

Supporting Information

Anchoring of Rare-earth based Single-Molecule Magnets on Single-Walled Carbon Nanotubes.

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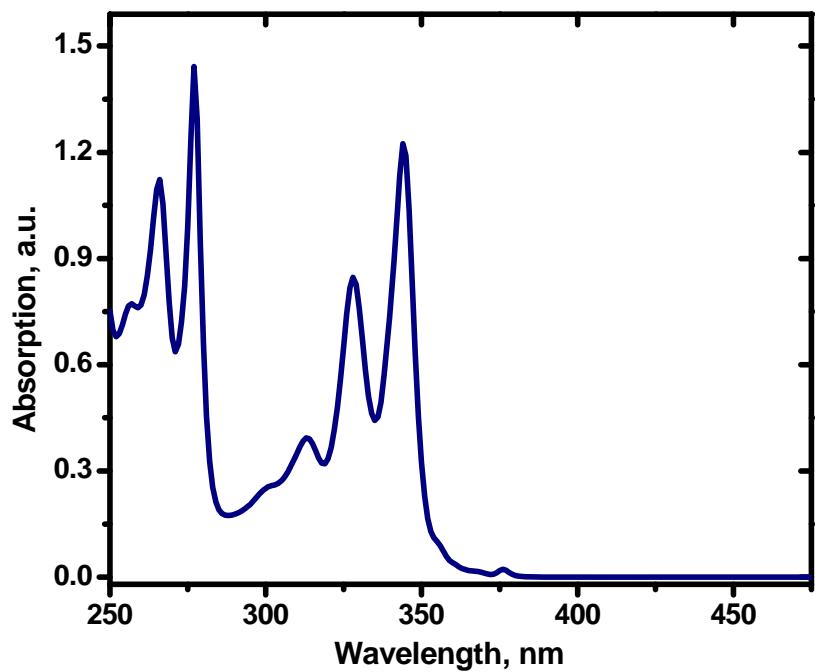


Figure 1S. UV-Vis spectrum of **8** in CH_2Cl_2 .

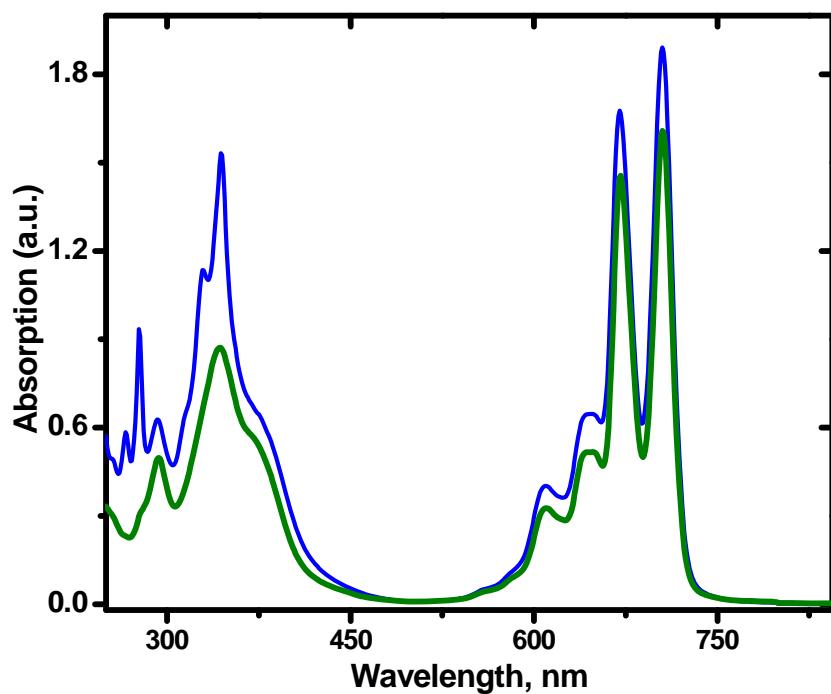
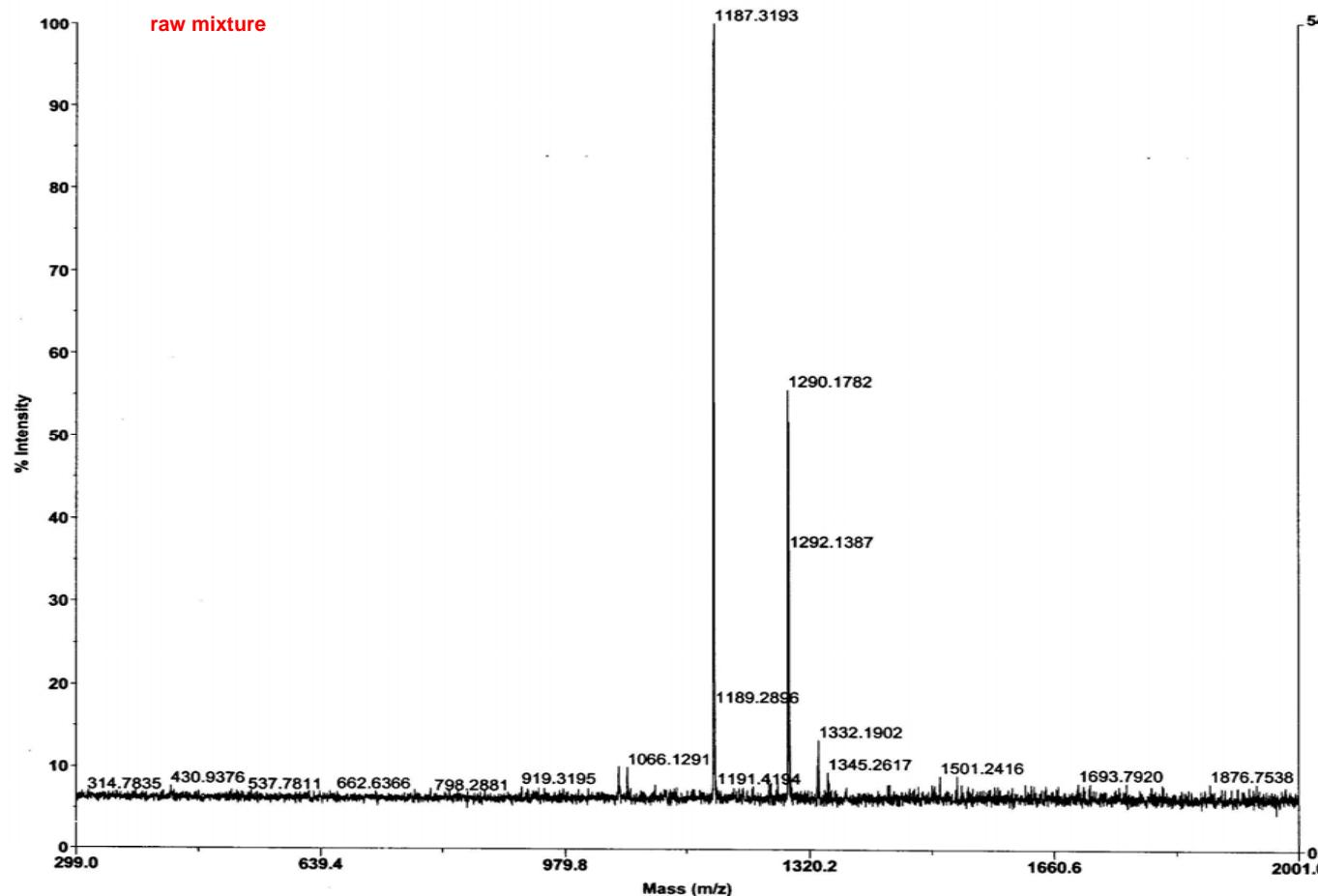


Figure 2S. UV-Vis spectrum of **A**₃**B** (**9**), blue line, and **A**₄ (**10**), green line; in CH_2Cl_2 .

Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1187.3, 5454]



Mode of operation:
Extraction mode:
Polarity:
Acquisition control:

Reflector
Delayed
Positive
Manual

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Extraction delay time: 100 nsec

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Laser Rep Rate: 3.0 Hz
Calibration type: Default
Calibration matrix: a-Cyano-4-hydroxycinnamic acid
Low mass gate: 200 Da
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Input bandwidth 0: 750 MHz

