Supplementary Materials

Highly luminescent 4*H*-1,2,4-triazole derivatives: synthesis, molecular structure and photophysical properties

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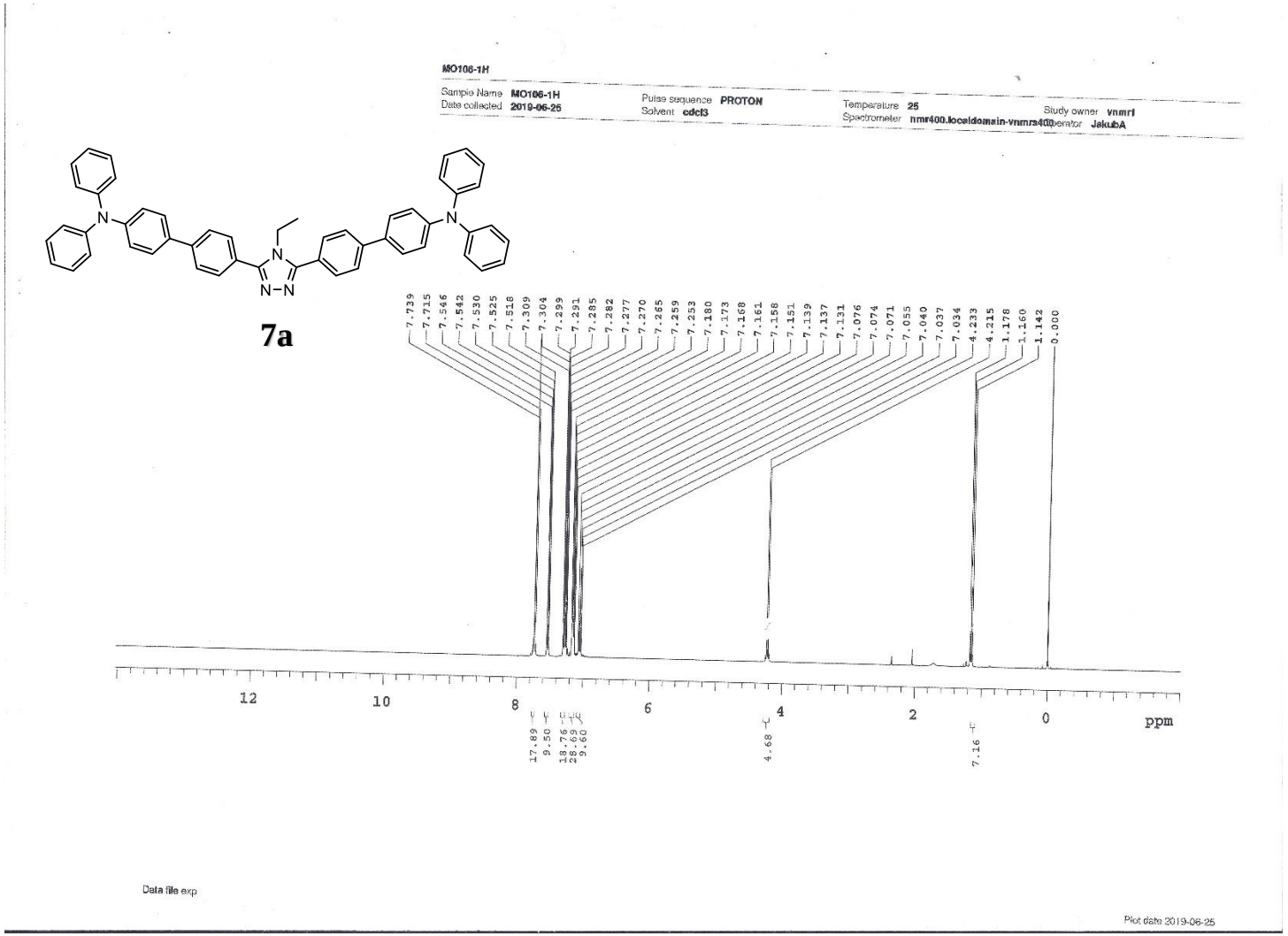
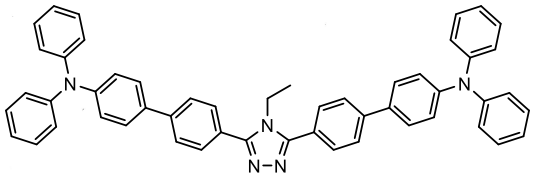
1. ^{1}H NMR and ^{13}C NMR spectra

4-Ethyl-3,5-bis[4′-(N,N-diphenylamino)biphenyl-4-yl]-4H-1,2,4-triazole (**7a**).

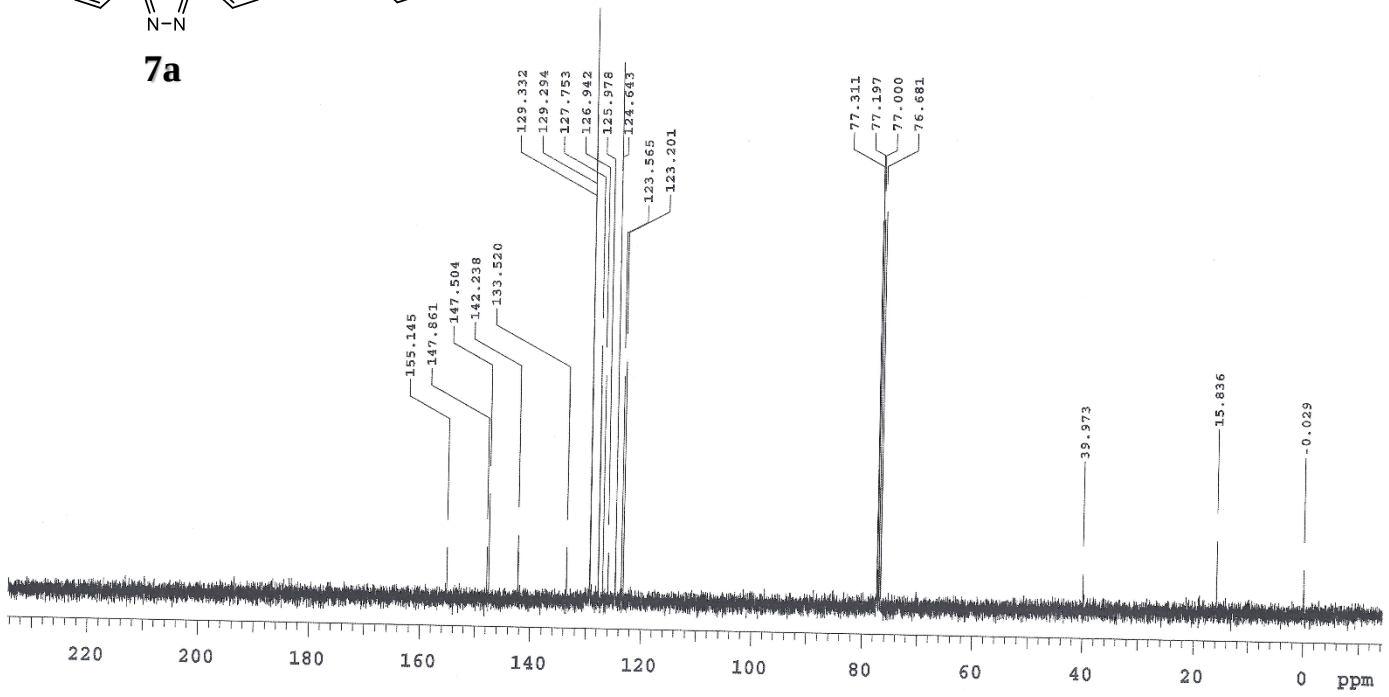




7a

MO106-13C

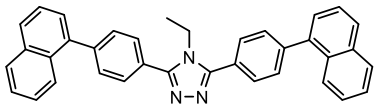
Sample Name MO106-13C
Date collected 2019-06-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA



Data file exp

Plot date 2019-06-25

4-Ethyl-3,5-bis[4-(naphthalen-1-yl)phenyl]-4H-1,2,4-triazole (**7b**).

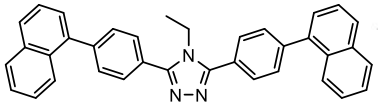


7b

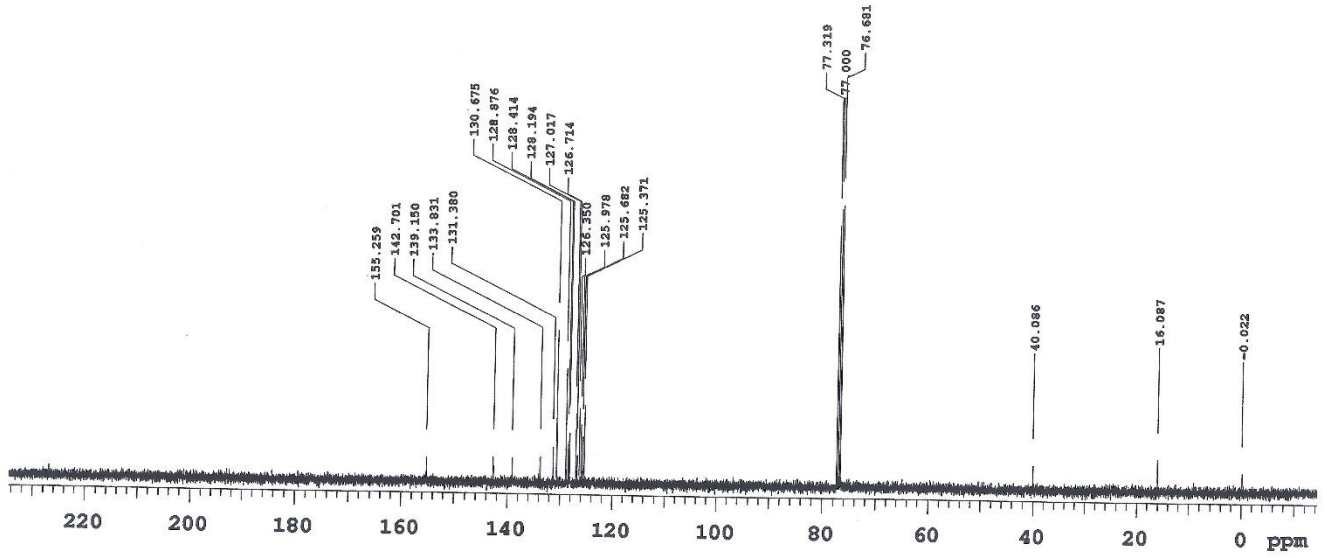
MO112-13C

Sample Name	MO112-13C	Pulse sequence	CARBON	Temperature	25
Date collected	2019-07-09	Solvent	cdcl3	Spectrometer	nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA



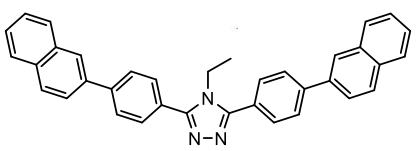
7b



Data file exp

Plot date 2019-07-09

4-Ethyl-3,5-bis[4-(naphthalen-2-yl)phenyl]-4H-1,2,4-triazole (**7c**)



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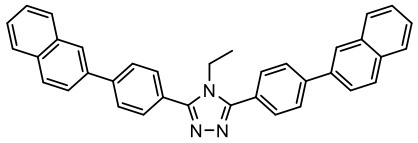
Sample Name MO-111
Date collected 2019-06-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA



7c

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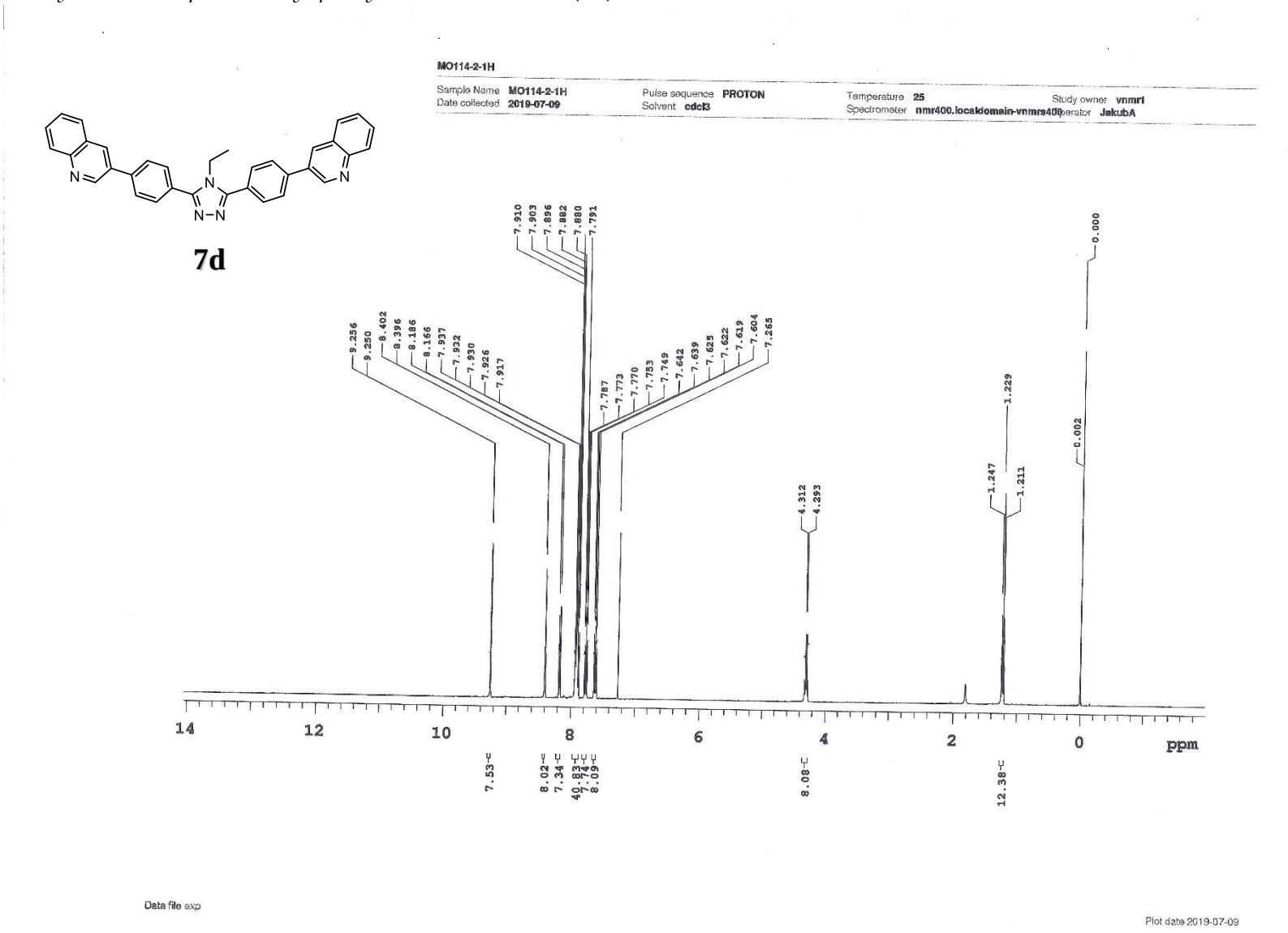
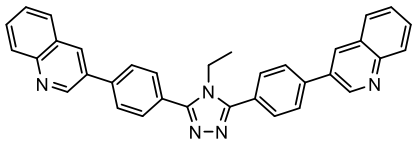
Plot date 2019-06-26

4-Ethyl-3,5-bis[4-(quinolin-3-yl)phenyl]-4H-1,2,4-triazole (**7d**).



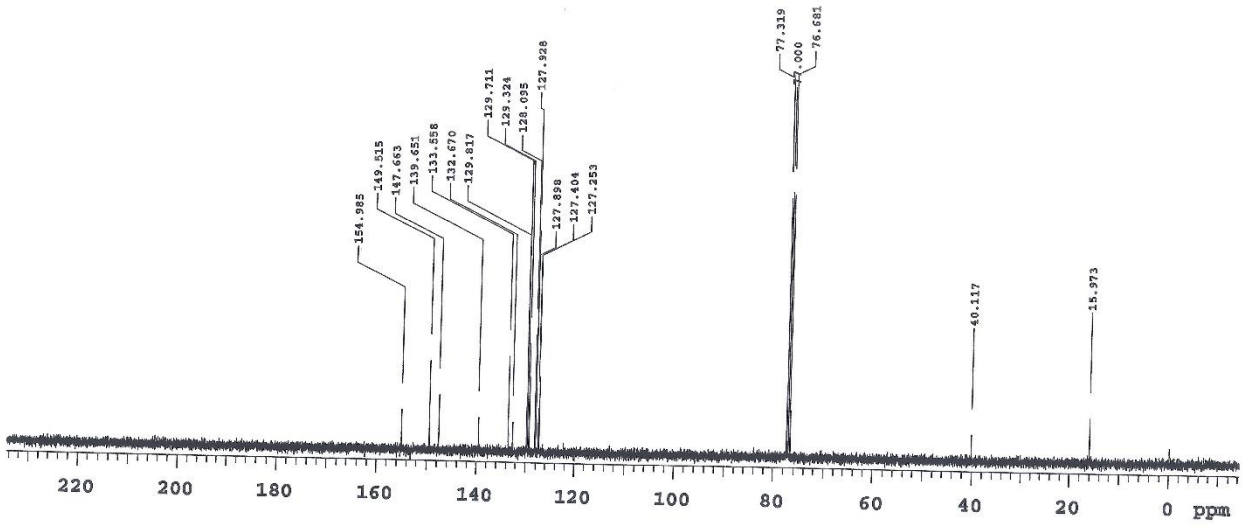


7d

MO114-2-13C

Sample Name	MO114-2-13C	Pulse sequence	CARBON	Temperature	25
Date collected	2019-07-09	Solvent	cdcl3	Spectrometer	nmr400.localdomain-vnmrs400

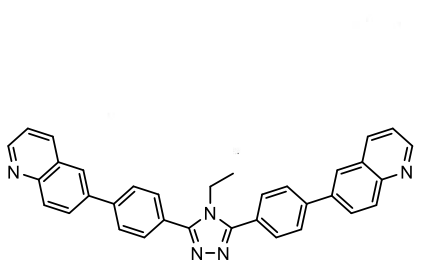
Study owner JakubA
Operator JakubA



Data file exp

Plot date 2019-07-09

4-Ethyl-3,5-bis[4-(quinolin-6-yl)phenyl]-4H-1,2,4-triazole (**7e**).



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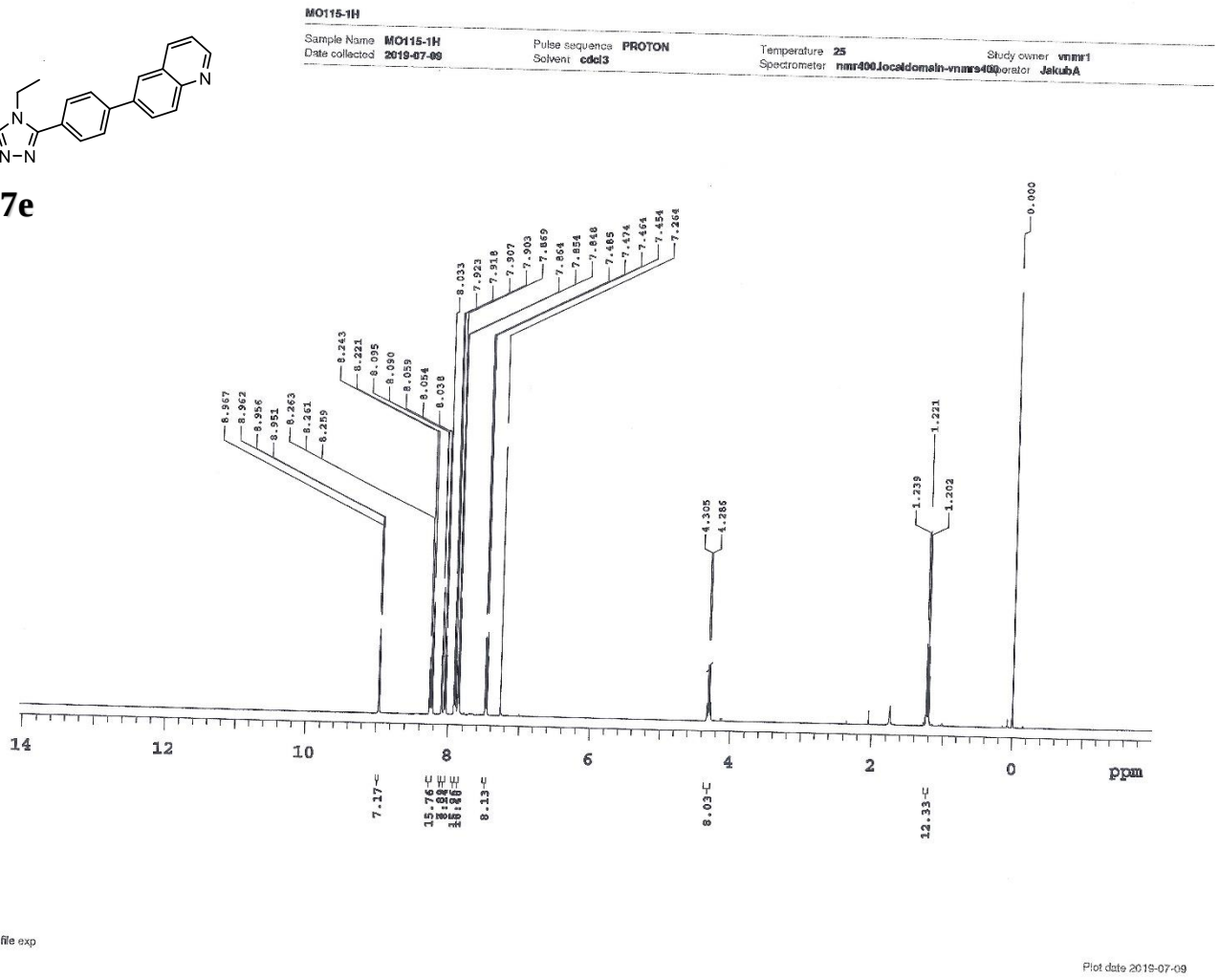
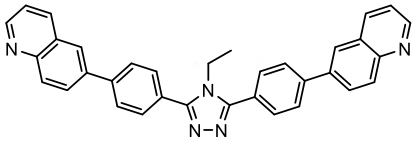


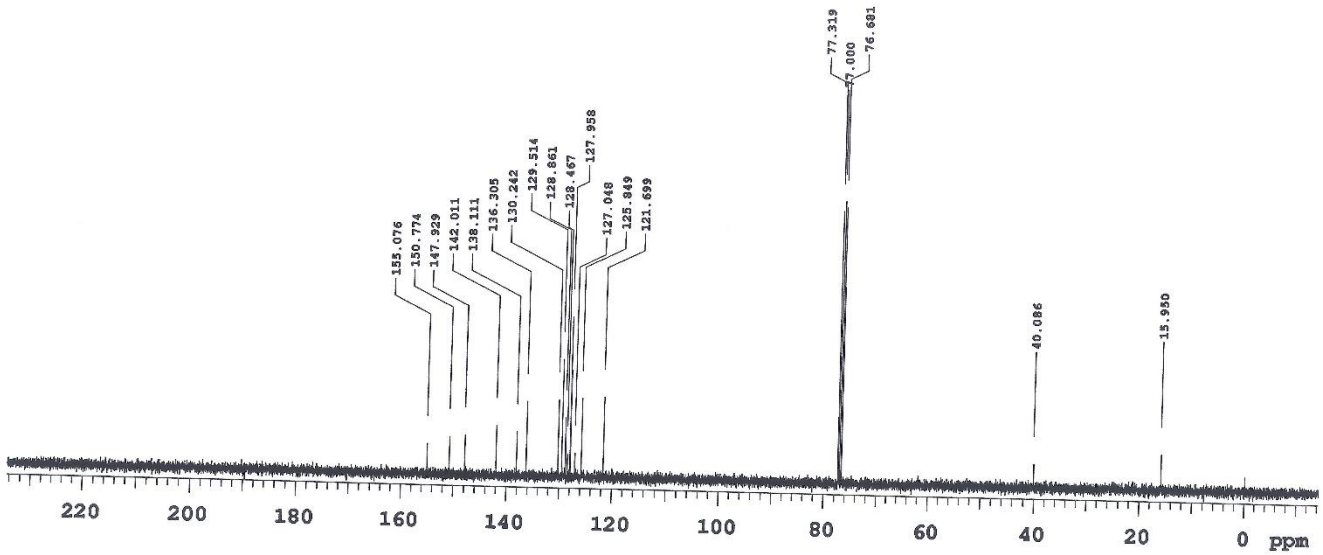


7e

MO115-13C

Sample Name	MO115-13C	Pulse sequence	CARBON	Temperature	25
Date collected	2019-07-09	Solvent	cdcl3	Spectrometer	nmr400.localdomain-vnmrs400

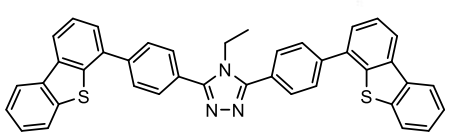
Study owner JakubA
Operator JakubA



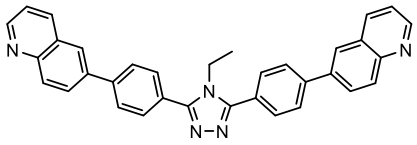
Data file exp

Plot date 2019-07-09

3,5-Bis[4-(dibenzothiophen-4-yl)phenyl]-4-ethyl-4H-1,2,4-triazole (**7f**).



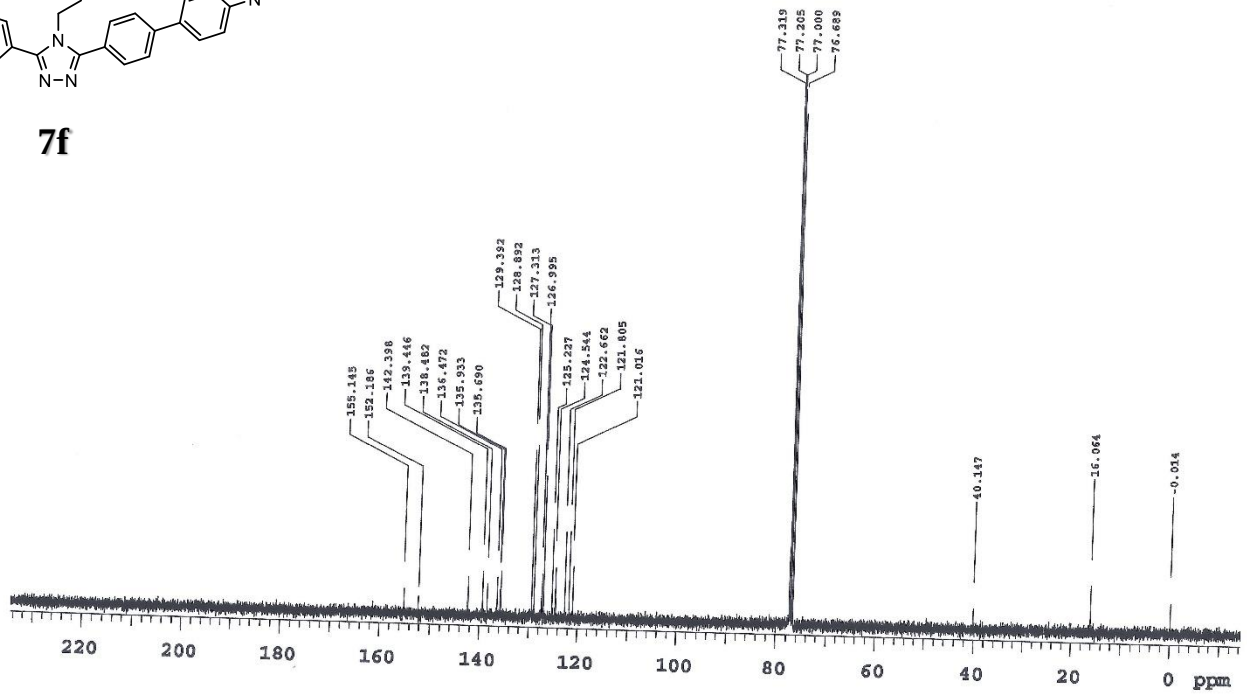
7f



7f

MO116-13C

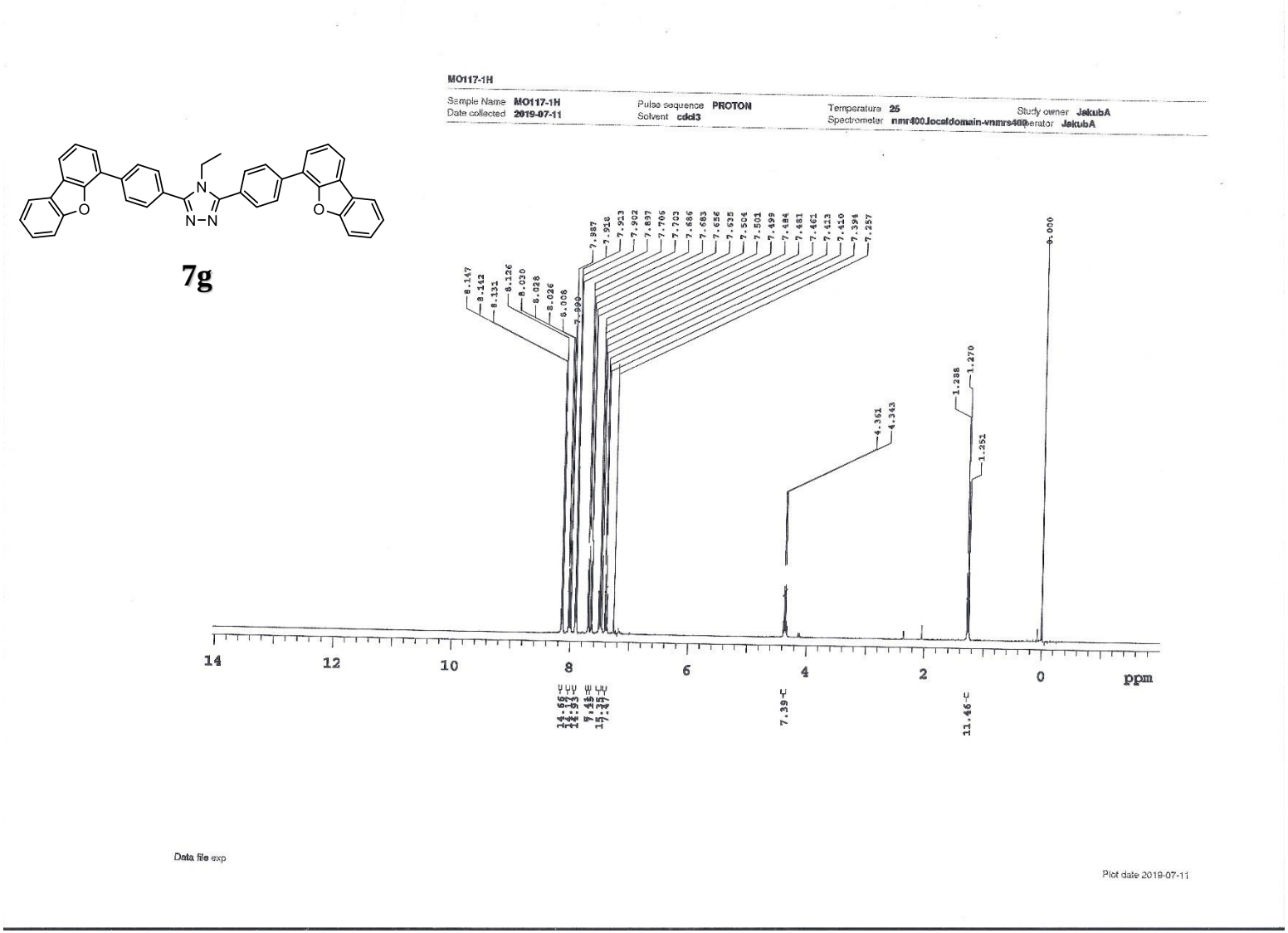
Sample Name MO116-13C
Date collected 2019-07-11
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA

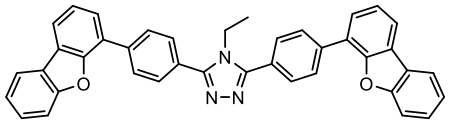


Data file exp

Plot date 2019-07-11

3,5-Bis[4-(dibenzofuran-4-yl)phenyl]-4-ethyl-4H-1,2,4-triazole (**7g**).



