

Supplementary Material

Some new 2,8-disubstituted-1,7-dicyano-3,9-diazaperylenes

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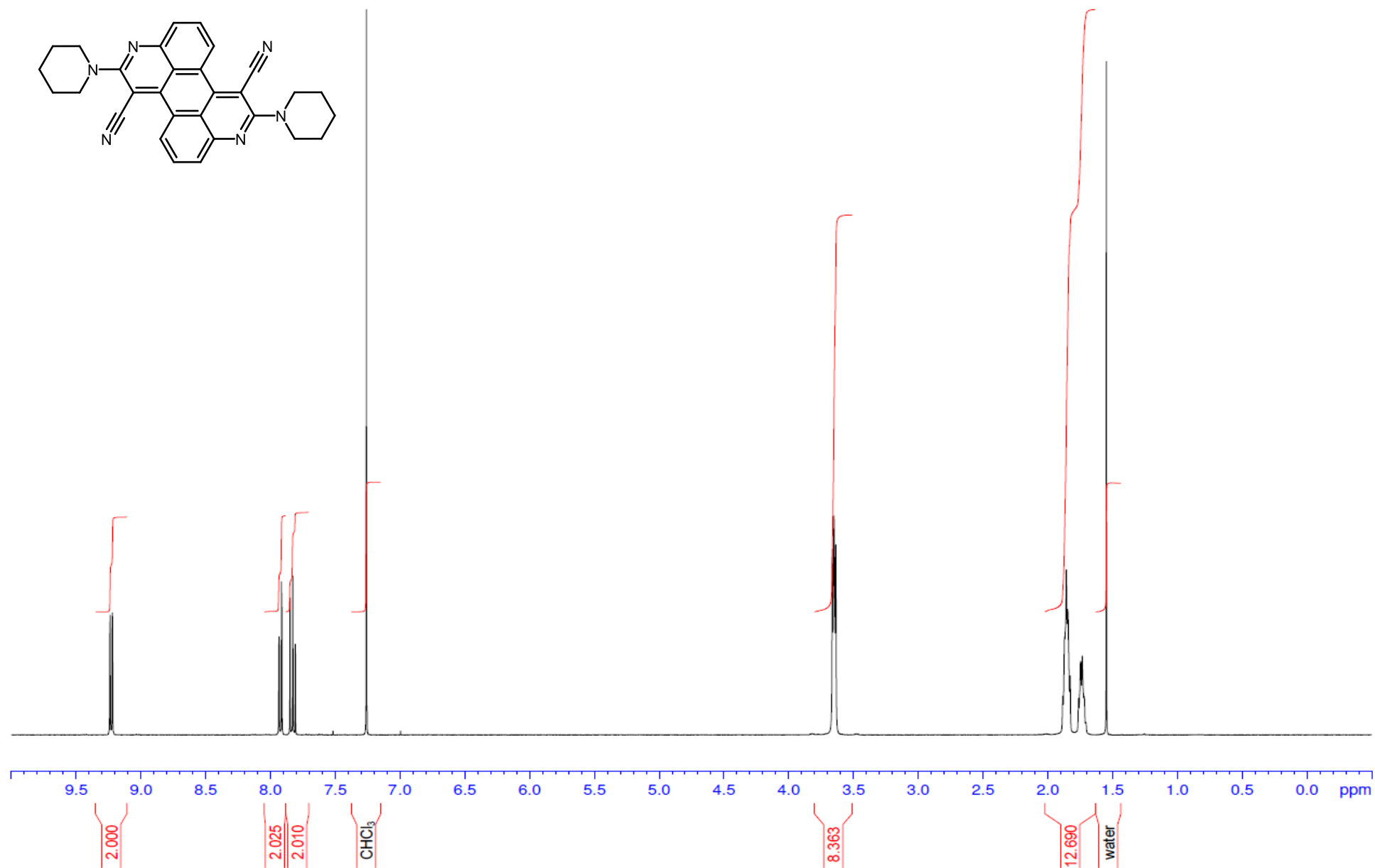
^c School of Chemistry, Monash University, Clayton, VIC 3800, Australia

Email: craig.francis@csiro.au

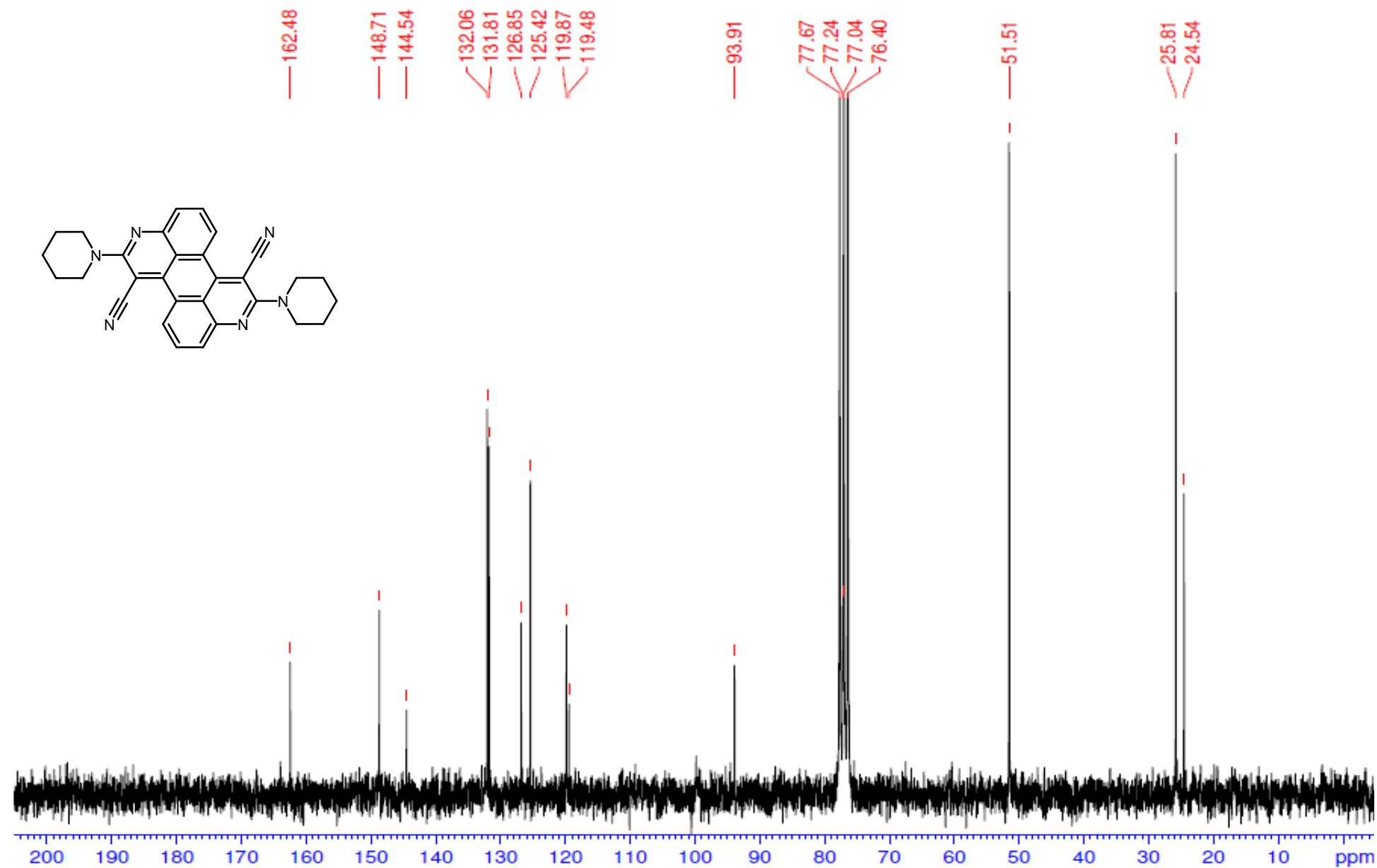
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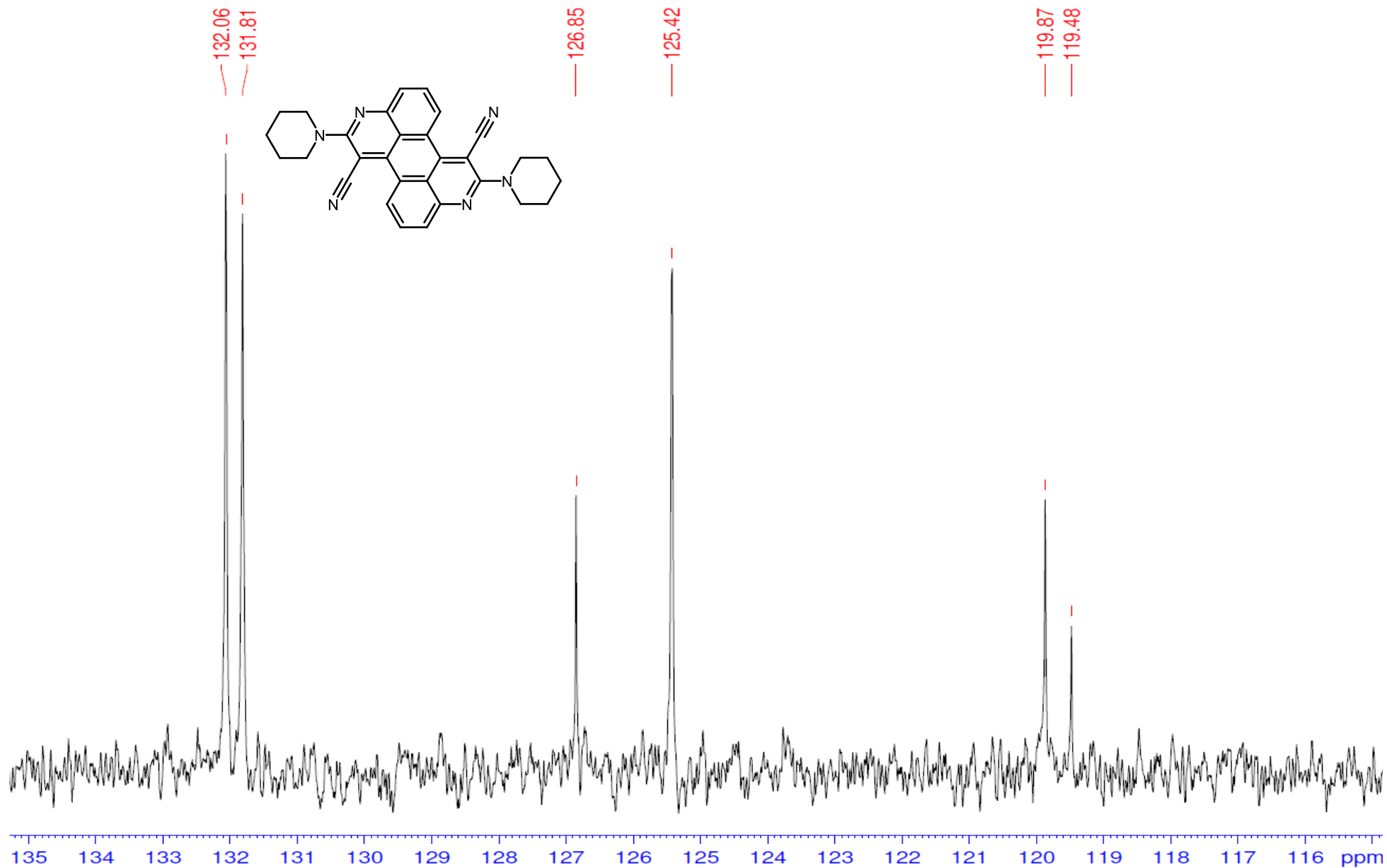
^1H NMR spectrum of **3b** (400 MHz; CDCl_3)



^{13}C NMR spectrum of **3b** (50 MHz; CDCl_3)



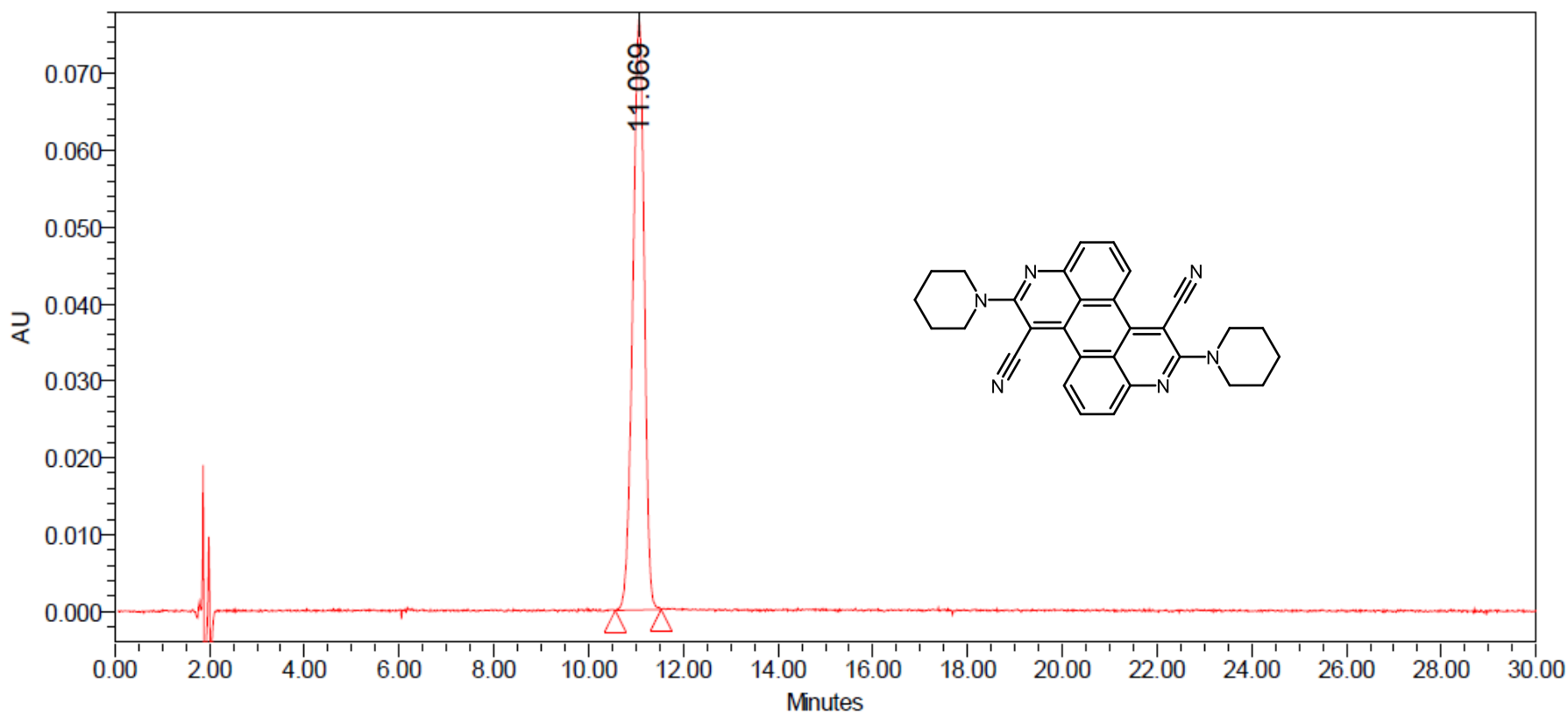
^{13}C NMR spectrum of **3b** (expansion 135-115 ppm)



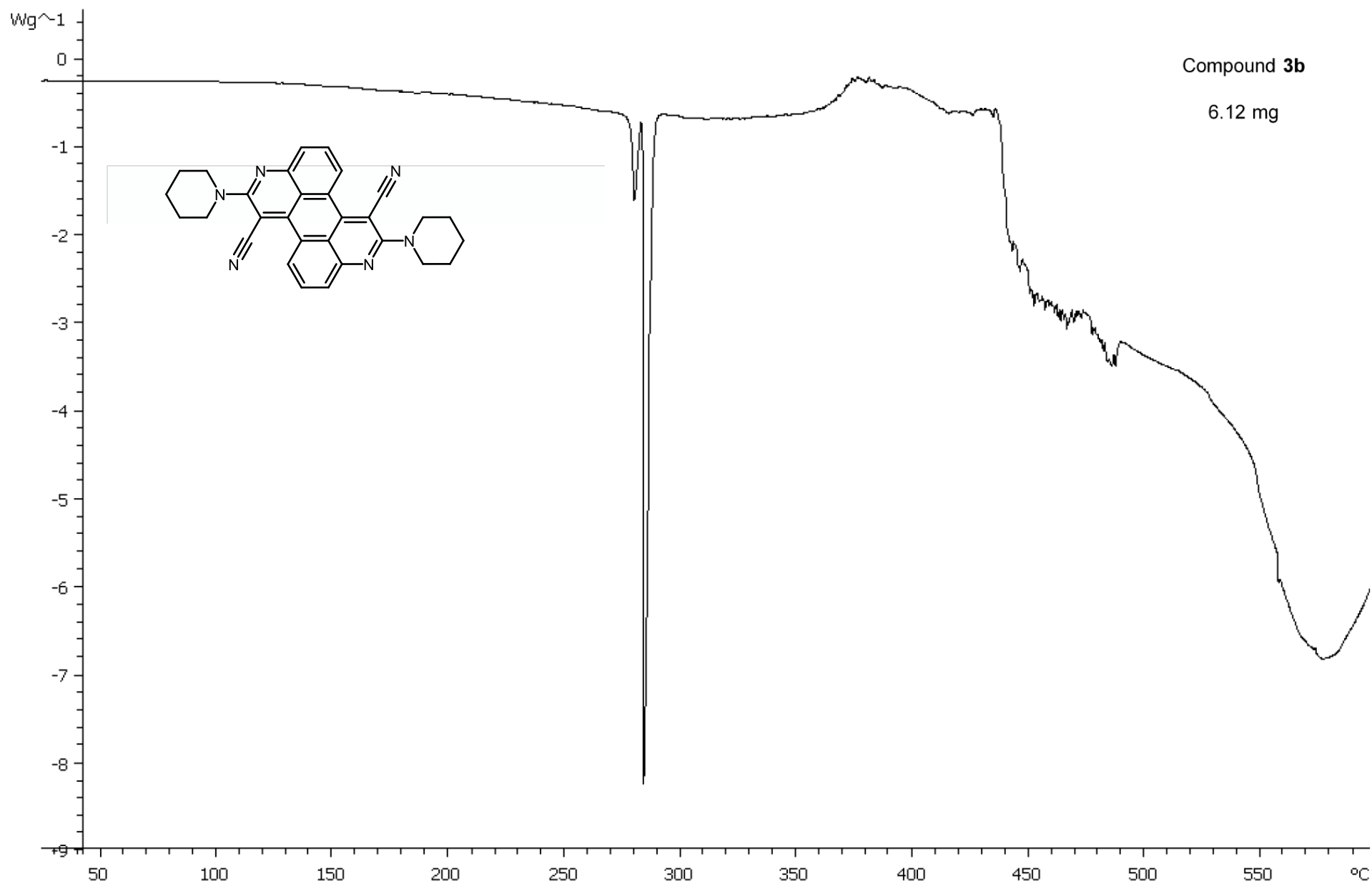
HPLC Chromatogram for **3b**

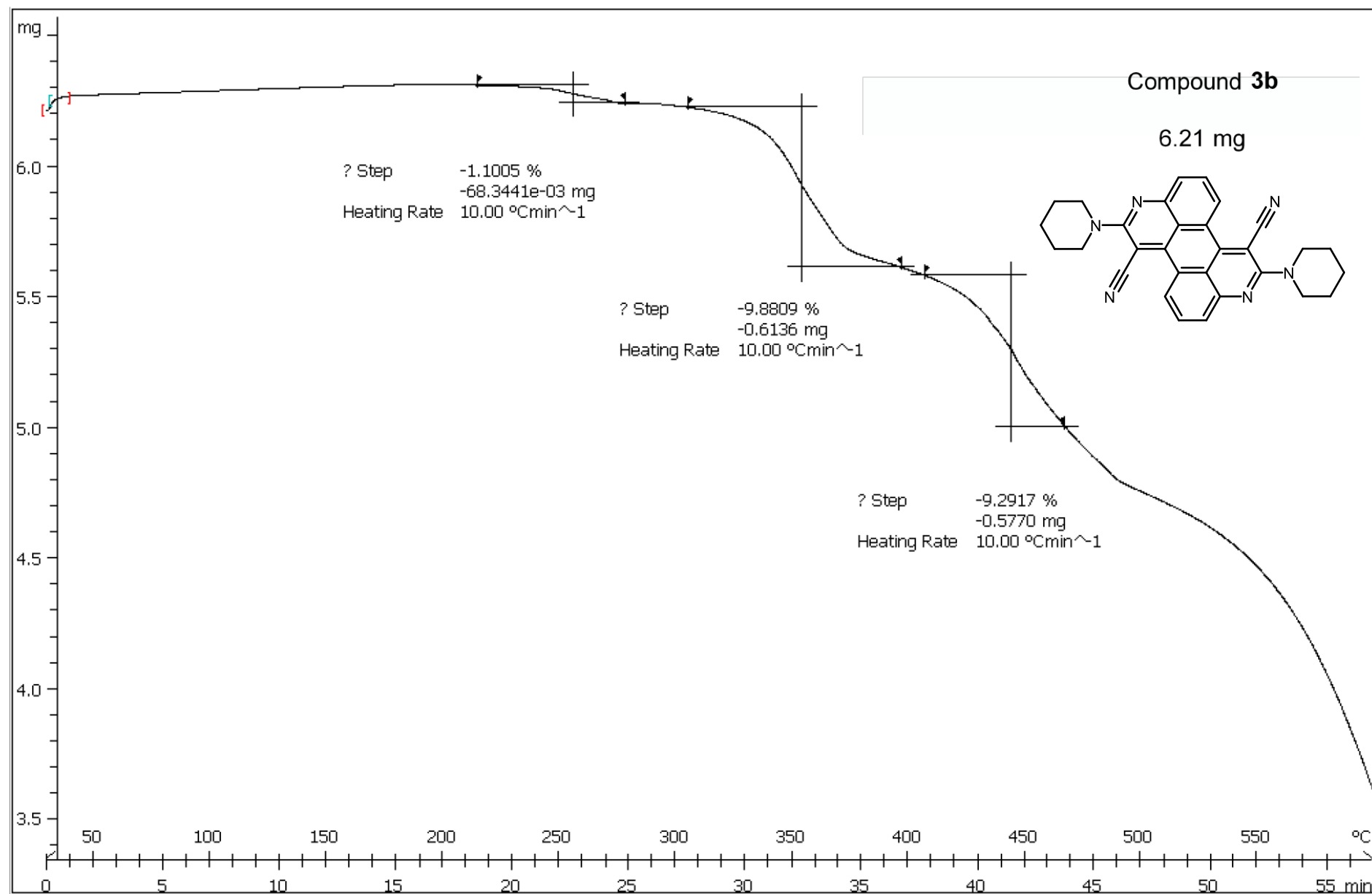
Sample Name: CLF 1455-68 xtls 95%ACN/H₂O
Detector: PDA 417.0 nm
HplcColumn 150x4.6mm Alltima HP C18
FlowRate: 1.0 mL / min
MobilePhase: 95% ACN / H₂O

Date Acquired: 19/11/2009 2:52:01 PM EST
Acq Method Set : AllianceE 100% A isocratic
Date Processed: 19/11/2009 3:36:44 PM EST
Processing Method: nkh