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Lab name: INT Karlsruhe

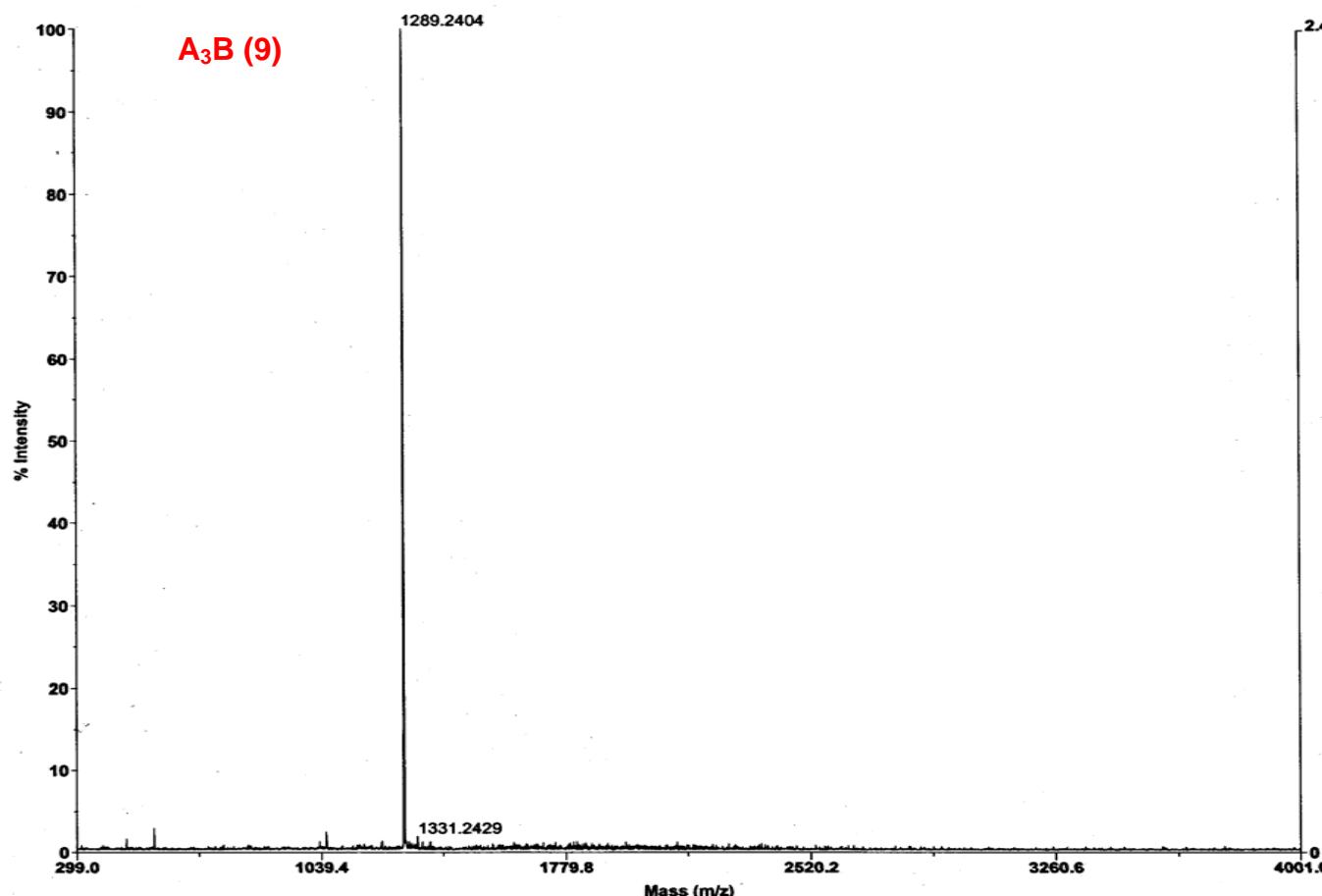
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Absolute y-position: 29887.9
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Relative y-position: -2179.65
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Mirror pressure: 2.986e-007
TC2 pressure: 0.00133
TIS gate width: 15
TIS flight length: 678

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Printed: 22:16, September 04, 2008

Applied Biosystems Voyager System 6059

Voyager Spec > [BP = 1289.2, 23798]



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Grid voltage:	64%
Mirror voltage ratio:	1.12
Guide wire 0:	0.012%
Extraction delay time:	50 nsec
Acquisition mass range:	300 – 4000 Da
Number of laser shots:	100/spectrum
Laser intensity:	2496
Laser Rep Rate:	3.0 Hz
Calibration type:	Default
Calibration matrix:	a-Cyano-4-hydroxycinnamic acid
Low mass gate:	200 Da
Timed ion selector:	Off
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Number of data points:	91718
Vertical scale 0:	1000 mV
Vertical offset:	-1%
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Serial number:	6059
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Plate type filename:	C:\VOYAGER\100 well plate.plt
Lab name:	INT Karlsruhe
Absolute x-position:	44093.9
Absolute y-position:	38405.1
Relative x-position:	1866.38
Relative y-position:	1257.6
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TIS flight length:	678

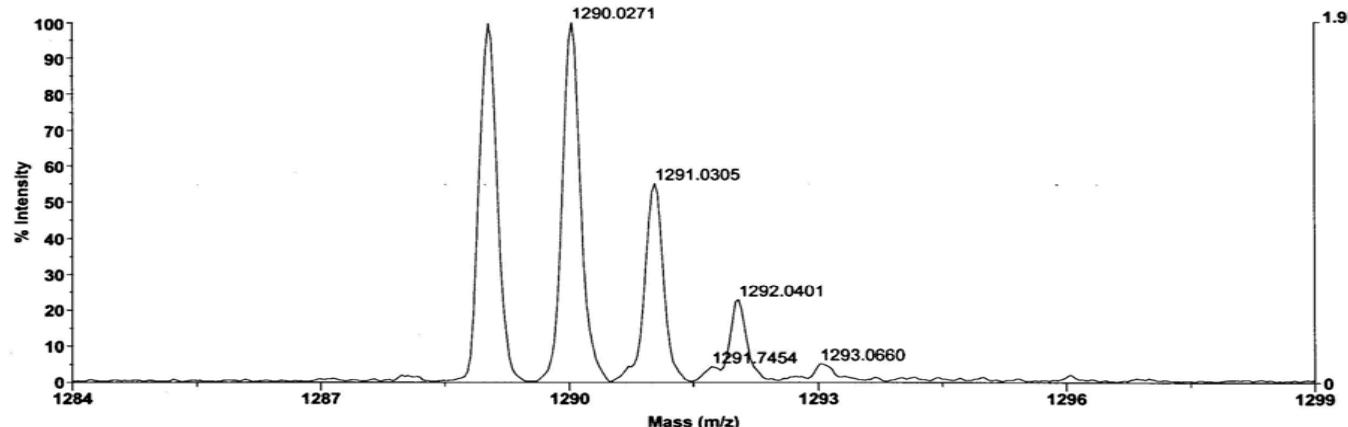
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Acquisition control:
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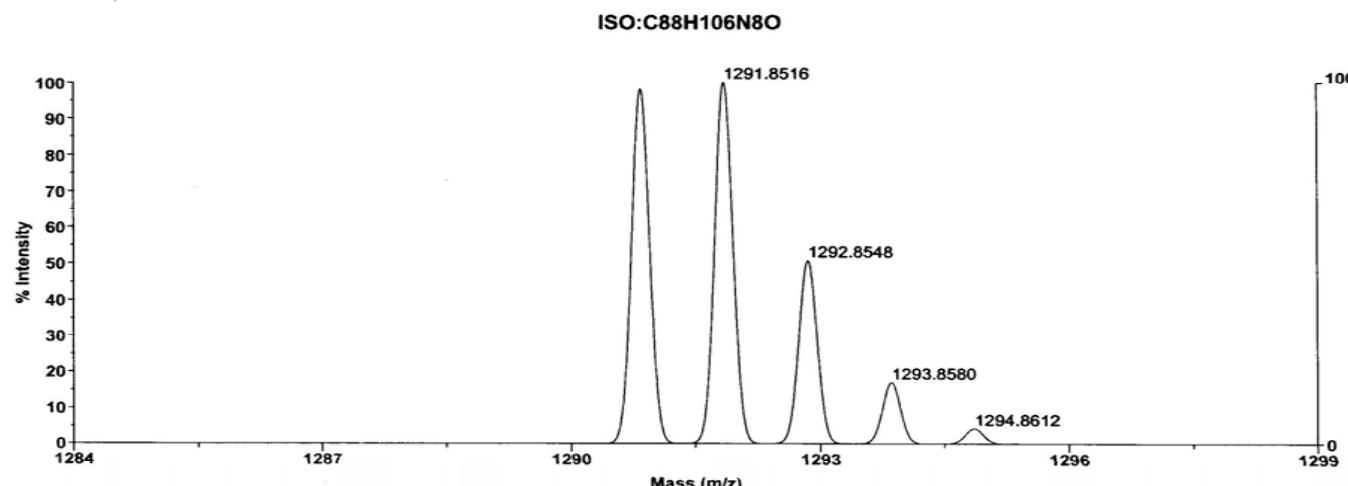
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Mirror voltage ratio: 1.12
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Laser intensity: 2496
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Calibration type: Default
Calibration matrix: a-Cyano-4-hydroxycinnamic acid
Low mass gate: 200 Da
Timed ion selector: Off

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Bin size: 0.5 nsec
Number of data points: 91717
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Vertical offset: -1%
Input bandwidth 0: 750 MHz

Sample well: 29
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Serial number: 6059
Instrument name: Voyager-DE PRO
Plate type filename: C:\VOYAGER\100 well plate.plt
Lab name: INT Karlsruhe

Absolute x-position: 40551.4
Absolute y-position: 37900.2
Relative x-position: -1676.15
Relative y-position: 752.729
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Mirror pressure: 9.197e-007
TC2 pressure: 0.00133
TIS gate width: 15
TIS flight length: 678



