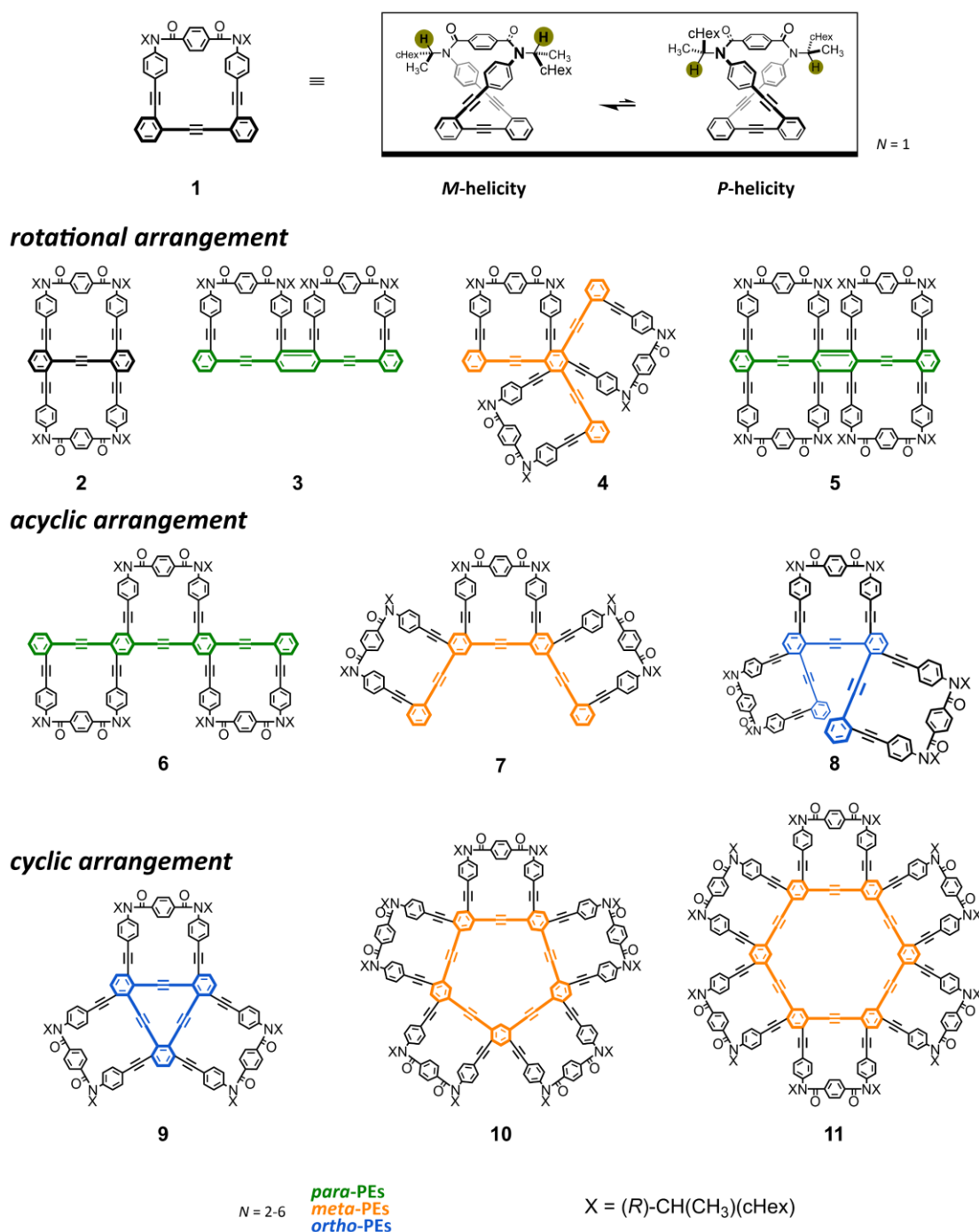


Electronic Supplementary Information_2

Consideration of optical rotation based on the molecular structure in fused oligomers of macrocycles

Ryo Katoono*, Yudai Obara, Kazuki Sakamoto and Rei Miyashita
Department of Chemistry, Faculty of Science, Hokkaido University

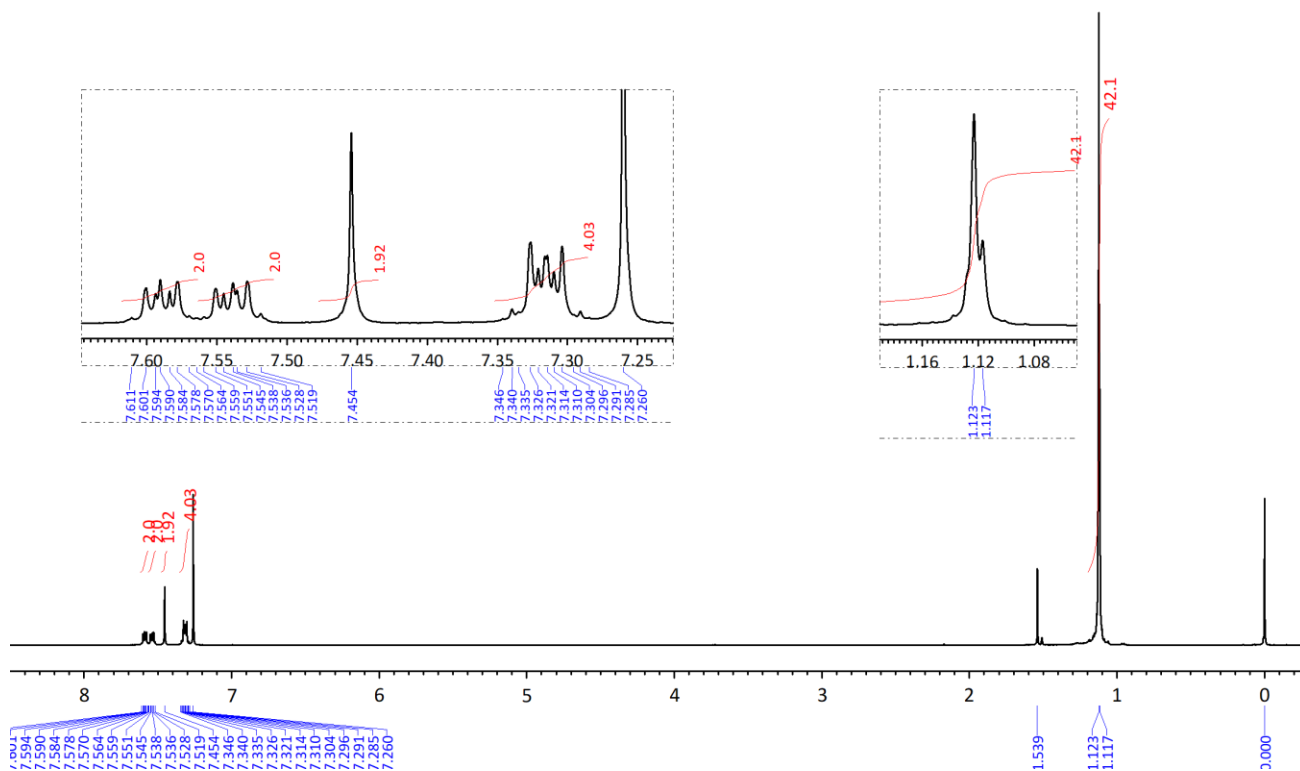


Contents (ESI_1)

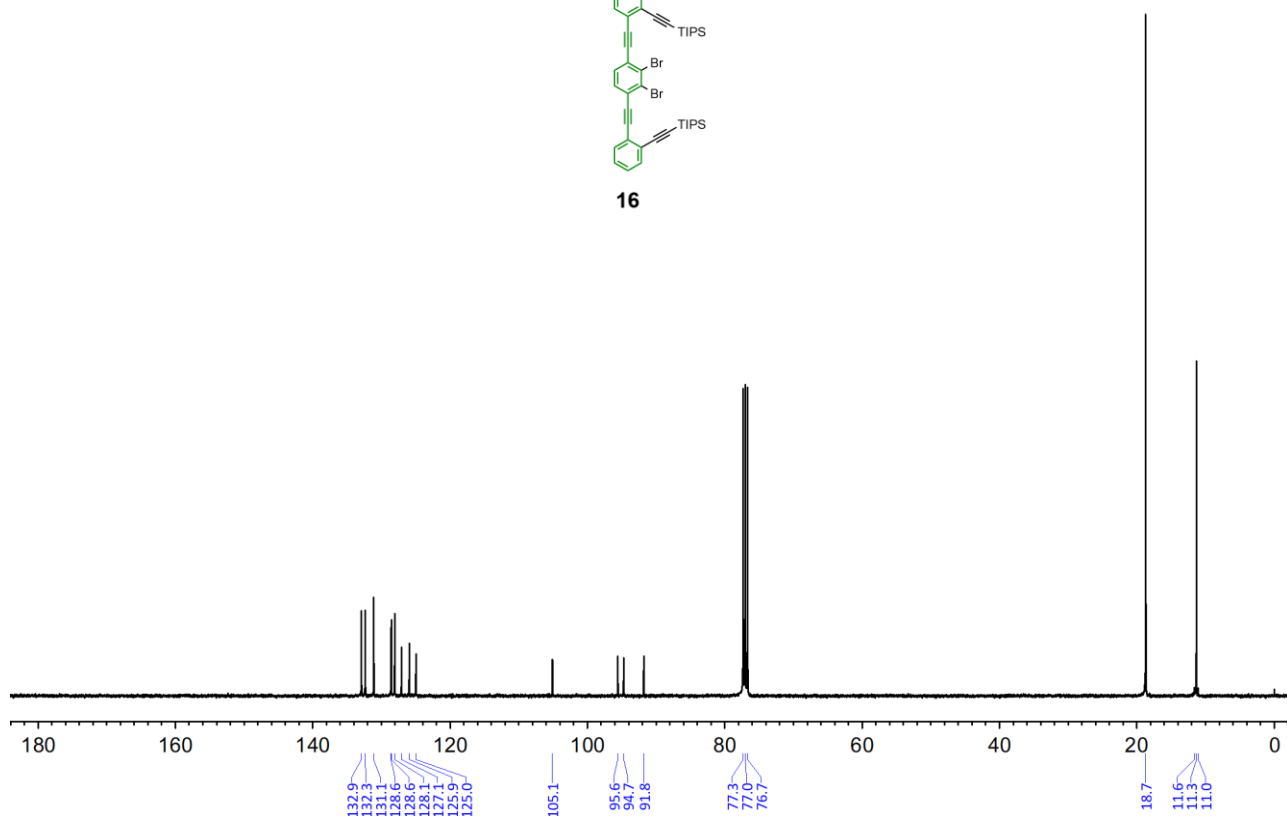
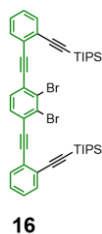
<u>Supplementary Figures (Figures S1-S27)</u>	page
Conformational searches using MacroModel software.	S3-S9
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Quantitative estimation of the diastereomeric ratio induced in 1, 2, 4, and 5 .	S17-S22
VT-CD spectra of 3, 6, 7, 8, and 9 .	S23-S24
UV spectra of 1-11 .	S25
Complexation experiment [X = butyl] with a chiral guest (14).	S26-S35
UV and CD spectra of 3, 6, 7, 8, and 9 in the presence of an achiral guest (13).	S36-S37
Plots of $\Delta\epsilon/\epsilon$ for 3, 6, 7, 8, and 9 before and after complexation (13).	S38
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Copies of ¹H/¹³C NMR spectra and LRMS of new compounds



¹H NMR spectrum (400 MHz) of **16**, measured in CDCl₃ at room temperature.

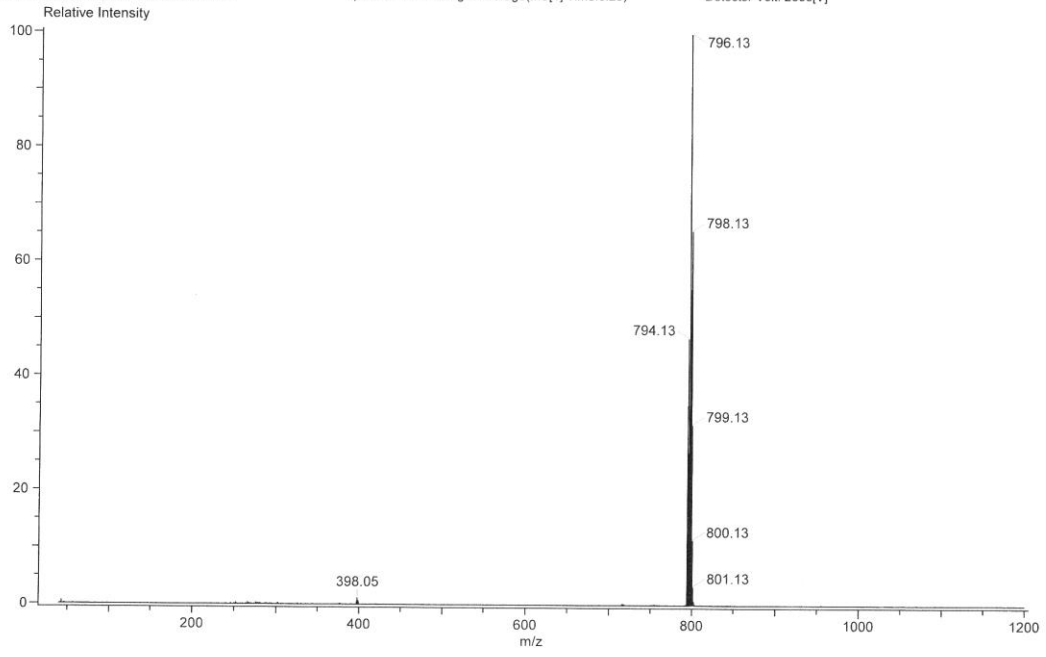


¹³C NMR spectrum (100 MHz) of **16**, measured in CDCl₃ at room temperature.

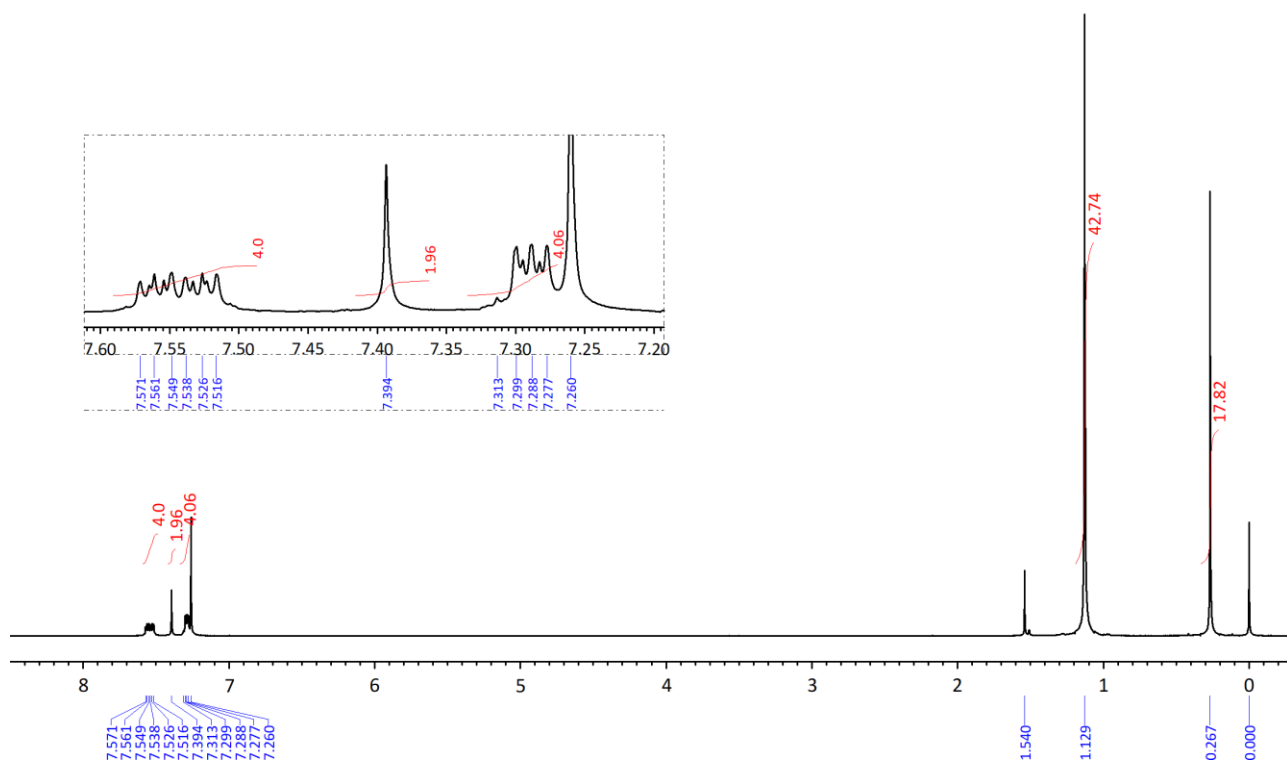
Data Name: common/Nov20/a51304-
Sample: u1 katoono / 16o339
Experiment Date/Time: 2023/11/20 10:08:20

Instrument: JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..3200
Spectrum Time Range: Average(MS[1] Time:0.25)

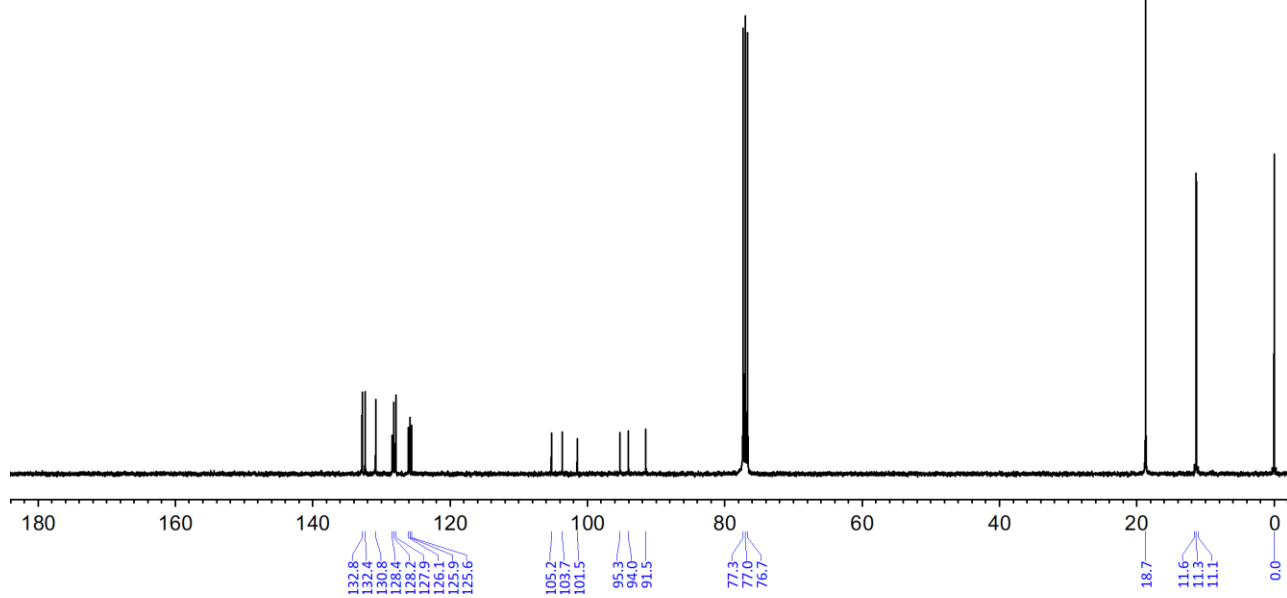
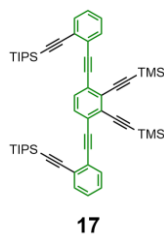
MS Tune Method Name: FD
GC: Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of 16.



¹H NMR spectrum (400 MHz) of **17**, measured in CDCl₃ at room temperature.

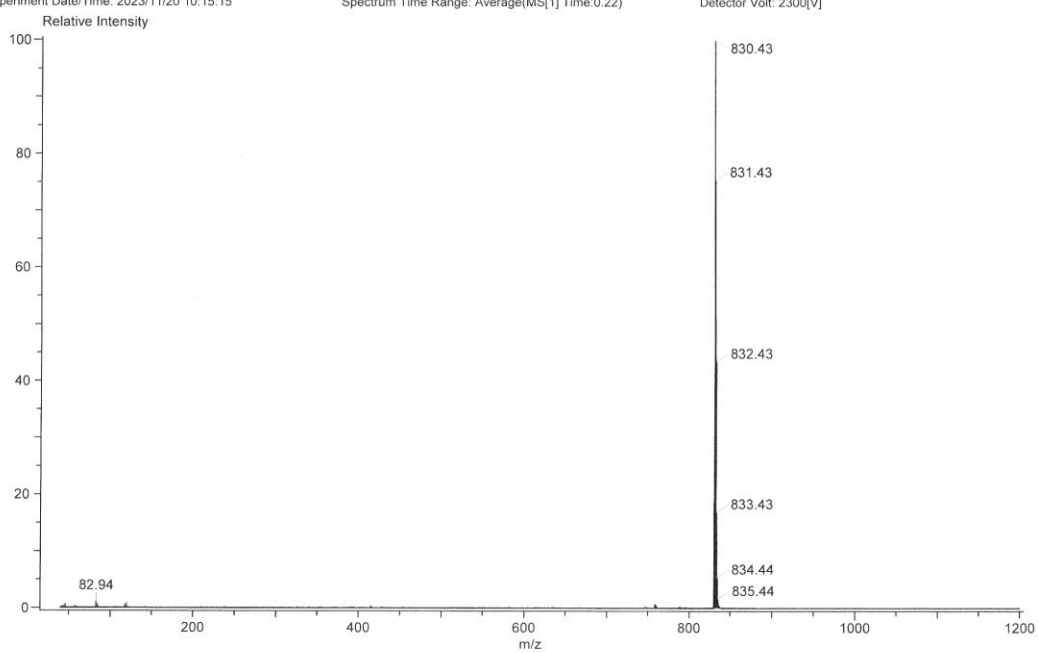


¹³C NMR spectrum (100 MHz) of **17**, measured in CDCl₃ at room temperature.

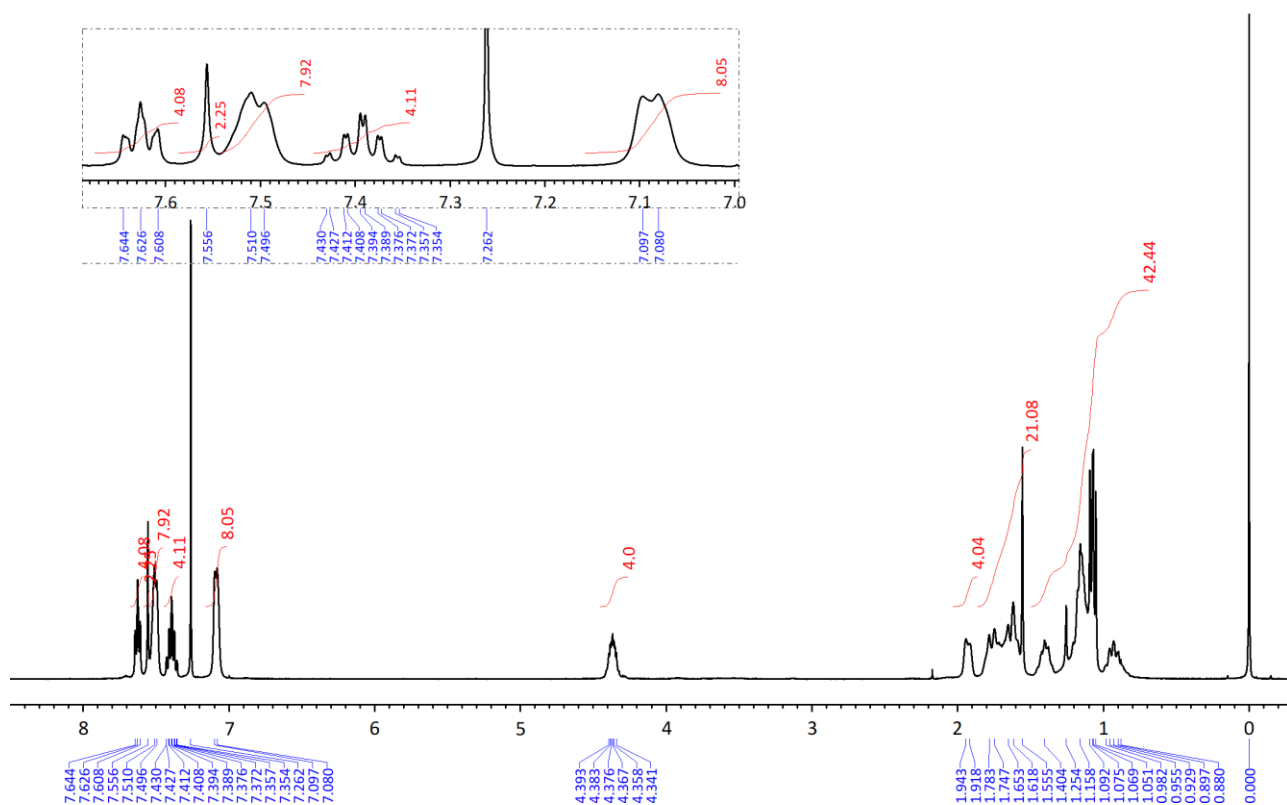
Data Name: common/Nov20/a51305-
Sample: u1 katoono / 17o398
Experiment Date/Time: 2023/11/20 10:15:15

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40.3200
Spectrum Time Range: Average(MS[1] Time:0.22)

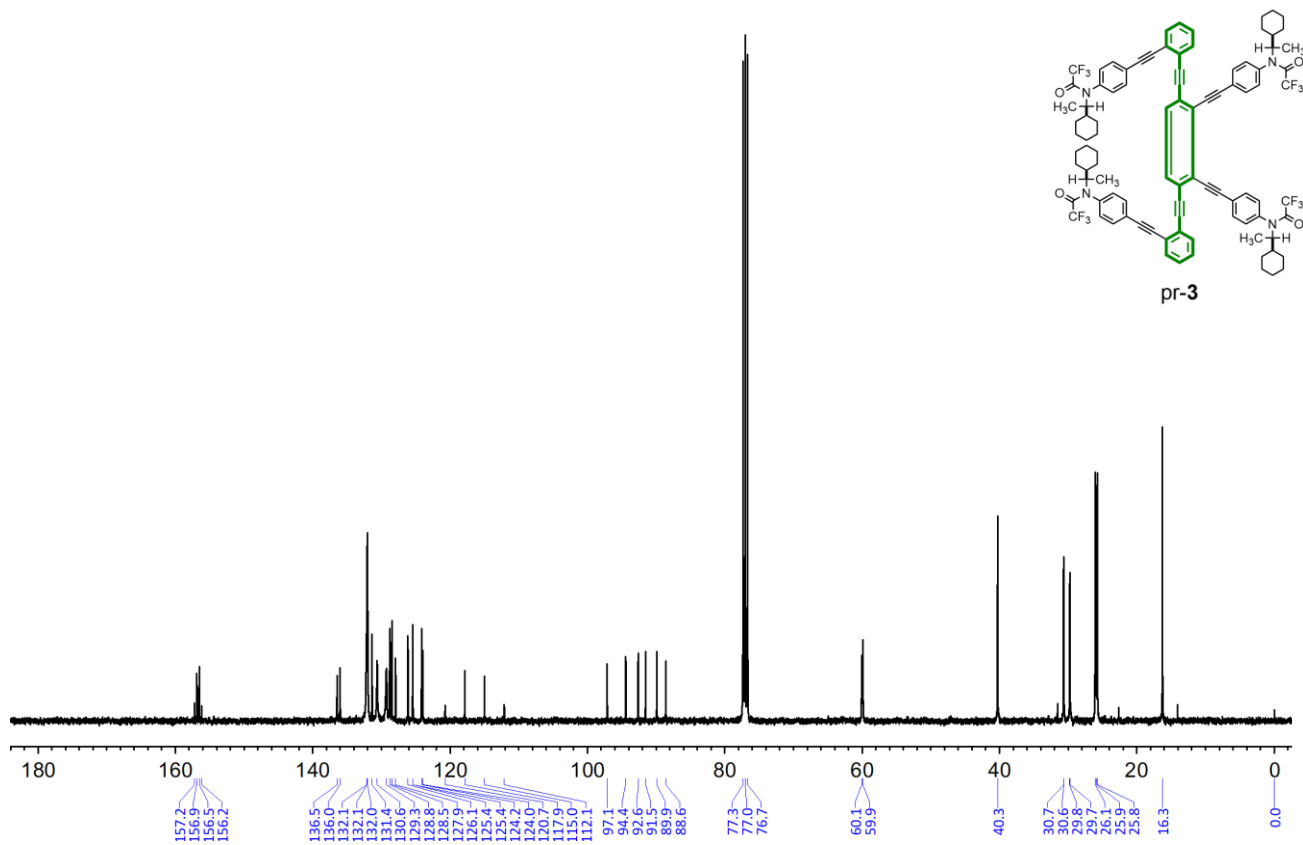
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of 17.



¹H NMR spectrum (400 MHz) of pr-3, measured in CDCl₃ at room temperature.

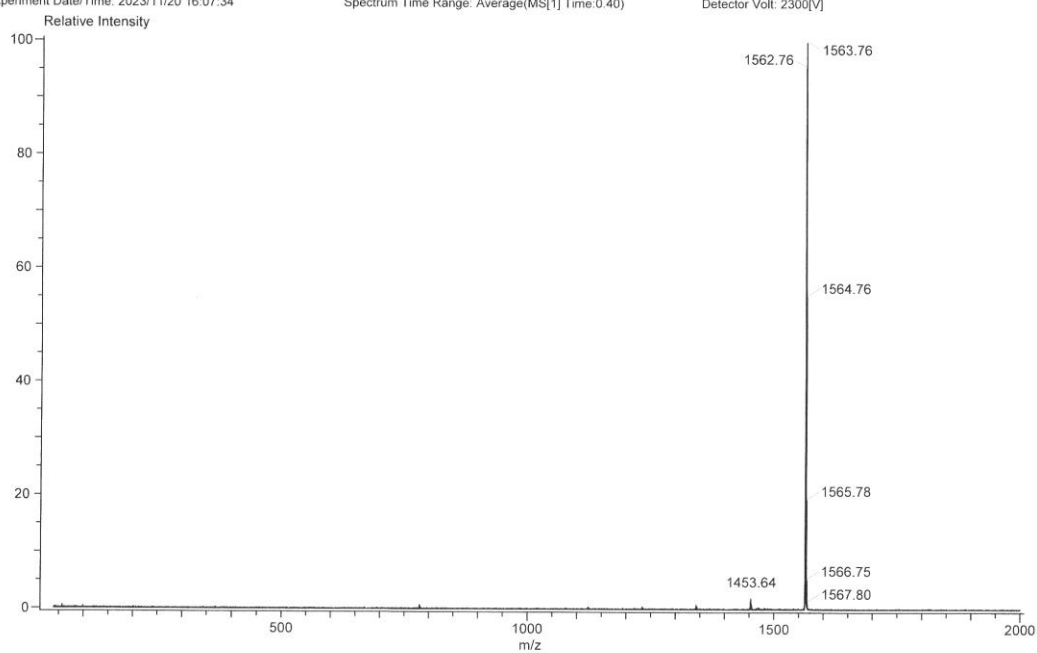


¹³C NMR spectrum (100 MHz) of pr-3, measured in CDCl₃ at room temperature.