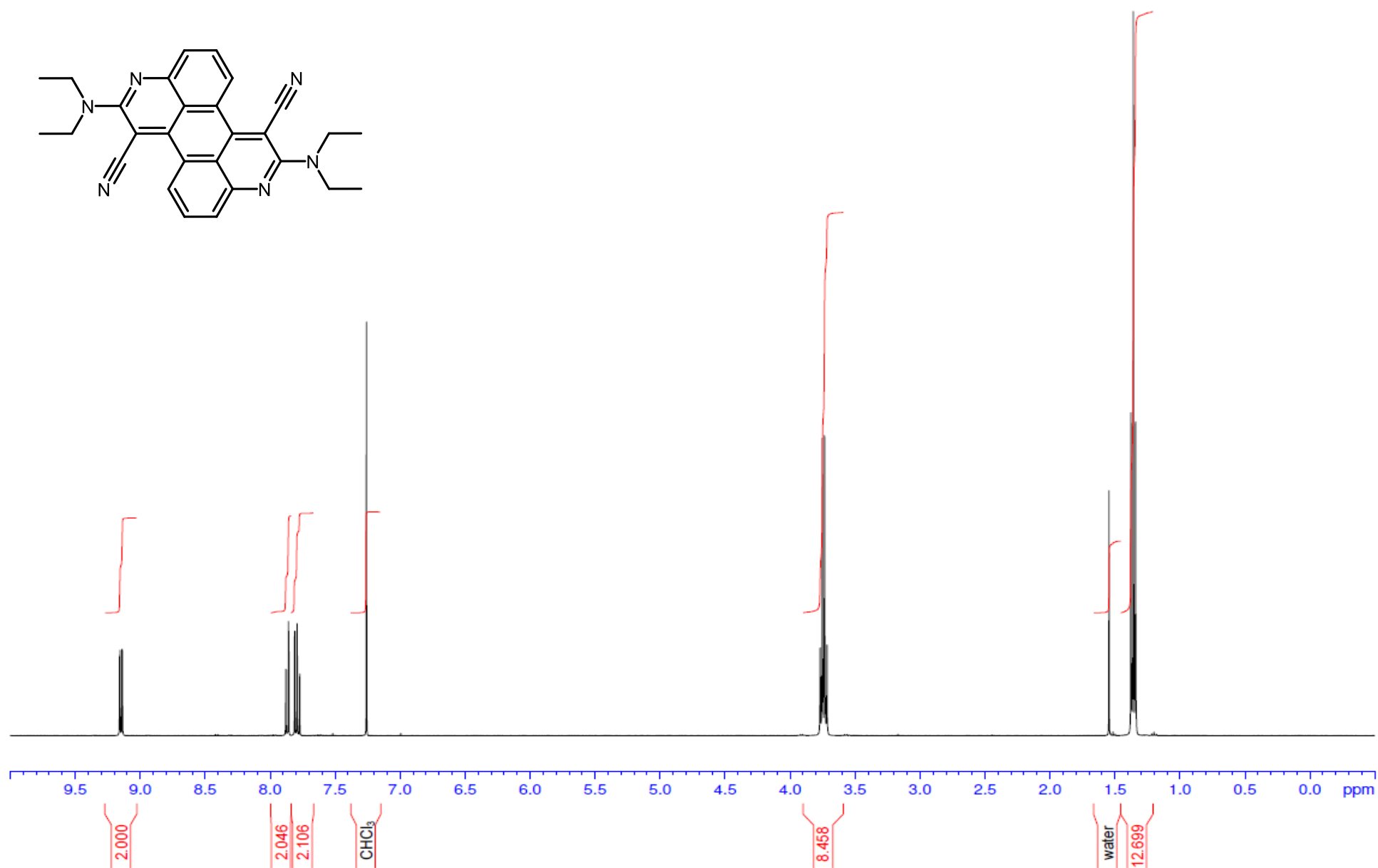


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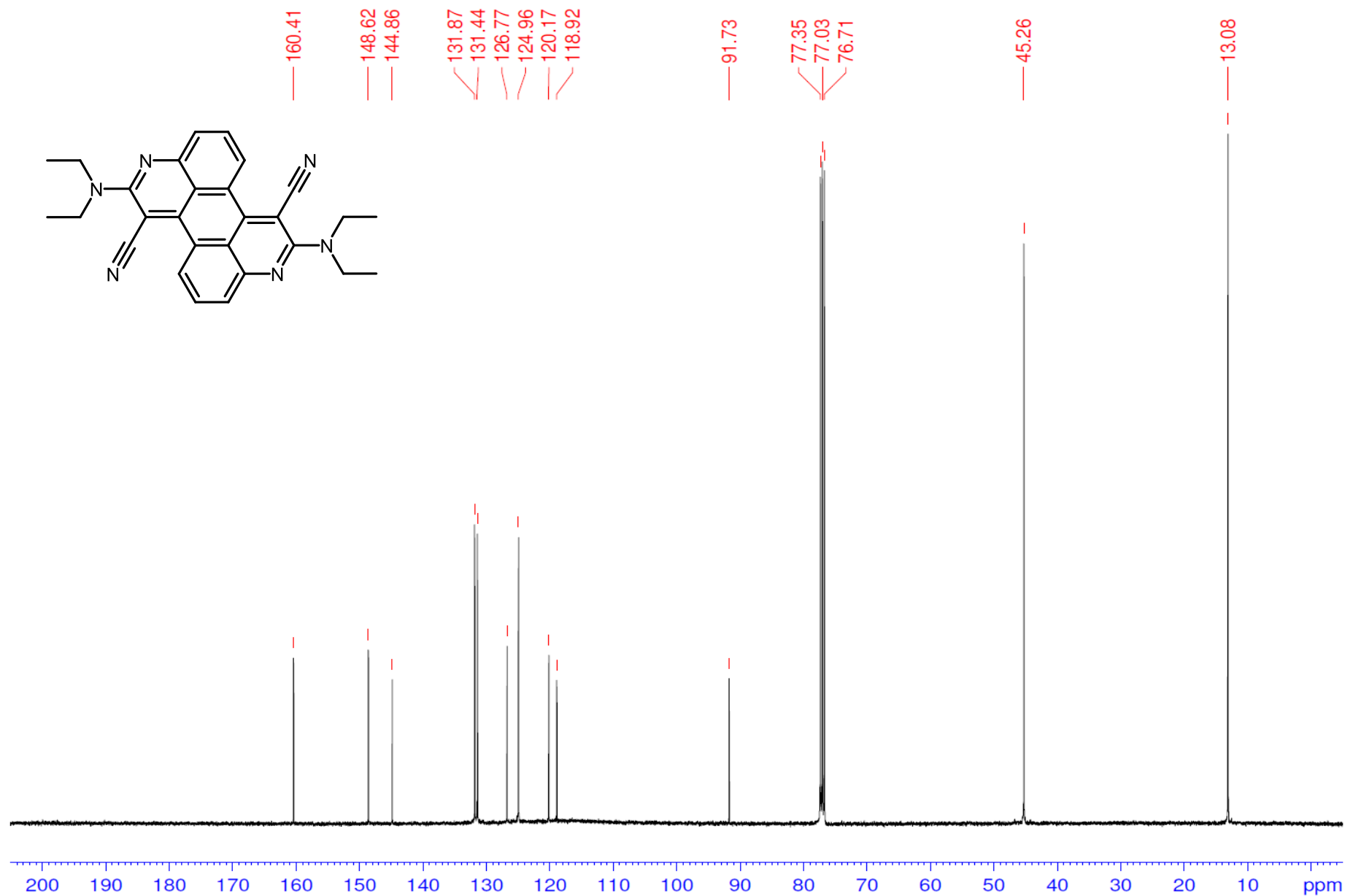
DSC curve for **3b**

TGA trace for **3b**

^1H NMR spectrum for **3c** (400 MHz; CDCl_3)



^{13}C NMR spectrum of **3c** (100 MHz; CDCl_3)



HPLC Chromatogram for **3c**Sample Name: CLF1455-90-2a 95%ACN/H₂O

Detector: PDA 269.0 nm

HplcColumn 150x4.6mm ALItima HP C18

FlowRate: 1.0 mL / min

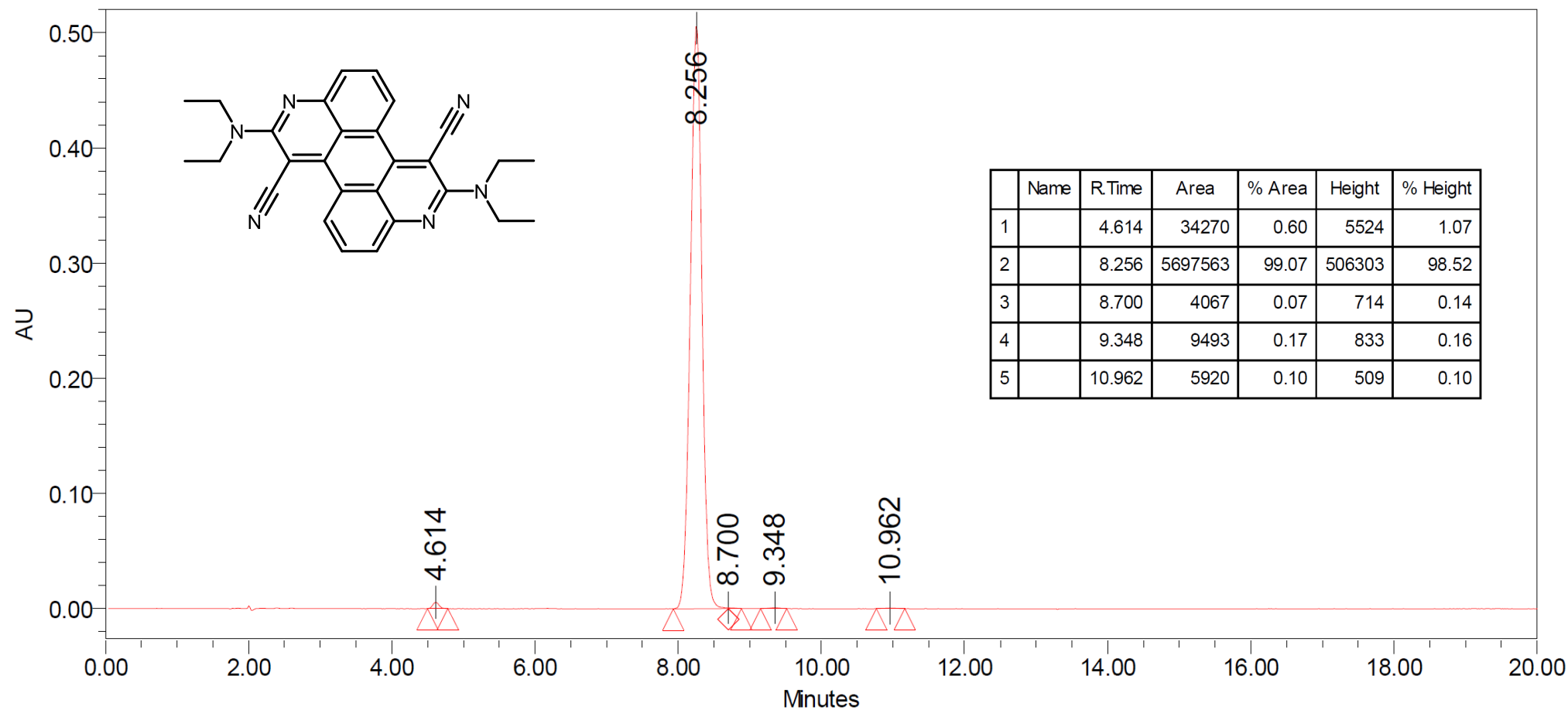
MobilePhase: 95% ACN / H₂O

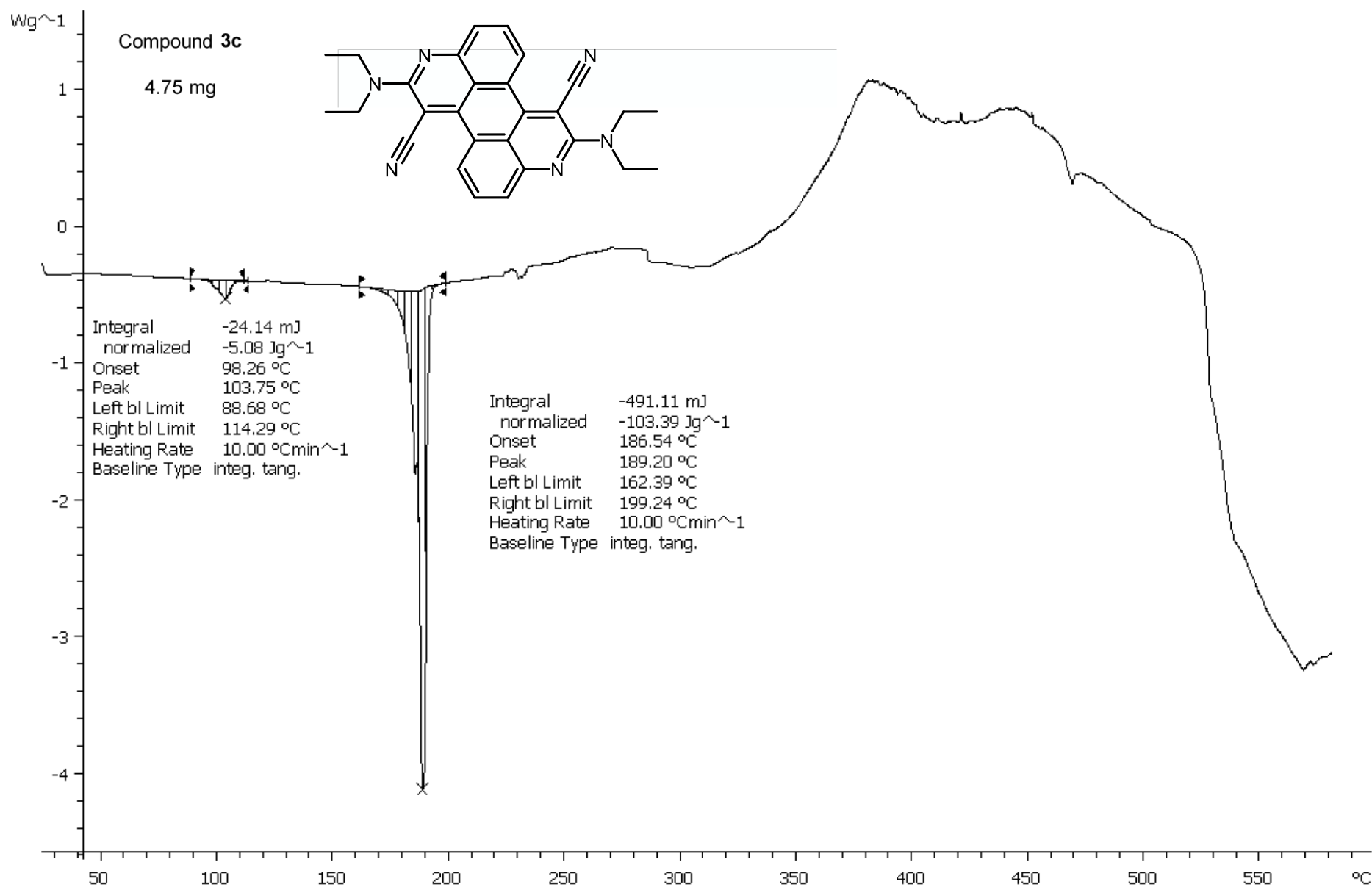
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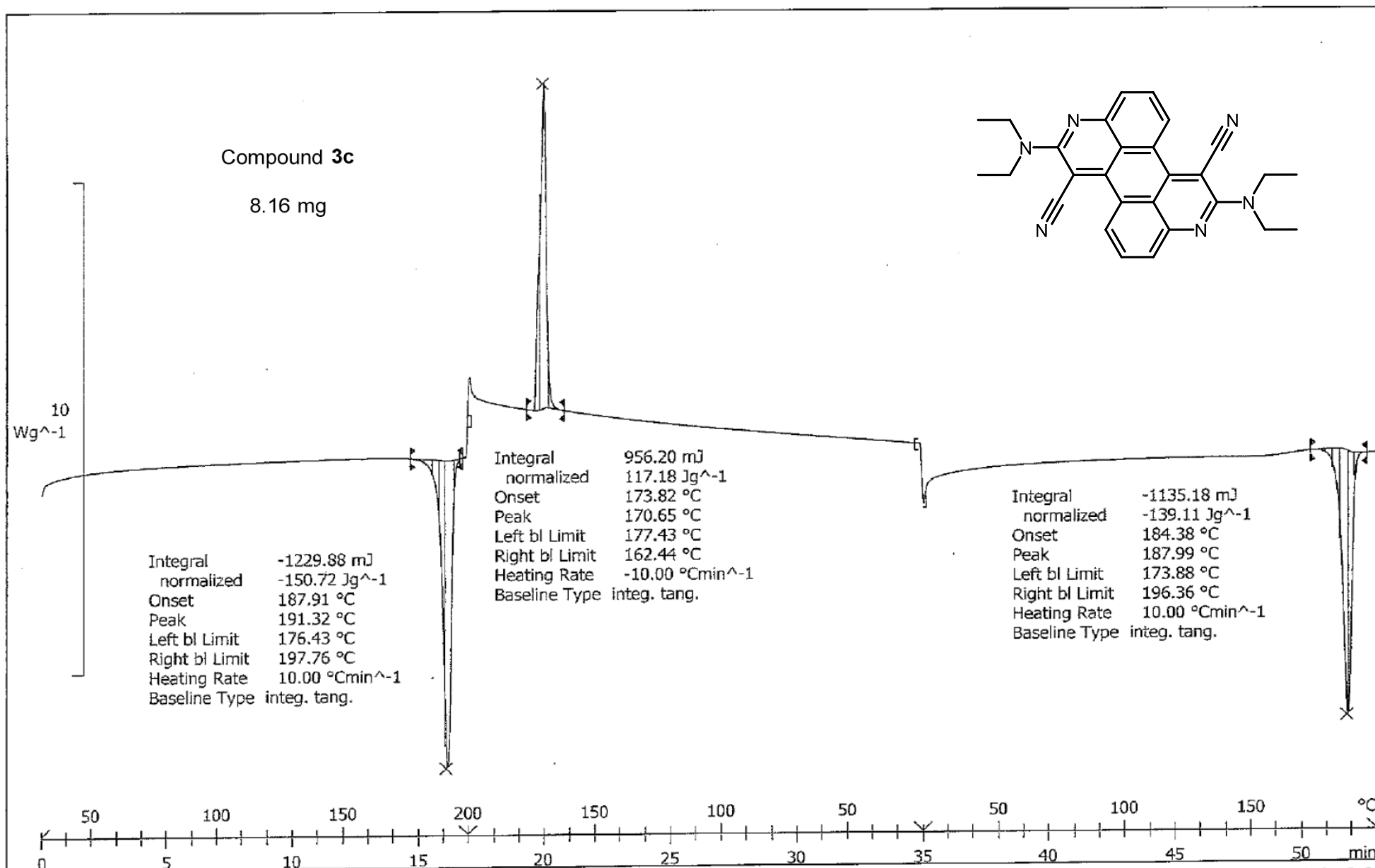
Acq Method Set : AllianceE 100% A isocratic

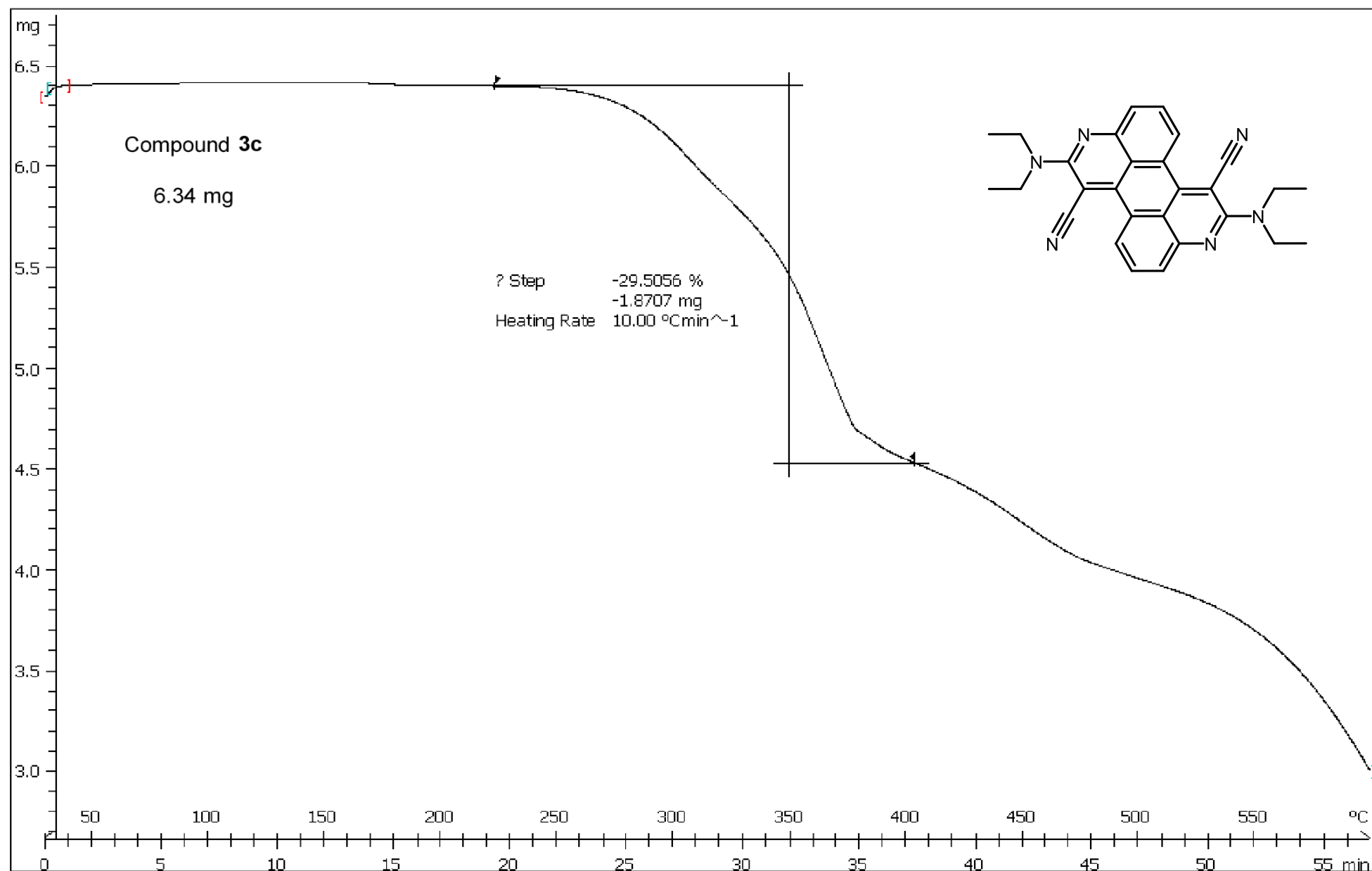
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Processing Method: nkh



DSC curve for **3c**

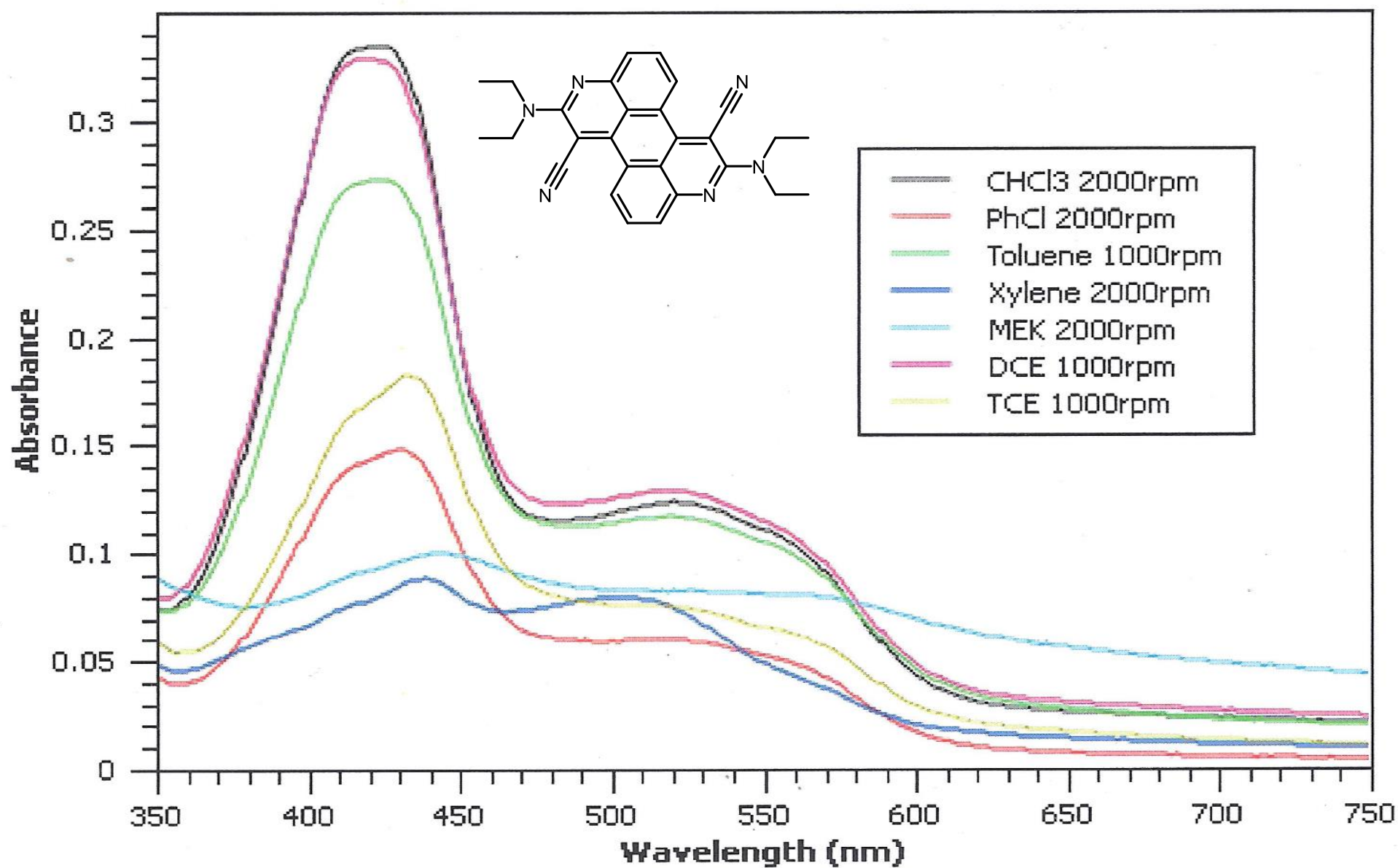
DSC curve for **3c** (two cycles)

TGA trace for **3c**

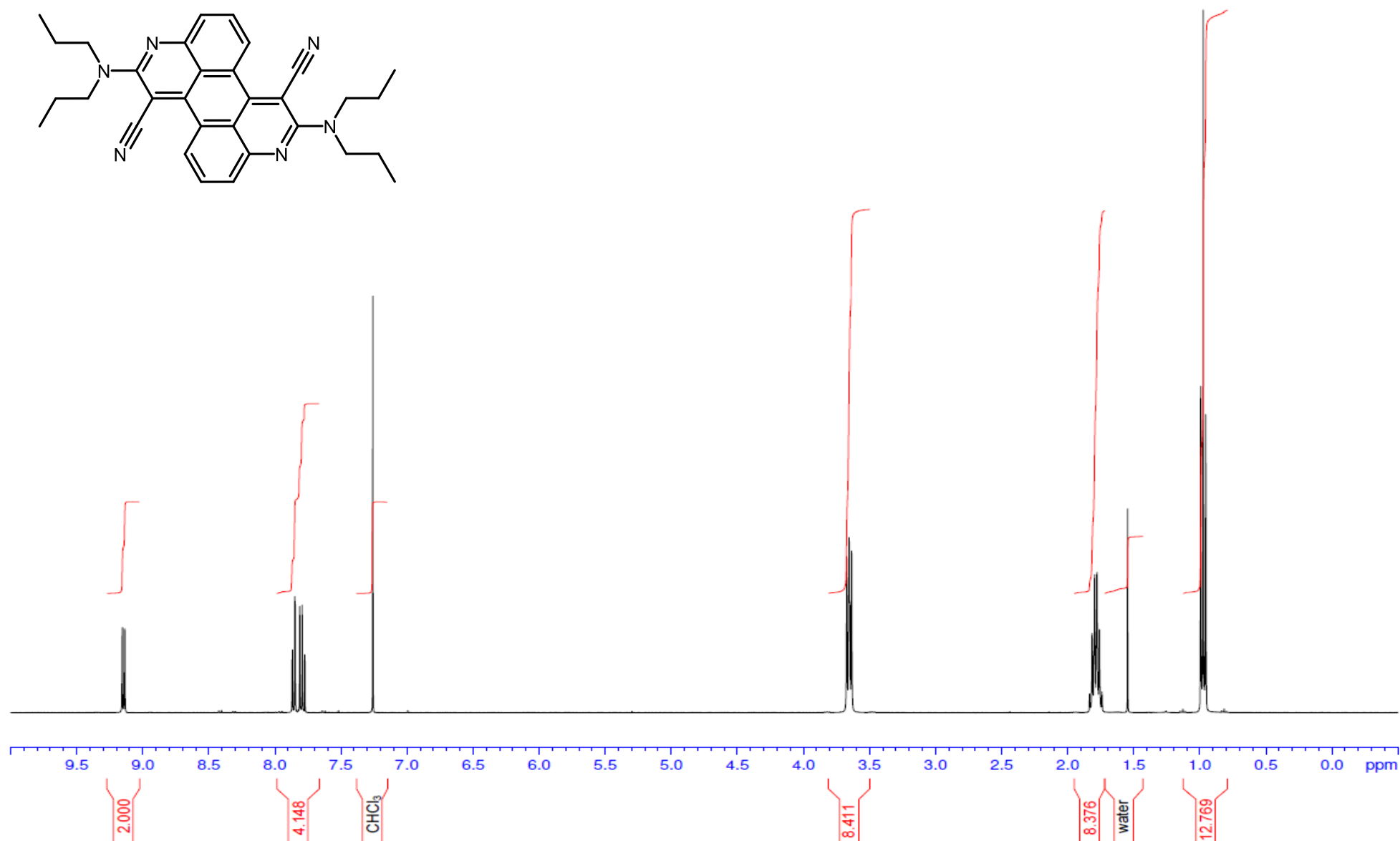
Test spin-coating conditions for films of **3c** from different solvents (CHCl₃, PhCl, xylene, toluene, MEK, dichloroethane (DCE) and tetrachloroethane (TCE)) on UV-ozone-cleaned glass

