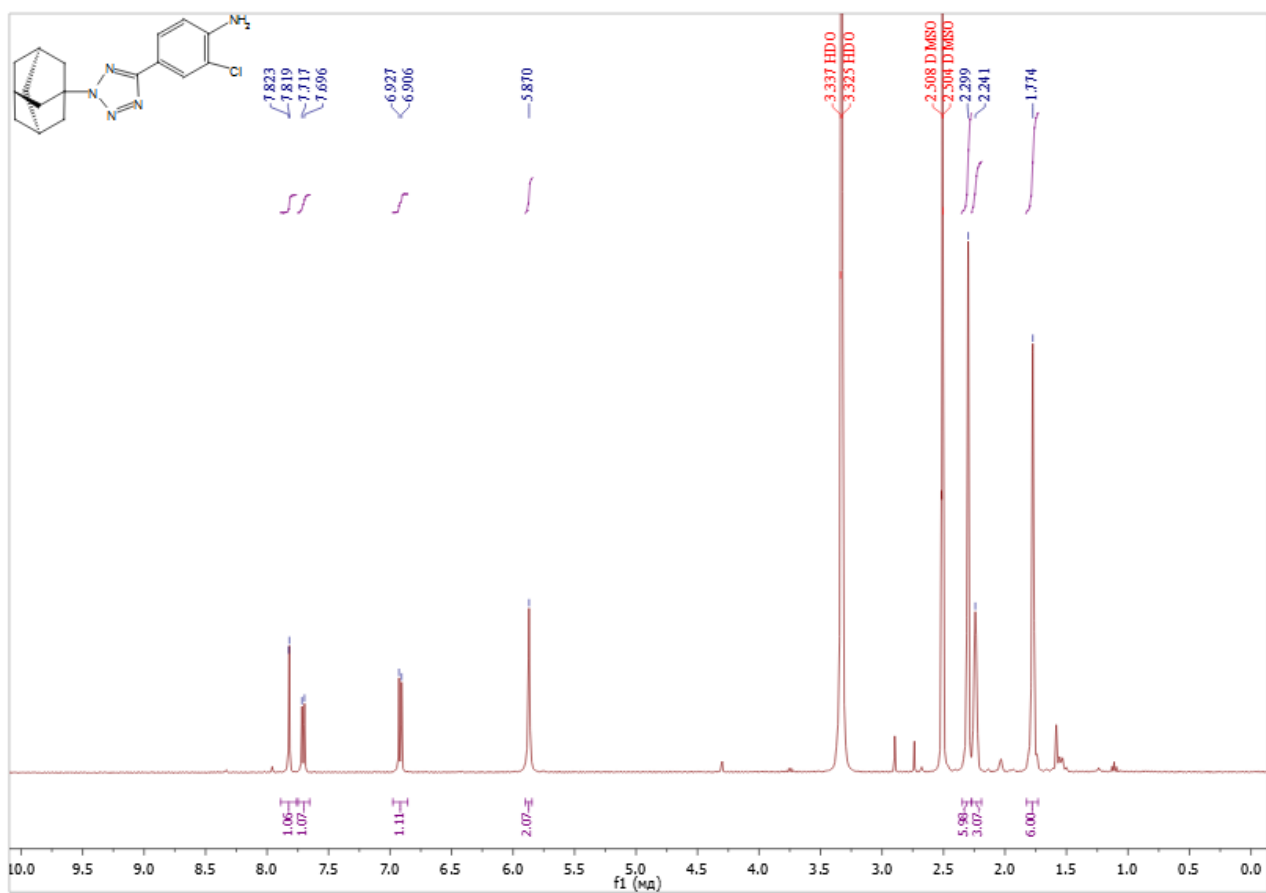


Fig. S17. ^1H spectra of **3e**

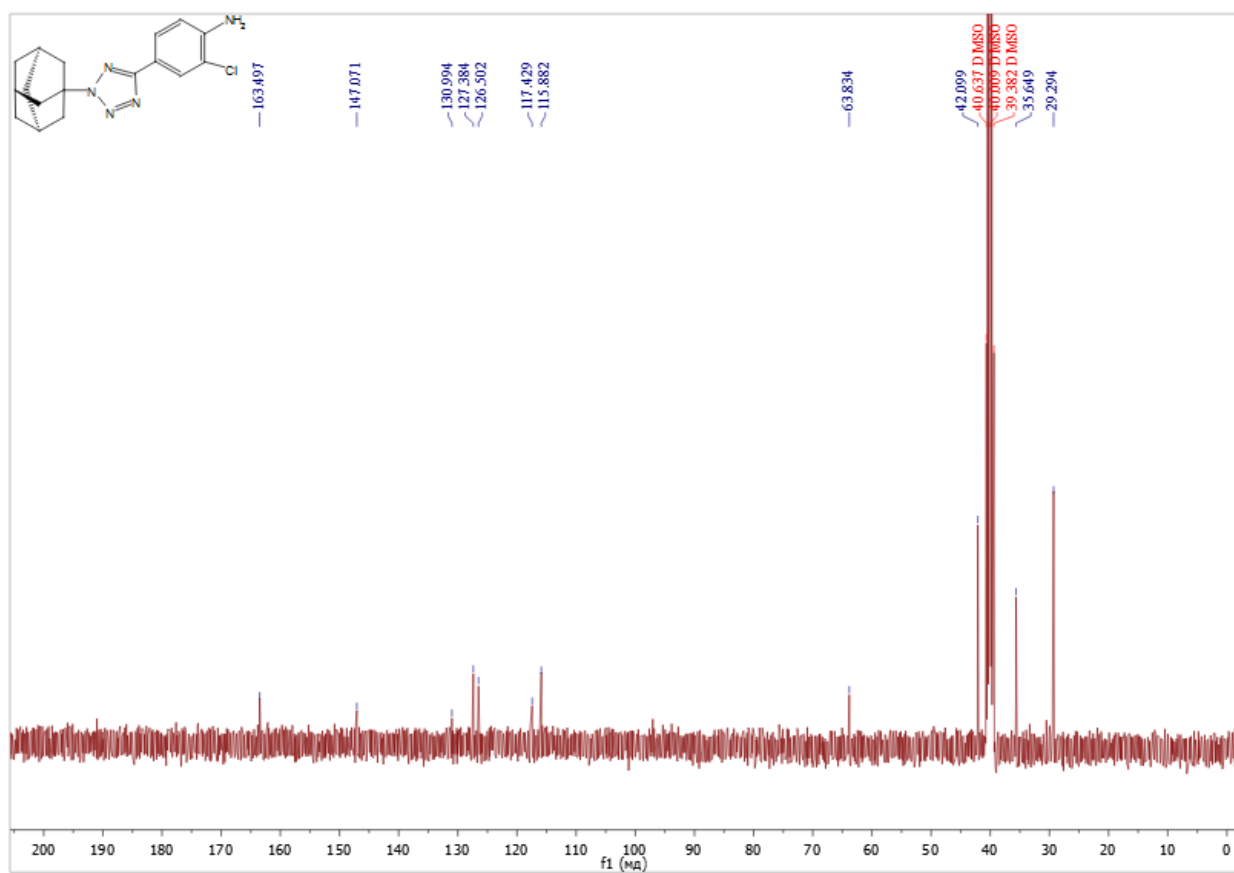


Fig. S18. $^{13}\text{C}\{^1\text{H}\}$ spectra of **3e**

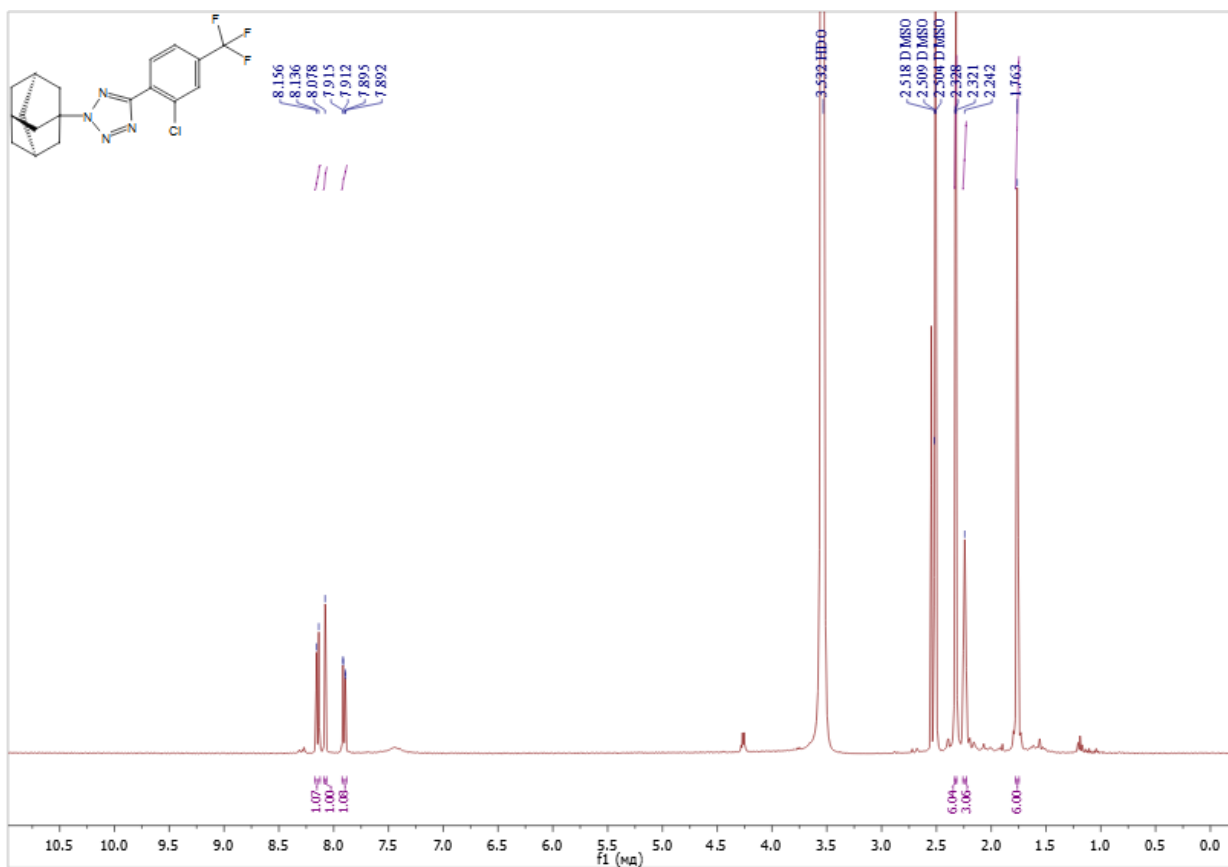


Fig. S19. ¹H spectra of **3f**

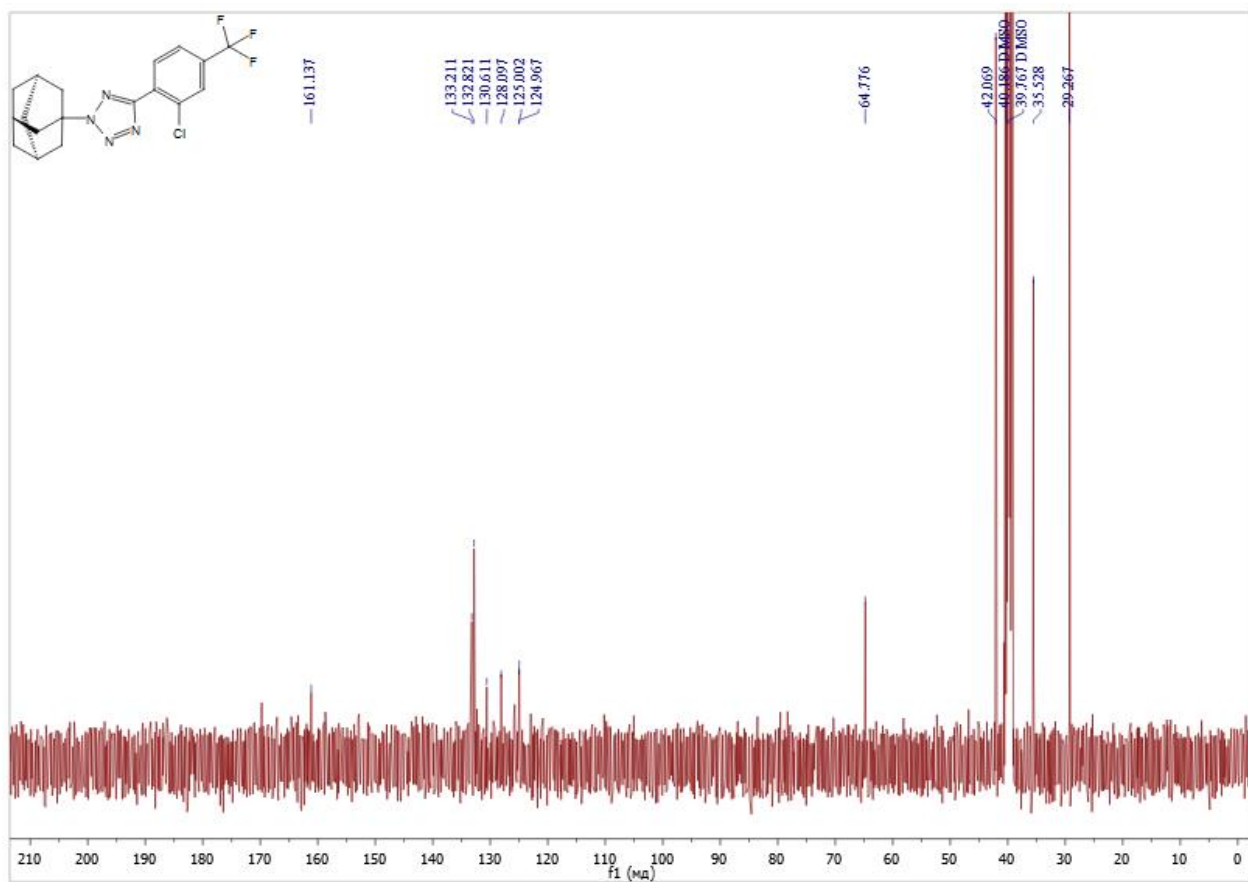


Fig. S20. ¹³C{¹H} spectra of **3f**

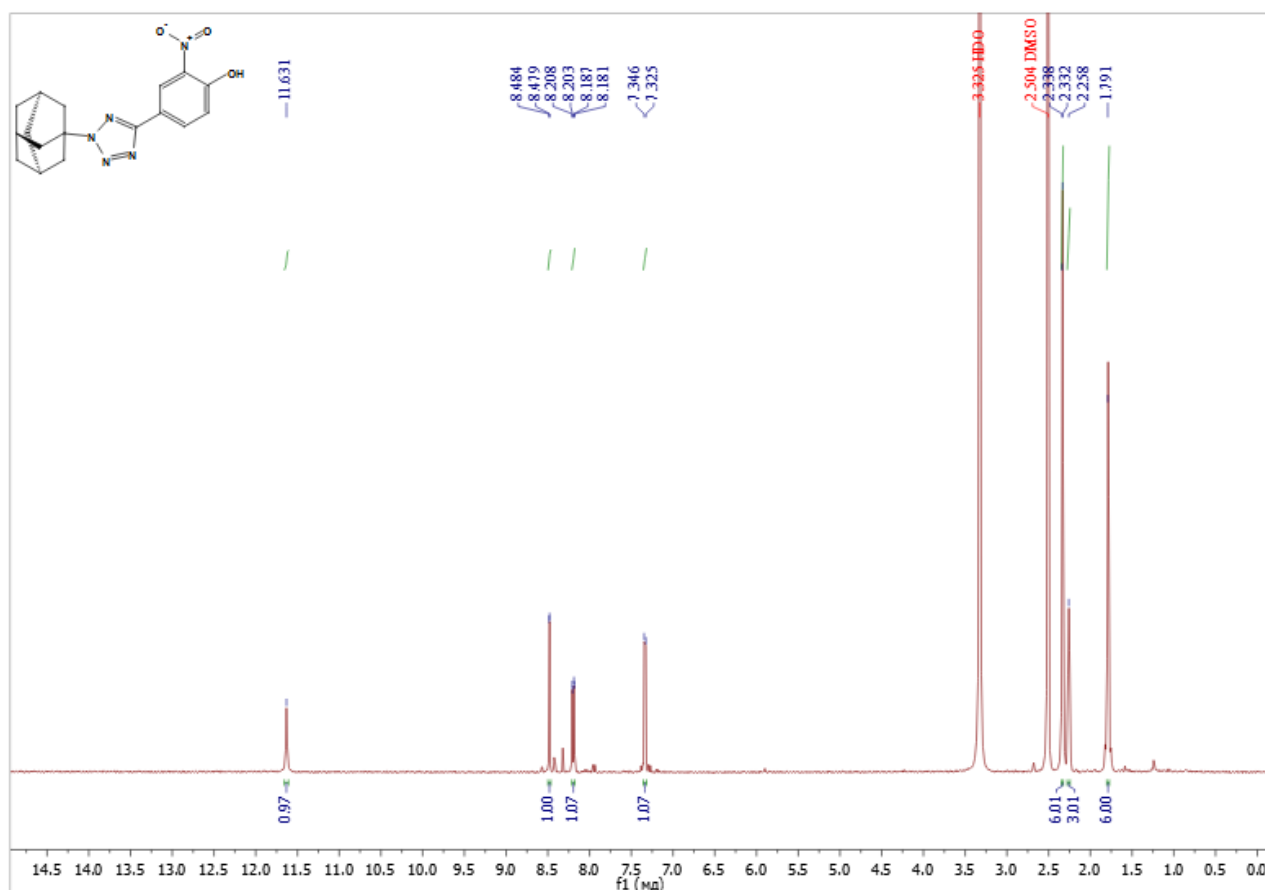


Fig. S21. ^1H spectra of **3g**

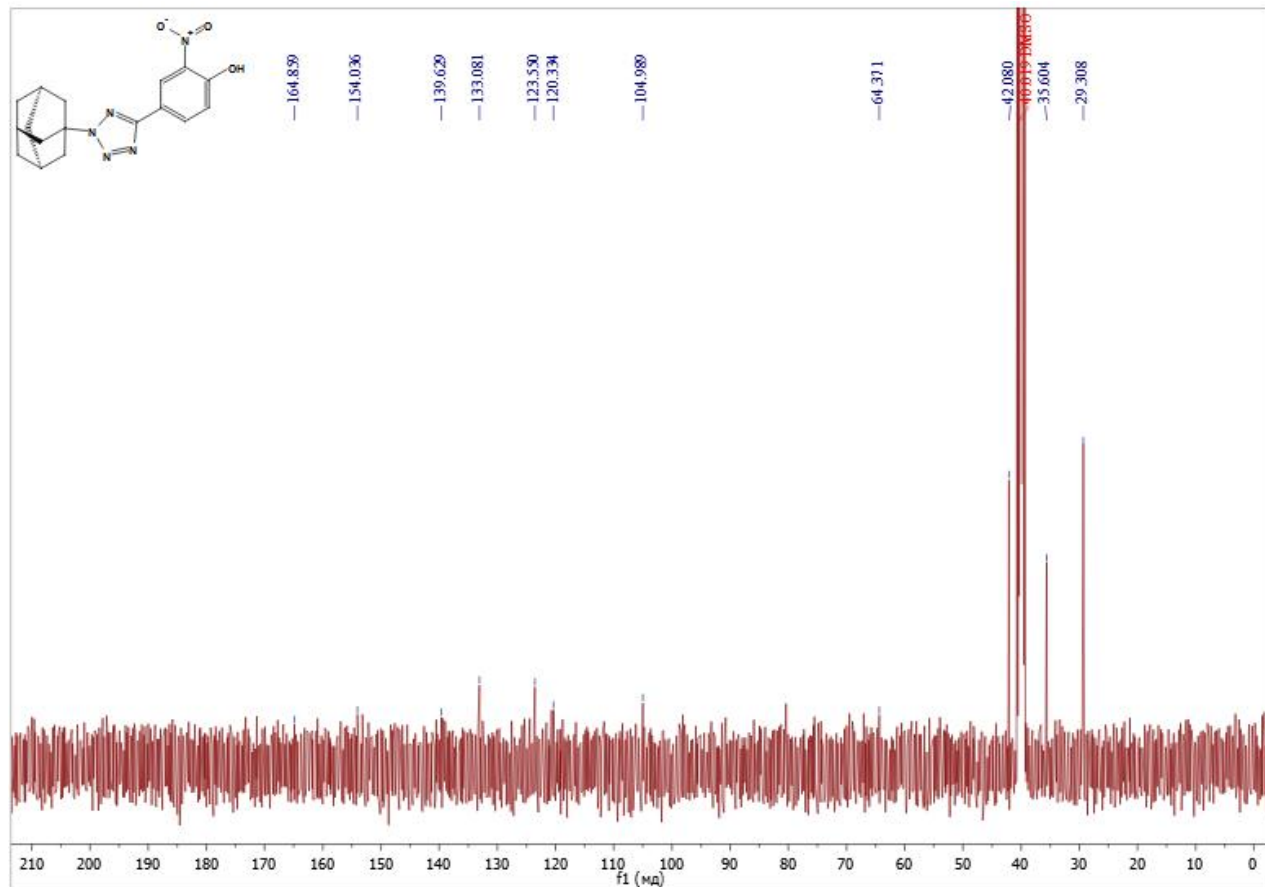


Fig. S22. $^{13}\text{C}\{^1\text{H}\}$ spectra of **3g**