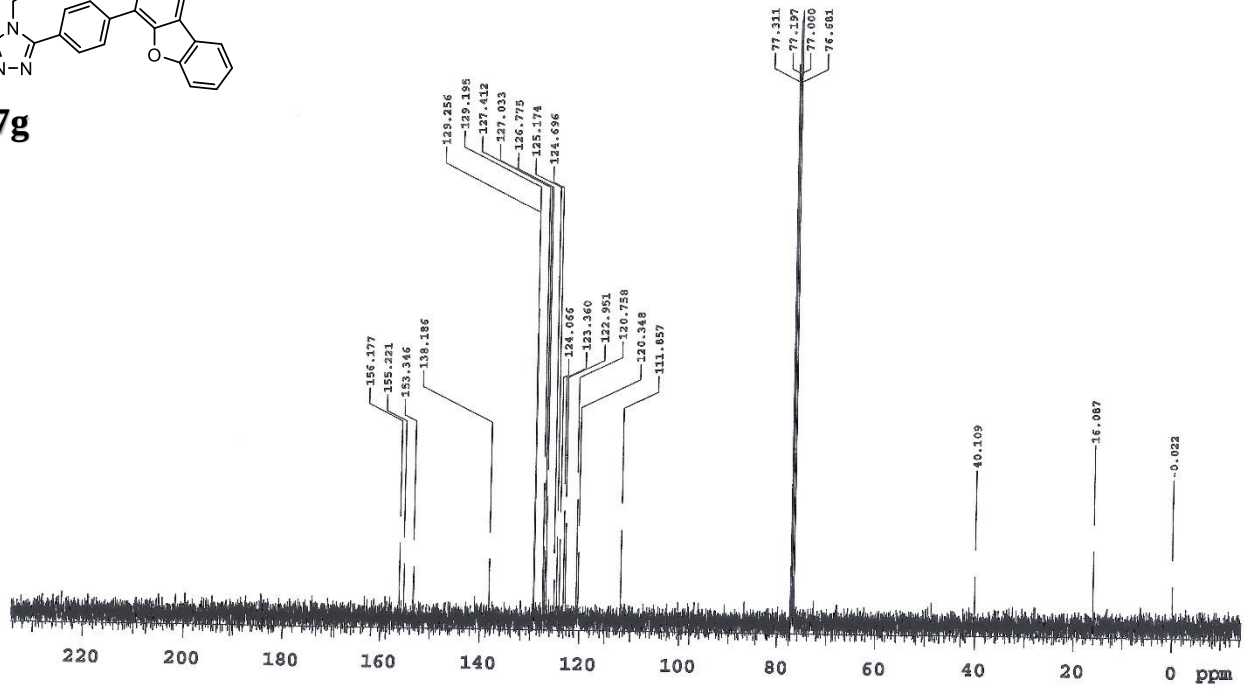


7g

MO117-13C

Sample Name	MO117-13C	Pulse sequence	CARBON	Temperature	25
Date collected	2019-07-11	Solvent	cdcl3	Spectrometer	nmr400.localdomain-vnmrs400

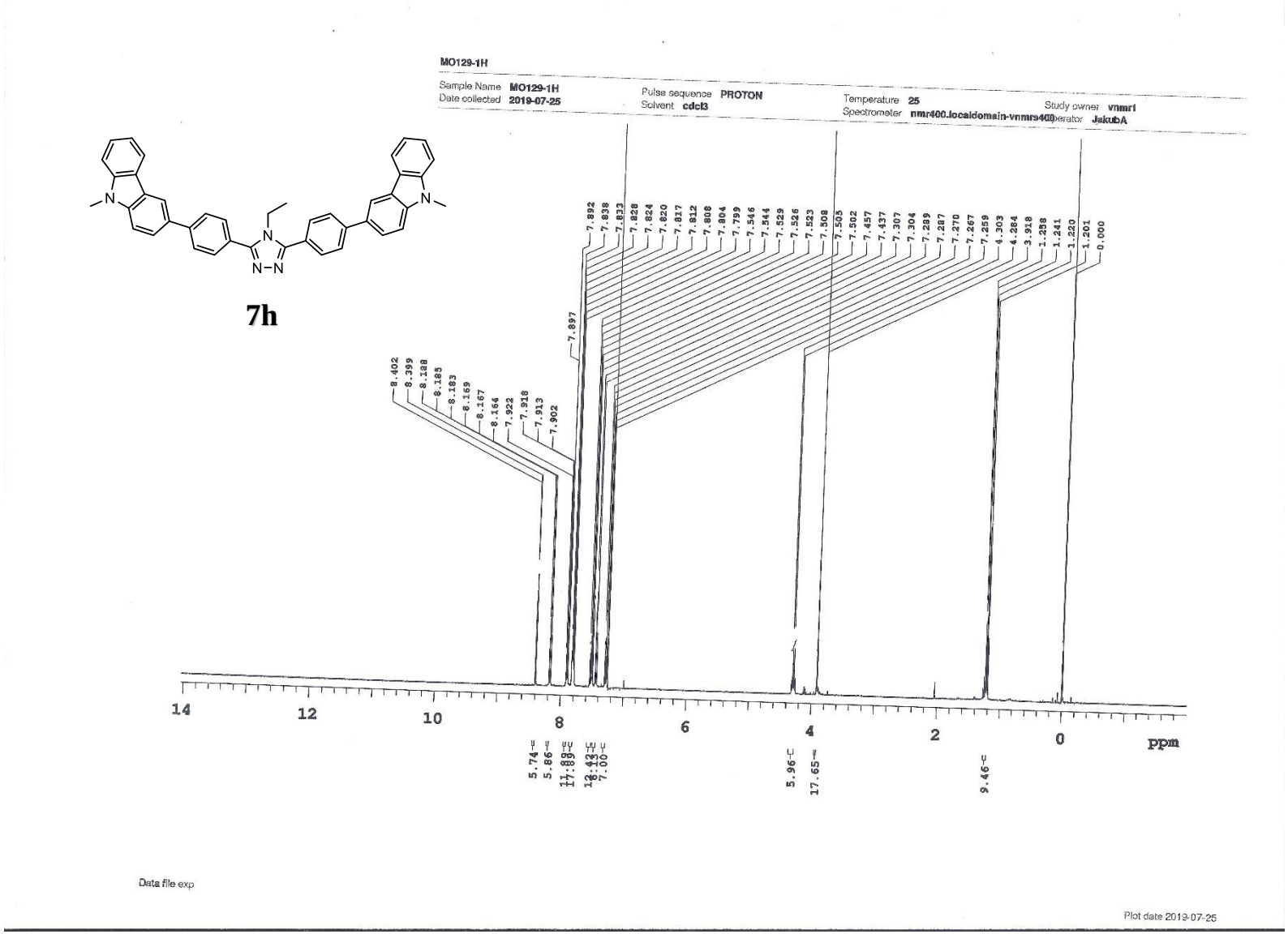
Study owner JakubA
Operator JakubA



Data file exp

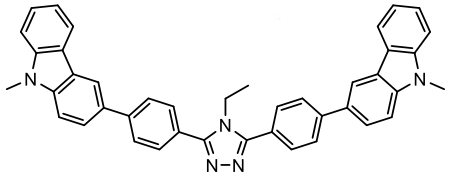
Plot date 2019-07-11

4-Ethyl-3,5-bis[4-(9-methyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**7h**).



MO129-13C

Sample Name MO129-13C
Date collected 2019-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA

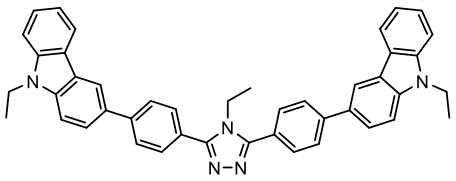


7h

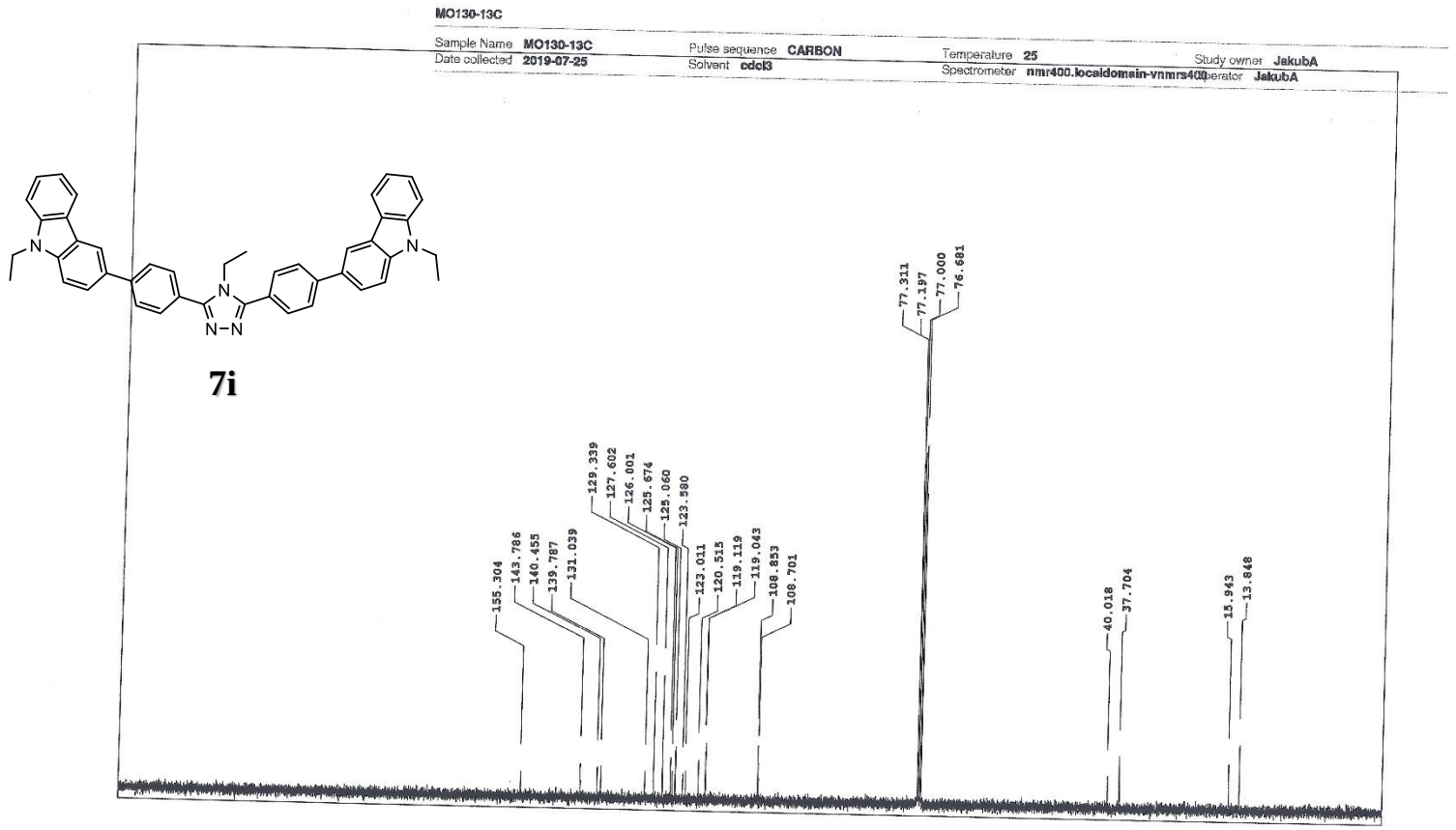
Data file exp

Plot date 2019-07-25

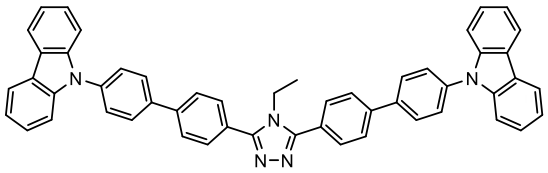
4-Ethyl-3,5-bis[4-(9-ethyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**7i**).



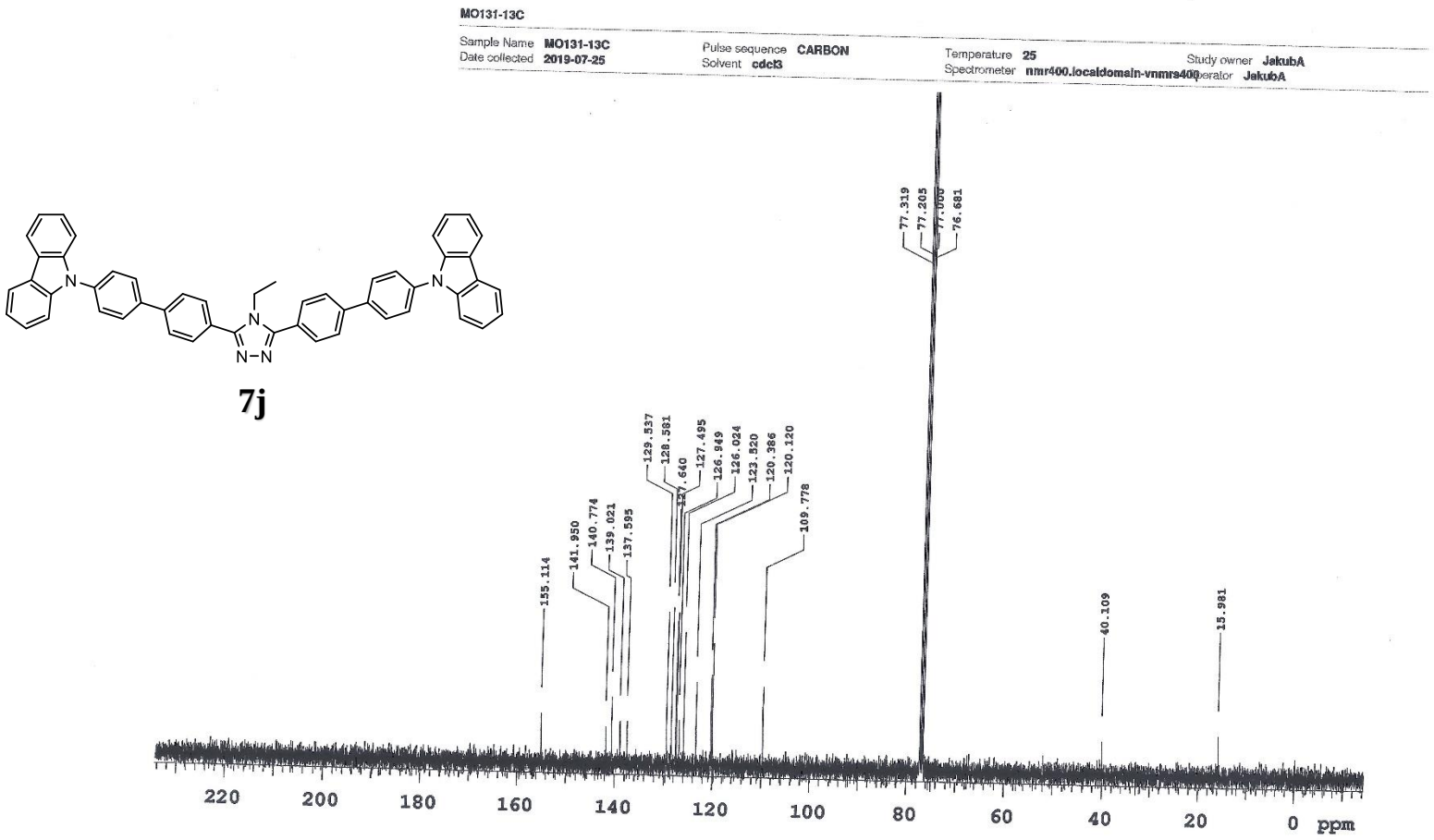
7i


MO130-13C
Sample Name MO130-13C
Date collected 2019-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA
7i
155.304
143.786
140.455
139.787
131.039
129.339
127.602
126.001
125.674
125.060
123.580
123.011
120.515
119.119
119.043
108.853
108.701
77.311
77.197
77.000
76.681
40.018
37.704
15.943
13.848
Data file exp
Plot date 2019-07-25

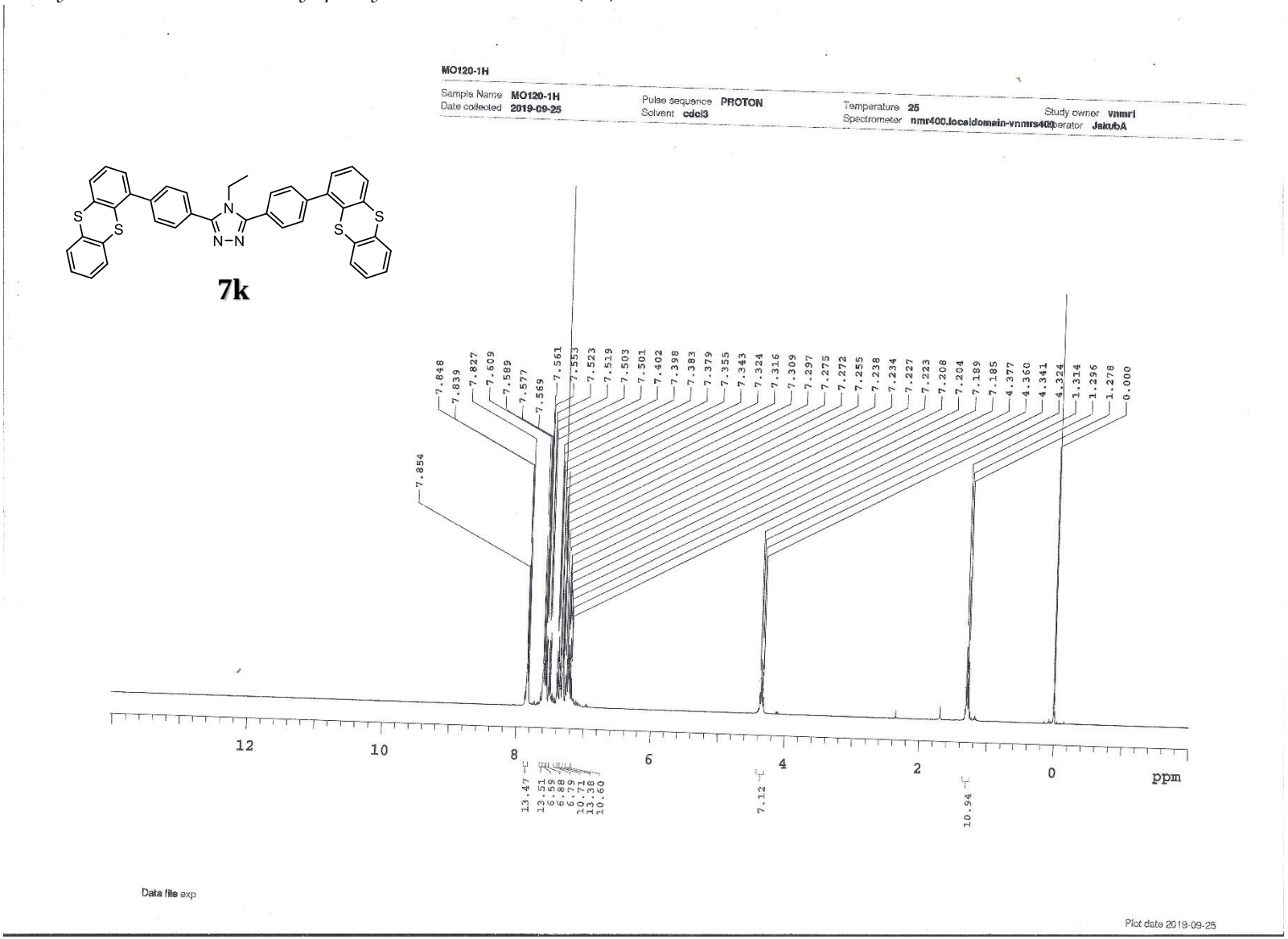
3,5-Bis[4′-(9H-carbazol-9-yl)biphenyl-4-yl]-4-ethyl-4H-1,2,4-triazole (**7j**).



7j

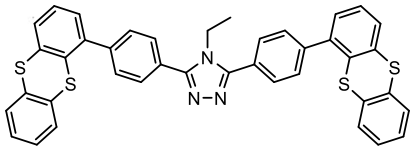

MO131-13C
Sample Name MO131-13C
Date collected 2019-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA
7j
155.114
141.950
140.774
139.021
137.595
129.537
128.581
127.640
127.495
126.949
126.024
123.520
120.386
120.120
109.778
77.319
77.205
76.681
40.109
15.981
220
200
180
160
140
120
100
80
60
40
20
0 ppm
Data file /home/vnmrj_4.2_A/fidlib/Data/AgnieszkaKudelko/2019/Lipiec/MO131-13c.fid
Plot date 2019-07-30

4-Ethyl-3,5-bis[4-(thiantren-1-yl)phenyl]-4H-1,2,4-triazole (**7k**).

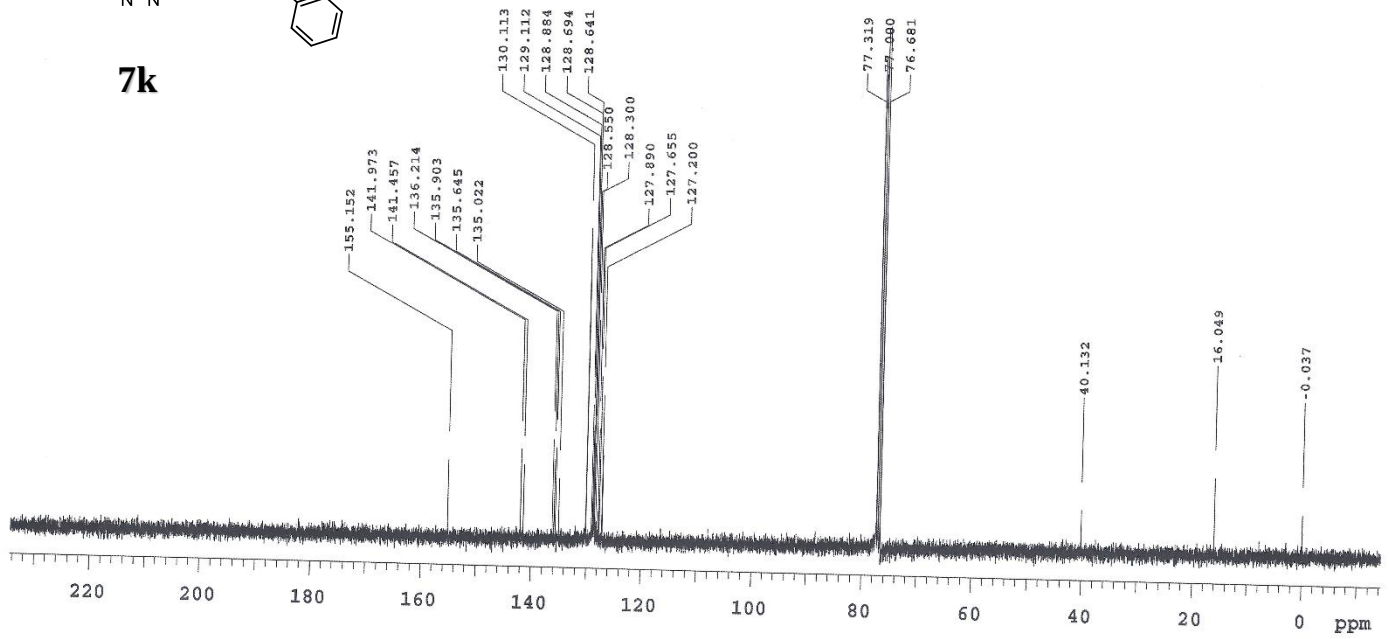


MO120-13C

Sample Name MO120-13C
Date collected 2019-09-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA



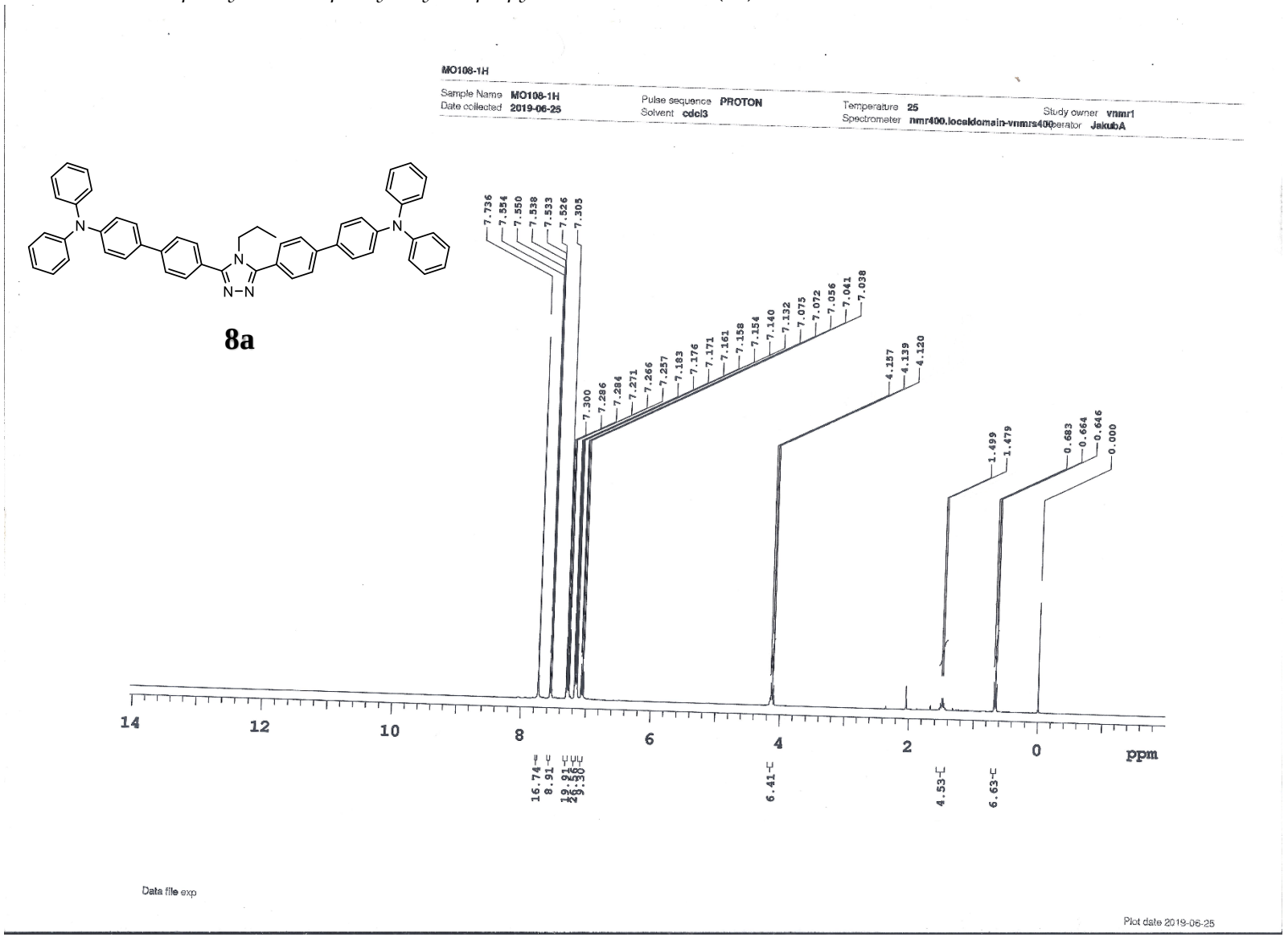
7k



Data file exp

Plot date 2019-09-25

3,5-Bis[4′-(N,N-diphenylamino)biphenyl-4-yl]-4-propyl-4H-1,2,4-triazole (**8a**).



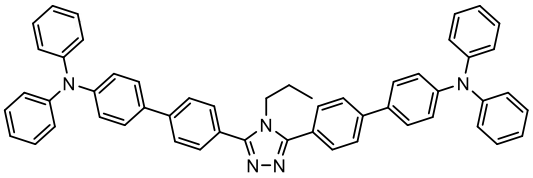
MO108-13C

Sample Name MO108-13C
Date collected 2019-06-25

Pulse sequence CARBON
Solvent cdcl3

Temperature 25
Spectrometer nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA

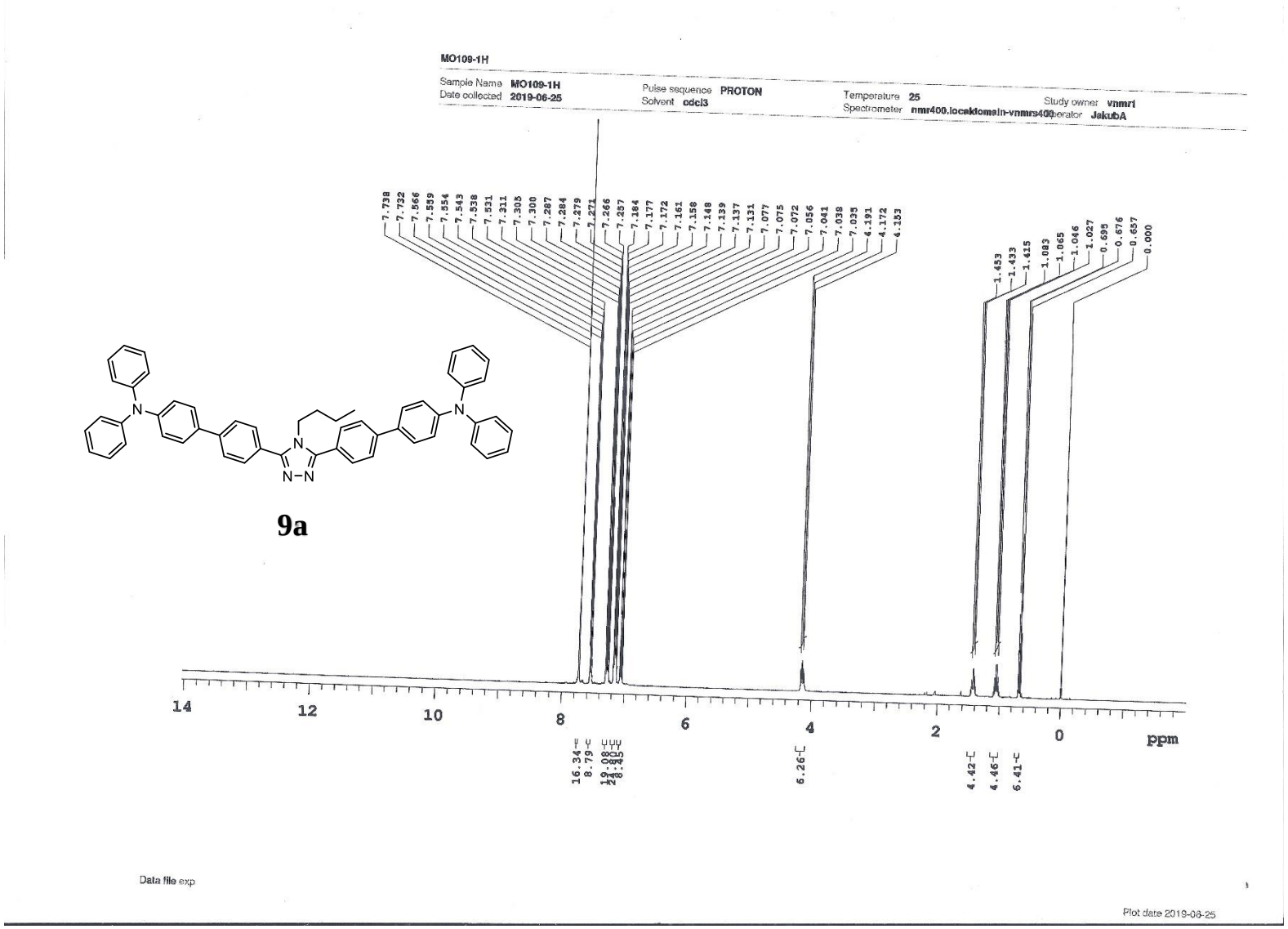


8a

Data file exp

Plot date 2019-06-25

4-Butyl-3,5-bis[4′-(N,N-diphenylamino)biphenyl-4-yl]-4H-1,2,4-triazole (**9a**).