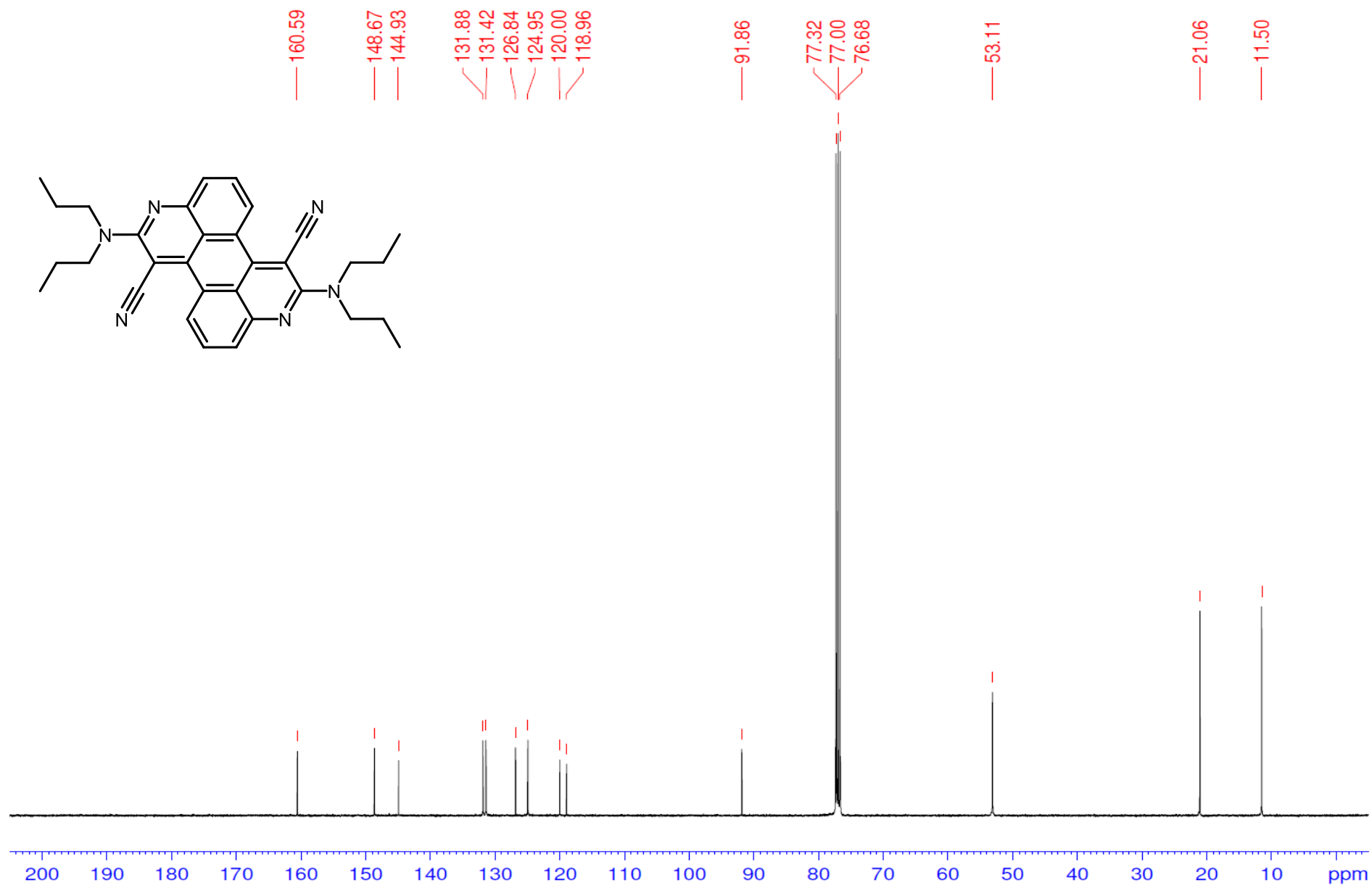
Film	Solvent	Spin-speed (rpm)	Vis. quality	UV@520nm	Thickness (nm)
1	CHCl ₃	4000	Good	0.103	79
2	CHCl ₃	2000	Good	0.124	99
3	PhCl	2000	Good	0.061	56
4	PhCl	1000	Good	0.086	35
5	Toluene	2000	Ok	0.085	50
6	Toluene	1000	Ok, bit hazy	0.117	88
7	Toluene	4000	Good	0.067	65
8	Xylene	2000	Hazy	0.075	42
9	Xylene	4000	Hazy	0.49	36
10	MEK	2000	Hazy	0.083	61
11	DCE	2000	Good	0.096	41
12	DCE	1000	Good	0.129	89
13	DCE	4000	Good	0.080	53
14	TCE	2000	Good	0.061	28
15	TCE	2000	Good	0.050	19
16	TCE	1000	Ok, bit hazy	0.075	42

UV spectra of thin films of **3c** spun from 15mg/mL solutions at different spin speeds. Absorption spectra shown are from the thickest films.



^1H NMR spectrum for **3d** (400 MHz; CDCl_3)



¹³C NMR spectrum of **3d** (100 MHz; CDCl₃)

HPLC Chromatogram for **3d**

Sample Name: 2010672JJ027 95%ACN/H2O

Date Acquired: 19/05/2010 6:07:45 PM EST

Detector: PDA 268.0 nm

Acq Method Set: AllianceE 100% A isocratic

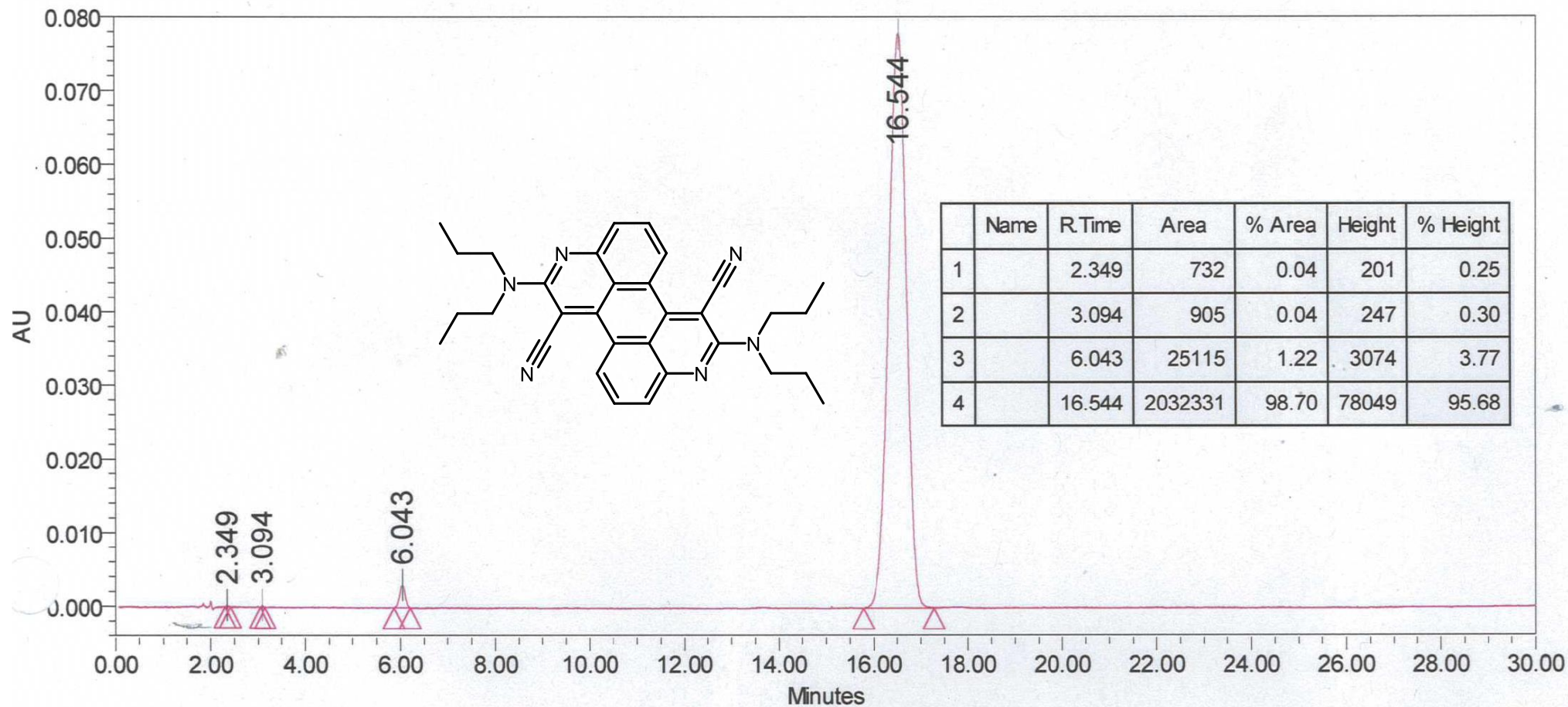
HplcColumn 150x4.6mm Alltima HP C18

Date Processed: 19/05/2010 6:51:14 PM EST

FlowRate: 1.0 mL / min

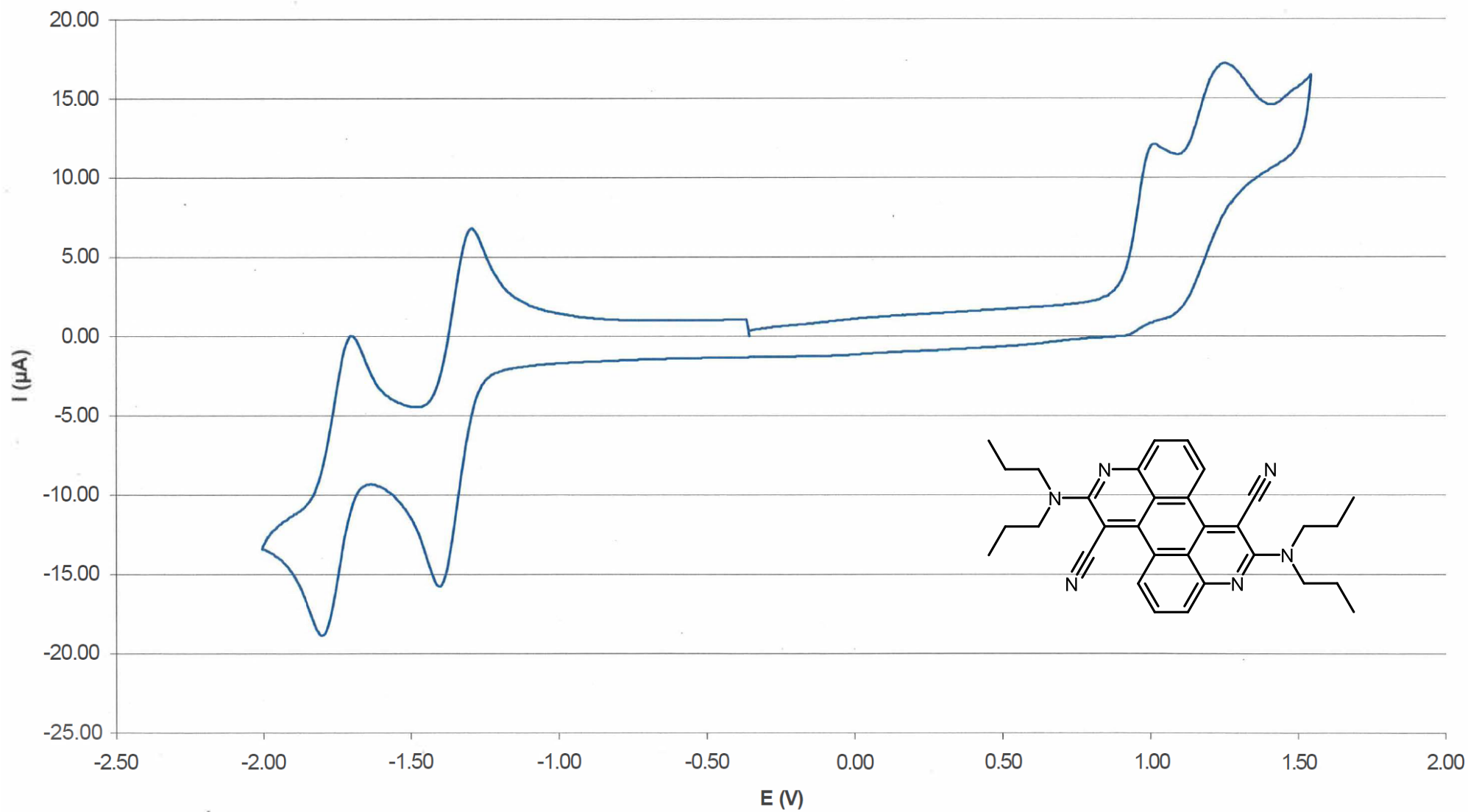
Processing Method: nkh

MobilePhase: 95% ACN H2O

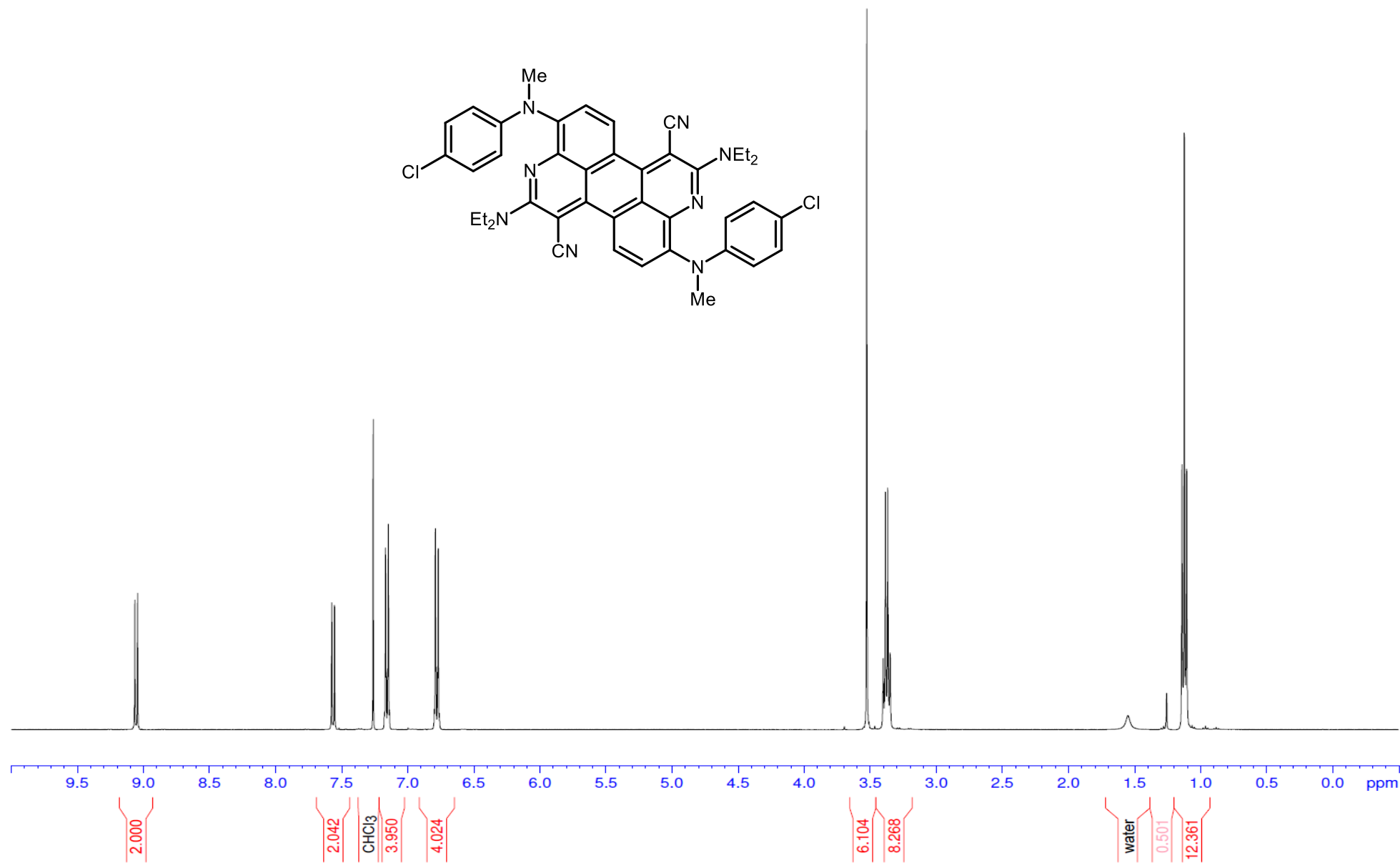


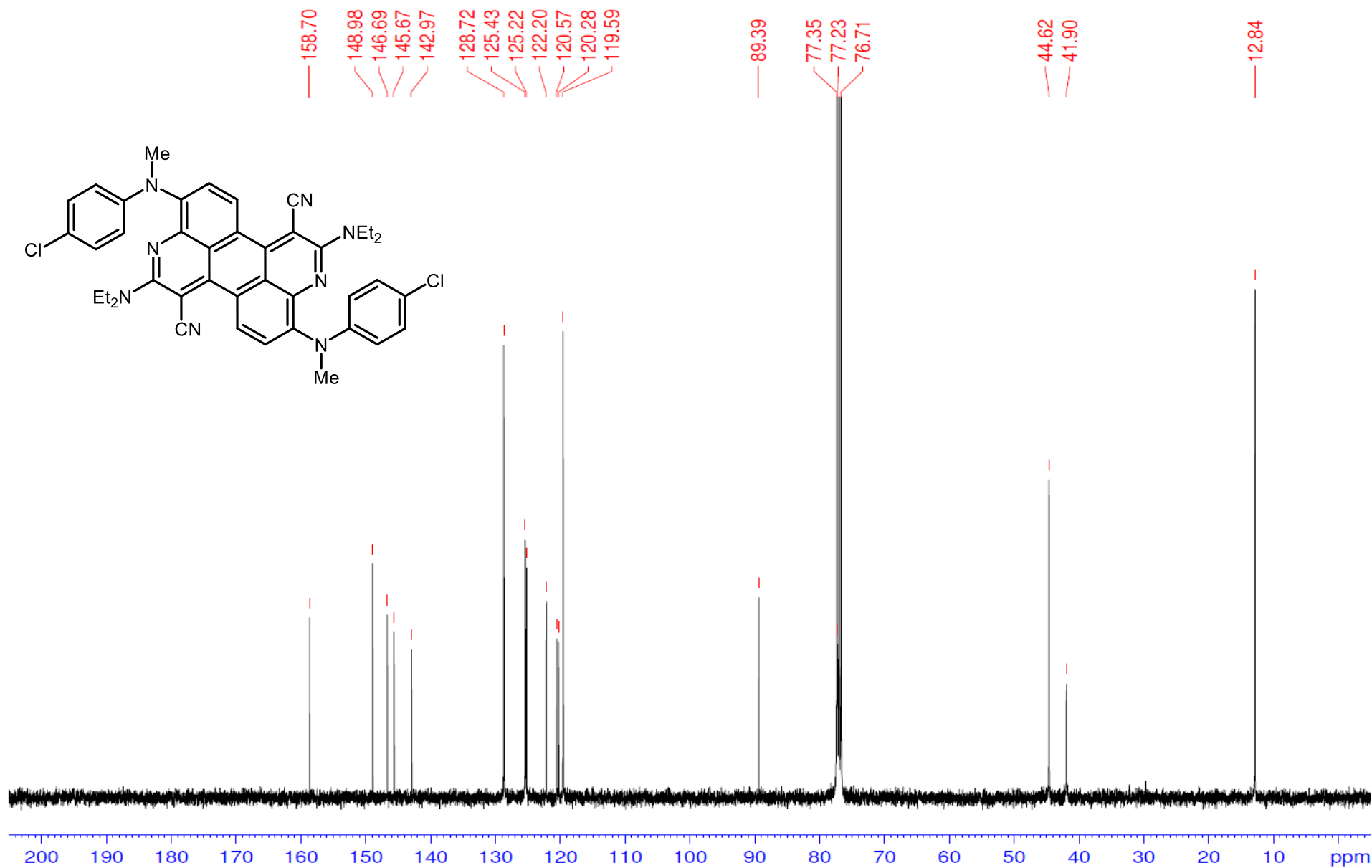
Cyclic voltammogram of **3d** showing two reversible reductions and an irreversible oxidation.

Compound 3d Vs Fe/Fe⁺



^1H NMR spectrum for **5** (400 MHz; CDCl_3)



¹³C NMR spectrum of **5** (100 MHz; CDCl₃)

HPLC Chromatogram for 5

Sample Name: CLF794-23-1 95%ACN/TFA

Detector: PDA 283.0 nm

HplcColumn 150x4.6mm Alltima HP C18

FlowRate: 1.0 mL / min

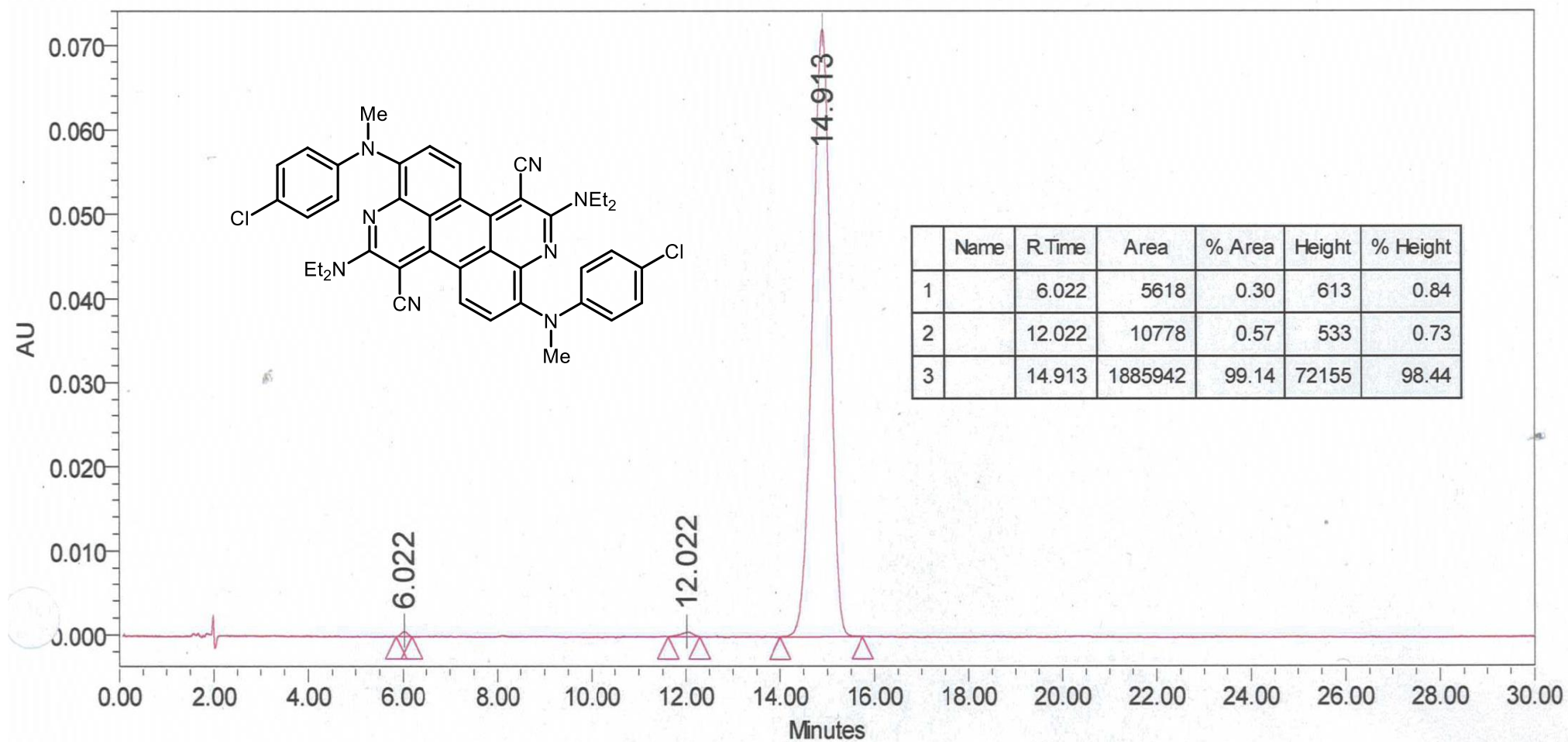
MobilePhase: 95% ACN / 0.1% TFA

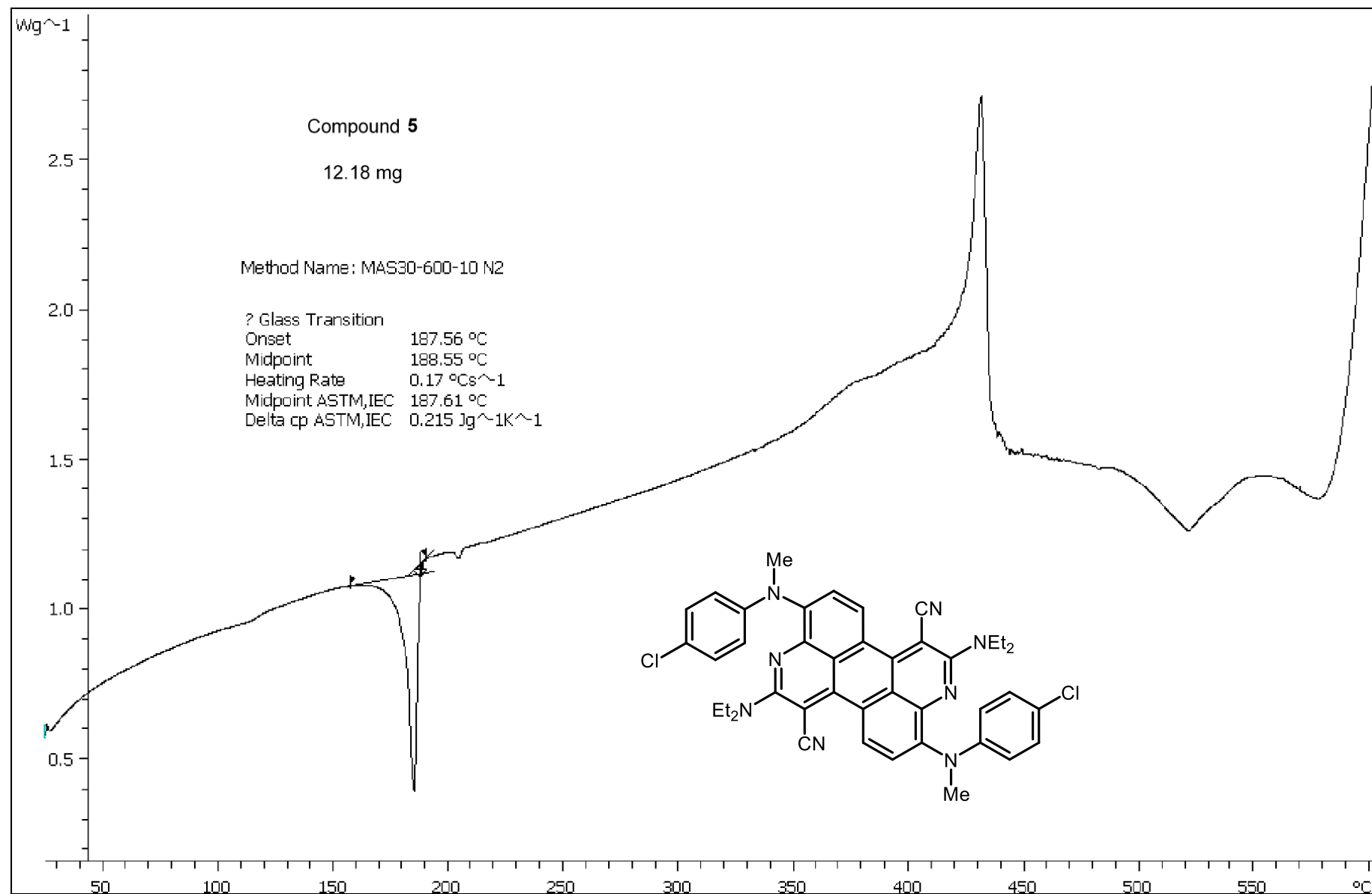
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Acq Method Set : AllianceE 100% A isocratic