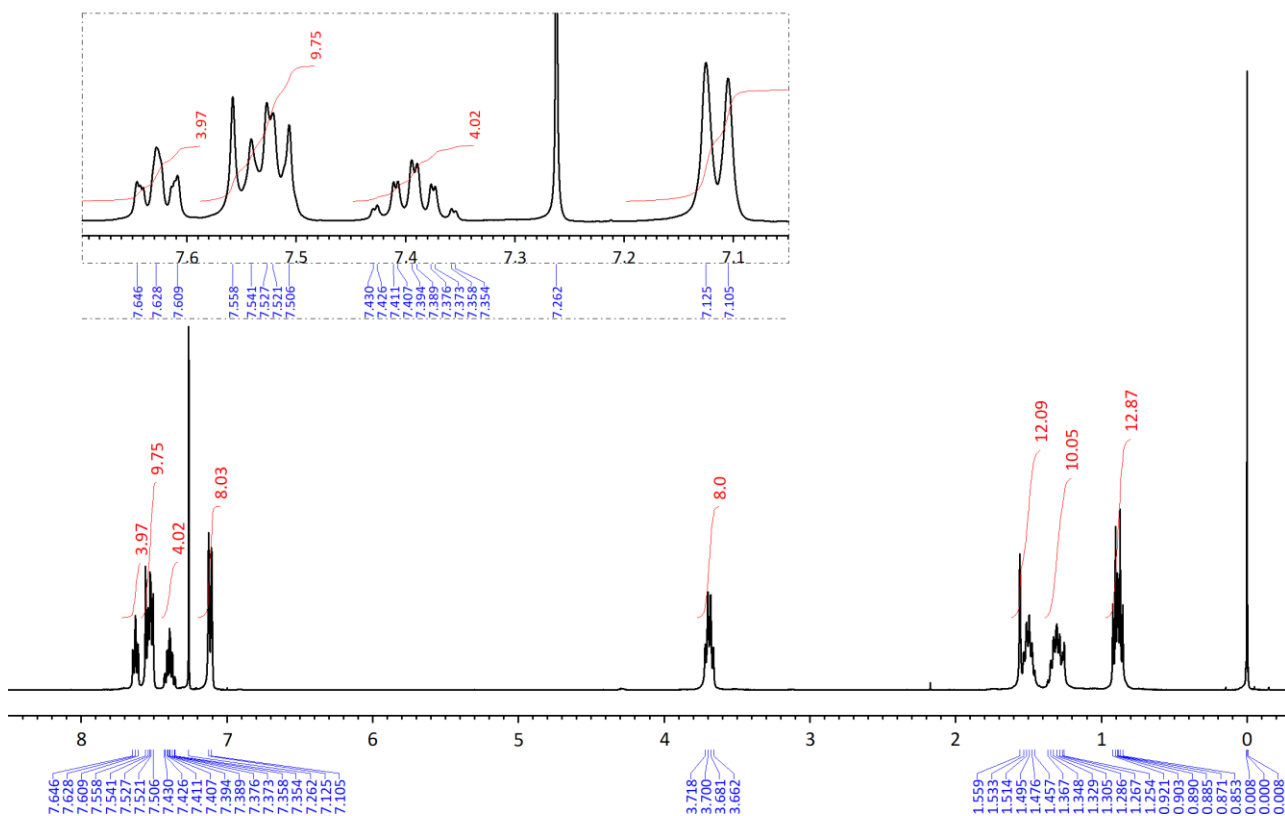
Data Name: common/Nov20 a51297-
Sample: u1 katoono / pr3o318
Experiment Date/Time: 2023/11/20 16:07:34

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40. 3200
Spectrum Time Range: Average(MS[1] Time:0.40)

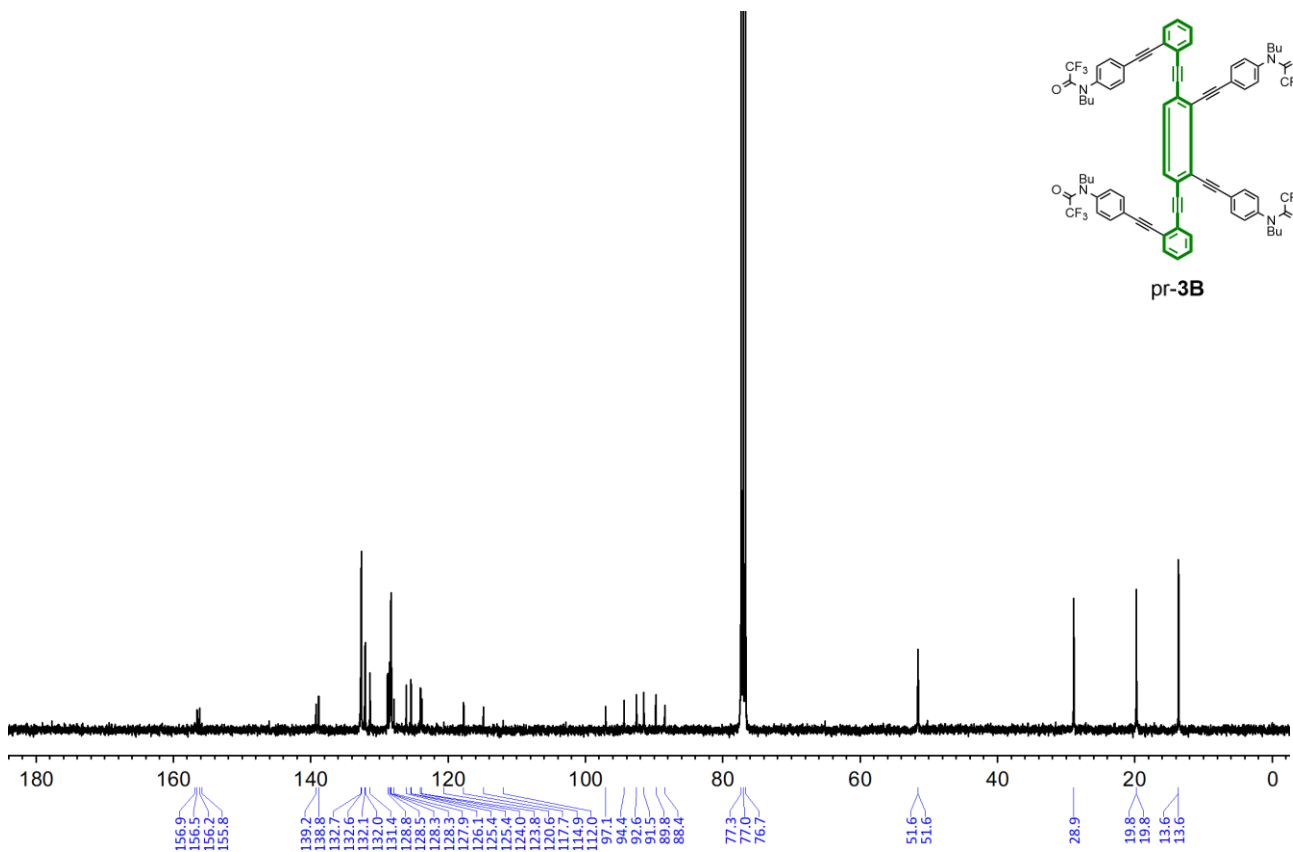
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of pr-3.



¹H NMR spectrum (400 MHz) of pr-3B, measured in CDCl₃ at room temperature.

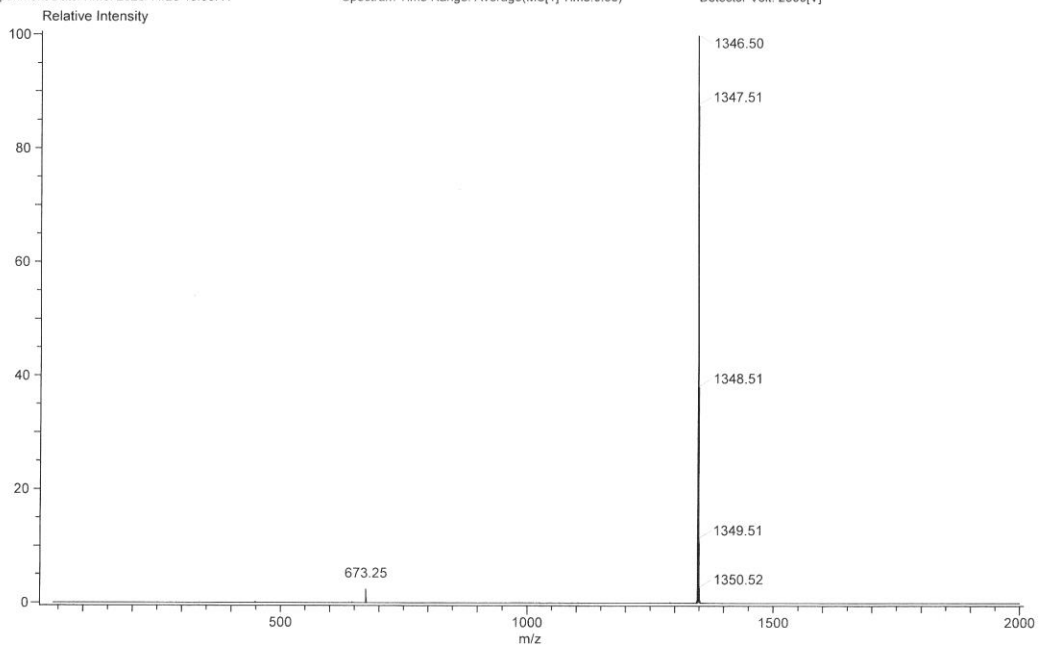


¹³C NMR spectrum (100 MHz) of pr-3B, measured in CDCl₃ at room temperature.

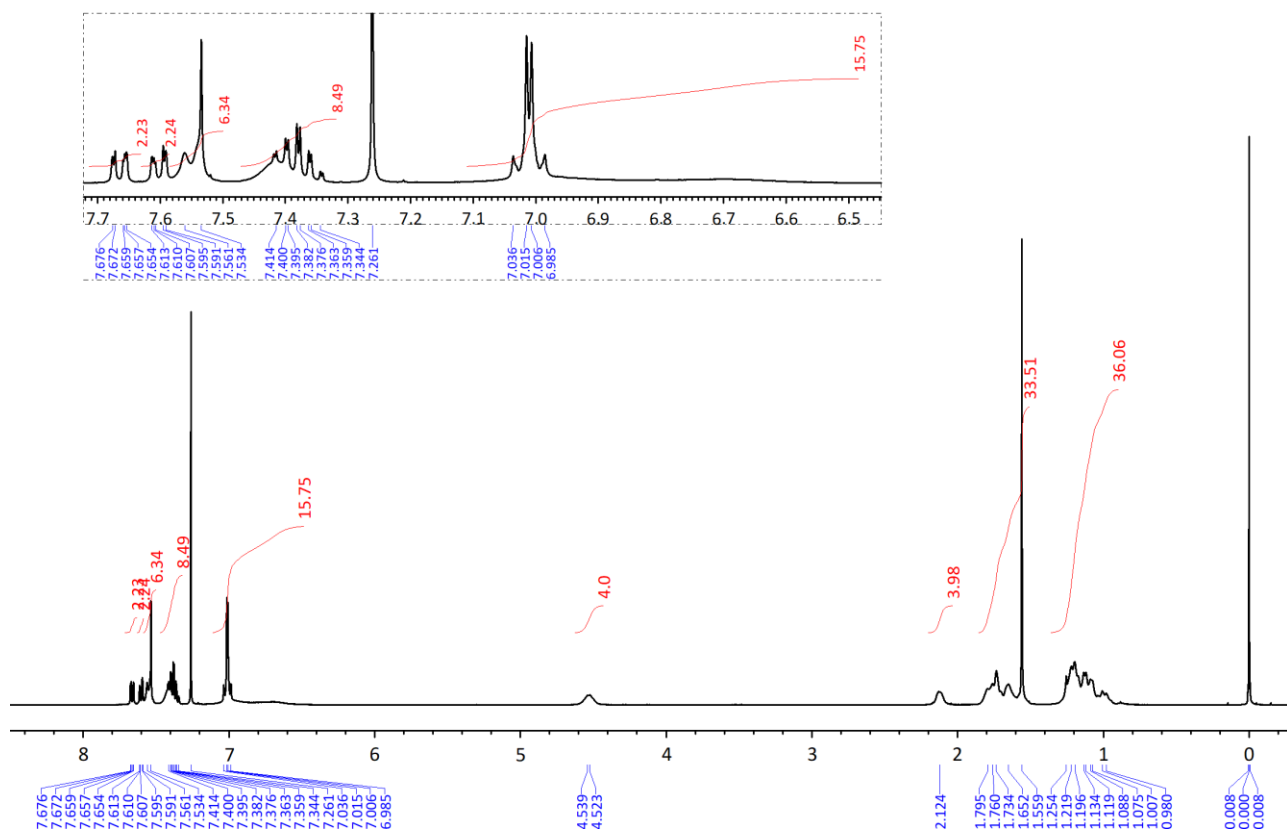
Data Name: common/Nov20_a51296-
Sample: u1 katoono / pr3Bc406
Experiment Date/Time: 2023/11/20 15:58:41

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..3200
Spectrum Time Range: Average(MS[1]) Time:0.38)

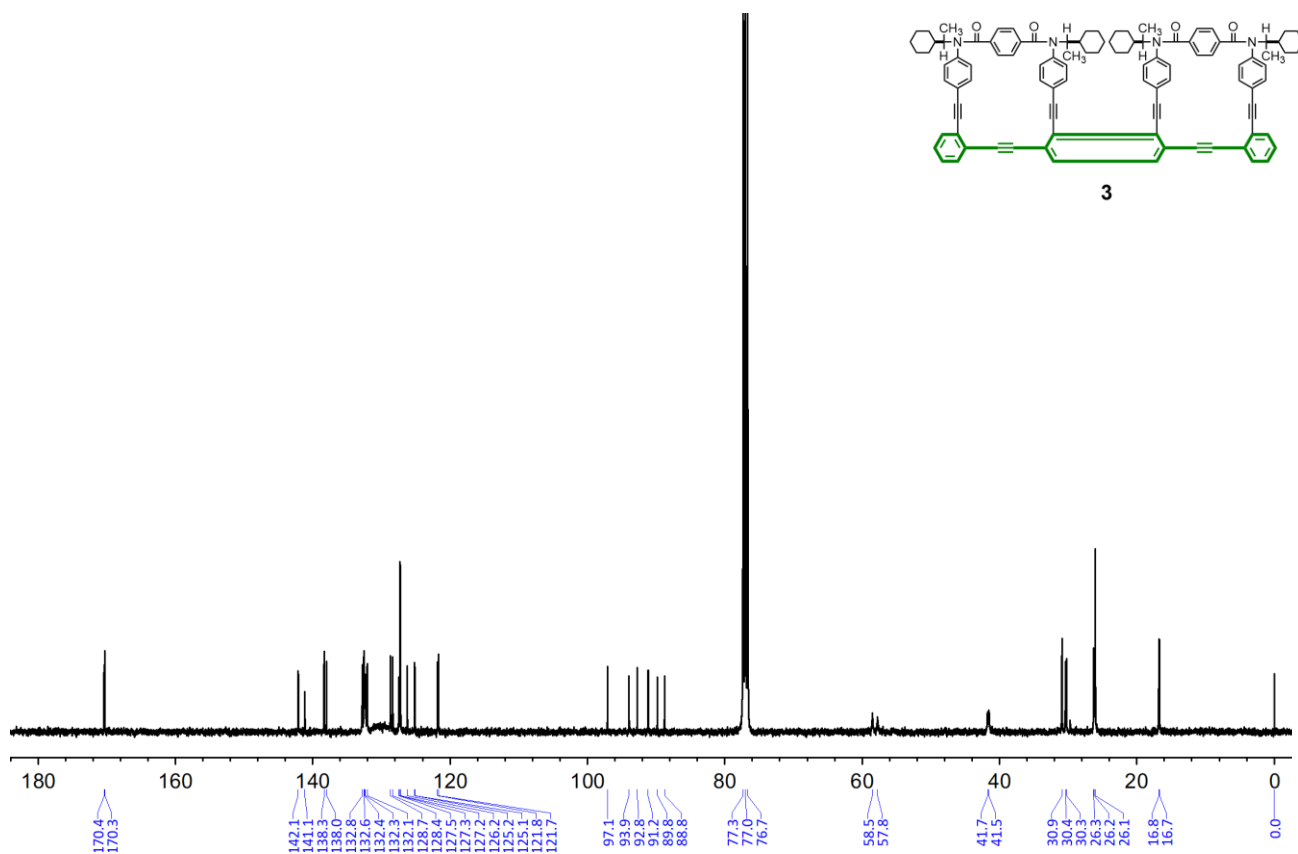
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of pr-3B.



¹H NMR spectrum (400 MHz) of **3**, measured in CDCl₃ at room temperature.

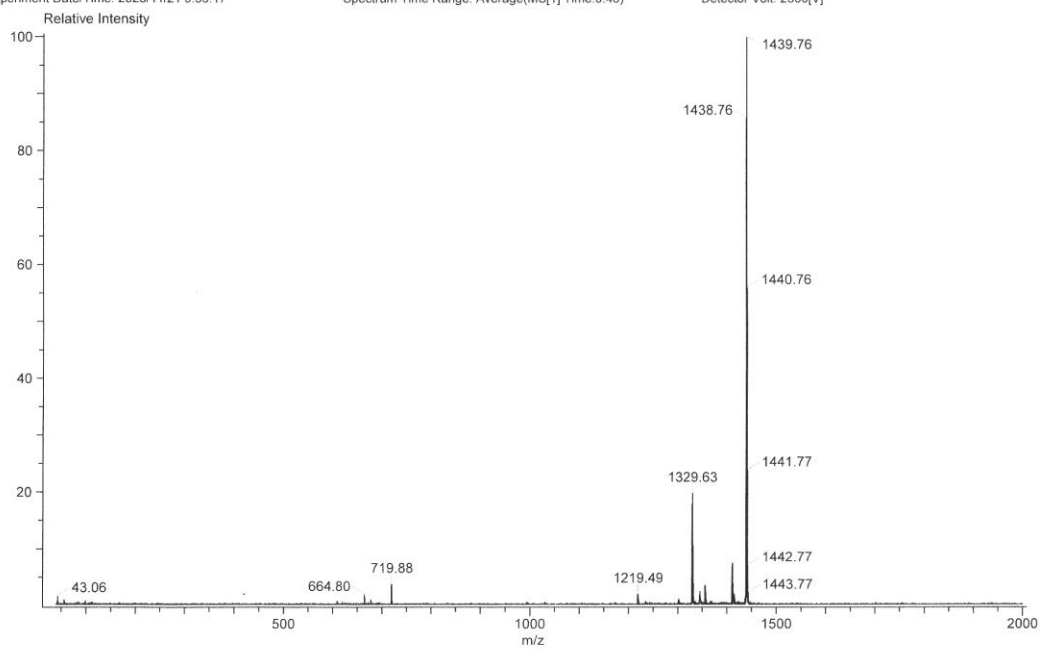


¹³C NMR spectrum (100 MHz) of **3**, measured in CDCl₃ at 313 K.

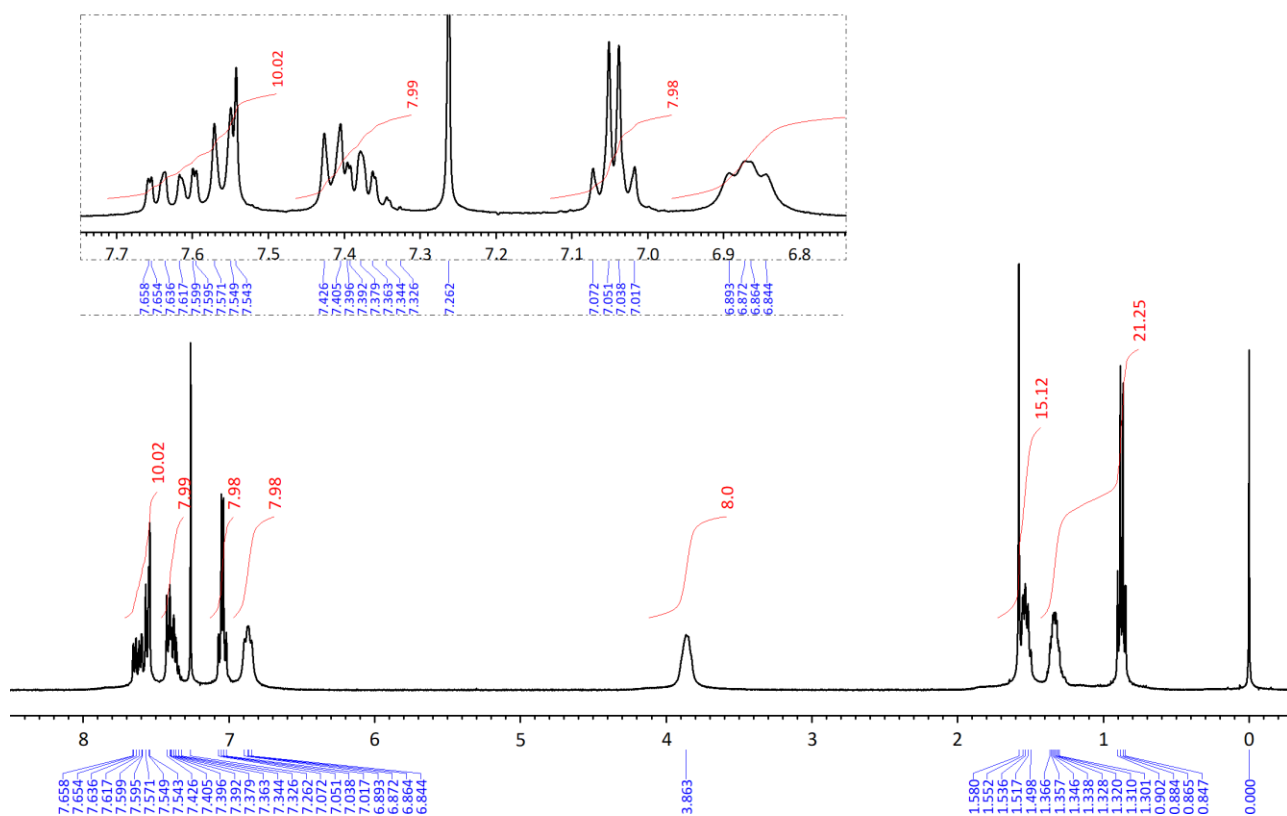
Data Name: common/Nov21_a51293-
Sample: u1 katoono / 3m44
Experiment Date/Time: 2023/11/21 9:56:17

Instrument: JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..3200
Spectrum Time Range: Average(MS[1] Time:0.46)

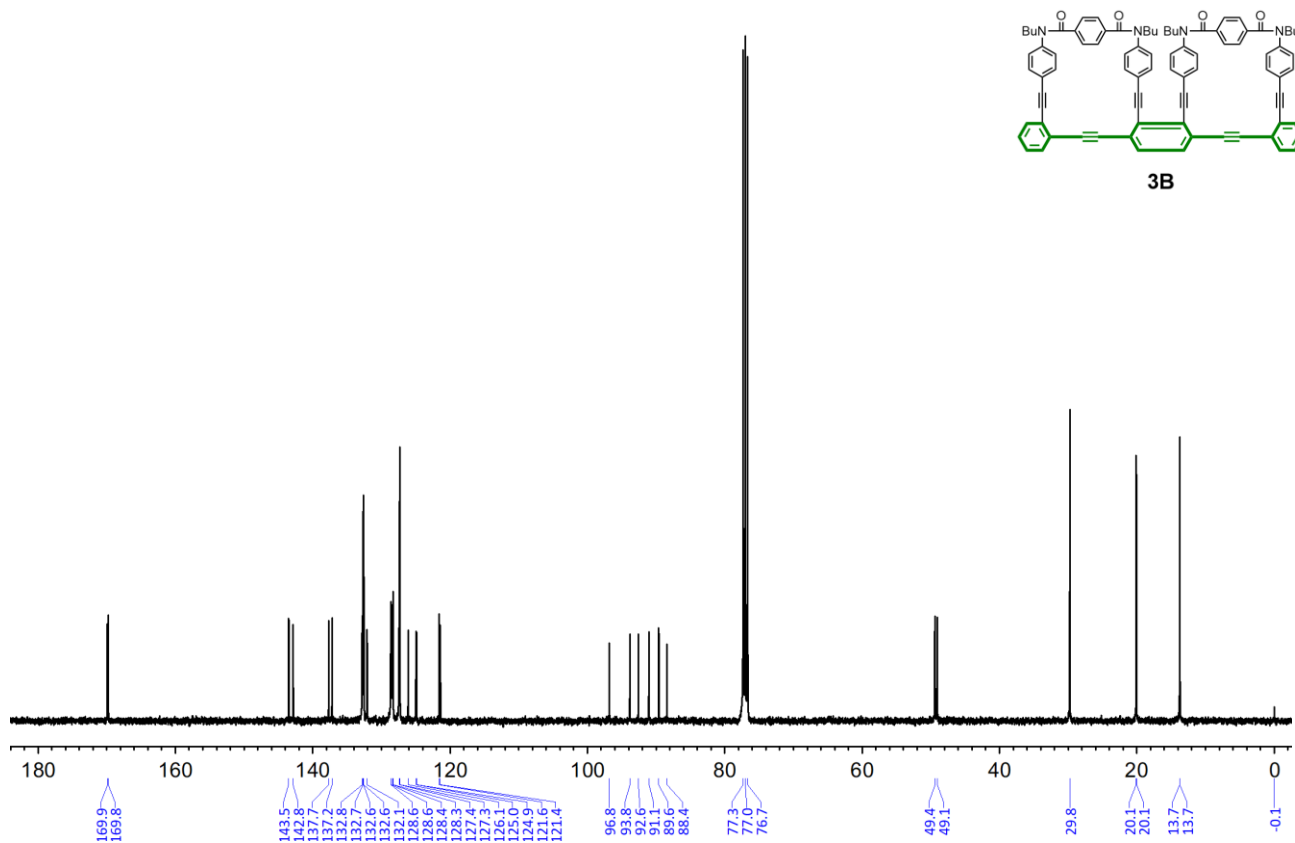
MS Tune Method Name: FD
GC: Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of 3.



¹H NMR spectrum (400 MHz) of **3B**, measured in CDCl₃ at room temperature.

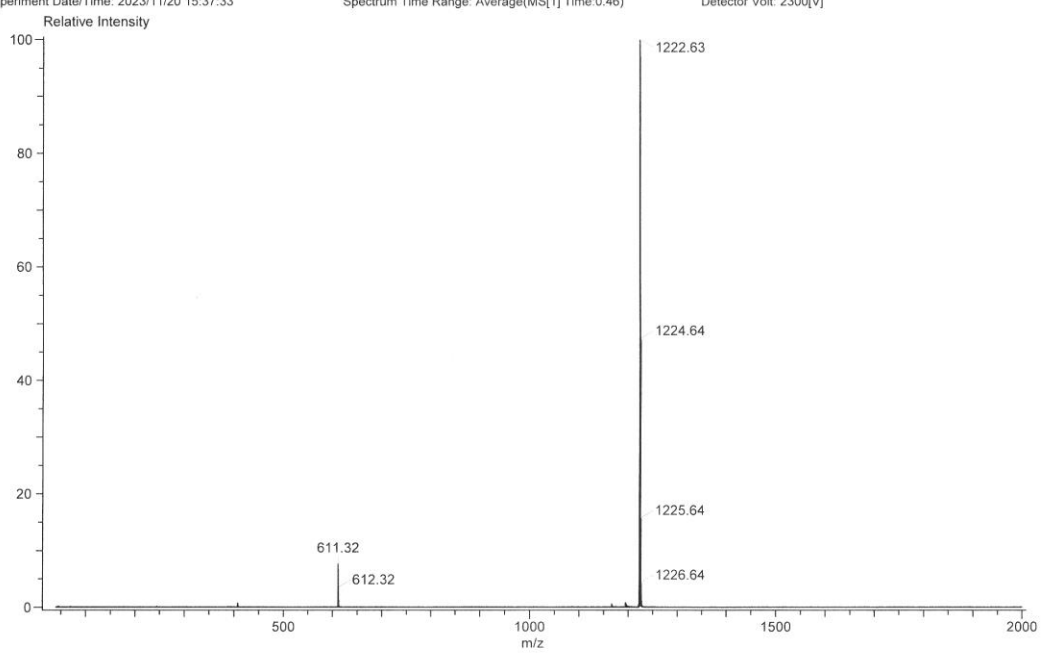


¹³C NMR spectrum (100 MHz) of **3**, measured in CDCl₃ at room temperature.

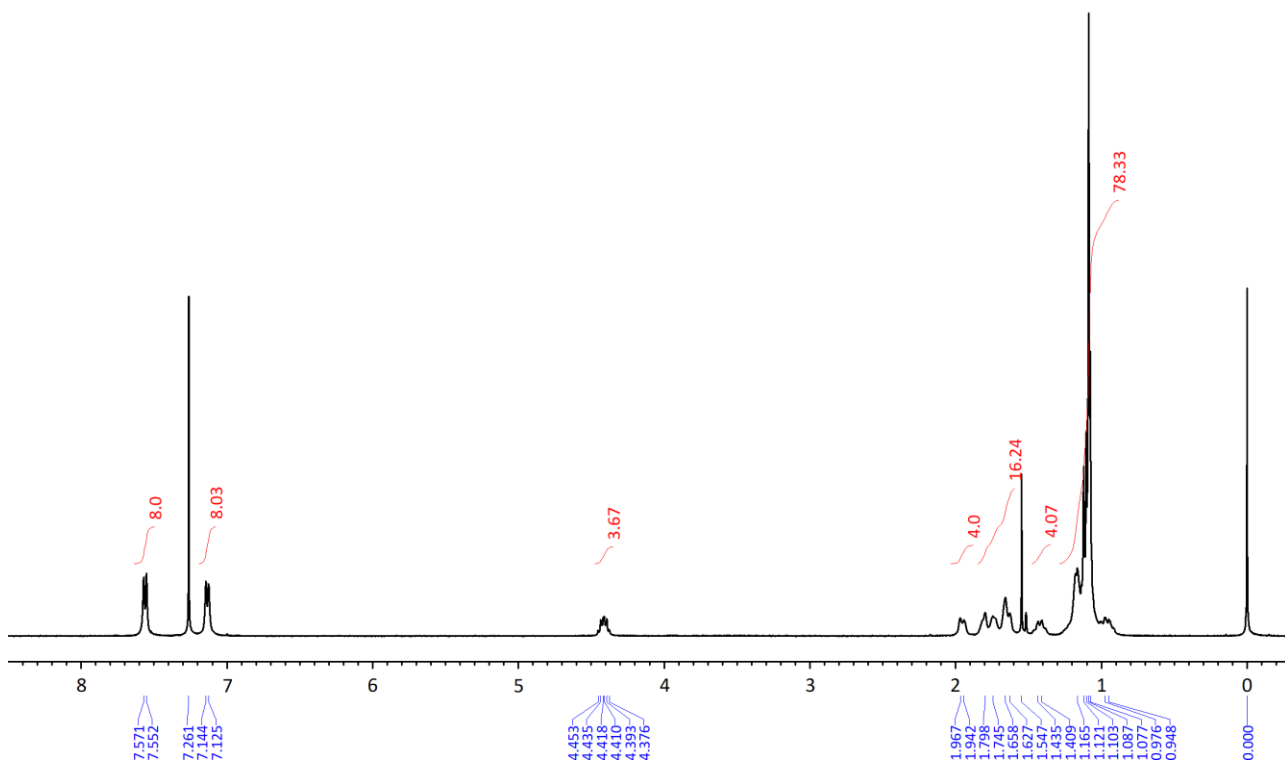
Data Name: common/Nov20_a51292-
Sample: u1 katoono / 38m39
Experiment Date/Time: 2023/11/20 15:37:33

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..3200
Spectrum Time Range: Average(MS[1] Time:0.46)

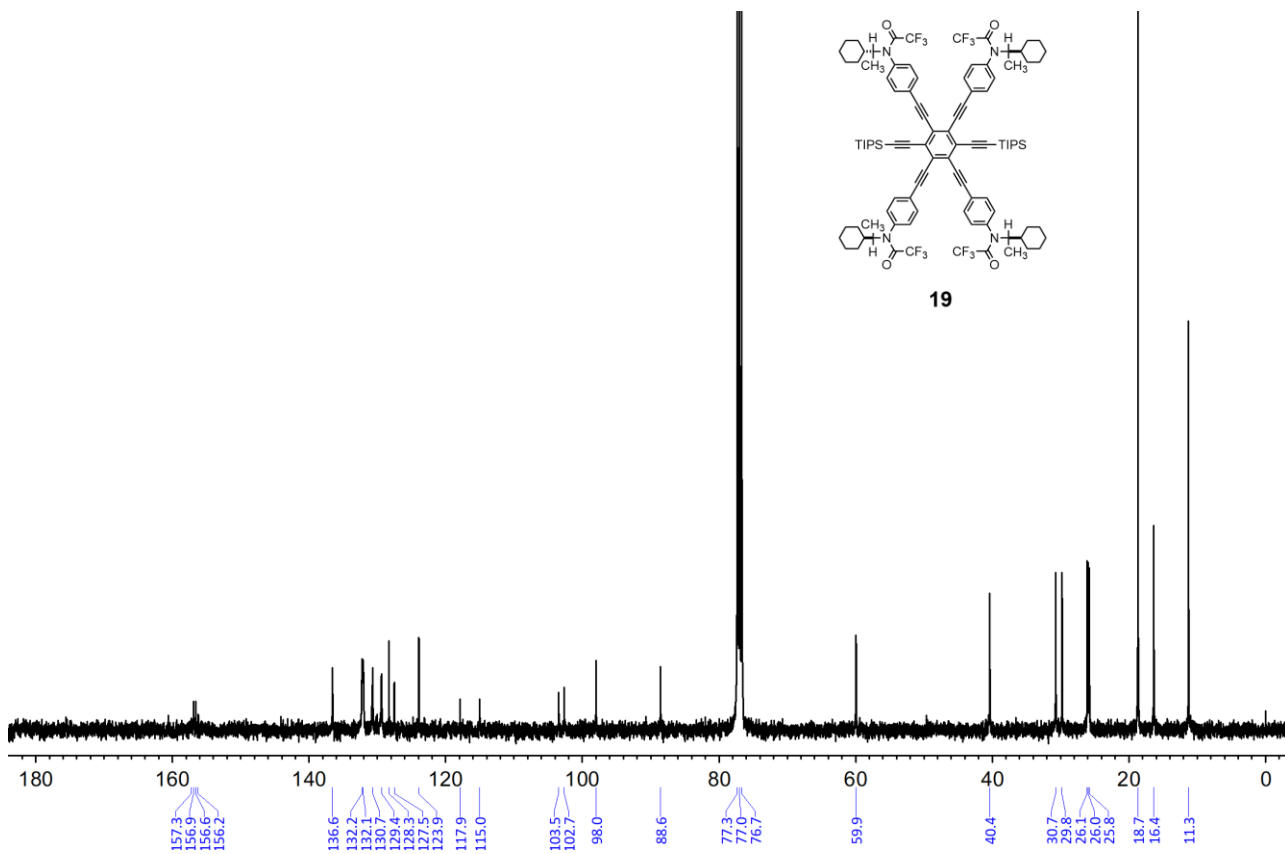
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **3B**.