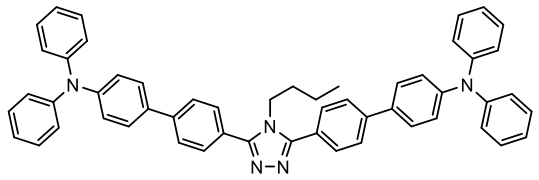
MO109-13C

Sample Name MO109-13C
Date collected 2019-06-25

Pulse sequence CARBON
Solvent cdcl3

Temperature 25
Spectrometer nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA

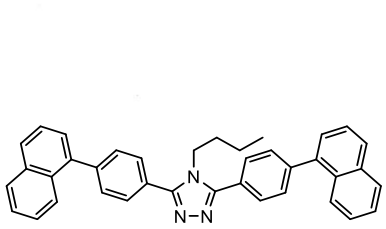


9a

Data file exp

Plot date 2019-06-25

4-Butyl-3,5-bis[4-(naphthalen-1-yl)phenyl]-4H-1,2,4-triazole (**9b**).

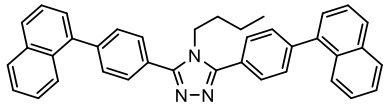


9b

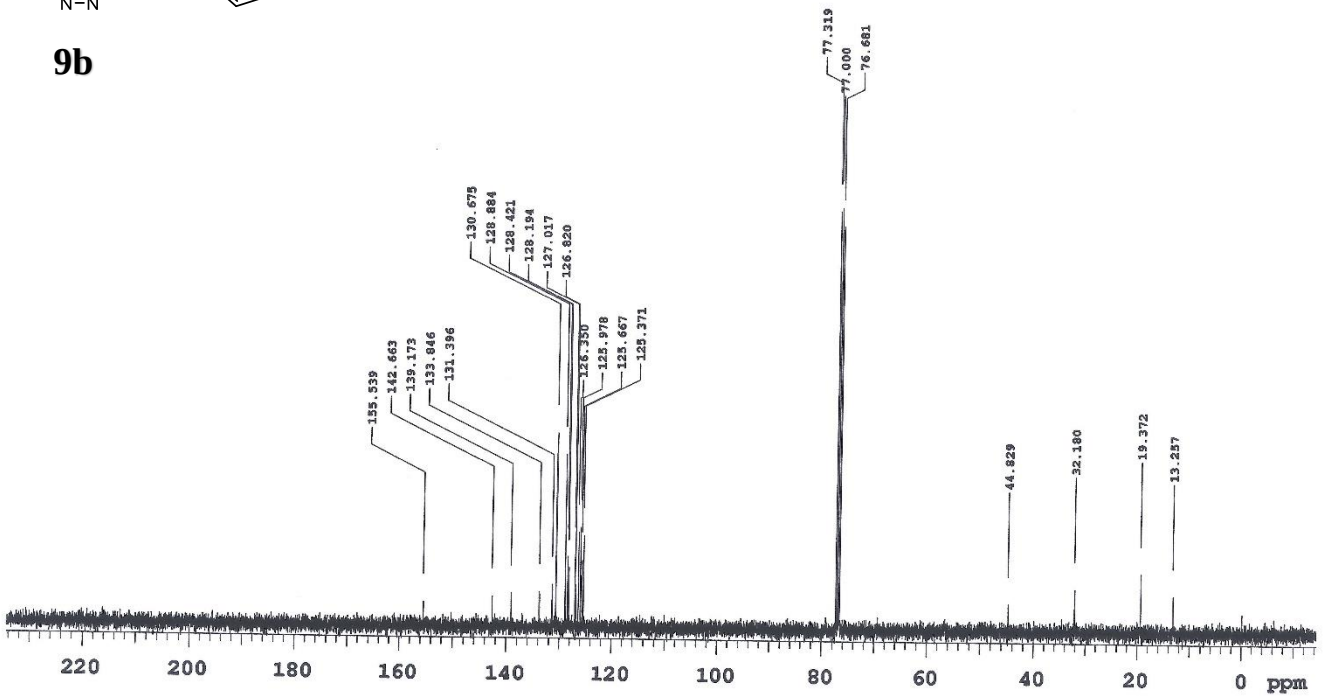
MO118-13C

Sample Name	MO118-13C	Pulse sequence	CARBON	Temperature	25
Date collected	2019-07-16	Solvent	cdcl3	Spectrometer	nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA



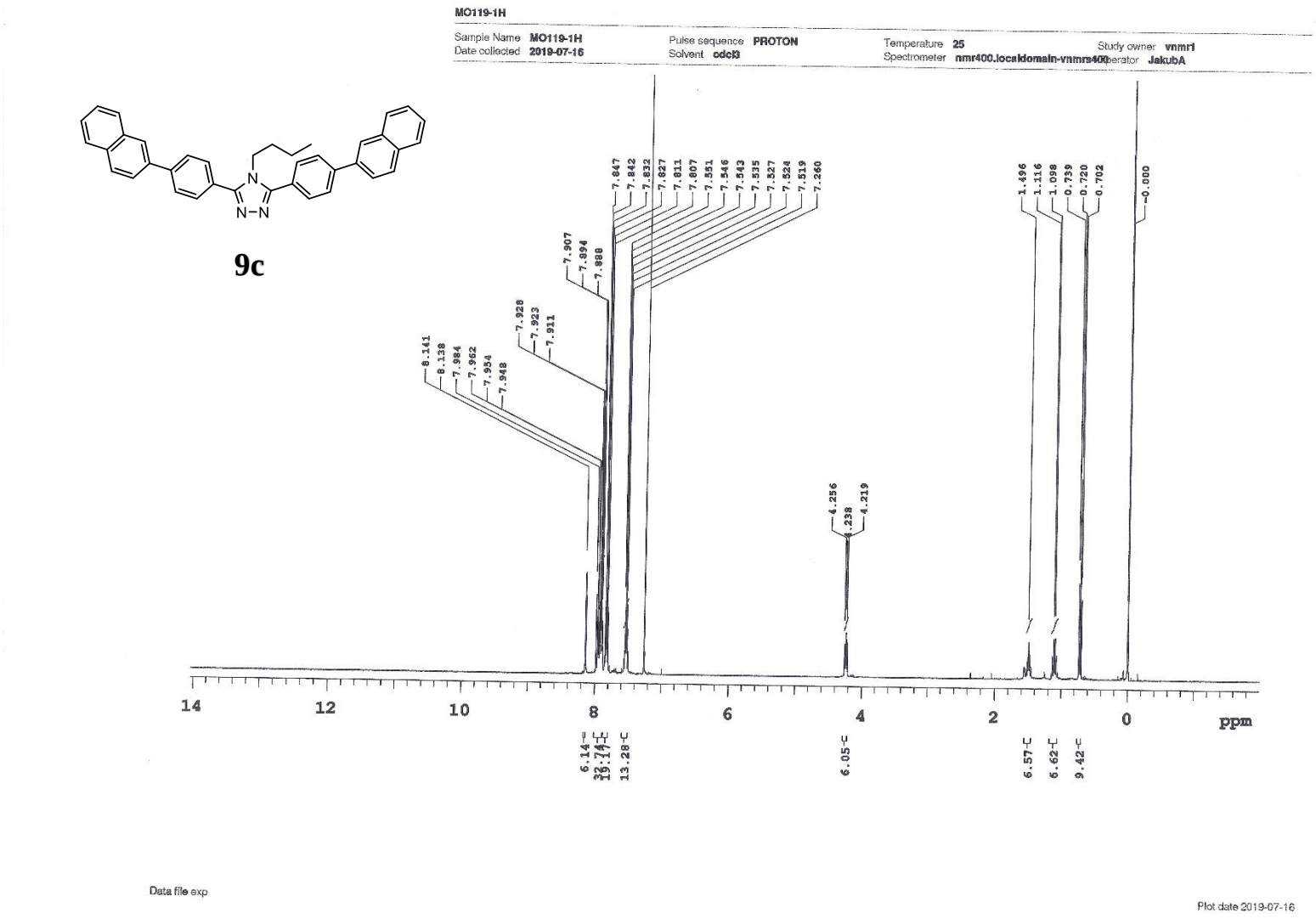
9b



Data file exp

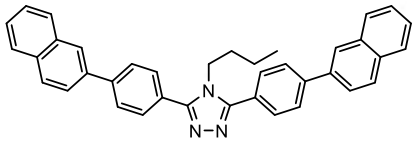
Plot date 2019-07-16

4-Butyl-3,5-bis[4-(naphthalen-2-yl)phenyl]-4H-1,2,4-triazole (**9c**).



MO119-13C

Sample Name **MO119-13C** Pulse sequence **CARBON** Temperature **25** Study owner **JakubA**
Date collected **2019-07-16** Solvent **cdcl3** Spectrometer **nmr400.localdomain-vnmrs400** Operator **JakubA**

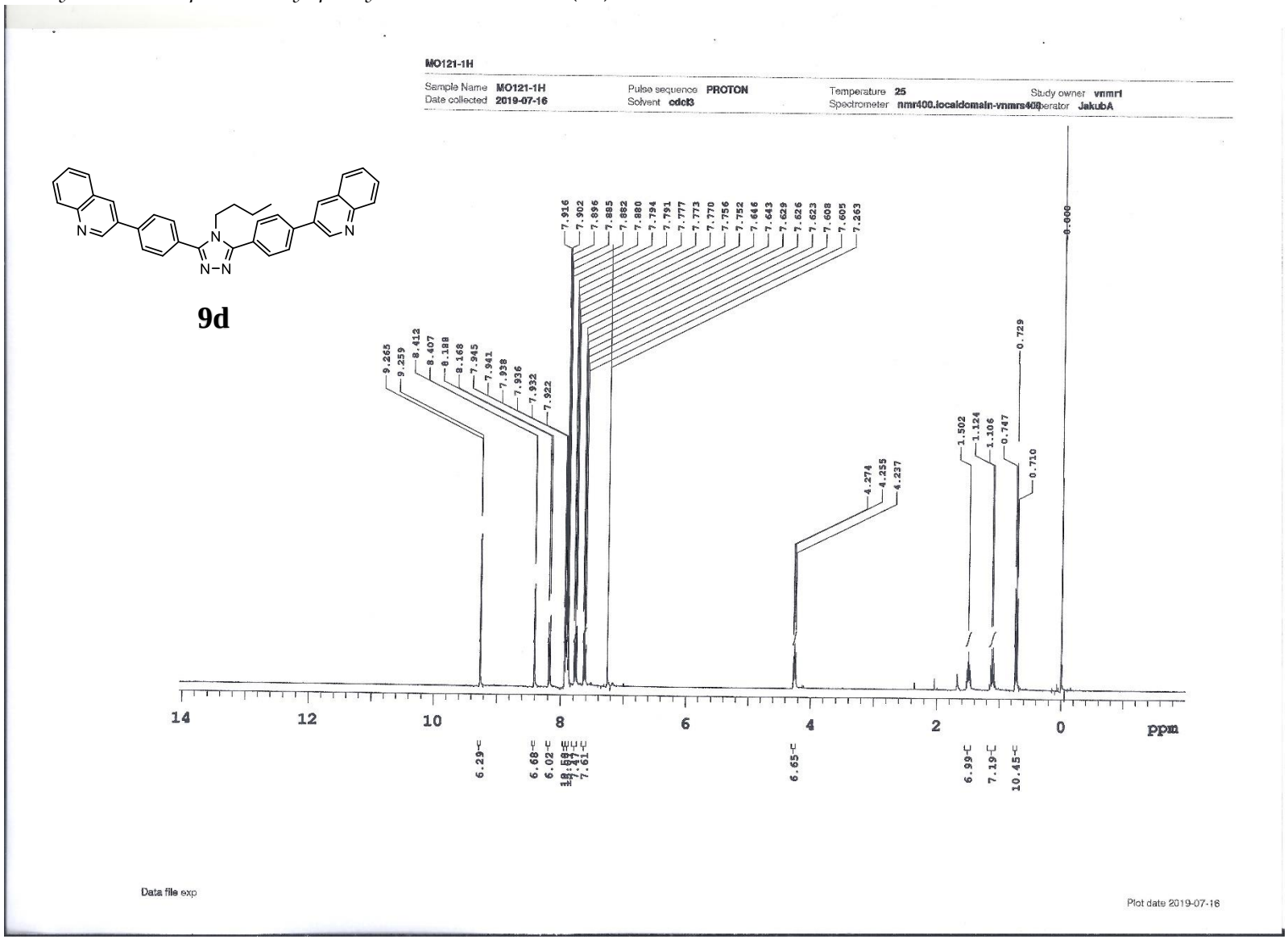


9c

Data file exp

Plot date 2019-07-16

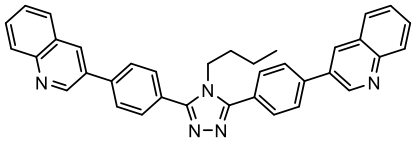
4-Butyl-3,5-bis[4-(quinolin-3-yl)phenyl]-4H-1,2,4-triazole (**9d**).



MO121-13C

Sample Name	MO121-13C	Pulse sequence	CARBON	Temperature	25
Date collected	2019-07-16	Solvent	cdcl3	Spectrometer	nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA

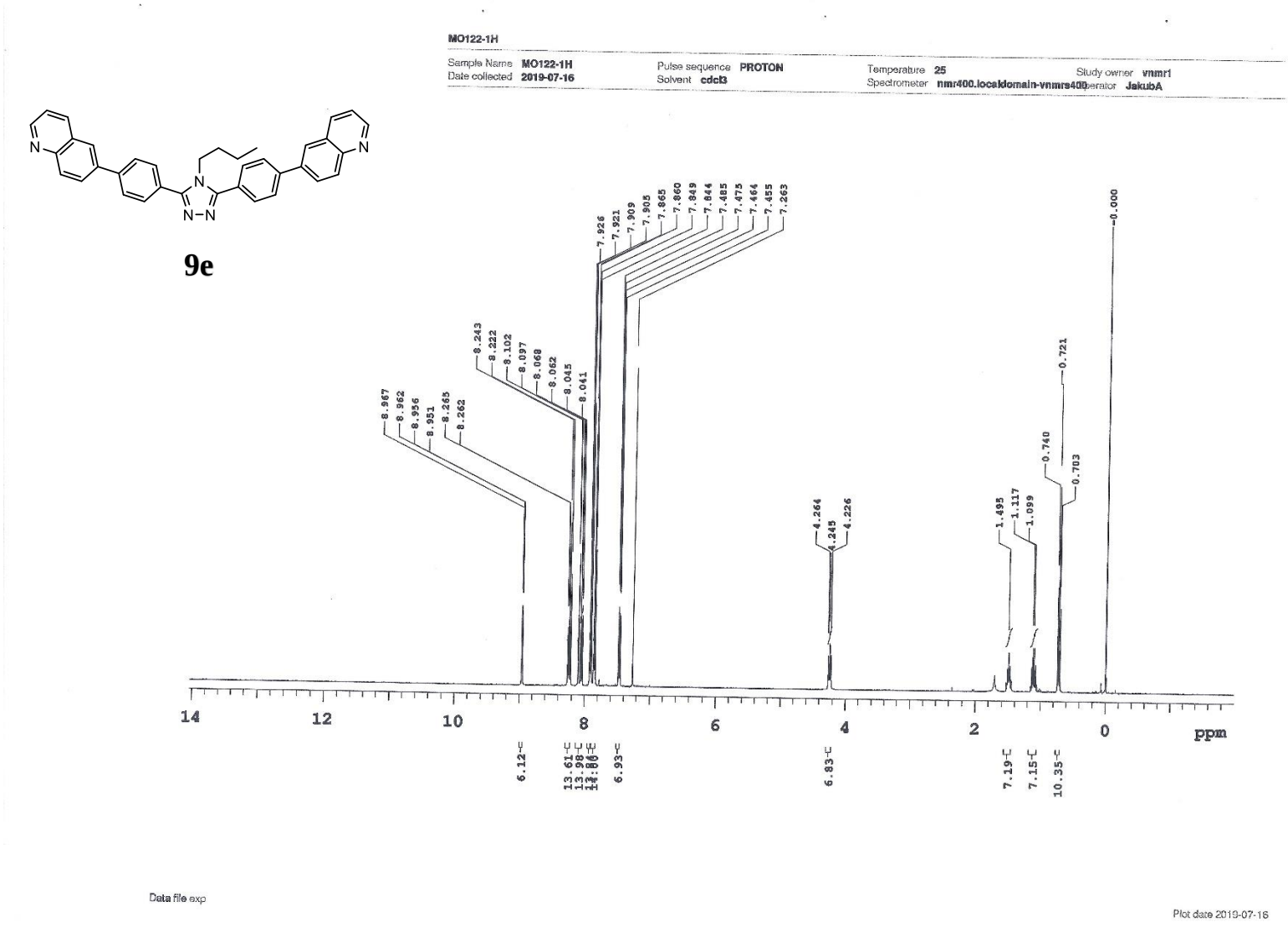


9d

Data file exp

Plot date 2019-07-16

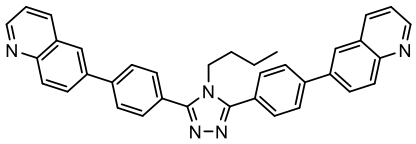
4-Butyl-3,5-bis[4-(quinolin-6-yl)phenyl]-4H-1,2,4-triazole (**9e**).



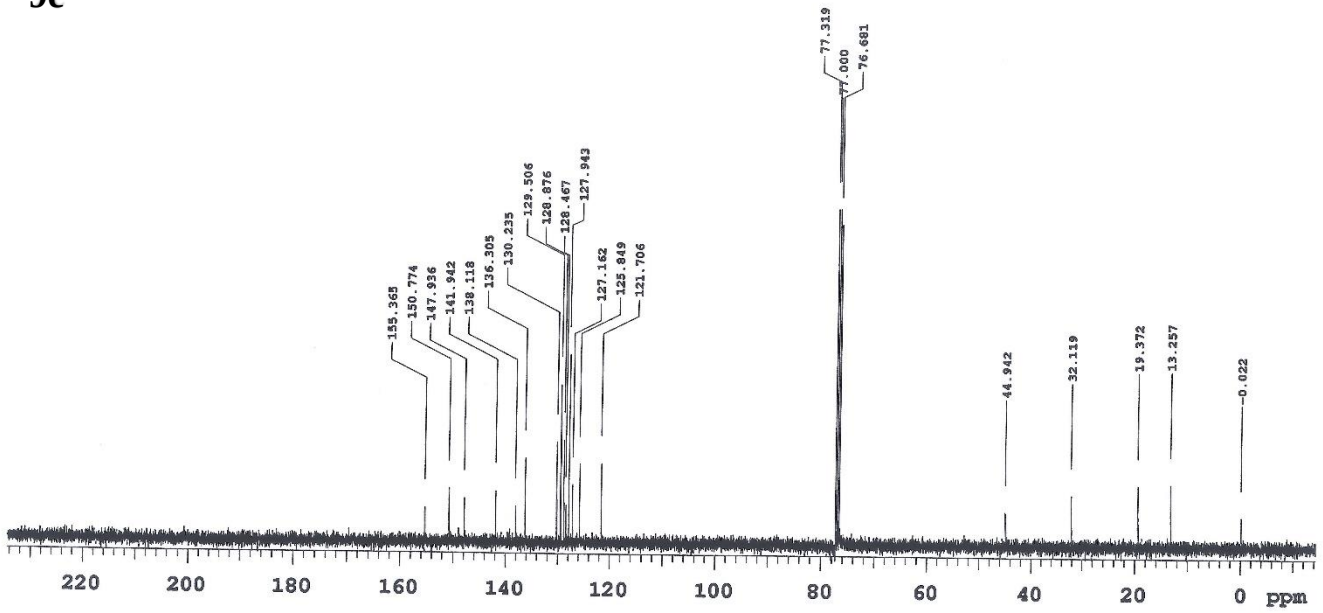
MO122-13C

Sample Name	MO122-13C	Pulse sequence	CARBON	Temperature	25
Date collected	2019-07-16	Solvent	cdcl3	Spectrometer	nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA



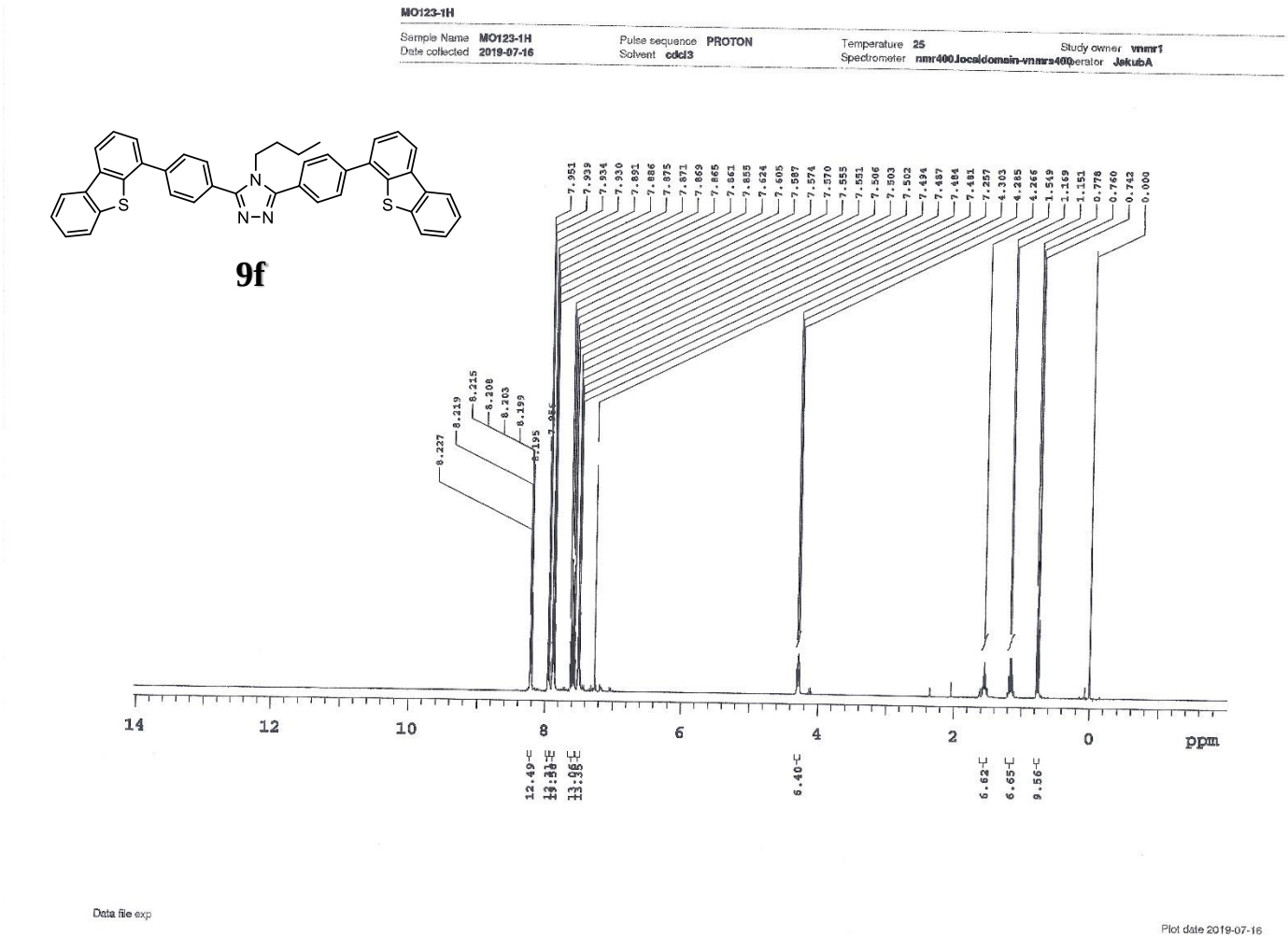
9e



Data file exp

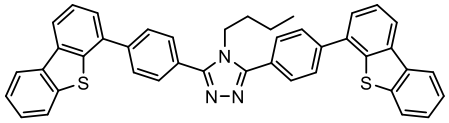
Plot date 2019-07-16

3,5-Bis[4-(dibenzothiophen-4-yl)phenyl]-4-butyl-4H-1,2,4-triazole (**9f**).



MO123-13C

Sample Name **MO123-13C**
Date collected **2019-07-16**
Pulse sequence **CARBON**
Solvent **cdcl3**
Temperature **25**
Spectrometer **nmr400.localdomain-vnmrs400**
Study owner **JakubA**
Operator **JakubA**

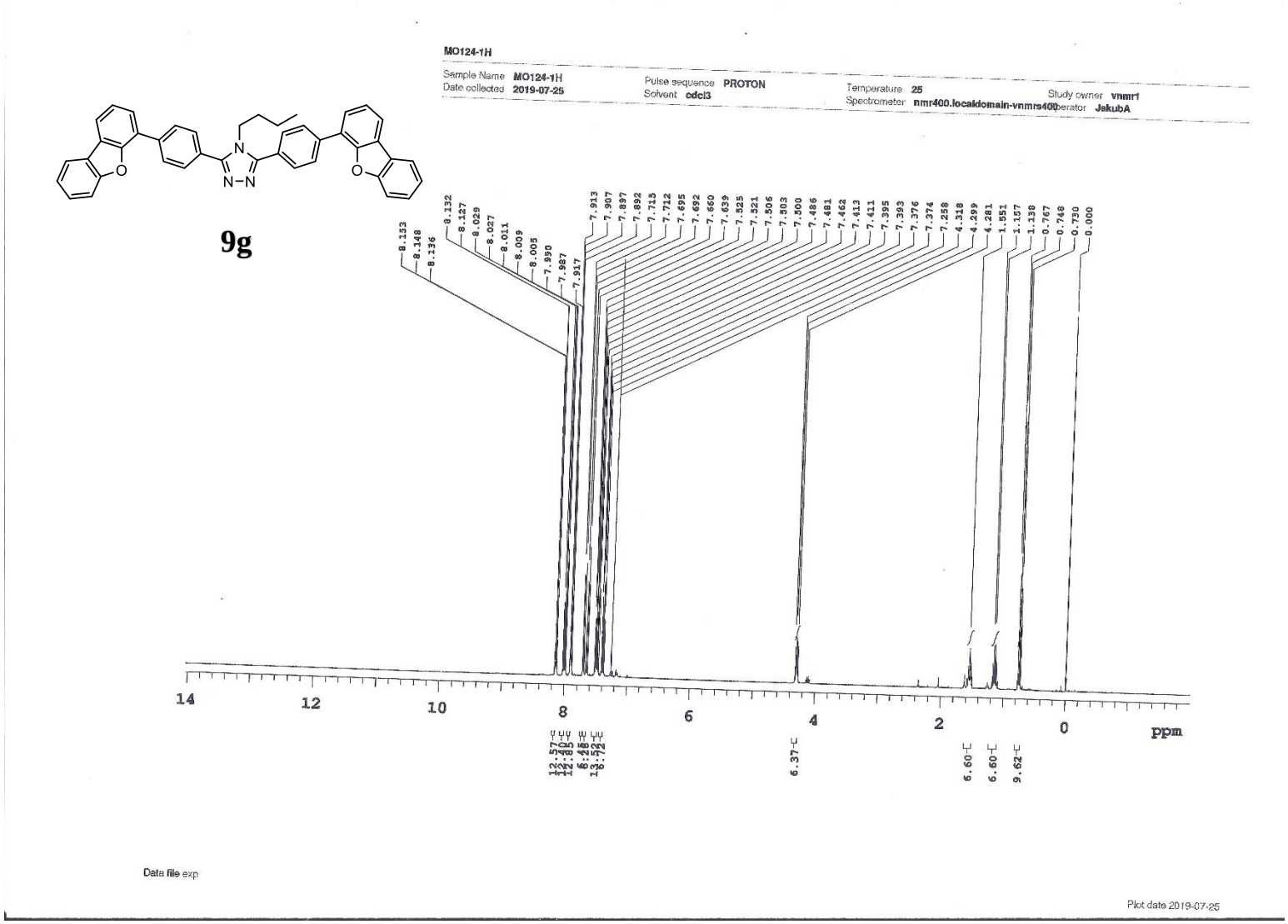


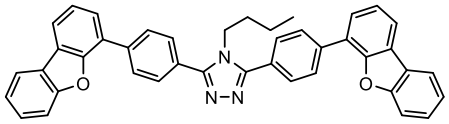
9f

Data file exp

Plot date 2019-07-16

3,5-Bis[4-(dibenzofuran-4-yl)phenyl]-4-butyl-4H-1,2,4-triazole (**9g**).