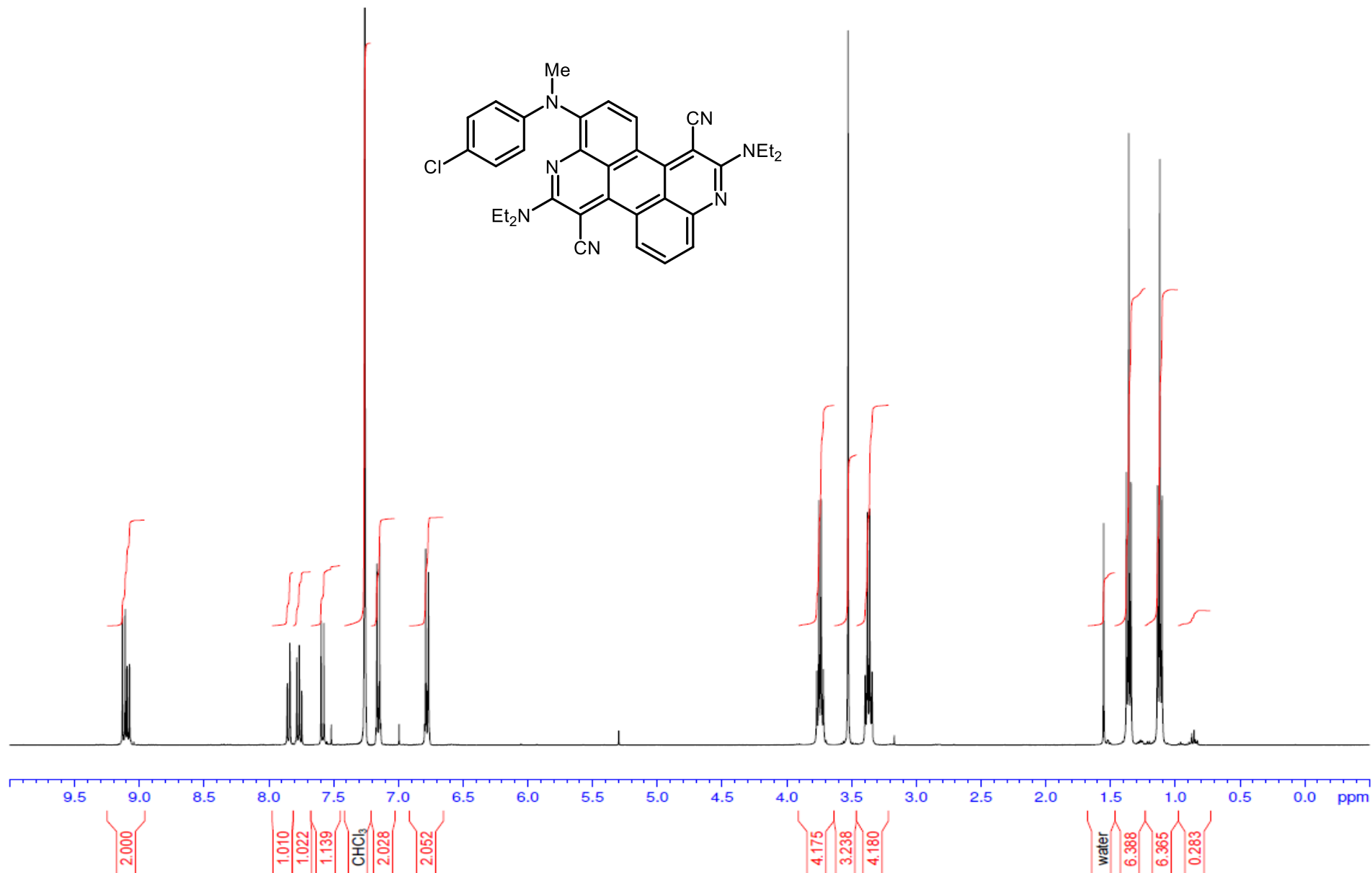
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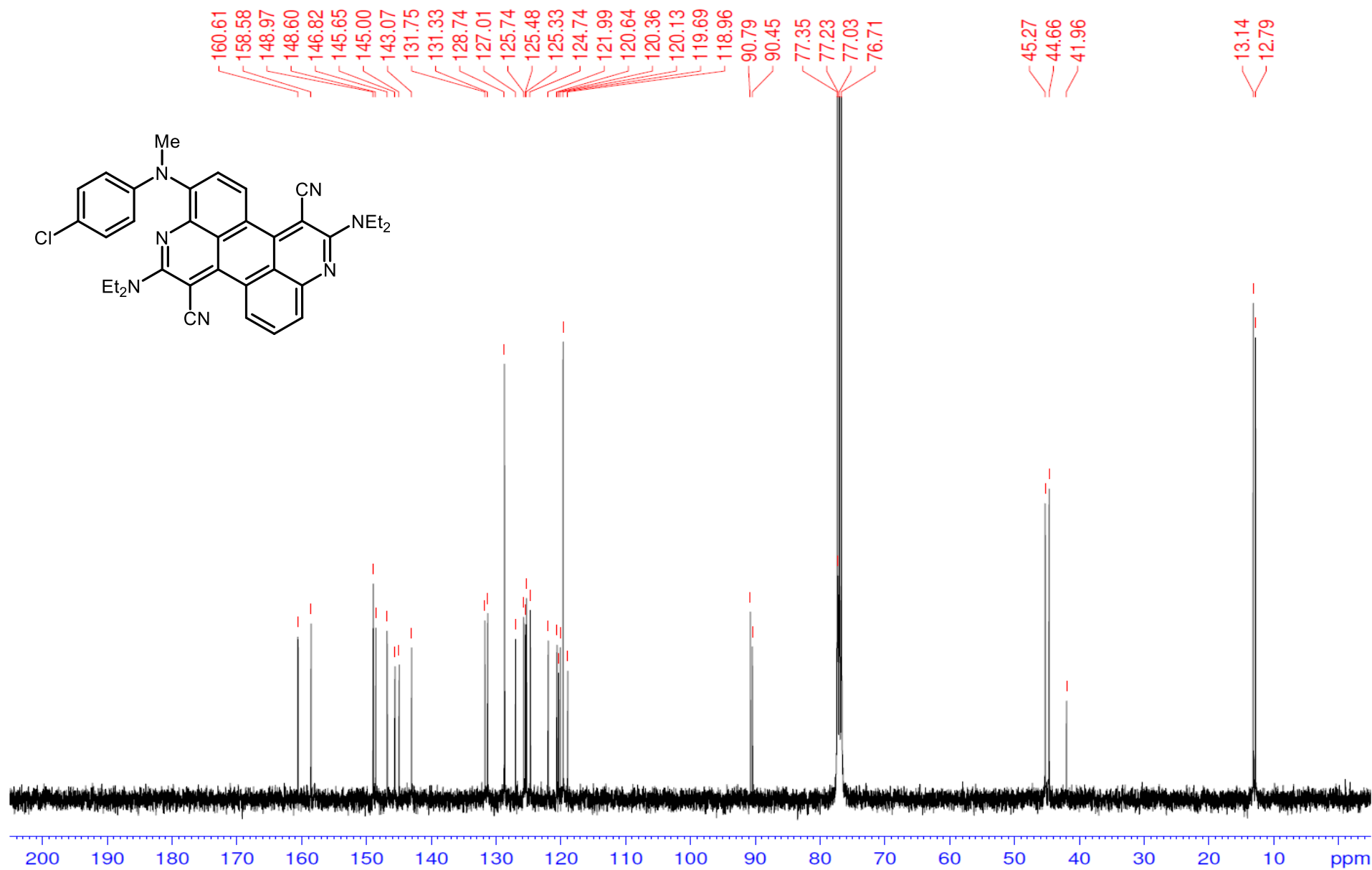
Processing Method: nkh



DSC curve for **5**

^1H NMR spectrum for **6** (400 MHz; CDCl_3)



¹³C NMR spectrum of **6** (100 MHz; CDCl₃)

HPLC Chromatogram for **6**

Sample Name: CLF794-37 combined 95%ACN/TFA Date Acquired: 3/12/2010 10:33:30 AM EST

Detector: PDA 283.0 nm

Acq Method Set : AllianceE 100% A isocratic

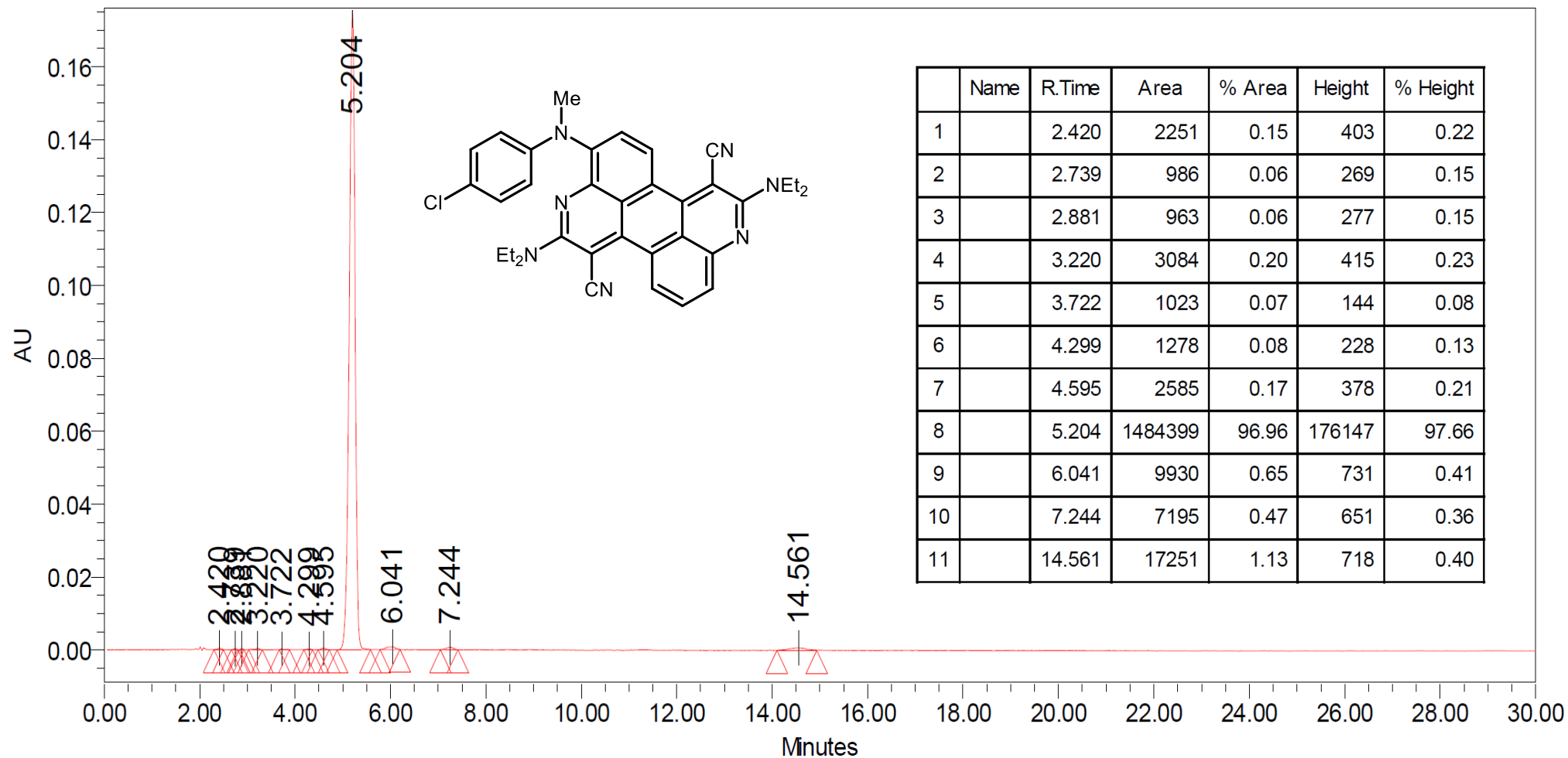
HplcColumn 150x4.6mm Alltima HP C18

Date Processed: 3/12/2010 12:31:32 PM EST

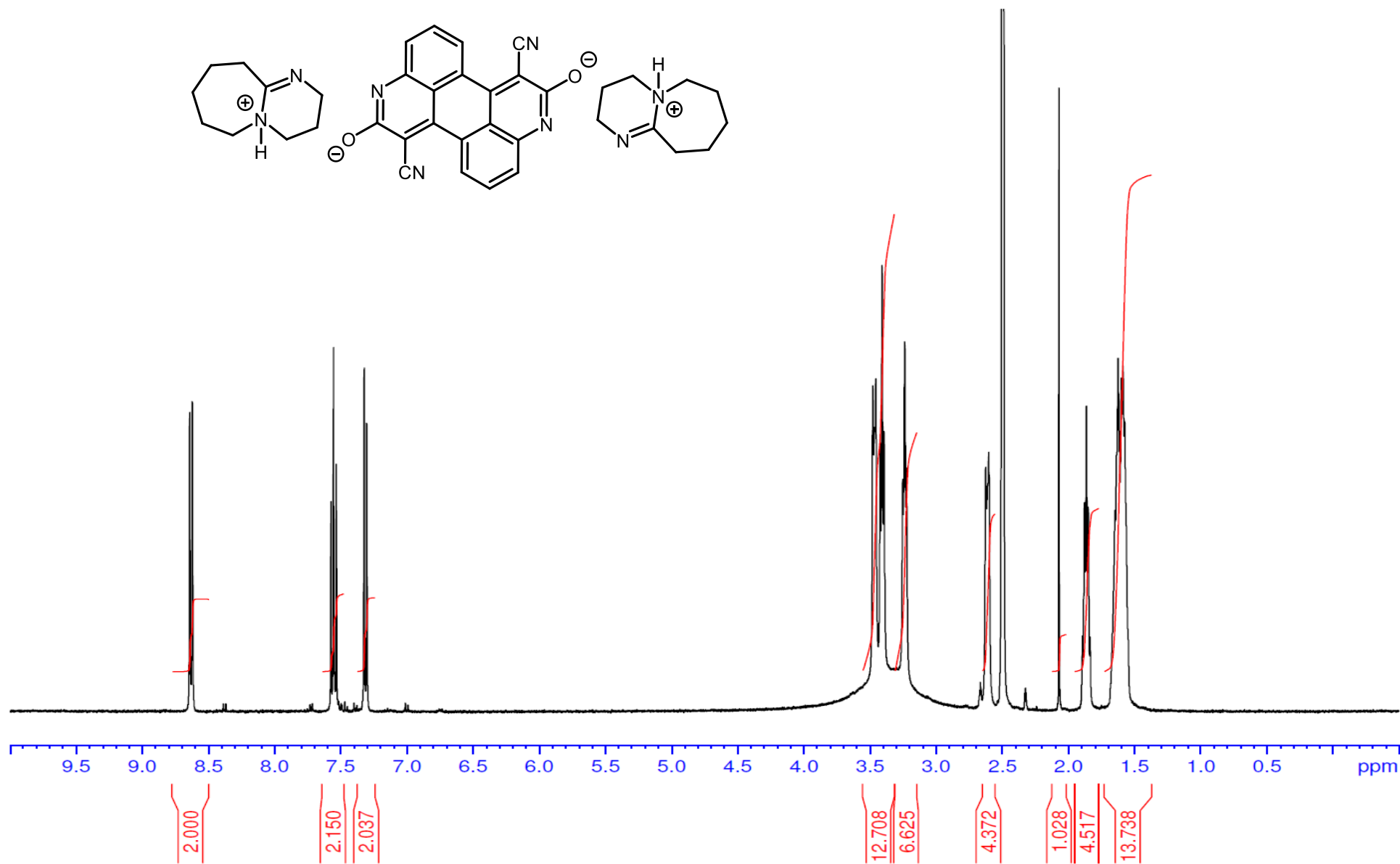
FlowRate: 1.0 mL / min

Processing Method: nkh

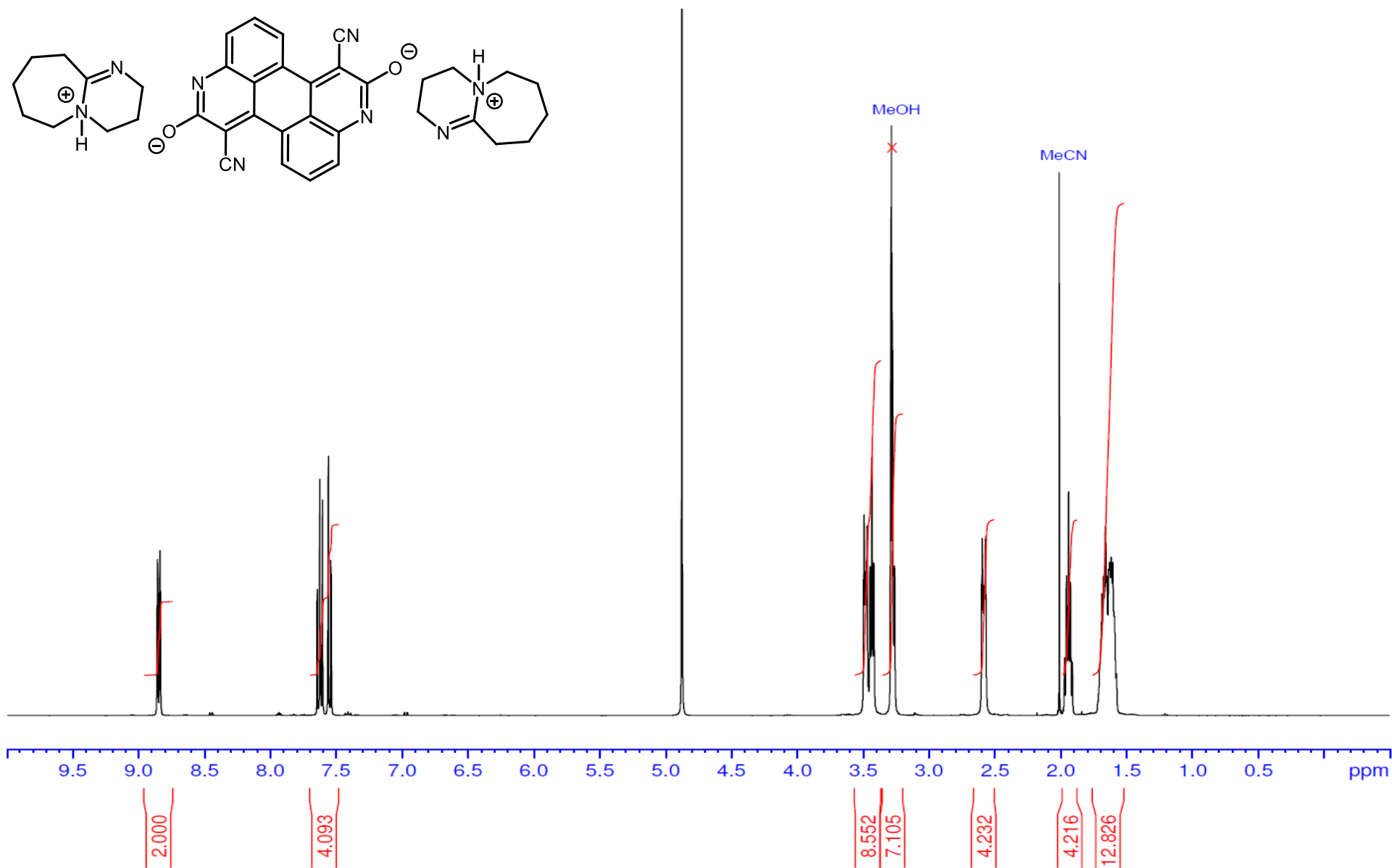
MobilePhase: 95% ACN / 0.1% TFA

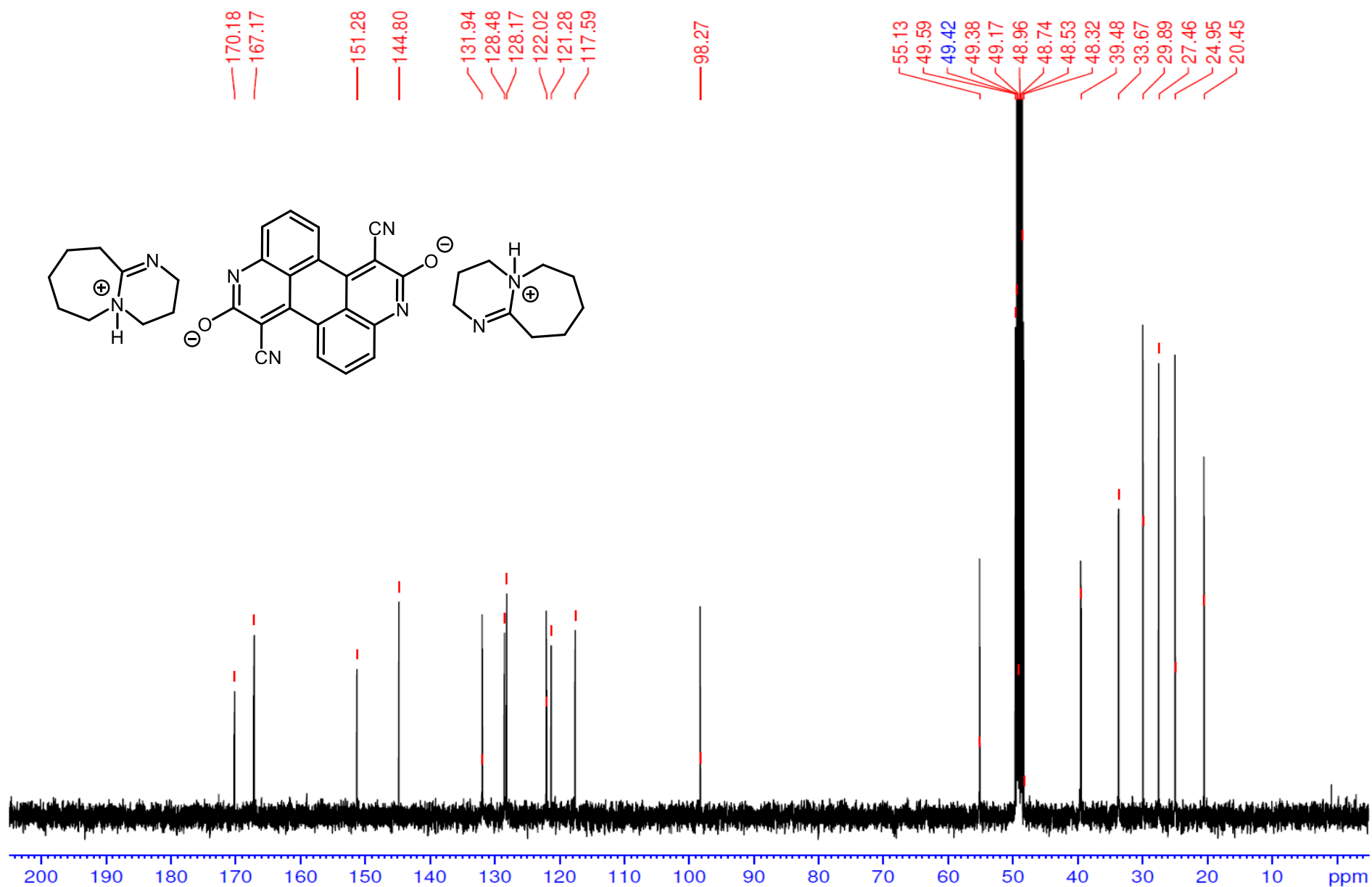


^1H NMR spectrum for **8** (400 MHz; DMSO- d_6)