^1H NMR spectrum (400 MHz) of **19**, measured in CDCl_3 at room temperature.

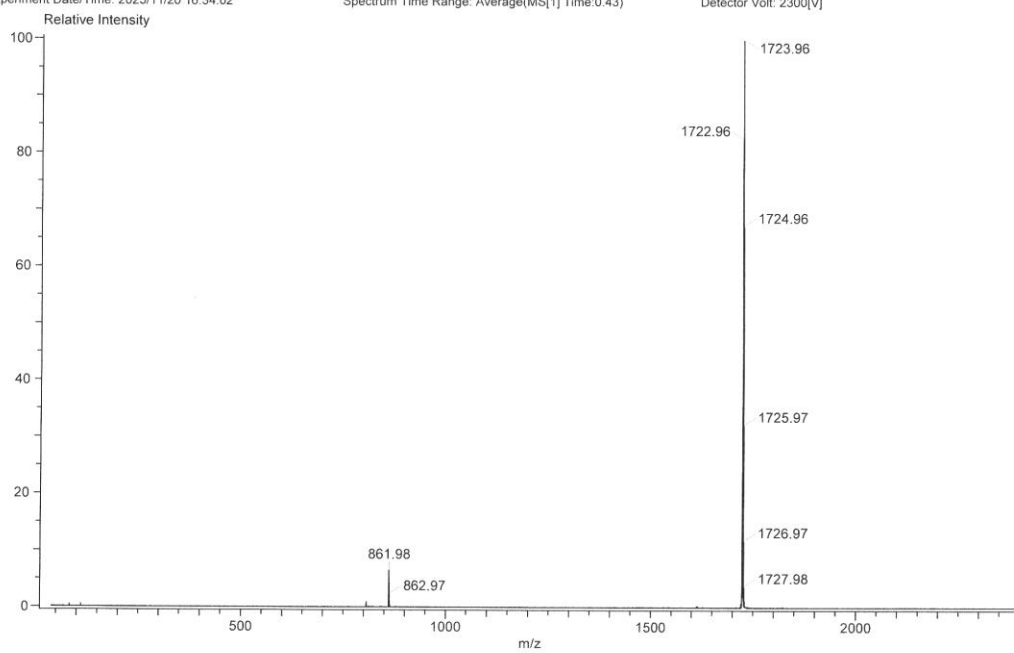


^{13}C NMR spectrum (100 MHz) of **19**, measured in CDCl_3 at room temperature.

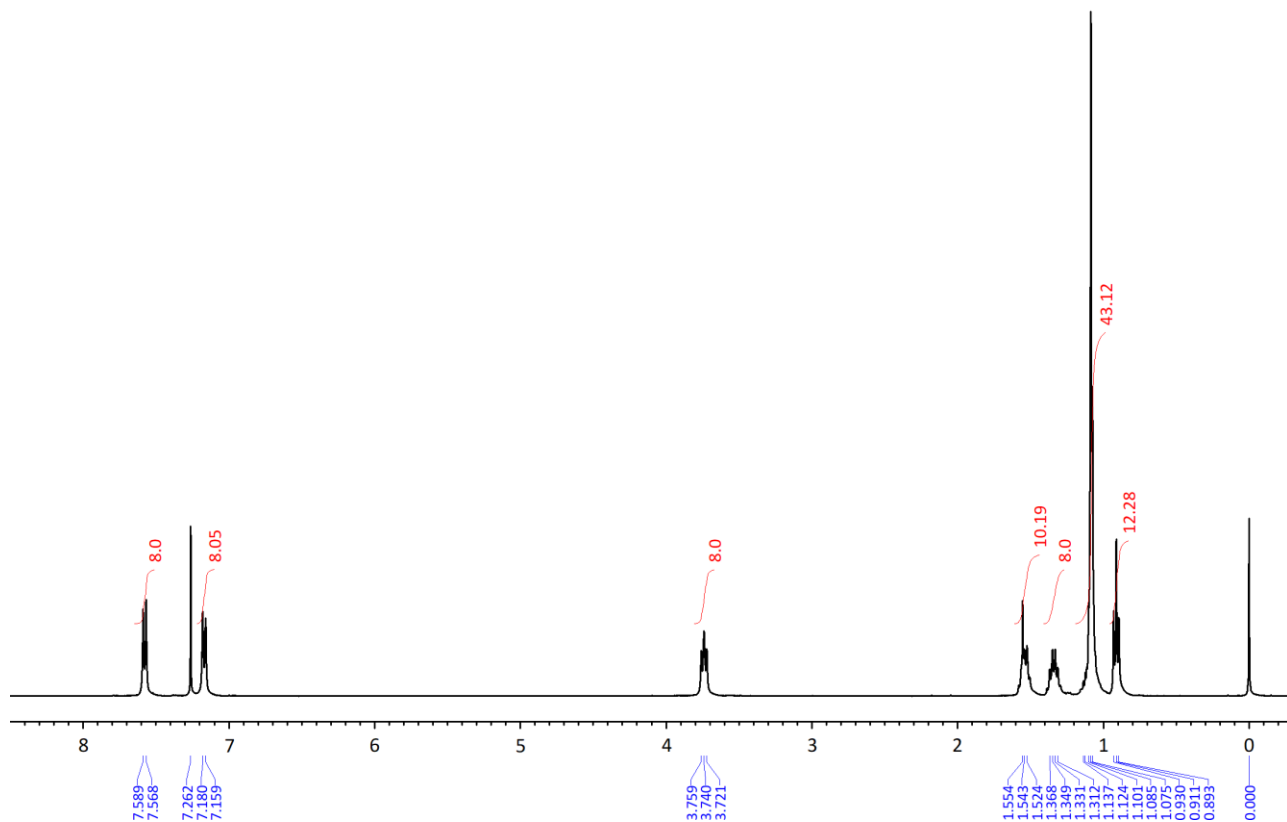
Data Name: common/Nov20.a51301-
Sample: u1 katoono / 19o396
Experiment Date/Time: 2023/11/20 16:34:02

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40. 6400
Spectrum Time Range: Average(MS[1] Time:0.43)

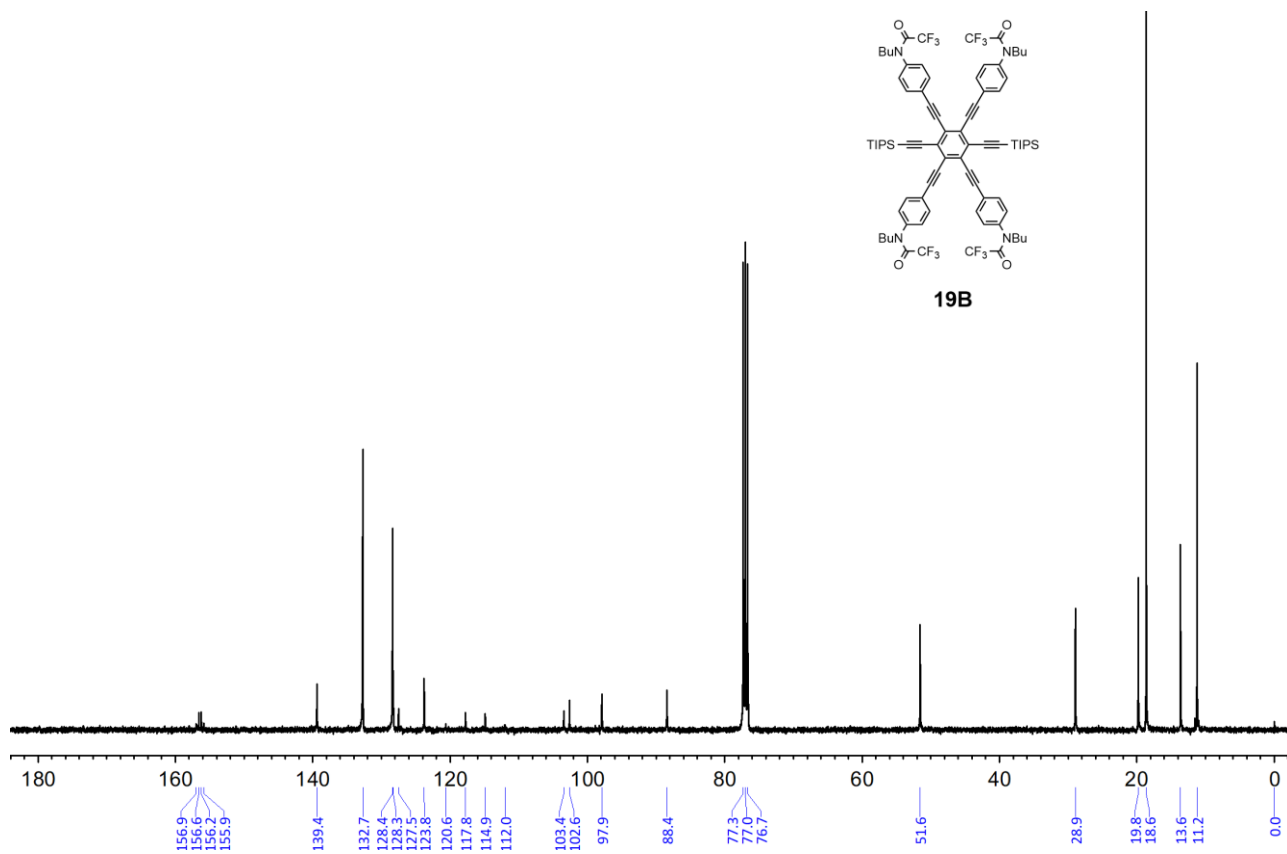
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **19**.



^1H NMR spectrum (400 MHz) of **19B**, measured in CDCl_3 at room temperature.

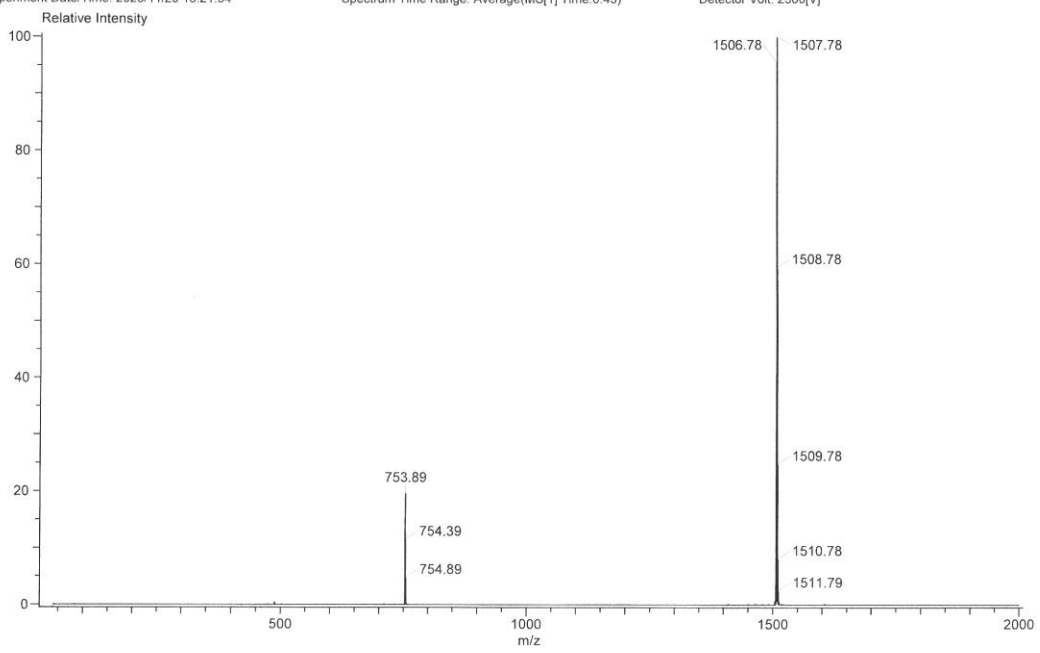


^{13}C NMR spectrum (100 MHz) of **19B**, measured in CDCl_3 at room temperature.

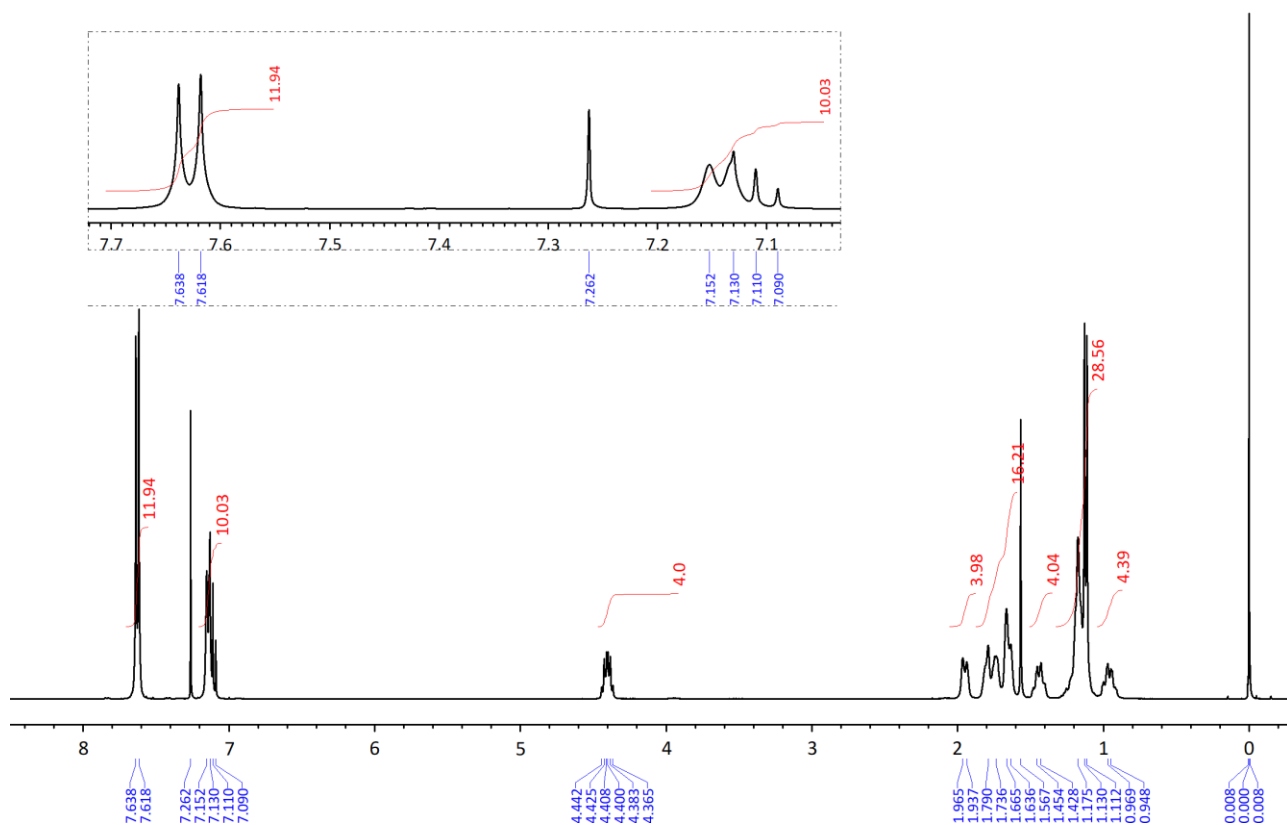
Data Name: common/Nov20_a51300-
Sample: u1 katoono / 19Bo378
Experiment Date/Time: 2023/11/20 16:21:54

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..3200
Spectrum Time Range: Average(MS[1]) Time:0.43

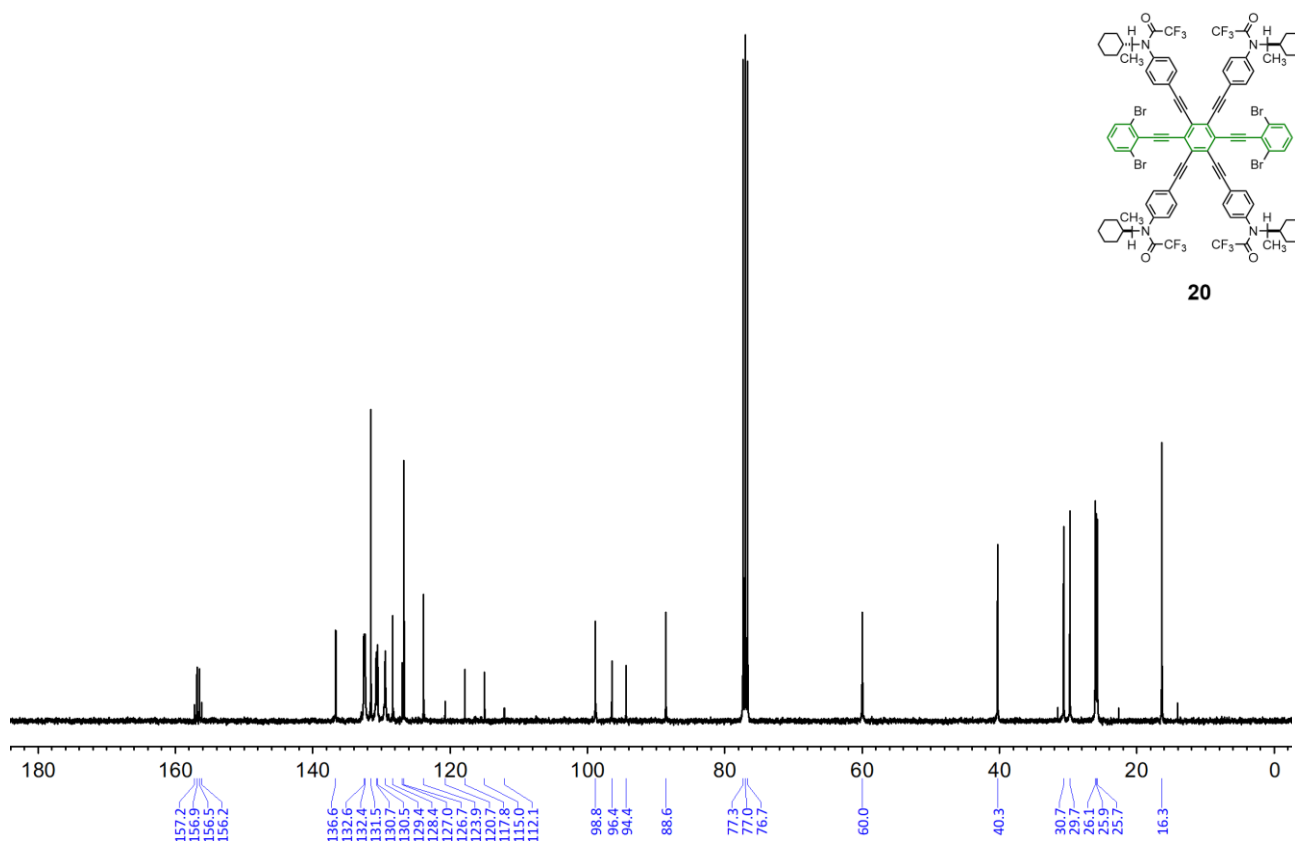
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **19B**.



¹H NMR spectrum (400 MHz) of **20**, measured in CDCl₃ at room temperature.

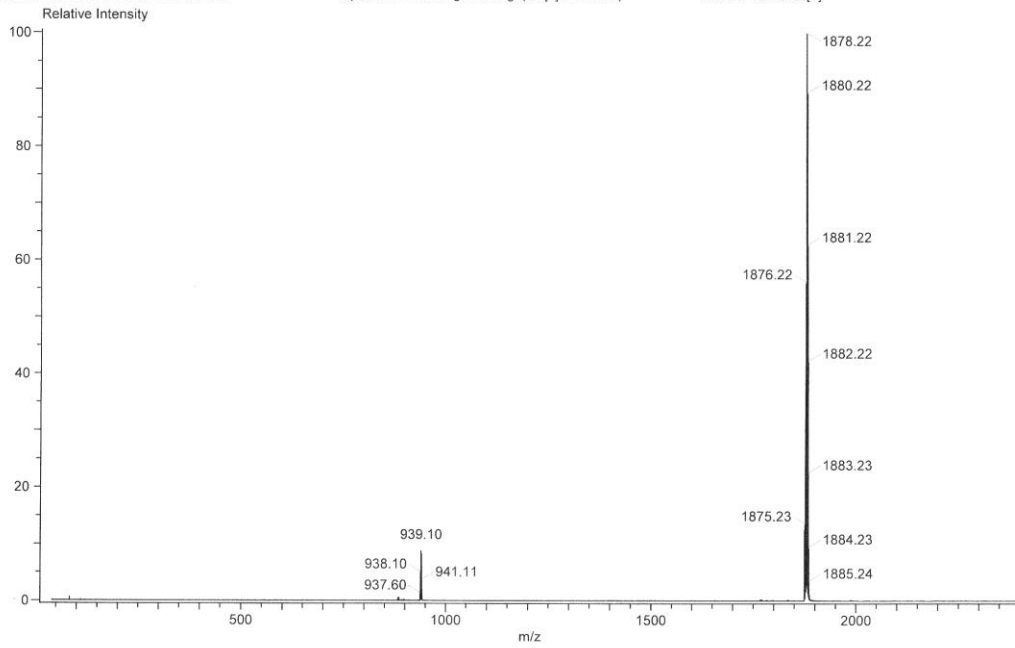


¹³C NMR spectrum (100 MHz) of **20**, measured in CDCl₃ at room temperature.

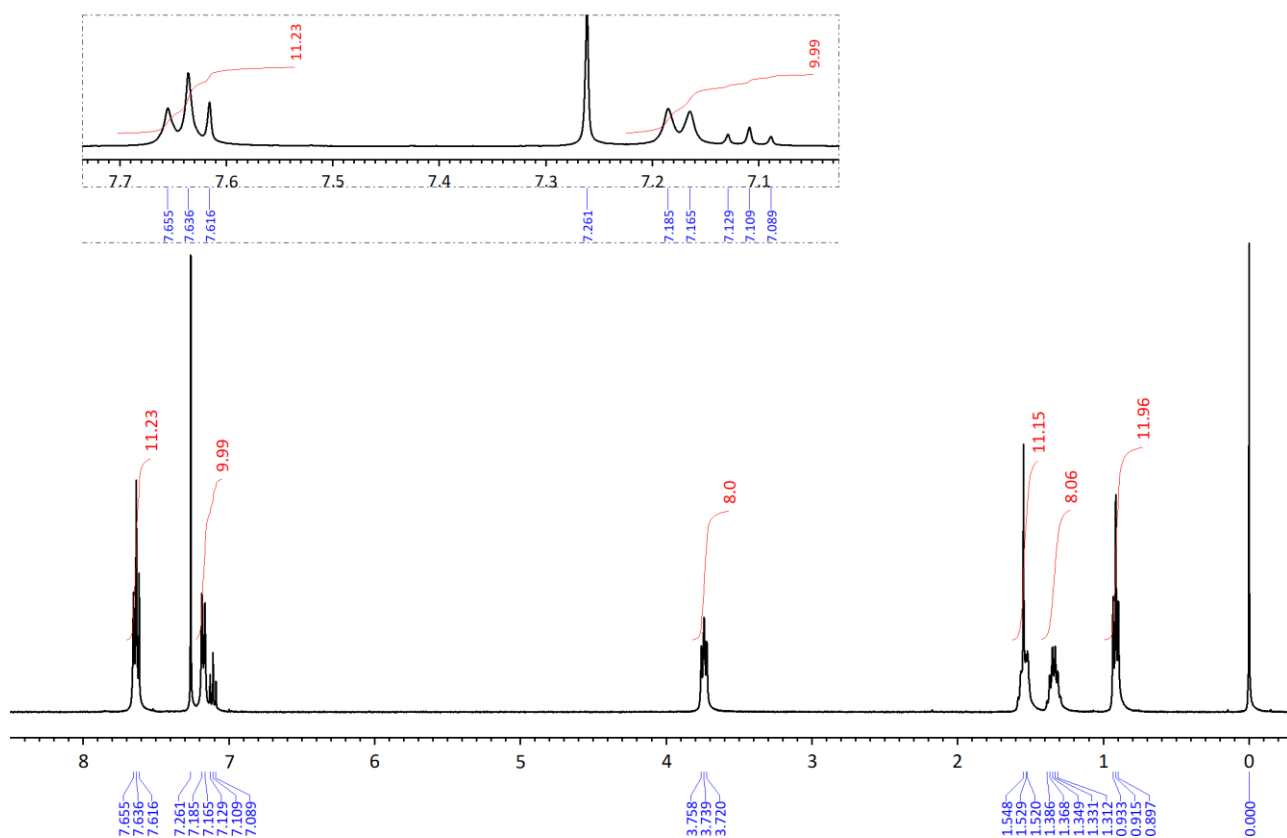
Data Name: common/Nov21_a51303-
Sample: r1 katonno / 20c404
Experiment Date/Time: 2023/11/21 9:44:32

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40_6400
Spectrum Time Range: Average(MS[1] Time:0.42)

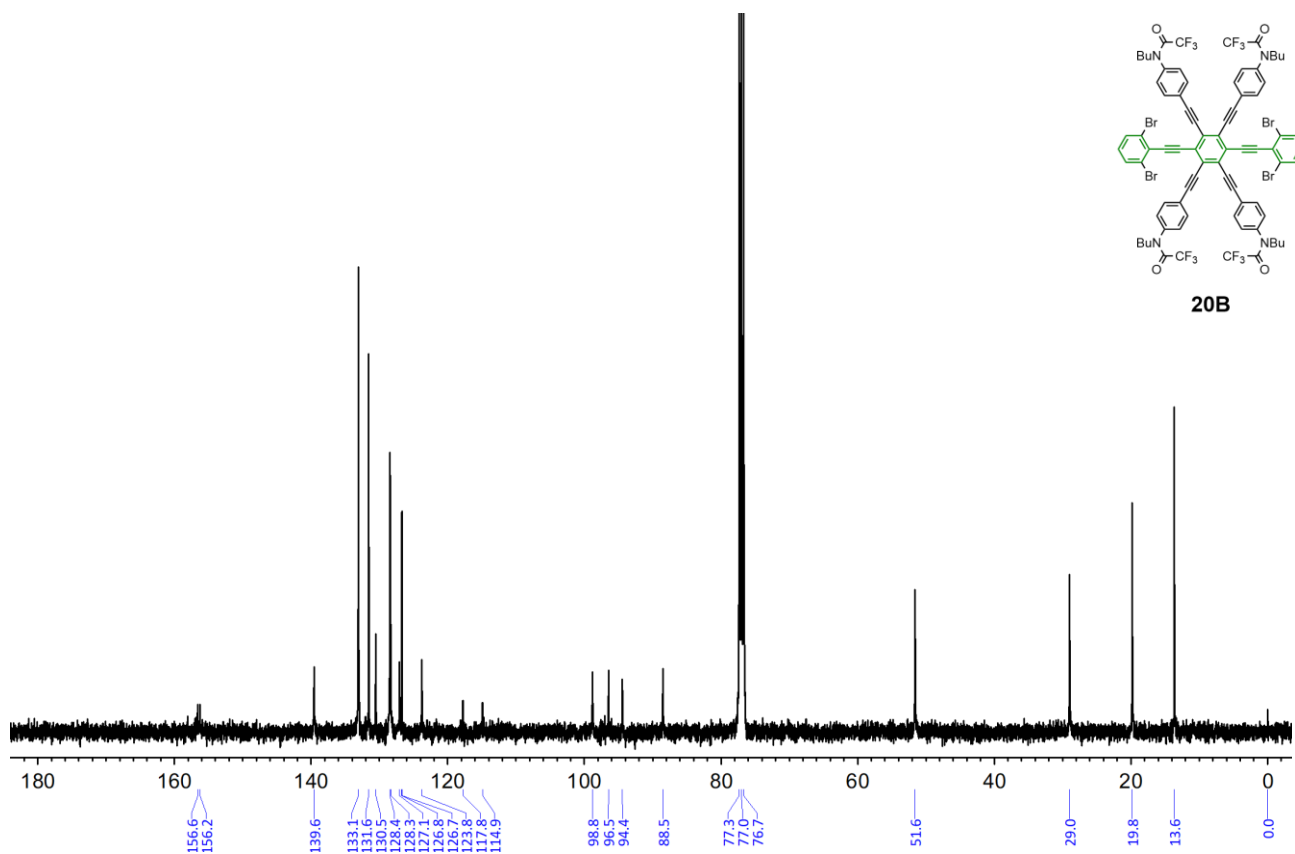
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **20**.



^1H NMR spectrum (400 MHz) of **20B**, measured in CDCl_3 at room temperature.

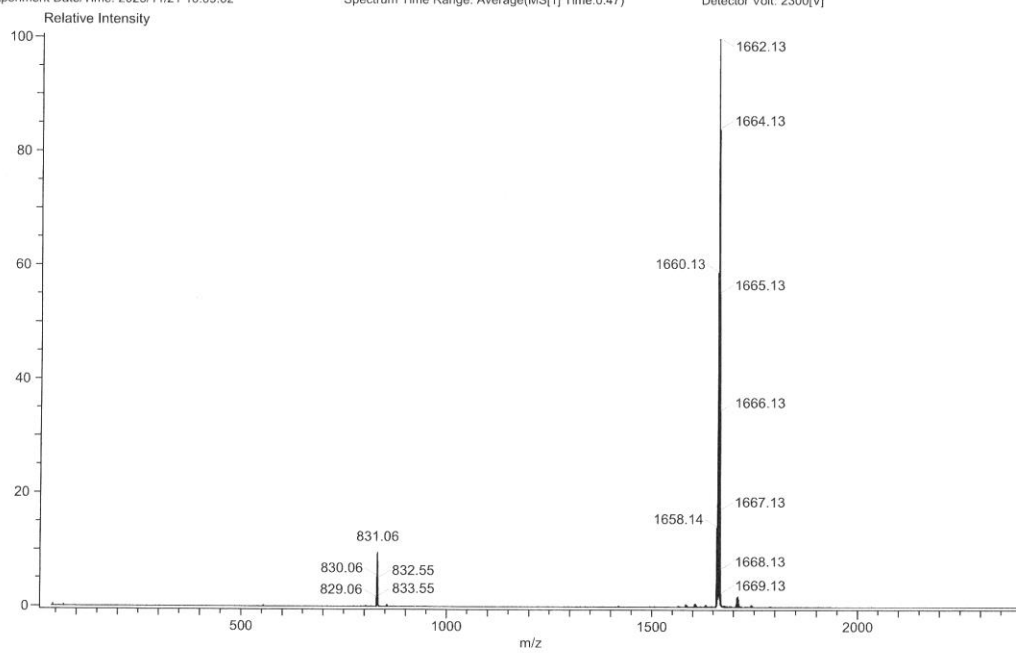


^{13}C NMR spectrum (100 MHz) of **20B**, measured in CDCl_3 at room temperature.