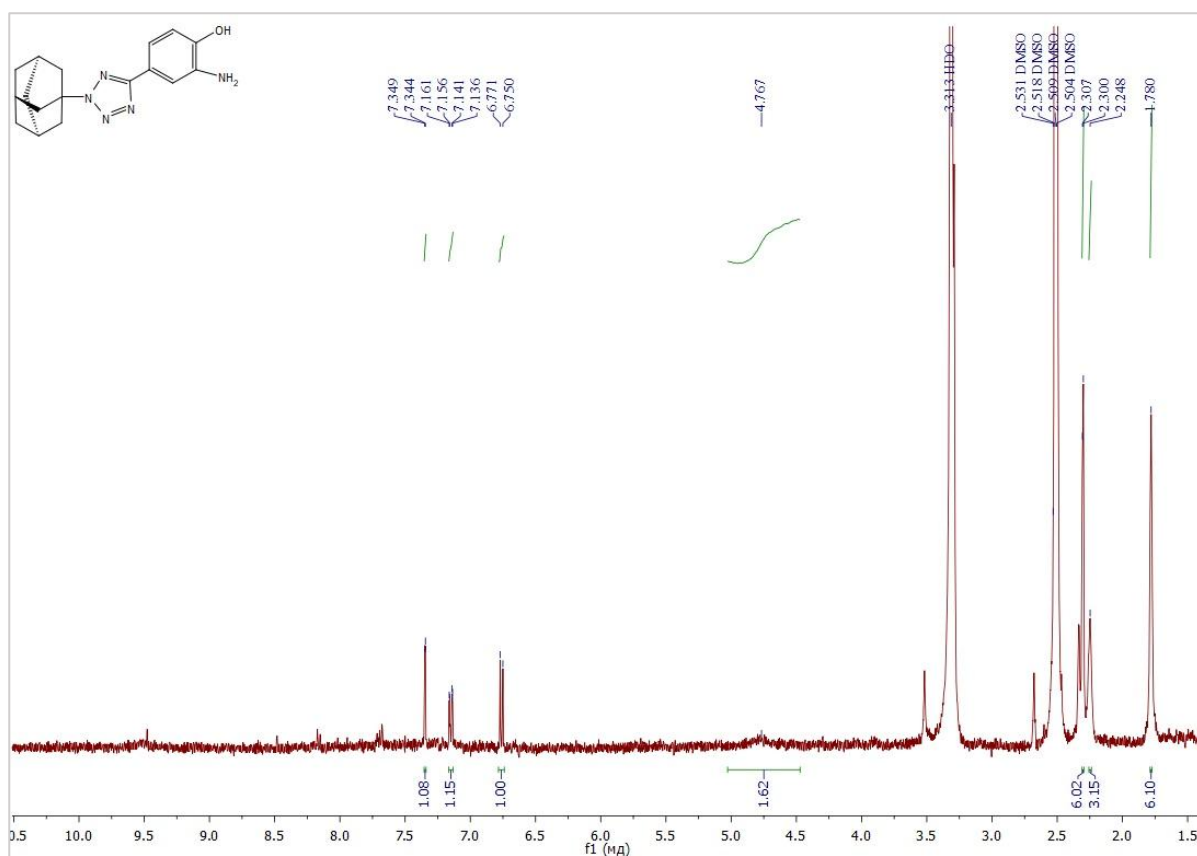


Fig. S23. ¹H spectra of **3h**

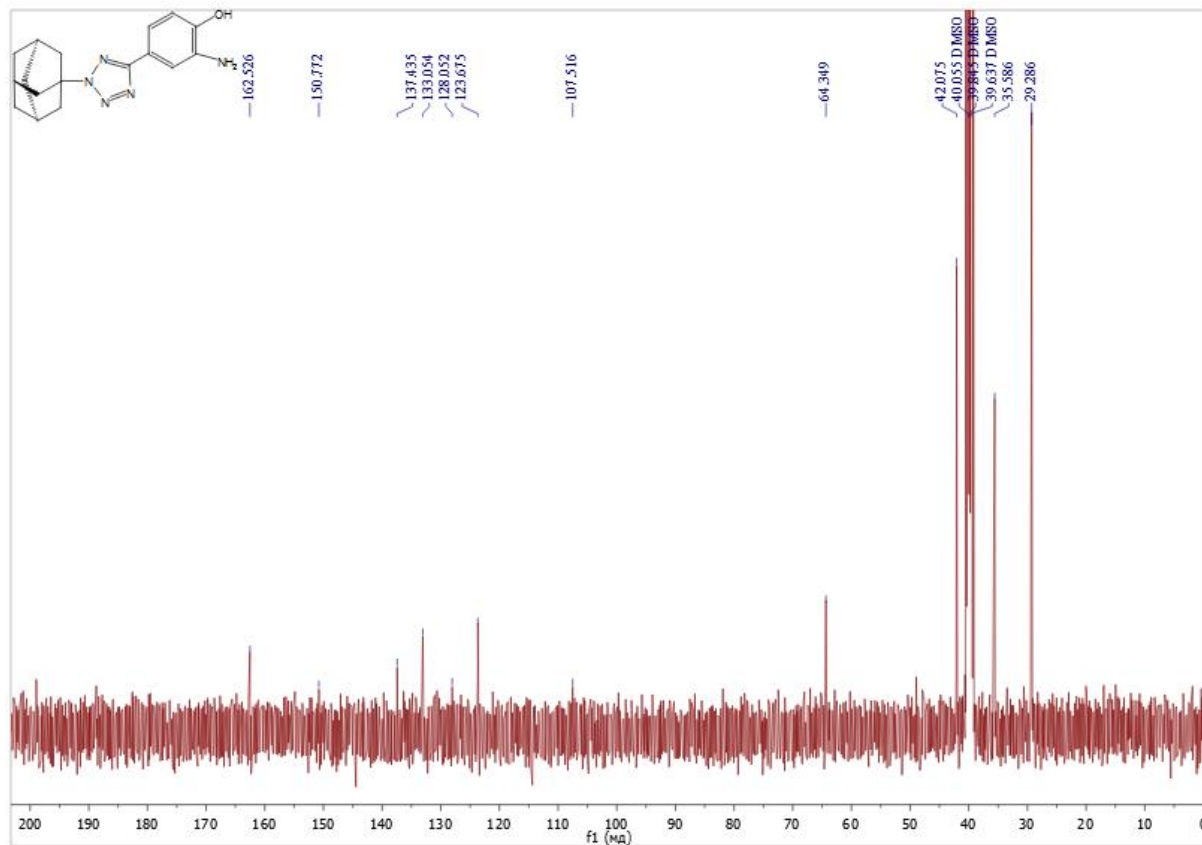


Fig. S24. ¹³C{¹H} spectra of **3h**

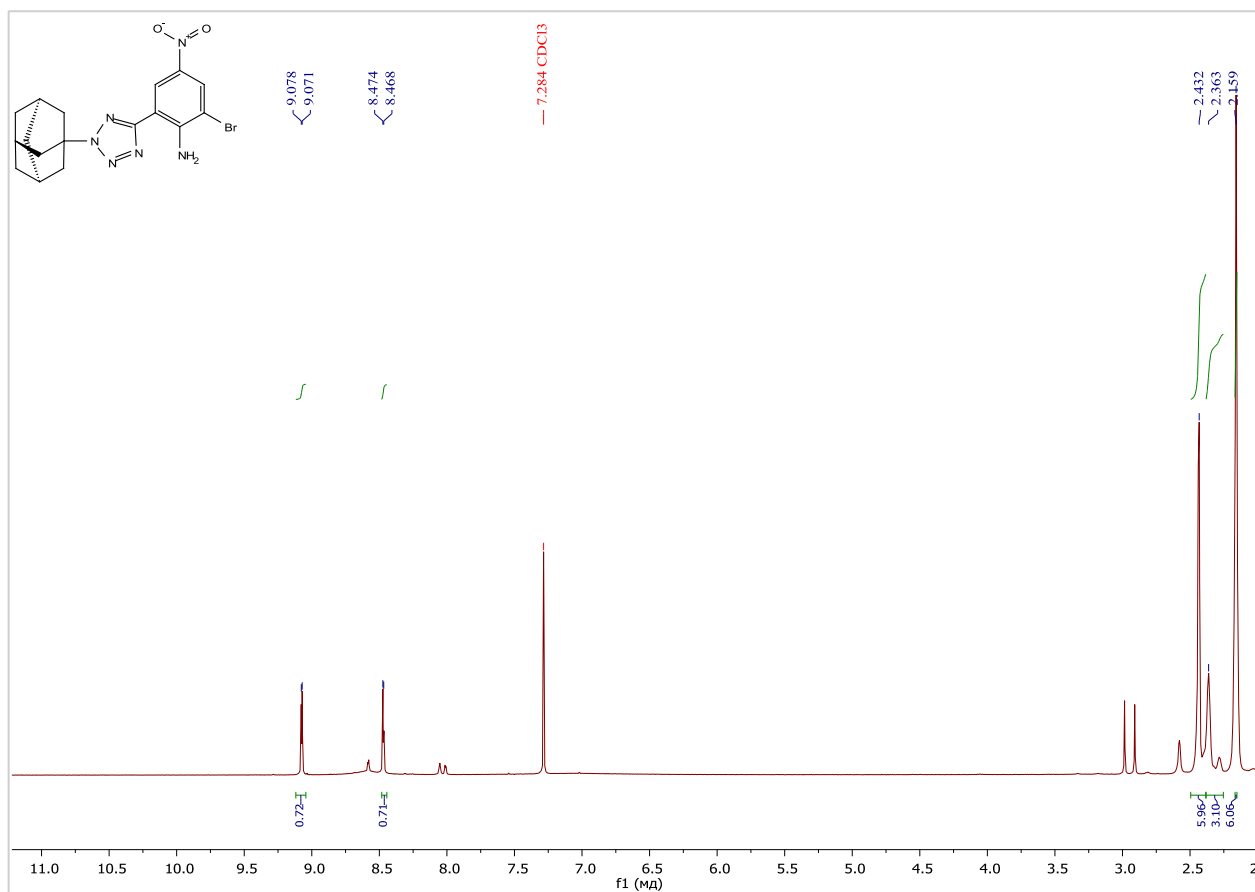


Fig. S25. ^1H spectra of **3i**

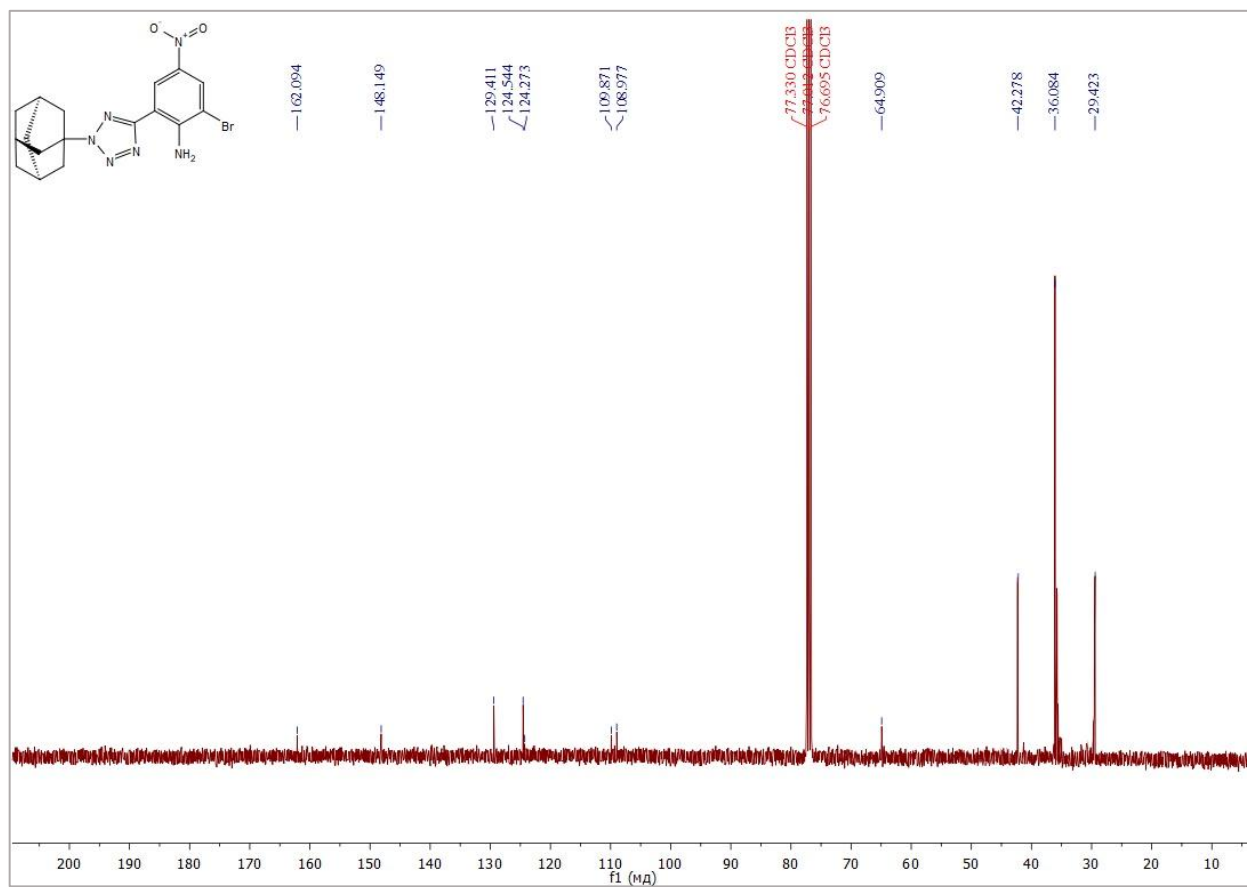


Fig. S26. $^{13}\text{C}\{^1\text{H}\}$ spectra of **3i**

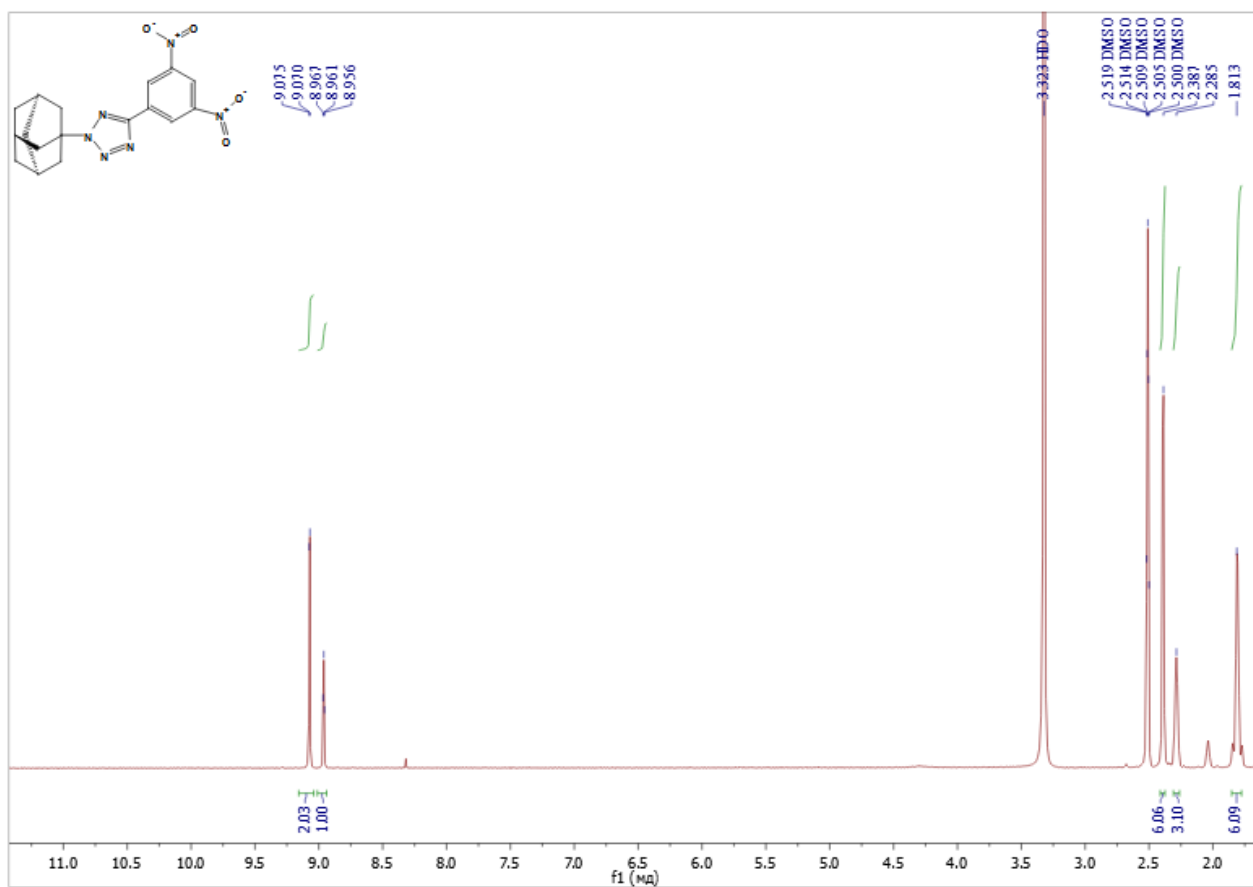


Fig. S27. ^1H spectra of **3j**

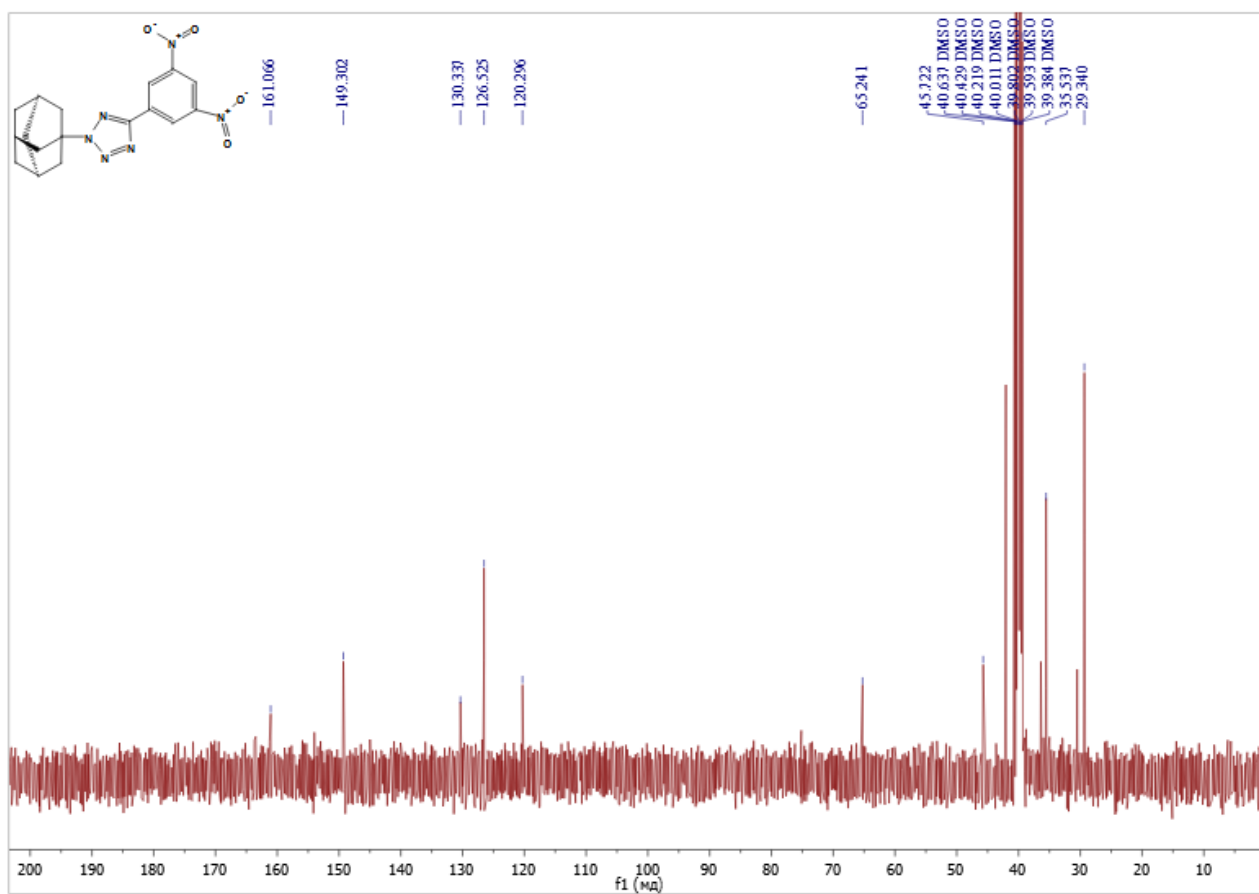


Fig. S28. $^{13}\text{C}\{^1\text{H}\}$ spectra of **3j**

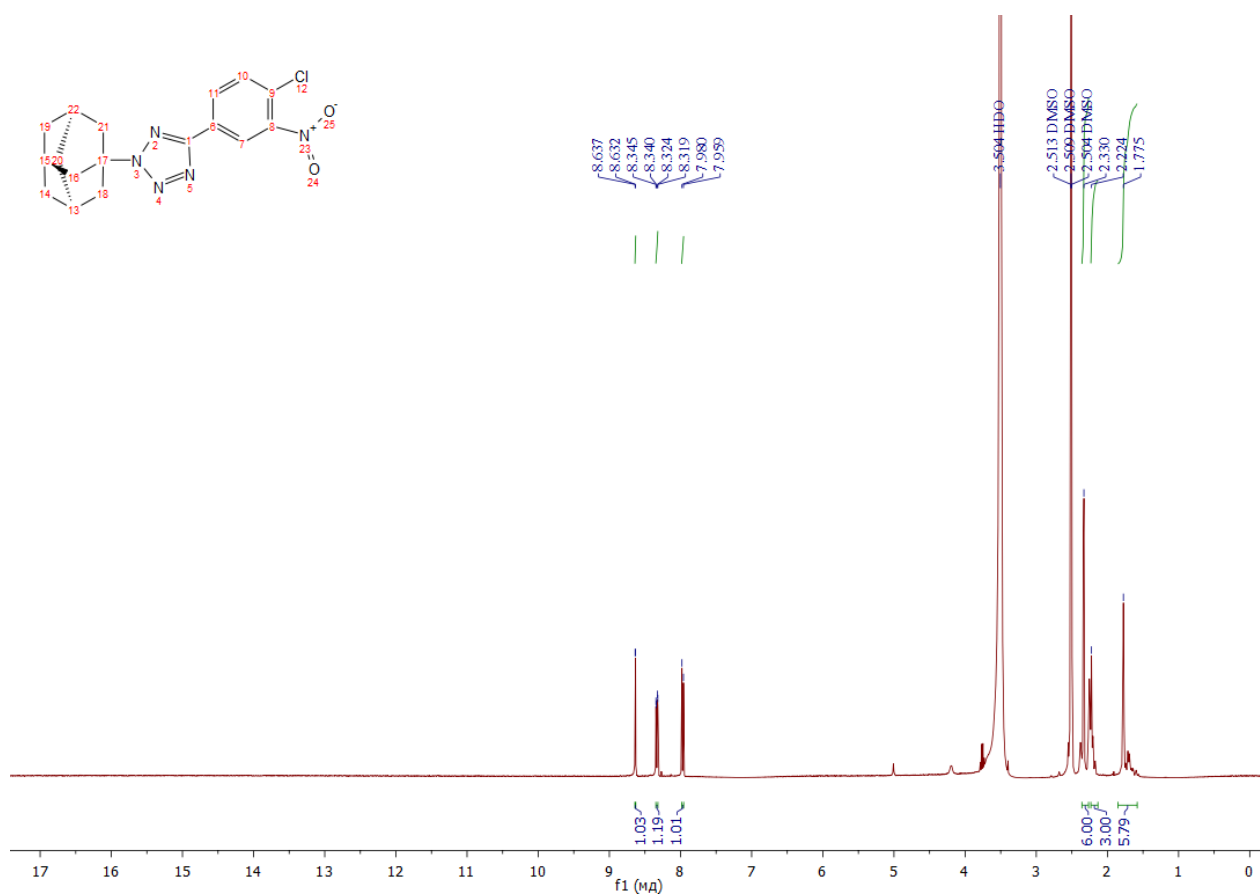