^1H NMR spectrum for **8** (400 MHz; CD_3OD)



¹³C NMR spectrum for **8** (100 MHz; CD₃OD)

HPLC Chromatogram for **8**Sample Name: KMM-276-29 DBU salt 30%ACN/H₂O

Date Acquired: 16/08/2011 4:37:15 PM EST

Detector: PDA 240.0 nm

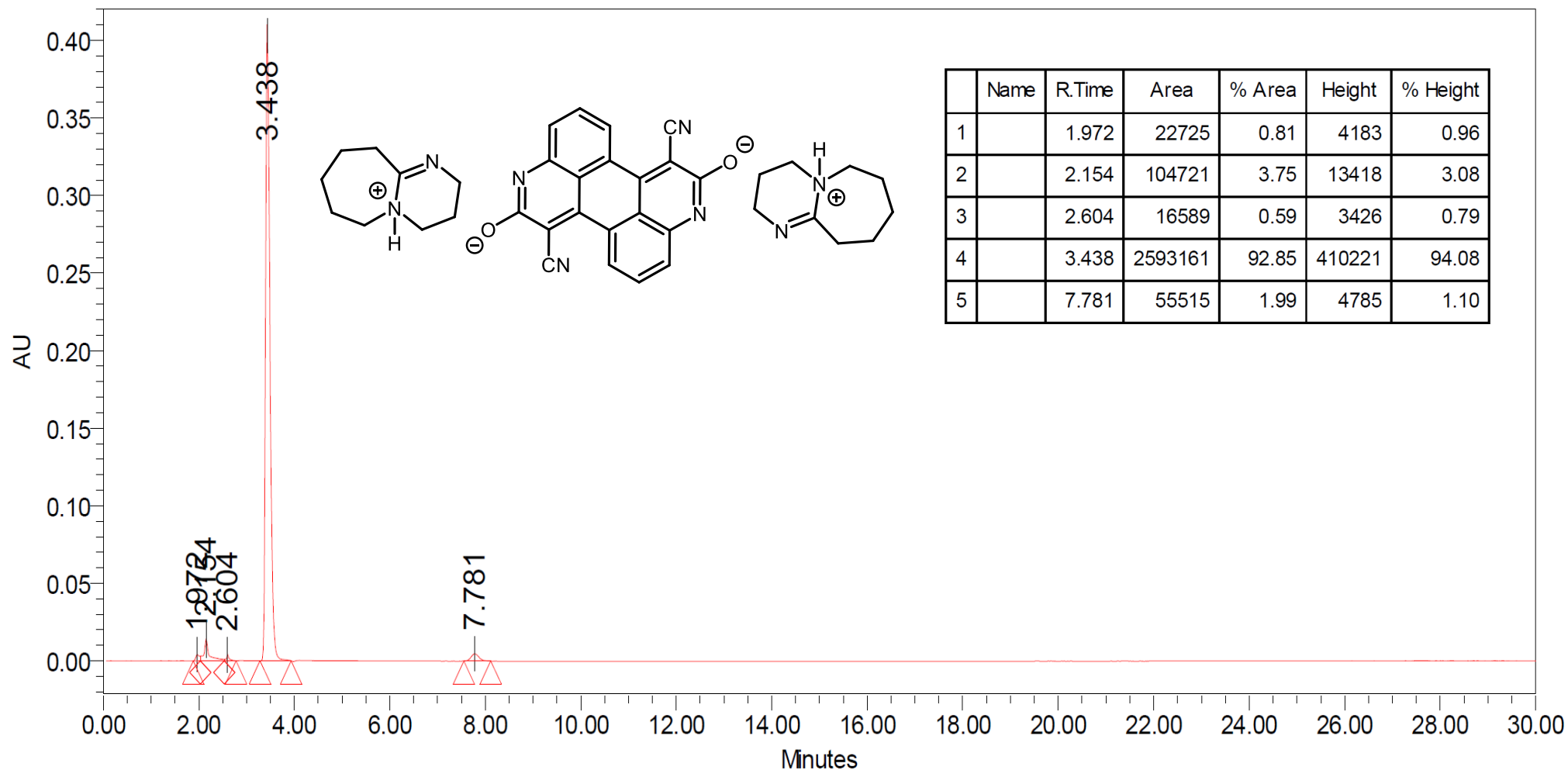
Acq Method Set : AllianceE 100% A isocratic

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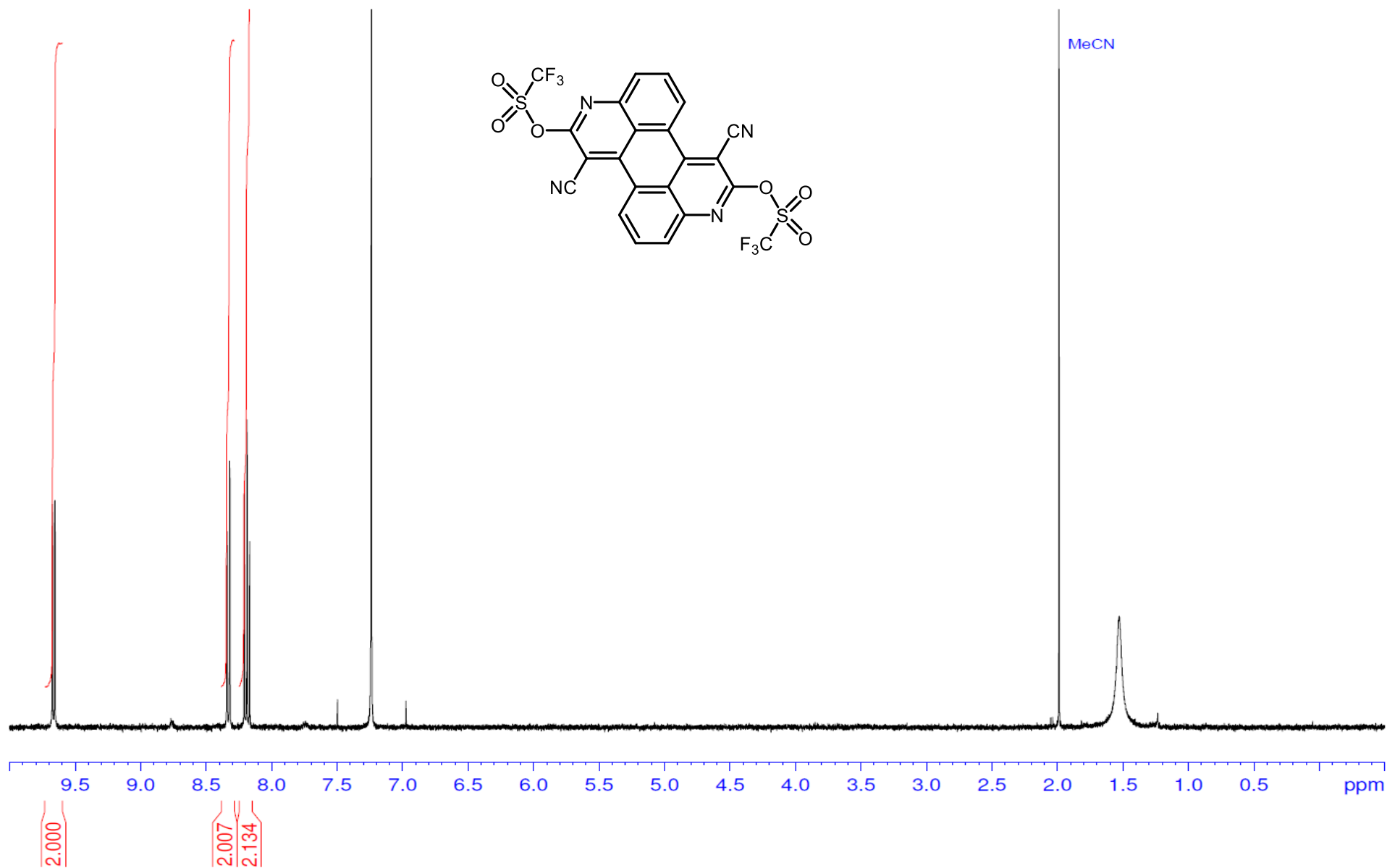
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FlowRate: 1.0 mL / min

Processing Method: nkh

MobilePhase: 30% ACN / H₂O

¹H NMR spectrum for **9** (400 MHz; CDCl₃)



HPLC Chromatogram for 9

Sample Name: KMM-276-54 80%ACN/H2O

Detector: PDA 343.0 nm

HplcColumn 150x4.6mm Allitm HP C18

FlowRate: 1.0 mL / min

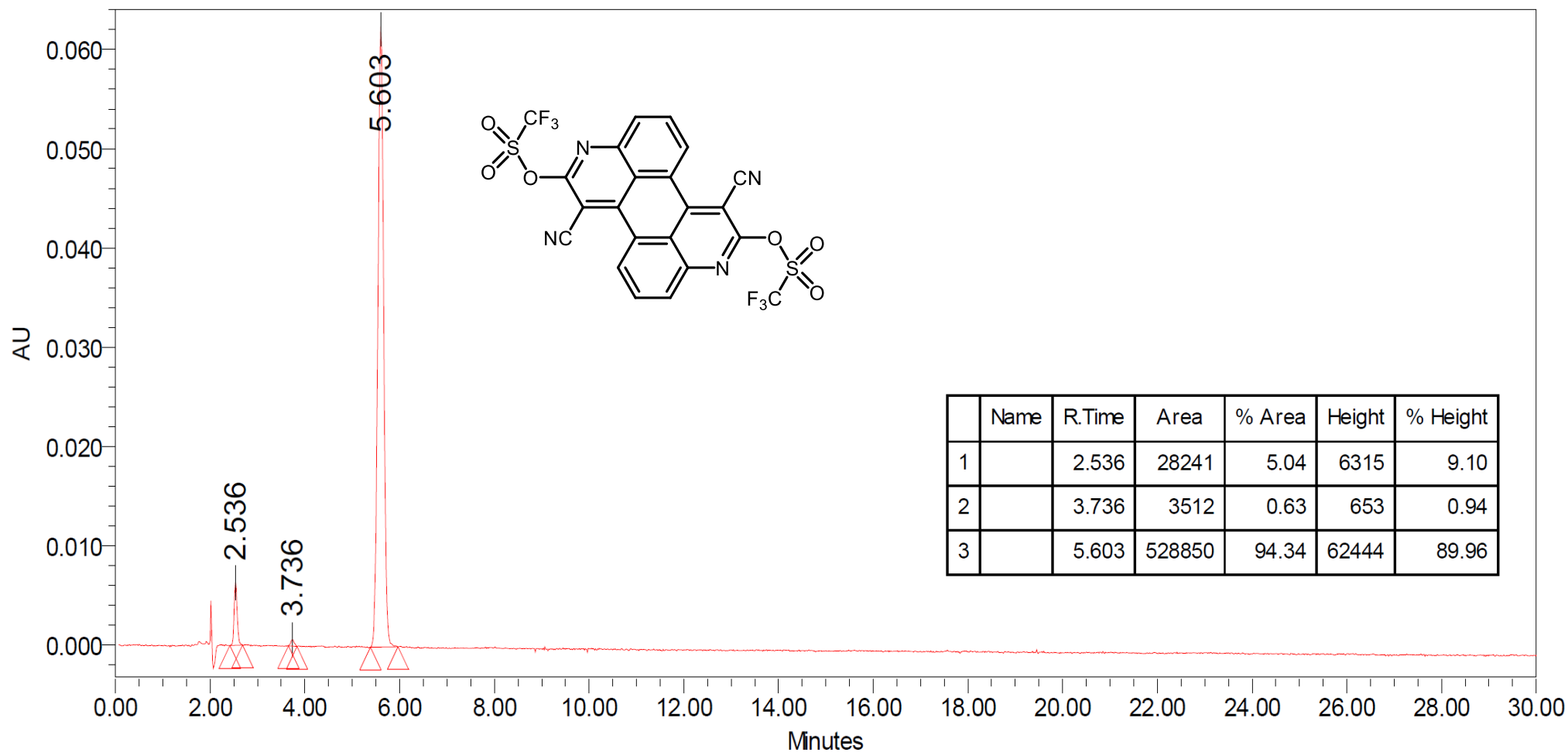
MobilePhase: 80% ACN / H2O

Date Acquired: 18/08/2011 10:33:24 AM EST

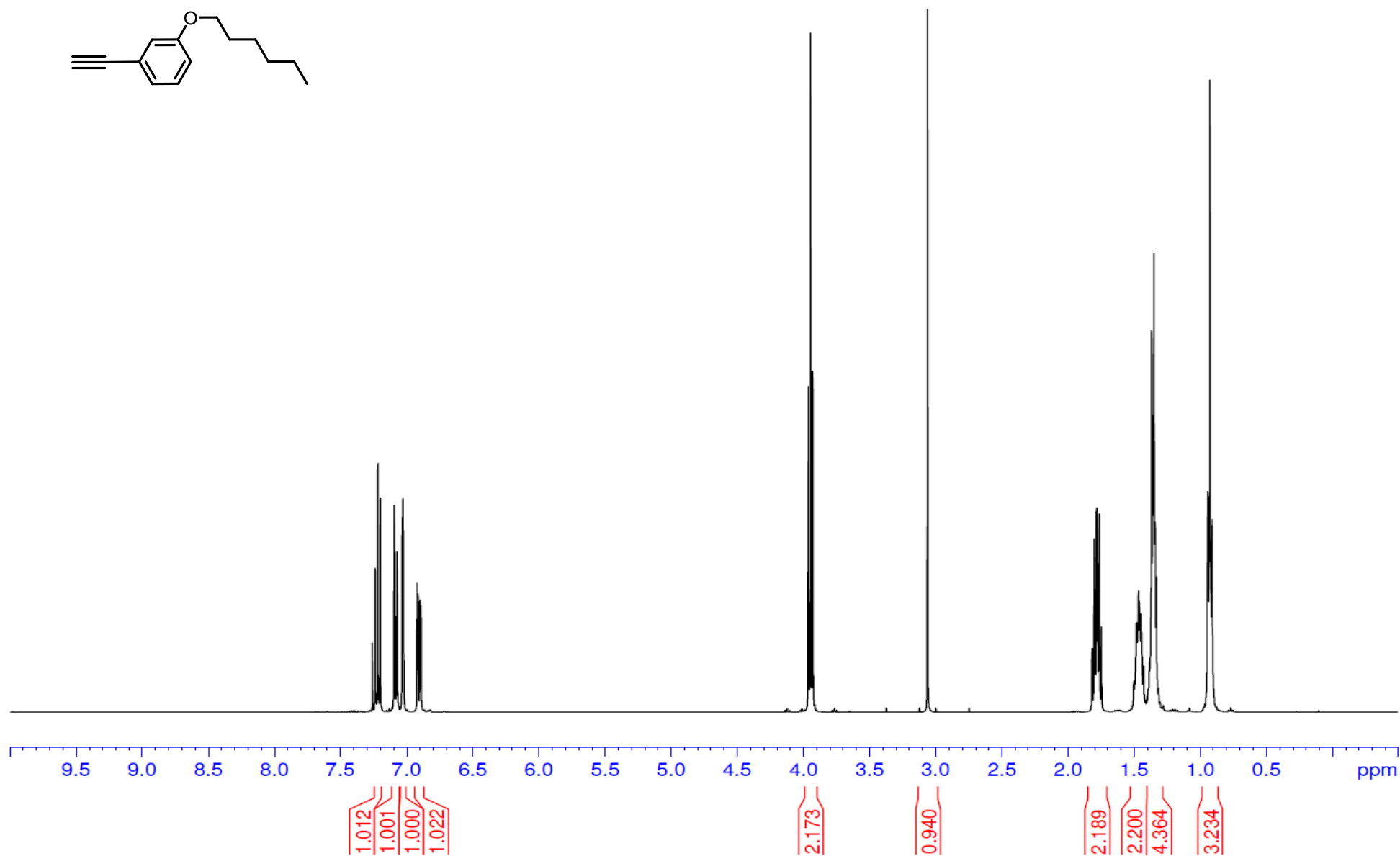
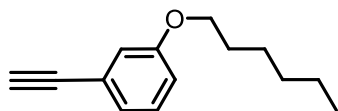
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Date Processed: 18/08/2011 11:43:31 AM EST

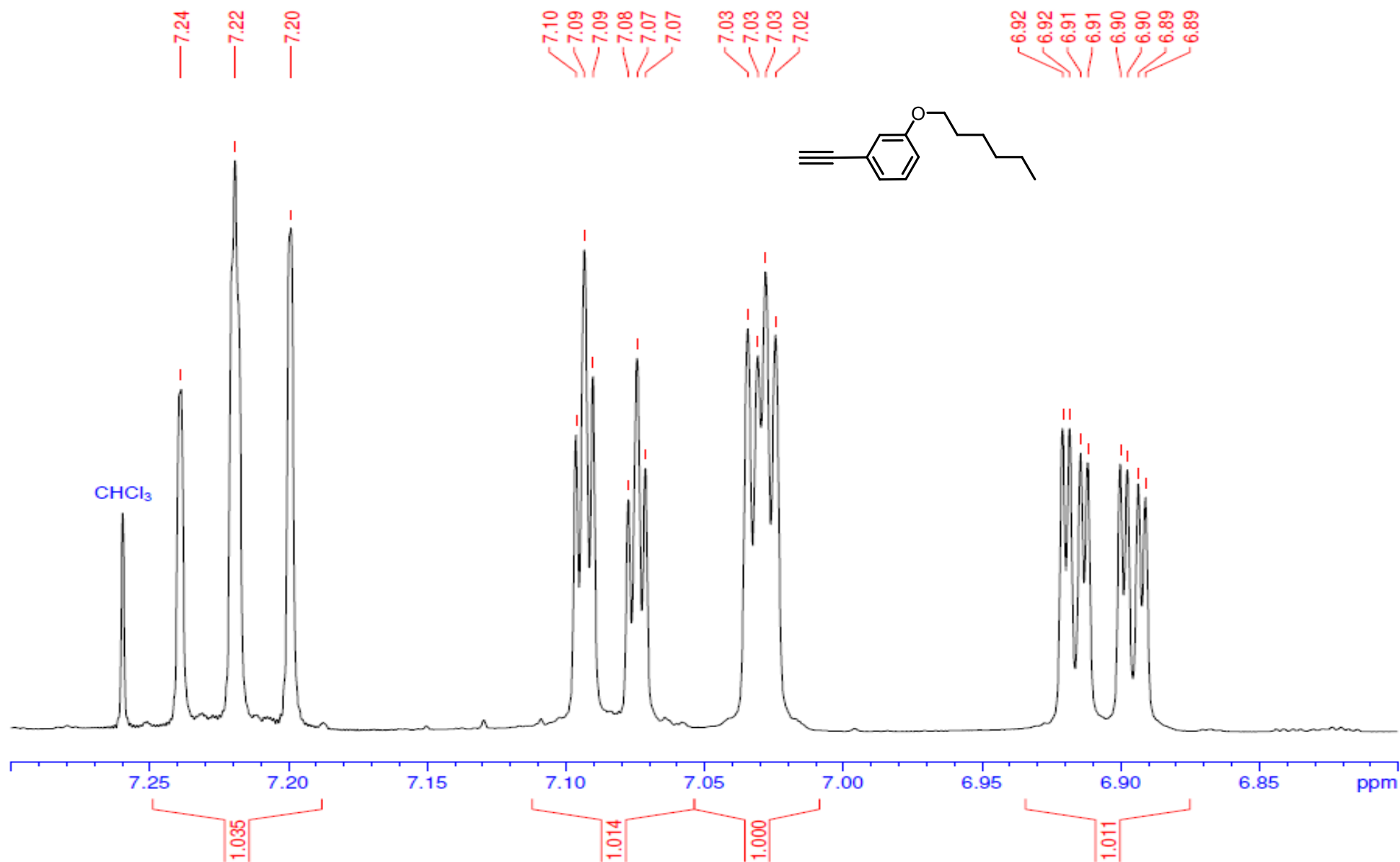
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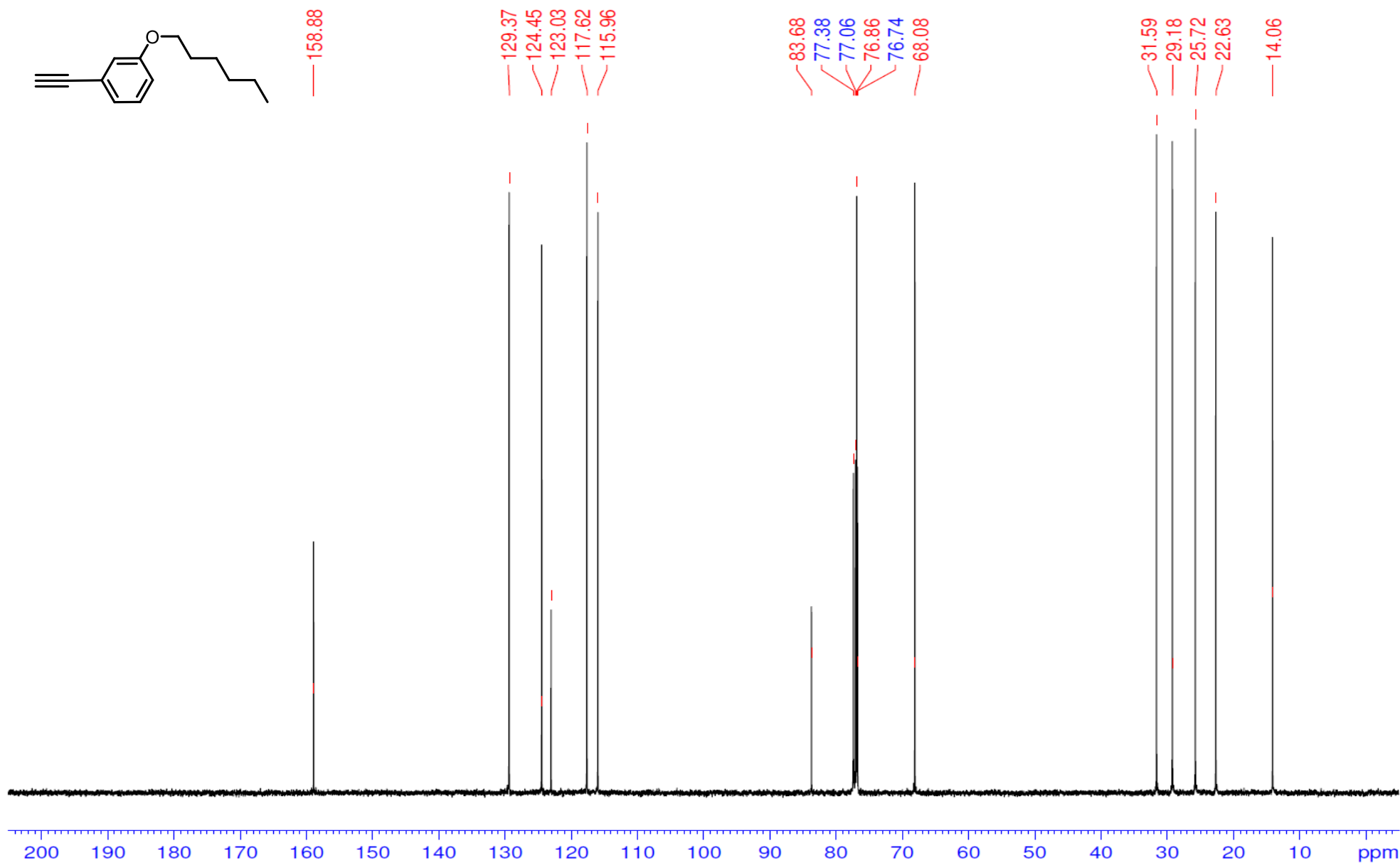


¹H NMR spectrum for **10b** (400 MHz; CDCl₃)



Expanded aromatic region of ^1H NMR spectrum for **10b** (400 MHz; CDCl_3)



¹³C NMR spectrum for **10b** (100 MHz; CDCl₃)

¹H NMR spectrum for **10c** (400 MHz; CDCl₃)