9g

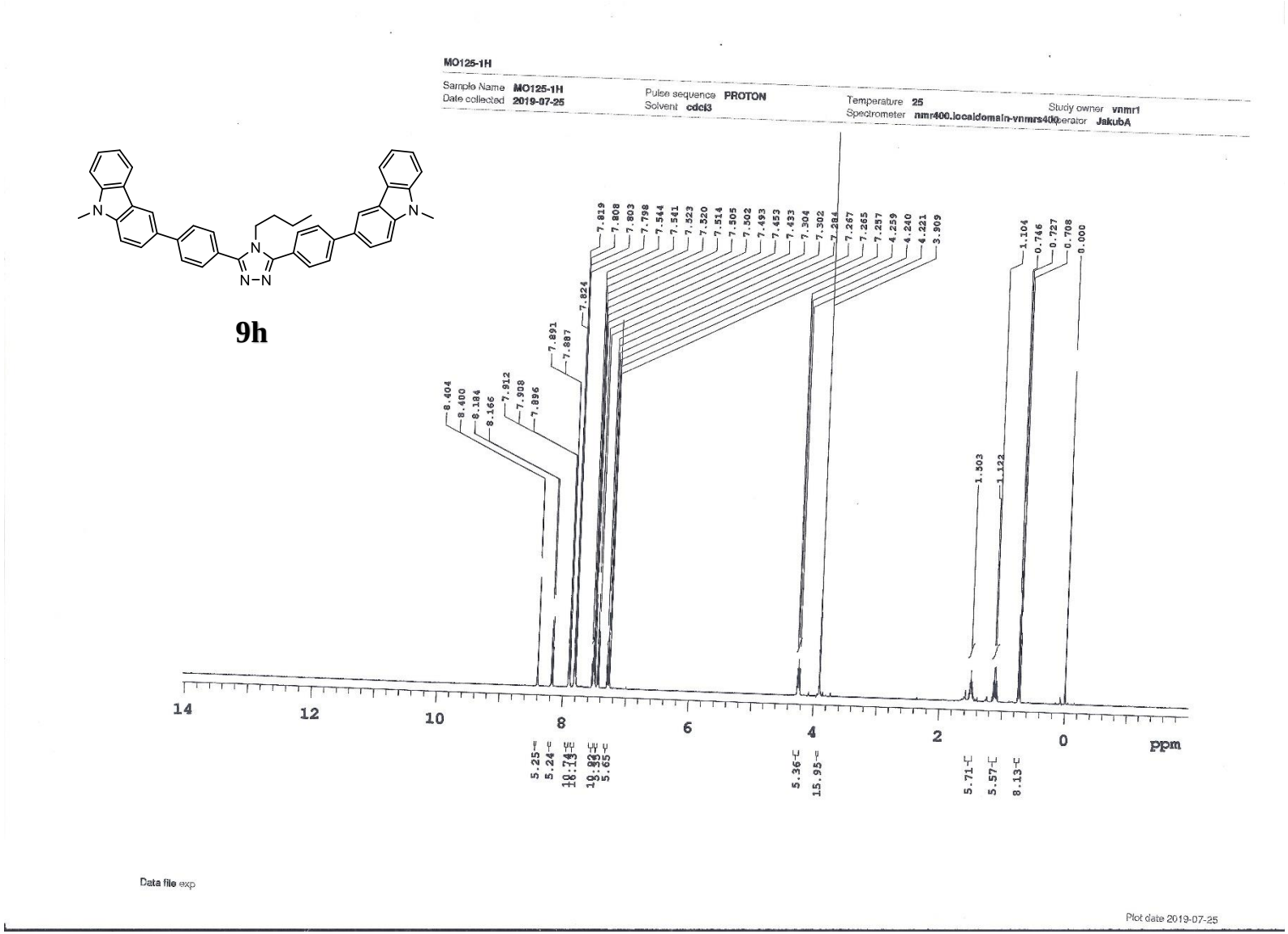
MO124-13C

Sample Name MO124-13C
Date collected 2019-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA

Data file exp

Plot date 2019-07-25

4-Butyl-3,5-bis[4-(9-methyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**9h**).



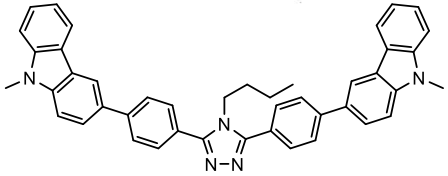
MO125-13C

Sample Name MO125-13C
Date collected 2019-07-25

Pulse sequence CARBON
Solvent cdcl3

Temperature 25
Spectrometer nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA

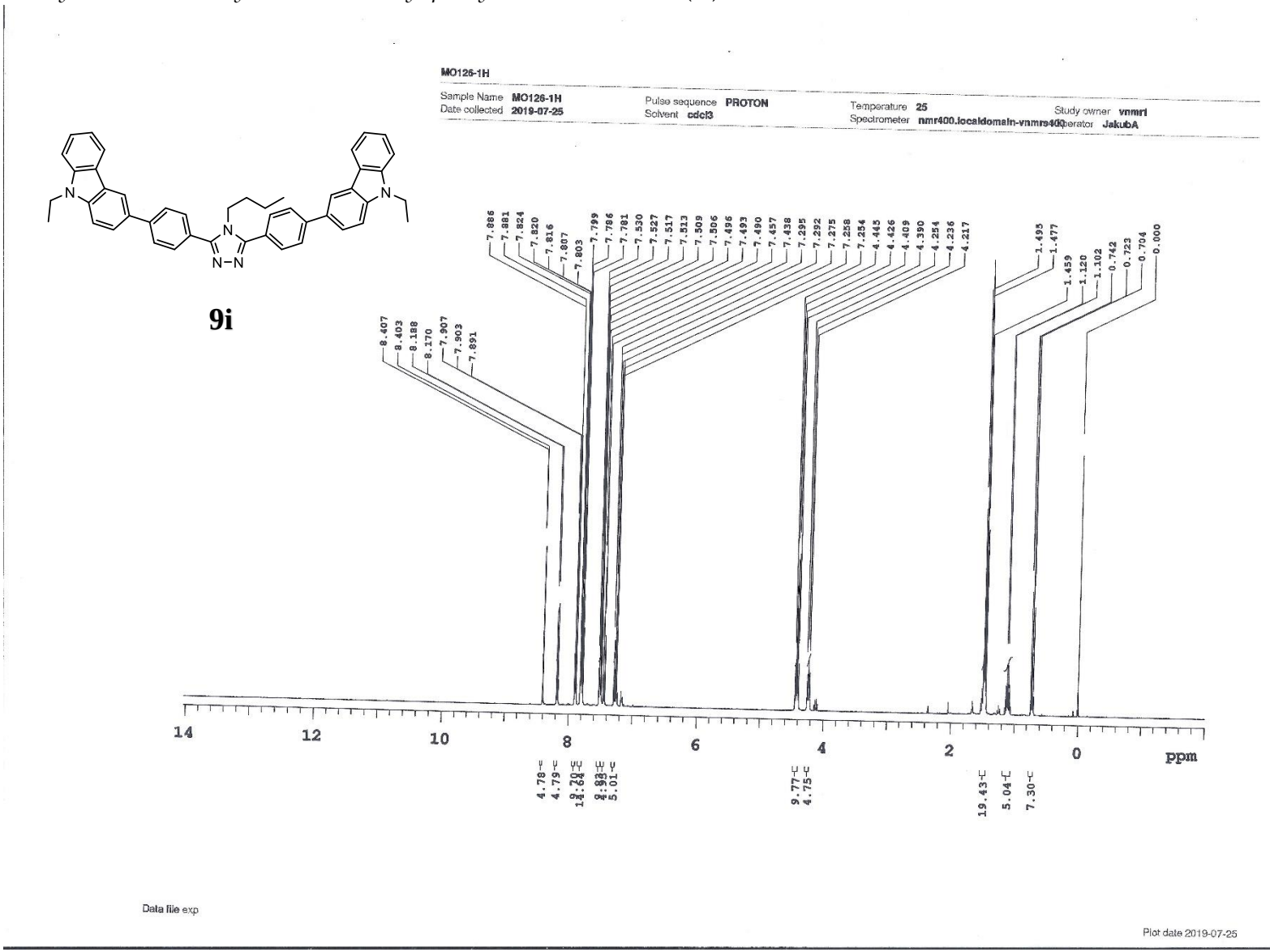


9h

Data file exp

Plot date 2019-07-25

4-Butyl-3,5-bis[4-(9-ethyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**9i**).



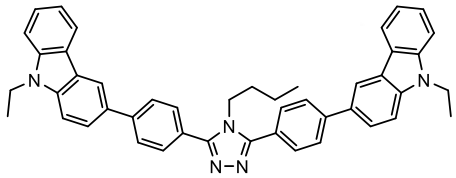
MO126-13C

Sample Name MO126-13C
Date collected 2019-07-25

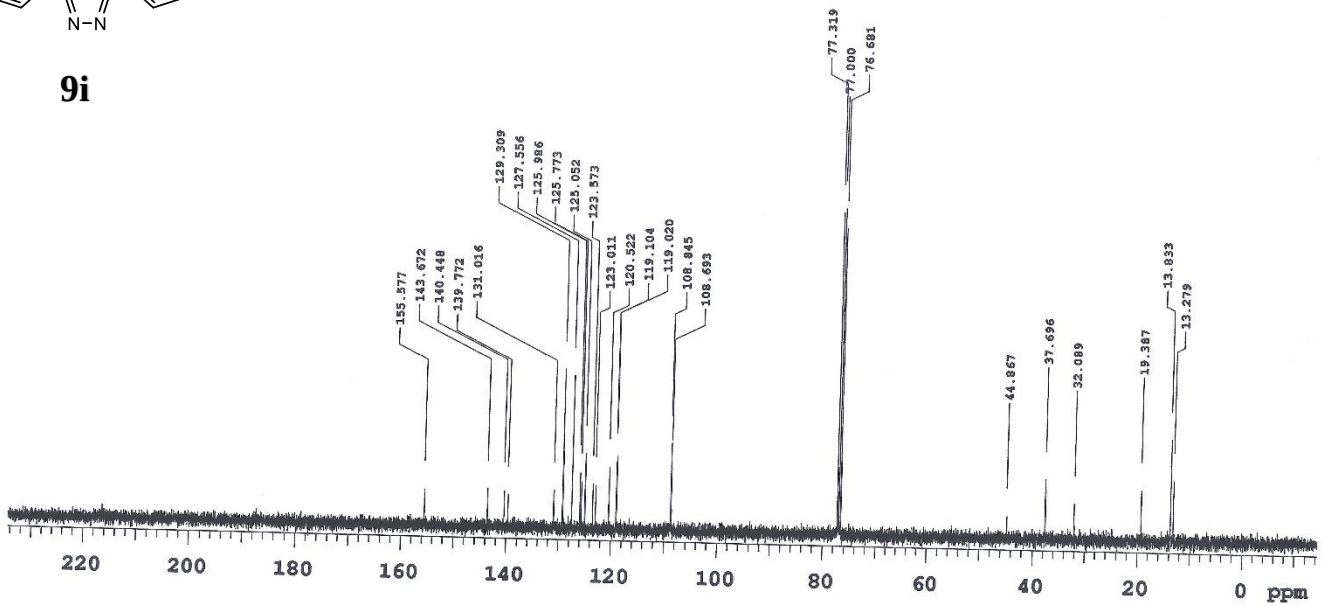
Pulse sequence CARBON
Solvent cdcl3

Temperature 25
Spectrometer nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA



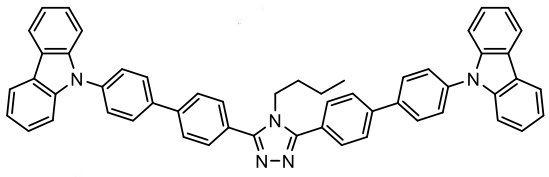
9i



Data file exp

Plot date 2019-07-25

4-Butyl-3,5-bis[4′-(9H-carbazol-9-yl)biphenyl-4-yl]-4H-1,2,4-triazole (**9j**).



9j

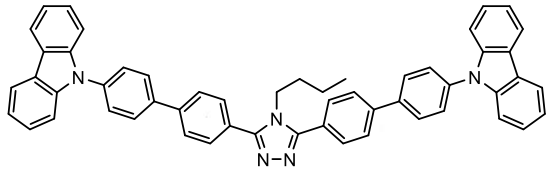
MO127-13C

Sample Name MO127-13C
Date collected 2019-07-30

Pulse sequence CARBON
Solvent cdcl3

Temperature 25
Spectrometer nmr400.localdomain-vnmrs400

Study owner JakubA
Operator JakubA

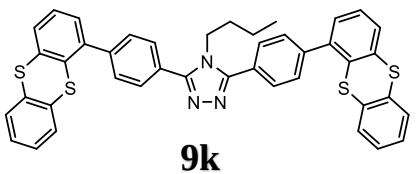


9j

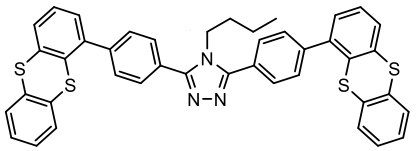
Data file /home/vnmrj_4.2_A/fidlib/Data/AgnieszkaKudelko/2019/Lipiec/MO127-13C.fid

Plot date 2019-07-31

4-Butyl-3,5-bis[4-(thiantren-1-yl)phenyl]-4H-1,2,4-triazole (**9k**).



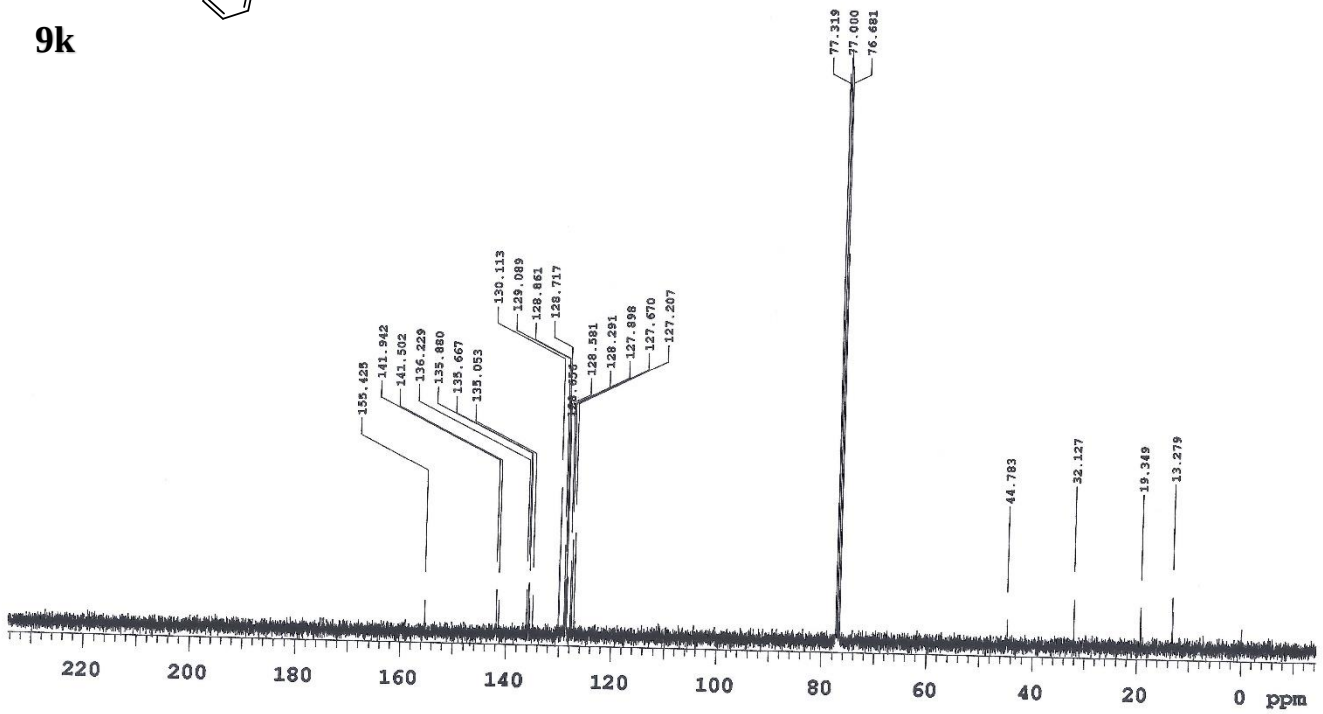
9k



9k

MO128-13C

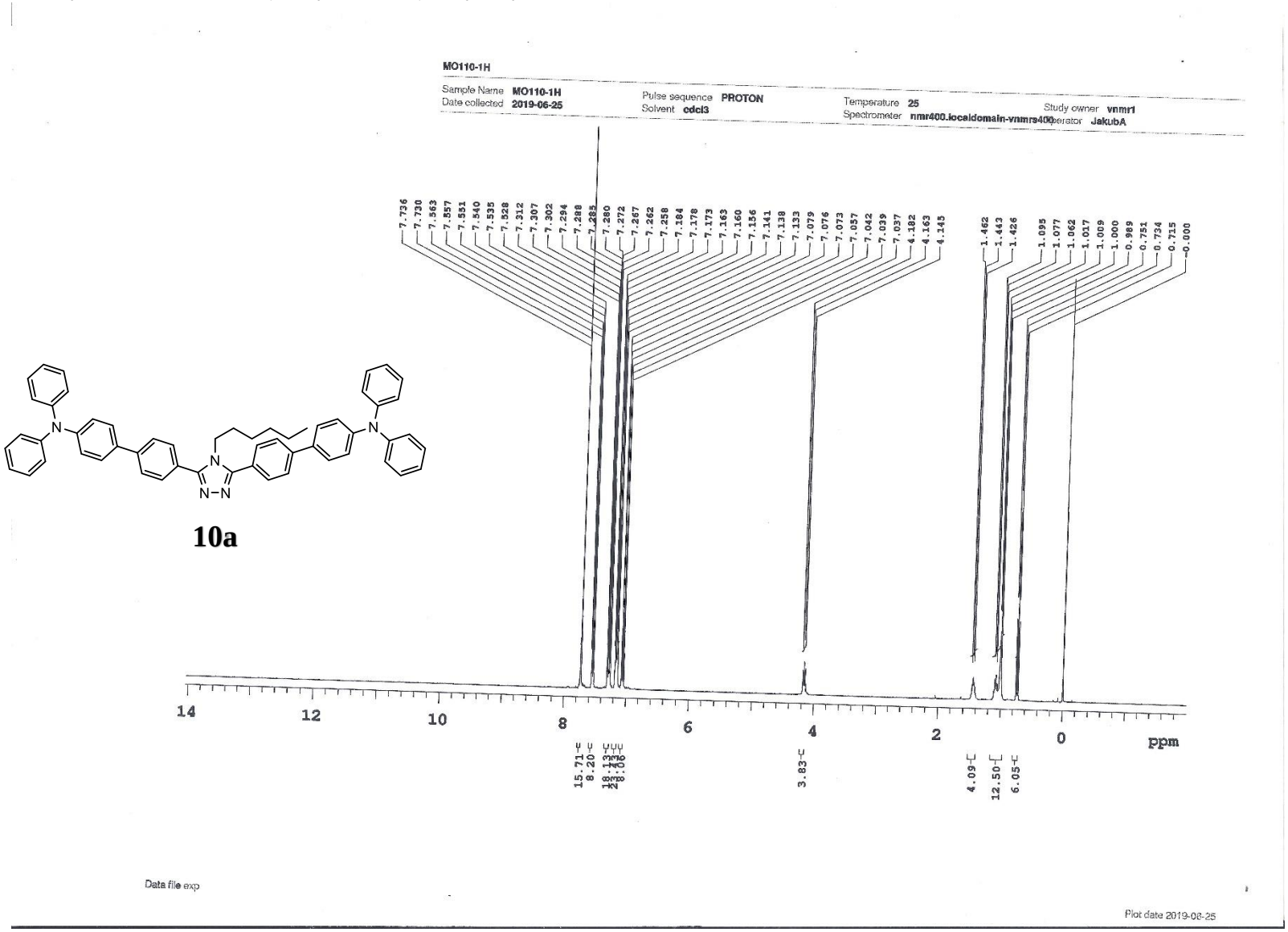
Sample Name MO128-13C
Date collected 2019-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA

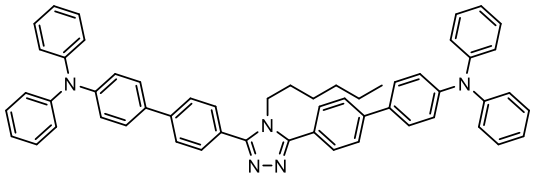


Data file exp

Plot date 2019-07-25

4-Hexyl-3,5-bis[4'-(N,N-diphenylamino)biphenyl-4-yl]-4H-1,2,4-triazole (**10a**).





10a

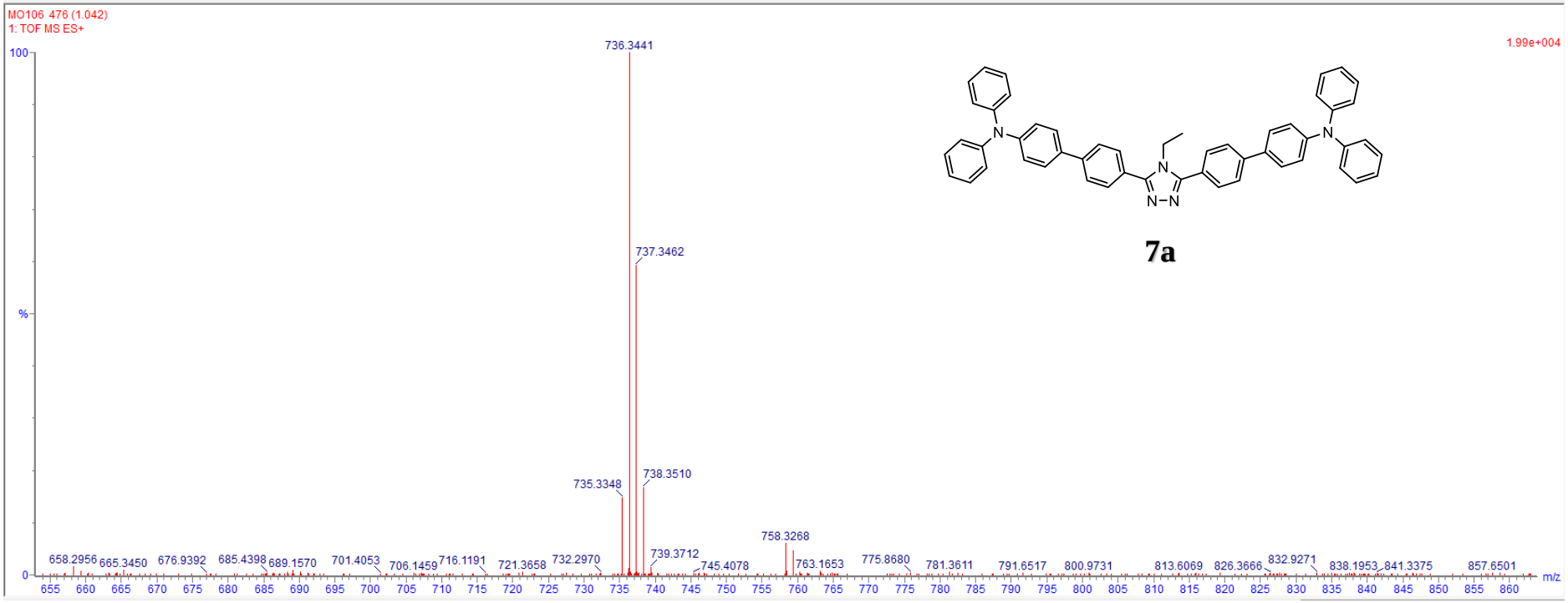
MO110-13C
Sample Name MO110-13C
Date collected 2019-06-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr400.localdomain-vnmrs400
Study owner JakubA
Operator JakubA
155.448
147.853
147.512
142.140
133.543
129.339
129.286
127.753
126.926
126.122
124.637
123.603
123.193
77.319
77.000
76.681
44.980
30.716
29.873
25.685
22.195
13.788
220
200
180
160
140
120
100
80
60
40
20
0 ppm
Data file exp
Plot date 2019-06-25

2. HRMS spectra

4-Ethyl-3,5-bis[4′-(N,N-diphenylamino)biphenyl-4-yl]-4H-1,2,4-triazole (**7a**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
186 formula(e) evaluated with 38 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
736.3441	100.00	736.3440	0.1	0.1	34.5	C52 H42 N5	89.8	1.252	28.60	52	42	5	
		736.3328	11.3	15.3	34.5	C53 H42 N3 O	89.7	1.162	31.27	53	42	3	1
		736.3579	-13.8	-18.7	33.5	C55 H46 N O	90.6	2.004	13.48	55	46	1	1
		736.3652	-21.1	-28.7	29.5	C49 H46 N5 O2	93.5	4.924	0.73	49	46	5	2
		736.3216	22.5	30.6	34.5	C54 H42 N O2	89.9	1.350	25.92	54	42	1	2
737.3462	59.22	737.3420	4.2	5.7	33.5	C55 H45 O2	102.7	1.453	23.40	55	45		2
		737.3532	-7.0	-9.5	33.5	C54 H45 N2 O	102.8	1.525	21.76	54	45	2	1
		737.3280	18.2	24.7	34.5	C52 H41 N4 O	102.9	1.634	19.52	52	41	4	1

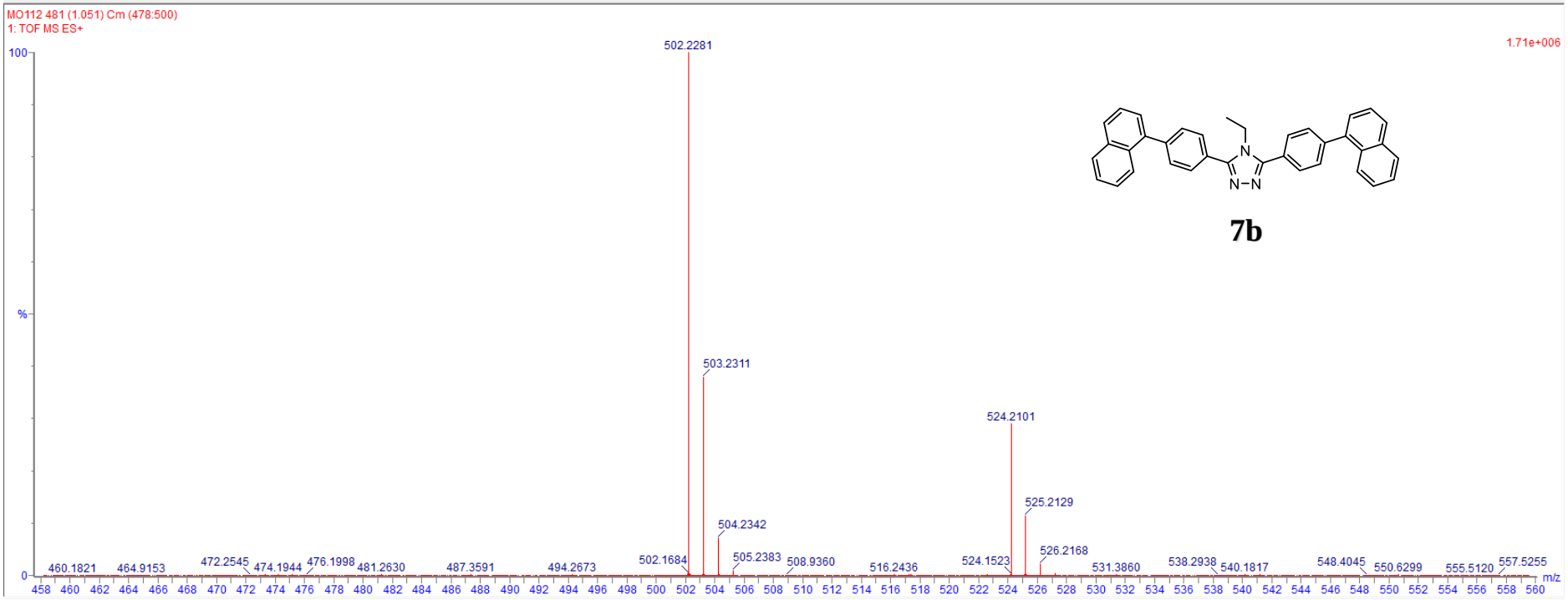


7a

4-Ethyl-3,5-bis[4-(naphthalen-1-yl)phenyl]-4H-1,2,4-triazole (**7b**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 7 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
502.2281	100.00	502.2283	-0.2	-0.4	24.5	C36 H28 N3	409.4	8.228	0.03	36	28	3
		502.2032	24.9	49.6	25.5	C34 H24 N5	406.8	5.678	0.34	34	24	5
		502.2535	-25.4	-50.6	23.5	C38 H32 N	411.1	9.967	0.00	38	32	1
		502.1596	68.5	136.4	30.5	C39 H20 N	413.3	12.112	0.00	39	20	1
		502.2971	-69.0	-137.4	18.5	C33 H36 N5	401.1	0.004	99.63	33	36	5

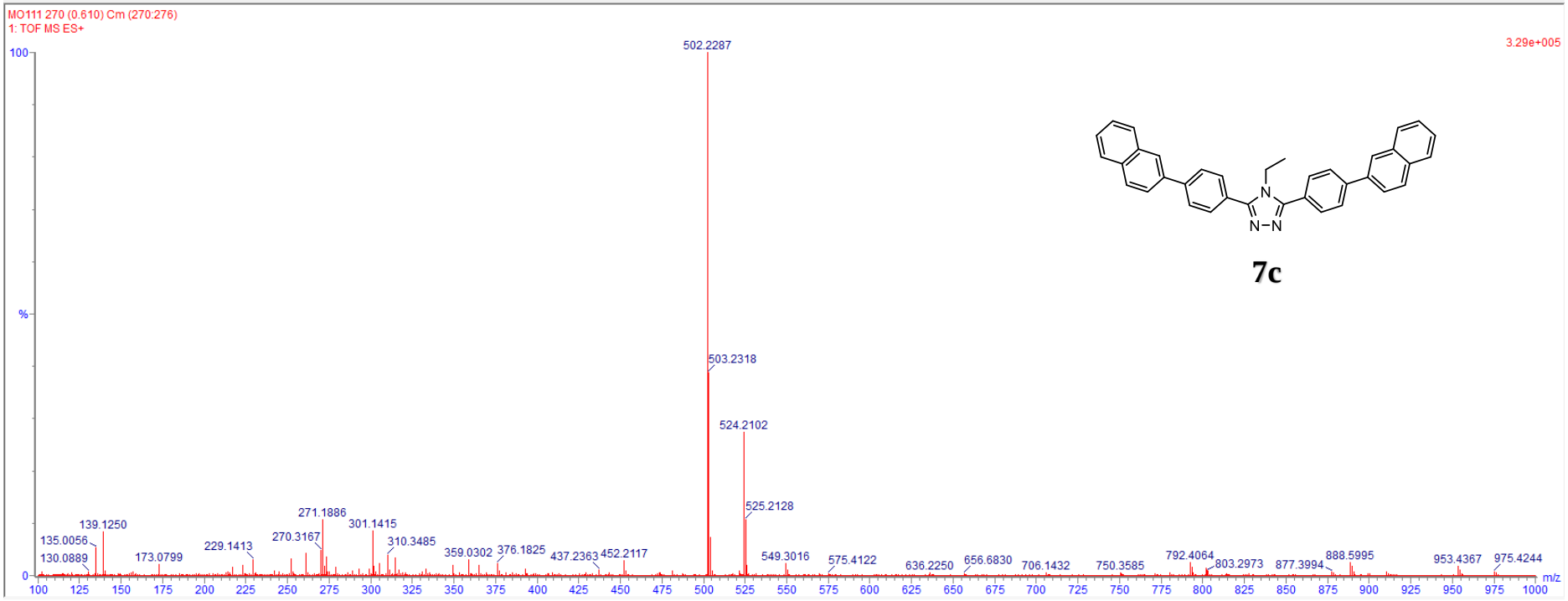


7b

4-Ethyl-3,5-bis[4-(naphthalen-2-yl)phenyl]-4H-1,2,4-triazole (**7c**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 7 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
502.2287	100.00	502.2283	0.4	0.8	24.5	C36 H28 N3	313.4	5.549	0.39	36	28	3
		502.2535	-24.8	-49.4	23.5	C38 H32 N	315.6	7.754	0.04	38	32	1
		502.2032	25.5	50.8	25.5	C34 H24 N5	307.9	0.010	98.97	34	24	5
		502.2971	-68.4	-136.2	18.5	C33 H36 N5	313.0	5.123	0.60	33	36	5
		502.1596	69.1	137.6	30.5	C39 H20 N	317.9	10.073	0.00	39	20	1