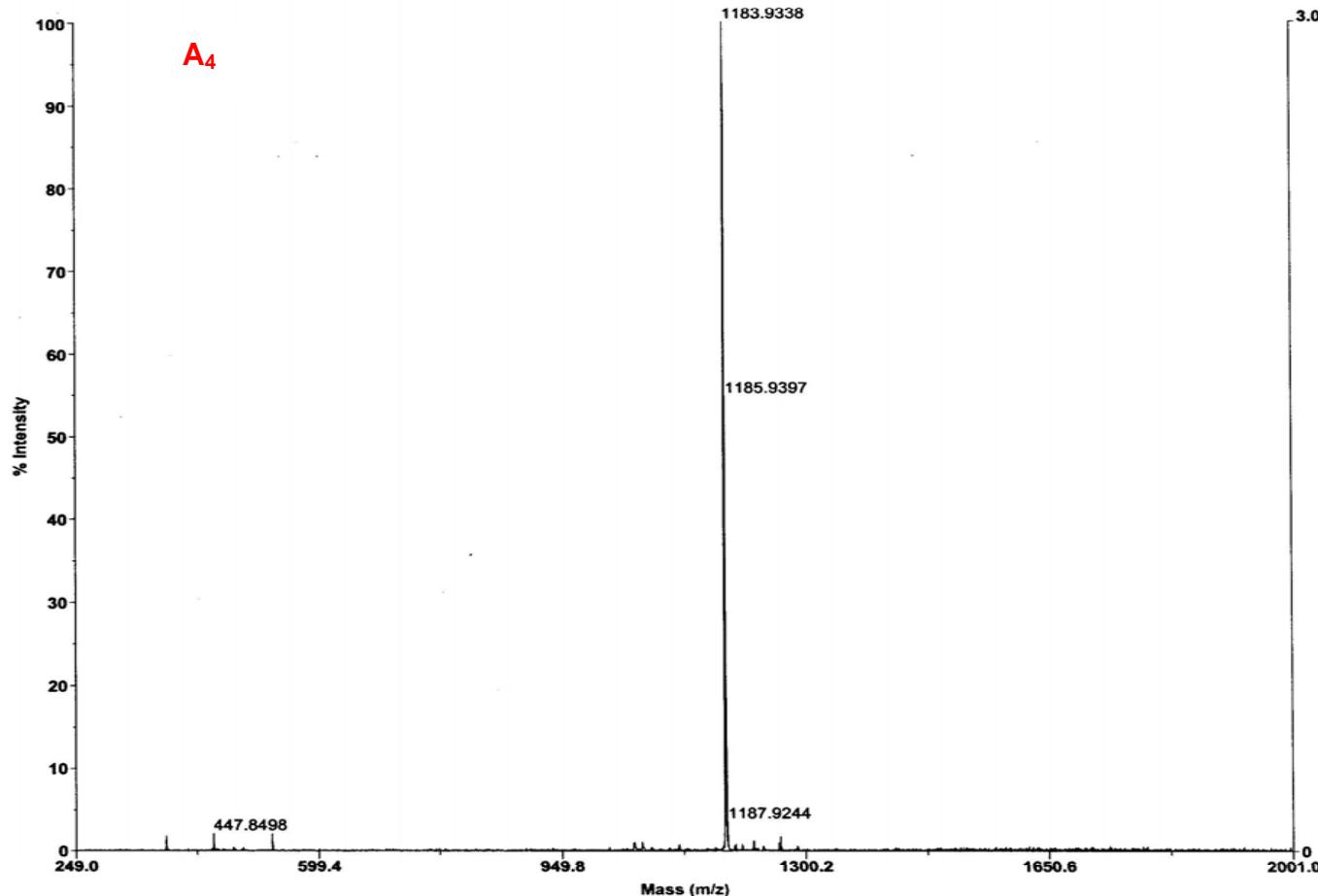
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Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1183.9, 29950]



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Extraction mode:	Delayed
Polarity:	Positive
Acquisition control:	Manual
3.0E+4 Accelerating voltage:	20000 V
Grid voltage:	60%
Mirror voltage ratio:	1.12
Guide wire 0:	0.015%
Extraction delay time:	150 nsec
Acquisition mass range:	250 – 2000 Da
Number of laser shots:	100/spectrum
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Laser Rep Rate:	3.0 Hz
Calibration type:	Default
Calibration matrix:	2,5-Dihydroxybenzoic acid
Low mass gate:	250 Da
Timed ion selector:	Off
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Serial number:	6059
Instrument name:	Voyager-DE PRO
Plate type filename:	C:\VOYAGER100 well plate.plt
Lab name:	INT Karlsruhe
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Absolute y-position:	33186.5
Relative x-position:	-318.311
Relative y-position:	1119.01
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Mirror pressure:	2.028e-007
TC2 pressure:	0.00133
TIS gate width:	15
TIS flight length:	678

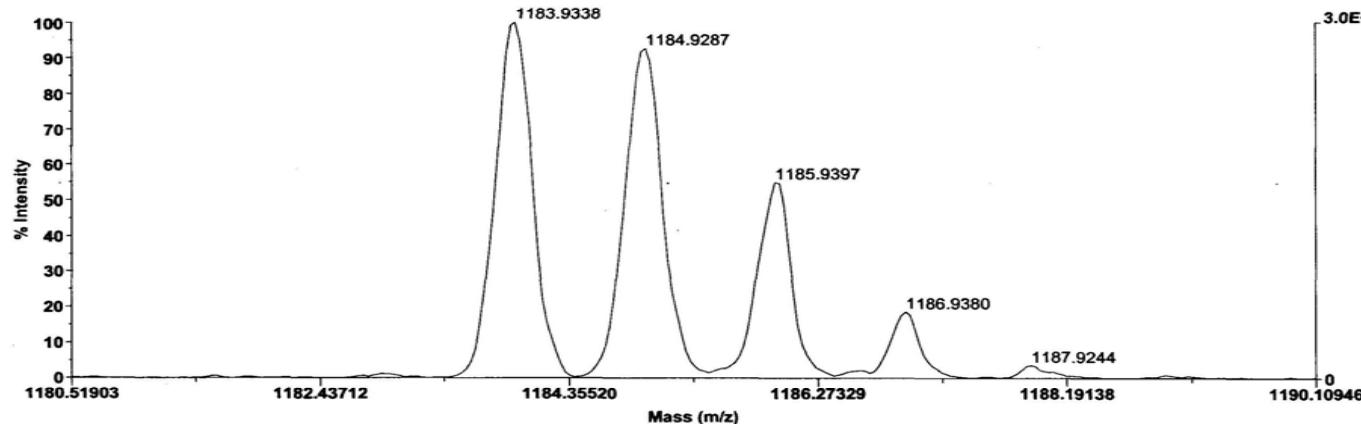
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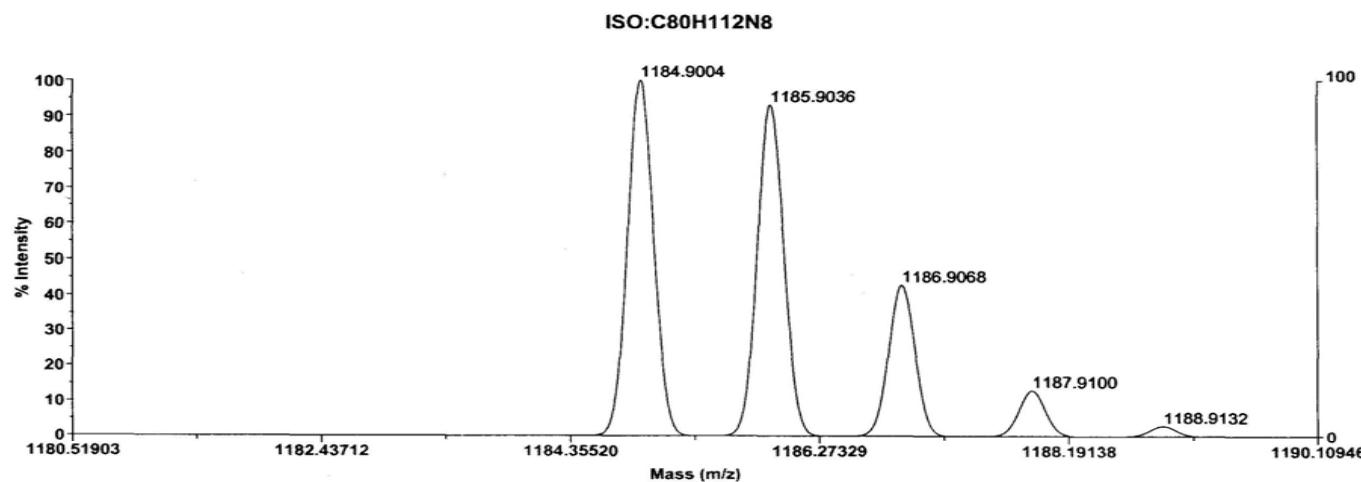
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Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1183.9, 29950]



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Extraction mode:	Delayed
Polarity:	Positive
Acquisition control:	Manual
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Accelerating voltage:	20000 V
Grid voltage:	60%
Mirror voltage ratio:	1.12
Guide wire 0:	0.015%
Extraction delay time:	150 nsec
Acquisition mass range:	250 – 2000 Da
Number of laser shots:	100/spectrum
Laser intensity:	3245
Laser Rep Rate:	3.0 Hz
Calibration type:	Default
Calibration matrix:	2,5-Dihydroxybenzoic acid
Low mass gate:	250 Da
Timed ion selector:	Off
Digitizer start time:	15.937
Bin size:	0.5 nsec
Number of data points:	57694
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Vertical offset:	-2.5%
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Serial number:	6059
Instrument name:	Voyager-DE PRO
Plate type filename:	C:\VOYAGER\100 well plate.plf
Lab name:	INT Karlsruhe
Absolute x-position:	41909.2
Absolute y-position:	33186.5
Relative x-position:	-318.311
Relative y-position:	1119.01
Shots in spectrum:	96
Source pressure:	2.164e-006
Mirror pressure:	2.028e-007
TC2 pressure:	0.00133
TIS gate width:	15
TIS flight length:	678



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Printed: 22:27, September 04, 2008

Figure 3S. MALDI-Tof spectra of A₃B (9) and A₄ (10).