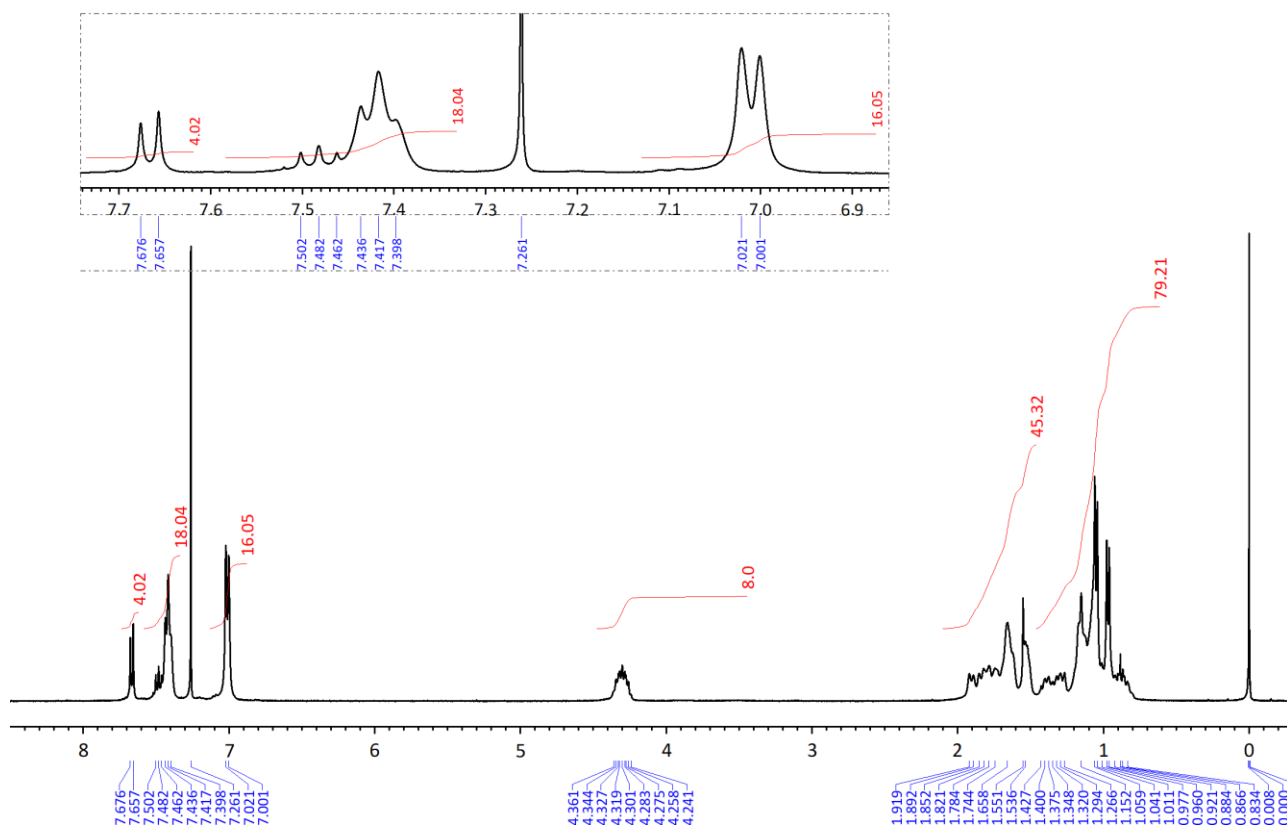
Data Name: common/Nov21_a51302-
Sample: u1 katoono / 20Bo387
Experiment Date/Time: 2023/11/21 10:09:02

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..6400
Spectrum Time Range: Average(MS[1] Time:0.47)

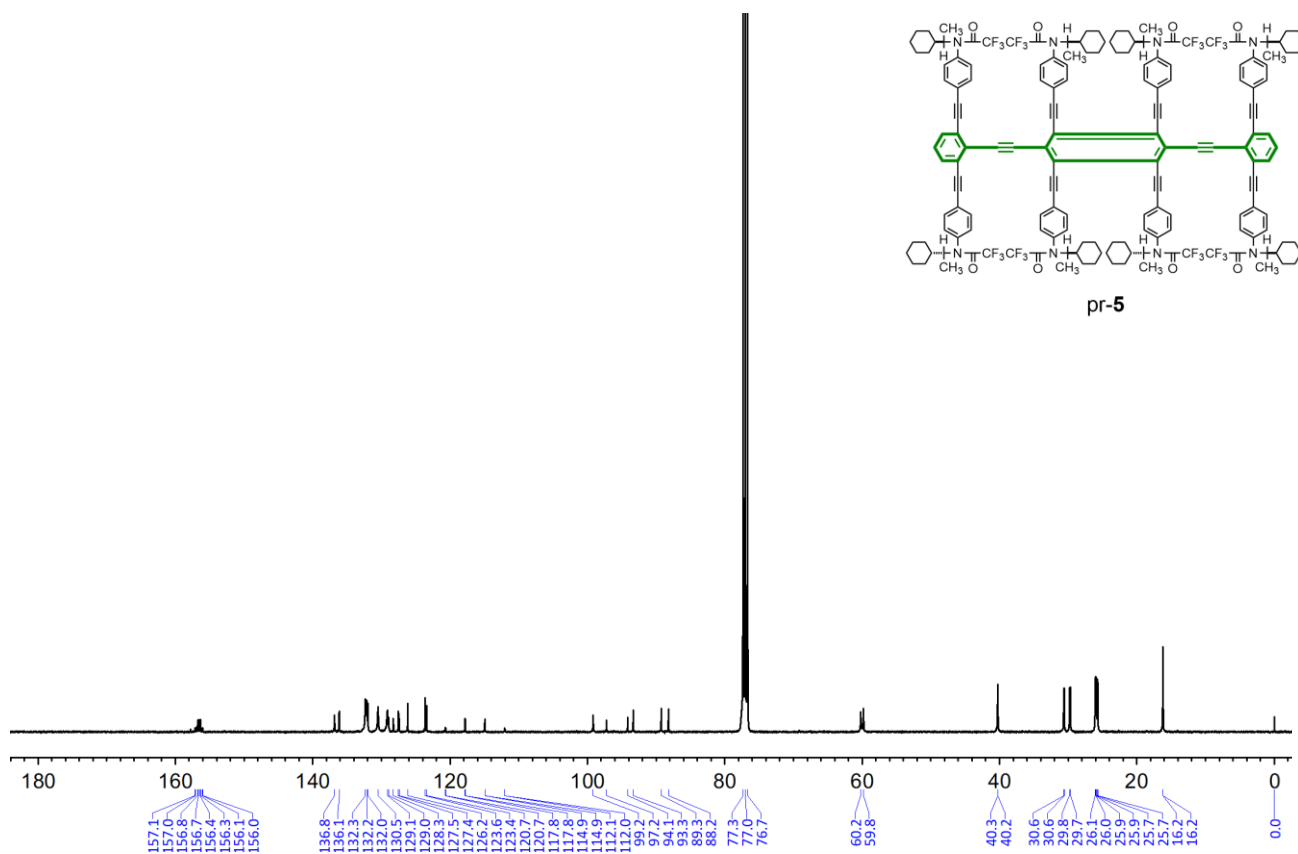
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **20B**.



¹H NMR spectrum (400 MHz) of pr-5, measured in CDCl₃ at room temperature.

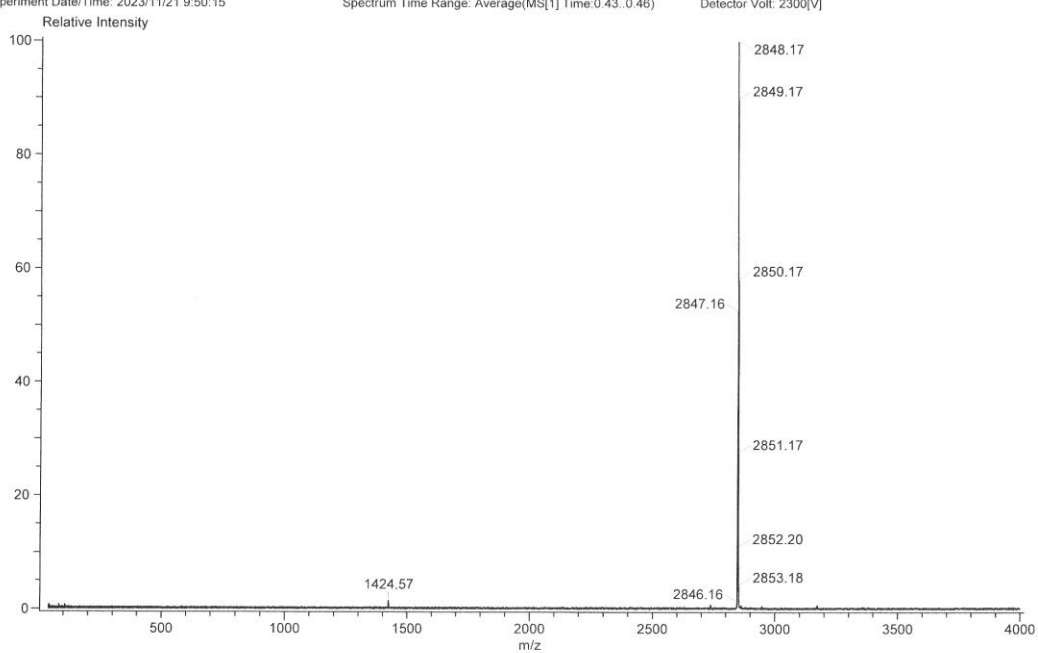


¹³C NMR spectrum (100 MHz) of pr-5, measured in CDCl₃ at room temperature.

Data Name: common/Nov21-a51299-
Sample: u1 katoono / pr5o409
Experiment Date/Time: 2023/11/21 9:50:15

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40. 6400
Spectrum Time Range: Average(MS[1] Time:0.43. 0.46)

MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]

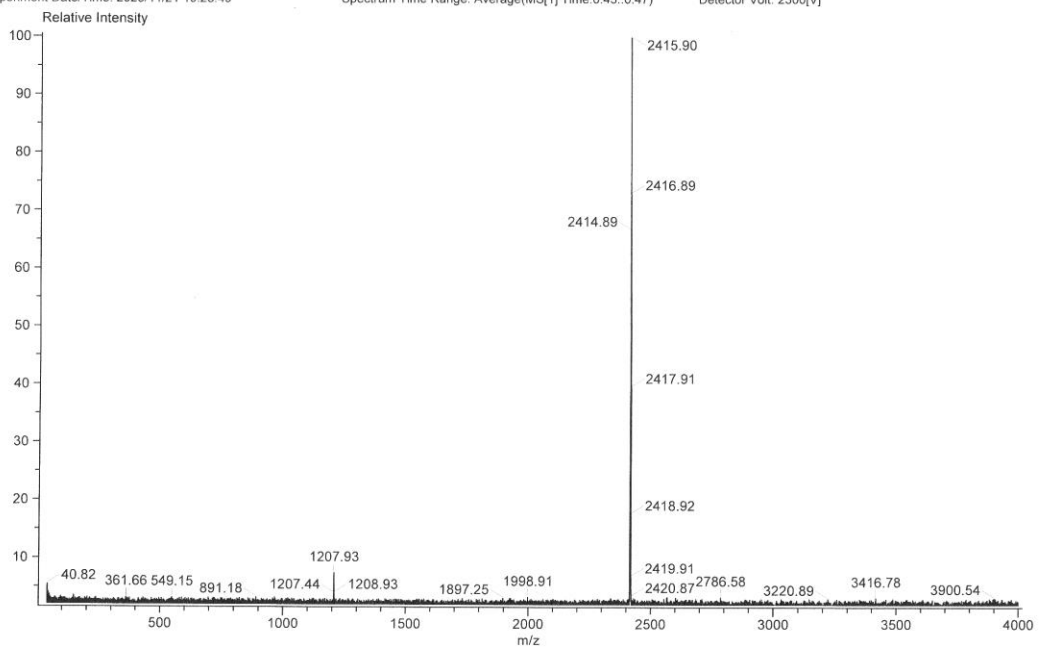


LRMS (FD) of pr-5.

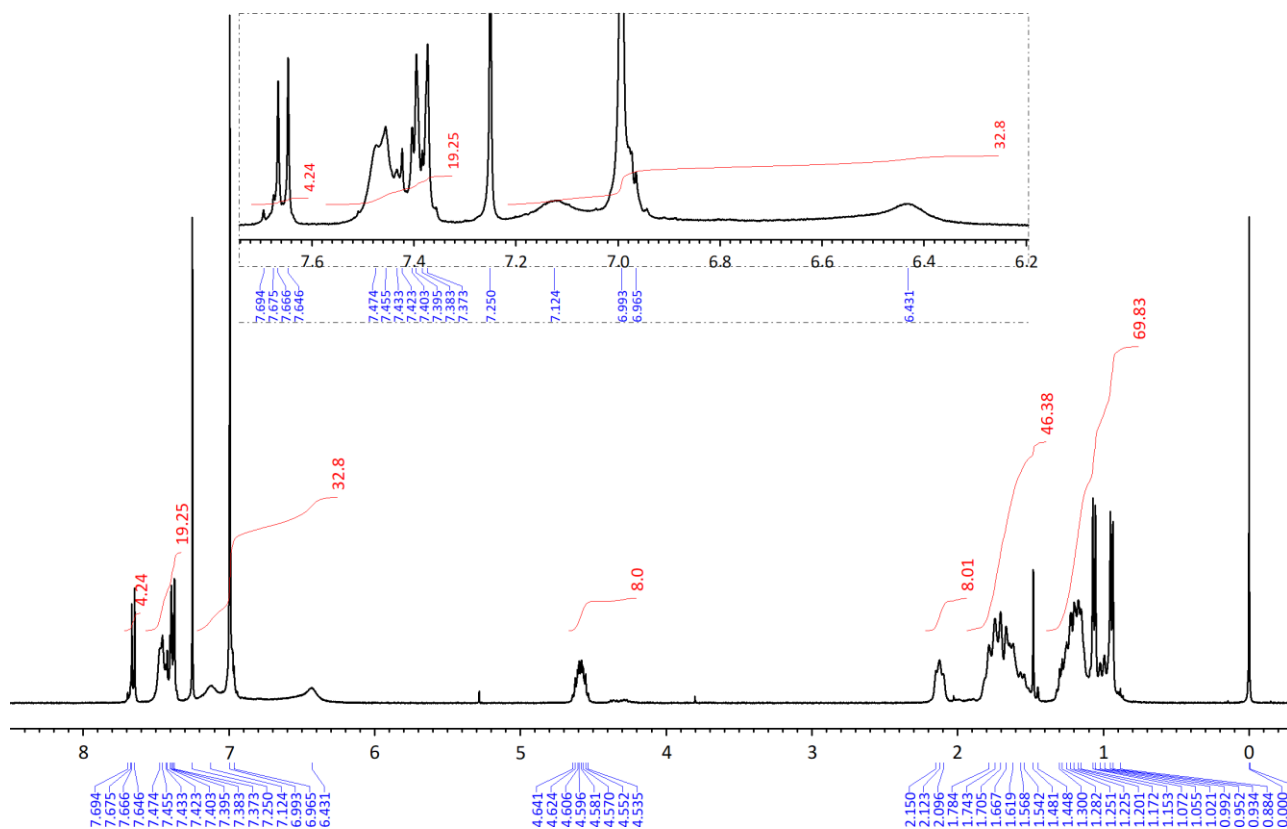
Data Name: common/Nov21_a51298-
Sample: u1 katoono / pr5B0408
Experiment Date/Time: 2023/11/21 10:28:49

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..6400
Spectrum Time Range: Average(MS[1]) Time:0.43..0.47)

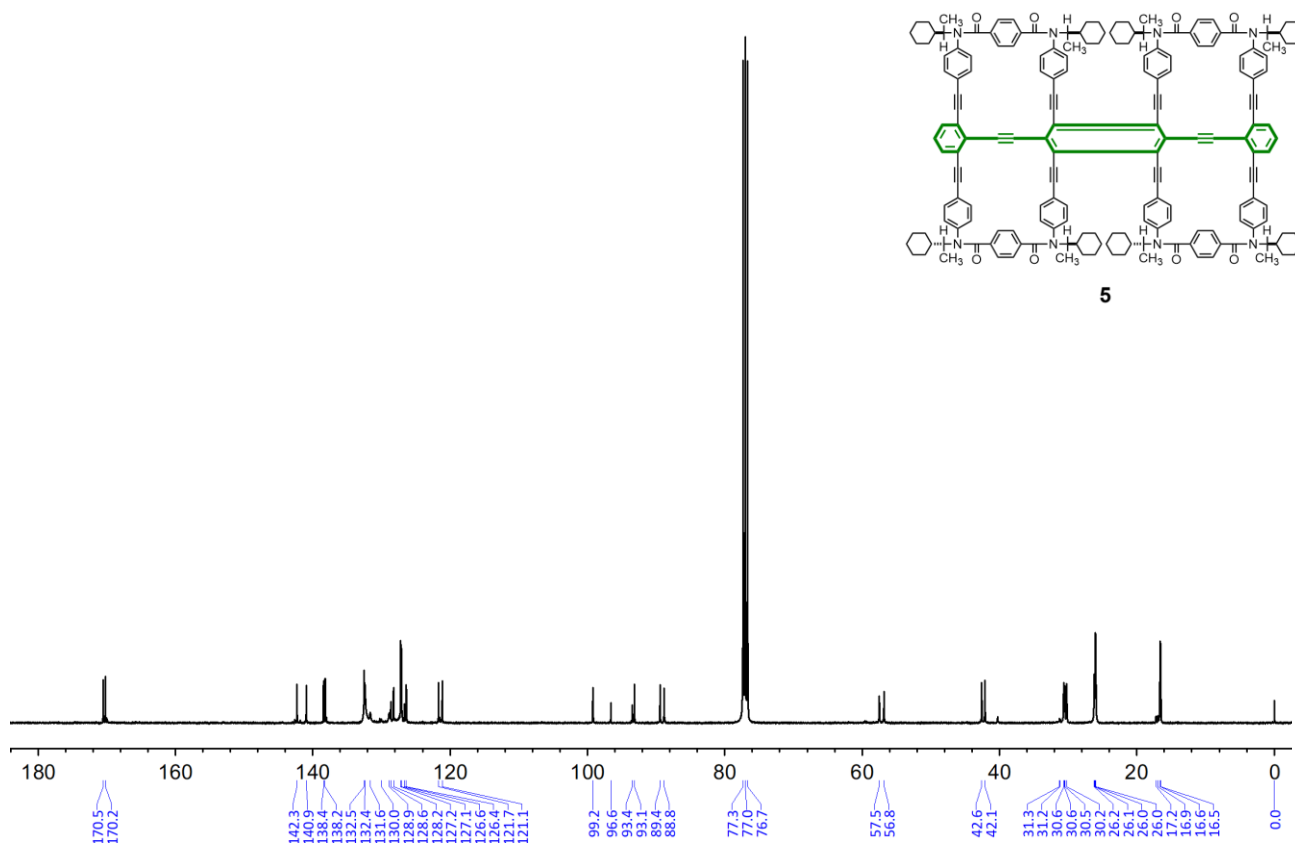
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of pr-5B.



¹H NMR spectrum (400 MHz) of **5**, measured in CDCl₃ at 323 K.

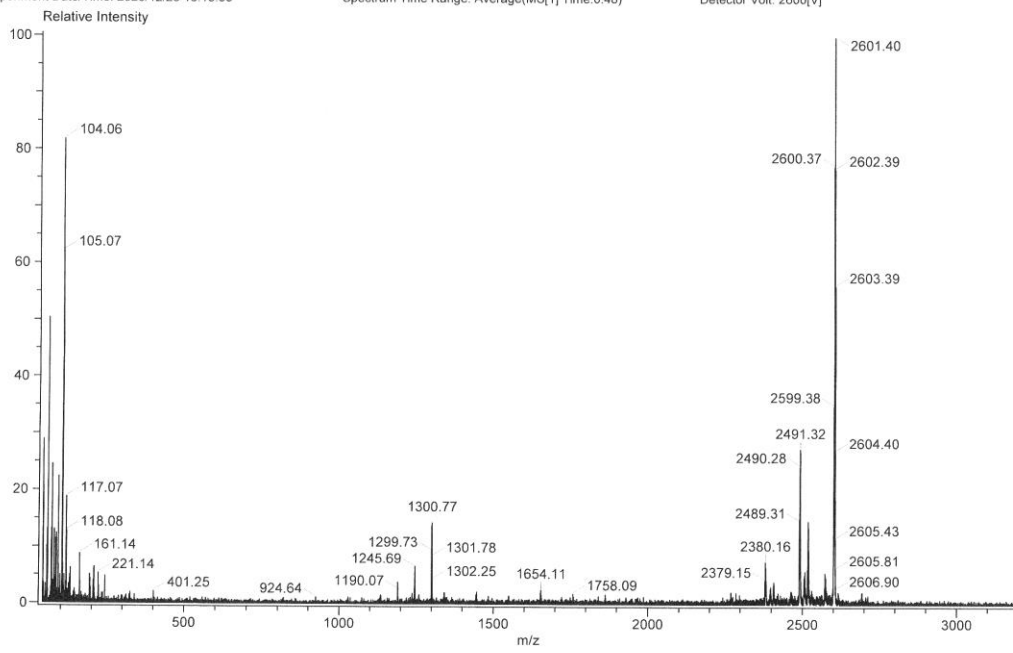


¹³C NMR spectrum (100 MHz) of **5**, measured in CDCl₃ at 313 K.

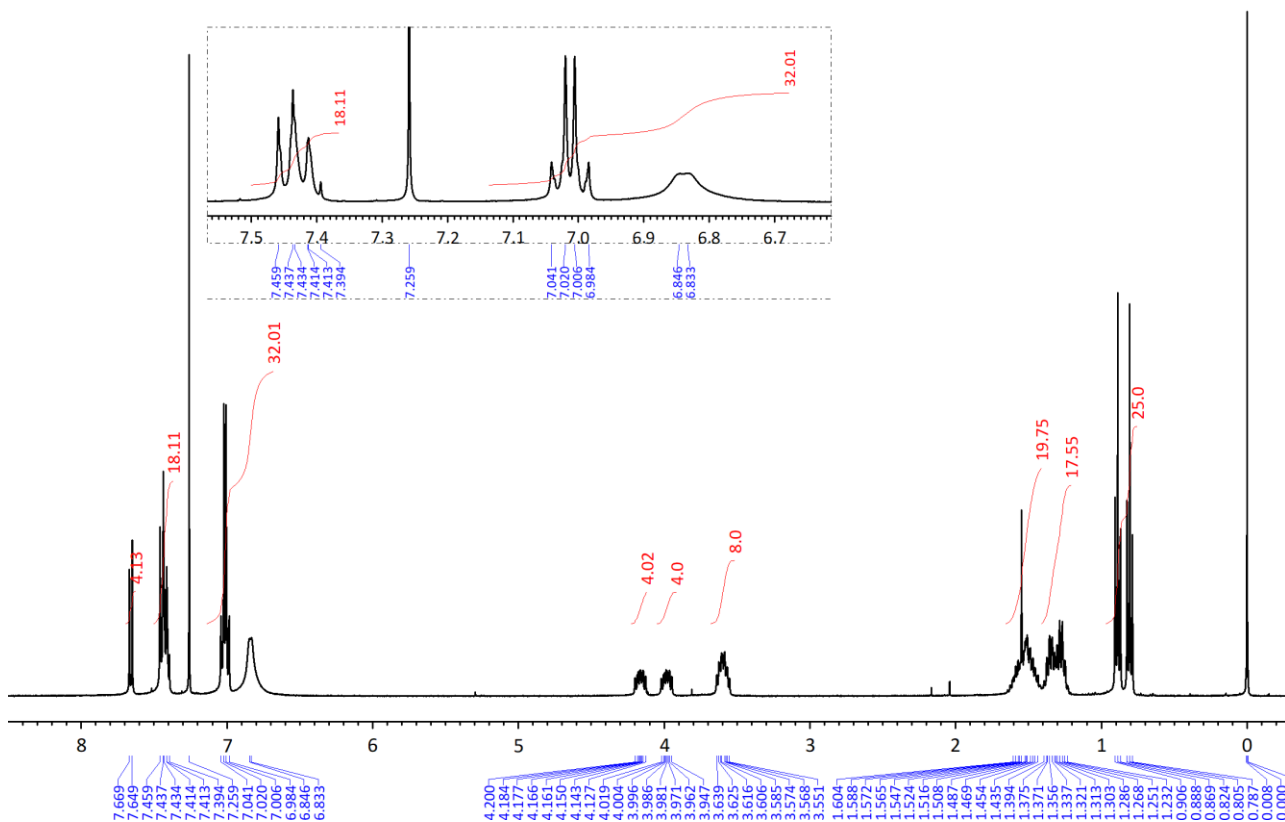
Data Name: common/Dec26 a51295-15
Sample: u1 katoono / 5o414
Experiment Date/Time: 2023/12/26 16:18:58

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..3200
Spectrum Time Range: Average(MS[1] Time:0.48)

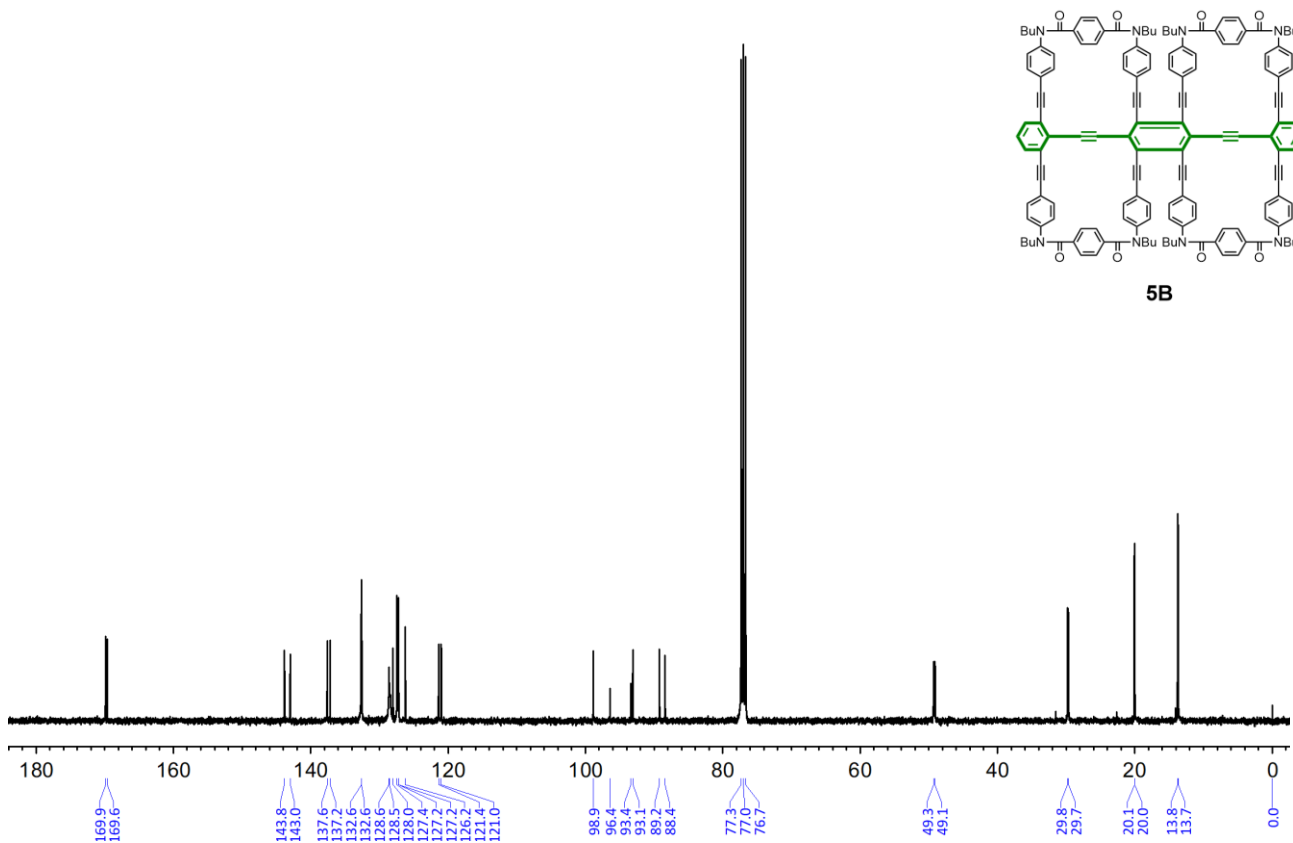
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2600[V]



LRMS (FD) of 5.



^1H NMR spectrum (400 MHz) of **5B**, measured in CDCl_3 at 303 K.

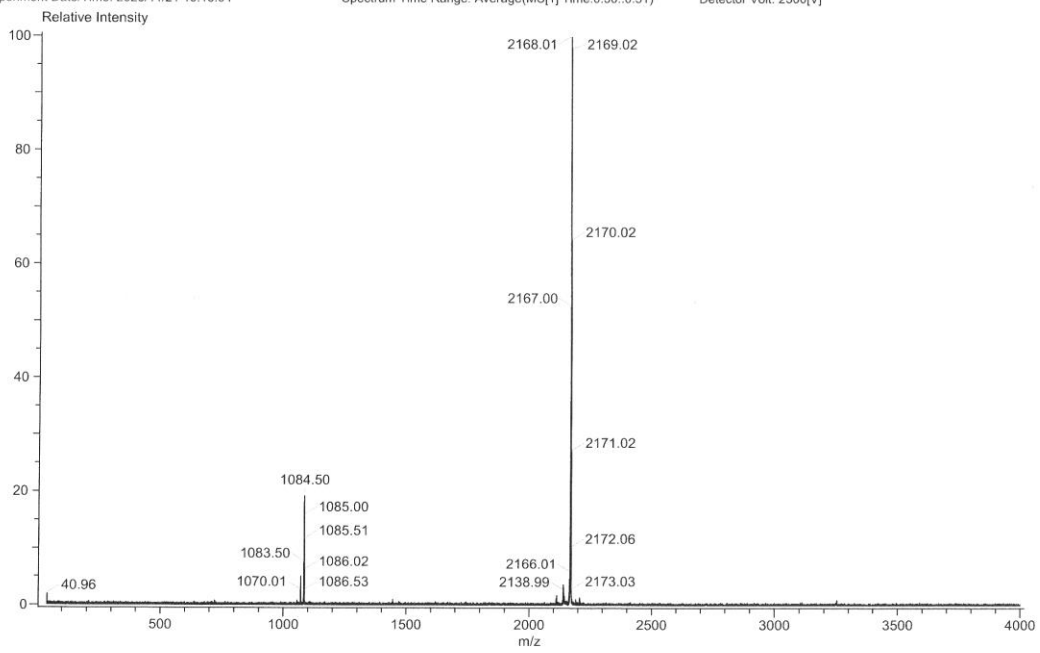


^{13}C NMR spectrum (100 MHz) of **5B**, measured in CDCl_3 at room temperature.