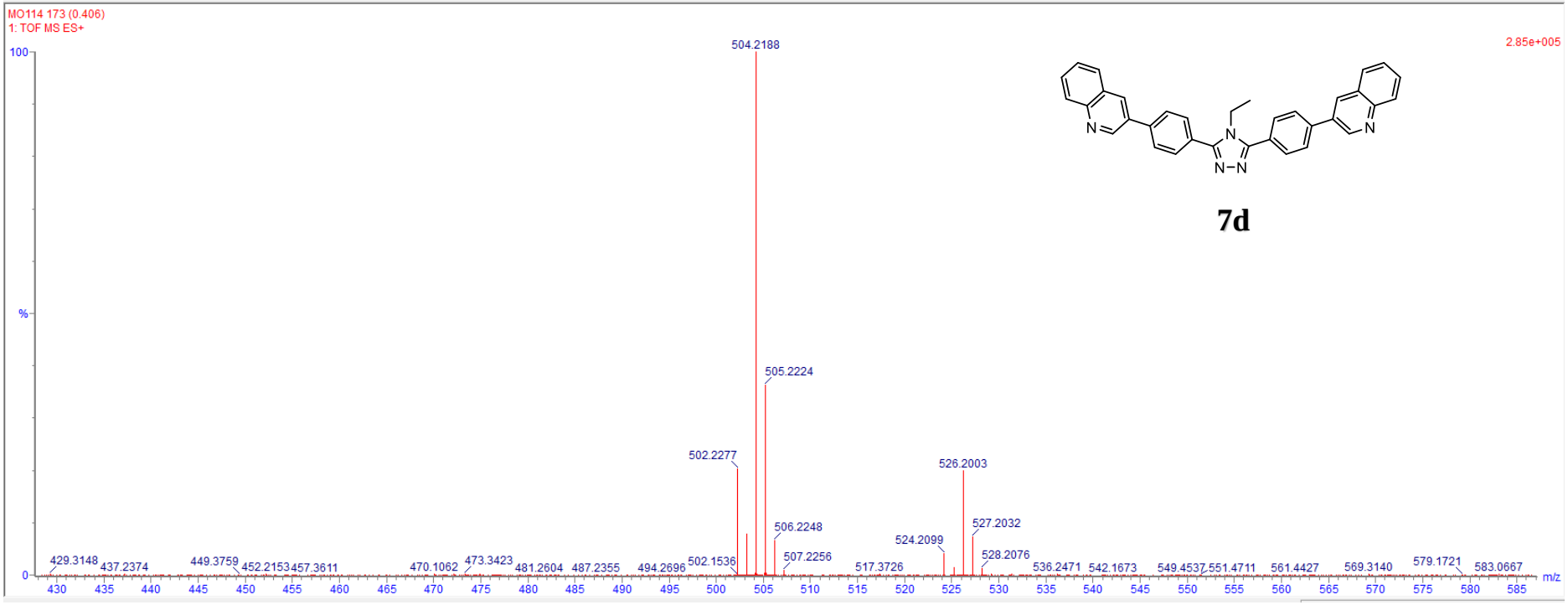


7c

4-Ethyl-3,5-bis[4-(quinolin-3-yl)phenyl]-4H-1,2,4-triazole (**7d**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 7 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
504.2188	100.00	504.2188	0.0	0.0	24.5	C34 H26 N5	293.5	0.302	73.92	34	26	5
		504.2440	-25.2	-50.0	23.5	C36 H30 N3	295.0	1.783	16.82	36	30	3
		504.1752	43.6	86.5	29.5	C39 H22 N	296.6	3.457	3.15	39	22	1
		504.2691	-50.3	-99.8	22.5	C38 H34 N	296.5	3.332	3.57	38	34	1
		504.1501	68.7	136.3	30.5	C37 H18 N3	296.9	3.674	2.54	37	18	3

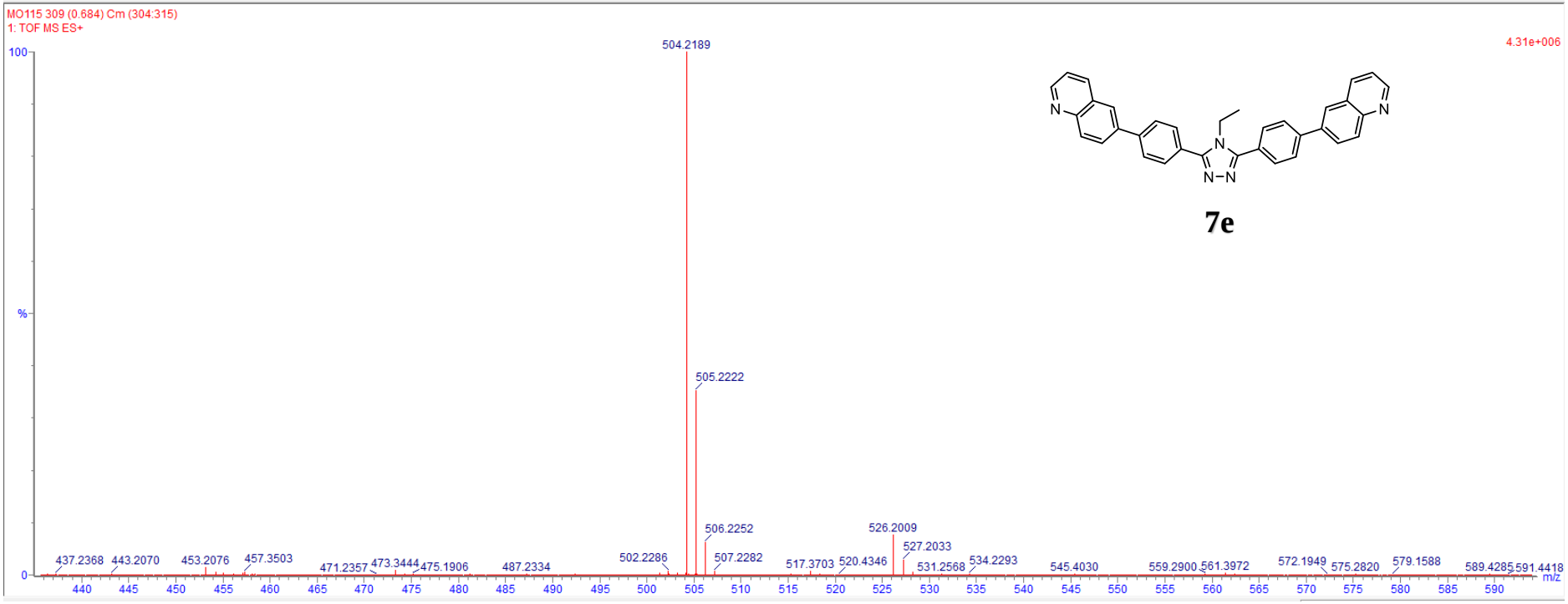


7d

4-Ethyl-3,5-bis[4-(quinolin-6-yl)phenyl]-4H-1,2,4-triazole (**7e**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 7 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
504.2189	100.00	504.2188	0.1	0.2	24.5	C34 H26 N5	479.8	0.373	68.87	34	26	5
		504.2440	-25.1	-49.8	23.5	C36 H30 N3	481.1	1.616	19.86	36	30	3
		504.1752	43.7	86.7	29.5	C39 H22 N	482.7	3.246	3.89	39	22	1
		504.2691	-50.2	-99.6	22.5	C38 H34 N	482.5	3.096	4.52	38	34	1
		504.1501	68.8	136.4	30.5	C37 H18 N3	483.0	3.555	2.86	37	18	3

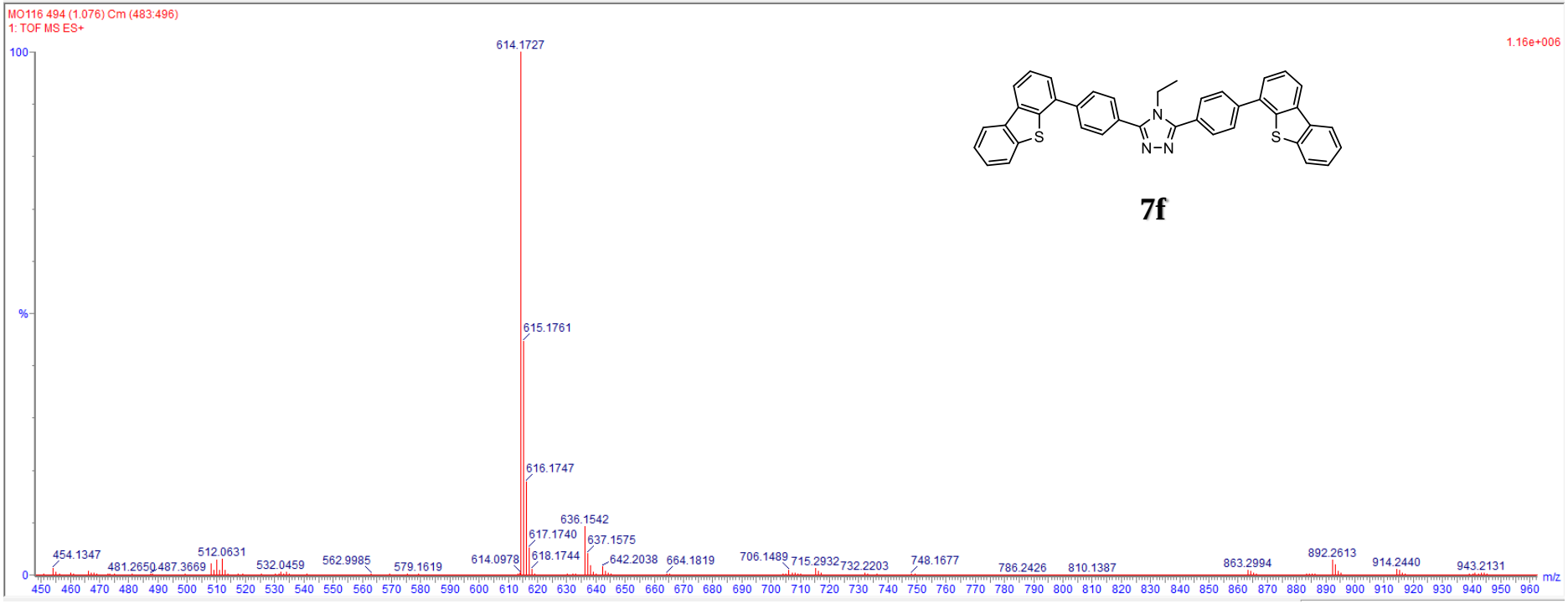


7e

3,5-Bis[4-(dibenzothiophen-4-yl)phenyl]-4-ethyl-4H-1,2,4-triazole (**7f**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
104 formula(e) evaluated with 23 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	S
614.1727	100.00	614.1725	0.2	0.3	28.5	C40 H28 N3 S2	396.5	2.108	12.15	40	28	3	2
		614.1758	-3.1	-5.0	23.5	C37 H32 N3 S3	394.6	0.156	85.57	37	32	3	3
		614.1691	3.6	5.9	33.5	C43 H24 N3 S	399.2	4.762	0.85	43	24	3	1
		614.1792	-6.5	-10.6	18.5	C34 H36 N3 S4	398.8	4.411	1.21	34	36	3	4
		614.1657	7.0	11.4	38.5	C46 H20 N3	400.5	6.122	0.22	46	20	3	

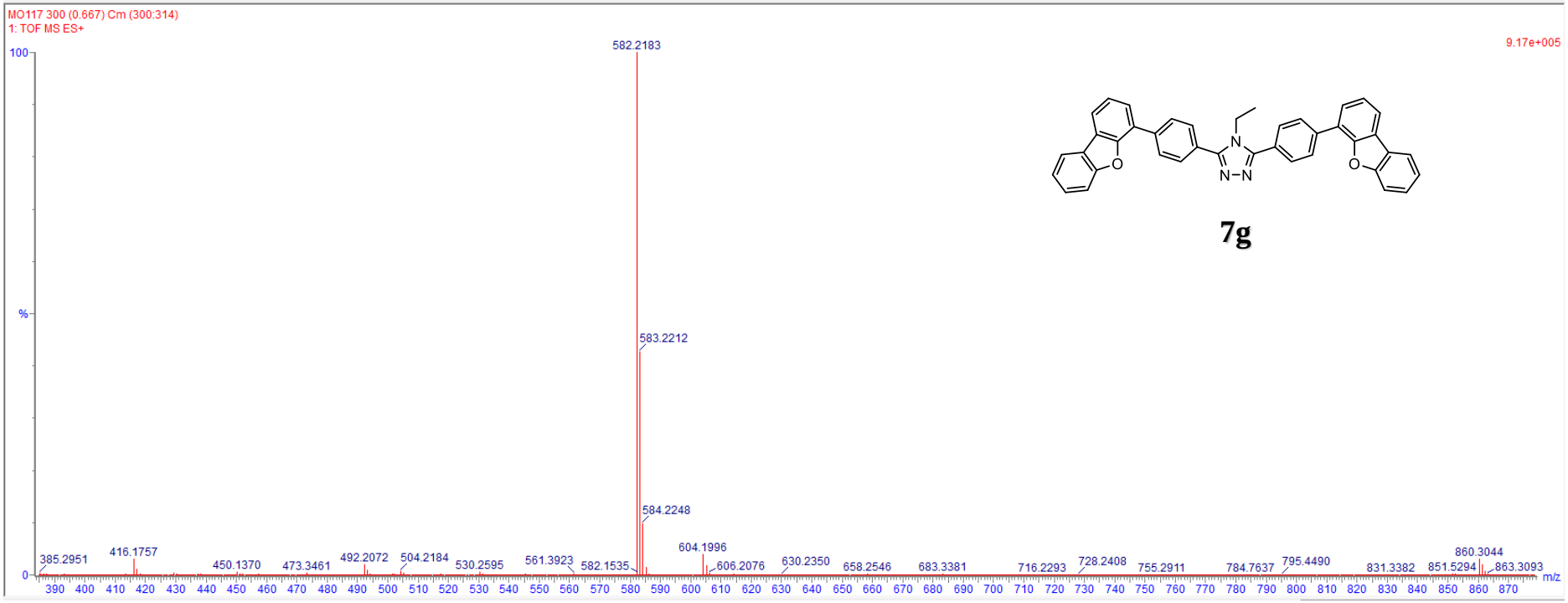


7f

3,5-Bis[4-(dibenzofuran-4-yl)phenyl]-4-ethyl-4H-1,2,4-triazole (**7g**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 20 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
582.2183	100.00	582.2182	0.1	0.2	28.5	C40 H28 N3 O2	366.1	1.155	31.51	40	28	3	2
		582.2222	-3.9	-6.7	32.5	C45 H28 N	369.7	4.760	0.86	45	28	1	
		582.2294	-11.1	-19.1	28.5	C39 H28 N5 O	365.4	0.482	61.73	39	28	5	1
		582.1970	21.3	36.6	33.5	C43 H24 N3	369.1	4.154	1.57	43	24	3	
		582.2433	-25.0	-42.9	27.5	C42 H32 N O2	368.1	3.140	4.33	42	32	1	2

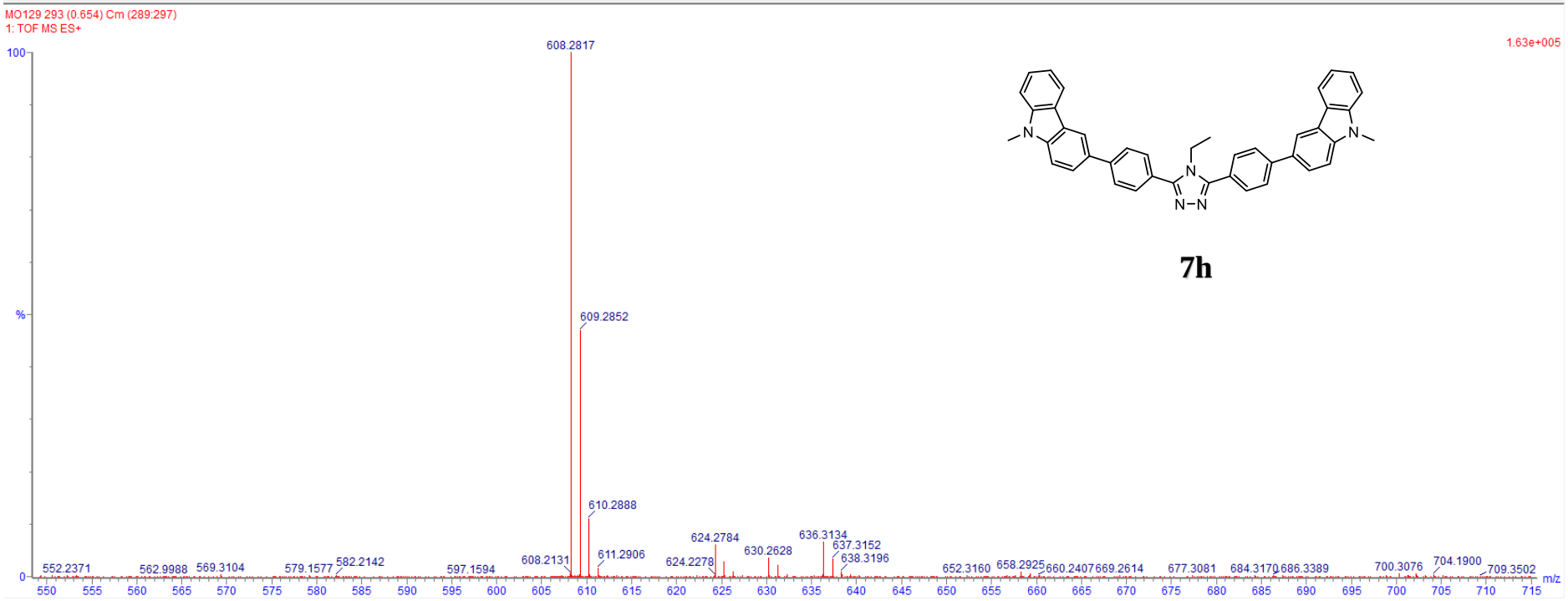


7g

4-Ethyl-3,5-bis[4-(9-methyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**7h**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 19 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
608.2817	100.00	608.2814	0.3	0.5	28.5	C42 H34 N5	236.4	0.344	70.91	42	34	5	
		608.2702	11.5	18.9	28.5	C43 H34 N3 O	237.7	1.633	19.54	43	34	3	1
		608.2953	-13.6	-22.4	27.5	C45 H38 N O	240.3	4.200	1.50	45	38	1	1
		608.3026	-20.9	-34.4	23.5	C39 H38 N5 O2	240.5	4.382	1.25	39	38	5	2
		608.2590	22.7	37.3	28.5	C44 H34 N O2	238.8	2.687	6.81	44	34	1	2

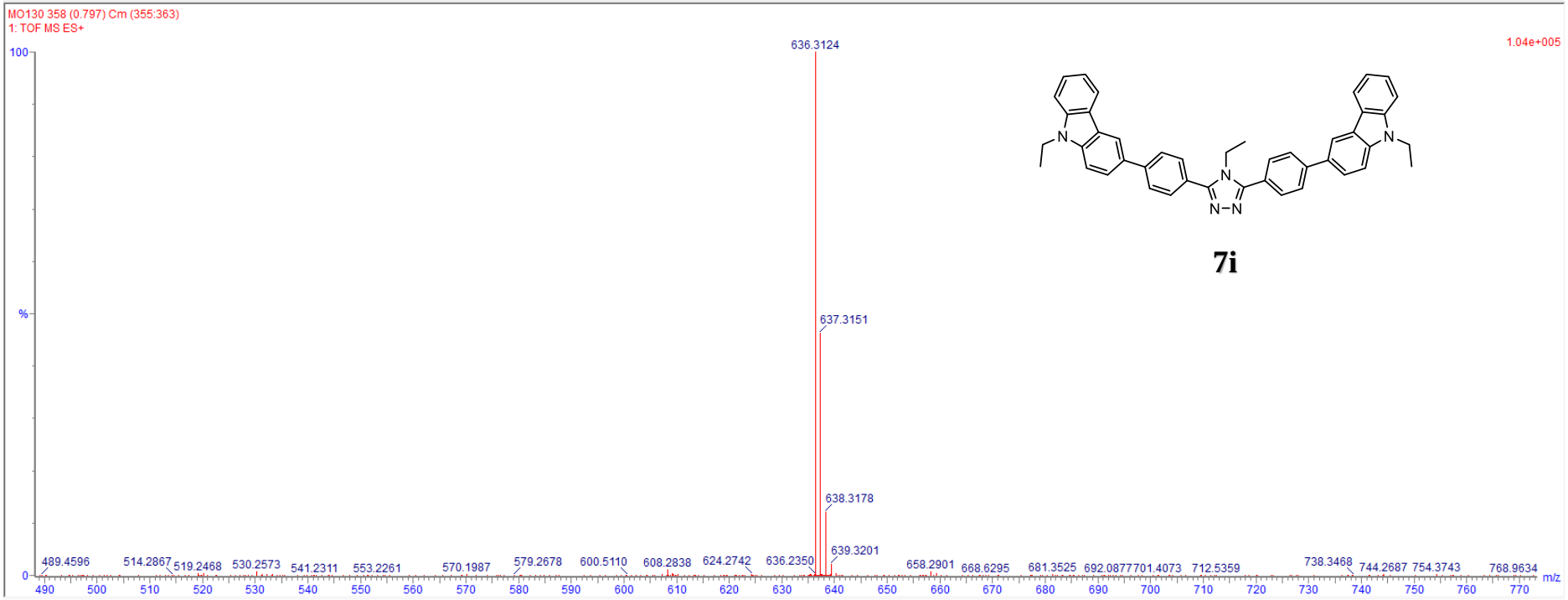


7h

4-Ethyl-3,5-bis[4-(9-ethyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**7i**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 19 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
636.3124	100.00	636.3127	-0.3	-0.5	28.5	C44 H38 N5	216.1	5.592	0.37	44	38	5	
		636.3015	10.9	17.1	28.5	C45 H38 N3 O	216.5	6.050	0.24	45	38	3	1
		636.3266	-14.2	-22.3	27.5	C47 H42 N O	217.5	7.043	0.09	47	42	1	1
		636.3339	-21.5	-33.8	23.5	C41 H42 N5 O2	210.5	0.008	99.16	41	42	5	2
		636.2903	22.1	34.7	28.5	C46 H38 N O2	217.0	6.555	0.14	46	38	1	2

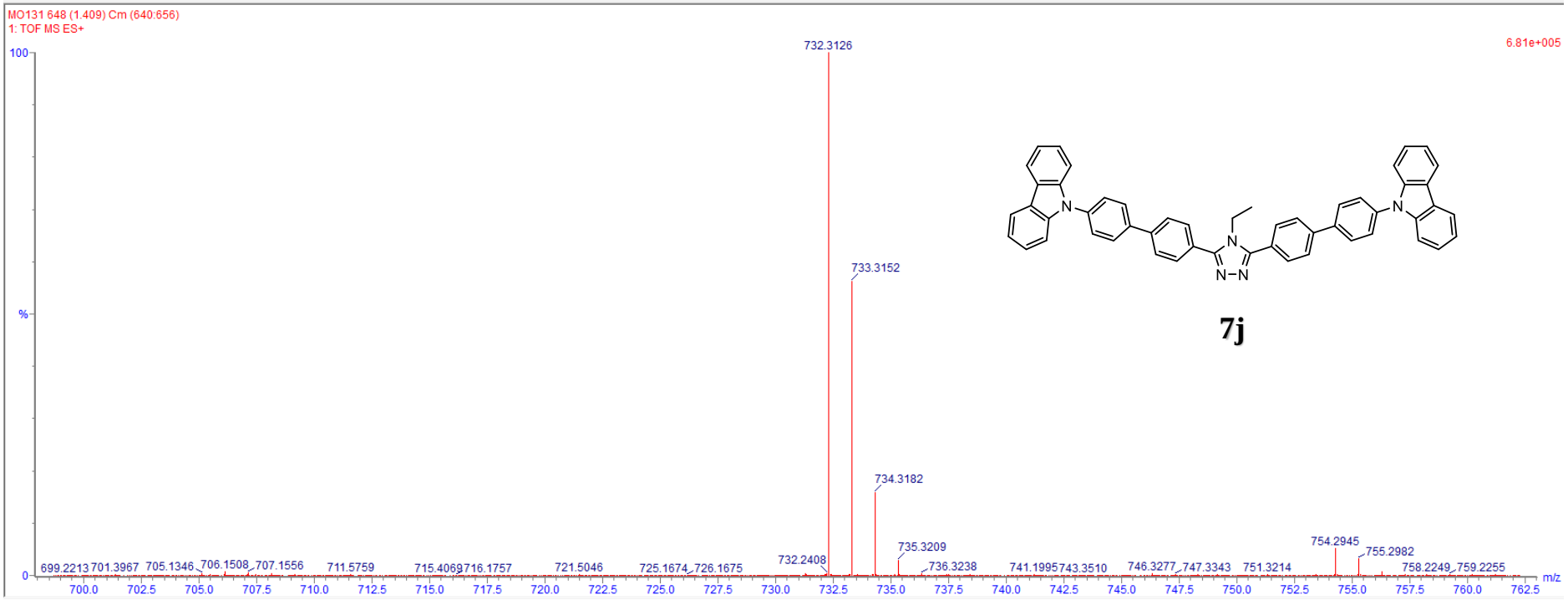


7i

3,5-Bis[4′-(9H-carbazol-9-yl)biphenyl-4-yl]-4-ethyl-4H-1,2,4-triazole (**7j**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
186 formula(e) evaluated with 38 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
732.3126	100.00	732.3127	-0.1	-0.1	36.5	C52 H38 N5	386.0	2.607	7.38	52	38	5	
		732.3015	11.1	15.2	36.5	C53 H38 N3 O	386.6	3.198	4.09	53	38	3	1
		732.3266	-14.0	-19.1	35.5	C55 H42 N O	388.0	4.579	1.03	55	42	1	1
		732.3339	-21.3	-29.1	31.5	C49 H42 N5 O2	383.6	0.158	85.34	49	42	5	2
		732.2903	22.3	30.5	36.5	C54 H38 N O2	387.3	3.832	2.17	54	38	1	2
733.3152	56.29	733.3107	4.5	6.1	35.5	C55 H41 O2	379.5	1.541	21.41	55	41		2
		733.3219	-6.7	-9.1	35.5	C54 H41 N2 O	379.5	1.495	22.43	54	41	2	1
		733.3331	-17.9	-24.4	35.5	C53 H41 N4	379.6	1.572	20.76	53	41	4	

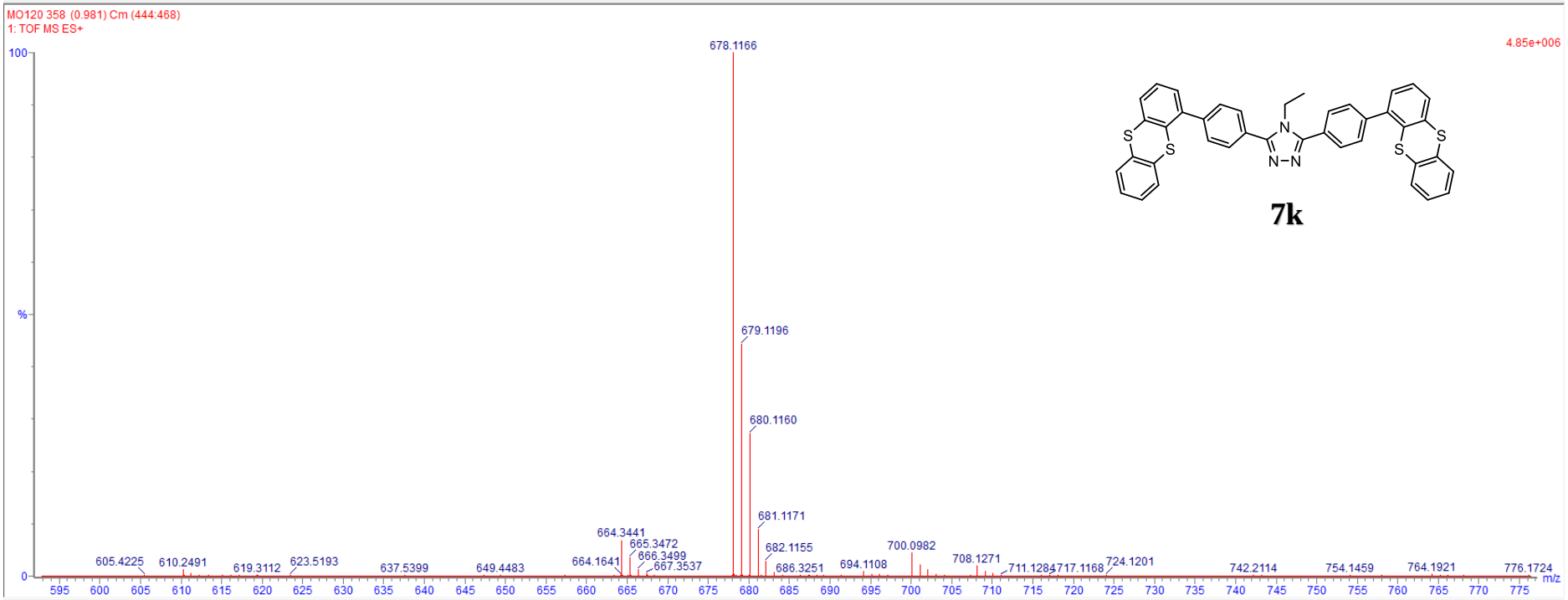


7j

4-Ethyl-3,5-bis[4-(thiantren-1-yl)phenyl]-4H-1,2,4-triazole (**7k**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
103 formula(e) evaluated with 21 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	S
678.1166	100.00	678.1166	0.0	0.0	28.5	C40 H28 N3 S4	537.1	0.300	74.08	40	28	3	4
		678.1132	3.4	5.0	33.5	C43 H24 N3 S3	538.7	1.829	16.05	43	24	3	3
		678.1099	6.7	9.9	38.5	C46 H20 N3 S2	539.7	2.827	5.92	46	20	3	2
		678.1065	10.1	14.9	43.5	C49 H16 N3 S	540.4	3.577	2.80	49	16	3	1
		678.1283	-11.7	-17.3	47.5	C54 H16 N	541.3	4.467	1.15	54	16	1	