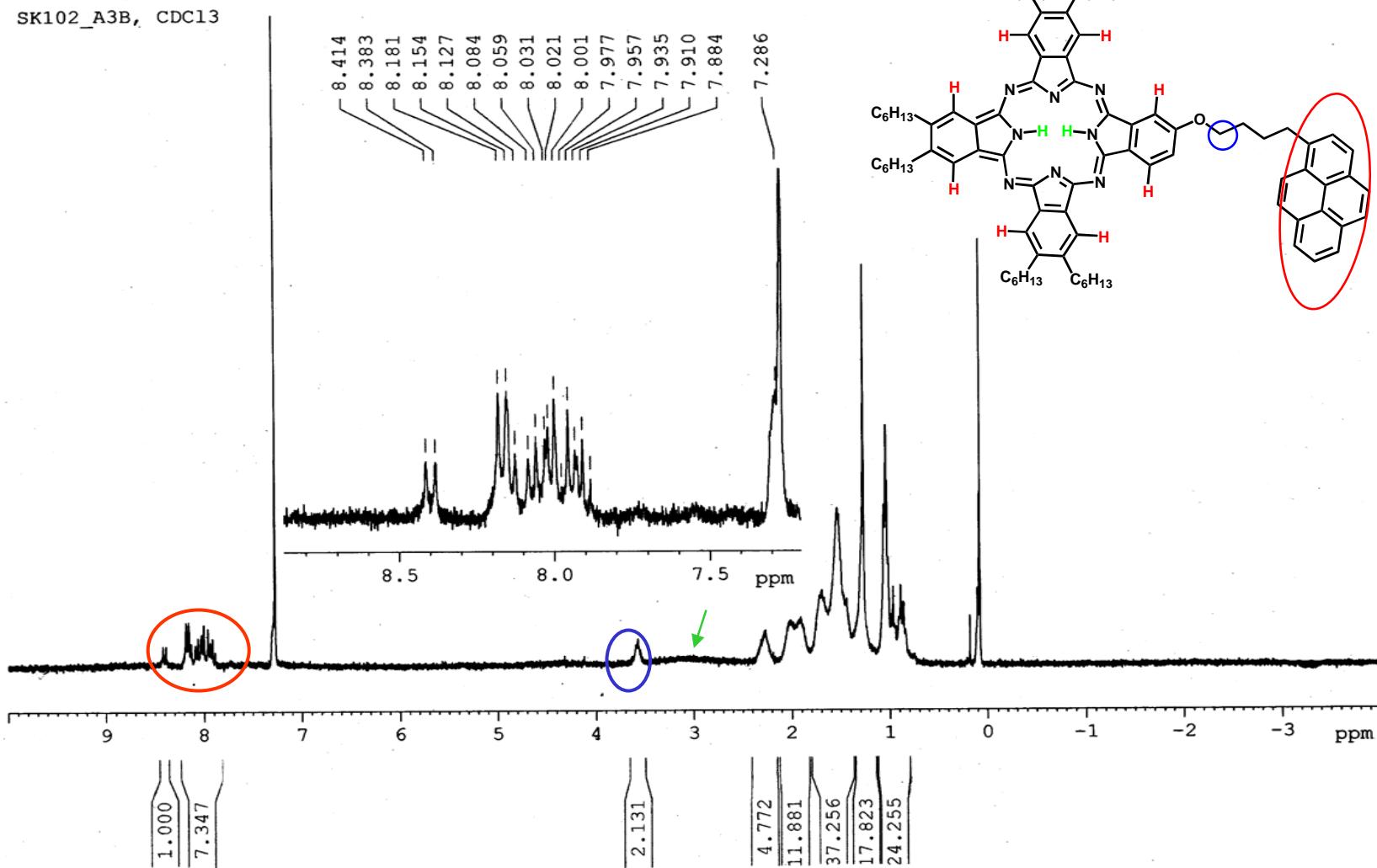


Figure 4S. ¹H NMR spectra of A₃B (9) (top) in CDCl₃.

SK102_A4, CDCl₃

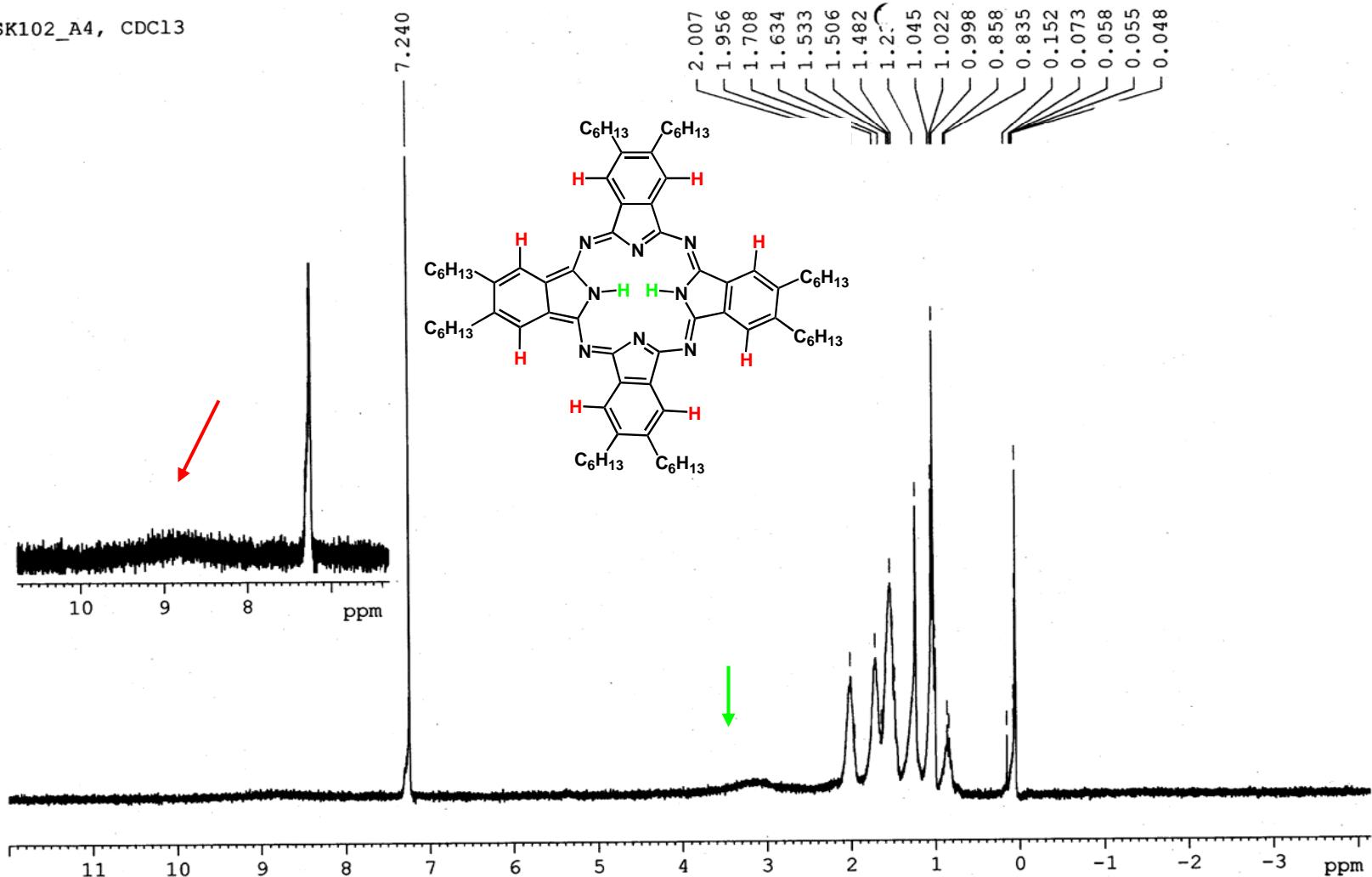


Figure 5S. ¹H NMR spectra of A₄ (10) in CDCl₃.

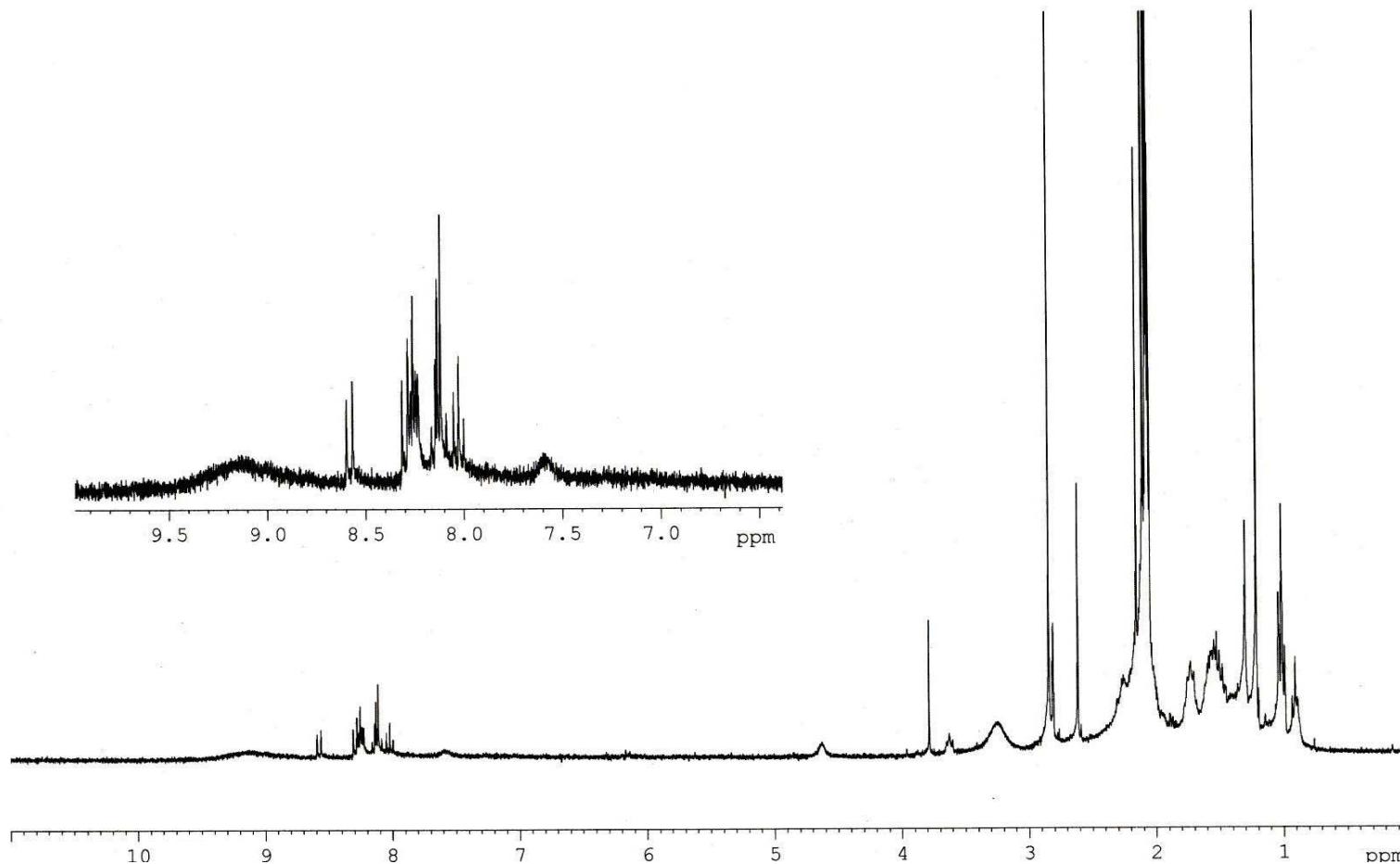
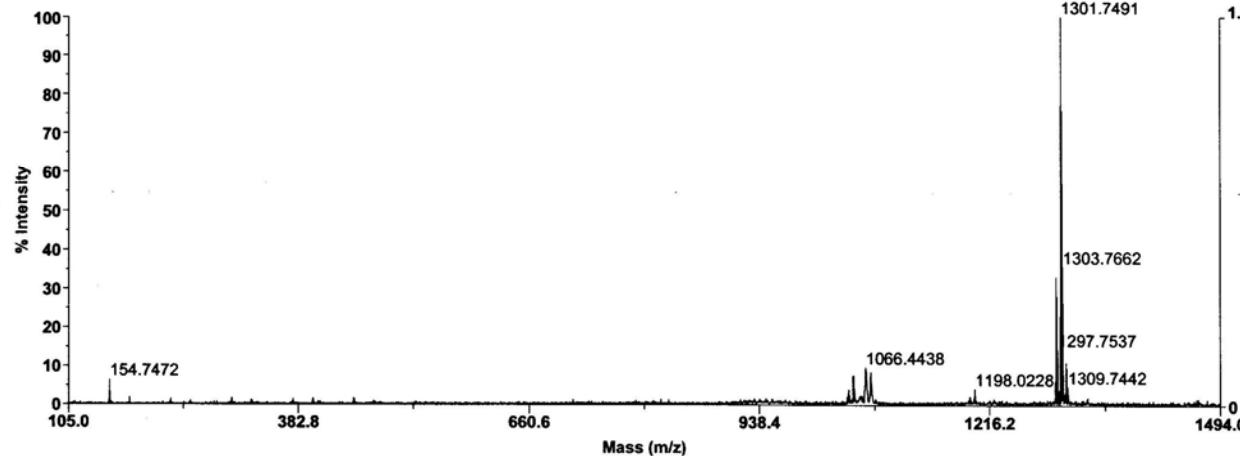