Fig. S29. ^1H spectra of **3k**

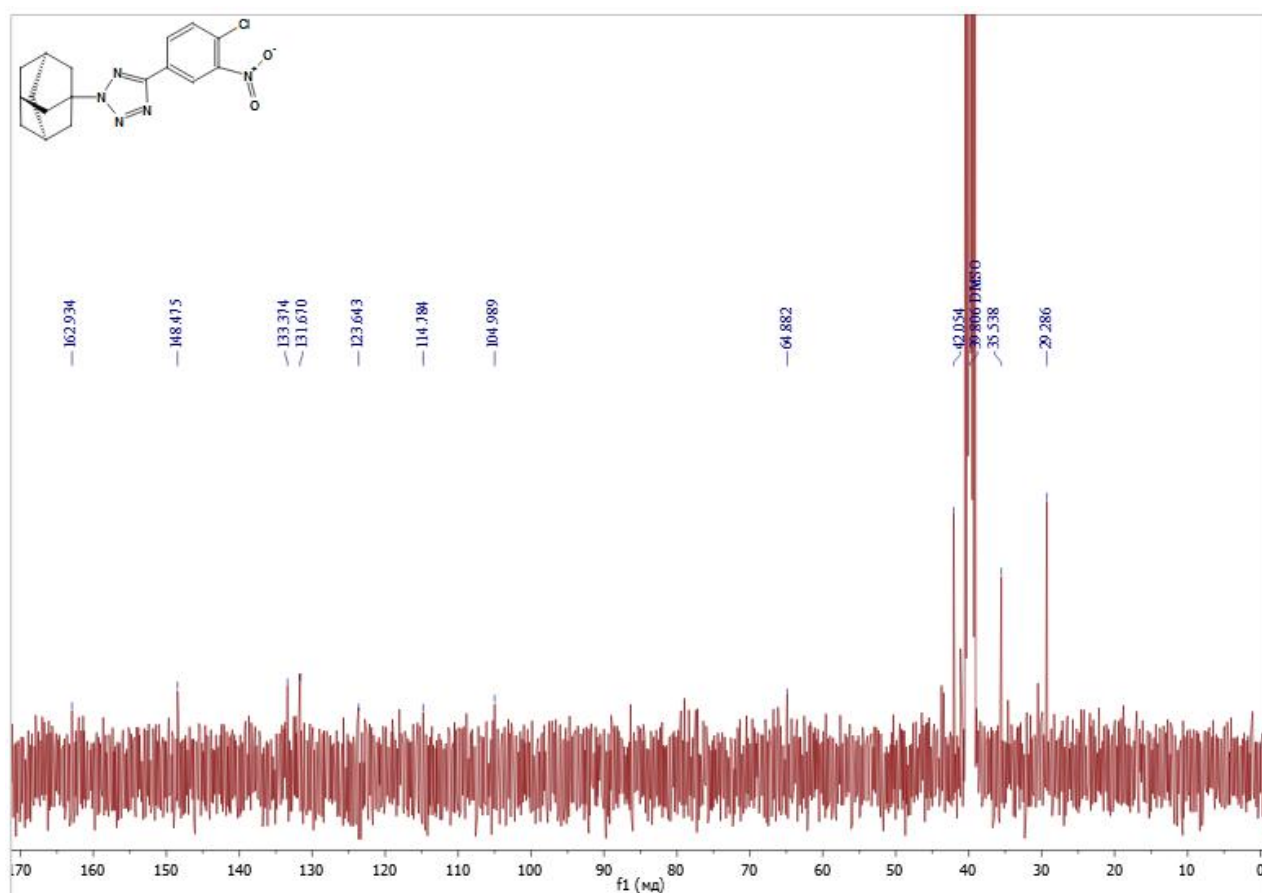


Fig. S30. $^{13}\text{C}\{^1\text{H}\}$ spectra of **3k**

2. Mass spectra of compounds

Display Report

Analysis Info

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Method tune_low_pos.m
Sample Name
Comment

Acquisition Date 18-Mar-19 11:42:47

Operator BDAL@DE
Instrument / Ser# maXis 62

Acquisition Parameter

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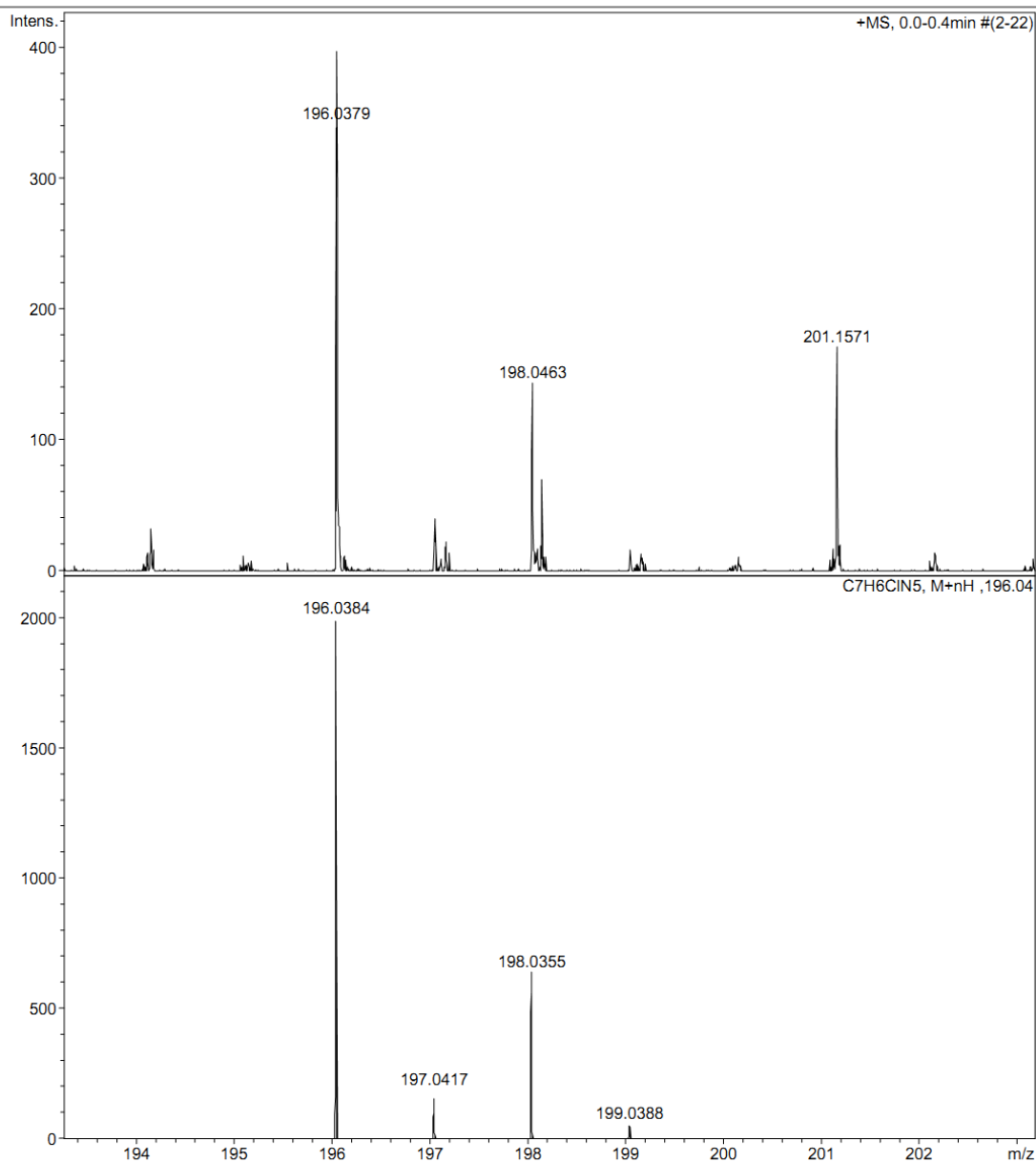


Fig. S31. Mass spectra of 2e