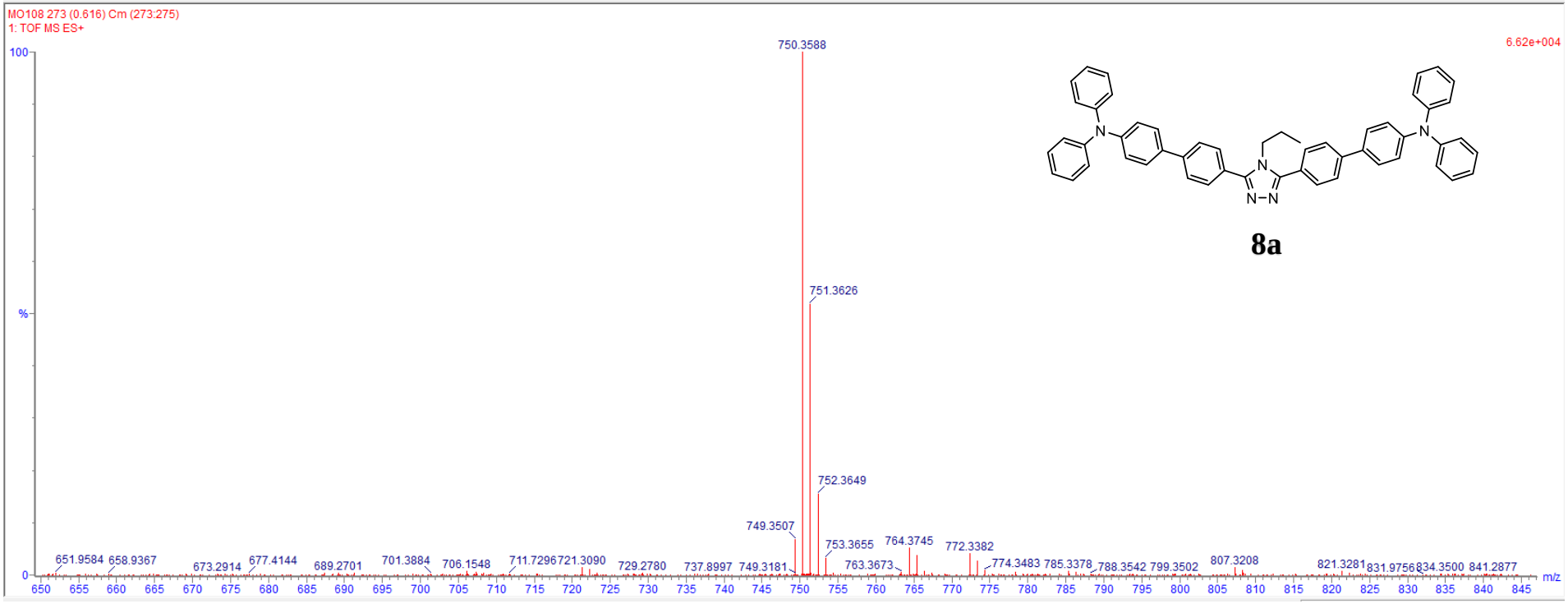


7k

3,5-Bis[4′-(N,N-diphenylamino)biphenyl-4-yl]-4-propyl-4H-1,2,4-triazole (**8a**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
62 formula(e) evaluated with 13 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
750.3588	100.00	750.3597	-0.9	-1.2	34.5	C53 H44 N5	207.1	0.635	53.02	53	44	5
		750.3848	-26.0	-34.7	33.5	C55 H48 N3	207.8	1.393	24.84	55	48	3
		750.3161	42.7	56.9	39.5	C58 H40 N	208.9	2.432	8.78	58	40	1
		750.4100	-51.2	-68.2	32.5	C57 H52 N	209.0	2.504	8.18	57	52	1
		750.2909	67.9	90.5	40.5	C56 H36 N3	209.4	2.960	5.18	56	36	3
751.3626	51.72	751.3801	-17.5	-23.3	33.5	C54 H47 N4	103.6	0.940	39.06	54	47	4
		751.3365	26.1	34.7	38.5	C59 H43	104.2	1.517	21.94	59	43	
		751.4052	-42.6	-56.7	32.5	C56 H51 N2	104.4	1.659	19.03	56	51	2

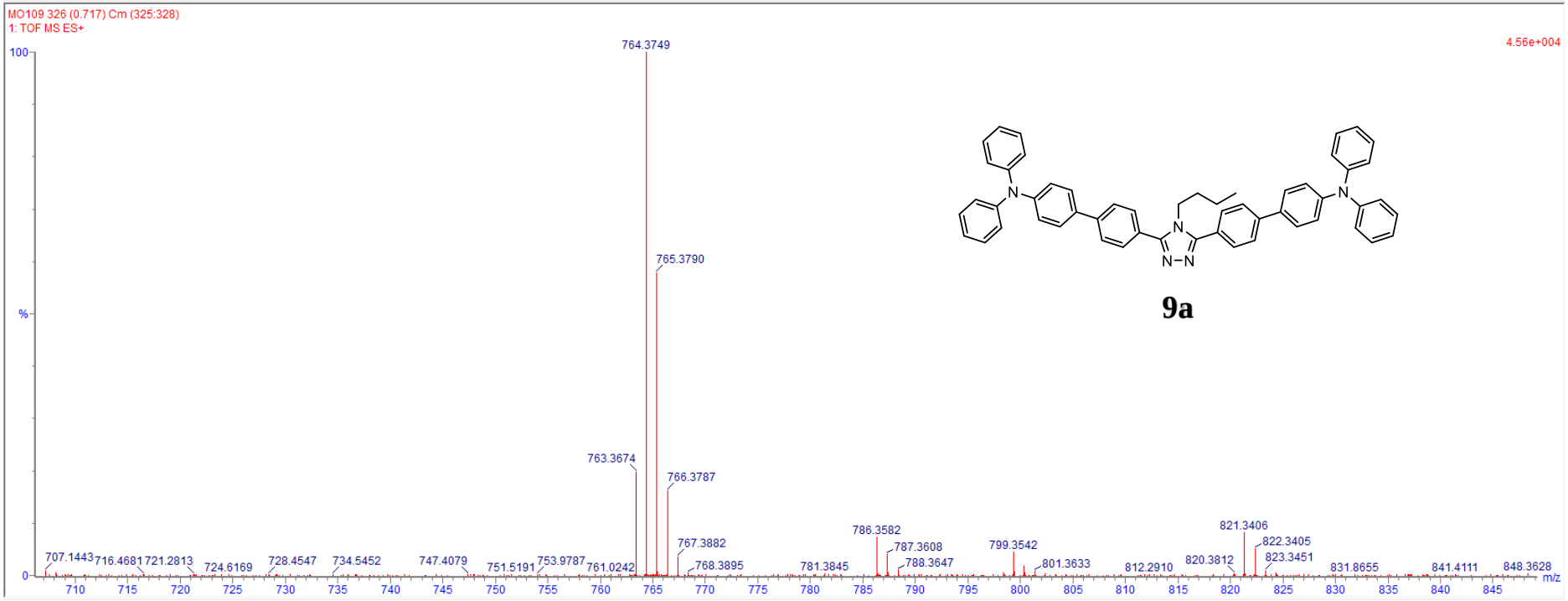


8a

4-Butyl-3,5-bis[4′-(N,N-diphenylamino)biphenyl-4-yl]-4H-1,2,4-triazole (**9a**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
62 formula(e) evaluated with 13 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
764.3749	100.00	764.3753	-0.4	-0.5	34.5	C54 H46 N5	185.1	0.325	72.23	54	46	5
		764.4005	-25.6	-33.5	33.5	C56 H50 N3	186.6	1.739	17.57	56	50	3
		764.3317	43.2	56.5	39.5	C59 H42 N	188.2	3.361	3.47	59	42	1
		764.4256	-50.7	-66.3	32.5	C58 H54 N	188.1	3.240	3.92	58	54	1
		764.3066	68.3	89.4	40.5	C57 H38 N3	188.4	3.570	2.81	57	38	3
765.3790	57.76	765.3957	-16.7	-21.8	33.5	C55 H49 N4	120.4	1.236	29.04	55	49	4
		765.3521	26.9	35.1	38.5	C60 H45	120.9	1.742	17.52	60	45	
		765.4209	-41.9	-54.7	32.5	C57 H53 N2	120.8	1.554	21.15	57	53	2

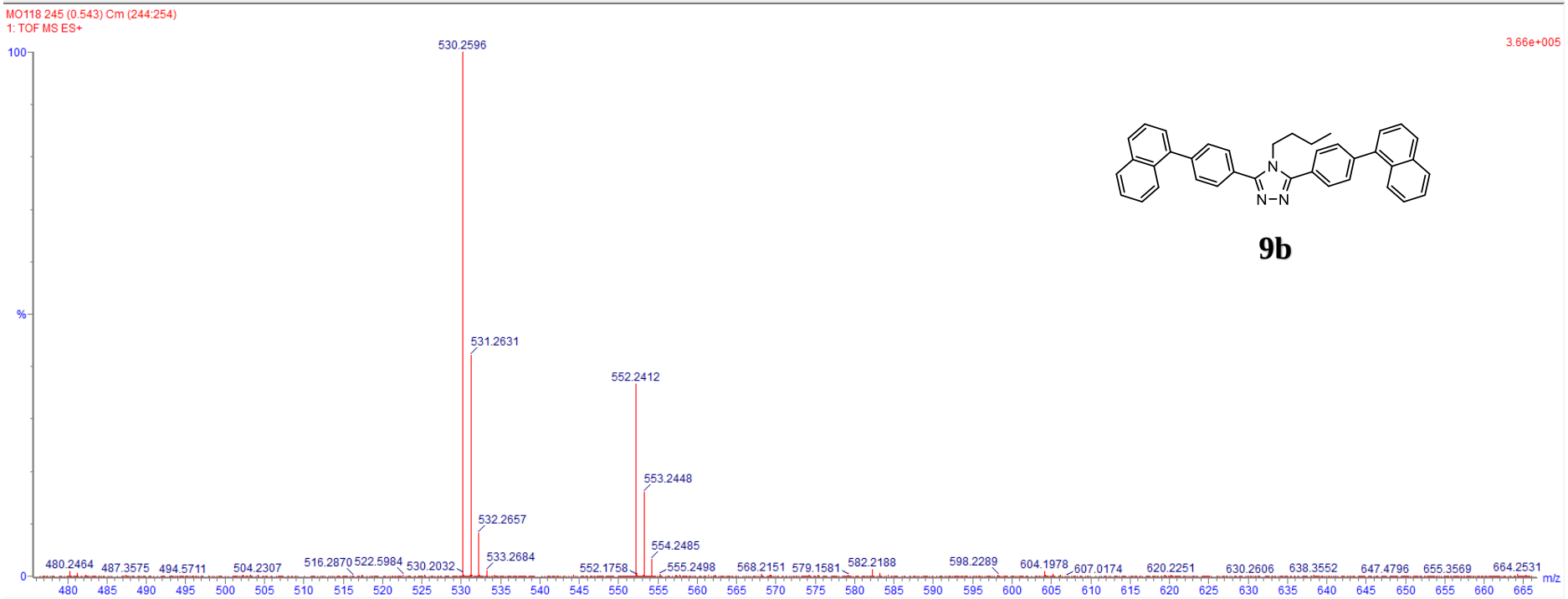


9a

4-Butyl-3,5-bis[4-(naphthalen-1-yl)phenyl]-4H-1,2,4-triazole (**9b**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 20 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
530.2596	100.00	530.2596	0.0	0.0	24.5	C38 H32 N3	257.7	0.187	82.98	38	32	3	
		530.2556	4.0	7.5	20.5	C33 H32 N5 O2	264.8	7.214	0.07	33	32	5	2
		530.2484	11.2	21.1	24.5	C39 H32 N O	259.6	2.058	12.77	39	32	1	1
		530.2808	-21.2	-40.0	19.5	C35 H36 N3 O2	263.5	5.983	0.25	35	36	3	2
		530.2345	25.1	47.3	25.5	C36 H28 N5	260.8	3.240	3.92	36	28	5	

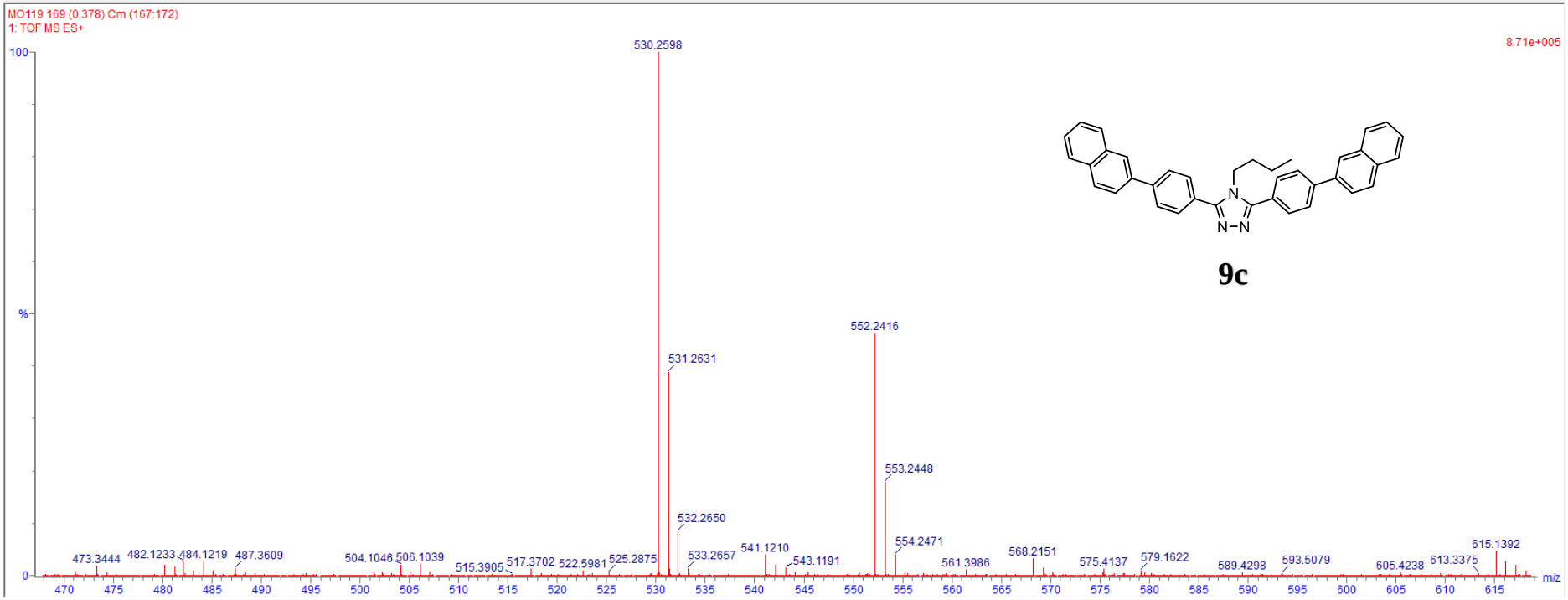


9b

4-Butyl-3,5-bis[4-(naphthalen-2-yl)phenyl]-4H-1,2,4-triazole (**9c**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 20 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
530.2598	100.00	530.2596	0.2	0.4	24.5	C38 H32 N3	387.0	5.431	0.44	38	32	3	
		530.2556	4.2	7.9	20.5	C33 H32 N5 O2	382.6	1.017	36.15	33	32	5	2
		530.2484	11.4	21.5	24.5	C39 H32 N O	387.4	5.761	0.31	39	32	1	1
		530.2808	-21.0	-39.6	19.5	C35 H36 N3 O2	382.1	0.463	62.97	35	36	3	2
		530.2848	-25.0	-47.1	23.5	C40 H36 N	388.3	6.663	0.13	40	36	1	

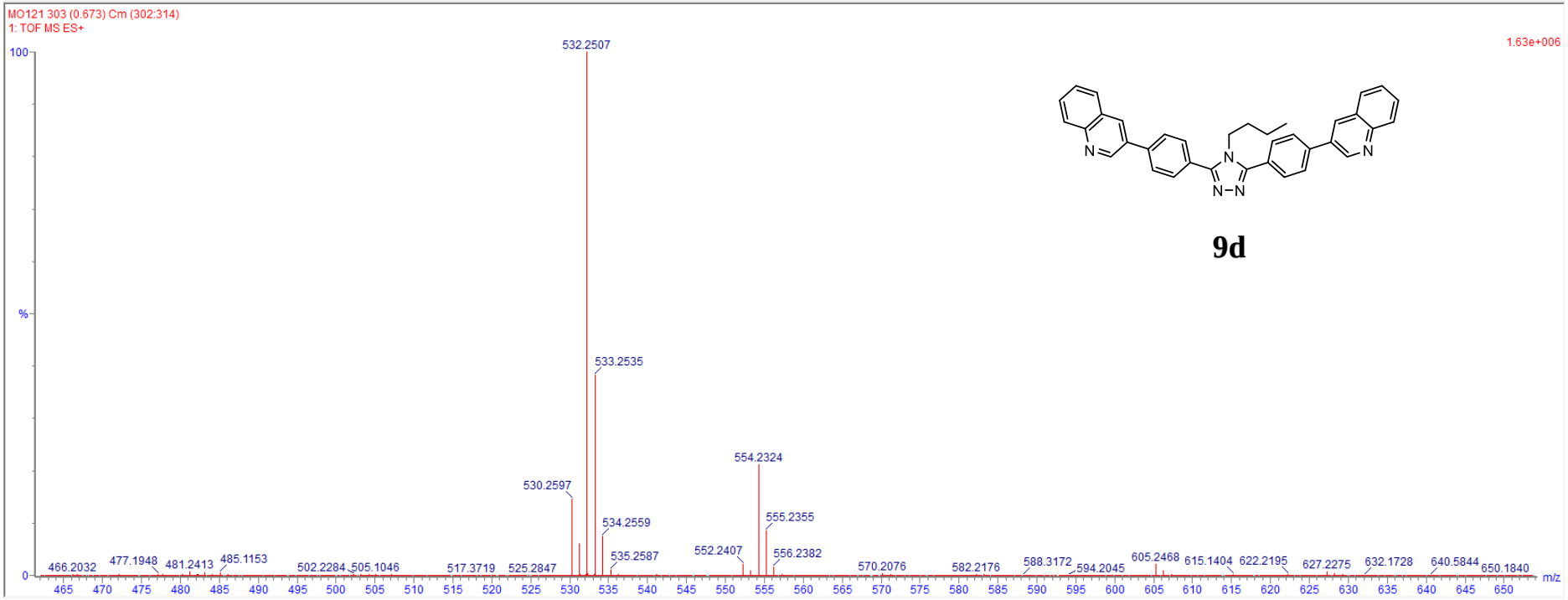


9c

4-Butyl-3,5-bis[4-(quinolin-3-yl)phenyl]-4H-1,2,4-triazole (**9d**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 19 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
532.2507	100.00	532.2501	0.6	1.1	24.5	C36 H30 N5	400.3	6.853	0.11	36	30	5	
		532.2389	11.8	22.2	24.5	C37 H30 N3 O	400.8	7.418	0.06	37	30	3	1
		532.2640	-13.3	-25.0	23.5	C39 H34 N O	402.0	8.620	0.02	39	34	1	1
		532.2713	-20.6	-38.7	19.5	C33 H34 N5 O2	393.4	0.002	99.78	33	34	5	2
		532.2277	23.0	43.2	24.5	C38 H30 N O2	401.4	8.008	0.03	38	30	1	2

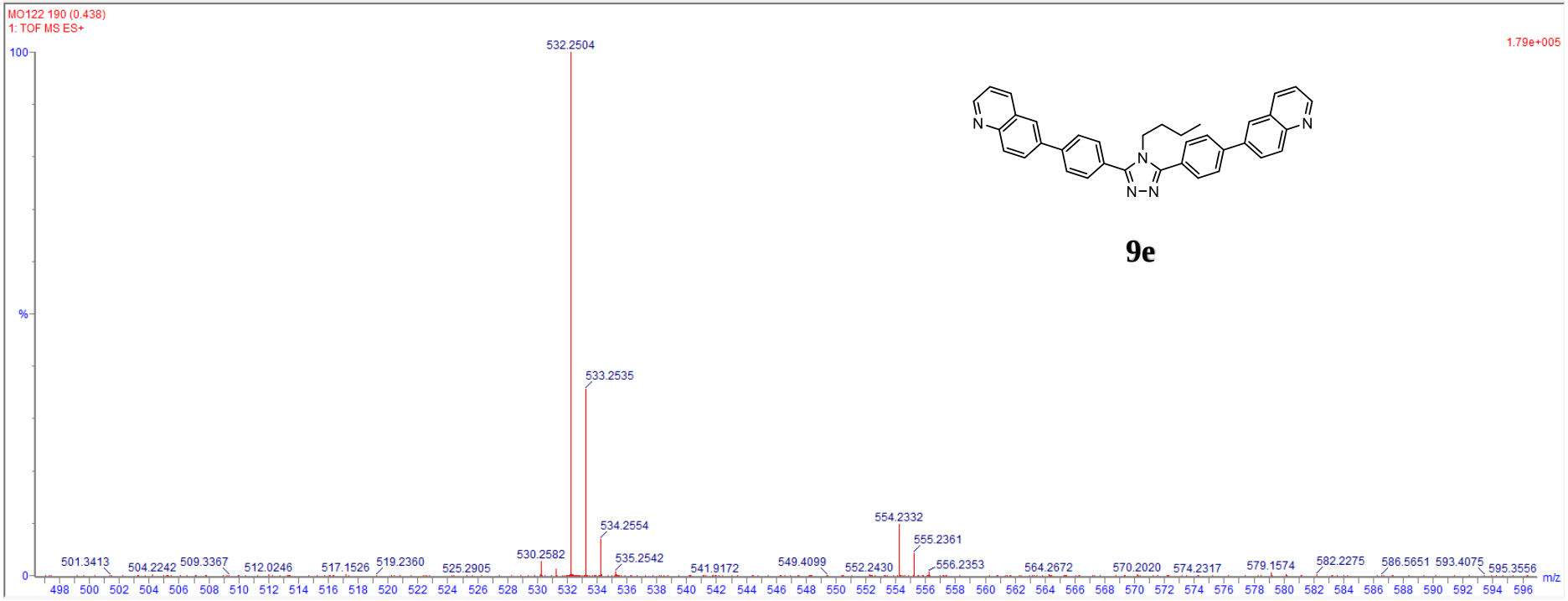


9d

4-Butyl-3,5-bis[4-(quinolin-6-yl)phenyl]-4H-1,2,4-triazole (**9e**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 19 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
532.2504	100.00	532.2501	0.3	0.6	24.5	C36 H30 N5	201.3	2.477	8.40	36	30	5	
		532.2389	11.5	21.6	24.5	C37 H30 N3 O	201.6	2.781	6.20	37	30	3	1
		532.2640	-13.6	-25.6	23.5	C39 H34 N O	202.3	3.488	3.06	39	34	1	1
		532.2713	-20.9	-39.3	19.5	C33 H34 N5 O2	199.1	0.246	78.21	33	34	5	2
		532.2277	22.7	42.6	24.5	C38 H30 N O2	202.0	3.186	4.13	38	30	1	2

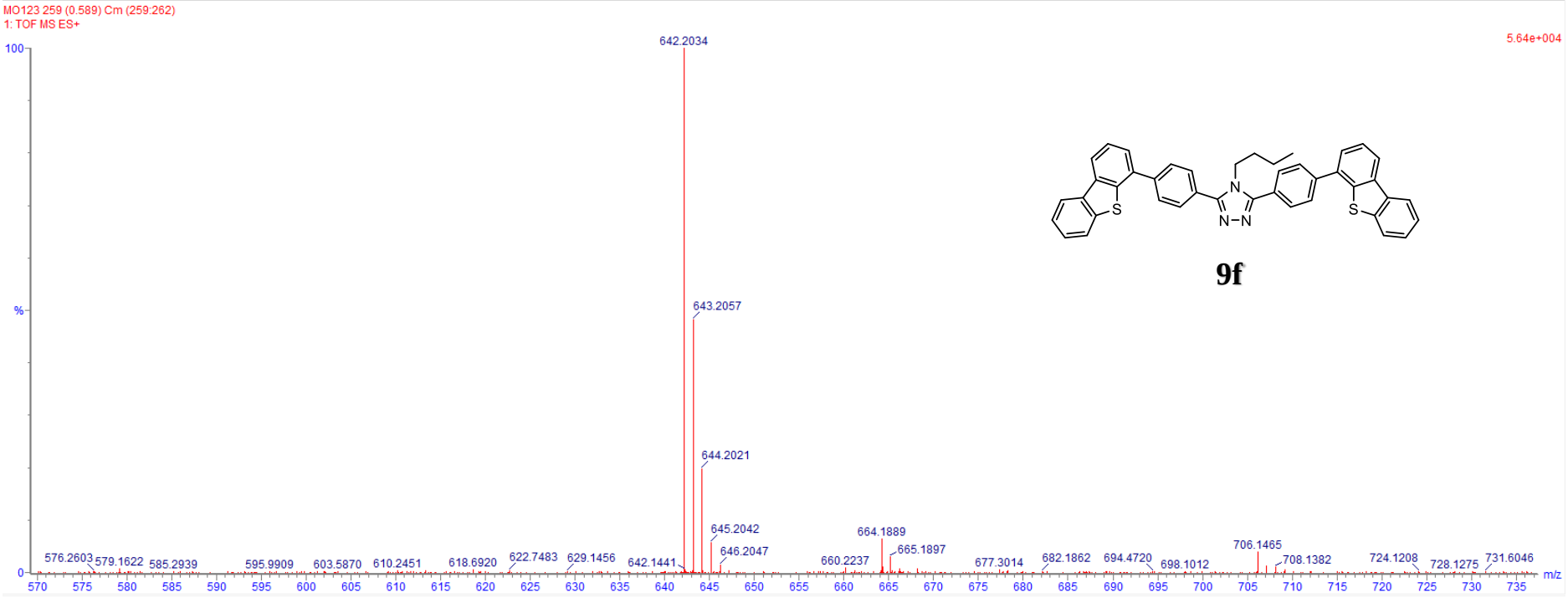


9e

3,5-Bis[4-(dibenzothiophen-4-yl)phenyl]-4-butyl-4H-1,2,4-triazole (**9f**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
103 formula(e) evaluated with 23 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	S
642.2034	100.00	642.2038	-0.4	-0.6	28.5	C42 H32 N3 S2	153.6	0.040	96.10	42	32	3	2
		642.2004	3.0	4.7	33.5	C45 H28 N3 S	158.1	4.623	0.98	45	28	3	1
		642.2071	-3.7	-5.8	23.5	C39 H36 N3 S3	157.2	3.678	2.53	39	36	3	3
		642.1970	6.4	10.0	38.5	C48 H24 N3	160.1	6.571	0.14	48	24	3	
		642.2105	-7.1	-11.1	18.5	C36 H40 N3 S4	159.5	5.977	0.25	36	40	3	4

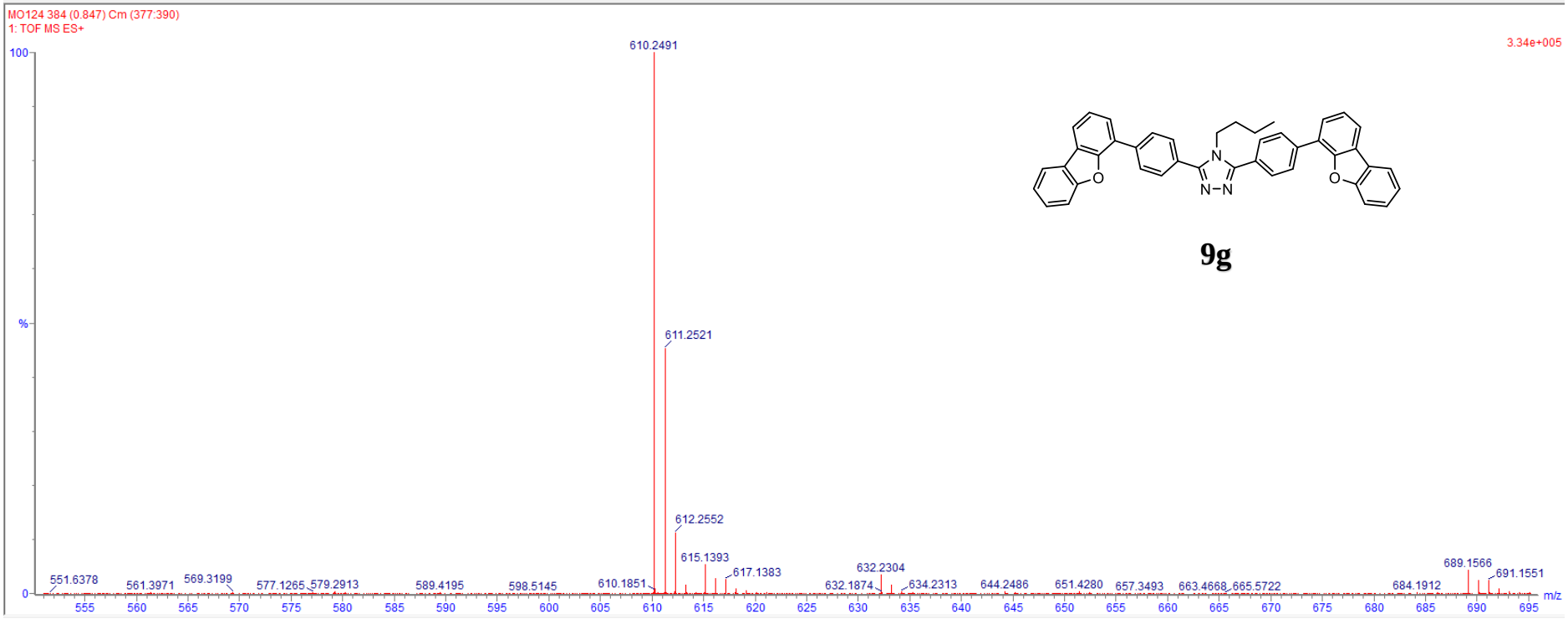


9f

3,5-Bis[4-(dibenzofuran-4-yl)phenyl]-4-butyl-4H-1,2,4-triazole (**9g**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
62 formula(e) evaluated with 14 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
610.2491	100.00	610.2495	-0.4	-0.7	28.5	C42 H32 N3 O2	309.4	0.171	84.29	42	32	3	2
		610.2535	-4.4	-7.2	32.5	C47 H32 N	313.4	4.119	1.63	47	32	1	
		610.2283	20.8	34.1	33.5	C45 H28 N3	312.8	3.482	3.07	45	28	3	
		610.2746	-25.5	-41.8	27.5	C44 H36 N O2	311.7	2.386	9.20	44	36	1	2
		610.2171	32.0	52.4	33.5	C46 H28 N O	313.3	4.010	1.81	46	28	1	1

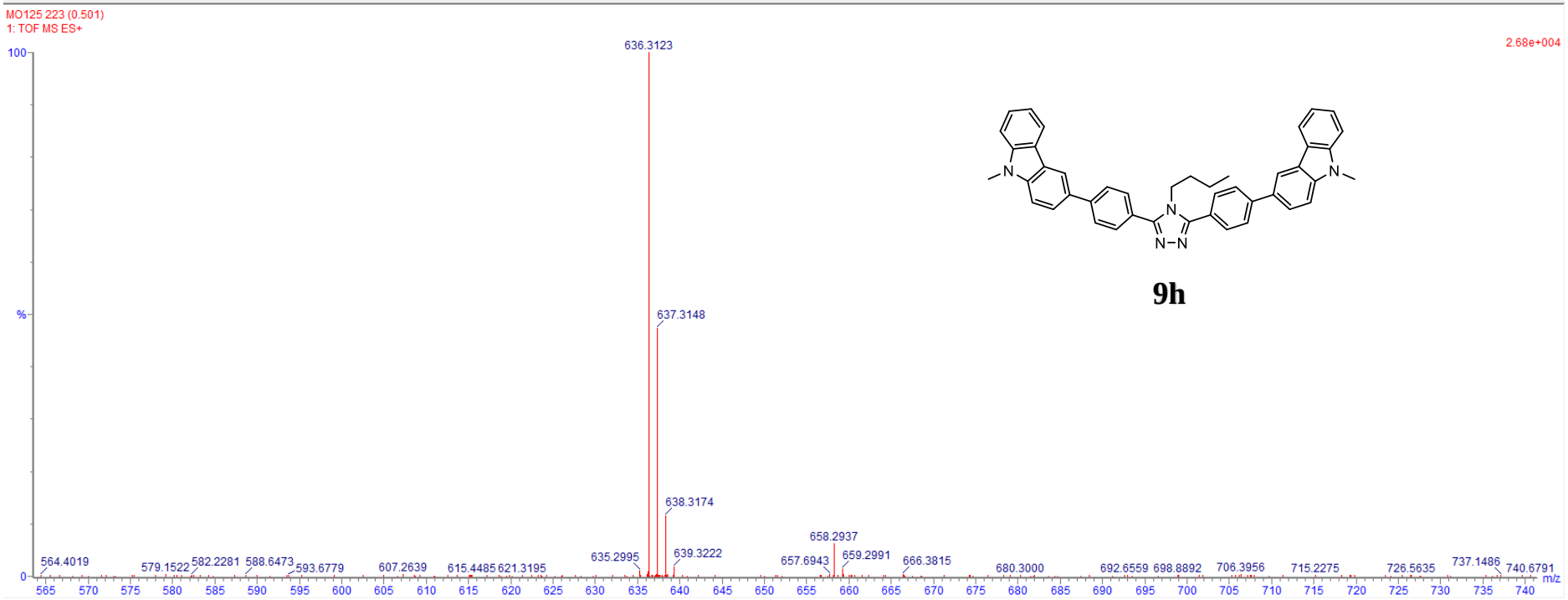


9g

4-Butyl-3,5-bis[4-(9-methyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**9h**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
93 formula(e) evaluated with 19 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
636.3123	100.00	636.3127	-0.4	-0.6	28.5	C44 H38 N5	111.3	2.953	5.22	44	38	5	
		636.3015	10.8	17.0	28.5	C45 H38 N3 O	111.9	3.566	2.83	45	38	3	1
		636.3266	-14.3	-22.5	27.5	C47 H42 N O	113.2	4.837	0.79	47	42	1	1
		636.3339	-21.6	-33.9	23.5	C41 H42 N5 O2	108.4	0.110	89.62	41	42	5	2
		636.2903	22.0	34.6	28.5	C46 H38 N O2	112.5	4.174	1.54	46	38	1	2