Figure 6S: ¹H NMR spectra of Lithium Phthalocyanine – $[A_3B\text{-Li}_2]$ (**2**) in Acetone- d_6 .

Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1301.8, 12079]



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Polarity:
Acquisition control:

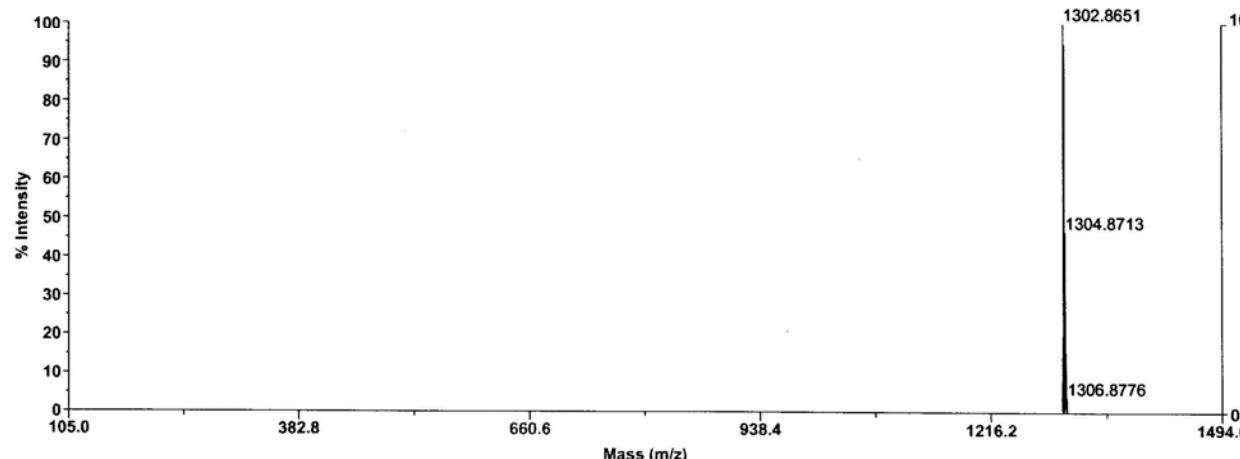
Reflector
Delayed
Positive
Manual

Accelerating voltage: 20000 V
Grid voltage: 64%
Mirror voltage ratio: 1.12
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Extraction delay time: 80 nsec

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Timed ion selector: Off

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Lab name: INT Karlsruhe

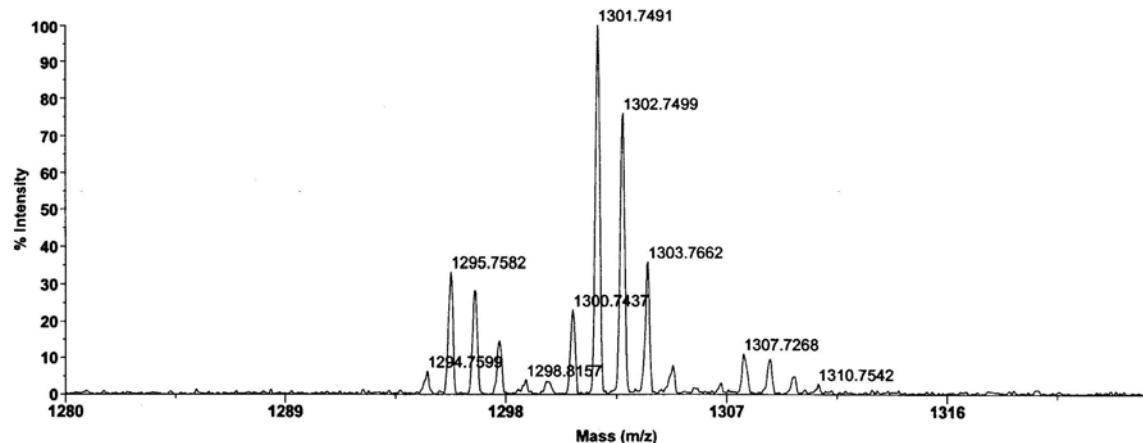
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Relative y-position: 738.417
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Mirror pressure: 1.05e-006
TC2 pressure: 0.00133
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Printed: 23:08, August 20, 2008

Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1301.8, 12079]



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Polarity: Positive
Acquisition control: Manual

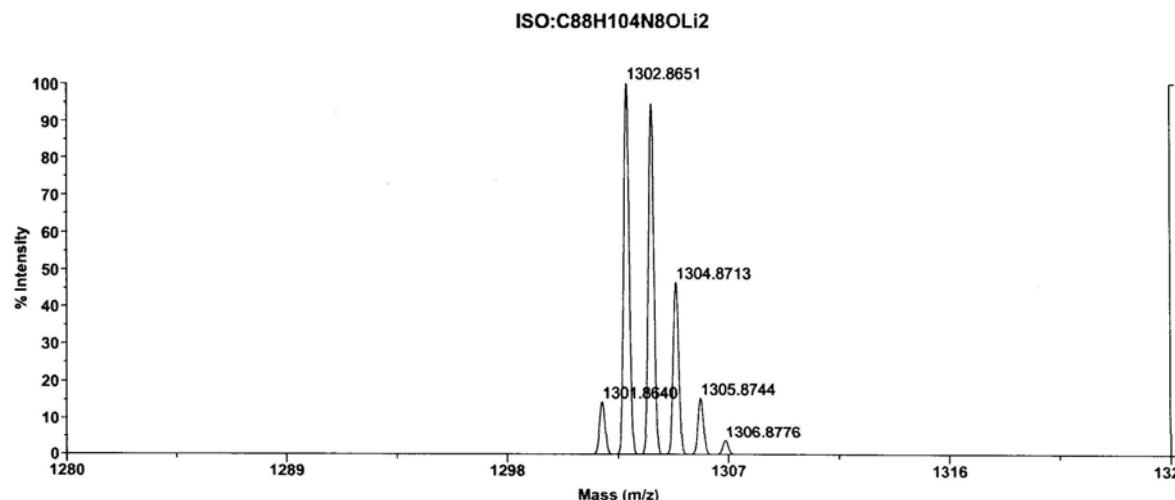
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Grid voltage: 64%
Mirror voltage ratio: 1.12
Guide wire 0: 0.015%
Extraction delay time: 80 nsec

Acquisition mass range: 100 – 1500 Da
Number of laser shots: 100/spectrum
Laser Intensity: 2746
Laser Rep Rate: 3.0 Hz
Calibration type: Default
Calibration matrix: 2,5-Dihydroxybenzoic acid
Low mass gate: 100 Da
Timed ion selector: Off

Digitizer start time: 10.122
Bin size: 0.5 nsec
Number of data points: 57371
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Vertical offset: -2.5%
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Plate ID: 100
Serial number: 6059
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Plate type filename: C:\VOYAGER100 well plate.plt
Lab name: INT Karlsruhe