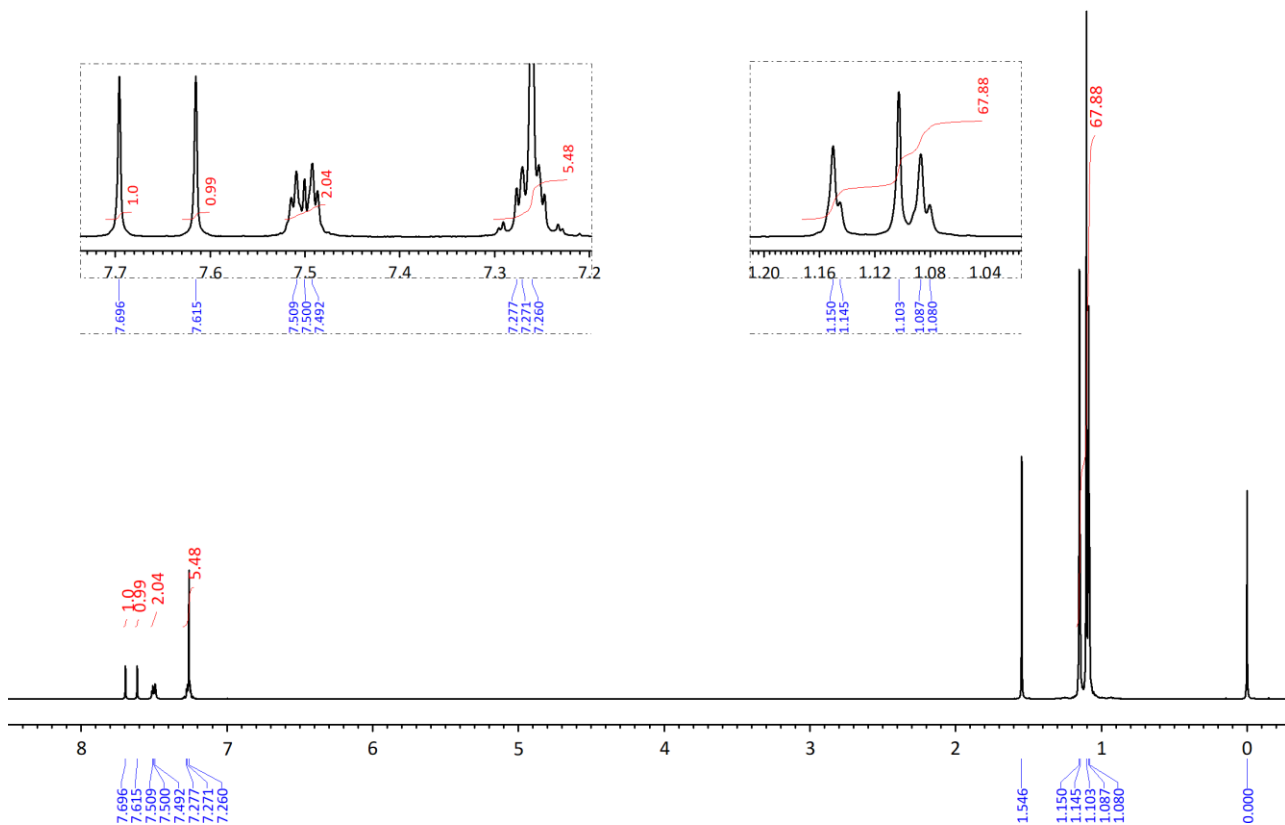
Data Name: common/Nov21-a51294-
Sample: u1 katoono / 5Bo412
Experiment Date/Time: 2023/11/21 10:16:04

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..6400
Spectrum Time Range: Average(MS[1] Time:0.50..0.51)

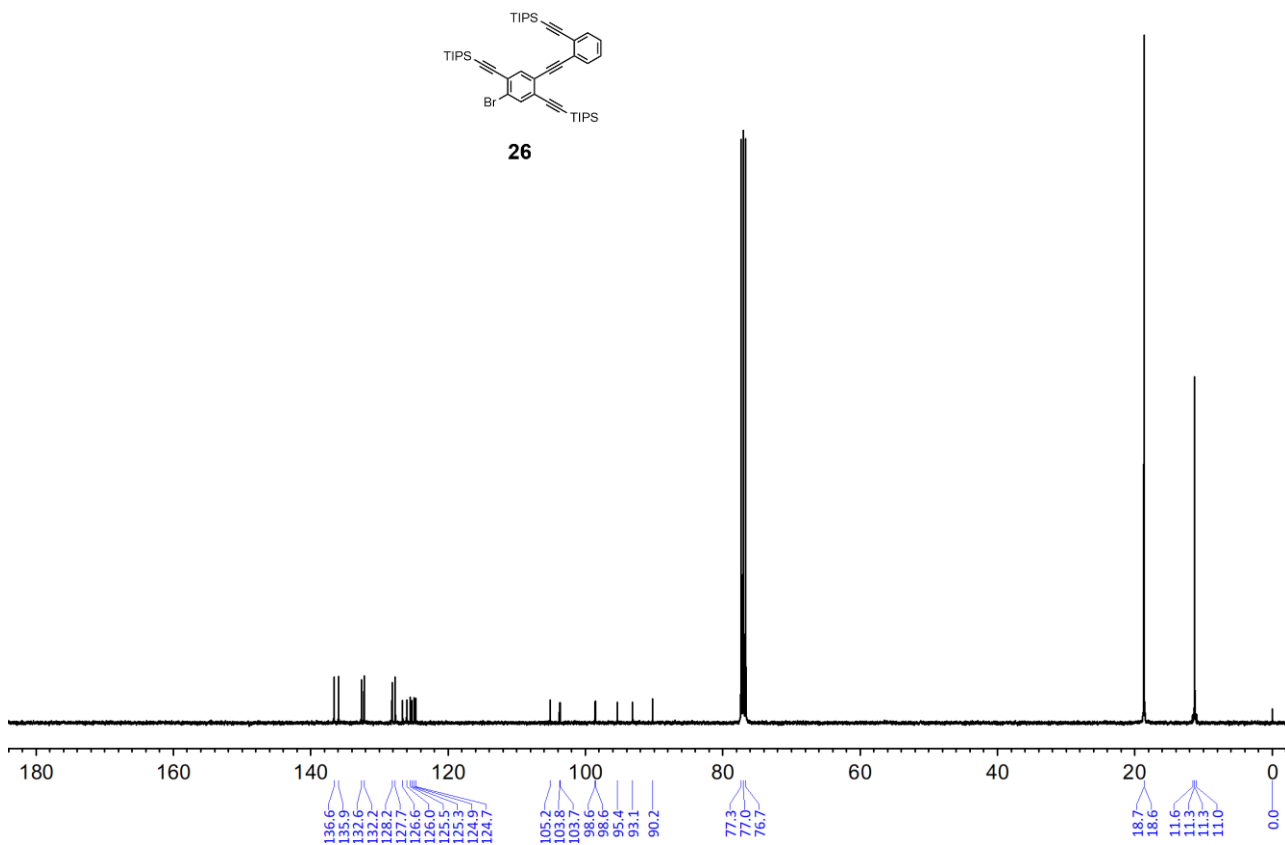
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **5B**.



¹H NMR spectrum (400 MHz) of **26**, measured in CDCl₃ at room temperature.

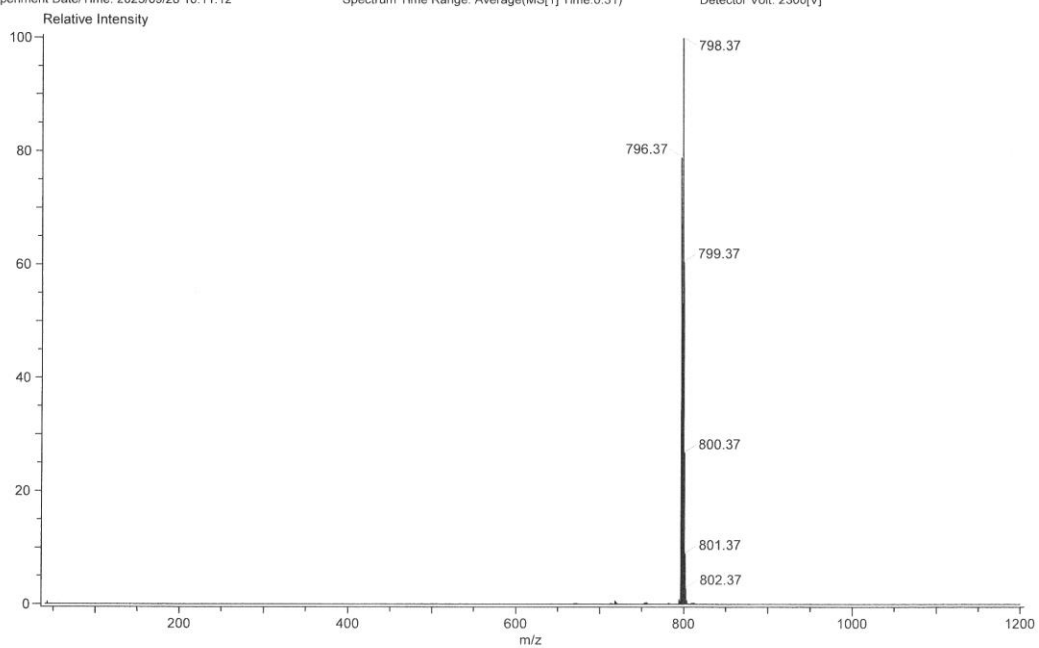


¹³C NMR spectrum (100 MHz) of **26**, measured in CDCl₃ at room temperature.

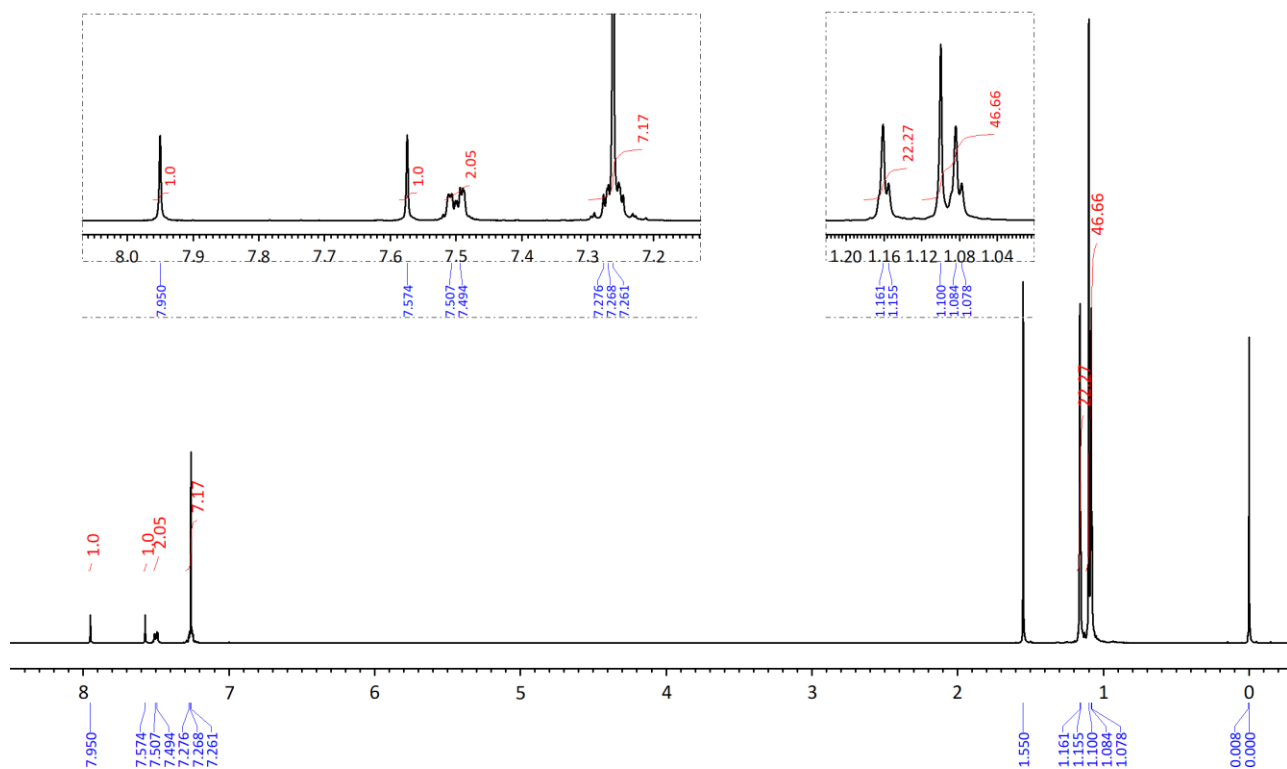
Data Name: common/Sep28.a51209-
Sample: u1 katono / 796
Experiment Date/Time: 2023/09/28 10:11:12

Instrument: JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40_3200
Spectrum Time Range: Average(MS[1]) Time: 0.31)

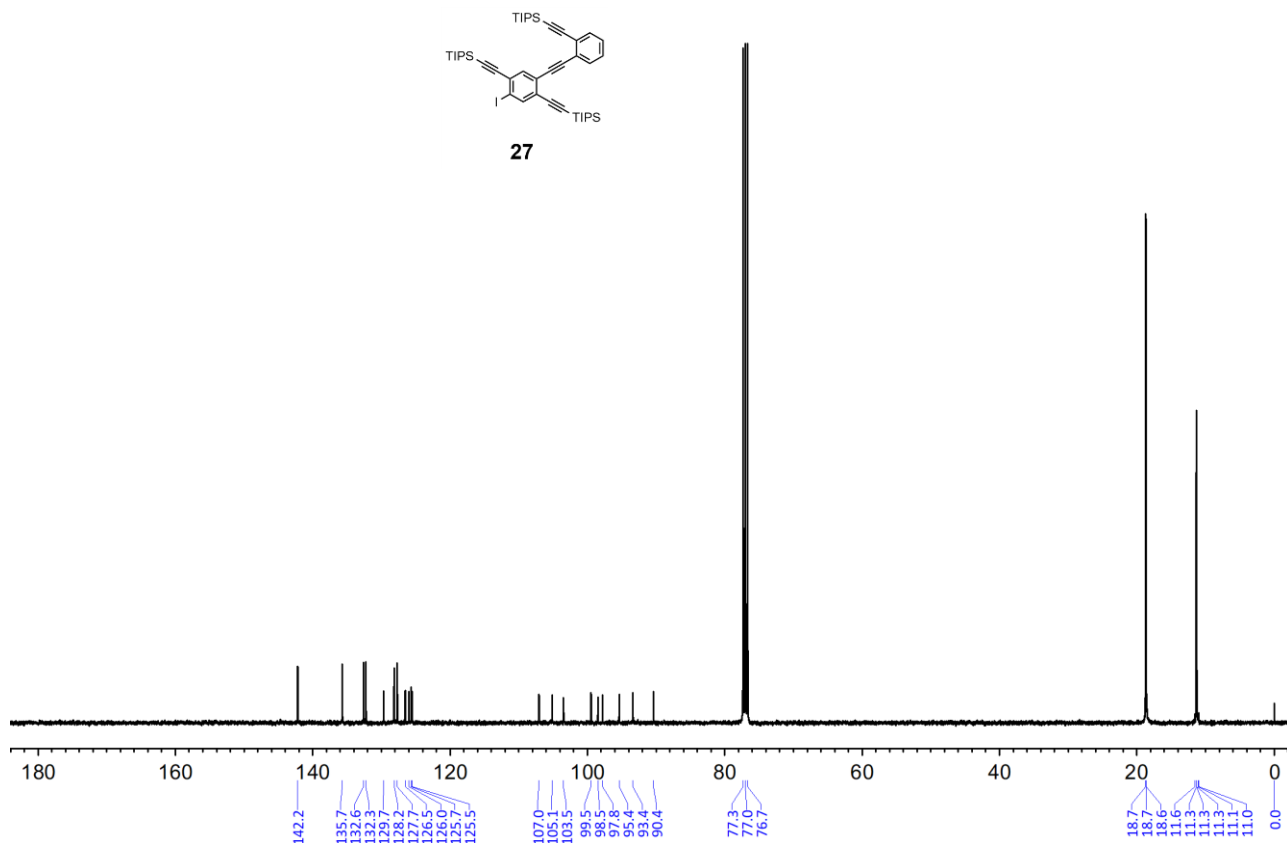
MS Tune Method Name: FD
GC: Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of 26.



¹H NMR spectrum (400 MHz) of **27**, measured in CDCl₃ at room temperature.

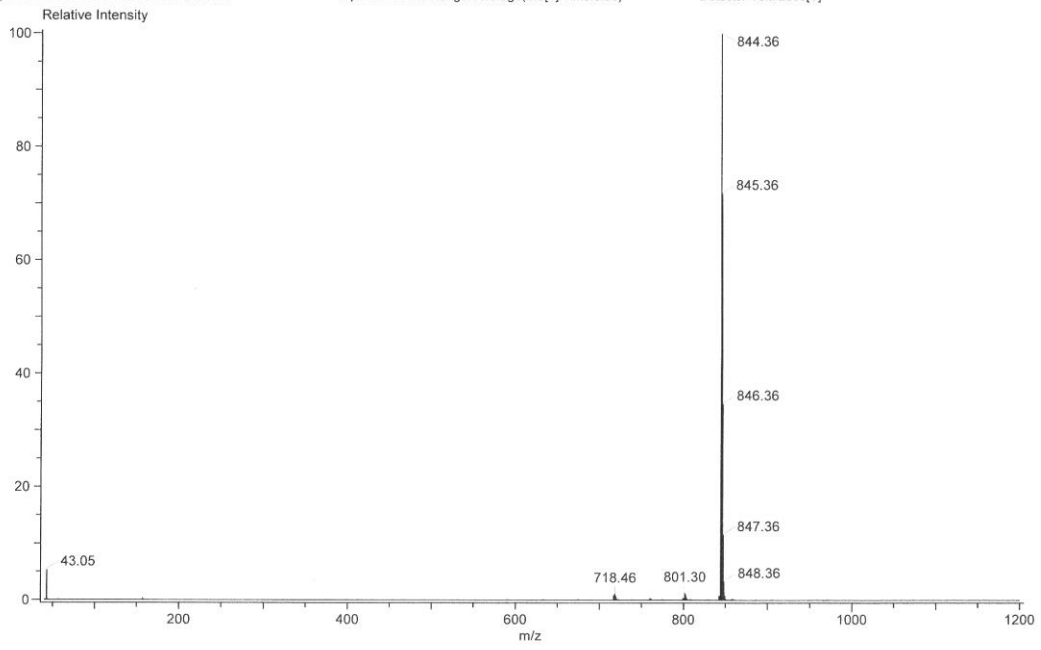


¹³C NMR spectrum (100 MHz) of **27**, measured in CDCl₃ at room temperature.

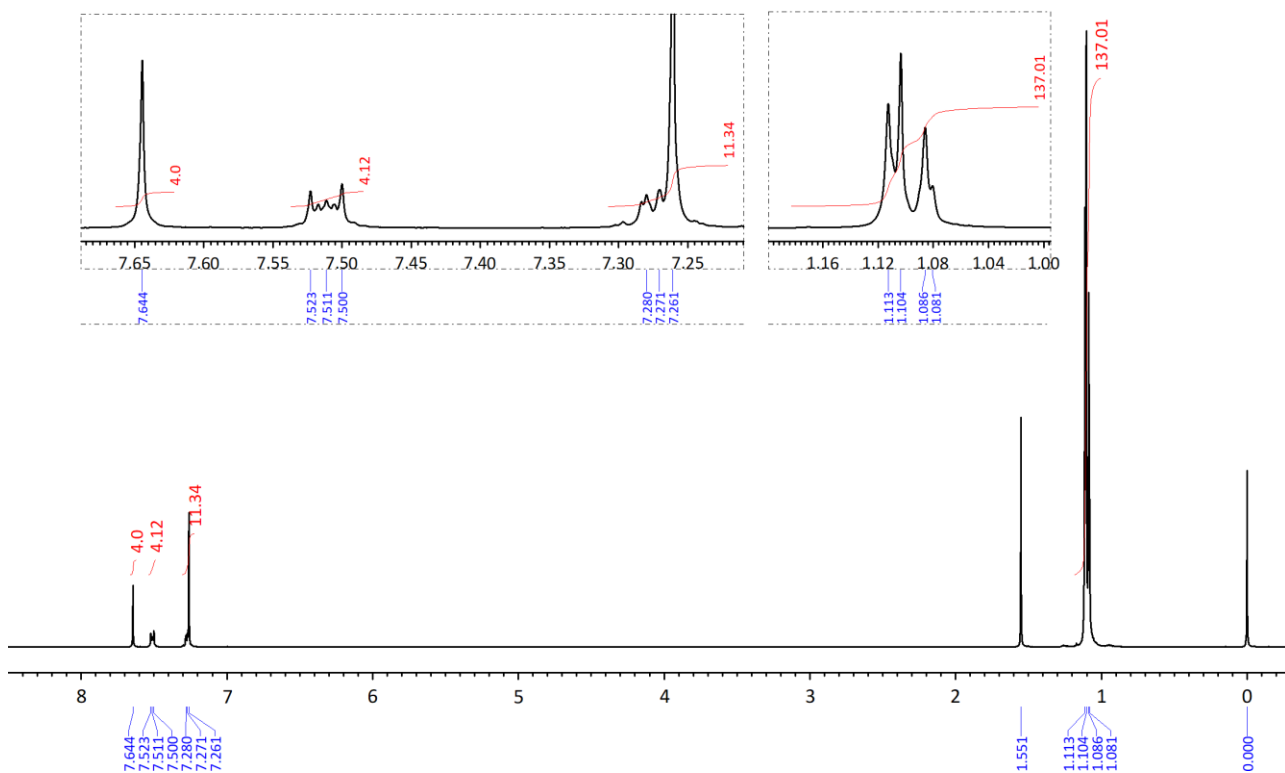
Data Name: common/Sep28.a51210-
Sample: u1 kalone / 1065
Experiment Date/Time: 2023/09/28 10:18:41

Instrument: JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40..3200
Spectrum Time Range: Average(MS[1]) Time:0.35)

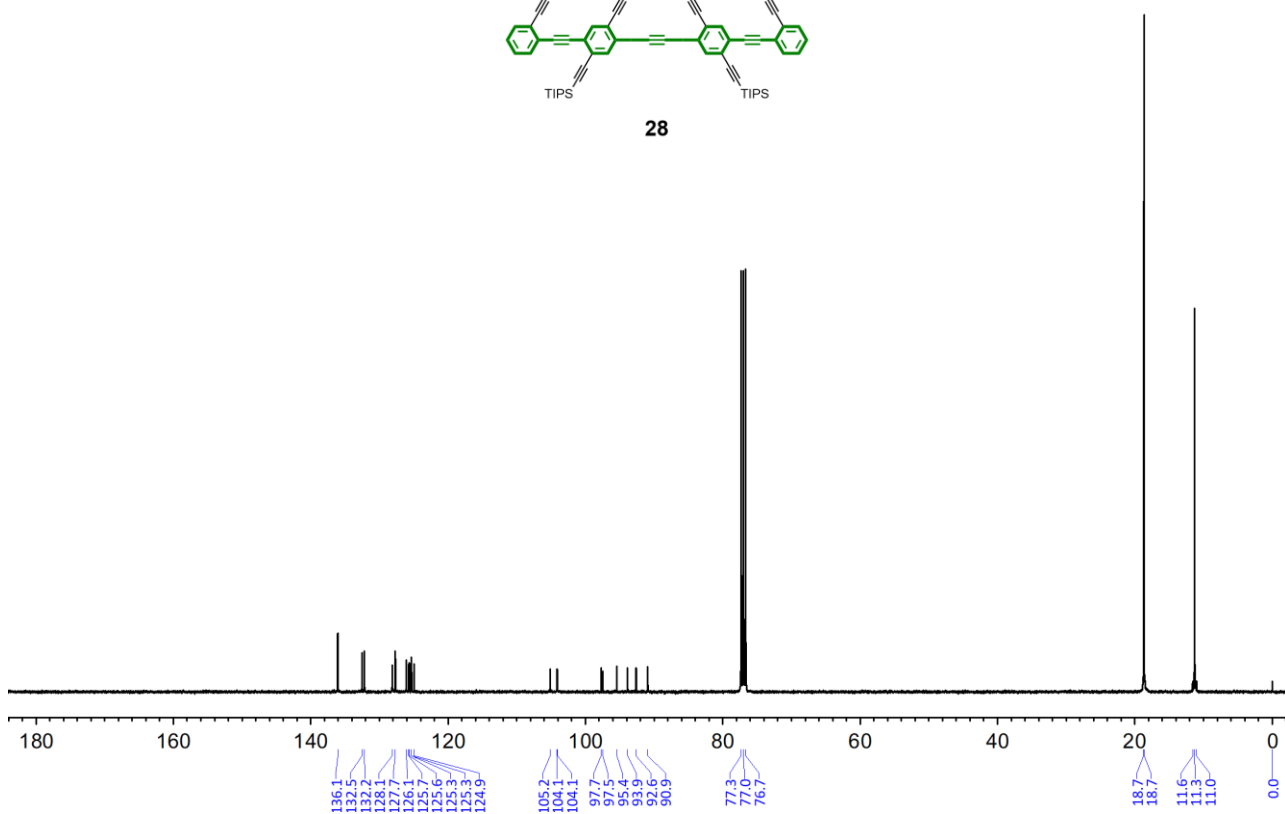
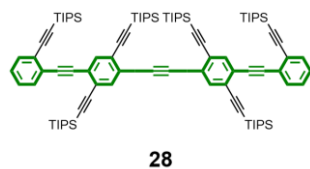
MS Tune Method Name: FD
GC: Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **27**.



¹H NMR spectrum (400 MHz) of **28**, measured in CDCl₃ at room temperature.

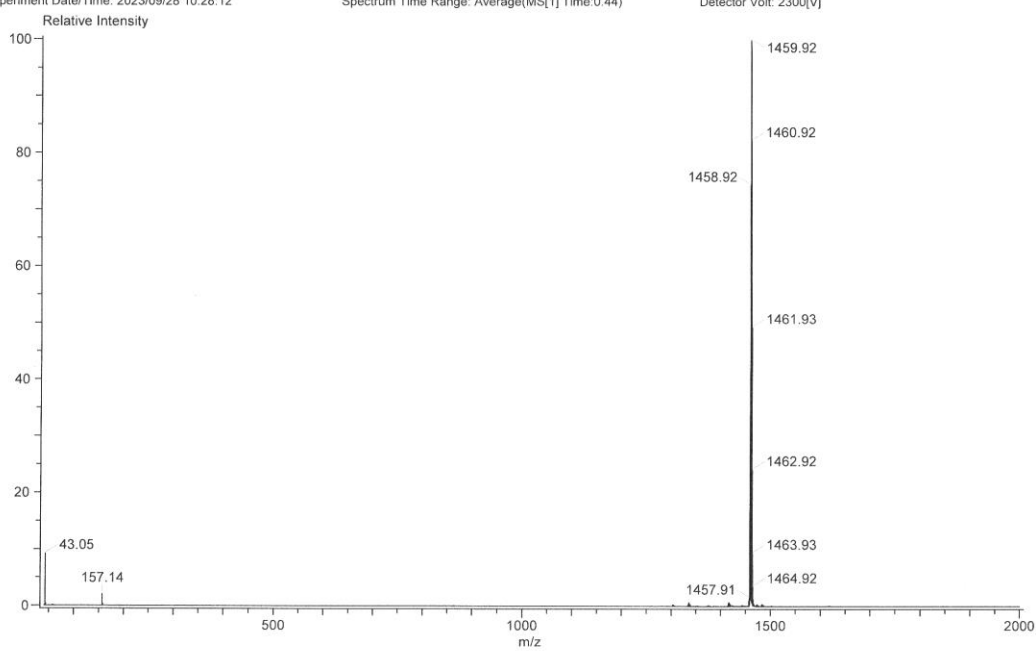


¹³C NMR spectrum (100 MHz) of **28**, measured in CDCl₃ at room temperature.

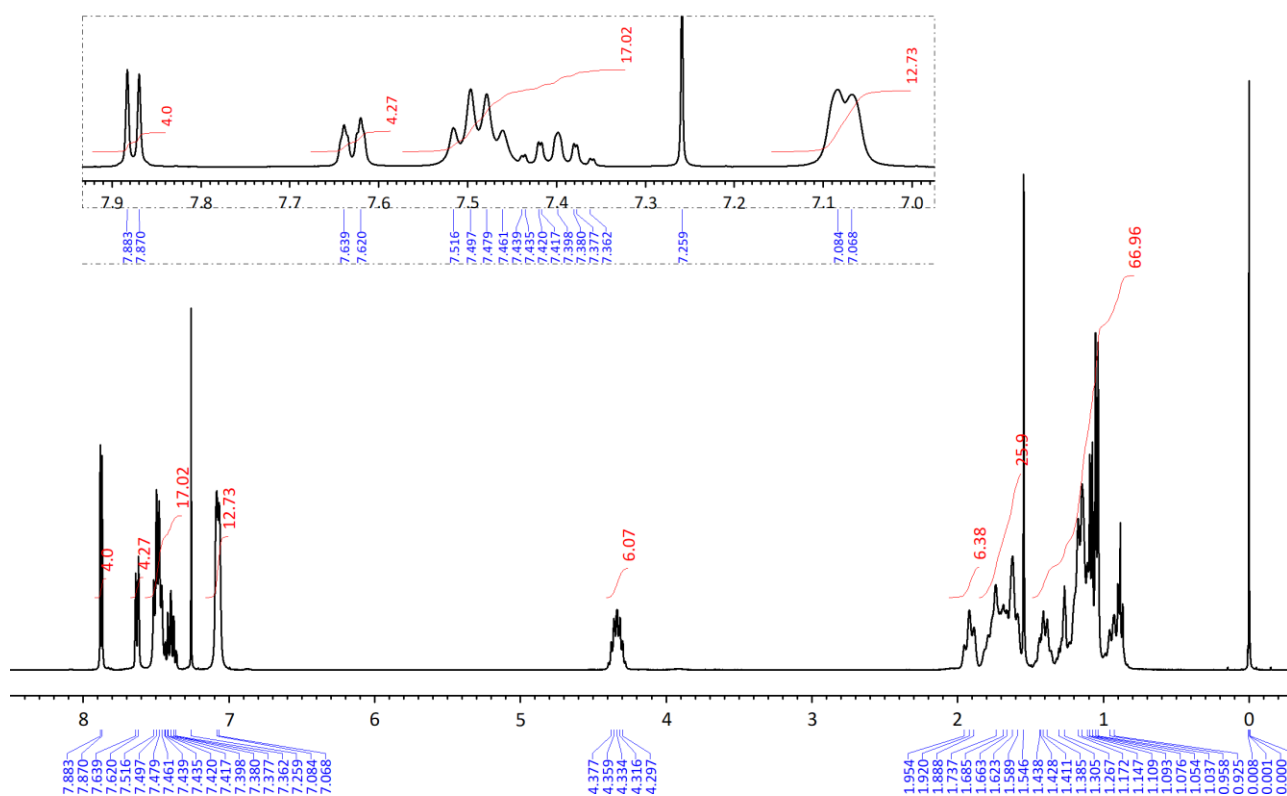
Data Name: common/Sep28.a51211-
Sample: u1 katonu / 1067
Experiment Date/Time: 2023/09/28 10:28:12

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40. 3200
Spectrum Time Range: Average(MS[1] Time 0.44)

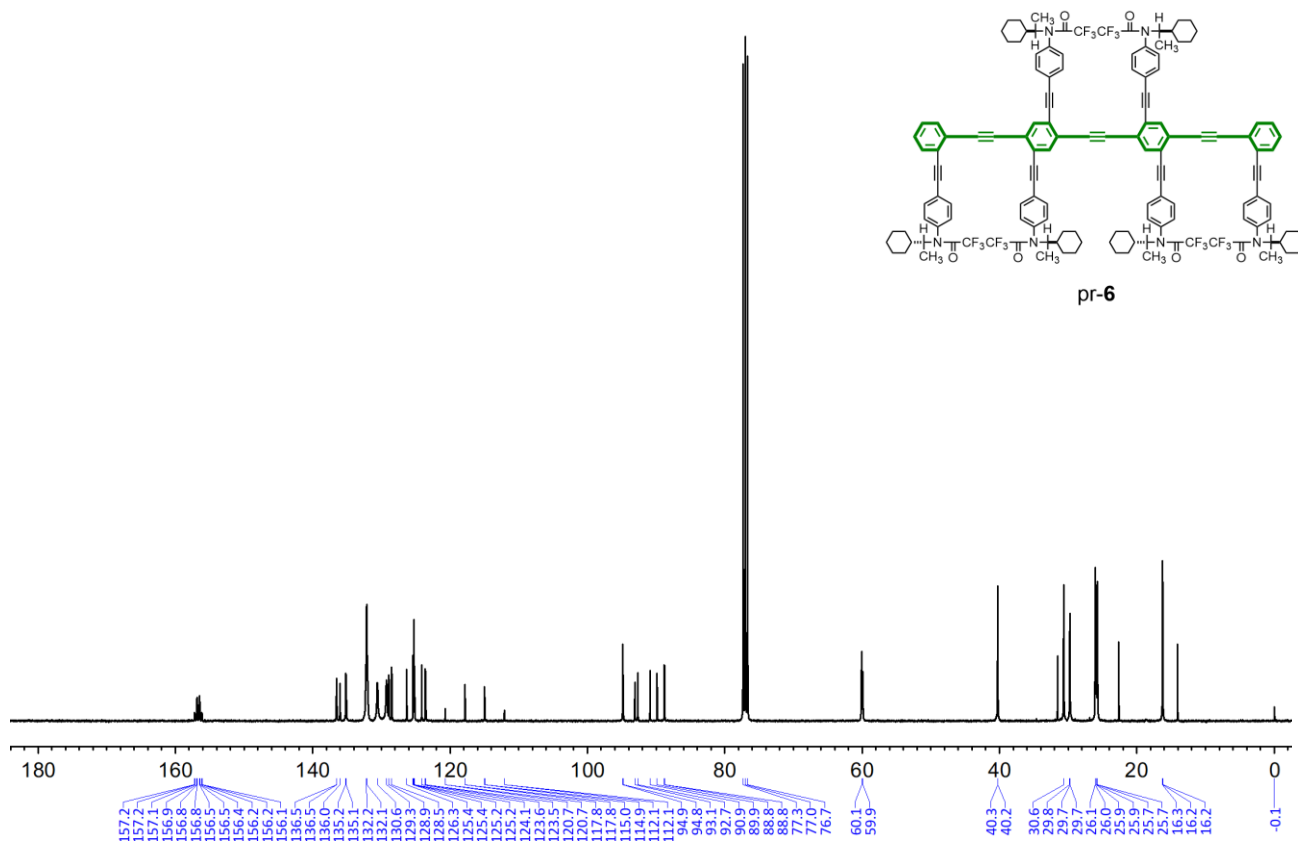
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of **28**.