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Sample Name
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Operator Bruker Customer
Instrument / Ser# micrOTOF 10223

Acquisition Parameter

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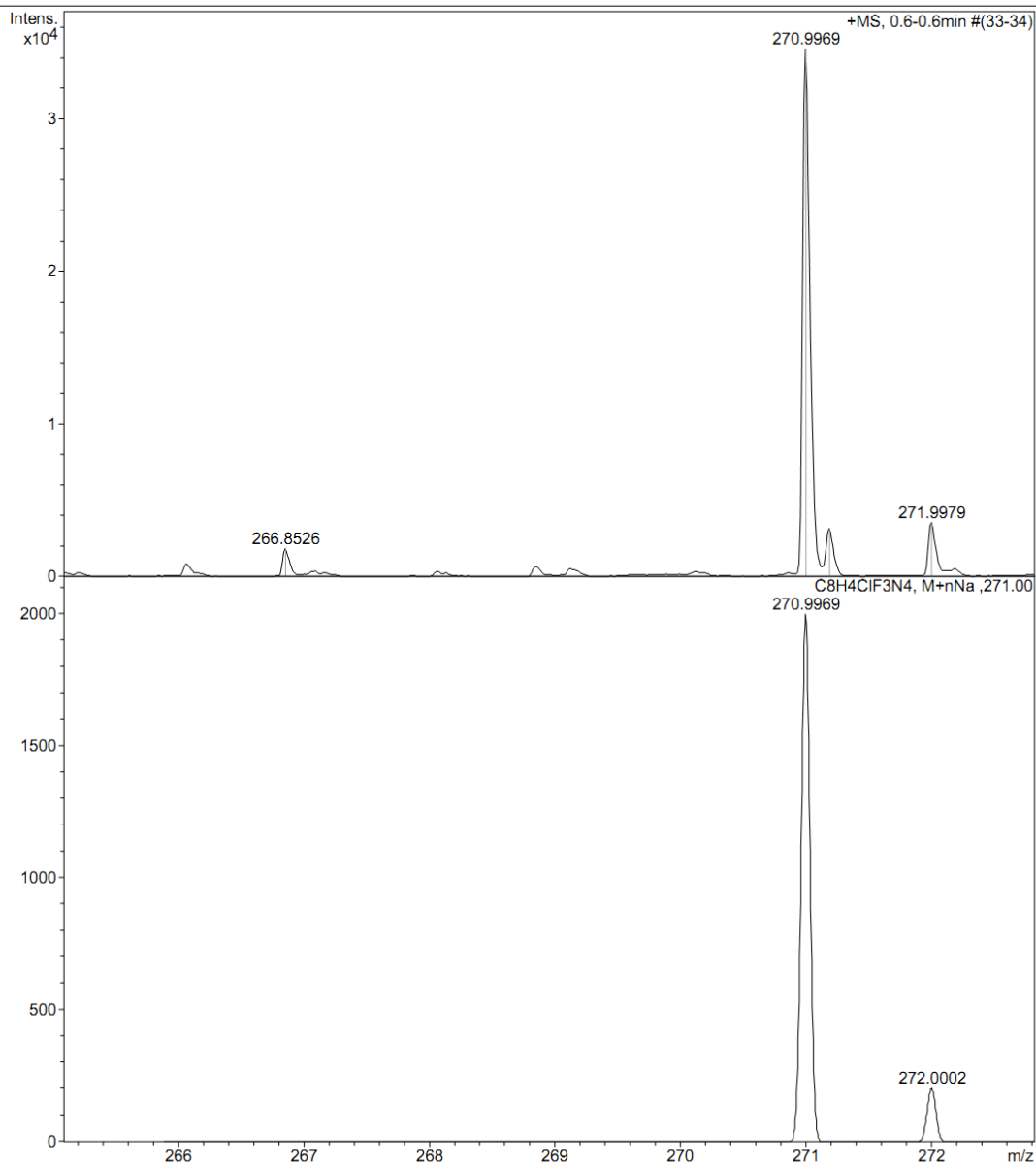


Fig. S32. Mass spectra of 2f

Display Report

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Sample Name
Comment

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Operator BDAL@DE
Instrument / Ser# maXis 62