Absolute x-position: 22476.5
Absolute y-position: 27725.9
Relative x-position: 568.969
Relative y-position: 738.417
Shots in spectrum: 100
Source pressure: 4.51e-006
Mirror pressure: 1.05e-006
TC2 pressure: 0.00133
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TIS flight length: 678



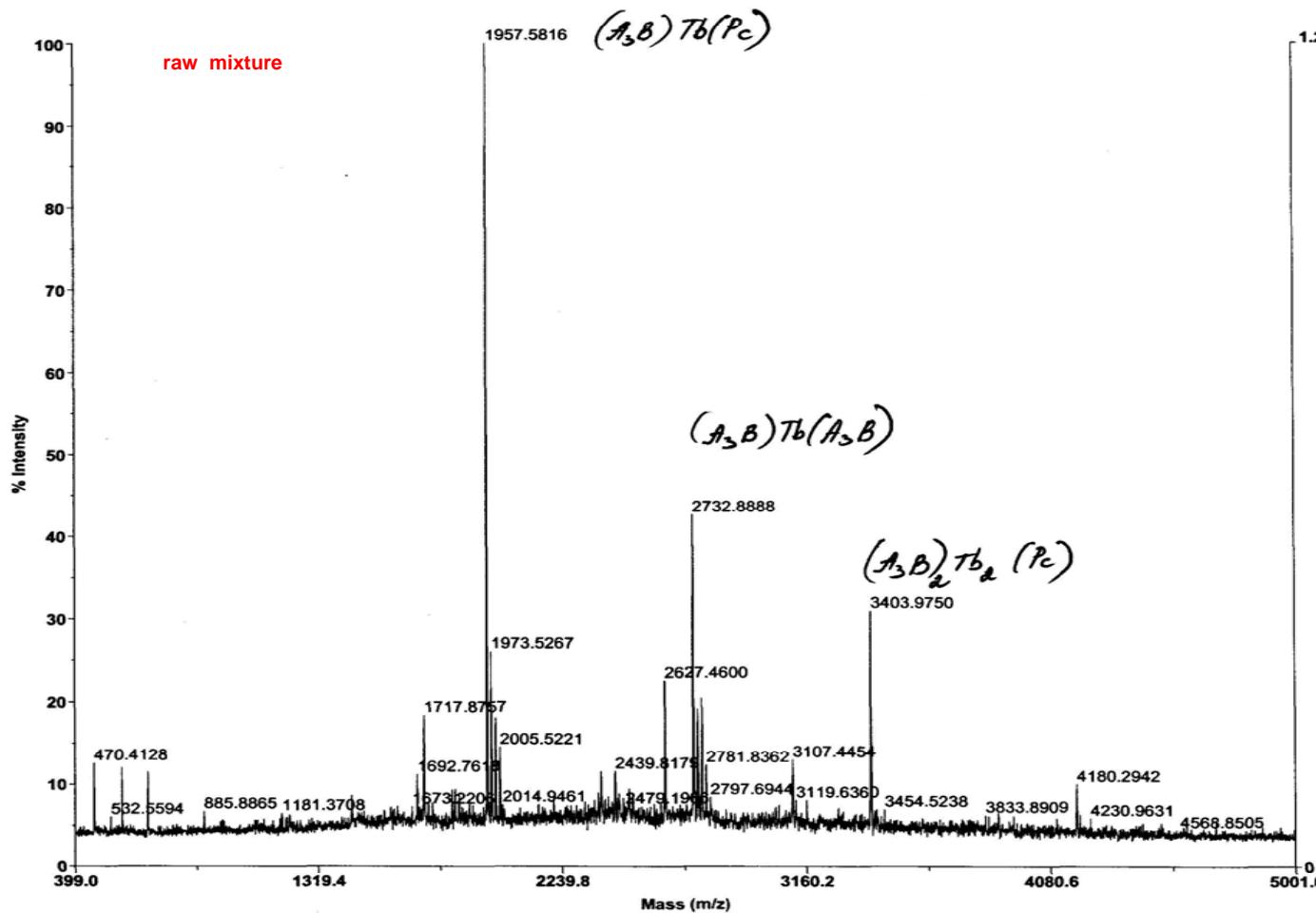
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Printed: 23:08, August 20, 2008

Figure 7S. MALDI-Tof spectra of 2.

Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1957.6, 11897]



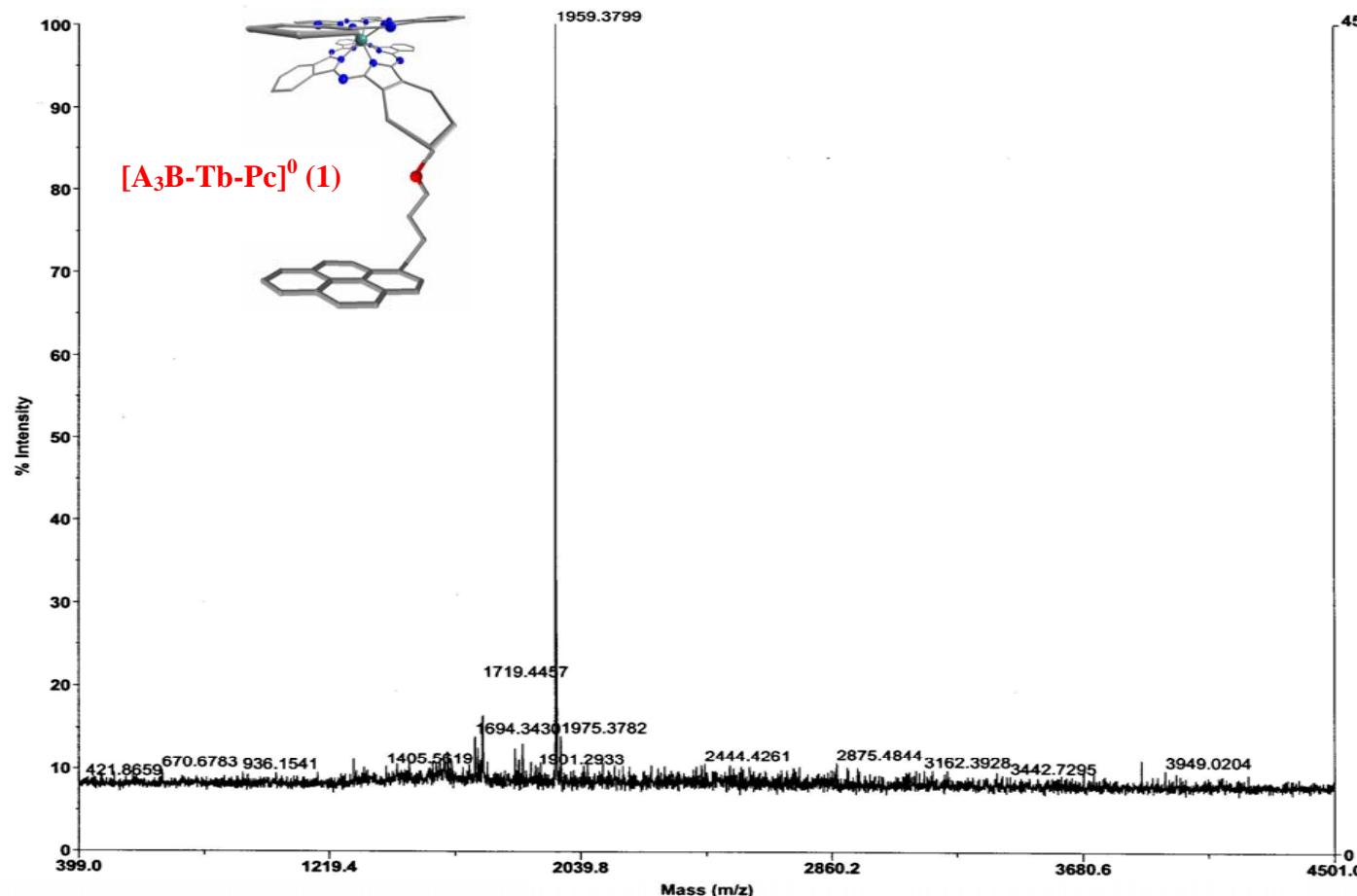
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Number of laser shots:	100/spectrum
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Laser Rep Rate:	3.0 Hz
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Calibration matrix:	Sinapinic acid
Low mass gate:	400 Da
Timed ion selector:	Off
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Bin size:	2 nsec
Number of data points:	25313
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Lab name:	INT Karlsruhe
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Absolute y-position:	21088.4
Relative x-position:	913.291
Relative y-position:	-819.116
Shots in spectrum:	100
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Mirror pressure:	3.144e-007
TC2 pressure:	0.00133
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Printed: 22:31, September 04, 2008

Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1959.3, 4511]