¹H NMR spectrum (400 MHz) of pr-6, measured in CDCl₃ at room temperature.

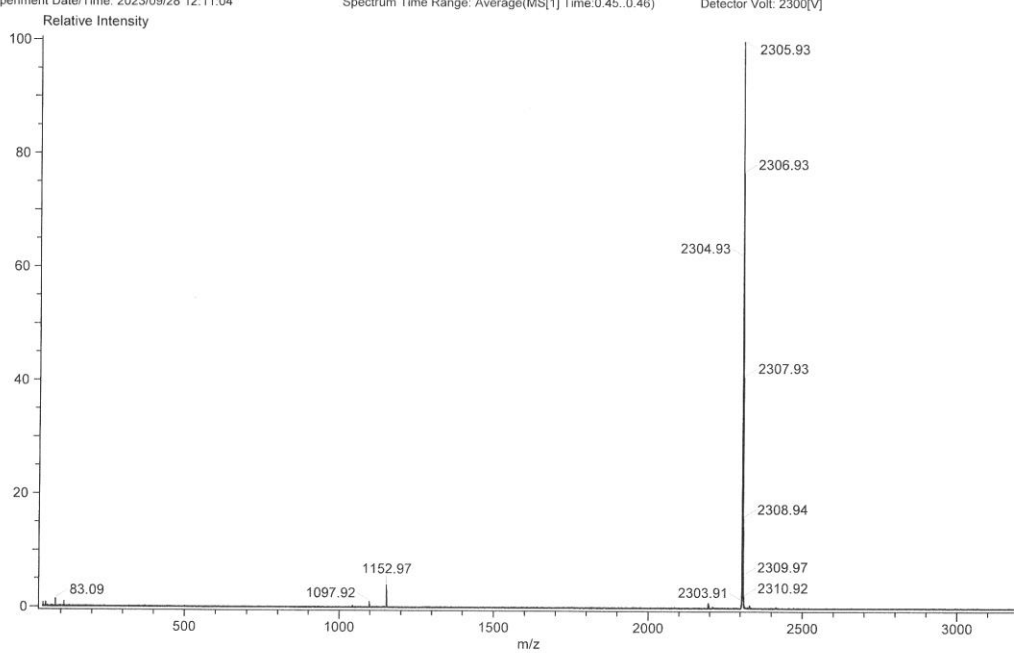


¹³C NMR spectrum (100 MHz) of pr-6, measured in CDCl₃ at 303 K.

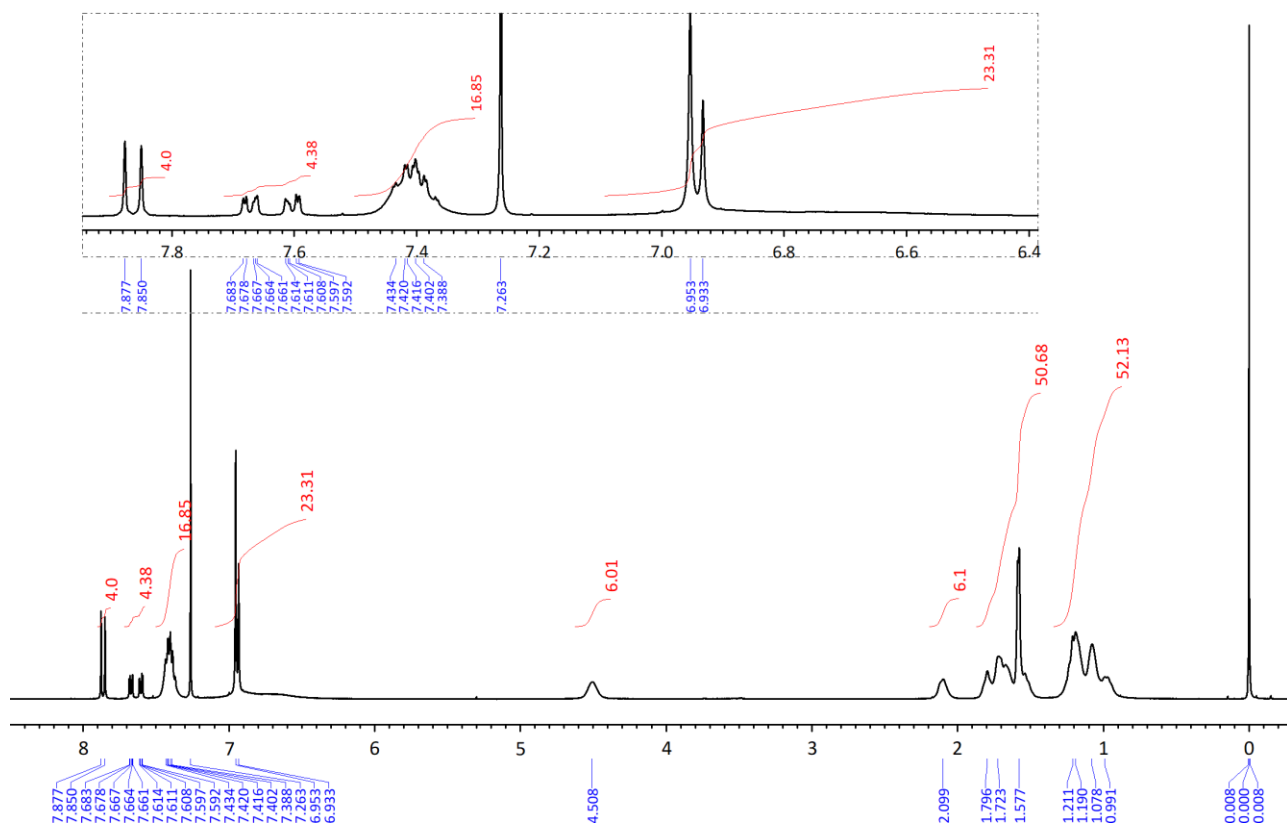
Data Name: common/Sep28.a51212-
Sample: u1 kato / 1071
Experiment Date/Time: 2023/09/28 12:11:04

Instrument:JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40. 3200
Spectrum Time Range: Average(MS[1]) Time:0.45. 0.46)

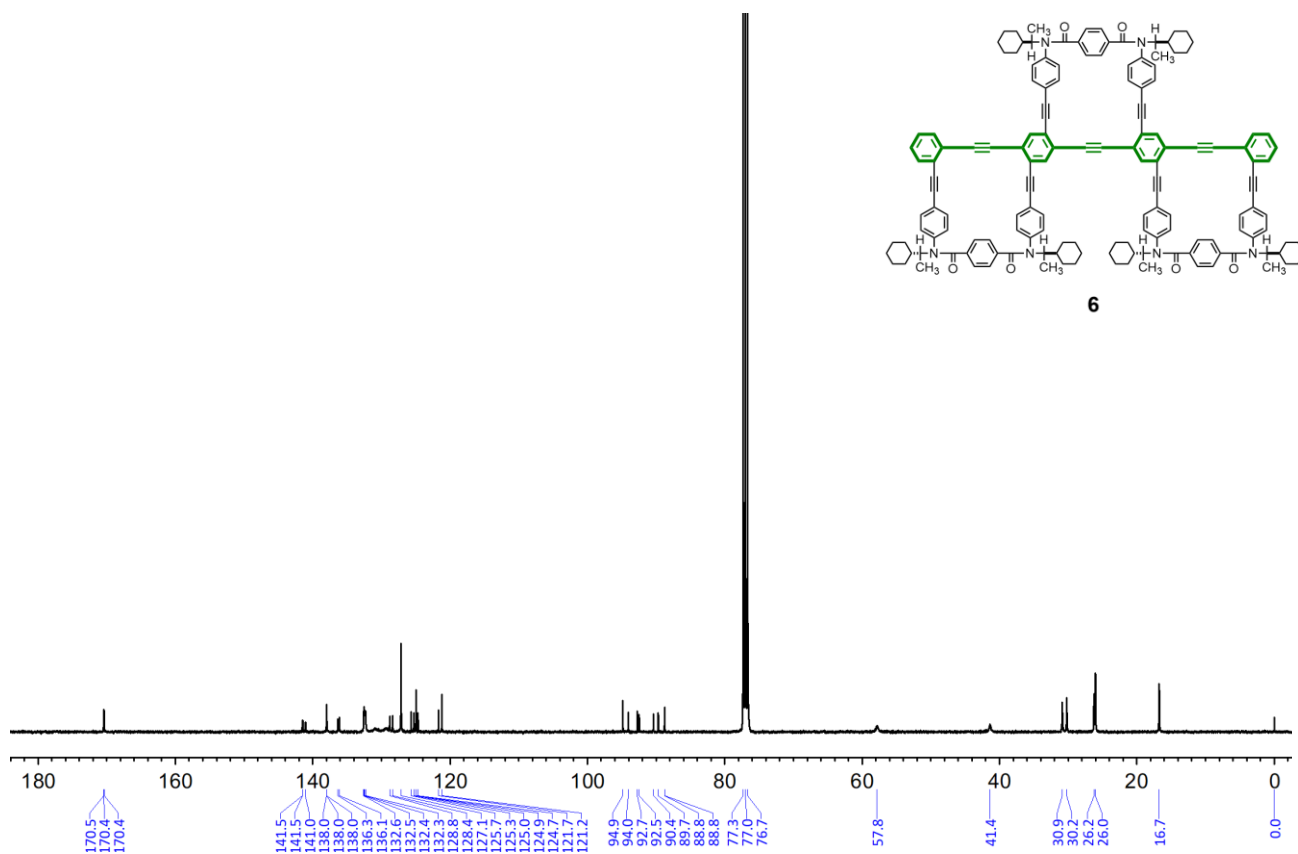
MS Tune Method Name: FD
GC:Agilent7890A, Method: -
Detector Volt: 2300[V]



LRMS (FD) of pr-6.



¹H NMR spectrum (400 MHz) of **6**, measured in CDCl₃ at 303 K.

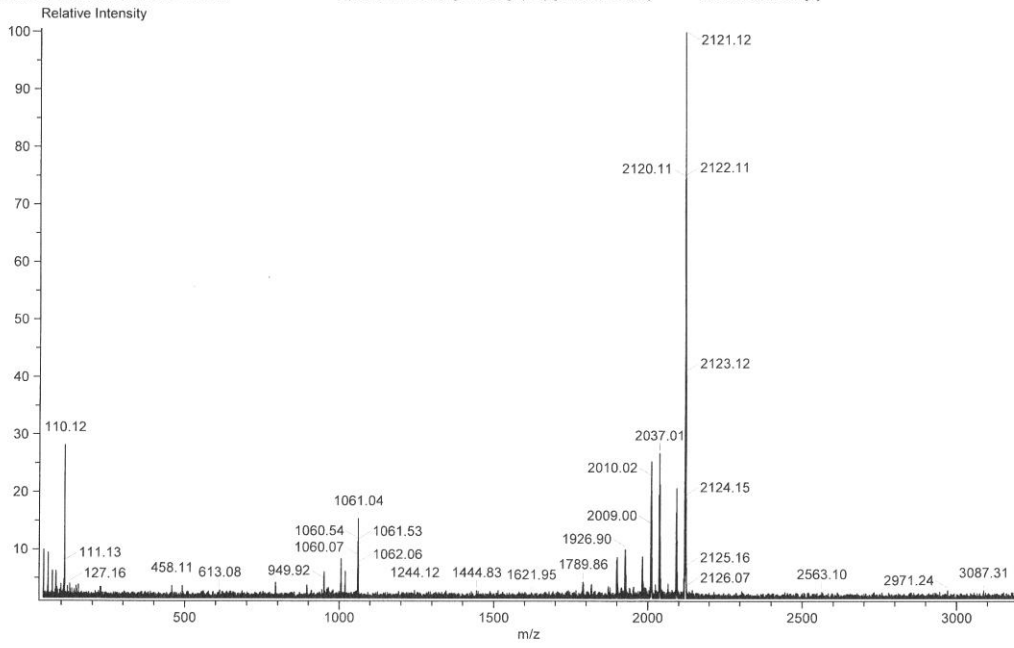


¹³C NMR spectrum (100 MHz) of **6**, measured in CDCl₃ at 303 K.

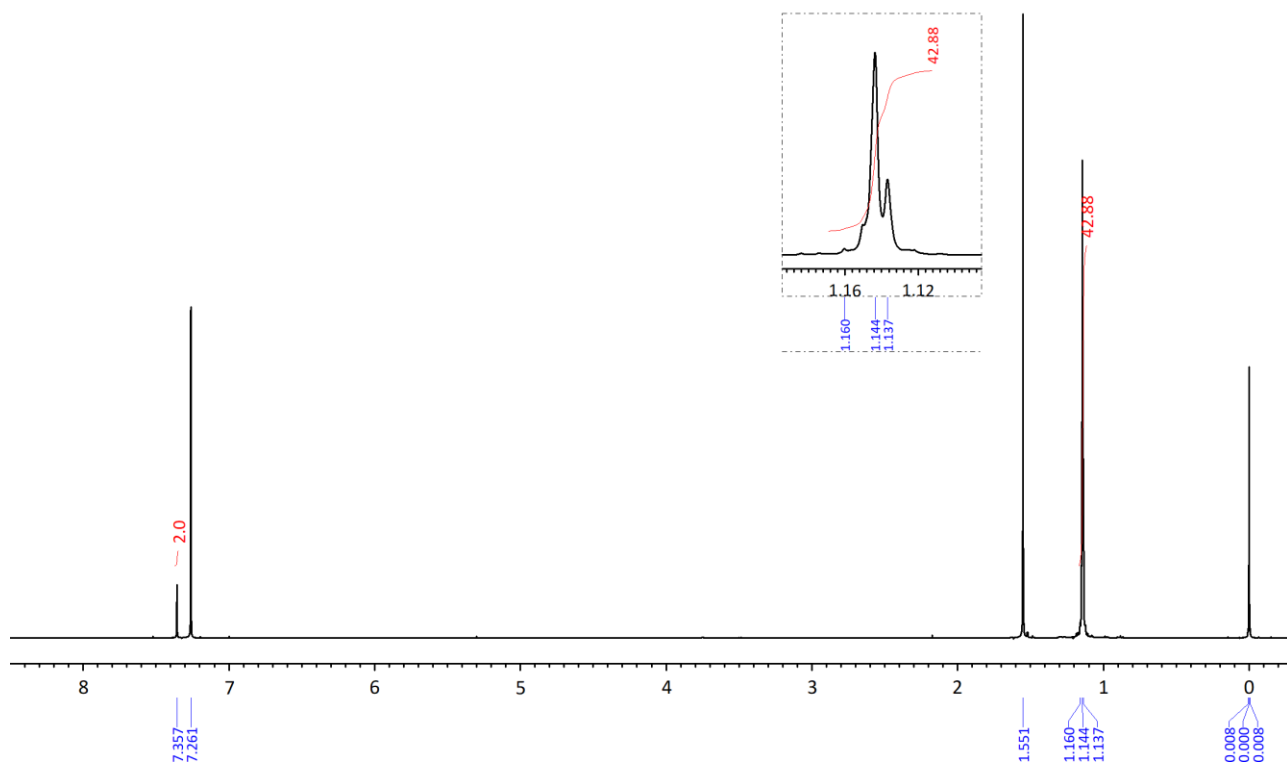
Data Name: common/Oct10_a51213-
Sample: u1 katoono / 1080
Experiment Date/Time: 2023/10/10 11:52:46

Instrument: JMST-100GCV, Ionization Mode: 1:FD+
Acquired m/z Range: 40. 3200
Spectrum Time Range: Average(MS[1]) Time:0.24..0.29

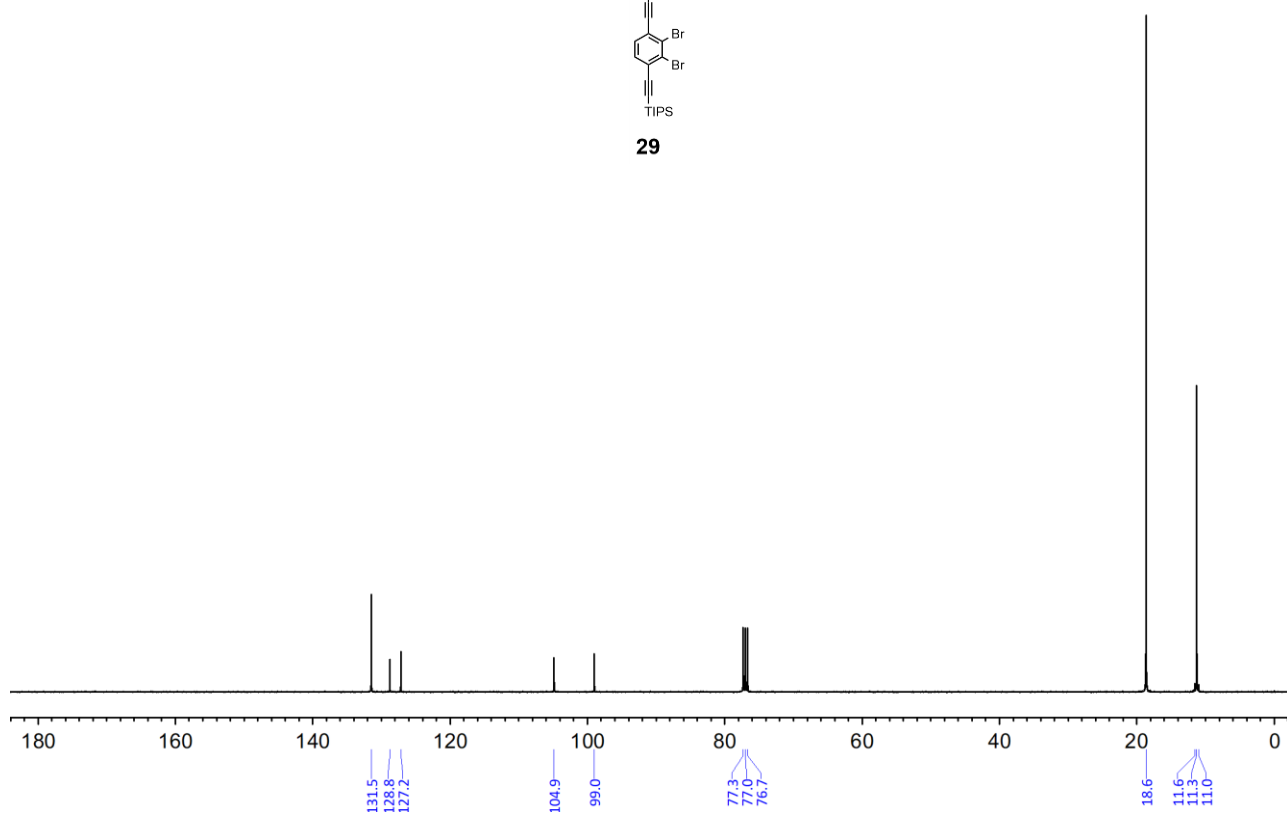
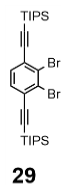
MS Tune Method Name: FD
GC: Agilent7890A, Method: -
Detector Volt: 2500[V]



LRMS (FD) of 6.



^1H NMR spectrum (400 MHz) of **29**, measured in CDCl_3 at room temperature.

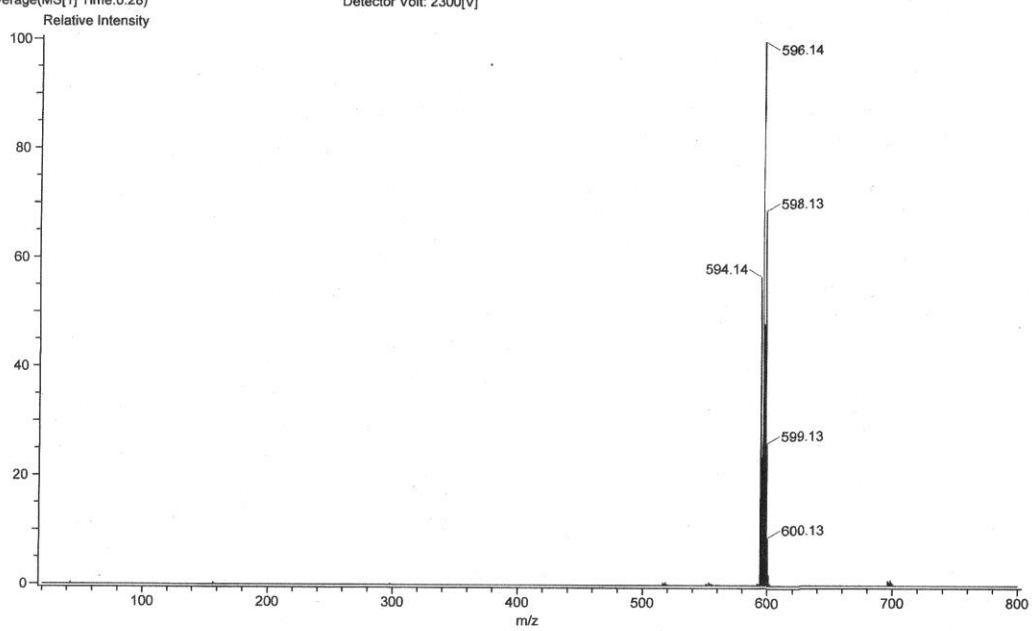


^{13}C NMR spectrum (100 MHz) of **29**, measured in CDCl_3 at room temperature.

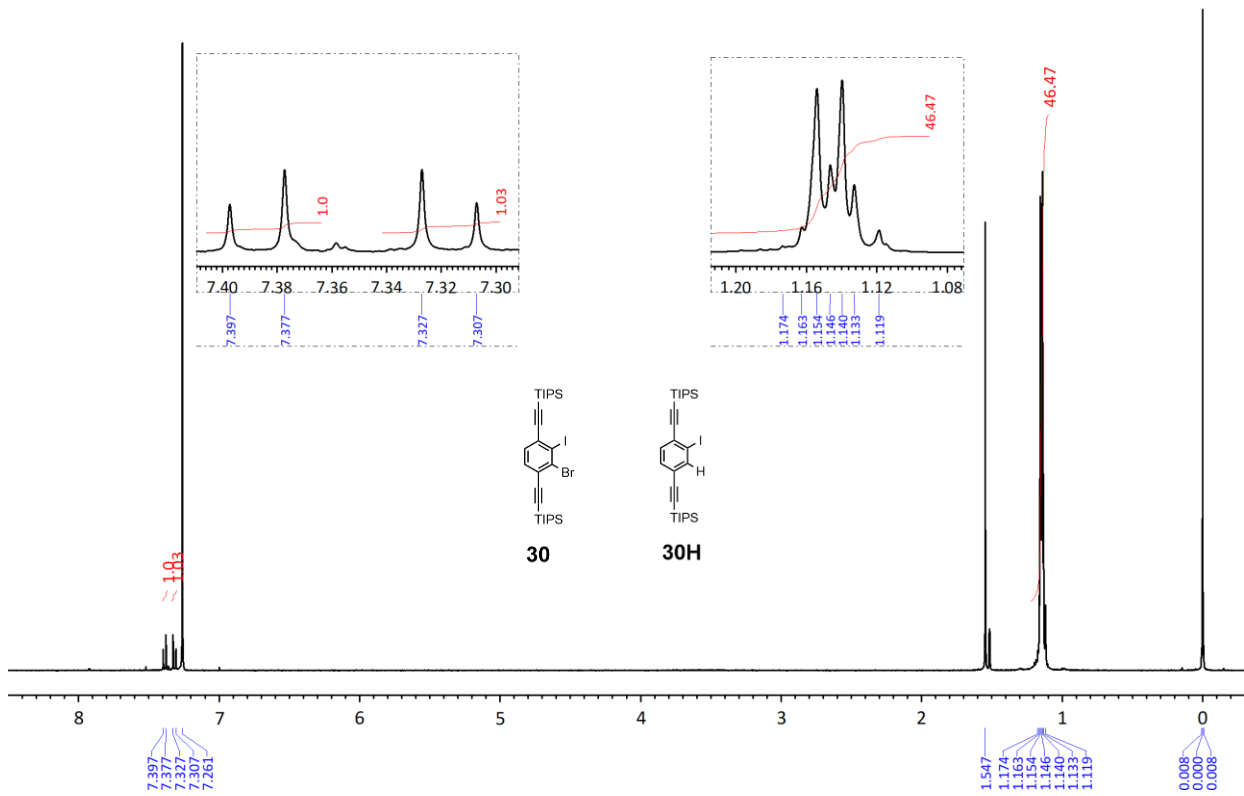
Data: common/May30:a90113-
Sample: 3396 Aoki / HA003-02
Experiment Date/Time: 2017/05/30 12:48:49
Average(MS[1] Time:0.28)

Instrument Configuration: FDプローブ,JMS-T100GCV
Ionization Mode: FD+
Acquired m/z Range: 20.00..1600.00
Detector Volt: 2300[V]

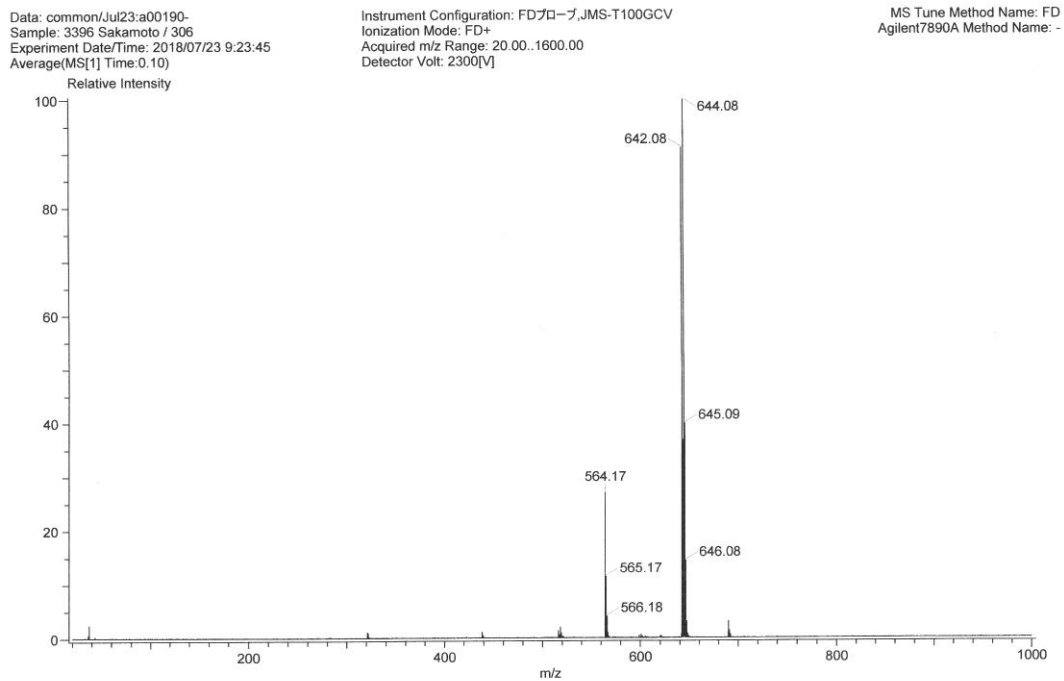
MS Tune Method Name: FD
Agilent7890A Method Name: -



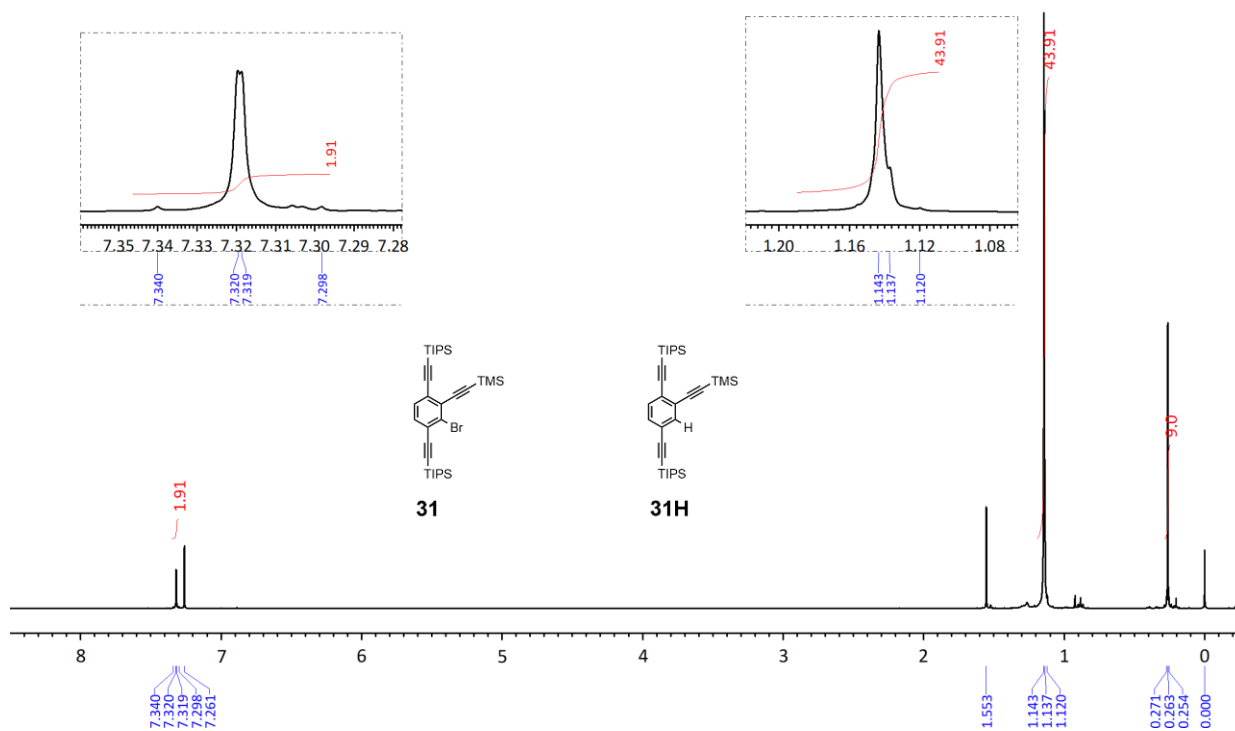
LRMS (FD) of **29**.



^1H NMR spectrum (400 MHz) of **30/30H**, measured in CDCl_3 at room temperature.



LRMS (FD) of **30/30H**.