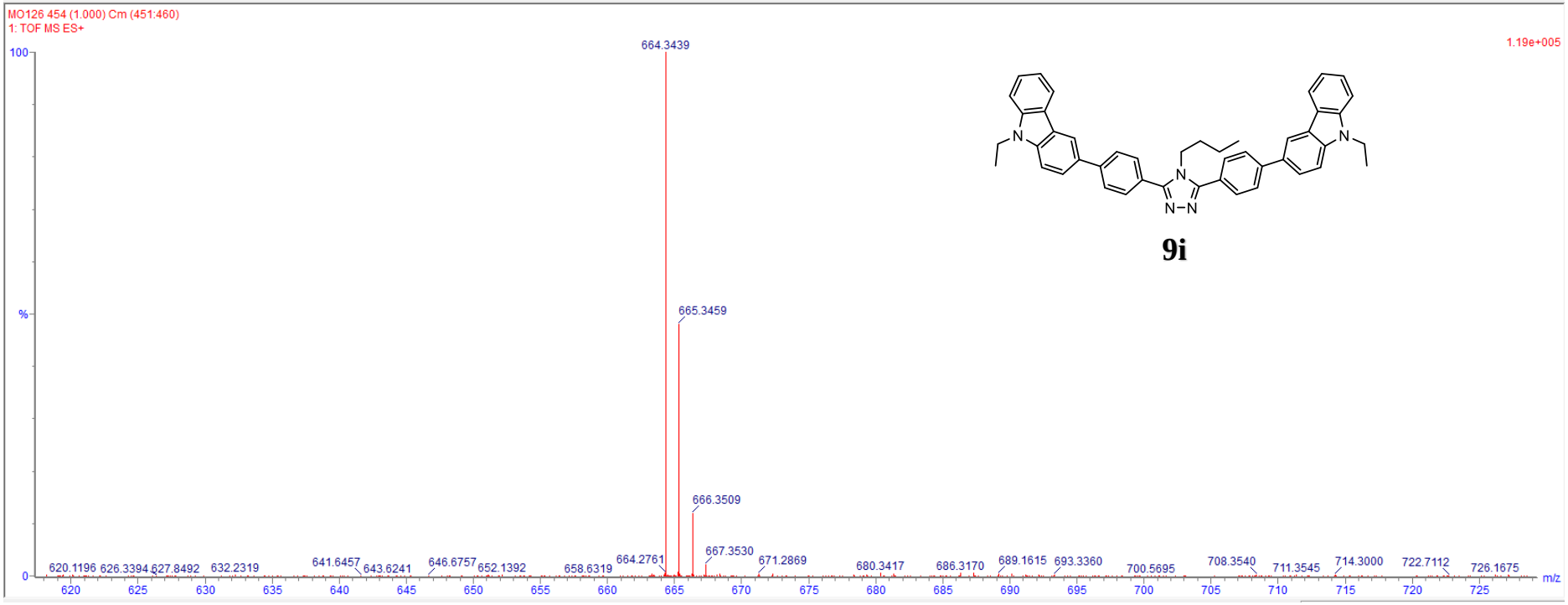


9h

4-Butyl-3,5-bis[4-(9-ethyl-9H-carbazol-3-yl)phenyl]-4H-1,2,4-triazole (**9i**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 7 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
664.3439	100.00	664.3440	-0.1	-0.2	28.5	C46 H42 N5	169.4	0.404	66.77	46	42	5
		664.3692	-25.3	-38.1	27.5	C48 H46 N3	170.5	1.601	20.18	48	46	3
		664.3004	43.5	65.5	33.5	C51 H38 N	172.2	3.297	3.70	51	38	1
		664.3943	-50.4	-75.9	26.5	C50 H50 N	171.9	2.907	5.46	50	50	1
		664.2753	68.6	103.3	34.5	C49 H34 N3	172.2	3.246	3.89	49	34	3

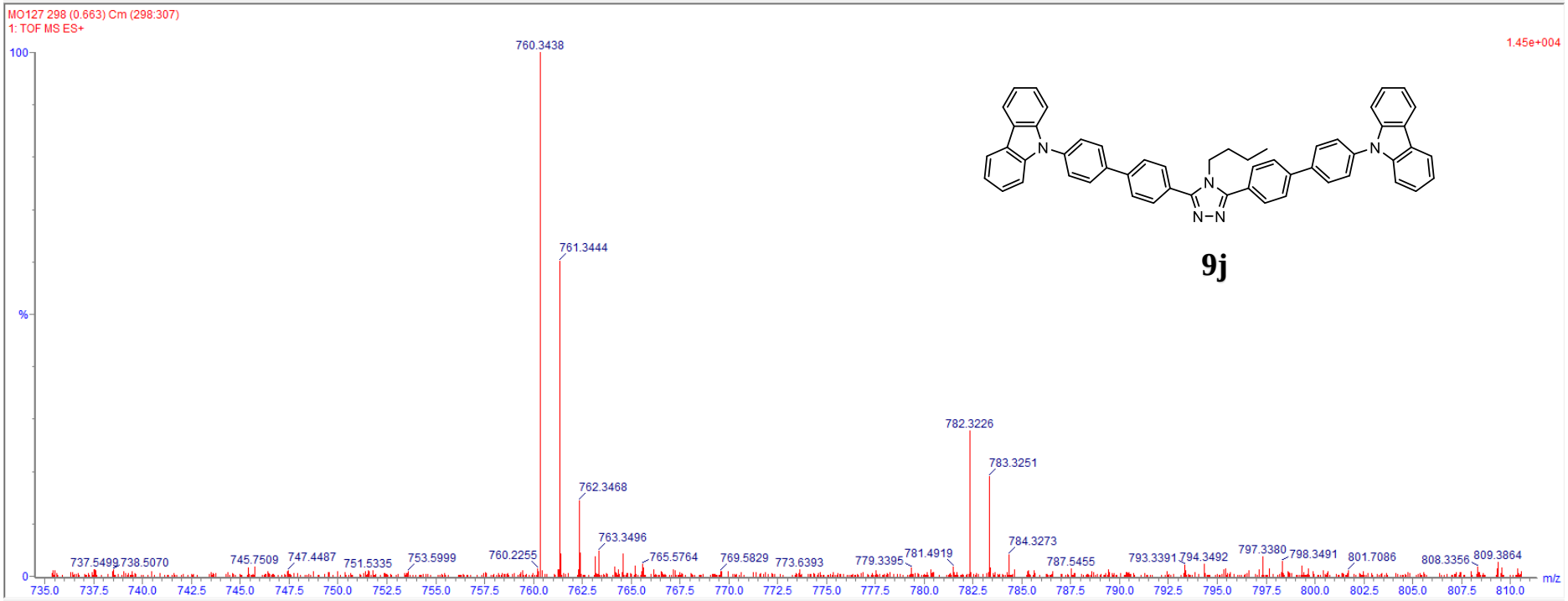


9i

4-Butyl-3,5-bis[4′-(9H-carbazol-9-yl)biphenyl-4-yl]-4H-1,2,4-triazole (**9j**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
186 formula(e) evaluated with 38 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
760.3438	100.00	760.3440	-0.2	-0.3	36.5	C54 H42 N5	143.2	0.878	41.58	54	42	5	
		760.3328	11.0	14.5	36.5	C55 H42 N3 O	143.6	1.234	29.11	55	42	3	1
		760.3579	-14.1	-18.5	35.5	C57 H46 N O	145.2	2.853	5.77	57	46	1	1
		760.3652	-21.4	-28.1	31.5	C51 H46 N5 O2	145.2	2.863	5.71	51	46	5	2
		760.3216	22.2	29.2	36.5	C56 H42 N O2	144.0	1.724	17.83	56	42	1	2
761.3444	60.12	761.3420	2.4	3.2	35.5	C57 H45 O2	136.0	1.565	20.90	57	45		2
		761.3532	-8.8	-11.6	35.5	C56 H45 N2 O	135.9	1.519	21.88	56	45	2	1
		761.3280	16.4	21.5	36.5	C54 H41 N4 O	135.9	1.449	23.49	54	41	4	1

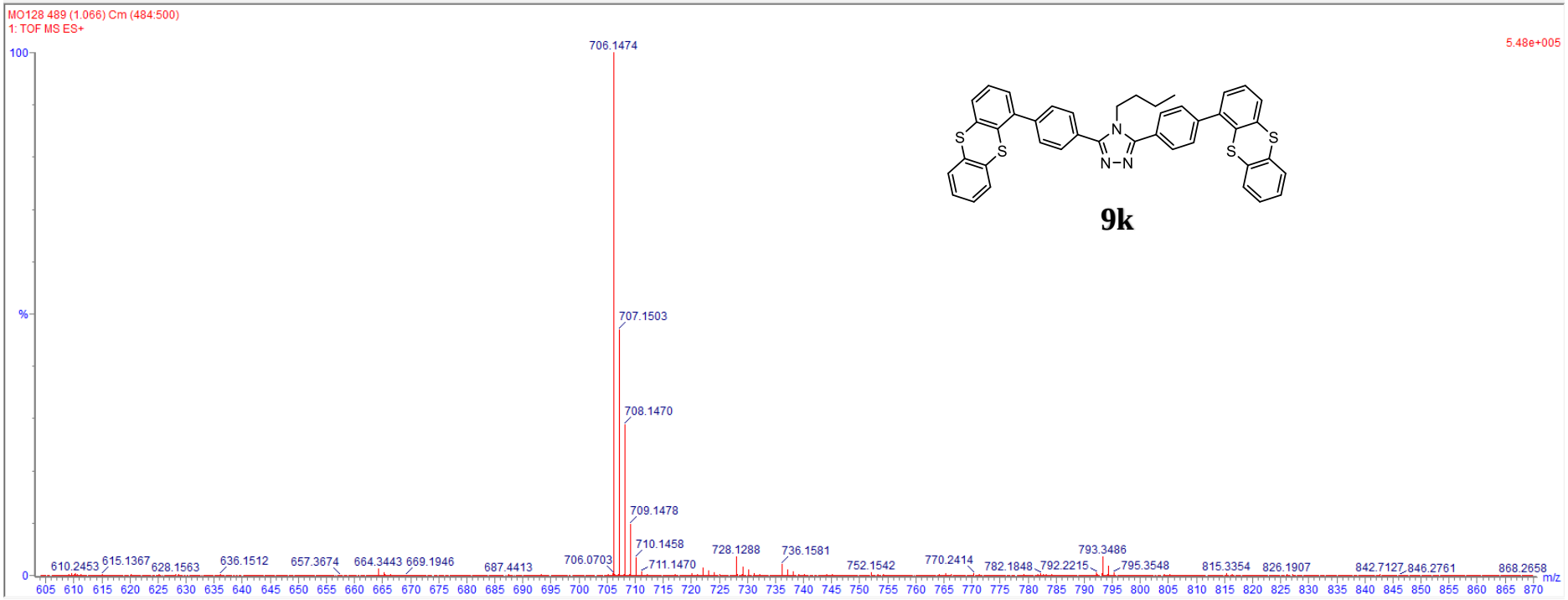


9j

4-Butyl-3,5-bis[4-(thiantren-1-yl)phenyl]-4H-1,2,4-triazole (**9k**).

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
103 formula(e) evaluated with 21 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	S
706.1474	100.00	706.1479	-0.5	-0.7	28.5	C42 H32 N3 S4	327.8	0.249	77.99	42	32	3	4
		706.1445	2.9	4.1	33.5	C45 H28 N3 S3	329.5	1.954	14.17	45	28	3	3
		706.1412	6.2	8.8	38.5	C48 H24 N3 S2	330.6	3.028	4.84	48	24	3	2
		706.1378	9.6	13.6	43.5	C51 H20 N3 S	331.4	3.824	2.18	51	20	3	1
		706.1596	-12.2	-17.3	47.5	C56 H20 N	332.4	4.805	0.82	56	20	1	

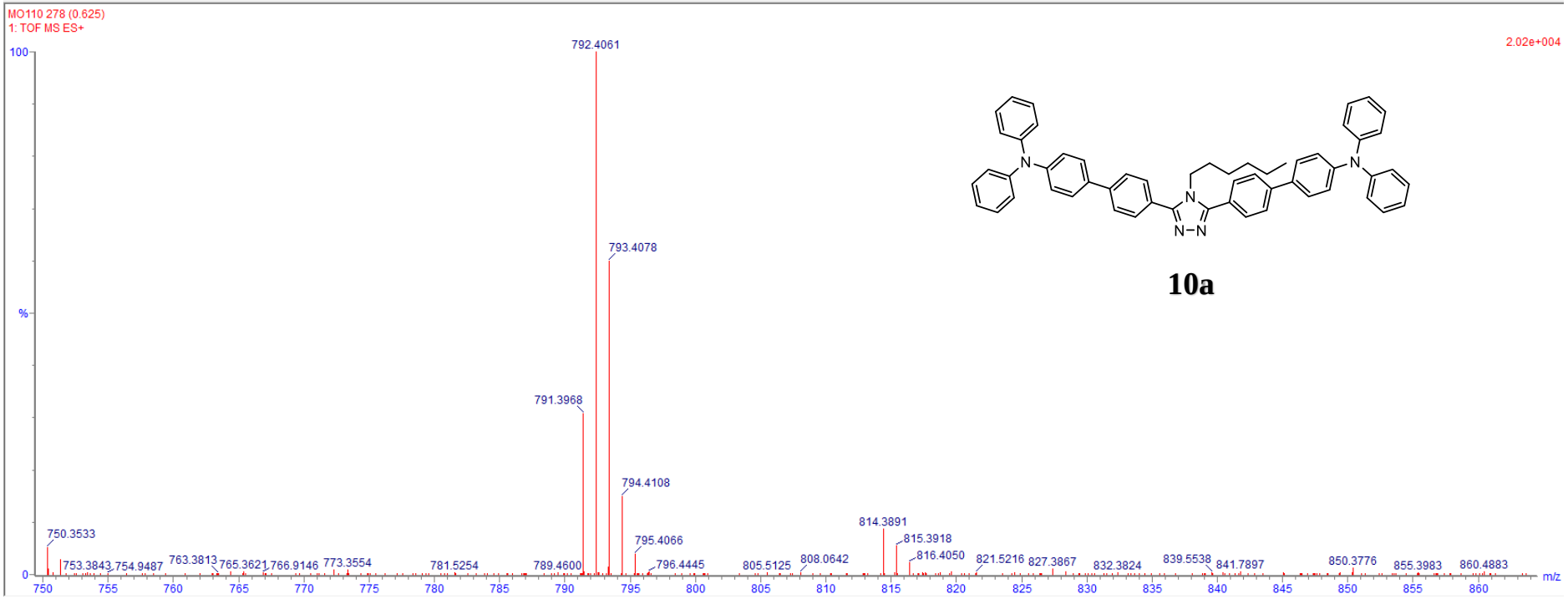


9k

4-Hexyl-3,5-bis[4'-(N,N-diphenylamino)biphenyl-4-yl]-4H-1,2,4-triazole (**10a**).

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 100.0 mDa / DBE: min = -10.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2
Monoisotopic Mass, Even Electron Ions
62 formula(e) evaluated with 11 results within limits (up to 5 closest results for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
792.4061	100.00	792.4066	-0.5	-0.6	34.5	C56 H50 N5	65.8	0.301	74.04	56	50	5
		792.4318	-25.7	-32.4	33.5	C58 H54 N3	67.3	1.835	15.96	58	54	3
		792.3630	43.1	54.4	39.5	C61 H46 N	69.1	3.570	2.82	61	46	1
		792.4569	-50.8	-64.1	32.5	C60 H58 N	68.7	3.252	3.87	60	58	1
		792.3379	68.2	86.1	40.5	C59 H42 N3	68.9	3.408	3.31	59	42	3
793.4078	60.02	793.4270	-19.2	-24.2	33.5	C57 H53 N4	53.2	0.996	36.92	57	53	4
		793.3834	24.4	30.8	38.5	C62 H49	53.5	1.320	26.71	62	49	
		793.4522	-44.4	-56.0	32.5	C59 H57 N2	54.0	1.768	17.07	59	57	2



10a

3. X-ray crystallography data

Crystal structure determination

X-ray intensity data of compounds **8a, 9a,** and **10a** were collected at 100.0(1) K, on a Rigaku Synergy Dualflex automatic diffractometer equipped with Pilatus 300K detector and micro-focus sealed PhotonJet X-ray tube. The mirror monochromated Cu$K\alpha$ (λ = 1.54184 Å) radiation and shutterless ω scan mode was used. Lorentz, polarization and numerical absorption (based on gaussian integration over a multifaceted crystal model) corrections were applied during the data reduction. The structure was solved by dual-space algorithm. All non-hydrogen atoms were refined anisotropically using full-matrix, least-squares technique on F^2. All hydrogen atoms were found from difference Fourier synthesis after ten cycles of anisotropic refinement. Hydrogen atoms were refined as "riding" on the adjacent atom with geometric idealization after each cycle of refinement. Individual isotropic displacement factors of non-methyl and methyl H atoms were set to be equal 1.2 and 1.5 times the value of equivalent displacement factors of the parent atoms, respectively. The SHELXT,[1] SHELXL[2] and SHELXTL[3] programs were used for all calculations. Atomic scattering factors were taken from International Tables for Crystallography.[4] Details concerning crystal data and refinement are given in Table S1.

The solvent molecules of **8a** and **9a** are disordered over three and two positions of asymmetric unit, respectively. The presence of one solvent atom in special position *d* of $P2_1/c$ space group (with site symmetry -1 and multiplicity 2) causes that one void containing a disordered solvent occupies two asymmetric units. Some atoms of three disordered ethanol molecules of **8a** occupy the same position of crystal net, causing formal presence of six atom sites in the refinement model (three sites contain atoms belonging to two molecules; Figure S5). The occupancy of individual molecules is 0.40, 0.25, 0.10, what totally gives 0.75 solvent molecule per **8a** molecule. The ethanol molecule in **9a** is simply disordered over two positions (with 0.5 participation of each domain) and form 1:1 solvate. Due to disorder and partial occupancy the positions of hydrogen atoms of solvent molecules could not be reliably determined thus these hydrogen atoms were not included into refinements. To asses influence of solvents electron density on results of refinement, structures of **8a** and **9a** were refined against squeezed data.[5] The convergence and fit parameters of squeezed and non- squeezed data (taken as measured) are similar (Table S1) what proves that solvent refinement models (including sites occupancy) were reasonable. The slightly larger values of difference Fourier synthesis global local peaks (smaller than 0.4 e•Å^{-3}) originate mainly from absence of solvents hydrogen atoms in refinement. Beside the solvent molecules, the part of alkyl substituents of compounds **9a** and **10a** are also disordered over two positions. In case of compound **9a** two terminal atoms are disordered with 0.6:0.4 participation of domains, while in compound **10a** five terminal atoms are disordered with 0.5:0.5 participation over domains.

CCDC 1999468-1999472 contain the supplementary crystallographic data for compounds **8a**, **9a**, and **10a**. These data can be obtained free of charge *via* http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk

(1) G.M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.* 2015, **71**, 3-8
(2) G.M. Sheldrick, *Acta Crystallogr., Sect. C: Struct. Chem.* 2015, **71**, 3-8
(3) G.M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.* 2008, **64**, 112-122
(4) *International Tables for Crystallography, Volume C: Mathematical, Physical and Chemical Tables,* ed. E. Prince, Kluwer Academic Publishers, Dordrecht, 3rd edition, 2004
(5) A. L. Spek, *Acta Crystallogr., Sect. E: Crystallogr. Commun.*, 2020, **76**, 1-11

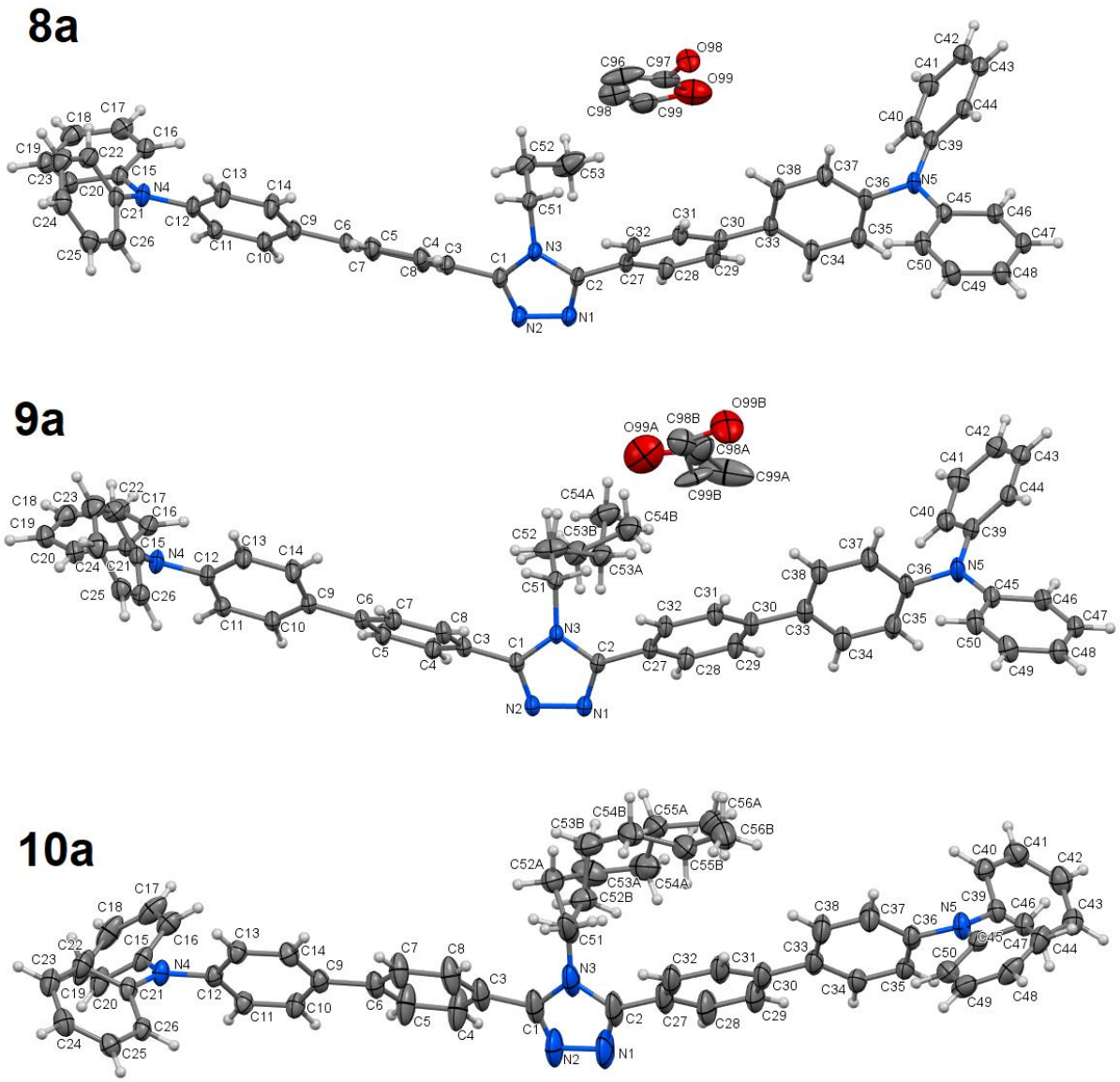


Figure S1. Complete asymmetric units of the structures of compounds **8a**, **9a**, and **10a**, with atom numbering scheme, plotted with 50% probability of displacement ellipsoids of non-hydrogen atoms. Hydrogen atoms are plotted as spheres of arbitrary radii.