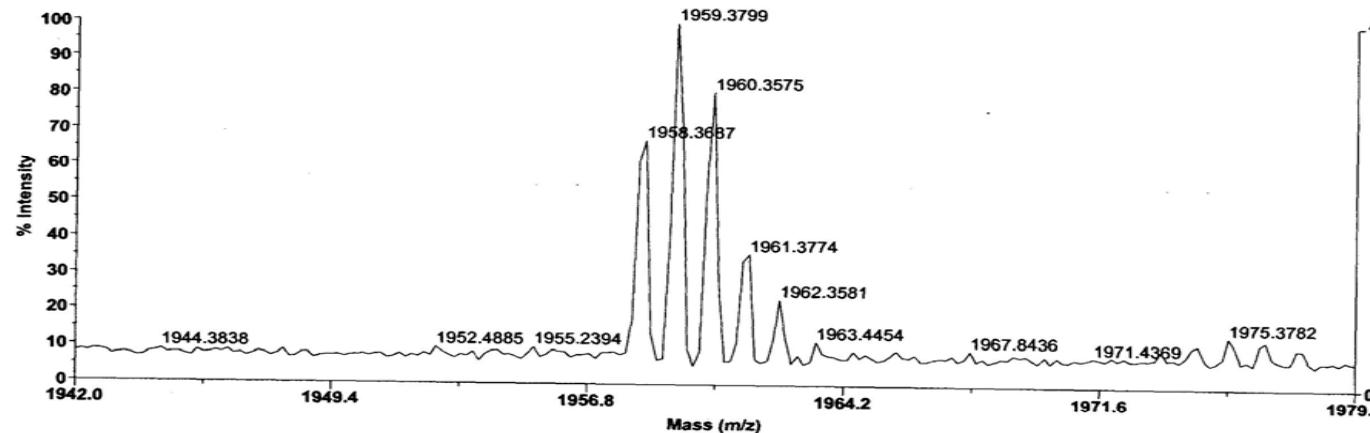
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	Guide wire 0: 0.015%
	Extraction delay time: 80 nsec
Acquisition mass range:	400 – 4500 Da
Number of laser shots:	100/spectrum
Laser intensity:	2083
Laser Rep Rate:	3.0 Hz
Calibration type:	Default
Calibration matrix:	a-Cyano-4-hydroxycinnamic acid
Low mass gate:	300 Da
Timed ion selector:	Off
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Lab name:	INT Karlsruhe
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Absolute y-position:	12925.1
Relative x-position:	-927.073
Relative y-position:	1177.57
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Mirror pressure:	1.053e-006
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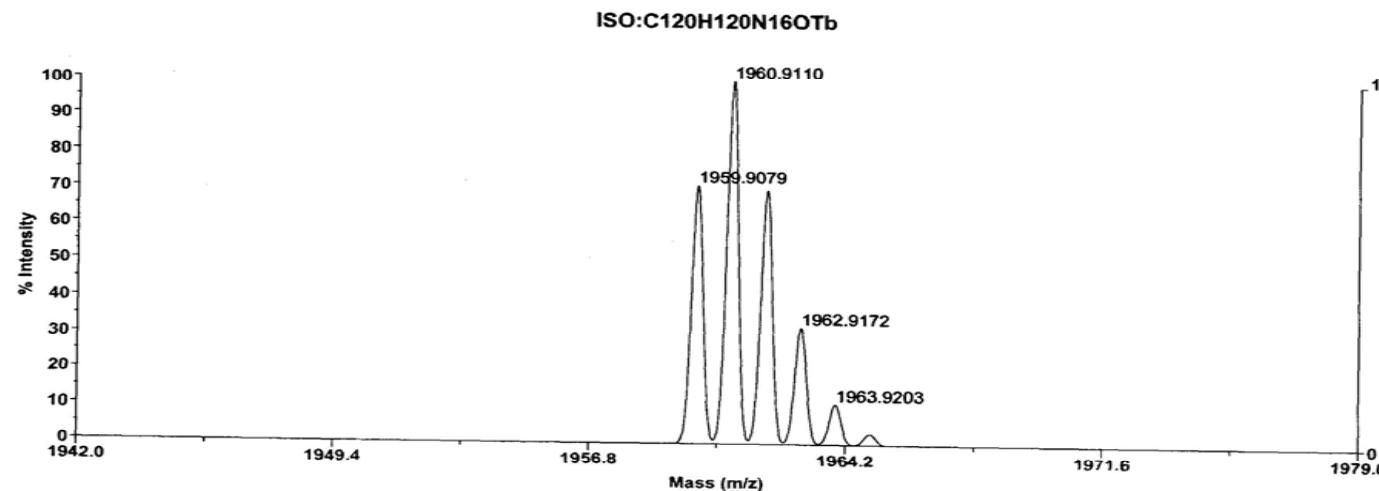
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Applied Biosystems Voyager System 6059

Voyager Spec #1[BP = 1959.3, 4511]



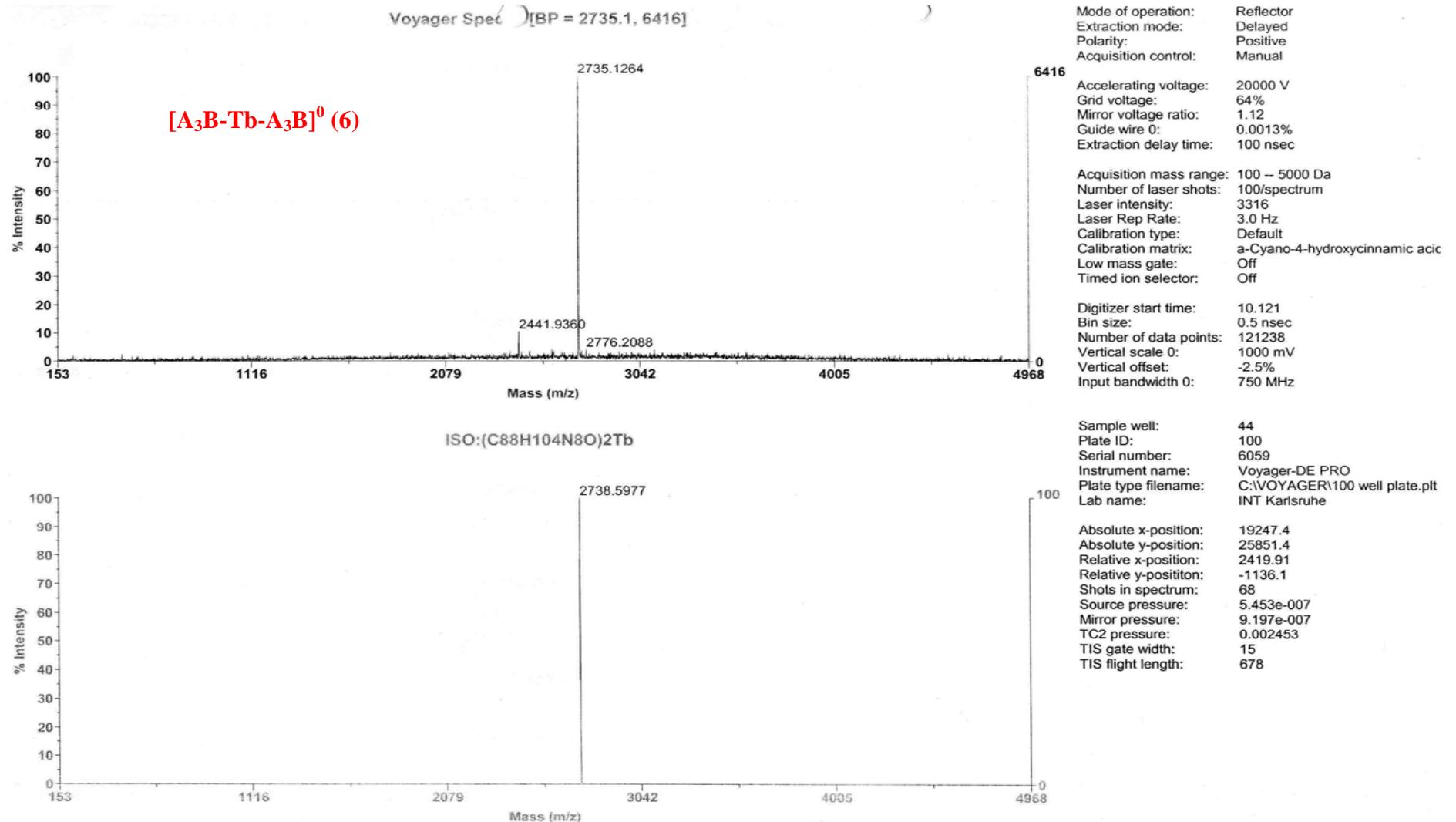
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Mirror voltage ratio:	1.12
Guide wire 0:	0.015%
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Acquisition mass range:	400 – 4500 Da
Number of laser shots:	100/spectrum
Laser intensity:	2063
Laser Rep Rate:	3.0 Hz
Calibration type:	Default
Calibration matrix:	a-Cyano-4-hydroxycinnamic acid
Low mass gate:	300 Da
Timed ion selector:	Off
Digitizer start time:	20.098
Bin size:	2 nsec
Number of data points:	23509
Vertical scale 0:	1000 mV
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Input bandwidth 0:	750 MHz