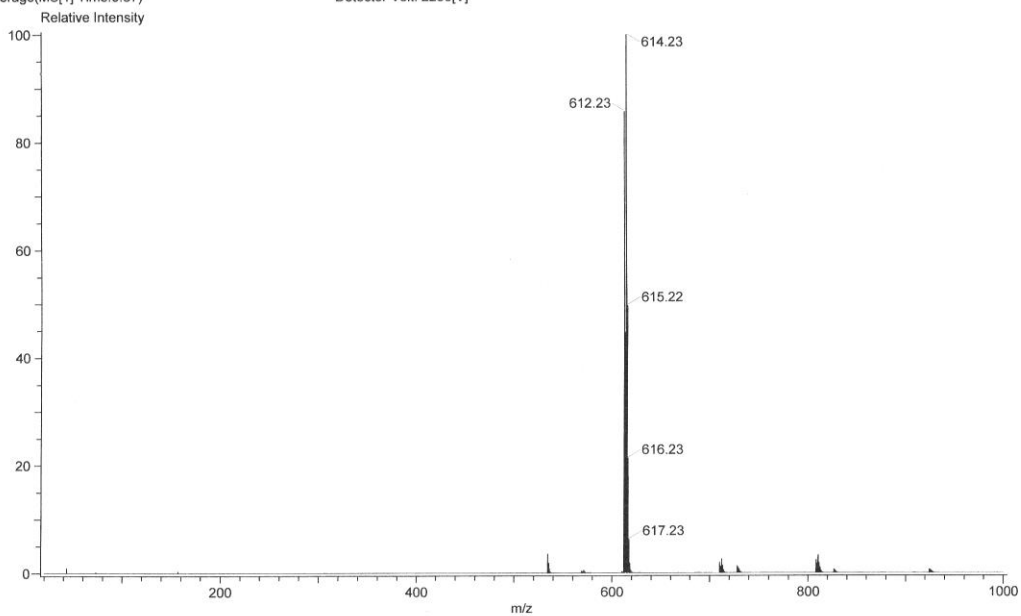


^1H NMR spectrum (400 MHz) of **31/31H**, measured in CDCl_3 at room temperature.

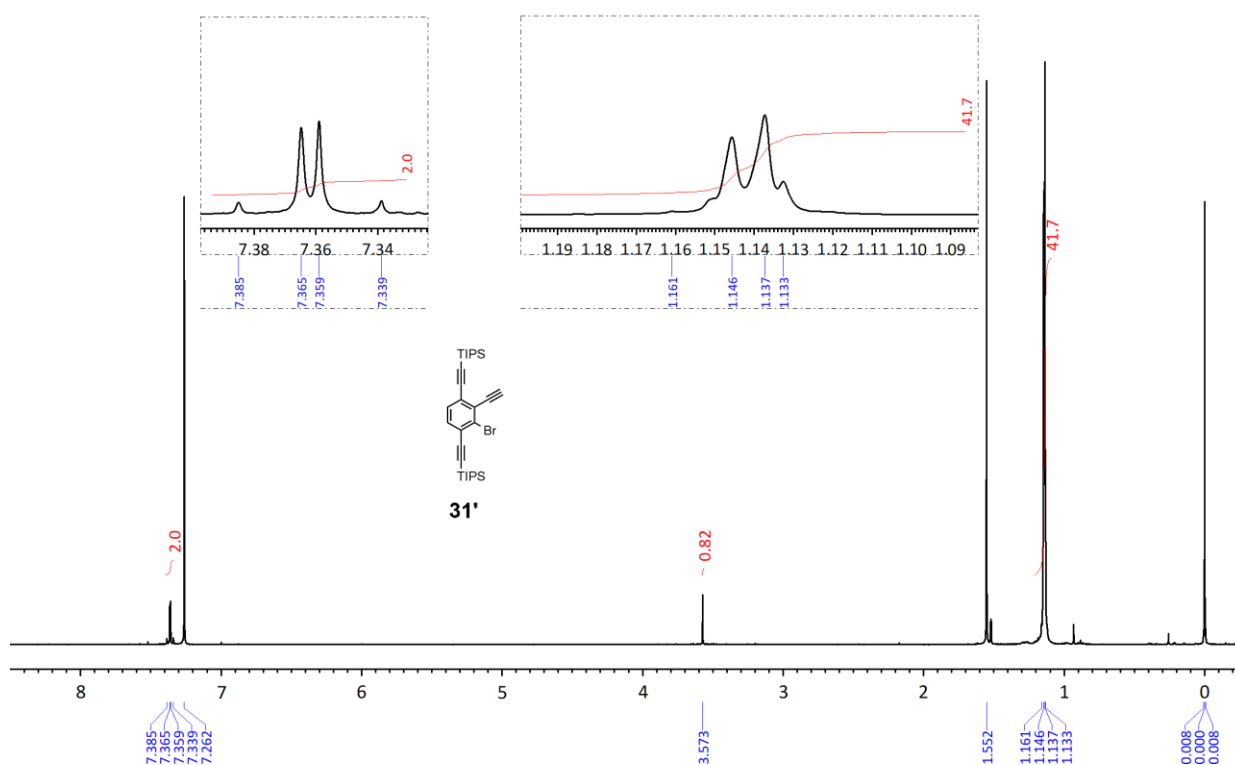
Data: common/Jul25:a00203-2
 Sample: 3396 Sakamoto / 307
 Experiment Date/Time: 2018/07/25 8:41:29
 Average(MS[1] Time:0.37)

Instrument Configuration: FDフロー-FJMS-T100GCV
 Ionization Mode: FD+
 Acquired m/z Range: 20.00..1600.00
 Detector Volt: 2250[V]

MS Tune Method Name: FD
 Agilent7890A Method Name: -



LRMS (FD) of **31/31H**.

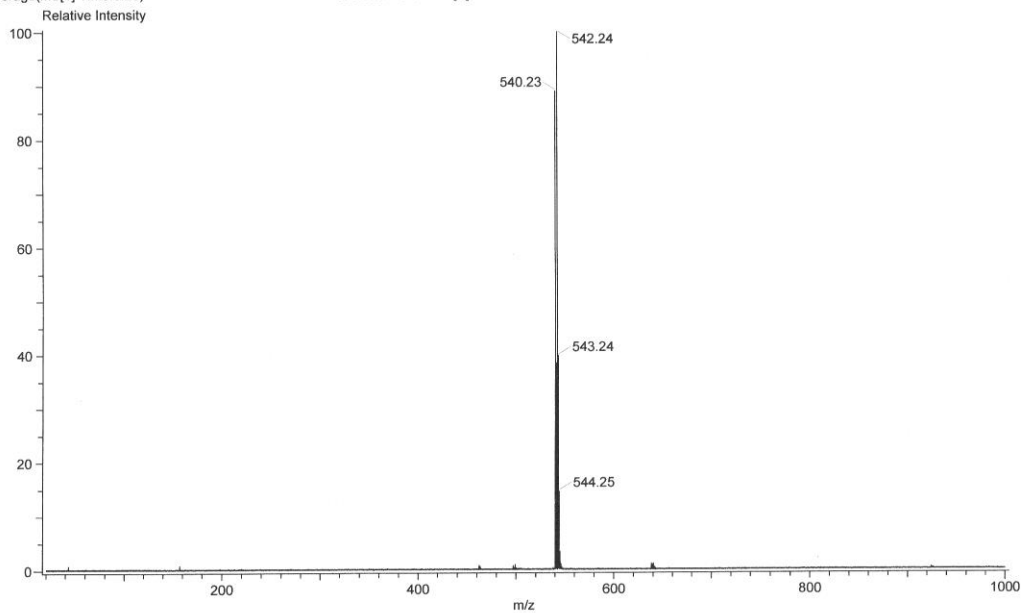


¹H NMR spectrum (400 MHz) of **31'**, measured in CDCl₃ at room temperature.

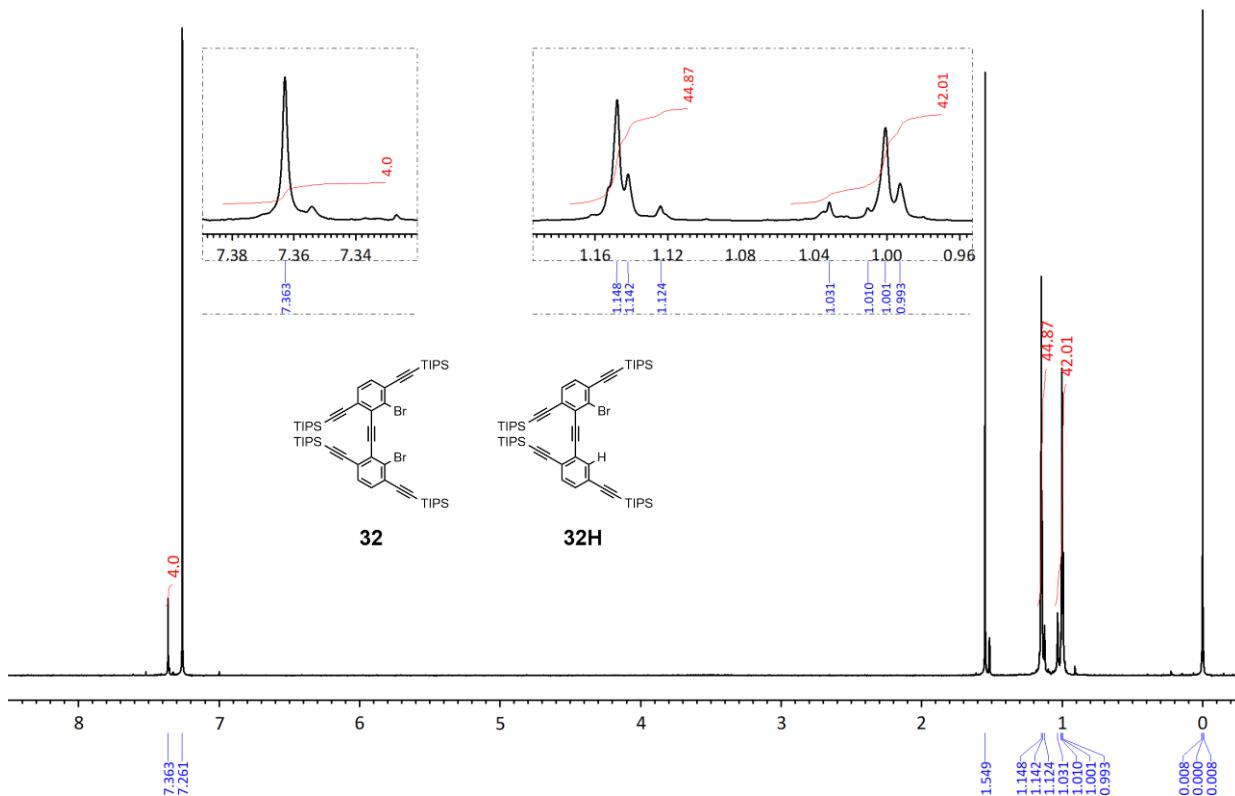
Data: common/Jul25:a00208-
 Sample: 3396 Sakamoto / 308
 Experiment Date/Time: 2018/07/25 15:43:04
 Average(MS[1] Time:0.28)

Instrument Configuration: FDフローブ,JMS-T100GCV
 Ionization Mode: FD+
 Acquired m/z Range: 20.00..1600.00
 Detector Volt: 2300[V]

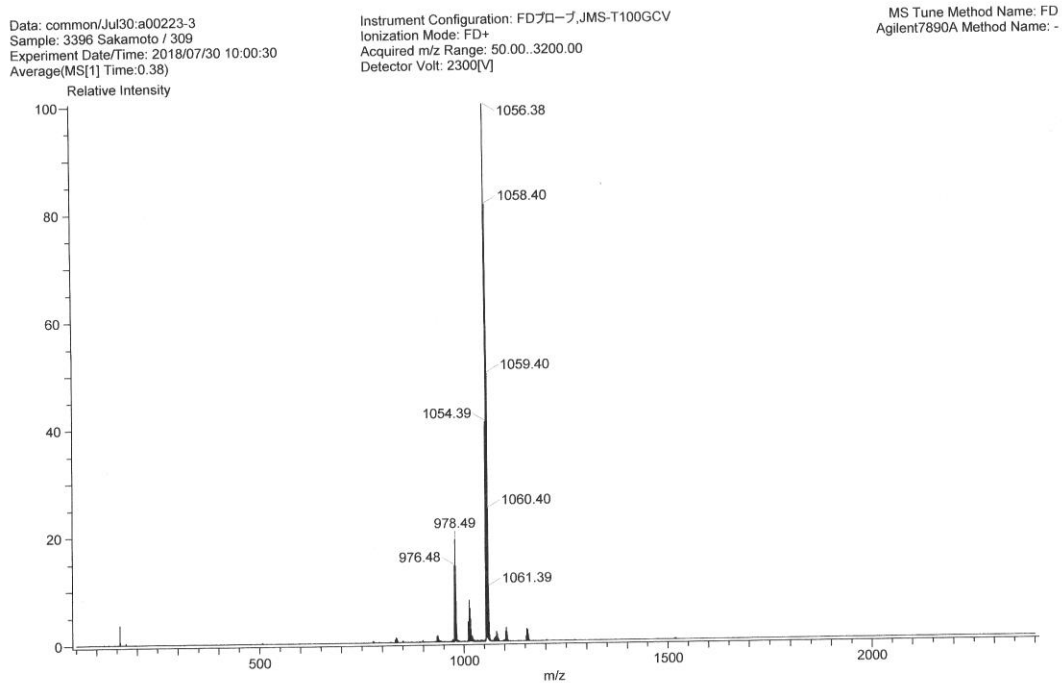
MS Tune Method Name: FD
 Agilent7890A Method Name: -



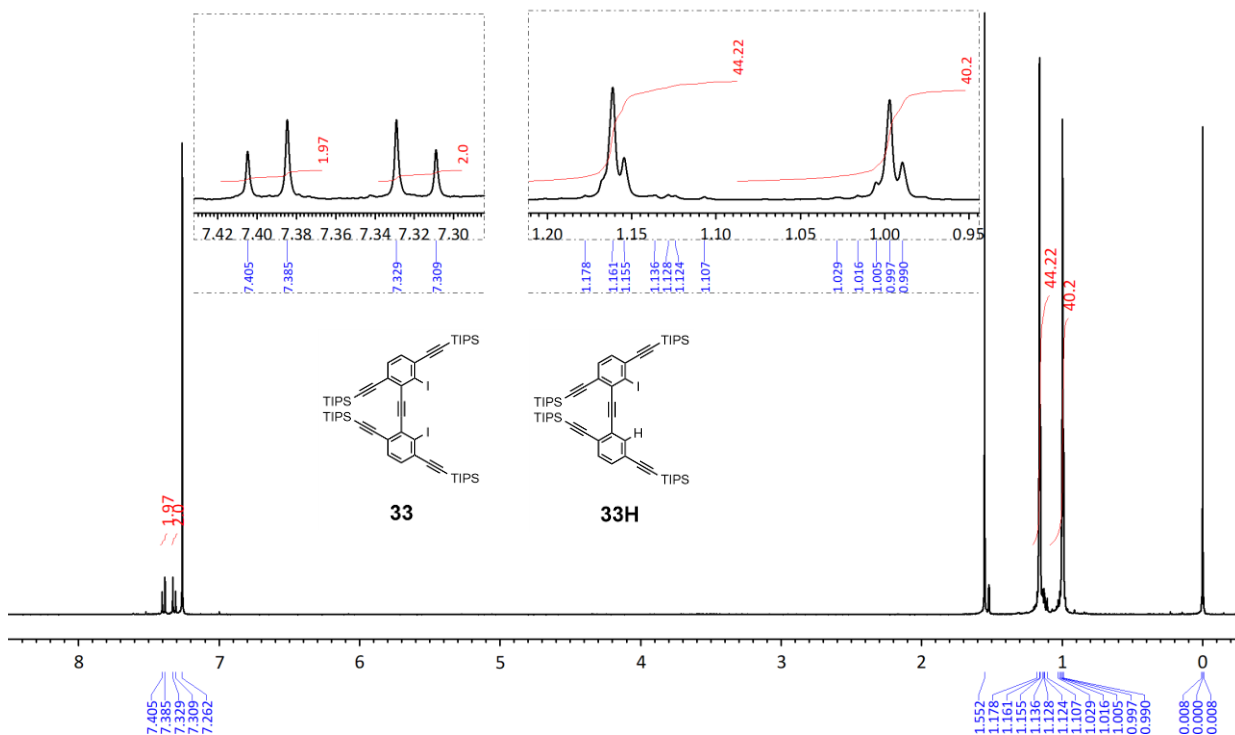
LRMS (FD) of **31'**.



^1H NMR spectrum (400 MHz) of **32/32H**, measured in CDCl_3 at room temperature.



LRMS (FD) of **32/32H**.

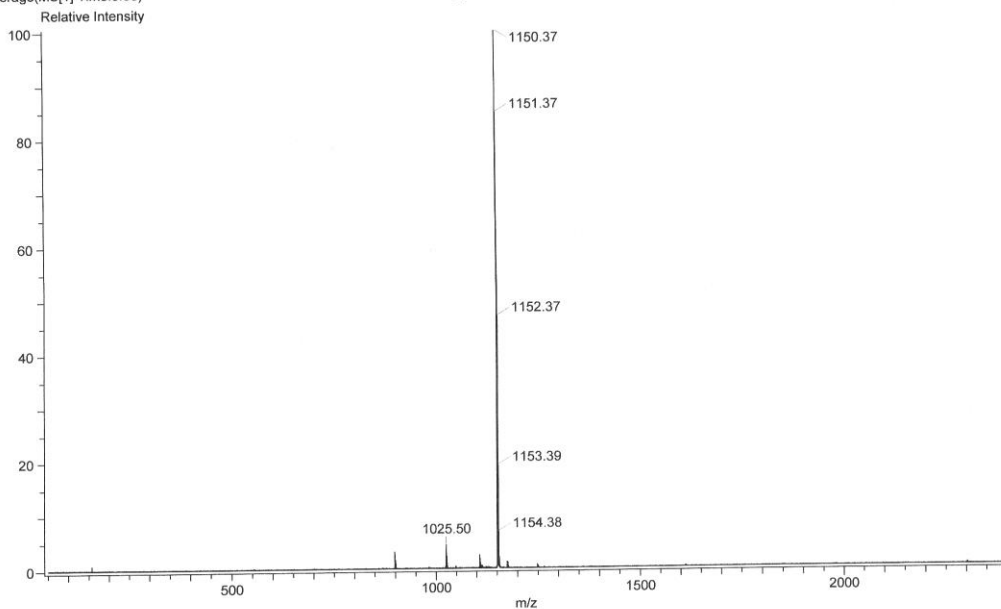


¹H NMR spectrum (400 MHz) of **33/33H**, measured in CDCl₃ at room temperature.

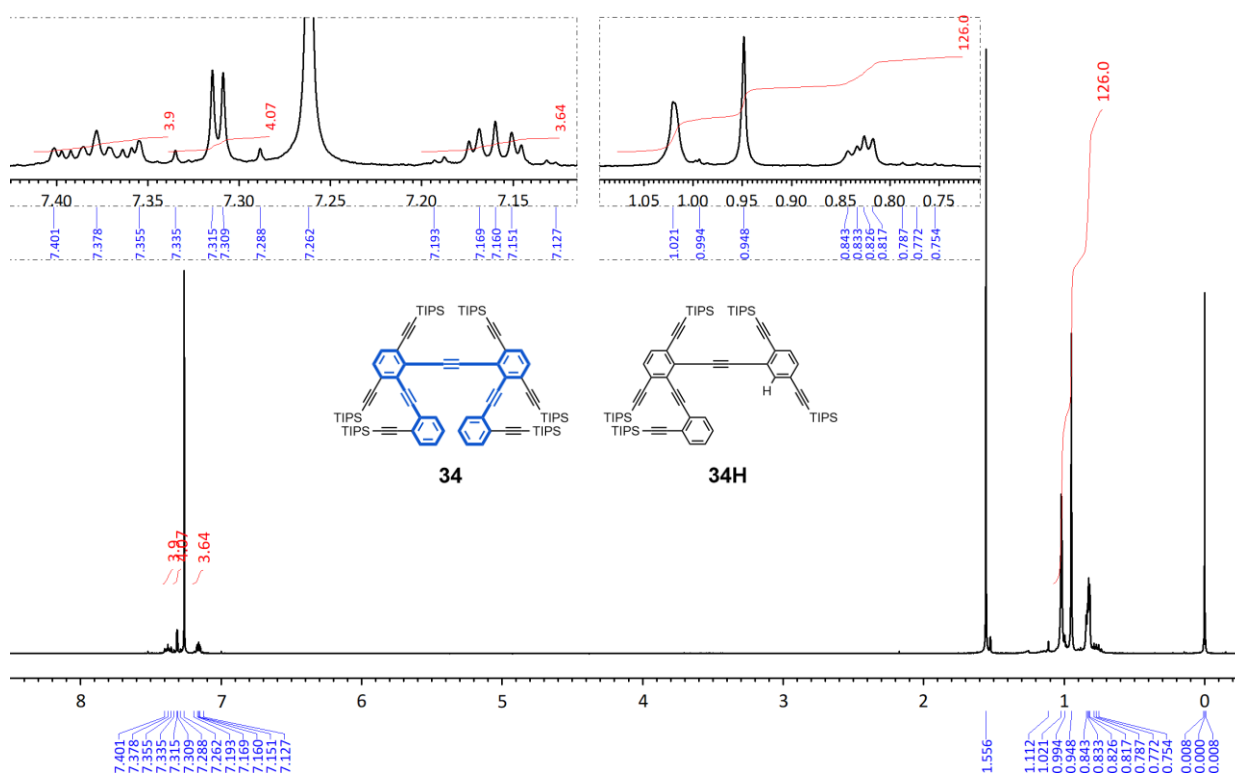
Data: common/Jul30:a00224-
 Sample: 3396 Sakamoto / 310
 Experiment Date/Time: 2018/07/30 10:15:31
 Average(MS[1] Time:0.33)

Instrument Configuration: FDプローブ,JMS-T100GCV
 Ionization Mode: FD+
 Acquired m/z Range: 50.00..3200.00
 Detector Volt: 2300[V]

MS Tune Method Name: FD
 Agilent7890A Method Name: -



LRMS (FD) of **33/33H**.

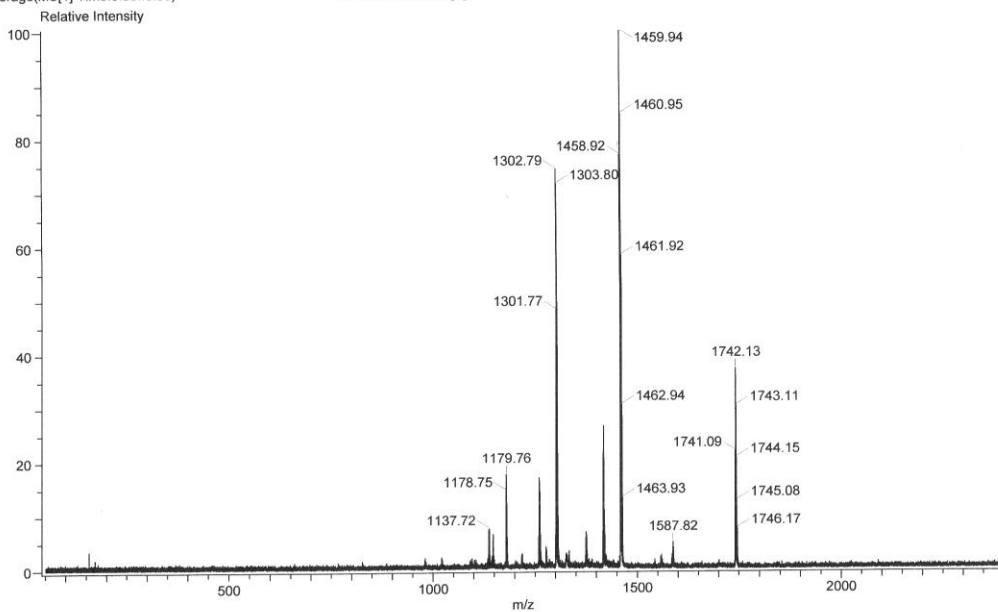


¹H NMR spectrum (400 MHz) of **34/34H**, measured in CDCl₃ at room temperature.

Data: common/Aug07:a00240-3
 Sample: 3396 Sakamoto / 312
 Experiment Date/Time: 2018/08/07 11:15:50
 Average(MS[1] Time:0.35..0.36)

Instrument Configuration: FDプローブ,JMS-T100GCV
 Ionization Mode: FD+
 Acquired m/z Range: 50.00..3200.00
 Detector Volt: 2600[V]

MS Tune Method Name: FD
 Agilent7890A Method Name: -

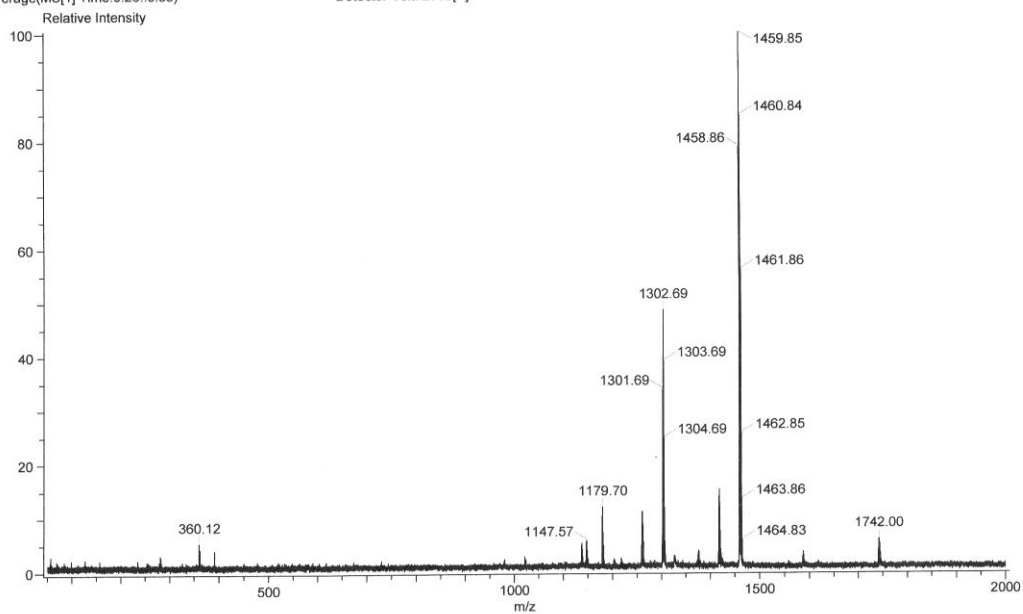


LRMS (FD) of **34/34H** (used to prepare **8**).

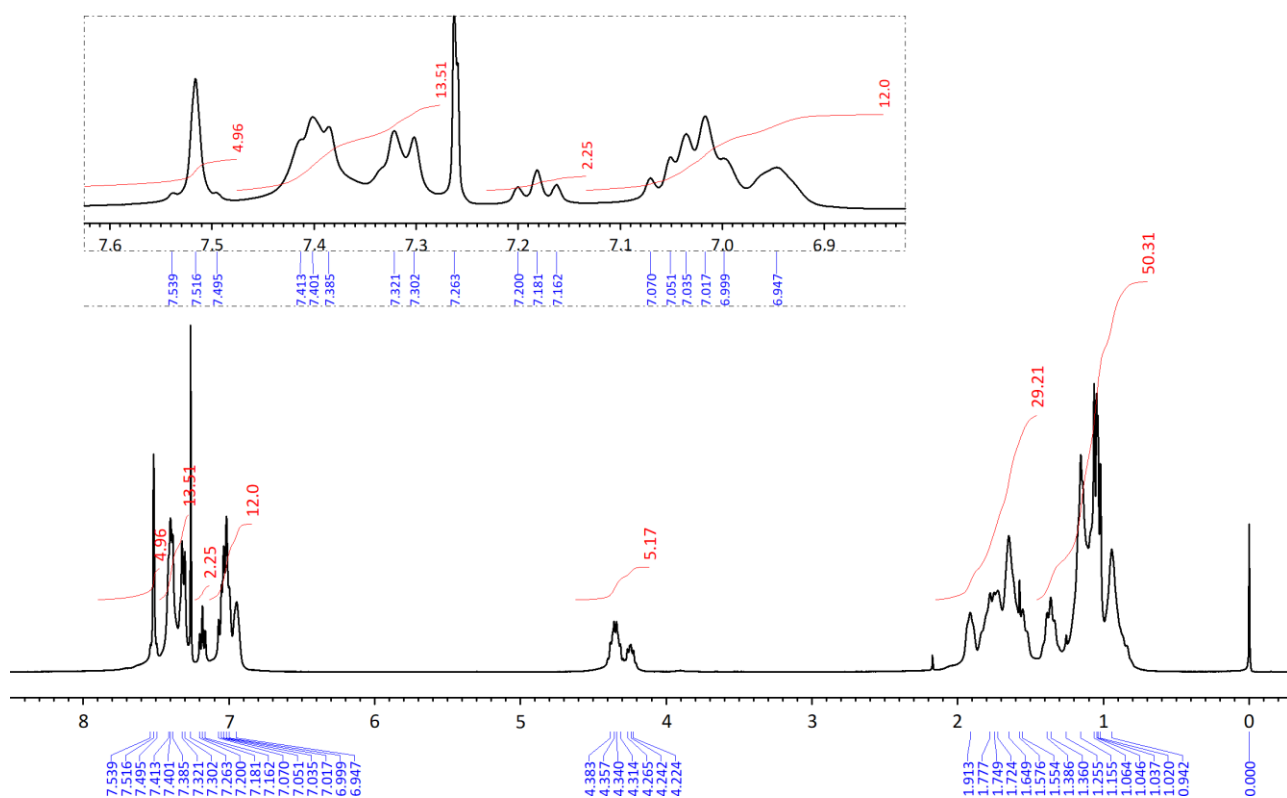
Data: common/Aug13:a00249-2
Sample: 3396 Sakamoto / 319
Experiment Date/Time: 2018/08/13 14:31:51
Average(MS[1] Time:0.26..0.35)

Instrument Configuration: FDプローブ,JMS-T100GCV
Ionization Mode: FD+
Acquired m/z Range: 50.00..3200.00
Detector Volt: 2300[V]

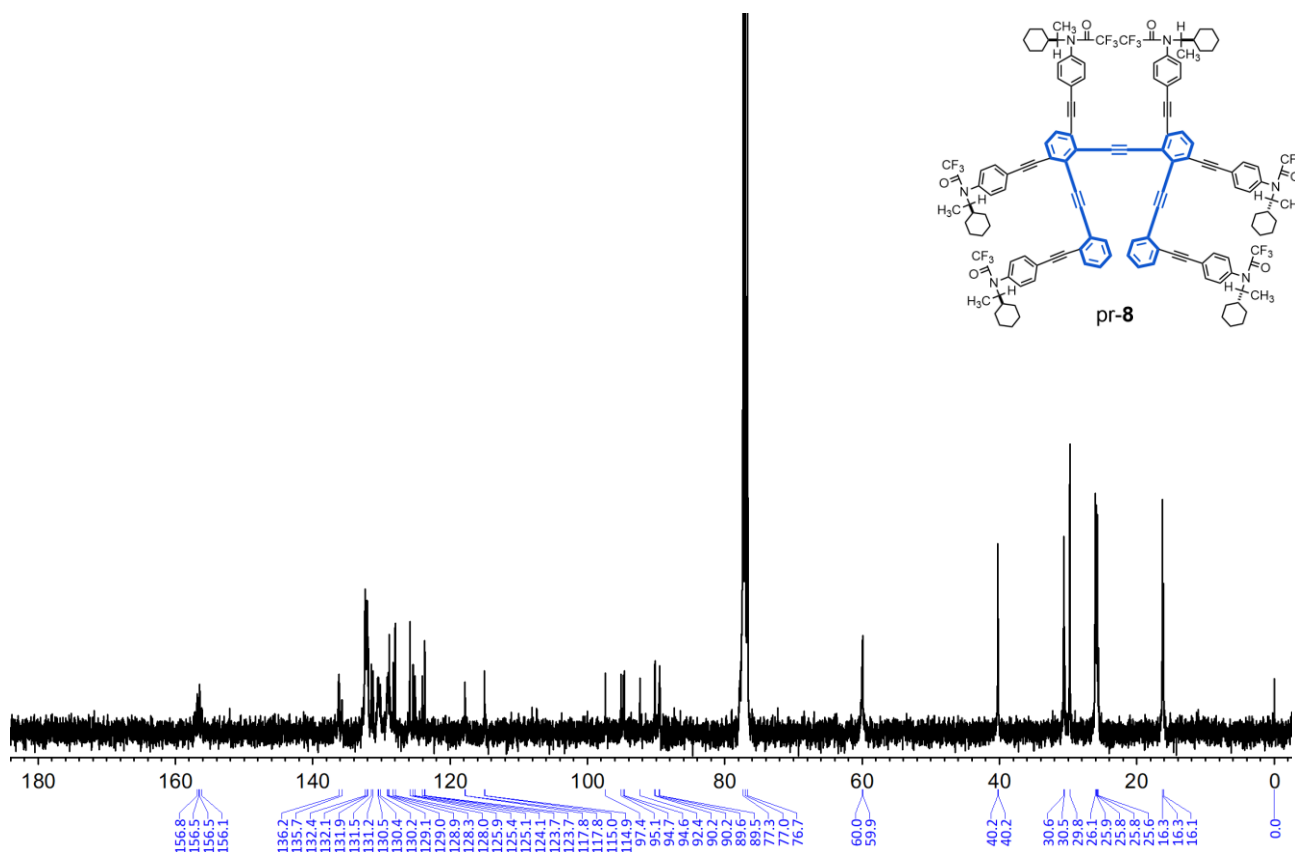
MS Tune Method Name: FD
Agilent7890A Method Name: -



LRMS (FD) of **34/34H** (used to prepare **8B**).