Username M. Ayer
MA233-27
Av400_1H CDCl₃

7.60
7.53

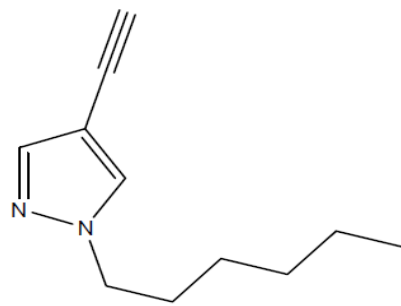
4.08

3.00

1.84

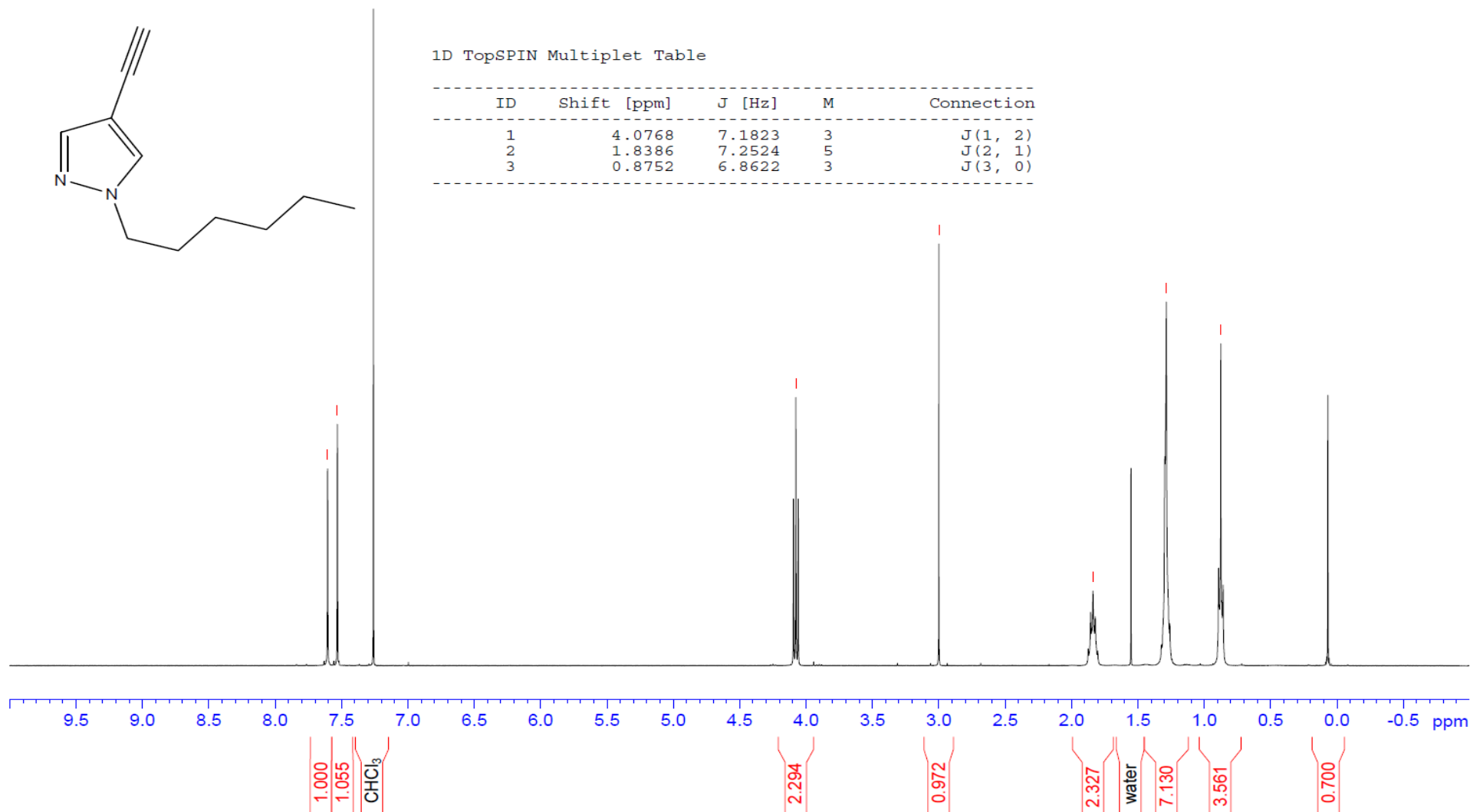
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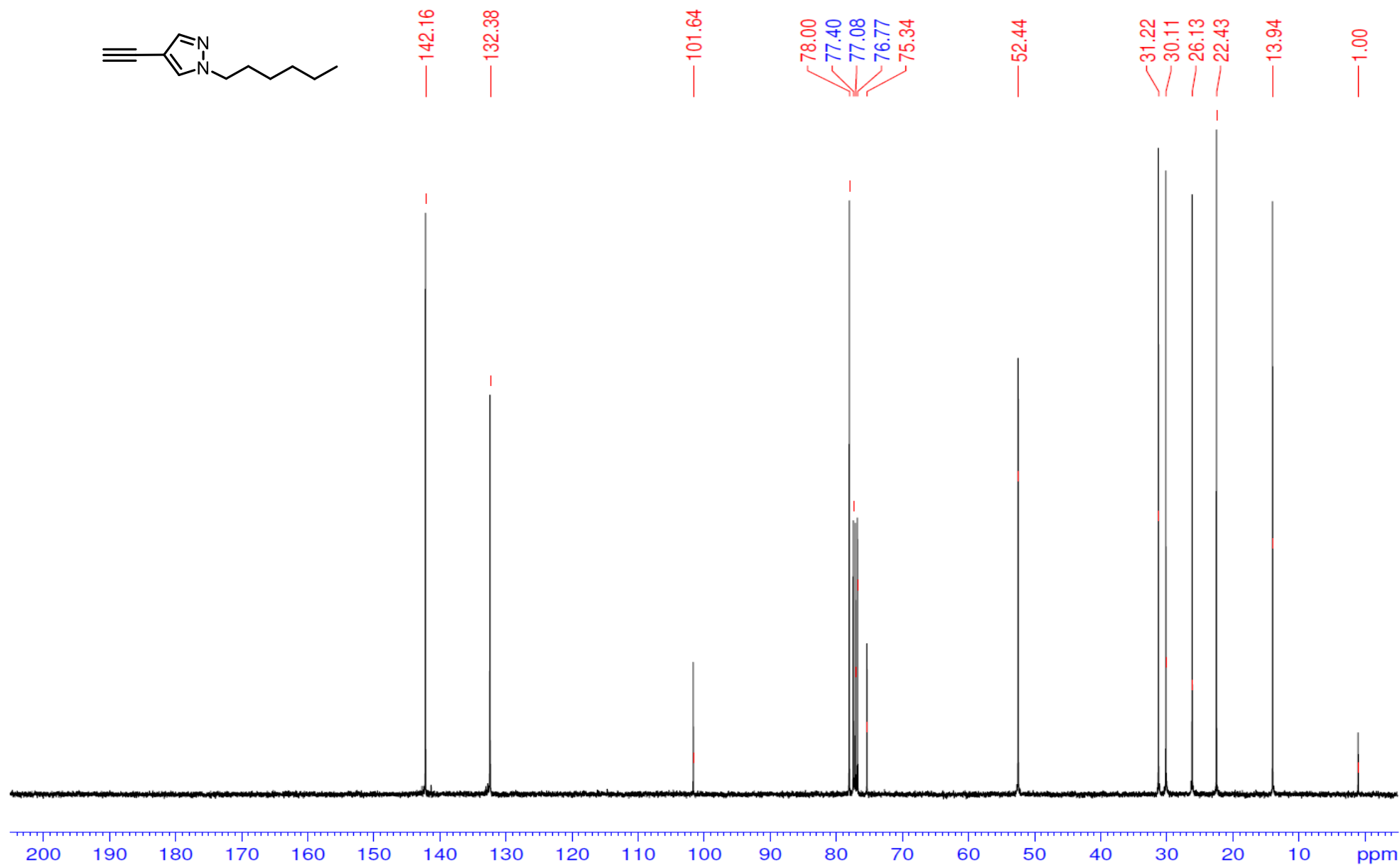
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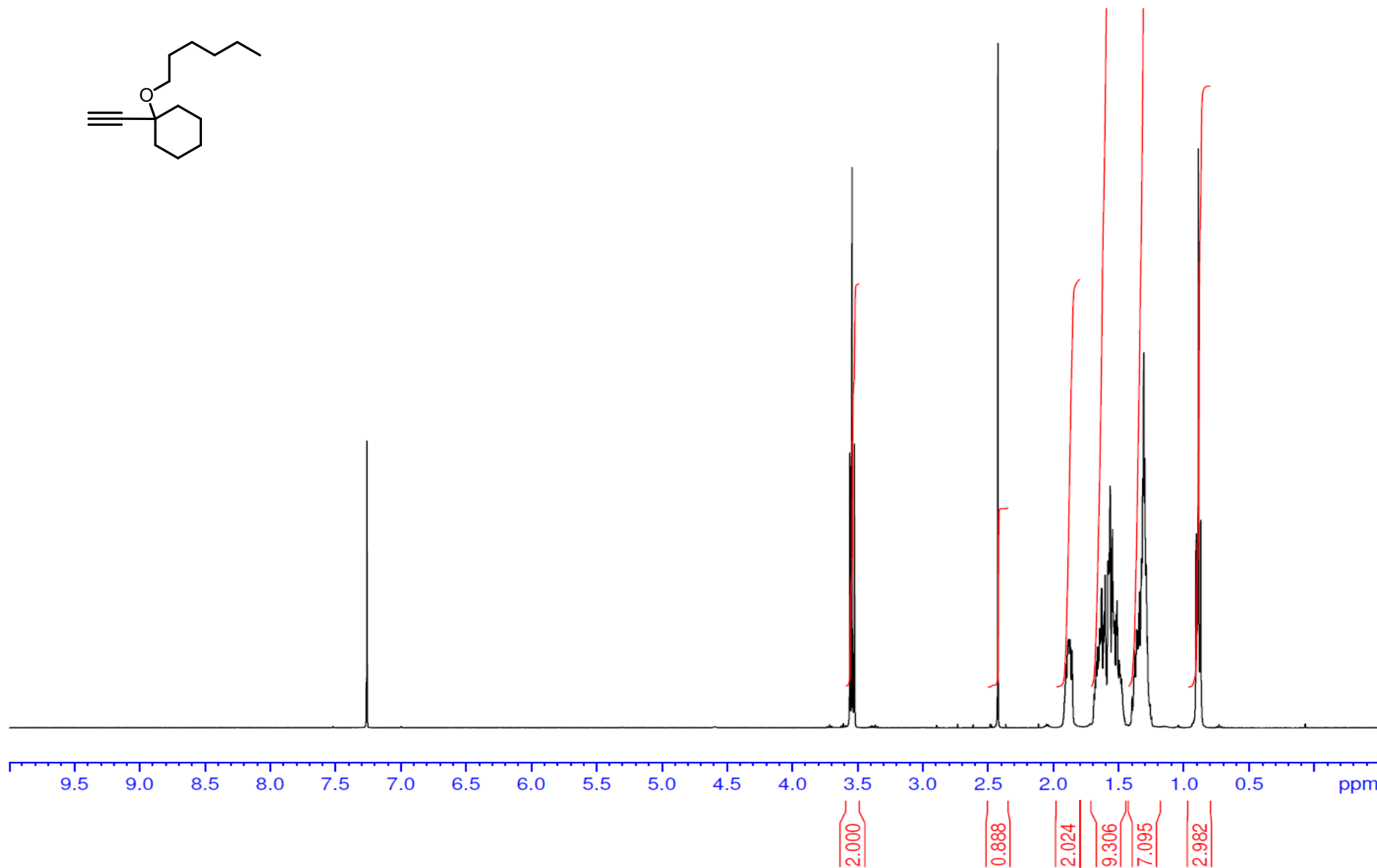
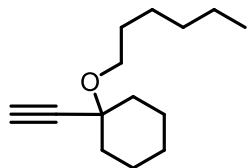
1D TopSPIN Multiplet Table

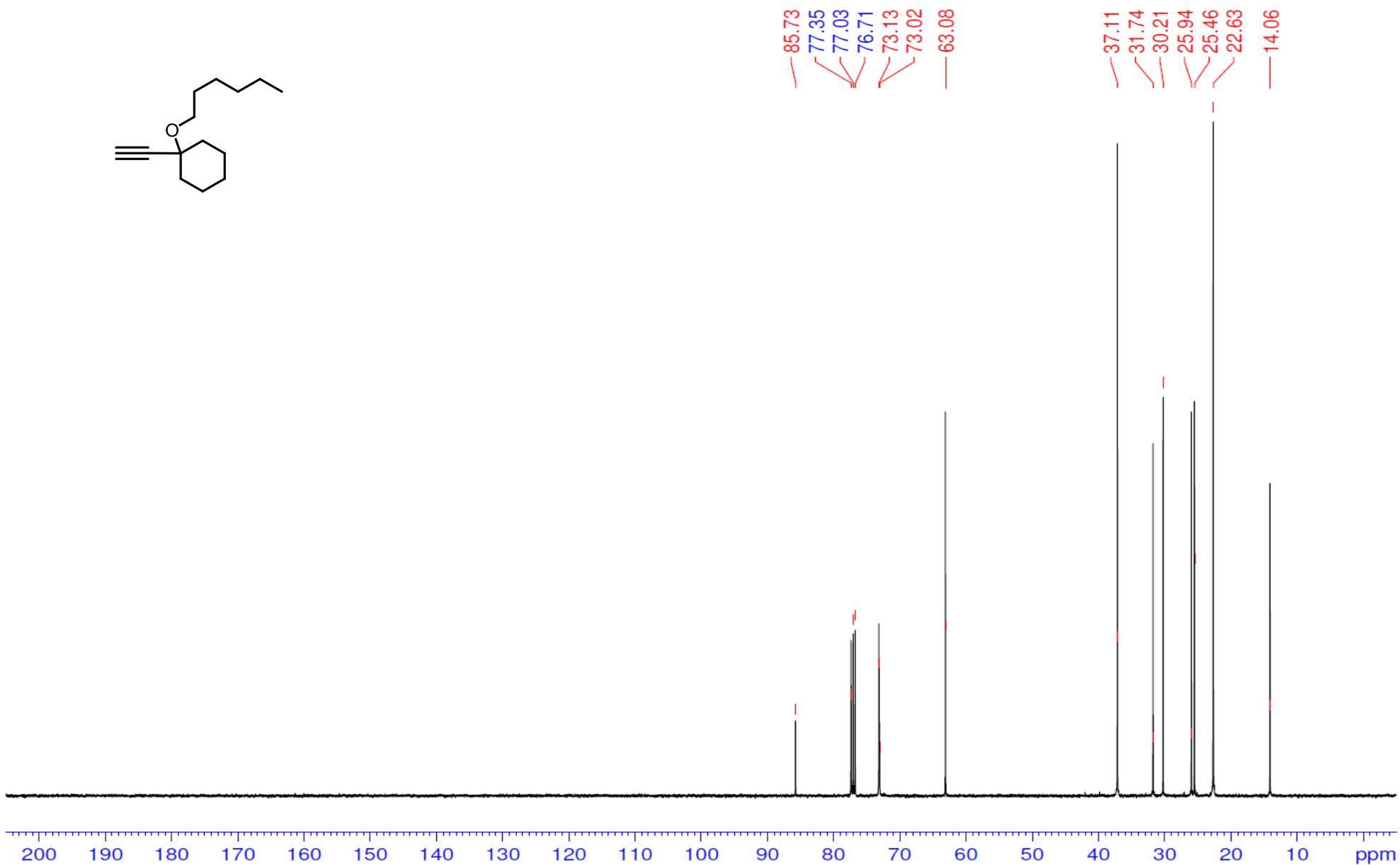
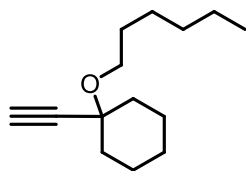
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2	1.8386	7.2524	5	J(2, 1)
3	0.8752	6.8622	3	J(3, 0)

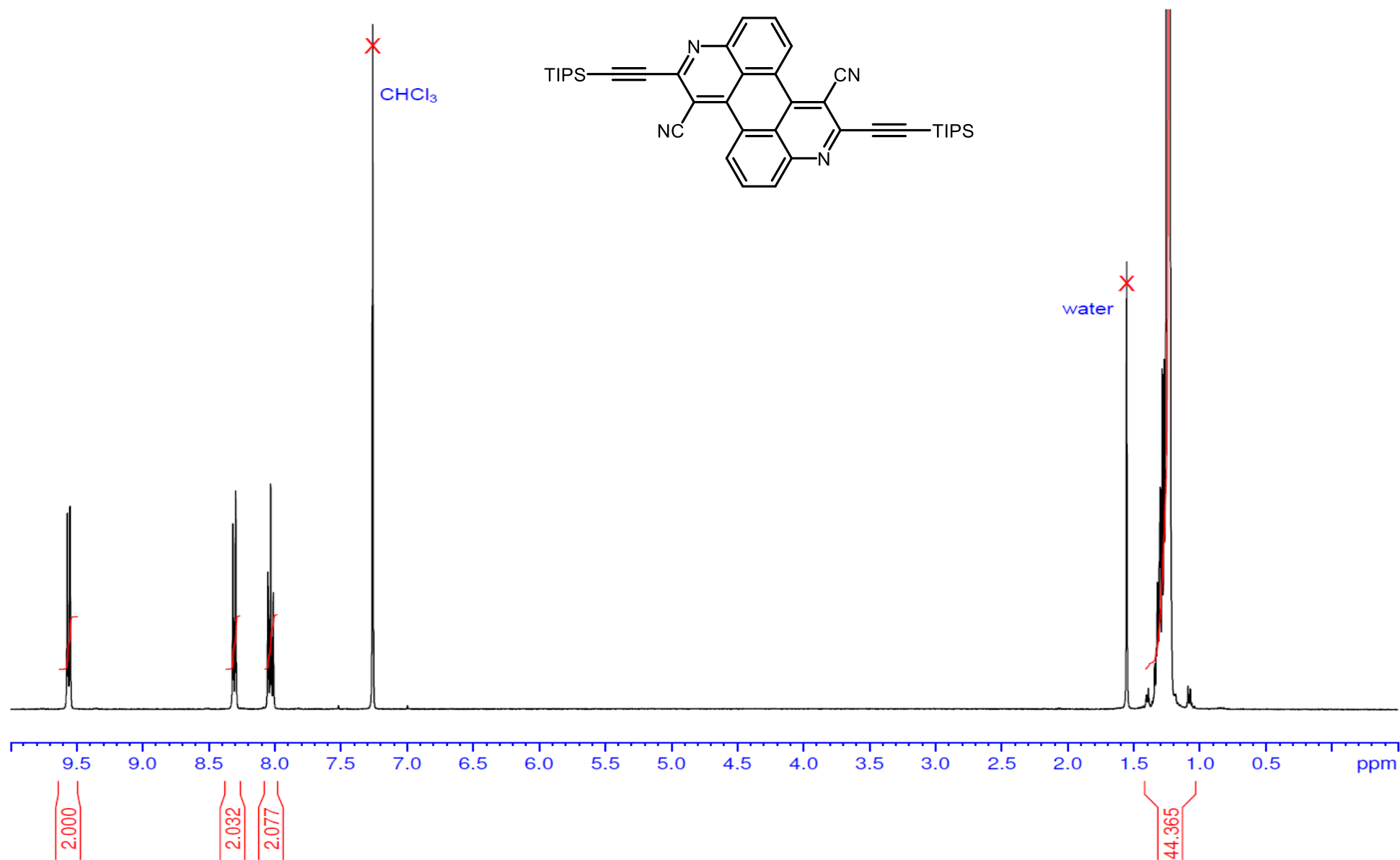


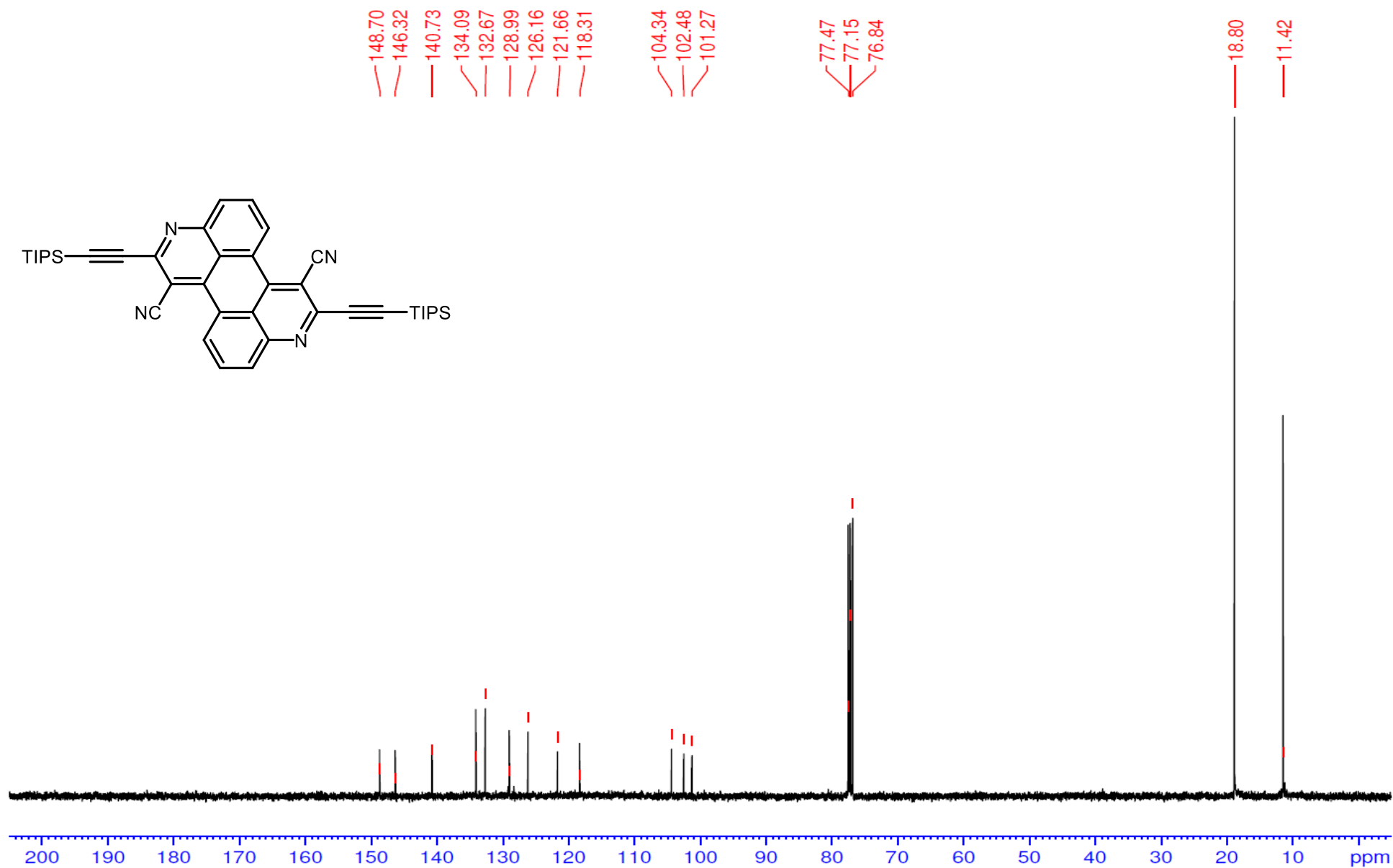
¹³C NMR spectrum for **10c** (100 MHz; CDCl₃)

^1H NMR spectrum for **10d** (400 MHz; CDCl_3)



¹³C NMR spectrum for **10d** (100 MHz; CDCl₃)

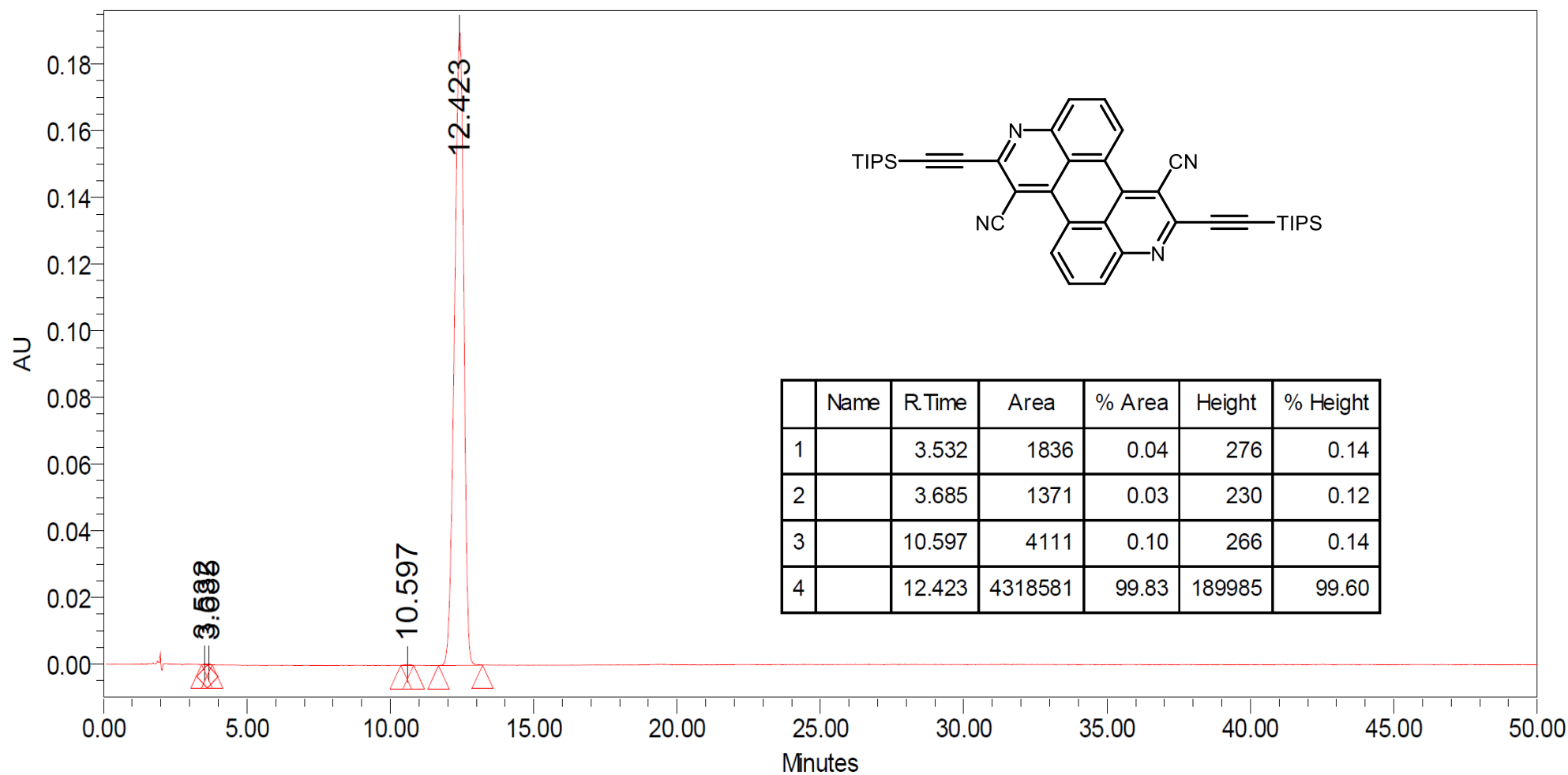
¹H NMR spectrum for **11a** (400 MHz; CDCl₃)