Acquisition Parameter

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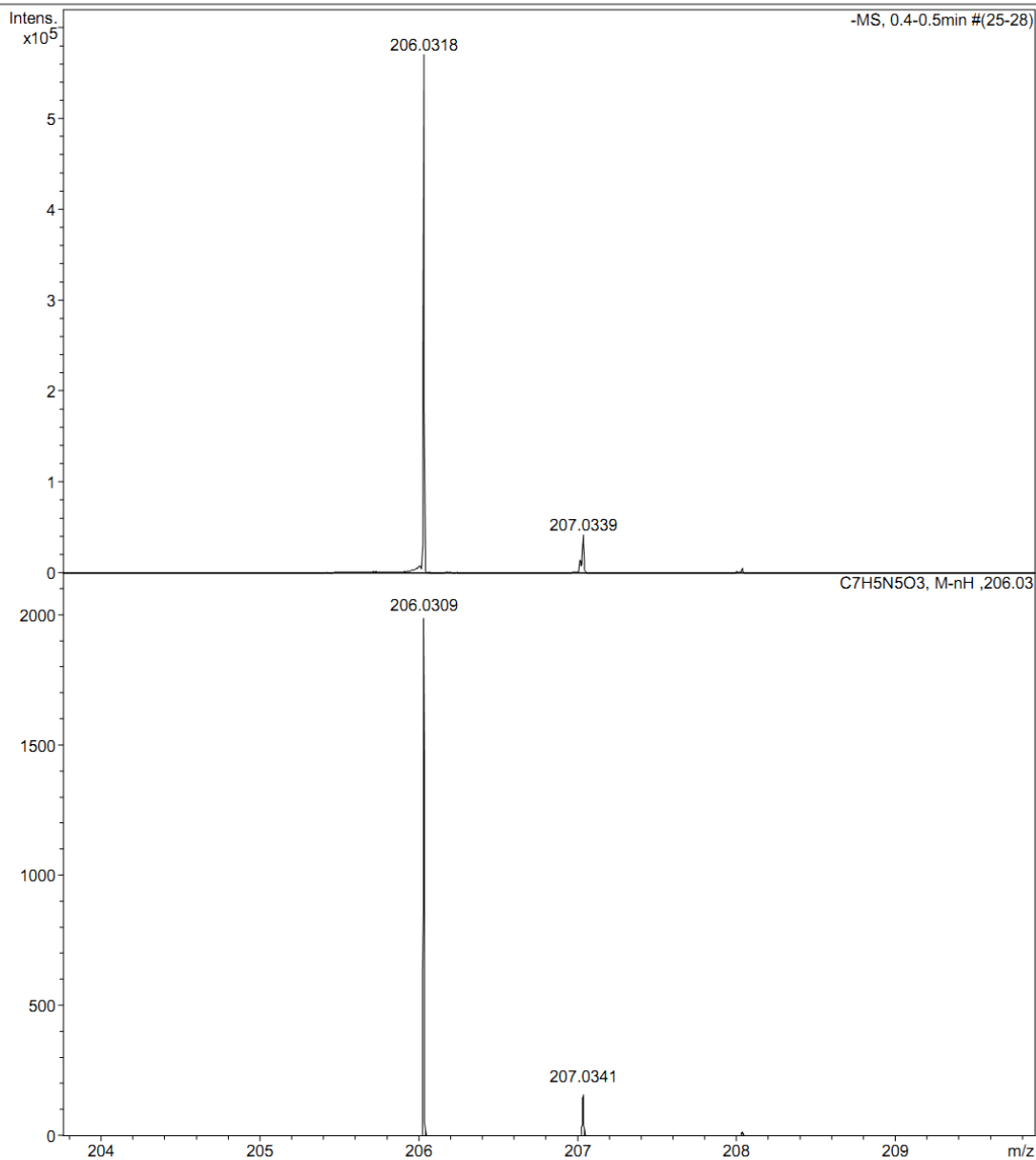


Fig. S33. Mass spectra of 2g

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Operator Bruker Customer
Instrument / Ser# micrOTOF 10223

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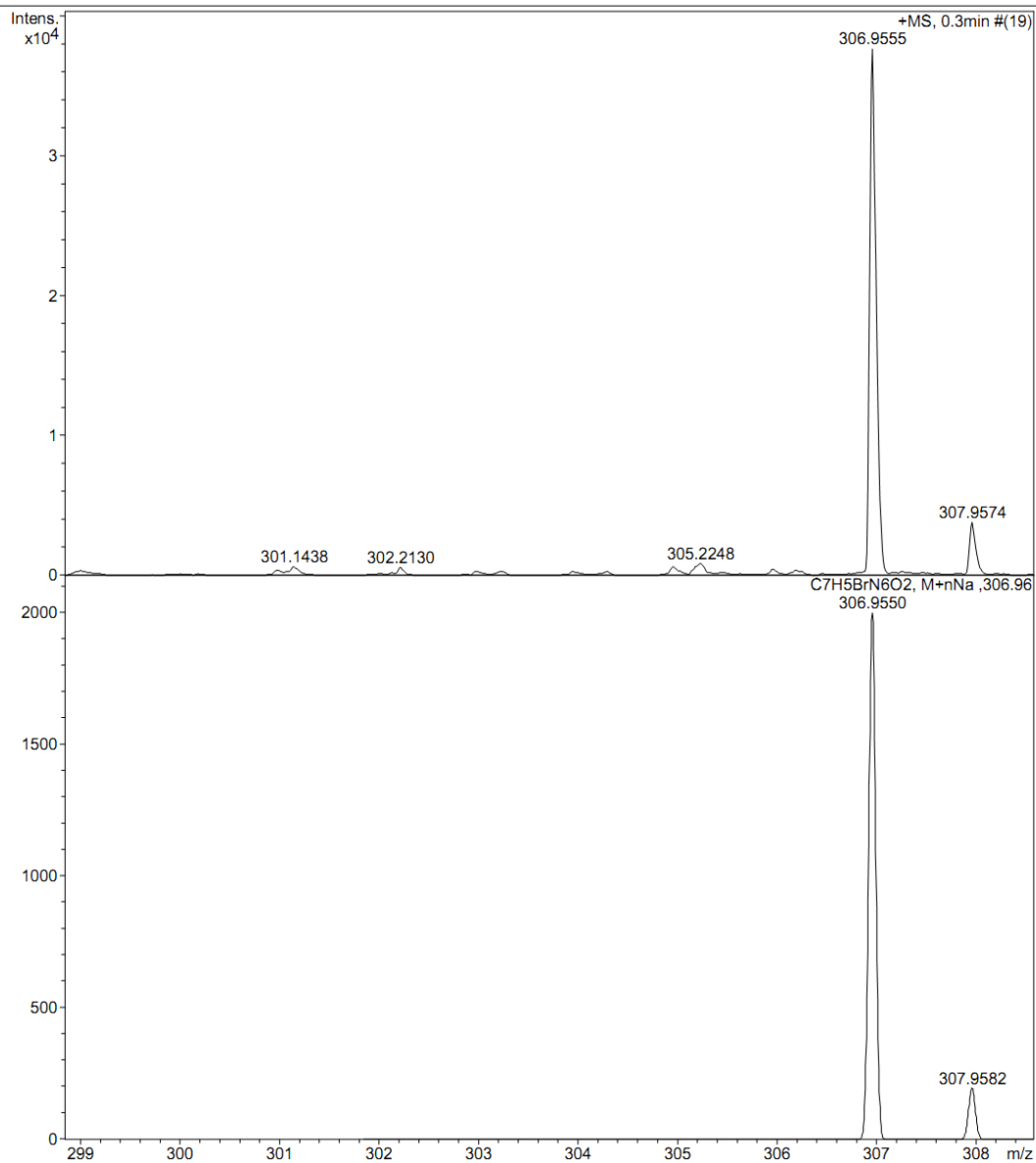


Fig. S34. Mass spectra of **2i**

Display Report

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Method tune_low.m
Sample Name
Comment

Acquisition Date 06-Nov-19 12:36:06

Operator BDAL@DE
Instrument / Ser# maXis 62

Acquisition Parameter

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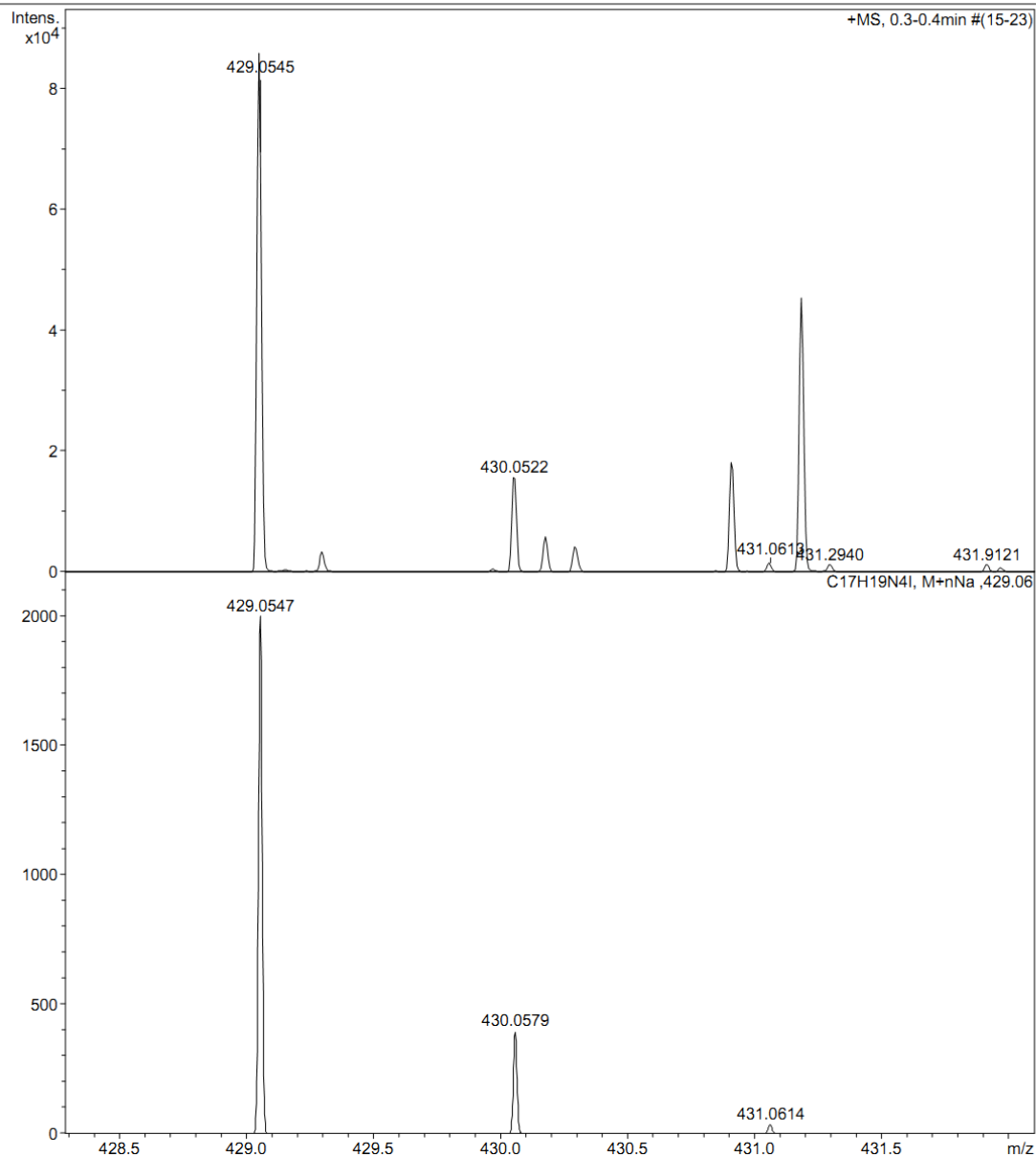


Fig. S35. Mass spectra of 3a

Display Report

Analysis Info

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Sample Name
Comment

Acquisition Date 25-Sep-19 10:07:28
Operator BDAL@DE
Instrument / Ser# maXis 62

Acquisition Parameter

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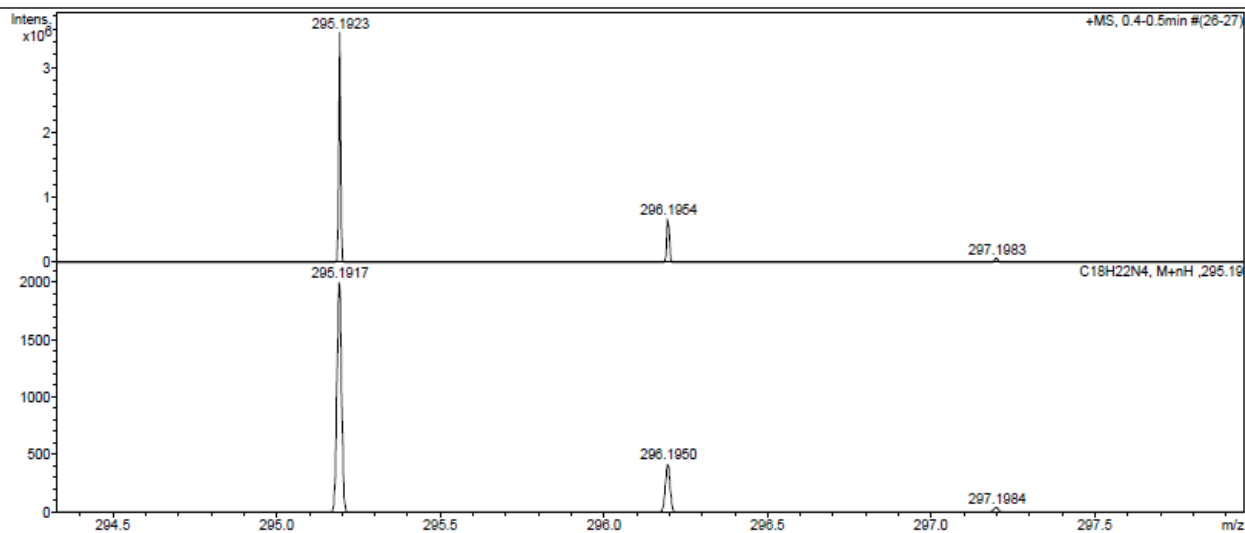


Fig. S36. Mass spectra of **3b**

Mass Spectrum Report

Analysis Info
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Sample Name
Comment

Acquisition Date 14.05.2019 15:41:28
Operator Bruker Customer
Instrument / Ser# microTOF 10223