^1H NMR spectrum (400 MHz) of pr-8, measured in CDCl_3 at room temperature.

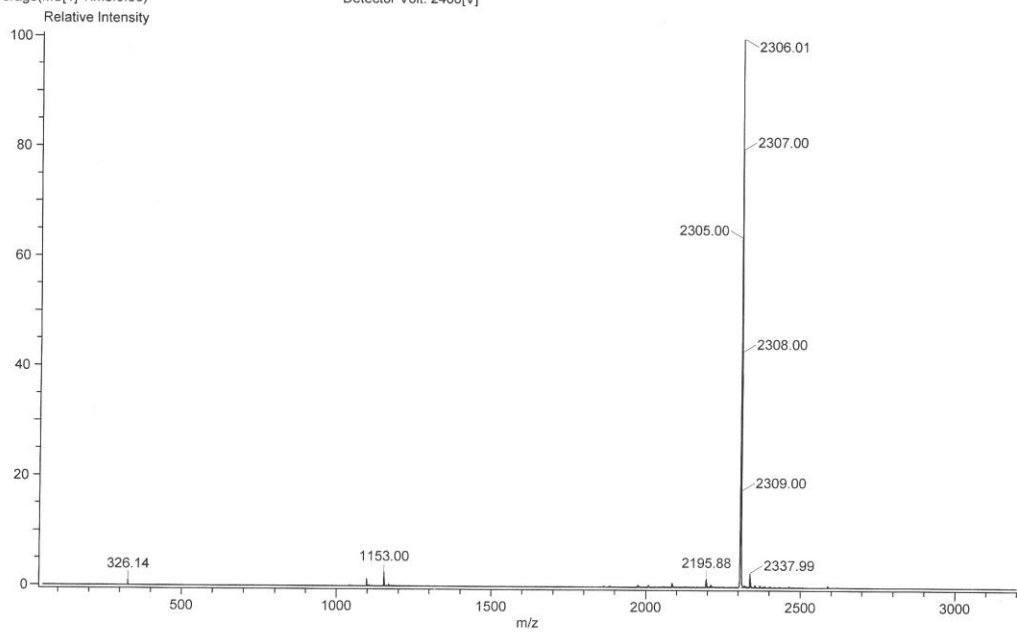


^{13}C NMR spectrum (100 MHz) of pr-8, measured in CDCl_3 at room temperature.

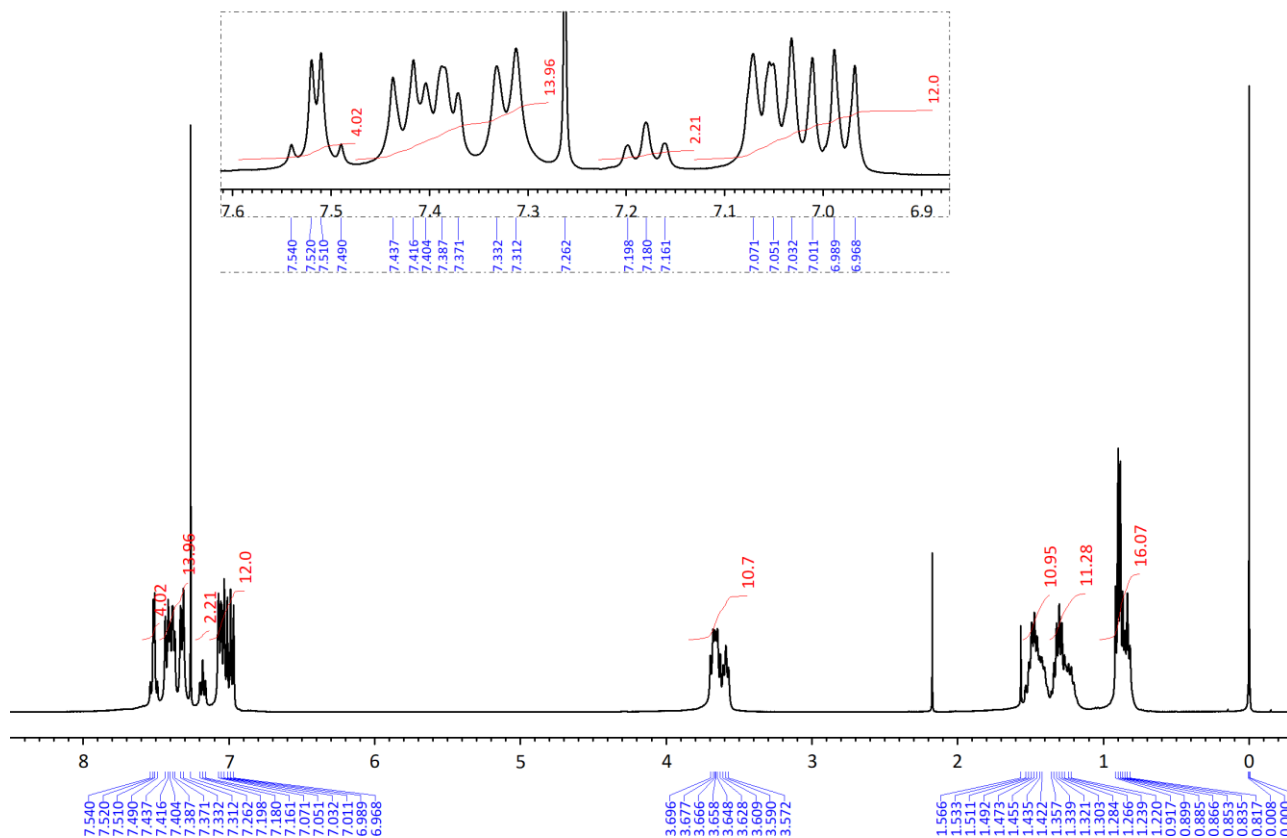
Data: common/Jan25.a00578-1
Sample: 3396 Sakamoto / 317data
Experiment Date/Time: 2019/01/25 11:19:17
Average(MS[1] Time:0.36)

Instrument Configuration: FDプローブ,JMS-T100GCV
Ionization Mode: FD+
Acquired m/z Range: 50.00..3200.00
Detector Volt: 2400[V]

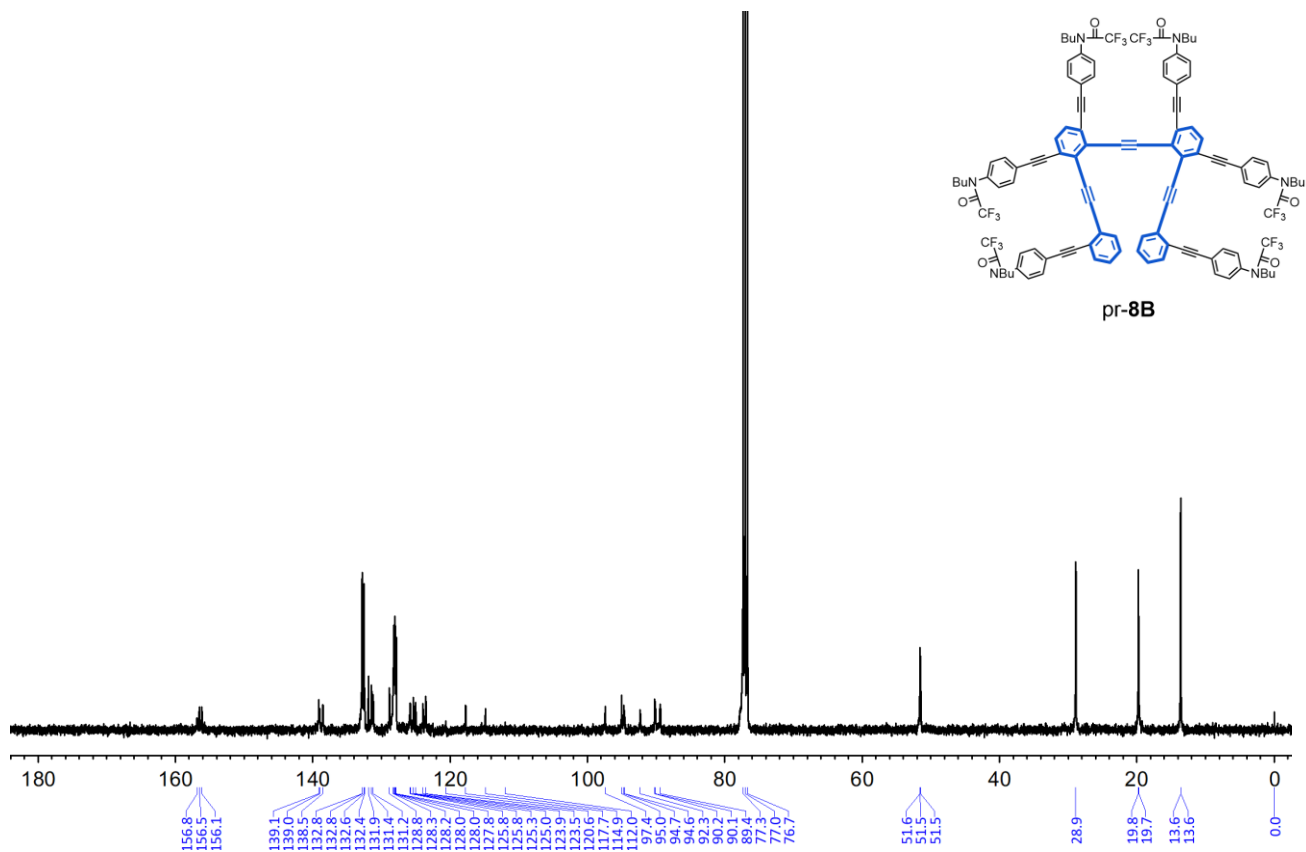
MS Tune Method Name: FD
Agilent7890A Method Name: -



LRMS (FD) of pr-8.



^1H NMR spectrum (400 MHz) of pr-**8B**, measured in CDCl_3 at room temperature.

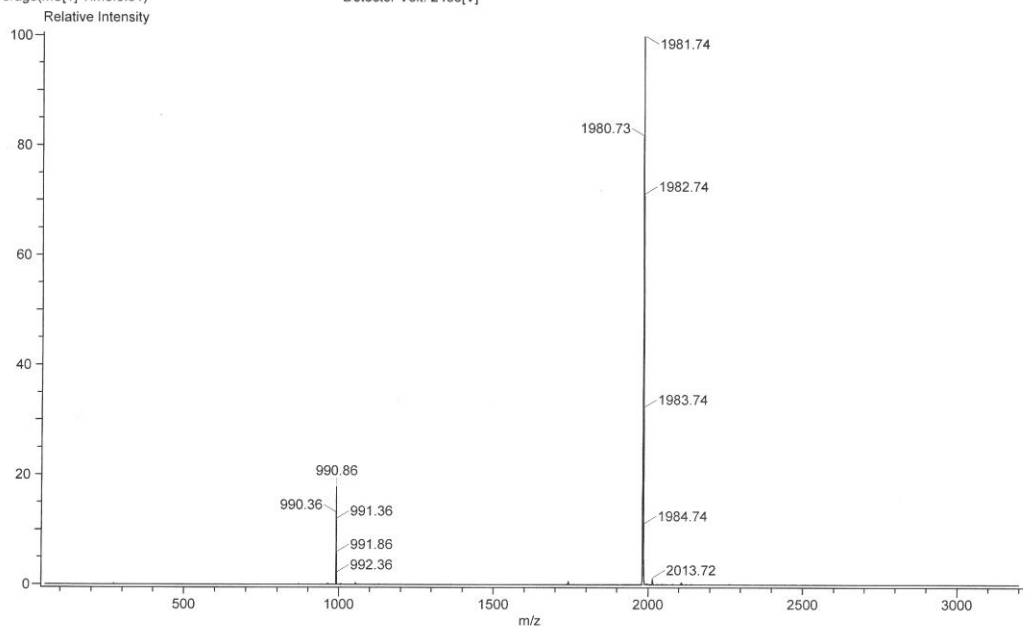


^{13}C NMR spectrum (100 MHz) of pr-**8B**, measured in CDCl_3 at room temperature.

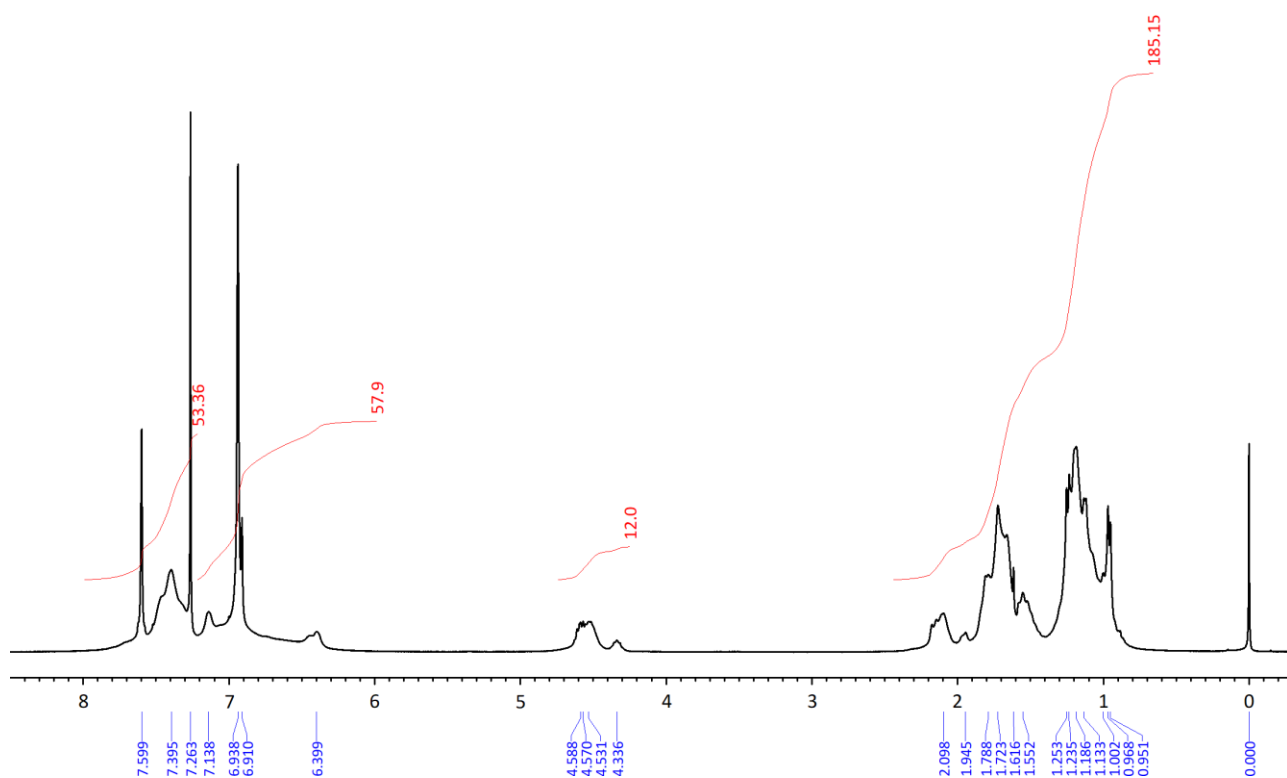
Data: common/Jan25_a00578-1
Sample: 3396 Sakamoto / 320data
Experiment Date/Time: 2019/01/25 10:44:51
Average(MS[1] Time:0.31)

Instrument Configuration: FDプローブ,JMS-T100GCV
Ionization Mode: FD+
Acquired m/z Range: 50.00..3200.00
Detector Volt: 2400[V]

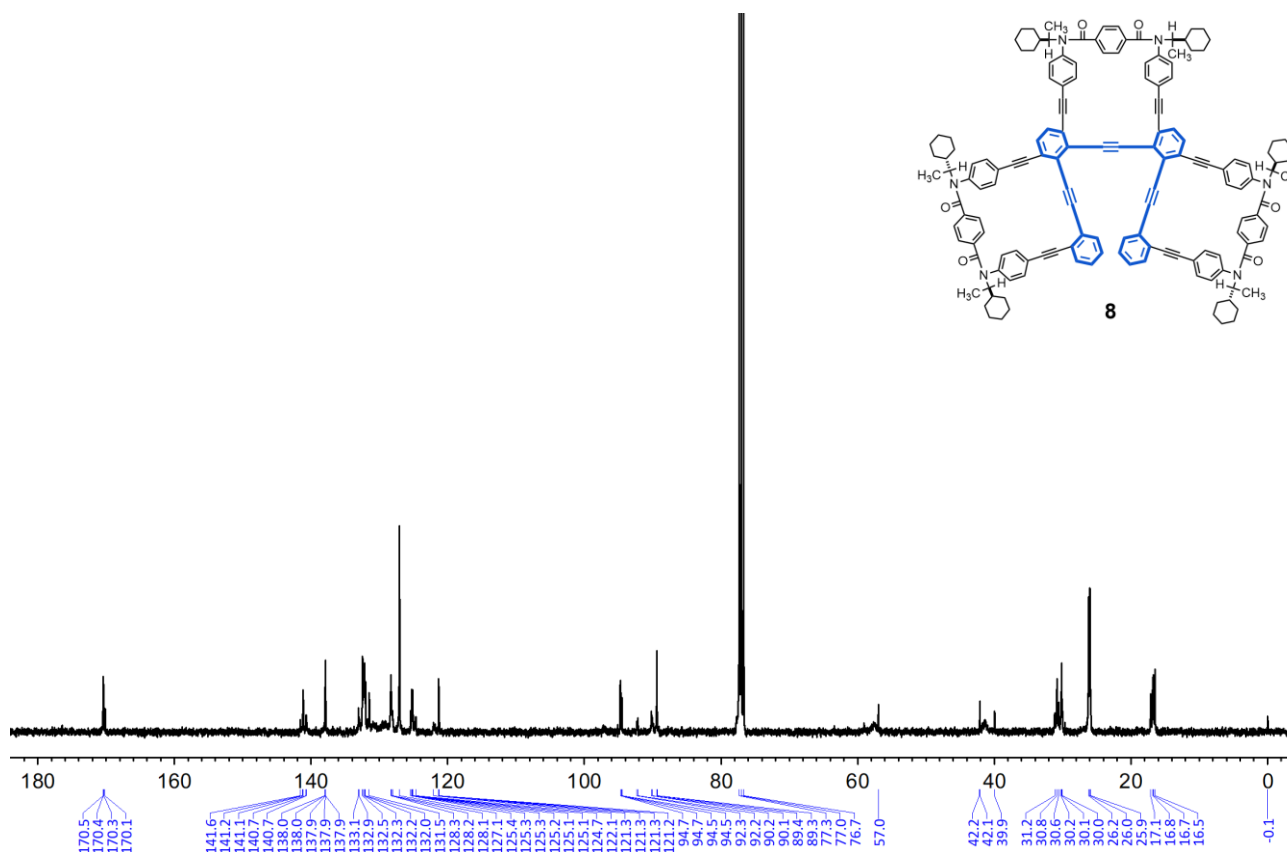
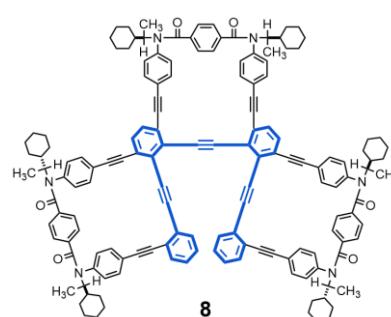
MS Tune Method Name: FD
Agilent7890A Method Name: -



LRMS (FD) of pr-8B.



^1H NMR spectrum (400 MHz) of **8**, measured in CDCl_3 at room temperature.

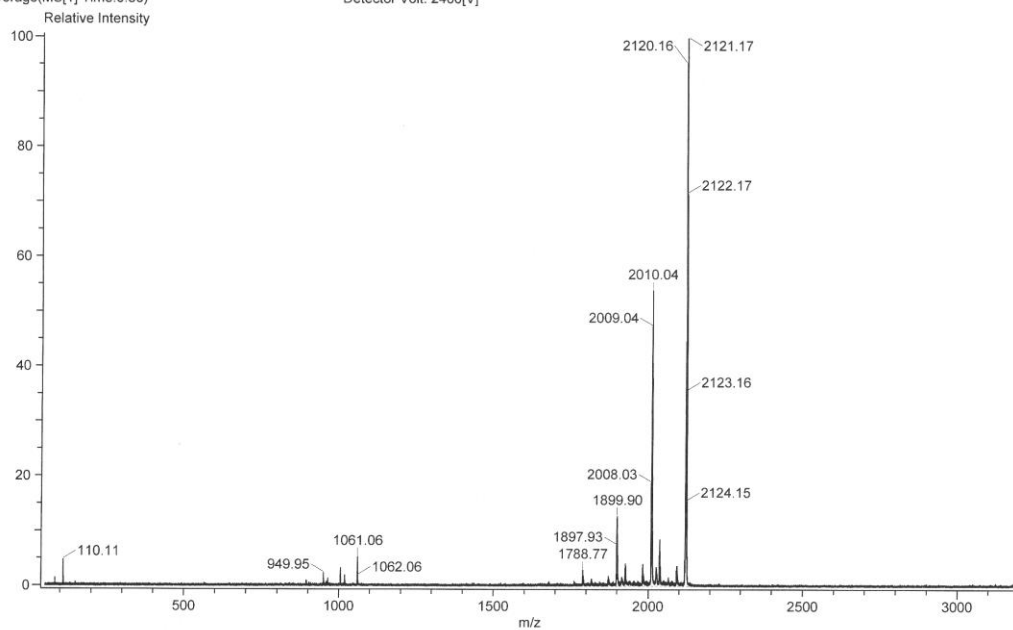


^{13}C NMR spectrum (100 MHz) of **8**, measured in CDCl_3 at room temperature.

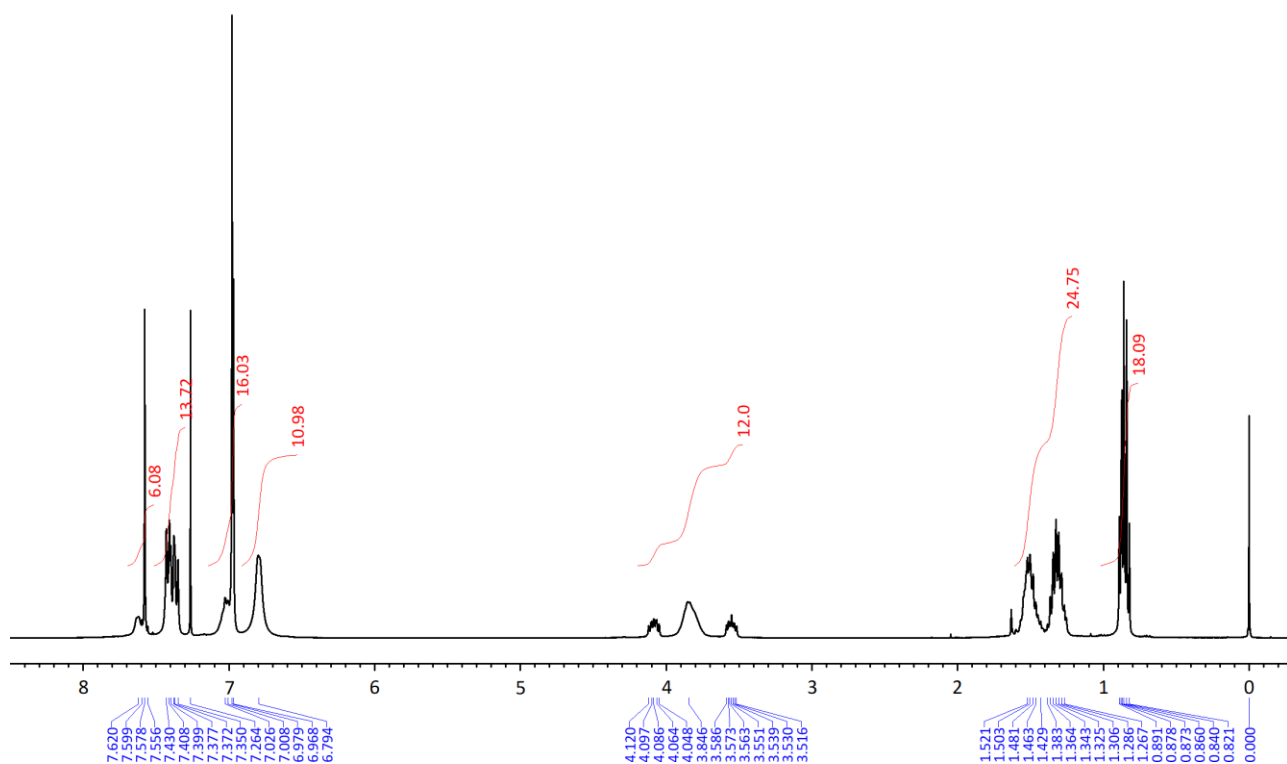
Data: common/Jan25:a00577-2
Sample: 3396 Sakamoto / 324data
Experiment Date/Time: 2019/01/25 11:08:45
Average(MS[1] Time:0.50)

Instrument Configuration: FDプローブ,JMS-T100GCV
Ionization Mode: FD+
Acquired m/z Range: 50.00..3200.00
Detector Volt: 2400[V]

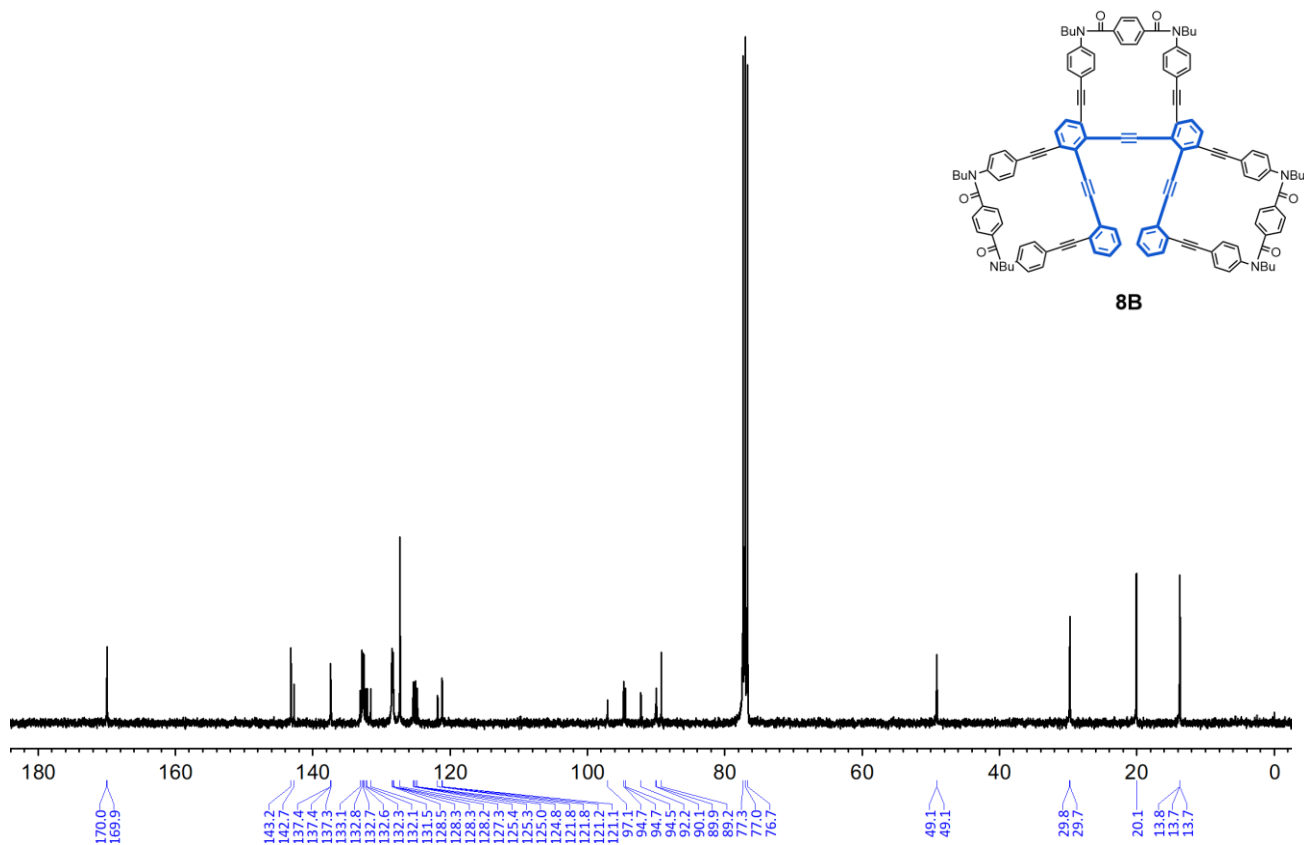
MS Tune Method Name: FD
Agilent7890A Method Name: -



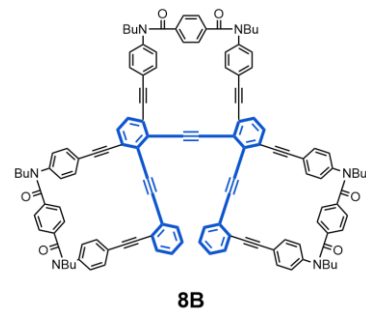
LRMS (FD) of 8.



^1H NMR spectrum (400 MHz) of **8B**, measured in CDCl_3 at room temperature.



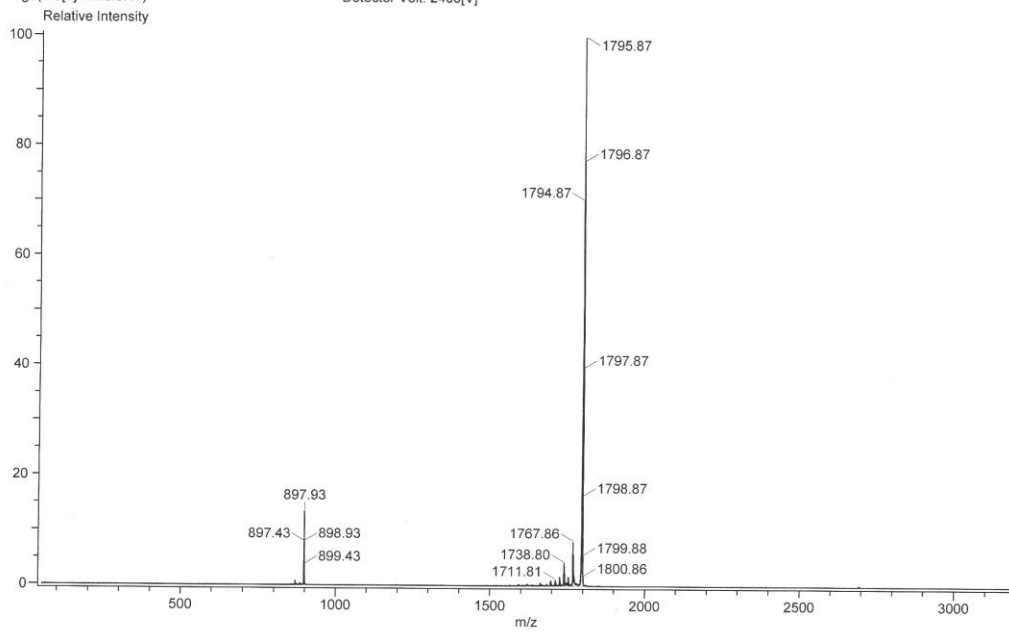
^{13}C NMR spectrum (100 MHz) of **8B**, measured in CDCl_3 at room temperature.



Data: common/Jan25.a00574-1
Sample: 3396 Sakamoto / 322data
Experiment Date/Time: 2019/01/25 10:22:02
Average(MS[1] Time:0.47)

Instrument Configuration: FDプロ-フ,JMS-T100GCV
Ionization Mode: FD+
Acquired m/z Range: 50.00..3200.00
Detector Volt: 2400[V]

MS Tune Method Name: FD
Agilent7890A Method Name: -



LRMS (FD) of **8B**.