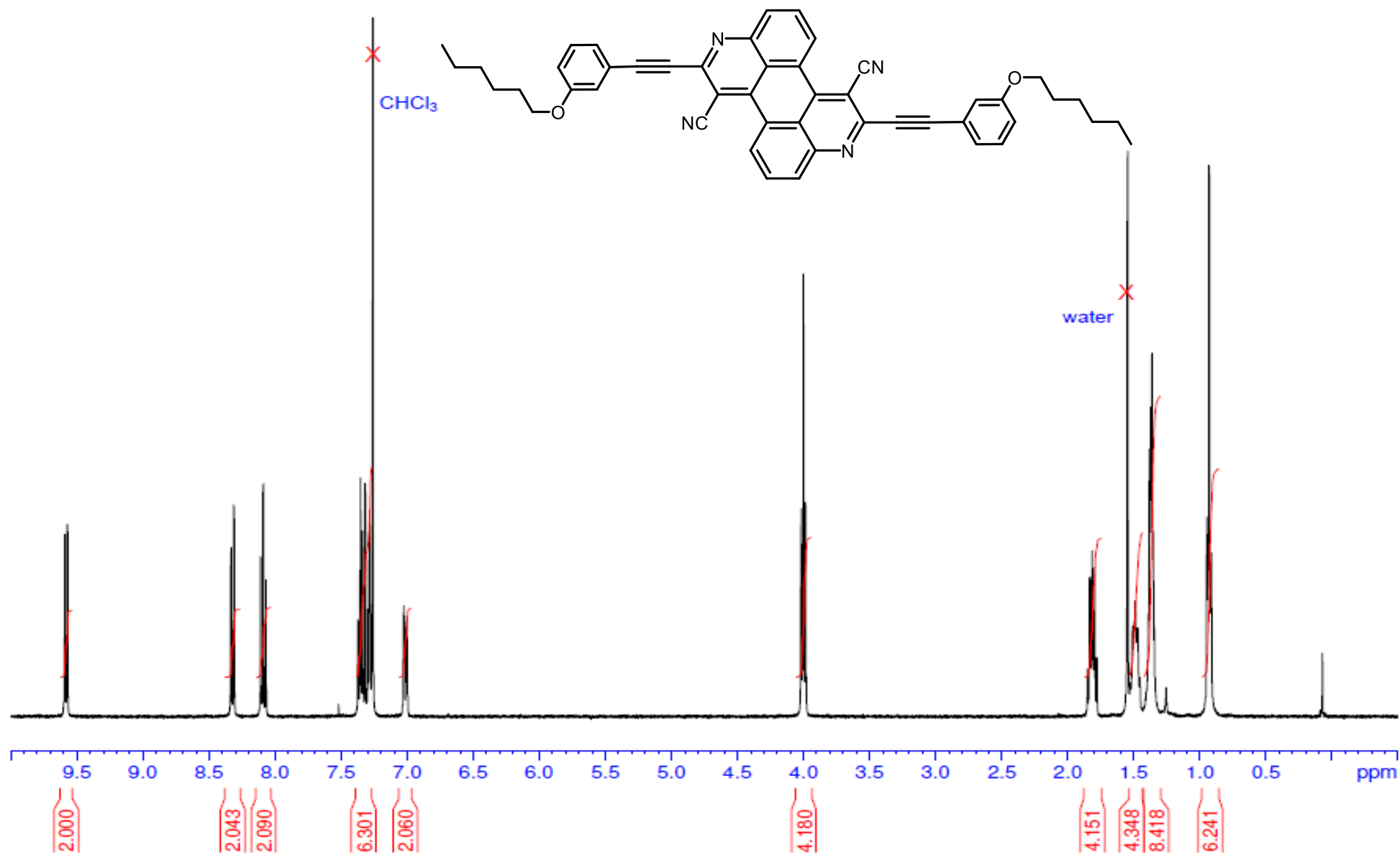
¹³C NMR spectrum for **11a** (100 MHz; CDCl₃)

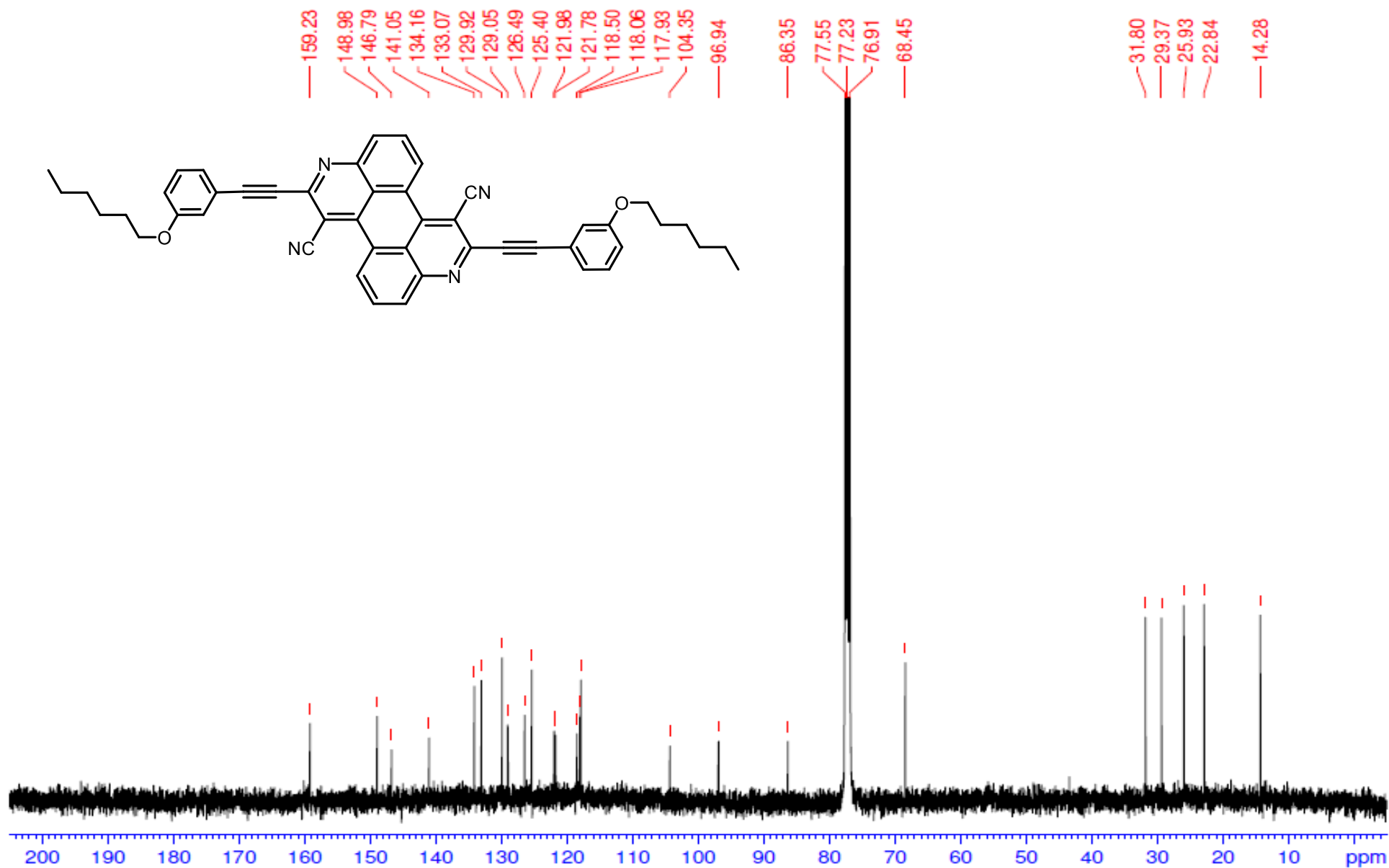
HPLC Chromatogram for **11a**

Sample Name: KMM-276-48-1 5%THF/ACN
Detector: PDA 280.0 nm
HplcColumn 150x4.6mm Alltima HP C18
FlowRate: 1.0 mL / min
MobilePhase: 5% THF / ACN

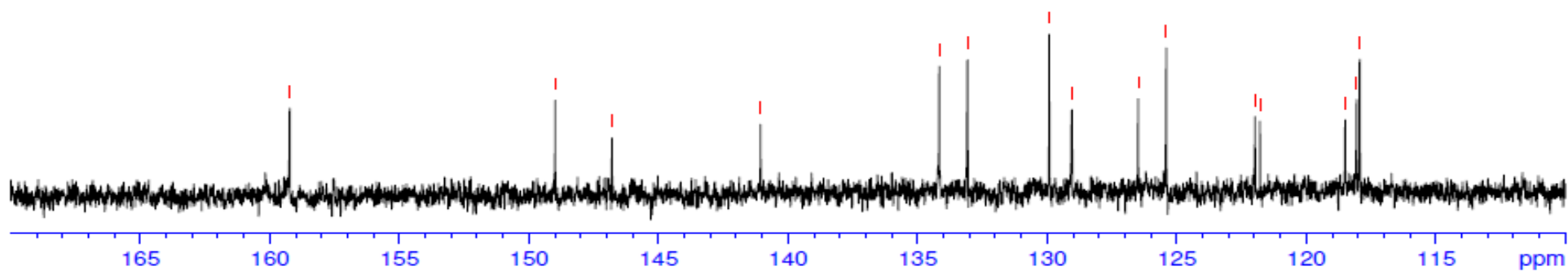
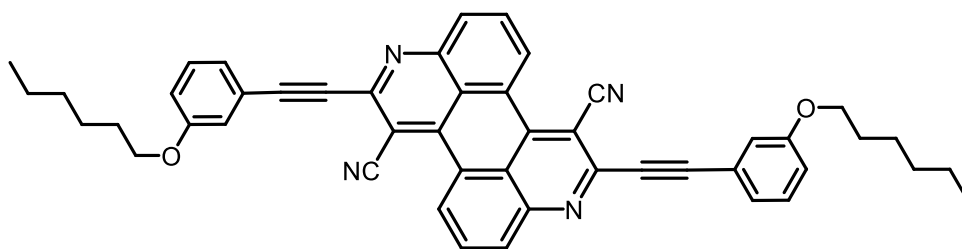
Date Acquired: 21/07/2011 2:52:47 PM EST
Acq Method Set : AllianceE 100% A isocratic
Date Processed: 21/07/2011 3:56:11 PM EST
Processing Method: nkh



¹H NMR spectrum for **11b** (400 MHz; CDCl₃)

¹³C NMR spectrum for **11b** (100 MHz; CDCl₃)

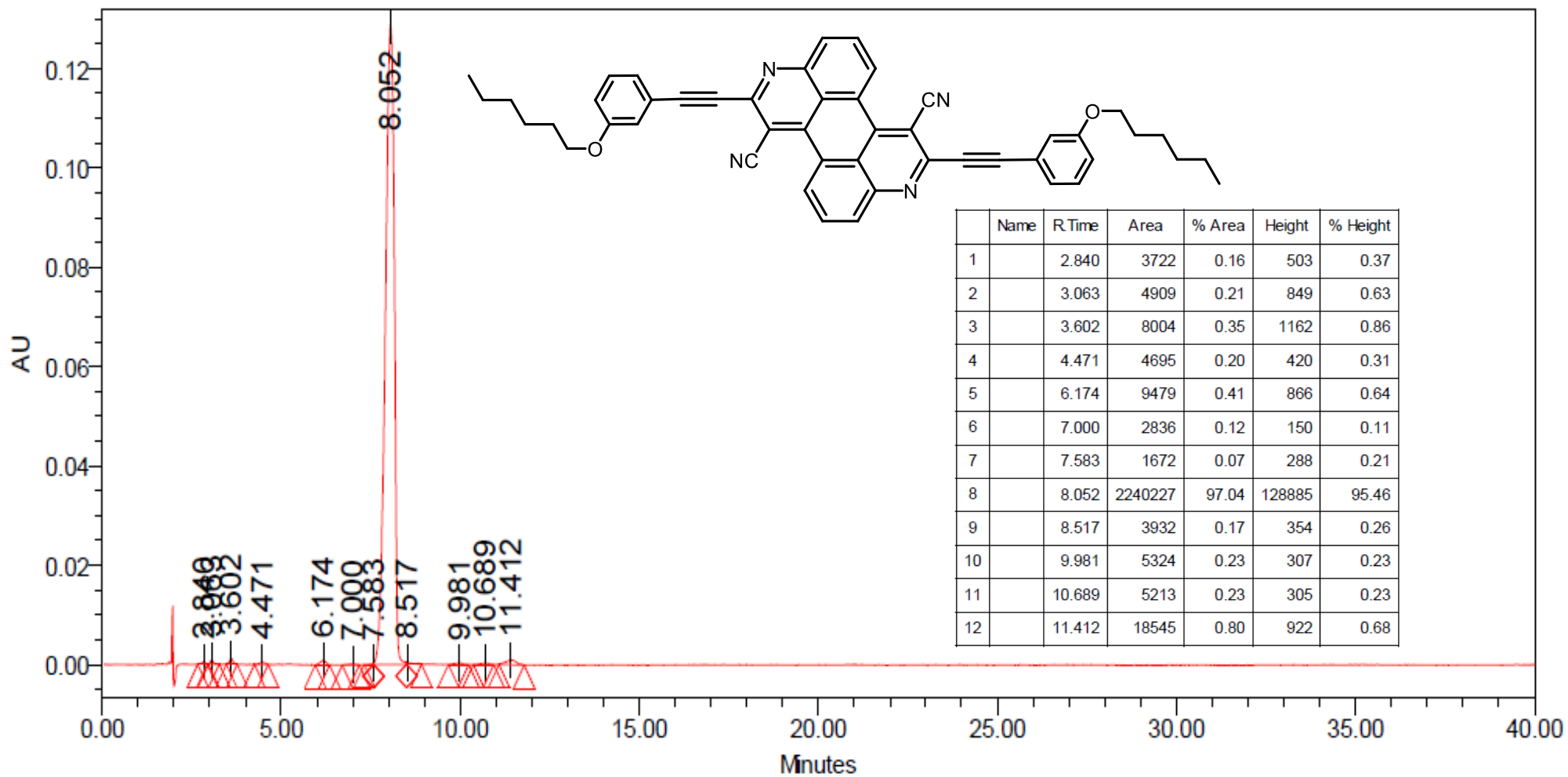
159.23	148.98	146.79	141.05	134.16	133.07	129.92	129.05	126.49	125.40	121.98	121.78	118.50	118.06	117.93
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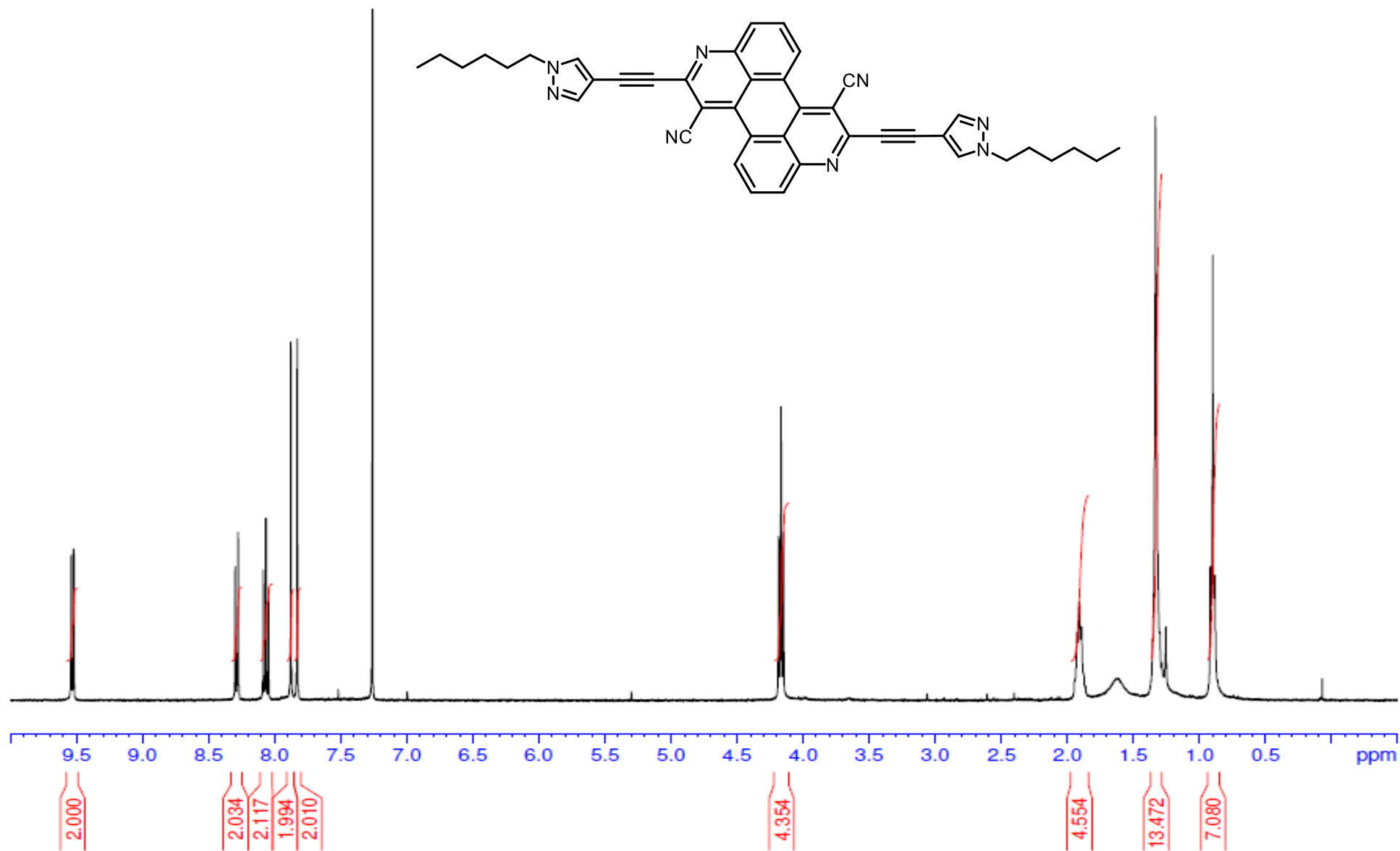


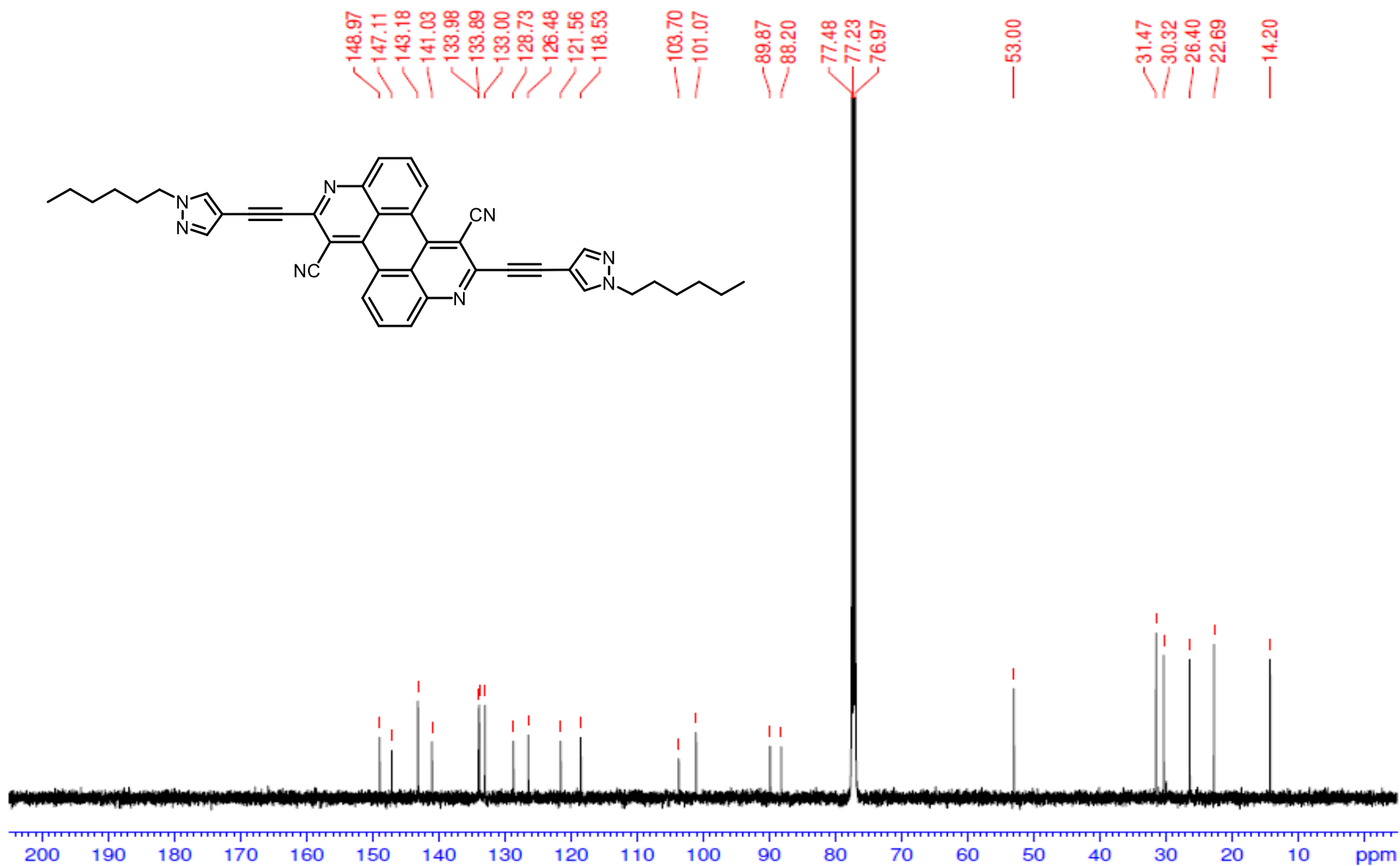
HPLC Chromatogram for **11b**

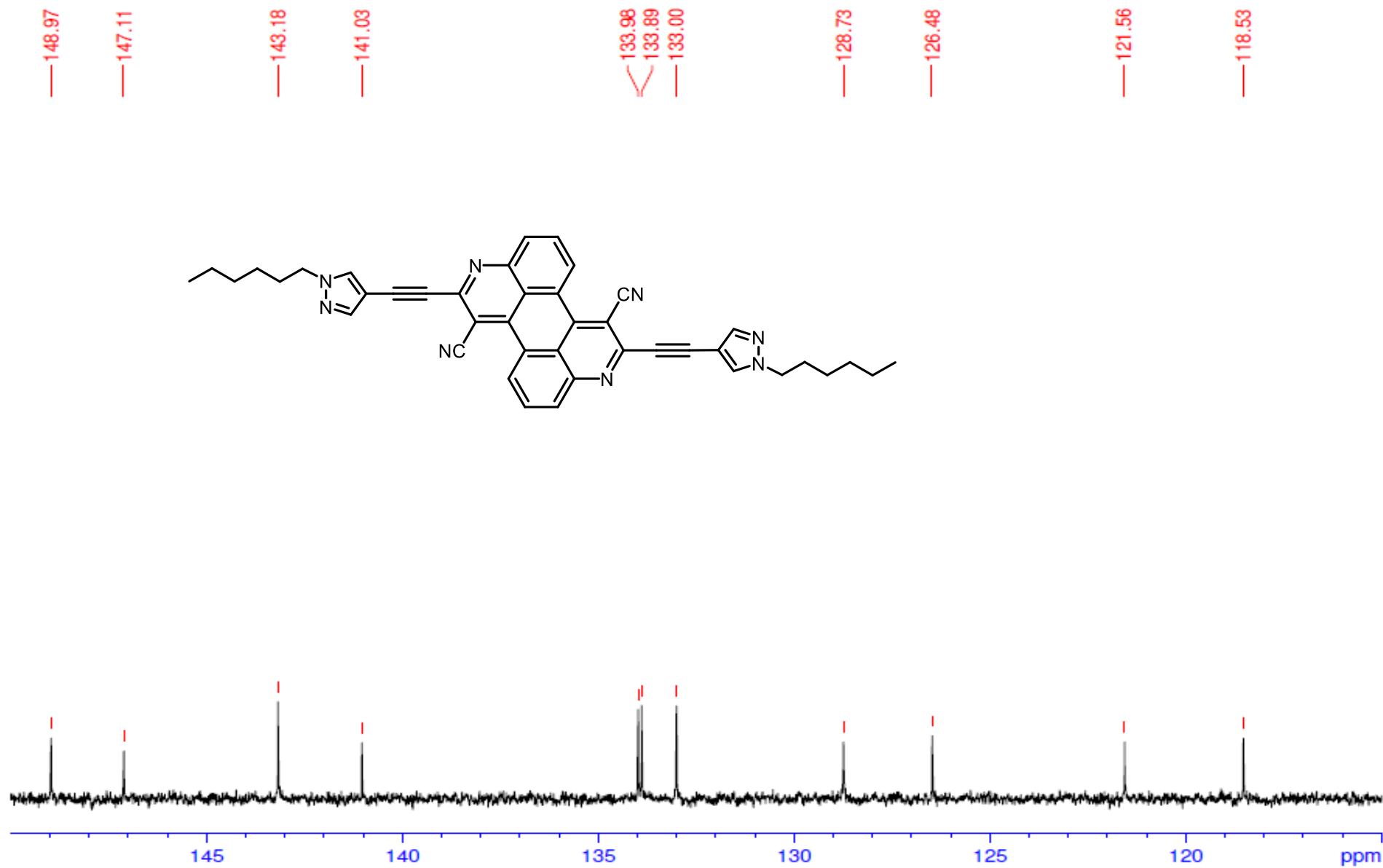
Sample Name: KMM-276-56 5%THF/ACN
Detector: PDA 305.0 nm
HplcColumn 150x4.6mm Alltima HP C18
FlowRate: 1.0 mL / min
MobilePhase: 5% THF / ACN

Date Acquired: 7/12/2011 6:08:12 PM EST
Acq Method Set : AllianceE 100% A isocratic
Date Processed: 8/12/2011 2:32:22 PM EST
Processing Method: nkh



¹H NMR spectrum for **11c** (400 MHz; CDCl₃)