Acquisition Parameter					
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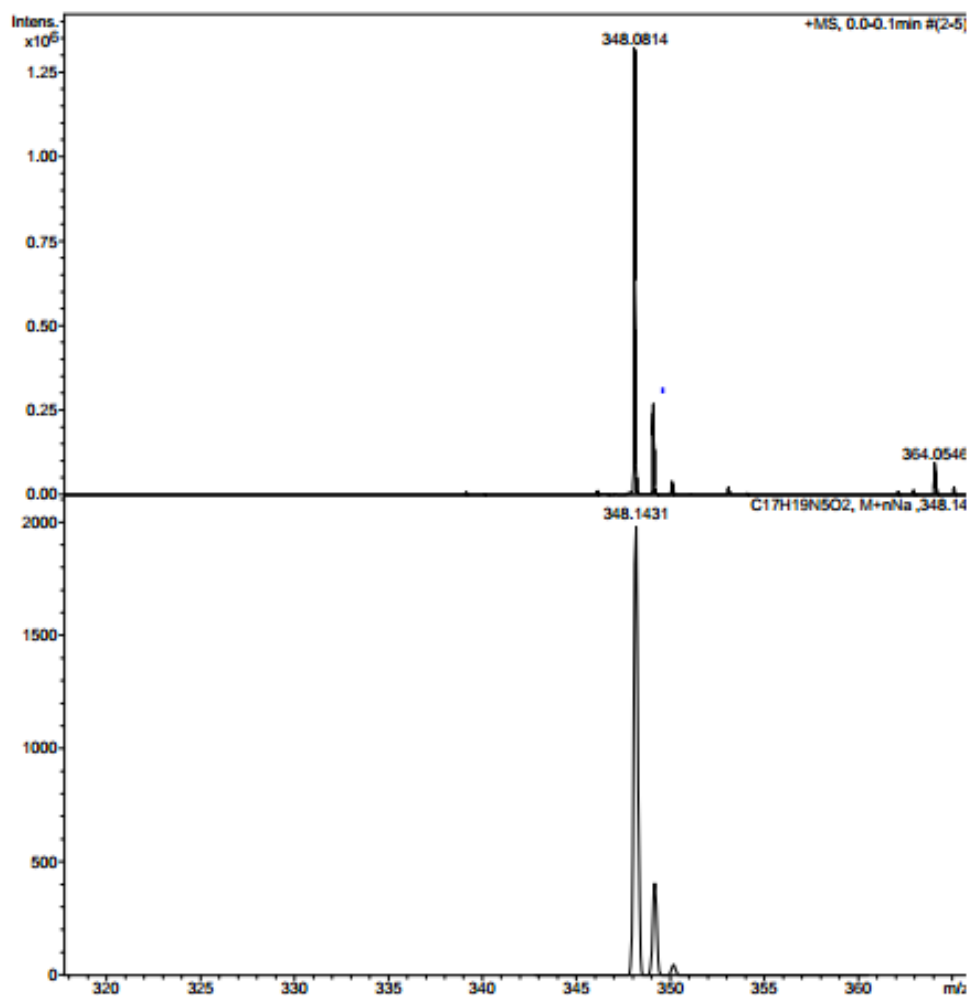


Fig. S37. Mass spectra of **3c**

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Method tune_low_pos_07neb.m
Sample Name
Comment

Acquisition Date 02-Nov-20 14:34:03

Operator BDAL@DE
Instrument / Ser# maXis 62

Acquisition Parameter

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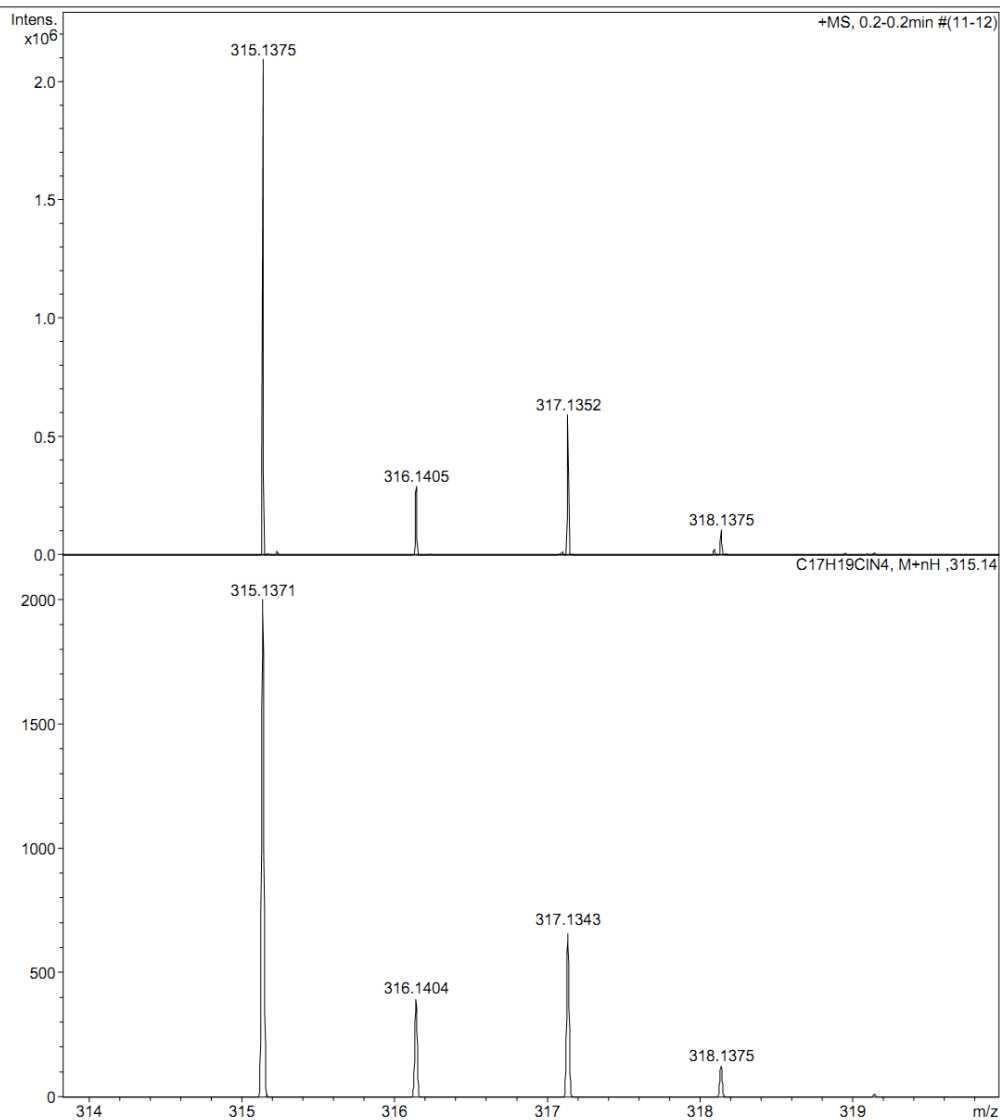


Fig. S38. Mass spectra of **3d**

Mass Spectrum Report

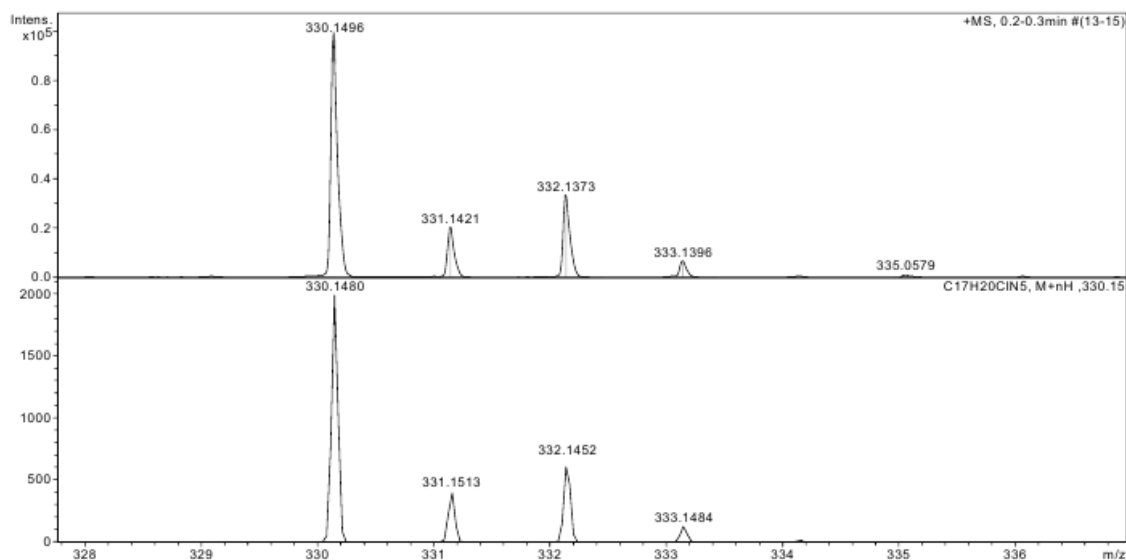
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Sample Name
Comment MeOH

Acquisition Date 17.04.2019 16:29:45
Operator Bruker Customer
Instrument / Ser# micrOTOF 10223

Acquisition Parameter

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Fig. S39. Mass spectra of 3e

Display Report

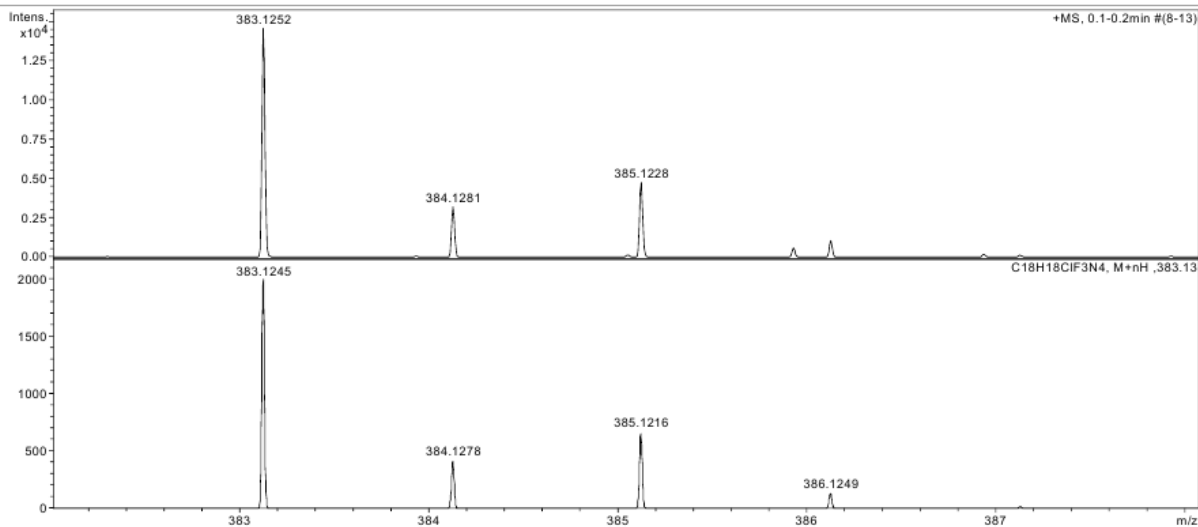
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Method tune_low.m
Sample Name
Comment

Acquisition Date 11-Oct-19 12:15:55
Operator BDAL@DE
Instrument / Ser# maXis 62

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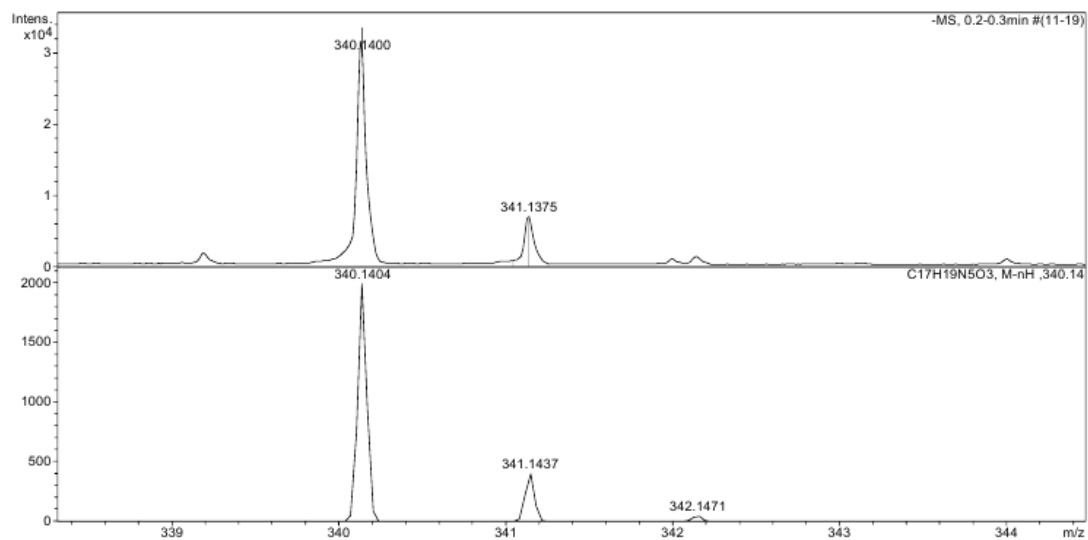
Page 1 of 1

Fig. S40. Mass spectra of 3f

Mass Spectrum Report

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Sample Name: MeOH
Comment: MeOH
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Operator: Bruker Customer
Instrument / Ser#: micrOTOF 10223

Acquisition Parameter
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Set End Plate Offset: -500 V
Set Nebulizer: 0.4 Bar
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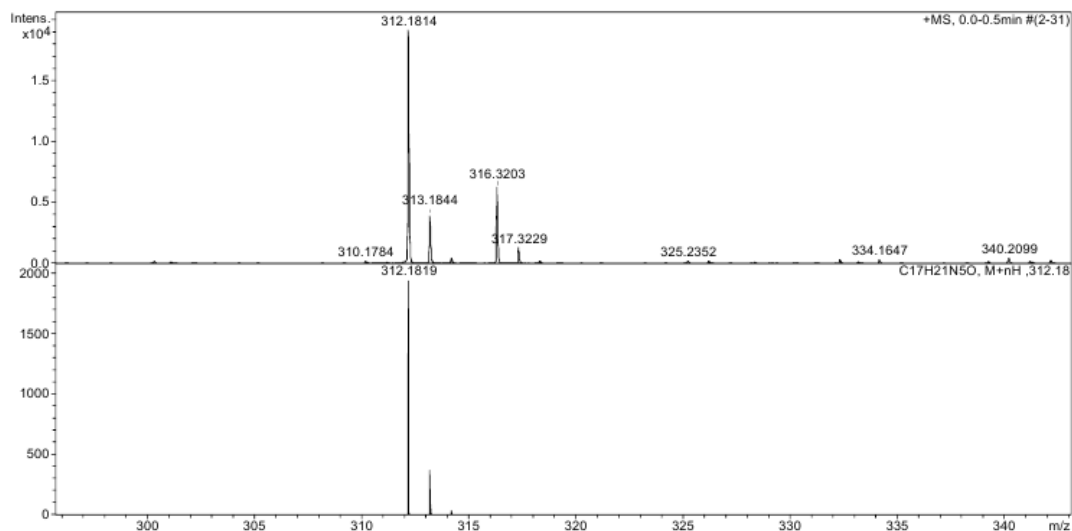
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Fig. S41. Mass spectra of **3g**