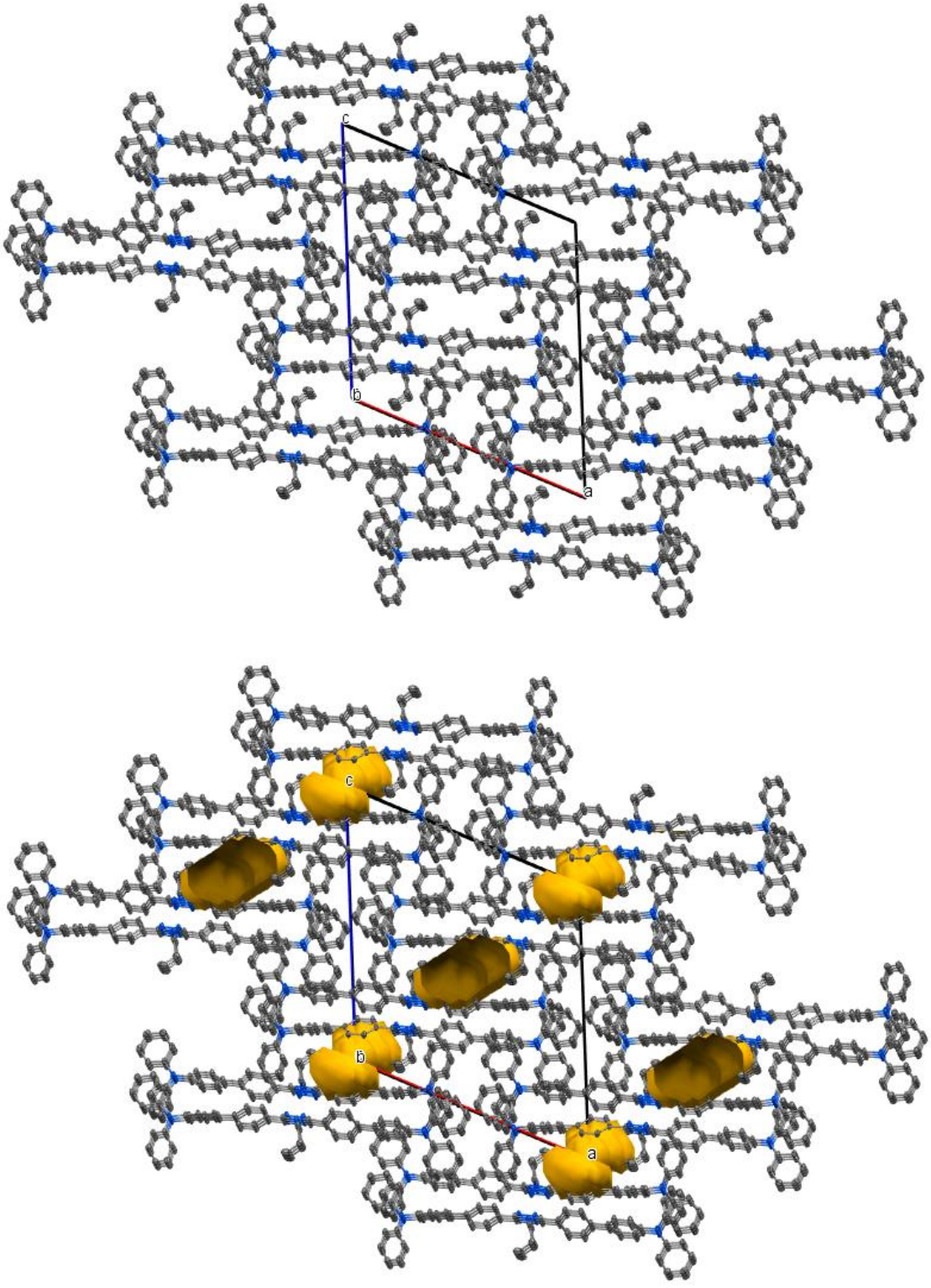


Figure S2. Solvent accessible voids within crystal structure of **8a**

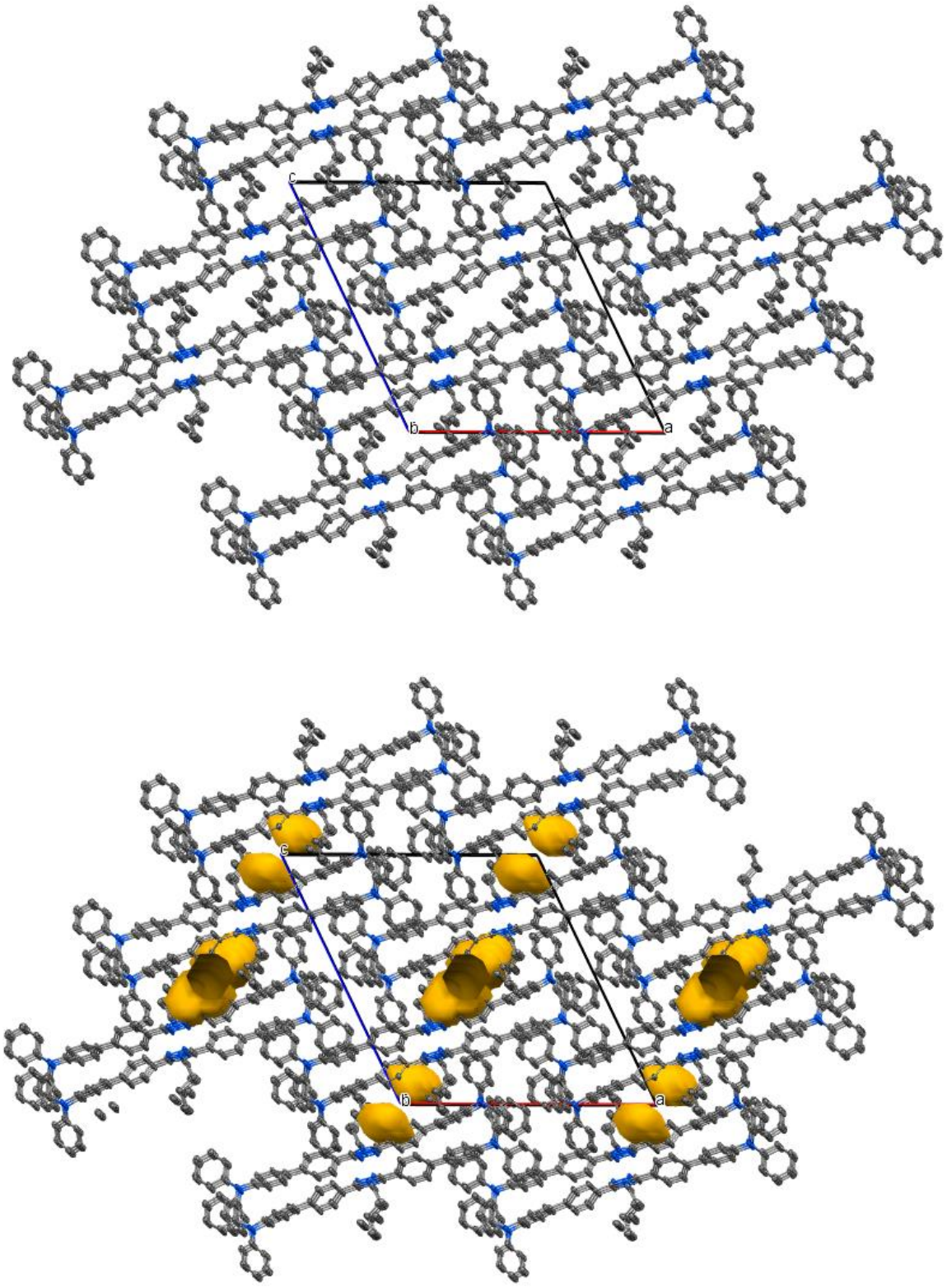


Figure S3. Solvent accessible voids within crystal structure of **9a**

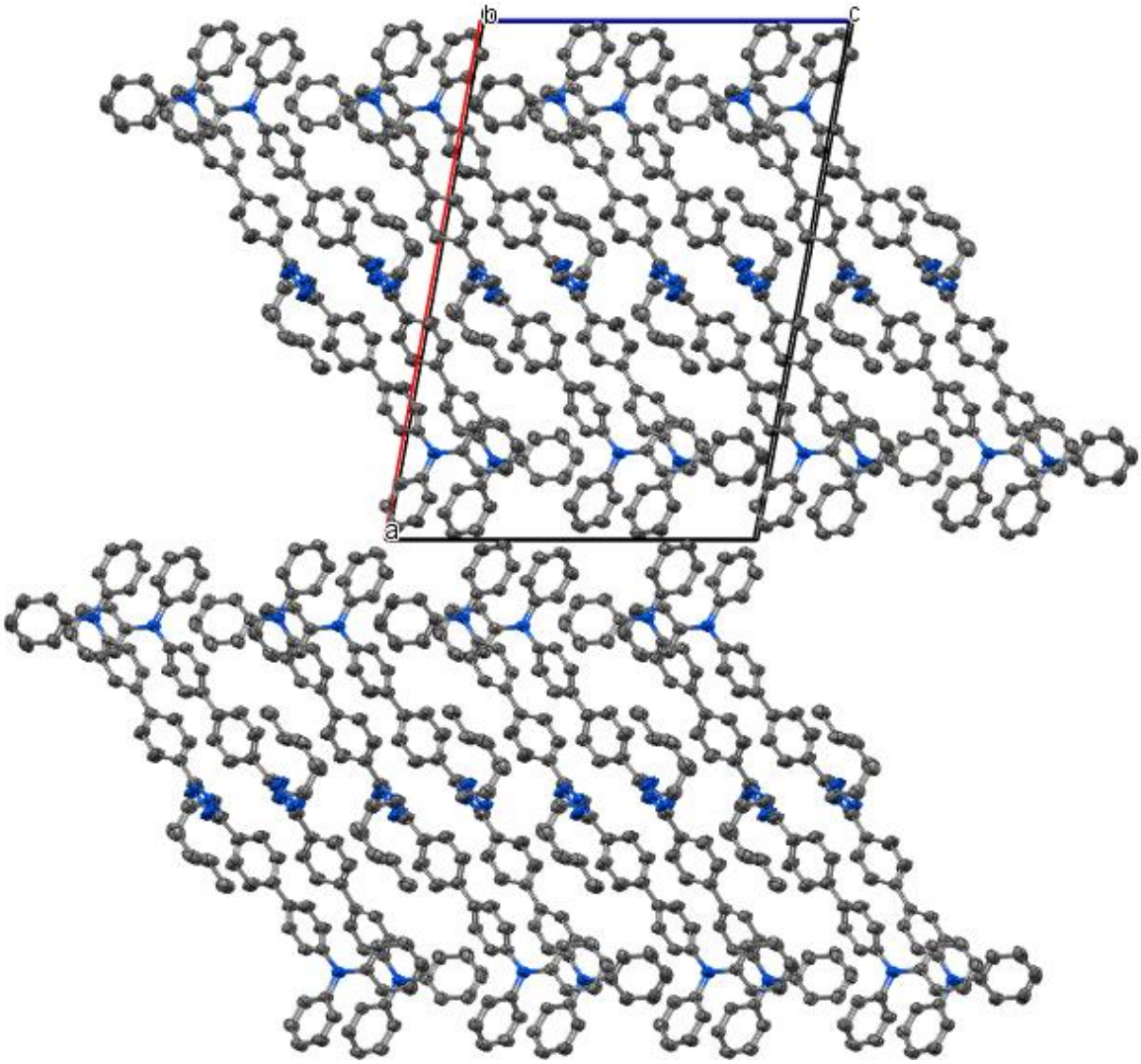


Figure S4. The part of crystal packing in **10a**

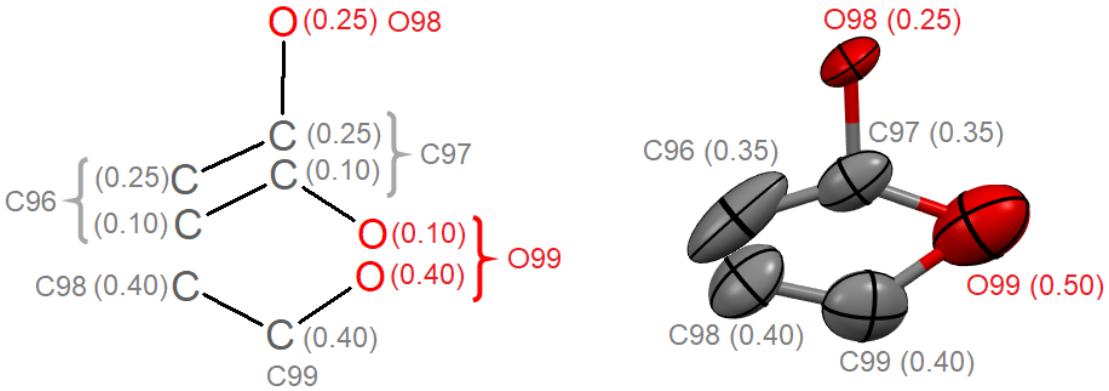


Figure S5. Disorder model of solvent in **8a.**

Table S1. Crystal data and structure refinement details for **8a**, **9a**, and **10a**. The structures of **8a** and **9a** were refined twice: against measured and squeezed data.

Compound	**8a**		**9a**		**10a**
Refinement data	as measured	squeezed	as measured	squeezed	as measured
CCDC number	1999469	1999471	1999470	1999472	1999468
Empirical formula	$C_{54.5}H_{43}N_5O_{0.75}$	$C_{53}H_{43}N_5$	$C_{56}H_{45}N_5O$	$C_{54}H_{45}N_5$	$C_{56}H_{49}N_5$
Formula weight	779.94	749.92	803.97	763.95	792.00
Crystal system	Monoclinic		Monoclinic		Monoclinic
Space group	$P2_1/n$ (No. 14)		$P2_1/n$ (No. 14)		$P2_1/c$ (No. 14)
Temperature (K)	100.0(1)		100.0(1)		100.0(1)
Wavelength (Å)	λ(Cu$K\alpha$) 1.54184		λ(Cu$K\alpha$) 1.54184		λ(Cu$K\alpha$) 1.54184
Unit cell dimensions					
a (Å)	21.1286(2)		21.1879(2)		26.7716(3)
b (Å)	9.6119(1)		9.7481(1)		8.6434(1)
c (Å)	23.0090(2)		22.9643(2)		18.7186(2)
α (°)	90		90		90
β (°)	115.057(1)		115.7160(1)		100.406(1)
γ (°)	90		90		90
Volume (Å^3)	4233.03(8)		4273.31(8)		4260.20(8)
Z	4		4		4
Calculated density (Mg/m^3)	1.224	1.177	1.250	1.187	1.235
Absorption coefficient (mm^{-1})	0.569	0.535	0.583	0.538	0.557
F(000)	1644	1584	1696	1616	1680
Crystal size (mm)	0.226 x 0.173 x 0.082		0.102 x 0.072 x 0.043		0.152 x 0.131 x 0.020
θ Range for data collection (°)	3.739 to 78.853		3.771 to 79.032		4.794 to 79.073
Index ranges	$-26 \le h \le 26$, $-12 \le k \le 10$, $-29 \le l \le 27$		$-13 \le h \le 26$, $-12 \le k \le 11$, $-28 \le l \le 23$		$-34 \le h \le 32$, $-10 \le k \le 8$, $-23 \le l \le 21$
Reflections collected / unique	70333 / 8633		44845 / 8827		44854 / 8789
R_{int}	0.0329	0.0330	0.0294	0.0297	0.0484
Completeness (%) θ = 67°	100.0		100.0		100.0
Min. and max. transmission	0.634 and 1.000		0.915 and 1.000		0.852 and 1.000
Data / restraints / parameters	8633 / 0 / 576	8633 / 0 / 525	8827 / 0 / 604	8827 / 0 / 553	8789 / 0 / 598
Goodness-of-fit on F^2	1.073	1.075	1.057	1.111	1.016
Final *R* indices [$I>2\sigma(I)$]	$R1$ = 0.0483, $wR2$ = 0.1504	$R1$ = 0.0423, $wR2$ = 0.1174	$R1$ = 0.0477, $wR2$ = 0.1303	$R1$ = 0.0434, $wR2$ = 0.1175	$R1$ = 0.0560, $wR2$ = 0.1372
R indices (all data)	$R1$ = 0.0525, $wR2$ = 0.1553	$R1$ = 0.0462, $wR2$ = 0.1196	$R1$ = 0.0574, $wR2$ = 0.1481	$R1$ = 0.0517, $wR2$ = 0.1339	$R1$ = 0.0716, $wR2$ = 0.1479
Largest diff. peak and hole (e•Å^{-3})	0.685 and -0.230	0.315 and -0.223	0.449 and -0.268	0.261 and -0.255	0.359 and -0.252

Table S2. Selected structural data of **8a**, **9a**, and **10a**.

i—j	d_{ij} (Å)		
	8a	**9a**	**10a**
N1—N2	1.3893(16)	1.3932(17)	1.385(2)
N1—C2	1.3132(19)	1.314(2)	1.311(4)
N2—C1	1.311(2)	1.316(2)	1.317(4)
N3—C1	1.3701(18)	1.3731(19)	1.376(3)
N3—C2	1.3699(17)	1.3725(19)	1.382(3)
N3—C51	1.4740(18)	1.470(2)	1.455(4)
C1—C3	1.4801(18)	1.474(2)	1.473(3)
C2—C27	1.4752(18)	1.472(2)	1.477(3)
N4—C12	1.4156(17)	1.4169(19)	1.4222(19)
N4—C15	1.416(2)	1.412(2)	1.421(2)
N4—C21	1.420(2)	1.425(2)	1.412(2)
N5—C36	1.4360(17)	1.433(2)	1.432(2)
N5—C39	1.416(2)	1.412(2)	1.430(2)
N5—C45	1.4102(19)	1.408(2)	1.416(2)
i—j—k	α_{ijk} (°)		
	8a	**9a**	**10a**
N1—C2—N3	110.63(12)	110.56(13)	110.96(18)
C2—N1—N2	107.22(11)	107.34(13)	107.2(2)
N1—N2—C1	107.07(12)	106.99(13)	107.5(2)
N2—C1—N3	110.84(12)	110.69(13)	110.63(19)
C1—N3—C2	104.24(12)	104.41(13)	103.7(2)
C1—N3—C51	125.98(11)	126.08(12)	127.44(19)
C2—N3—C51	127.65(12)	127.52(12)	127.04(19)
N2—C1—C3	124.63(13)	124.76(14)	121.6(2)
N3—C1—C3	124.49(13)	124.51(14)	127.8(3)
N1—C2—C27	123.91(12)	124.04(14)	122.8(2)
N3—C2—C27	125.46(13)	125.39(14)	126.3(3)
C12—N4—C15	121.25(13)	121.35(14)	118.13(14)
C12—N4—C21	119.19(12)	118.77(13)	119.29(13)
C15—N4—C21	119.02(11)	119.28(13)	122.12(13)
C36—N5—C39	116.77(12)	116.59(14)	115.53(14)
C36—N5—C45	119.22(12)	119.36(14)	120.45(14)
C39—N5—C45	123.44(12)	123.87(13)	122.10(13)

Table S3. Dihedral angles (°) between ring least squares planes in **8a**, **9a**, and **10a**. Each ring is indicated by one atom, which belongs solely to this ring.

8a

	N1	C3	C9	C15	C21	C27	C33	C39
N1								
C3	54.83(5)							
C9	31.83(5)	23.01(8)						
C15	88.73(6)	40.45(6)	61.11(6)					
C21	84.44(6)	59.81(6)	74.27(6)	65.52(5)				
C27	42.78(5)	25.79(7)	20.77(8)	49.57(6)	85.55(5)			
C33	11.73(5)	47.94(5)	25.62(5)	81.28(6)	83.12(5)	31.95(6)		
C39	77.76(6)	71.15(5)	83.41(5)	38.51(5)	78.79(4)	63.67(5)	89.43(5)	
C45	81.09(6)	44.14(5)	67.09(6)	18.06(3)	48.78(6)	61.46(5)	89.02(6)	52.80(5)

9a

	N1	C3	C9	C15	C21	C27	C33	C39
N1								
C3	54.70(6)							
C9	29.44(5)	25.34(8)						
C15	88.84(7)	40.28(6)	62.83(7)					
C21	85.80(6)	60.01(6)	75.98(6)	66.52(6)				
C27	45.01(6)	26.30(8)	23.19(8)	47.79(7)	86.30(5)			
C33	17.11(5)	43.74(6)	19.91(6)	75.89(7)	85.08(6)	28.51(7)		
C39	74.57(6)	73.95(5)	87.22(6)	40.60(6)	76.67(5)	64.41(6)	88.68(6)	
C45	81.02(7)	44.36(6)	69.54(7)	17.31(3)	50.87(7)	60.15(6)	86.18(7)	53.10(5)

10a

	N1	C3	C9	C15	C21	C27	C33	C39
N1								
C3	36.3(1)							
C9	24.8(1)	12.3(1)						
C15	85.21(8)	63.32(7)	71.51(5)					
C21	84.22(7)	65.48(7)	77.22(5)	61.31(5)				
C27	40.8(1)	12.0(1)	16.7(1)	54.83(6)	70.26(6)			
C33	23.4(1)	17.7(1)	6.7(1)	71.47(6)	83.14(5)	17.8(1)		
C39	85.51(7)	67.75(7)	79.18(5)	65.62(5)	4.4(1)	73.23(6)	85.31(5)	
C45	88.76(8)	57.73(7)	67.03(5)	8.38(8)	54.06(5)	50.50(6)	67.90(6)	58.43(6)

Table S4. Non-classic hydrogen bonds and the first level graph motifs in the studied compounds (Å, °).

D-H•••A	d(D-H)	d(H•••A)	d(D•••A)	<(DHA)	$G_d^a(n)$
		8a			
C8—H8•••N1^{i}	0.95	2.59	3.492(2)	158	C(6)
C32—H32•••N2^{i}	0.95	2.76	3.702(2)	174	C(6)
C41—H41•••N2^{ii}	0.95	2.79	3.481(2)	130	C(16)
C51—H51B•••N1^{i}	0.99	2.80	3.575(2)	136	C(5)
		9a			
C8—H8•••N1^{i}	0.95	2.68	3.573(2)	157	C(6)
C32—H32•••N2^{i}	0.95	2.69	3.640(2)	175	C(6)
C41—H41•••N2^{ii}	0.95	2.90	3.572(2)	129	C(16)
C51—H51B•••N1^{i}	0.99	2.81	3.529(2)	130	C(5)
		10a			
C32—H32•••N1^{iii}	0.95	2.55	3.470(2)	164	C(5)
C32—H32•••N2^{iii}	0.95	2.43	3.163(2)	134	C(6)

Symmetry transformations used to generate equivalent atoms: (i) -x+1.5, y-0.5, -z+1.5; (ii) -x+1, -y+1, -z+1; (iii) -x+1, y+0.5, -z+1.5.

Table S5. Stacking interactions in the studied compounds. Each ring is indicated by one atom, which belongs solely to this ring. The α is a dihedral angle between planes I and J, β is an angle between Cg(I)-Cg(J) vector and normal to plane I, d_p is a perpendicular distance of Cg(I) on ring J plane.

R(I)•••R(J)	d(Cg•••Cg) (Å)	α (°)	β (°)	d_p (Å)
		8a		
C15•••C45^{i}	4.8776(10)	5.60(8)	45.6	3.1070(7)
C45•••C15^{ii}	4.8776(10)	5.60(8)	50.4	3.4134(7)
C21•••C21^{iii}	5.7439(11)	0.02(9)	56.6	3.1589(7)
C45•••C45^{iv}	4.7511(10)	0.00(8)	45.9	3.3089(7)
		9a		
C15•••C45^{i}	4.9048(11)	6.31(9)	44.4	3.1458(8)
C45•••C15^{ii}	4.9050(11)	6.31(9)	50.1	3.5026(8)
C21•••C21^{iii}	5.7876(12)	0.00(10)	55.9	3.2444(8)
C45•••C45^{iv}	4.8010(11)	0.02(9)	45.0	3.3964(8)
		10a		
N1•••N1^{v}	5.4759(13)	0.00(13)	42.9	4.0097(9)
C21•••C39^{vi}	5.3990(10)	4.41(9)	47.0	3.9724(7)
C39•••C21^{vii}	5.3991(10)	4.41(9)	42.6	3.6798(8)

Symmetry transformations used to generate equivalent atoms: (i) -x+1.5, y+0.5, -z+1.5; (ii) -x+1.5, y-0.5, -z+1.5; (iii) -x+3, -y, -z+2; (iv) -x, -y, -z+1; (v) -x+1, -y+1, -z+1; (vi) x-1, y, z-1; (vii) x+1, y, z+1.

4. Absorption and emission spectrometry data

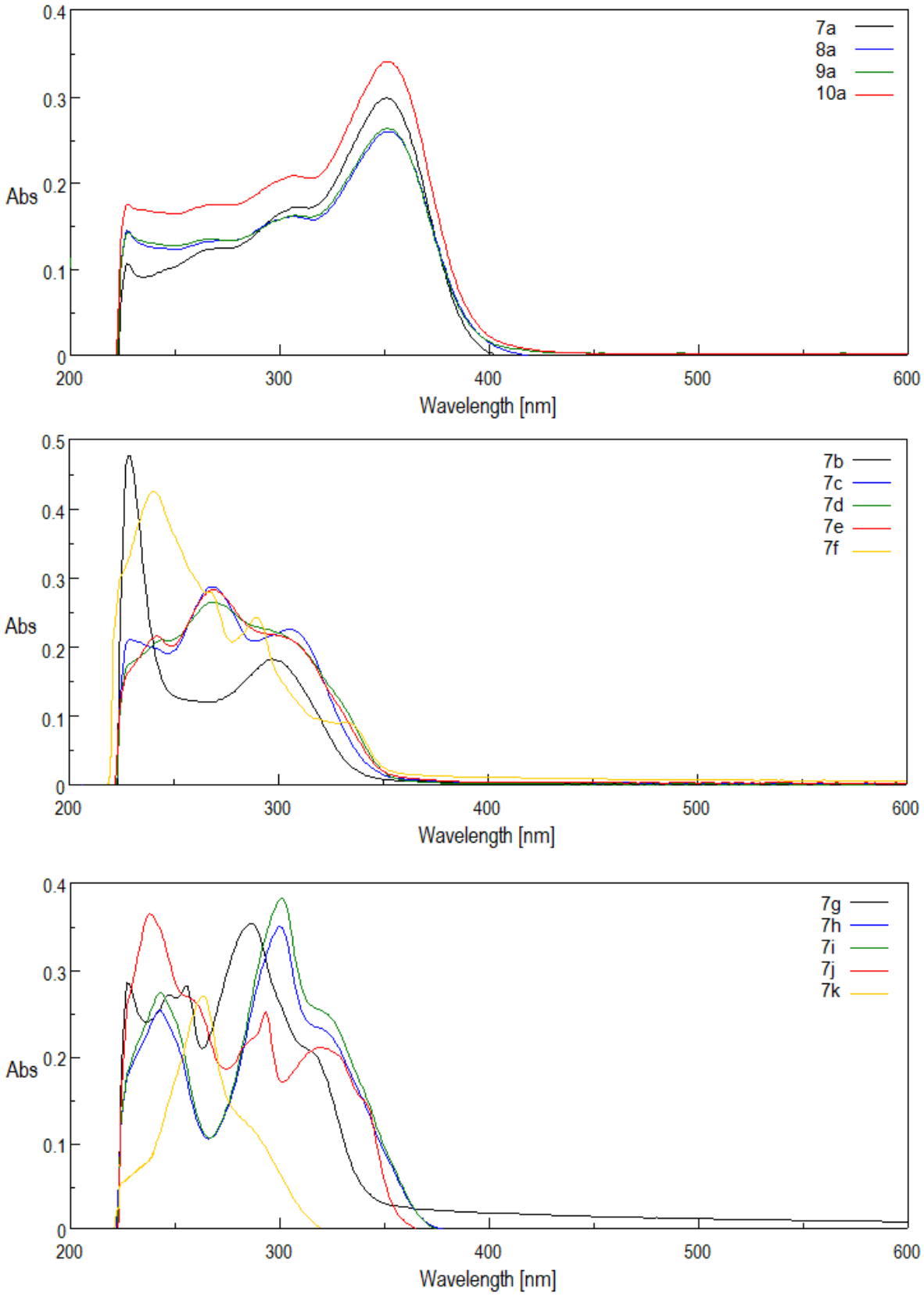


Figure S6. UV-Vis spectra of **7a-10a** and **7b-7k**.

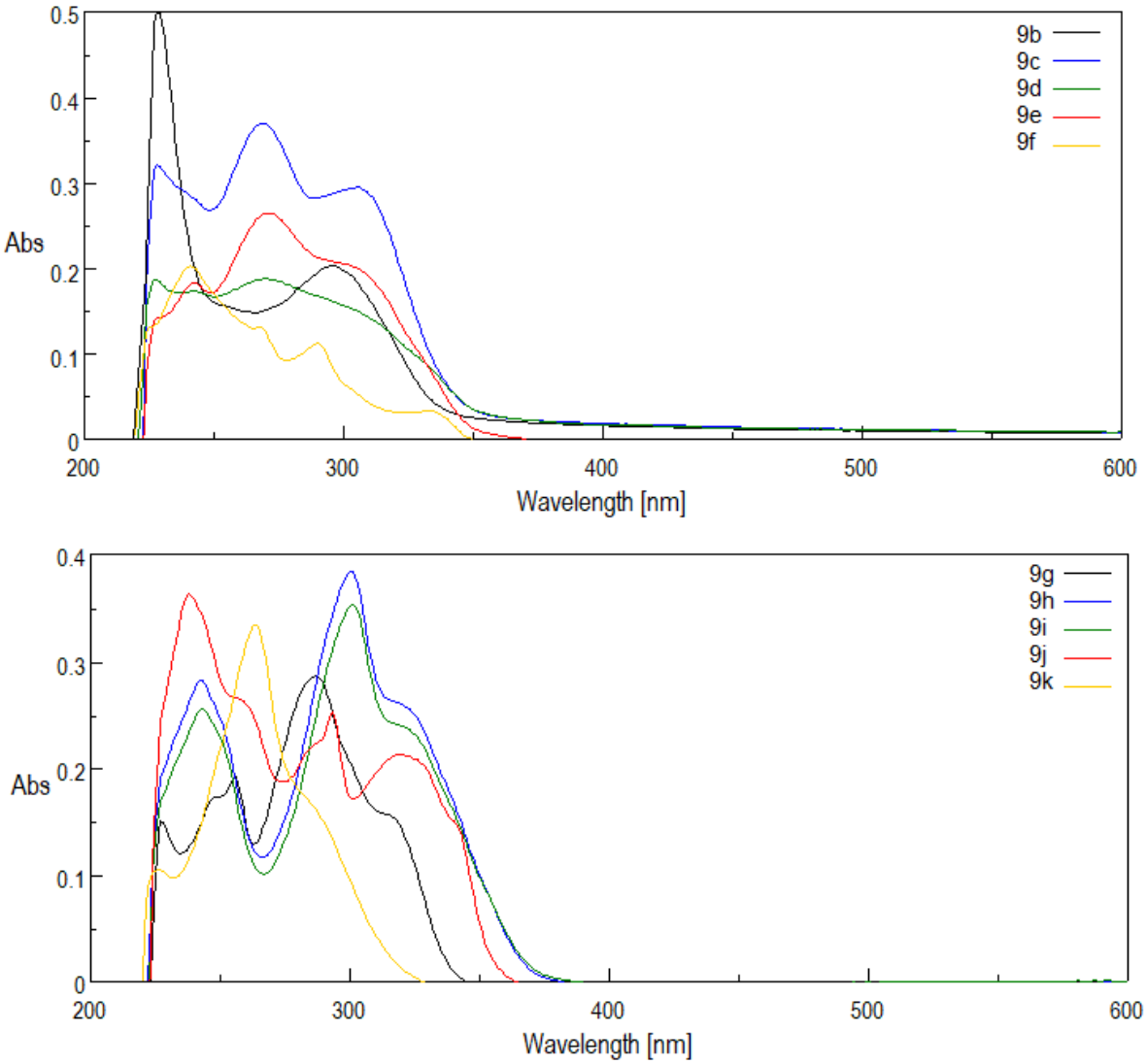


Figure S7. UV-Vis spectra of **9b-9k**.

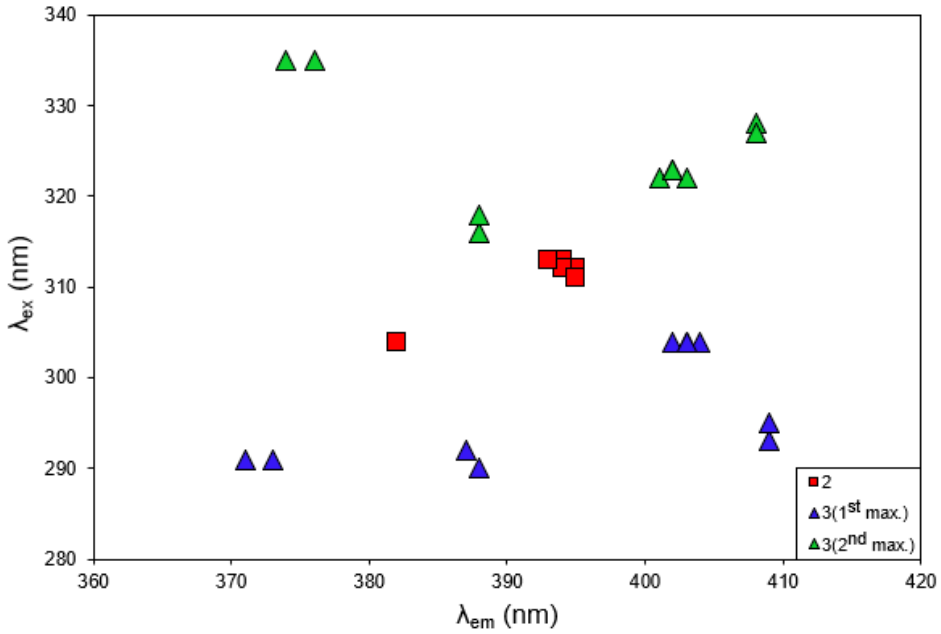


Figure S8. Positions of global maxima for studied compounds (divided into groups containing 2 or 3 rings at the ends of 4-alkyl-3,5-bis(phenyl)-4*H*-1,2,4-triazole core). "1st max." and "2nd max." indicate the first (for smaller excitation wavelengths) and the second (for larger excitation wavelengths) maxima on three-dimensional fluorescence spectra.

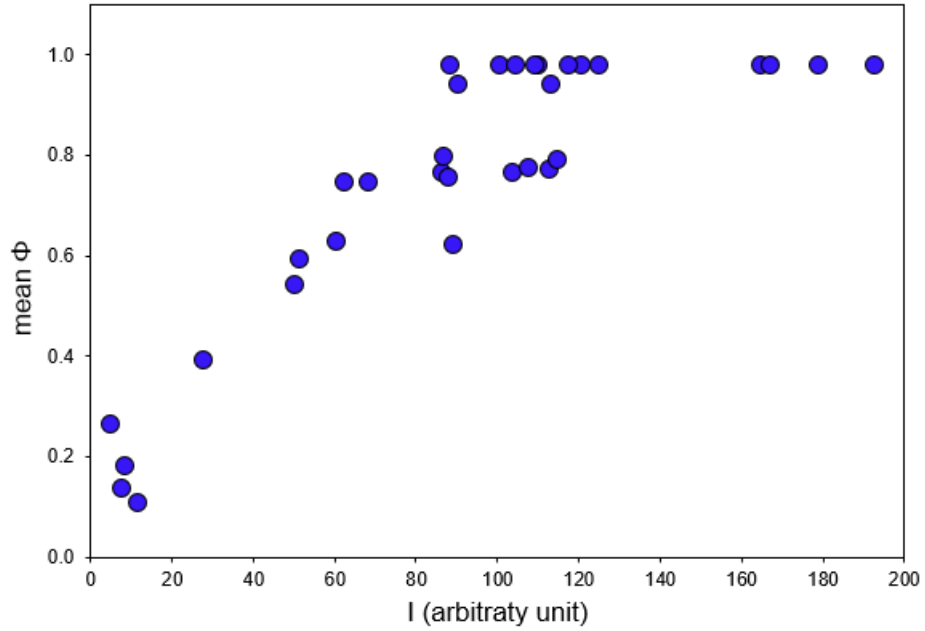


Figure S9. Quantum yield of studied compounds as a function of fluorescence intensity at global and local maximum.

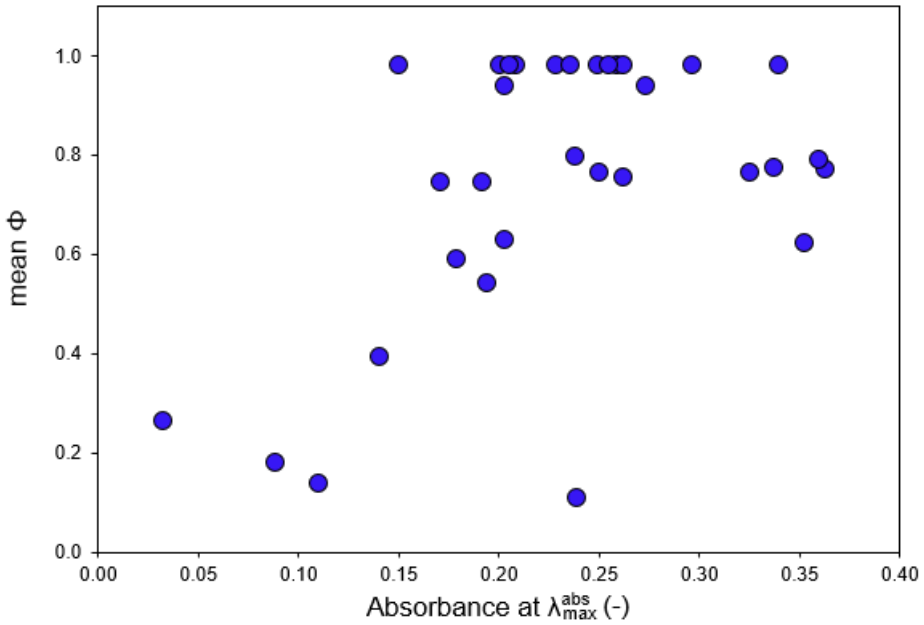


Figure S10. Quantum yield of studied compounds in relation to absorption at global and local maximum of fluorescence.