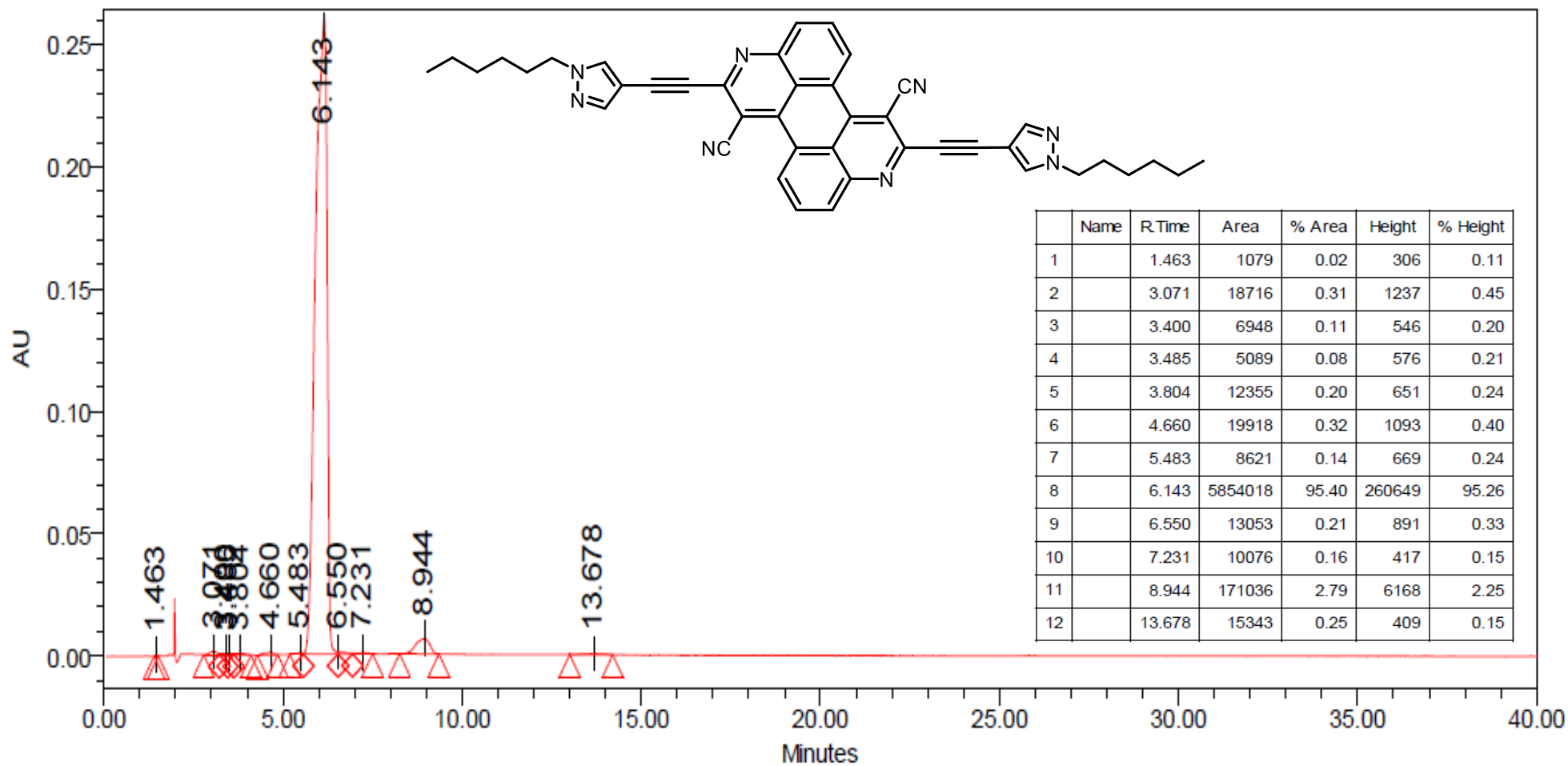
¹³C NMR spectrum for **11c** (100 MHz; CDCl₃)

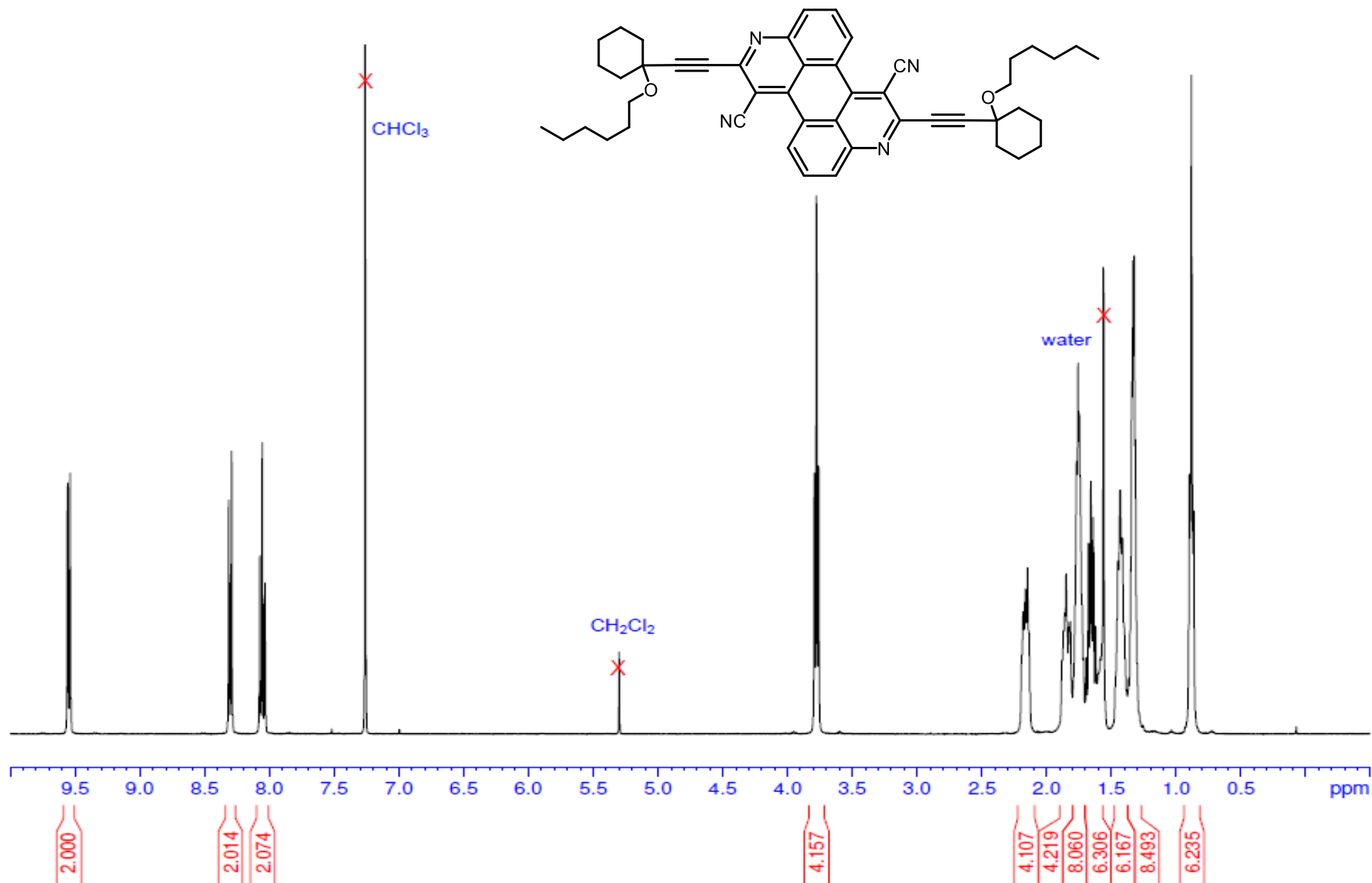
¹³C NMR spectrum for **11c** (expansion 150-115 ppm)

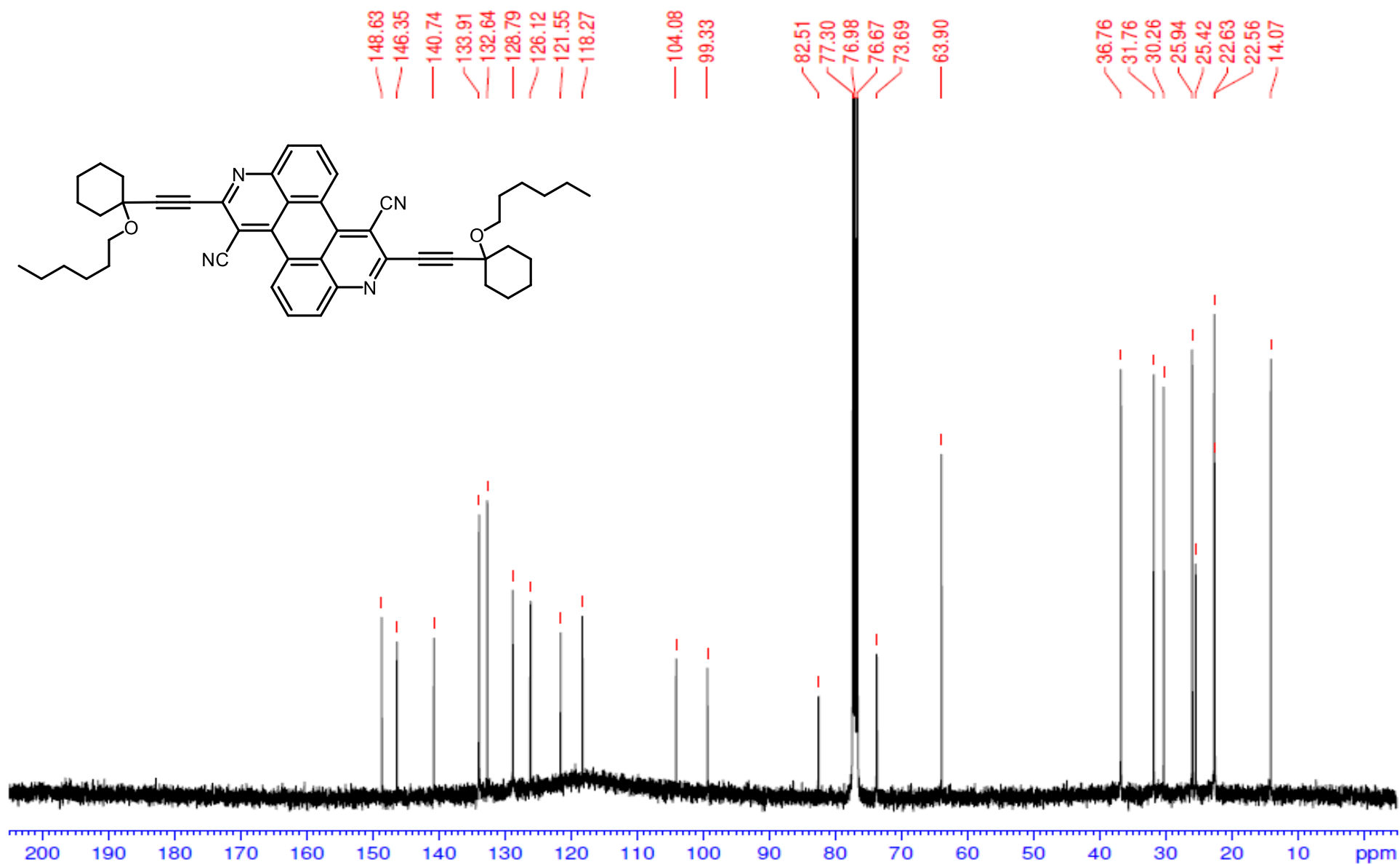
HPLC Chromatogram for **11c**

Sample Name: KMM-276-57 95%ACN/TFA
Detector: PDA 312.0 nm
HplcColumn 150x4.6mm Alltima HP C18
FlowRate: 1.0 mL / min
MobilePhase: 95% ACN / 0.1% TFA

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Date Processed: 8/12/2011 2:31:20 PM EST
Processing Method: nkh



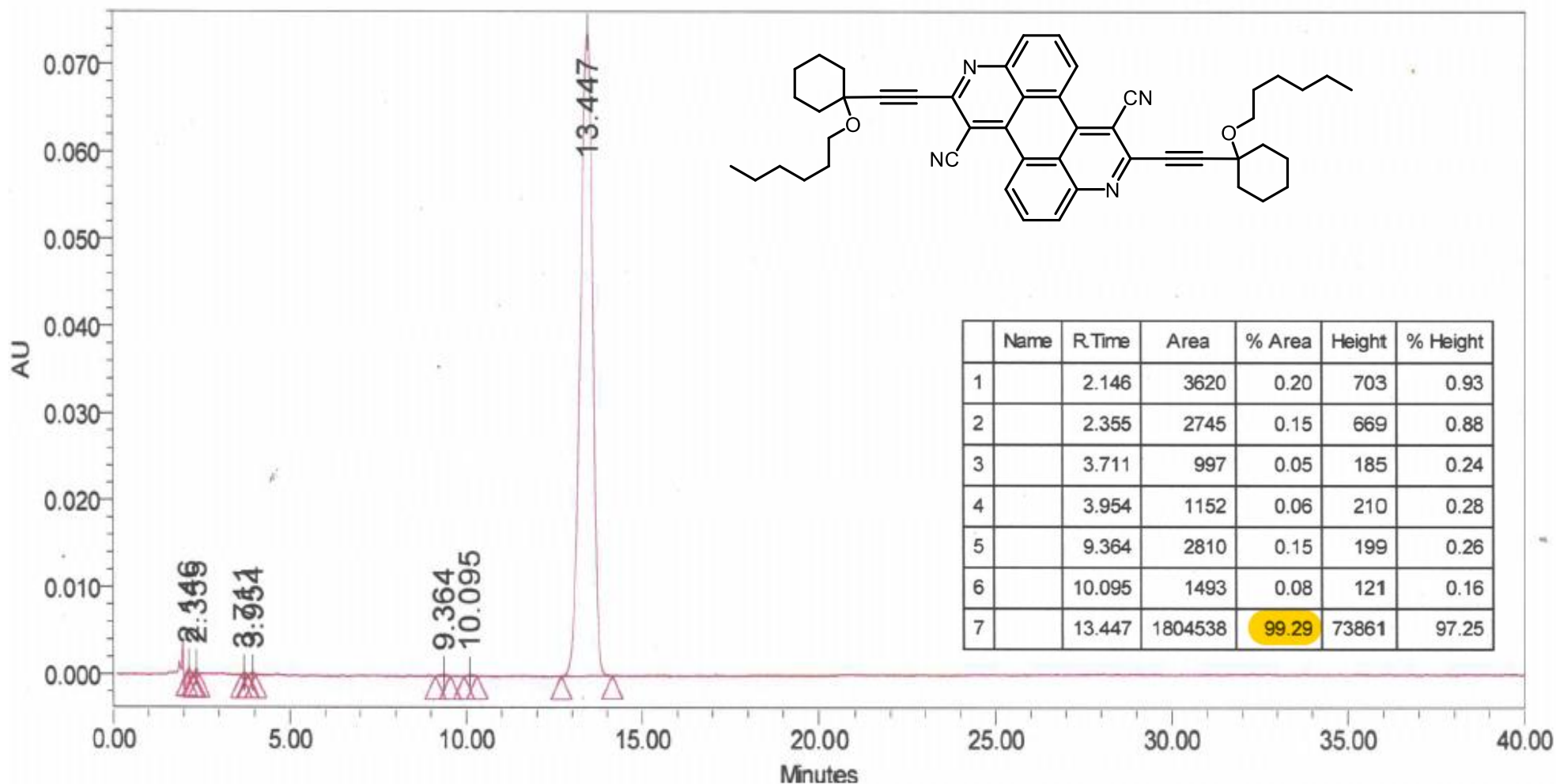
¹H NMR spectrum for **11d** (400 MHz; CDCl₃)

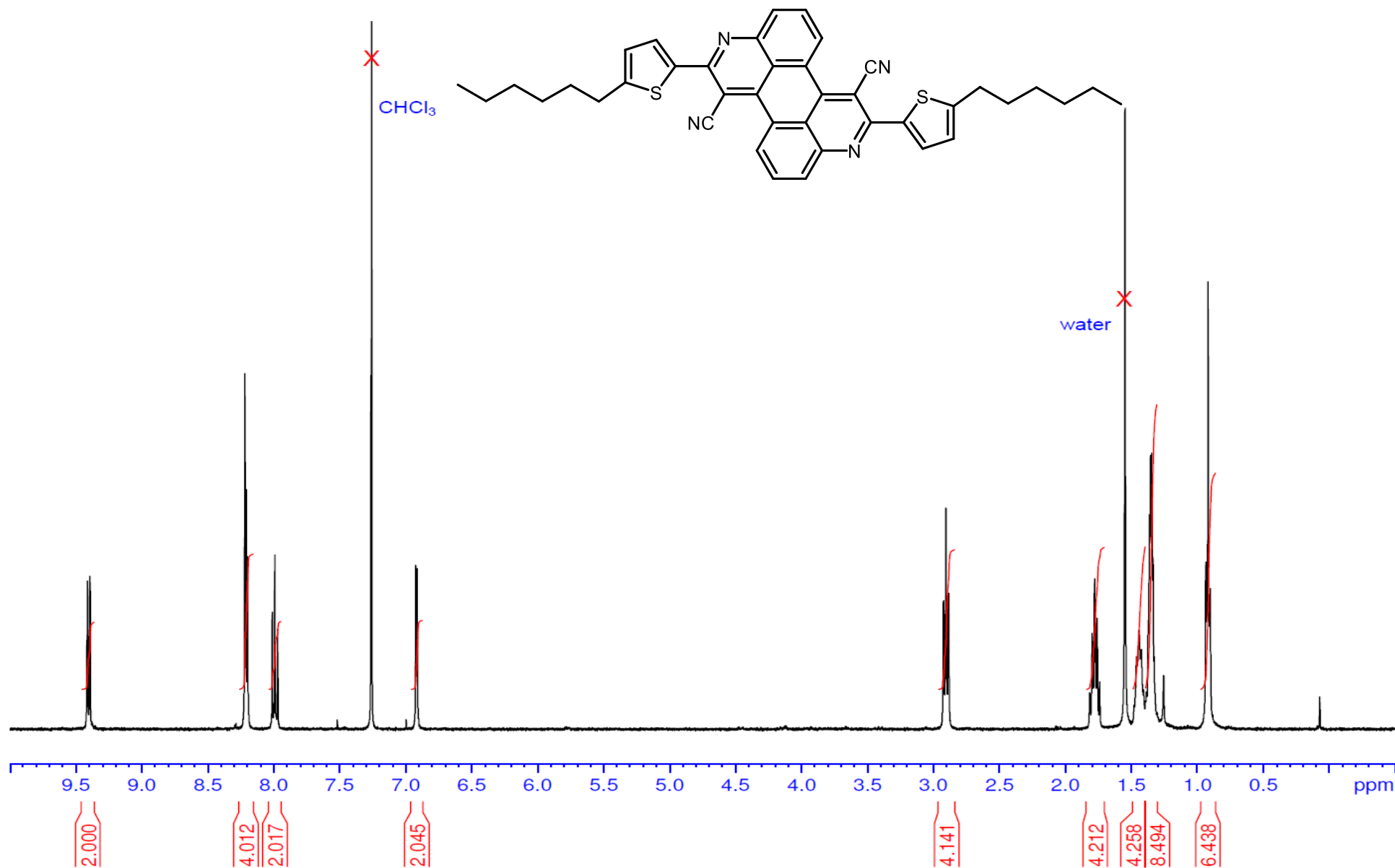
¹³C NMR spectrum for **11d** (100 MHz; CDCl₃)

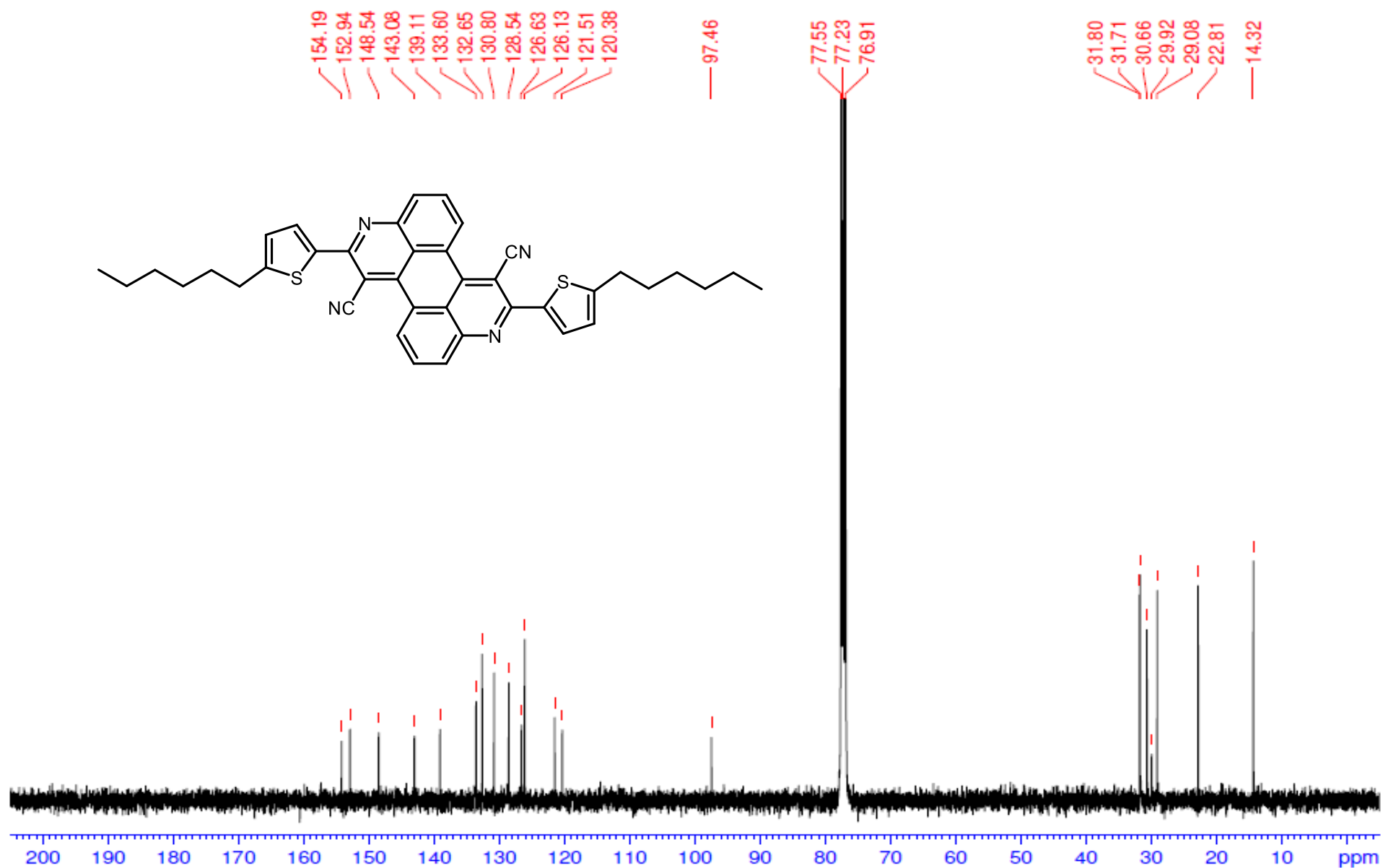
HPLC Chromatogram for **11d**

Sample Name: KMM-276-60-fr5-7 5%THF/ACN
Detector: PDA 287.0 nm
HplcColumn 150x4.6mm Alltima HP C18
FlowRate: 1.0 mL / min
MobilePhase: 5% THF / ACN

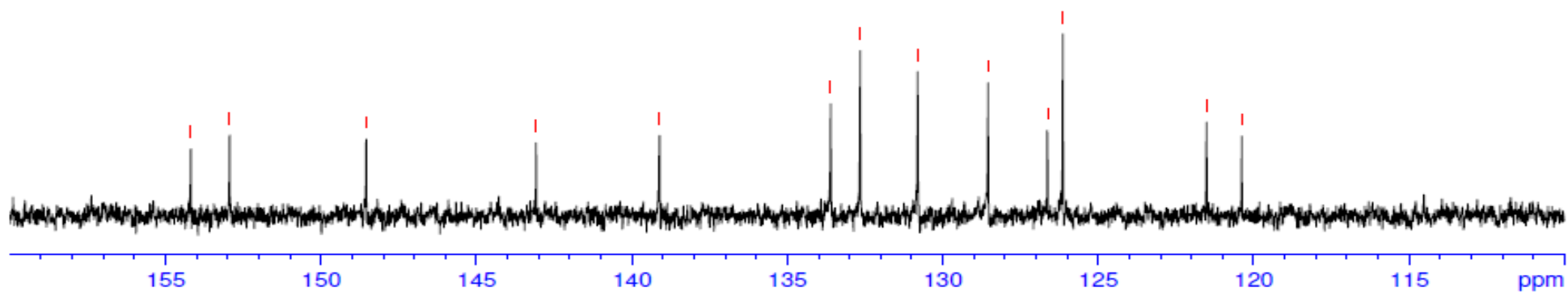
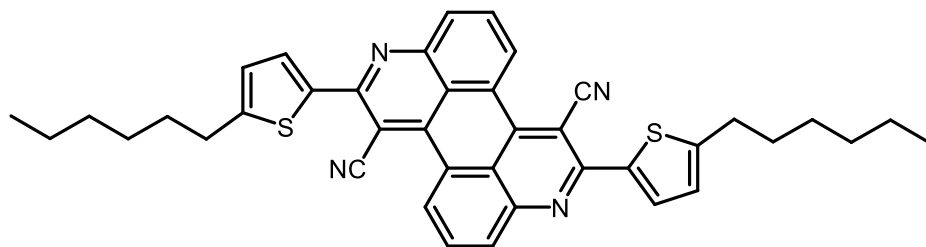
Date Acquired: 10/02/2012 1:43:08 PM EST
Acq Method Set : AllianceE 100% A isocratic
Date Processed: 22/02/2012 4:10:30 PM EST
Processing Method: nkh



¹H NMR spectrum for **12** (400 MHz; CDCl₃)

¹³C NMR spectrum for **12** (100 MHz; CDCl₃)

—	154.19
—	152.94
—	148.54
—	143.08
—	139.11
—	133.60
—	132.65
—	130.80
—	128.54
—	126.63
—	126.13
—	121.51
—	120.38



HPLC Chromatogram for **12**

Sample Name: KMM-276-64 pure 5%THF/ACN
Detector: PDA 321.0 nm
HplcColumn 150x4.6mm Alltima HP C18
FlowRate: 1.0 mL / min
MobilePhase: 5% THF / ACN

Date Acquired: 25/01/2012 12:43:00 PM EST
Acq Method Set : AllianceE 100% A isocratic
Date Processed: 25/01/2012 5:18:10 PM EST
Processing Method: nkh