Mass Spectrum Report

Analysis Info
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Method: tune_low.m
Sample Name: DSV16Ad
Comment: MeOH
Acquisition Date: 28.05.2019 12:33:44
Operator: Bruker Customer
Instrument / Ser#: micrOTOF 10223

Acquisition Parameter
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Focus: Not active
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Scan End: 3000 m/z
Ion Polarity: Positive
Set Capillary: 4500 V
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Set Dry Heater: 180 °C
Set Dry Gas: 8.0 l/min
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printed: 28.05.2019 12:38:03

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Fig. S42. Mass spectra of **3h**

Display Report

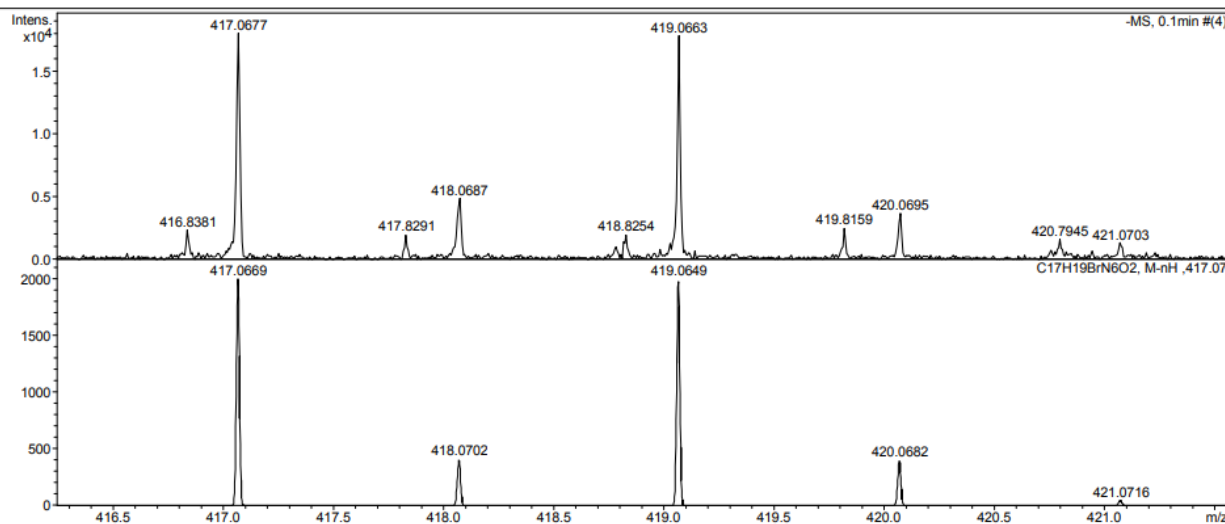
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 Sample Name
 Comment

Acquisition Date 25-Sep-19 10:10:02
 Operator BDAL@DE
 Instrument / Ser# maXis 62

Acquisition Parameter

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Bruker Compass DataAnalysis 4.0

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Fig. S43. Mass spectra of **3i**

Display Report

Analysis Info

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 Method tune_low.m
 Sample Name ABB420
 Comment

Acquisition Date 11.04.2019 9:39:39
 Operator Bruker Customer
 Instrument / Ser# micrOTOF 10223

Acquisition Parameter

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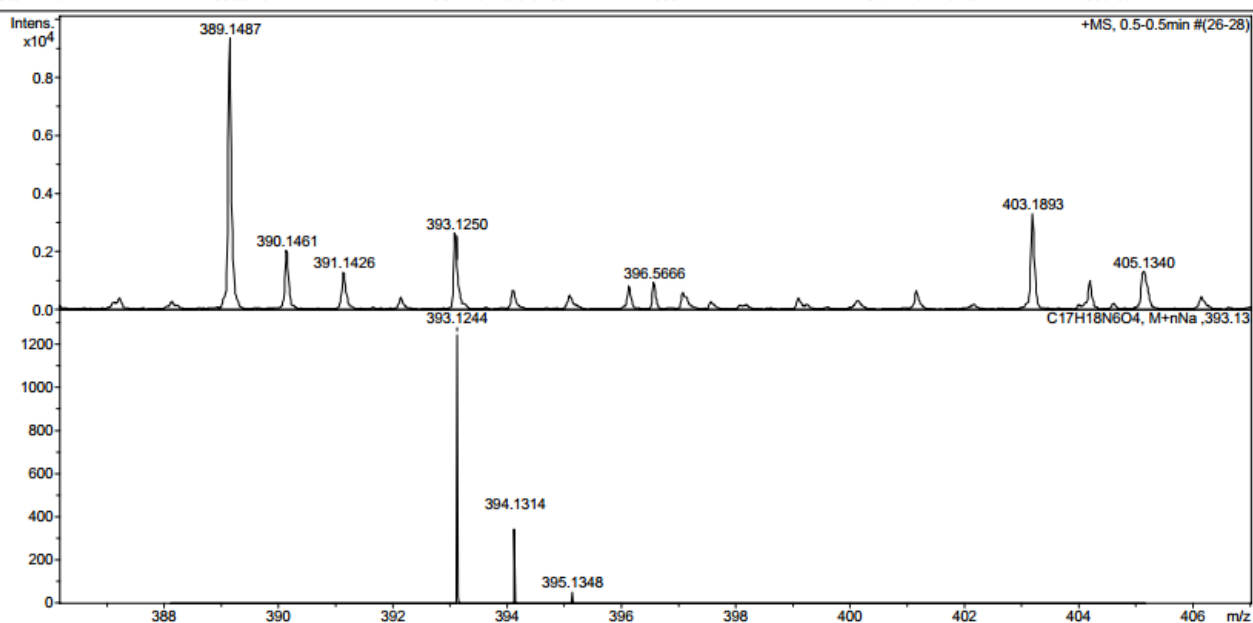


Fig. S44. Mass spectra of **3j**

Display Report

Analysis Info

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Method tune_low_pos_07neb.m
Sample Name
Comment

Acquisition Date 02-Nov-20 14:36:39

Operator BDAL@DE
Instrument / Ser# maXis 62

Acquisition Parameter

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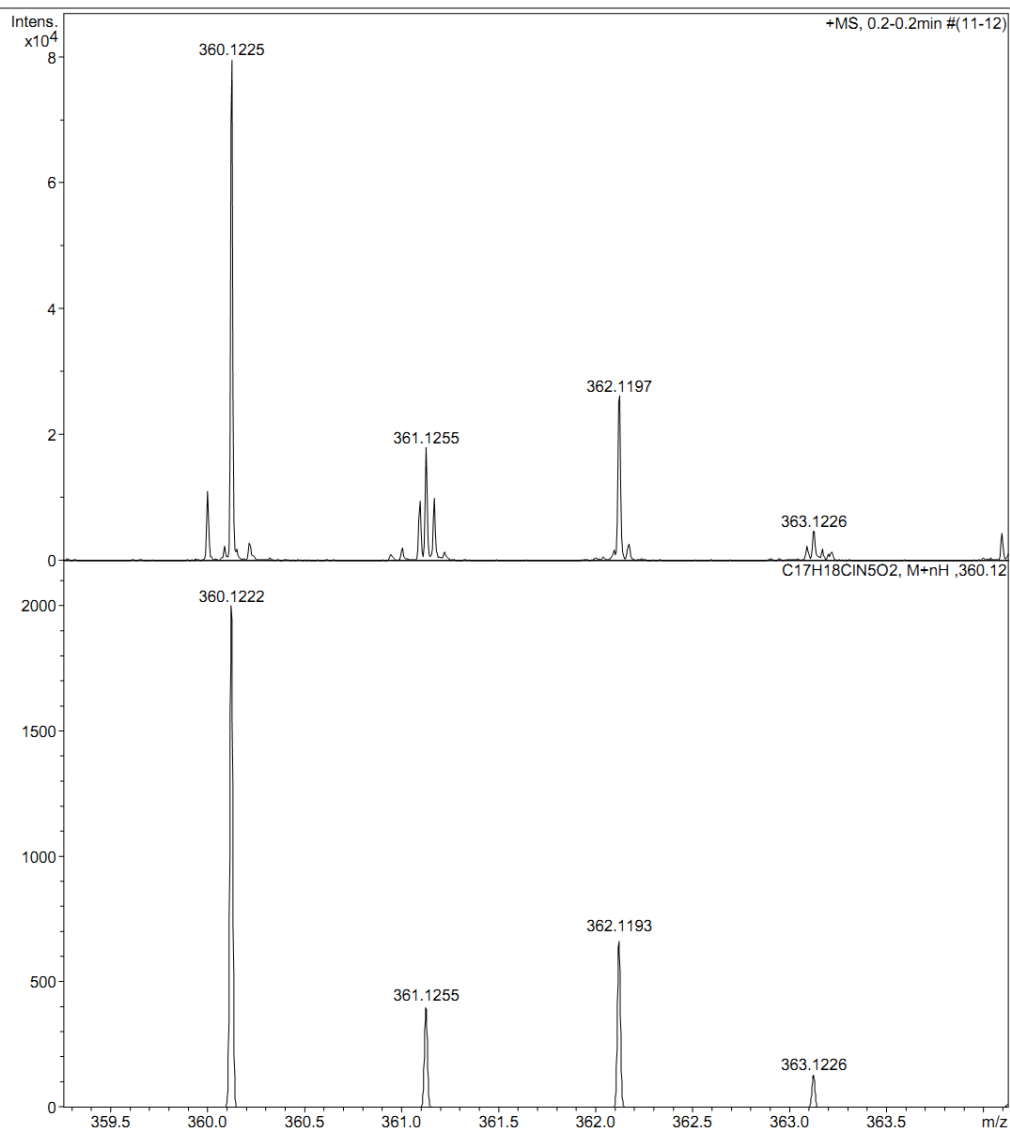
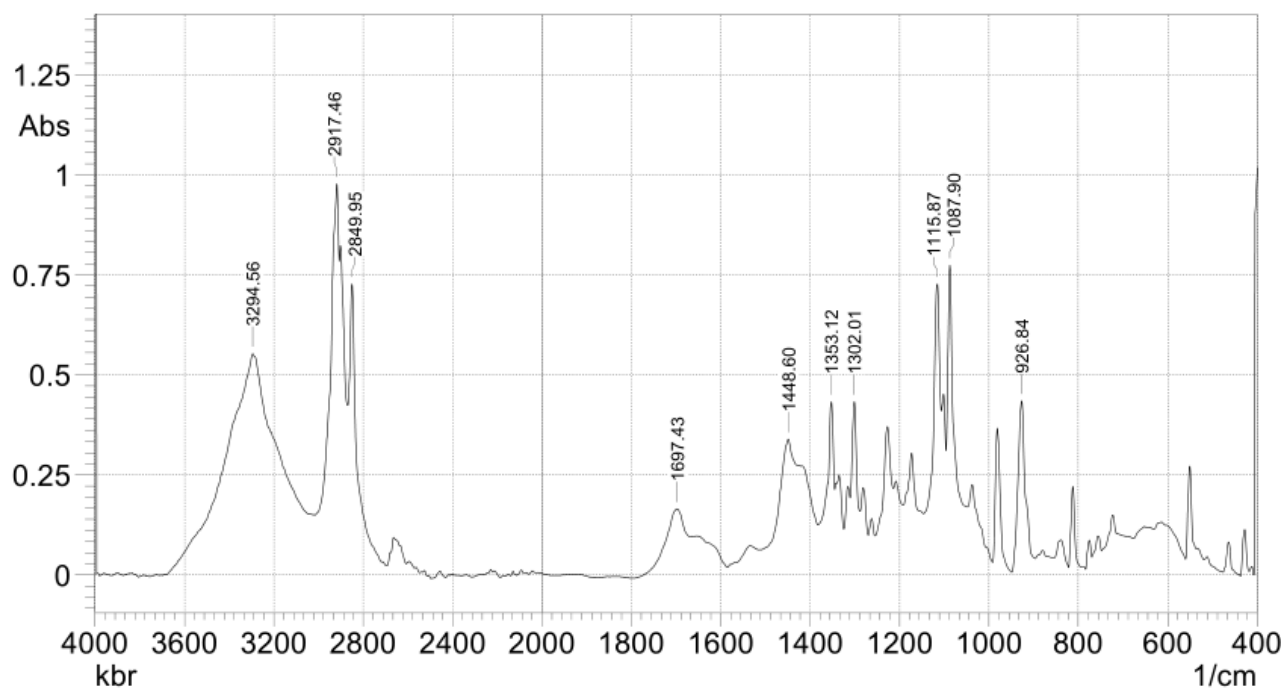


Fig. S45. Mass spectra of **3k**

3. IR spectra of compounds

SHIMADZU



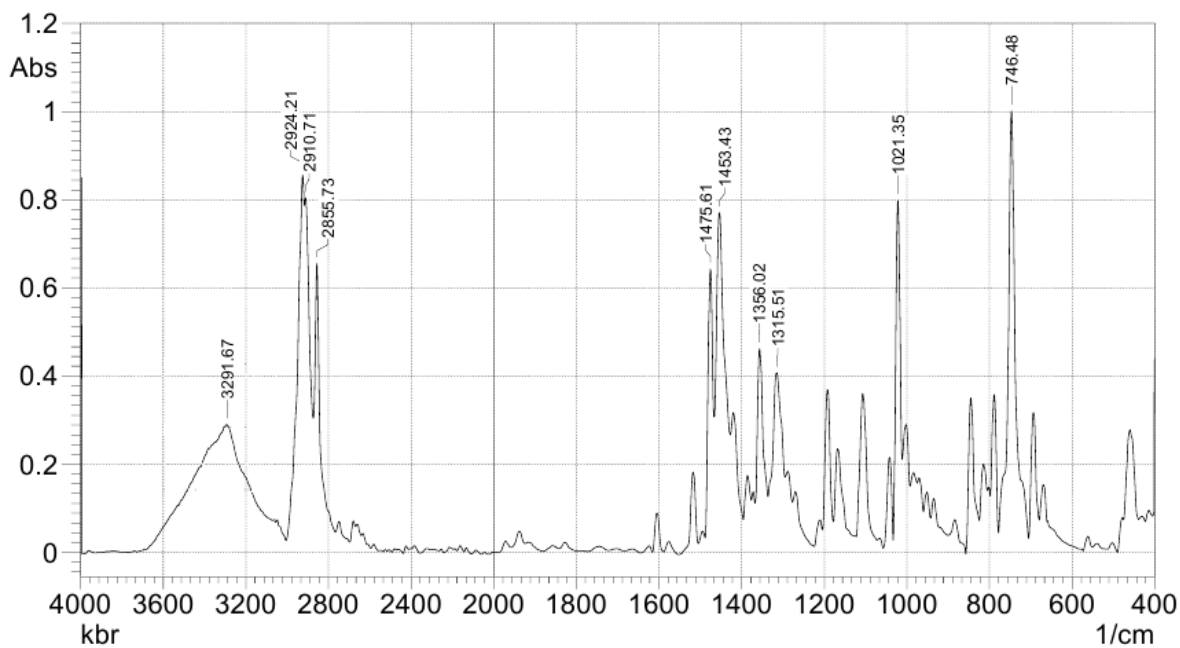
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No. of Scans;
Resolution;
Apodization;

Date/Time: 07 10 2020 16:50:06
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Fig. S46. IR spectra of **3a**

SHIMADZU

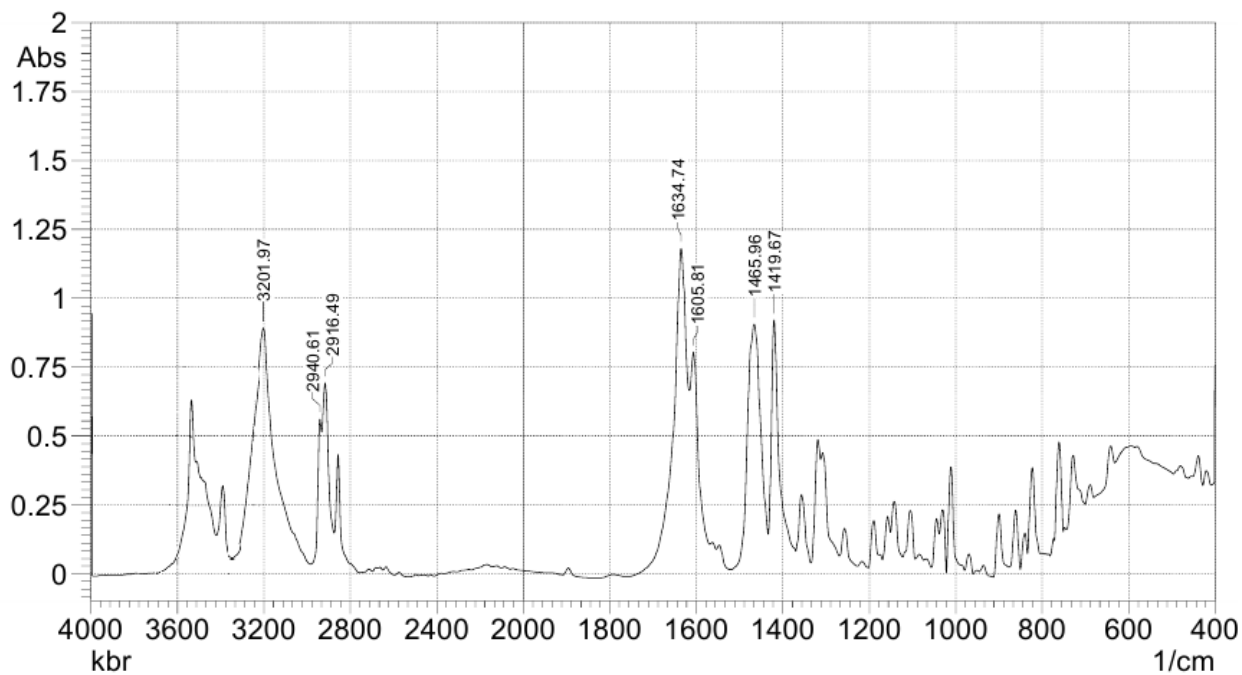


Comment;
kbr

No. of Scans;
Resolution;
Apodization;

Date/Time: 01 10 2020 15:28:12
Григорьев Я.М.; User

Fig. S47. IR spectra of **3b**

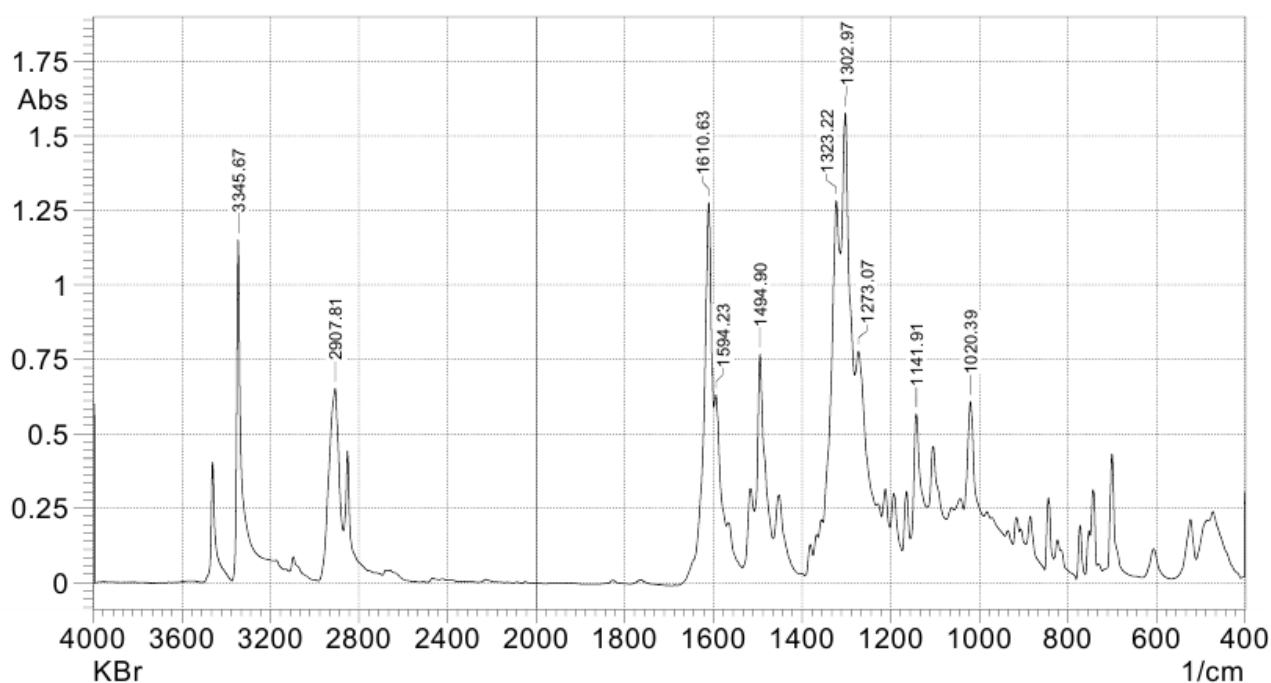


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kbr

No. of Scans:
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Apodization:

Date/Time: 01 10 2020 15:38:42
Григорьев Я.М.; User

Fig. S48. IR spectra of **3e**



Comment:
KBr

No. of Scans:
Resolution;
Apodization:

Date/Time: 21 10 2020 17:20:24
Григорьев Я.М.; User

Fig. S49. IR spectra of **3i**

5. XRD Data

Bond precision: C-C = 0.0023 Å Wavelength=1.54184

Cell: a=9.8279(2) b=12.8485(2) c=12.7327(3)
 alpha=90 beta=104.543(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1556.29(6)	1556.29(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C18 H22 N4	C18 H22 N4
Sum formula	C18 H22 N4	C18 H22 N4
Mr	294.40	294.39
Dx, g cm-3	1.257	1.256
Z	4	4
Mu (mm-1)	0.597	0.597
F000	632.0	632.0
F000'	633.65	
h, k, lmax	12, 16, 16	12, 15, 16
Nref	3251	3172
Tmin, Tmax	0.867, 0.971	0.713, 1.000
Tmin'	0.867	

Correction method= # Reported T Limits: Tmin=0.713 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.976 Theta(max)= 76.085

R(reflections)= 0.0565(2749) wR2(reflections)= 0.1639(3172)

S = 1.111 Npar= 200

Fig. S50. XRD data of **3b**

Bond precision: C-C = 0.0035 Å Wavelength=1.54184

Cell: a=7.2294(1) b=21.6410(3) c=10.2631(2)
 alpha=90 beta=91.291(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1605.27(4)	1605.27(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C17 H18.48 Cl N5	C17 H18.48 Cl N5
Sum formula	C17 H18.48 Cl N5	C17 H18.48 Cl N5
Mr	328.30	328.30
Dx, g cm-3	1.358	1.358
Z	4	4
Mu (mm-1)	2.154	2.154
F000	689.9	690.0
F000'	693.08	
h, k, lmax	8, 26, 12	8, 26, 12
Nref	3078	3073
Tmin, Tmax	0.643, 0.724	0.765, 1.000
Tmin'	0.568	

Correction method= # Reported T Limits: Tmin=0.765 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 70.478

R(reflections)= 0.0530(2818) wR2(reflections)= 0.1504(3073)

S = 1.082 Npar= 243

Fig. S51. XRD data of **3c**

Bond precision: C-C = 0.0019 Å Wavelength=1.54184

Cell: a=7.0477(1) b=17.9831(3) c=14.1252(3)
 alpha=90 beta=104.454(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1733.56(6)	1733.56(6)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H18 Cl F3 N4	C18 H18 Cl F3 N4
Sum formula	C18 H18 Cl F3 N4	C18 H18 Cl F3 N4
Mr	382.81	382.81
Dx, g cm ⁻³	1.467	1.467
Z	4	4
Mu (mm ⁻¹)	2.320	2.320
F000	792.0	792.0
F000'	795.99	
h, k, lmax	8, 22, 17	8, 22, 17
Nref	3617	3429
Tmin, Tmax	0.455, 0.740	0.680, 1.000
Tmin'	0.292	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.948 Theta(max)= 76.124

R(reflections)= 0.0332(3286) wR2(reflections)= 0.0906(3429)

S = 1.063 Npar= 235

Fig. S52. XRD data of **3f**

Bond precision: C-C = 0.0063 Å Wavelength=1.54184

Cell: a=31.7414(6) b=15.3710(3) c=6.4665(2)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	3154.99(13)	3154.99(13)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	C17 H19 N5 O3	2 (C17 H19 N5 O3)
Sum formula	C17 H19 N5 O3	C34 H38 N10 O6
Mr	341.37	682.74
Dx, g cm ⁻³	1.437	1.437
Z	8	4
Mu (mm ⁻¹)	0.841	0.841
F000	1440.0	1440.0
F000'	1444.54	
h, k, lmax	38, 18, 7	38, 18, 7
Nref	6103[3503]	6032
Tmin, Tmax	0.868, 0.992	0.334, 1.000
Tmin'	0.824	

Correction method= # Reported T Limits: Tmin=0.334 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.99 Theta(max)= 71.085

R(reflections)= 0.0683(5508) wR2(reflections)= 0.1392(6032)

S = 1.103 Npar= 454

Fig. S53. XRD data of **3g**

6. DSC/TG analysis of compound 3g

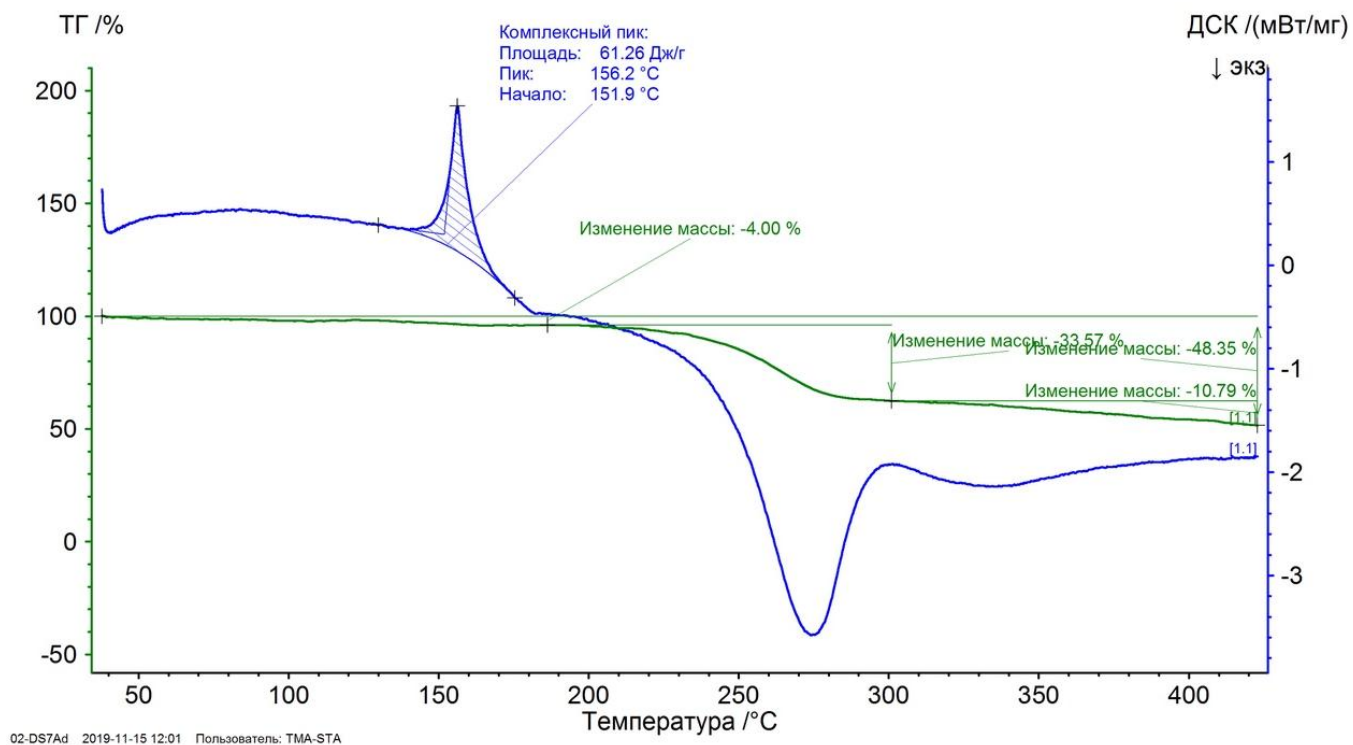


Fig. S54. DSC/TG analysis of compound of **3g**