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Lab name:	INT Karlsruhe
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Absolute y-position:	12925.1
Relative x-position:	-927.073
Relative y-position:	1177.57
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Mirror pressure:	1.053e-006
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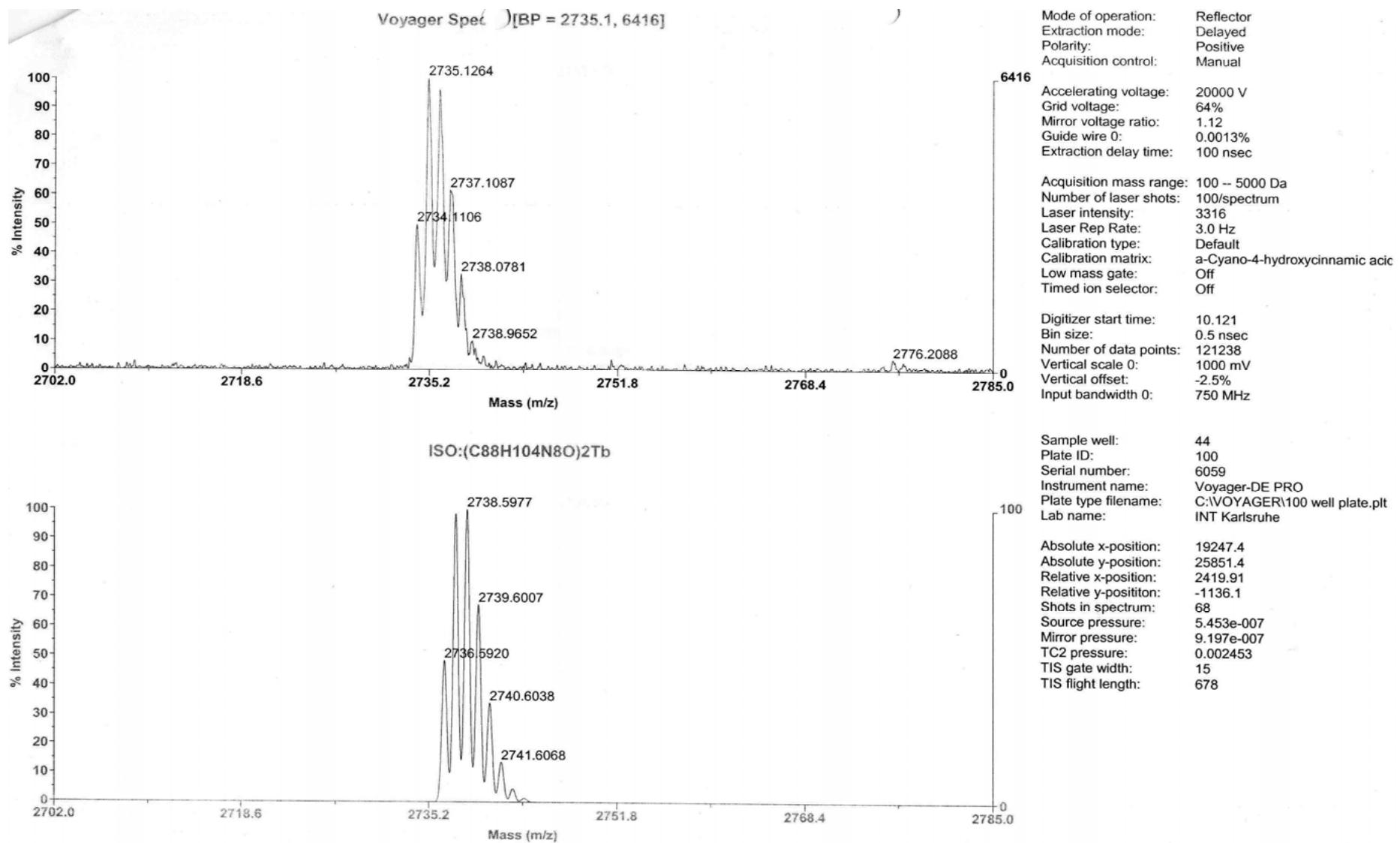


Figure 8S. MALDI-Tof spectra of **1** and **6**.

Table 1S. The MALDI-TOF mass spectral data.

Compound	Mass (m/z)	
	Calculated value	Measured value
$[A_3B\text{-Tb-Pc}]^0$ (1)	1960.9110 (for $C_{120}H_{120}N_{16}OTb$)	1959.3799
$A_3B\text{-Li}_2$ (2)	1301.7491 (for $C_{88}H_{104}N_8OLi_2$)	1302.8651
PcLi ₂ (4)	526.1814 (for $C_{32}H_{16}N_8Li_2$)	526.7666
$[A_3B\text{-Tb-A}_3B]^0$ (6)	2735.1264 (for $C_{176}H_{208}N_{16}O_2Tb$)	2736.9281
A_3B (9)	1291.8516 (for $C_{88}H_{106}N_8O$)	1290.0271
A_4 (10)	1184.9004 (for $C_{88}H_{112}N_8$)	1183.9338

SK120-3, CD₂Cl₂

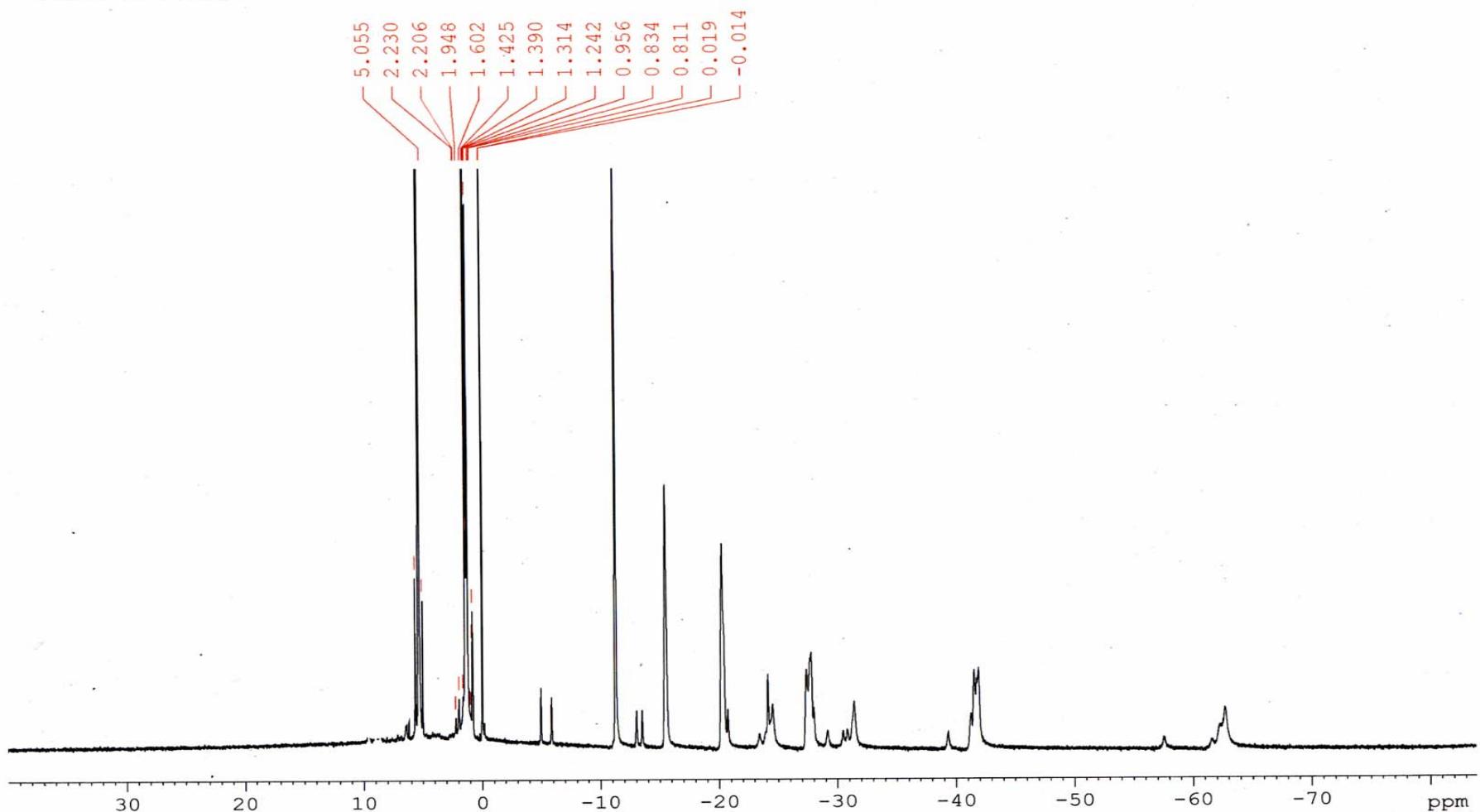


Figure 9S. Paramagnetic ¹H NMR spectrum of **1** in CD₂Cl₂ / 1% hydrazine hydrate.

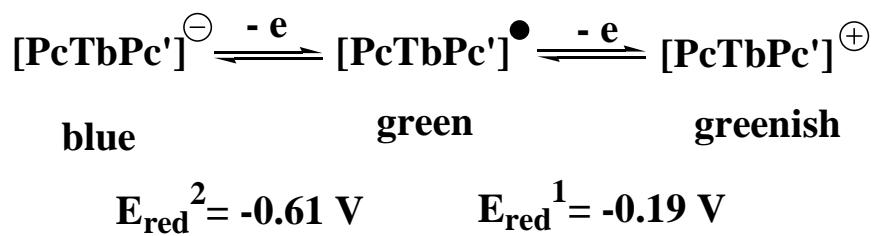
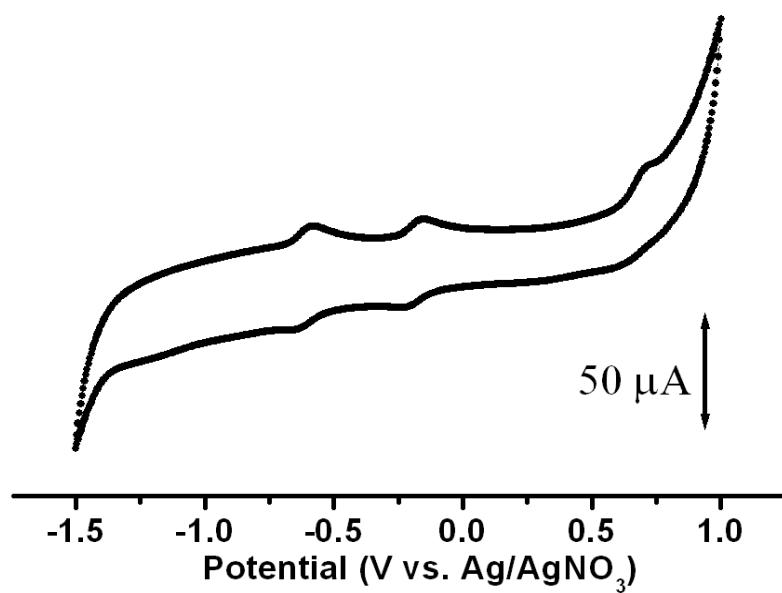


Figure 10S. Cyclic voltammogram of the complex (**1**) in CH₂Cl₂ containing 0.1 M (n-Bu₄N)PF₆, using ferrocene as a referent. A scan rate of 0.1 V s⁻¹ was used. Complex **1** exhibiting two quasi-reversible mono-electronic redox waves and an irreversible oxidation of the pyrene moiety (Pc' = double deprotonated ligand **9**).

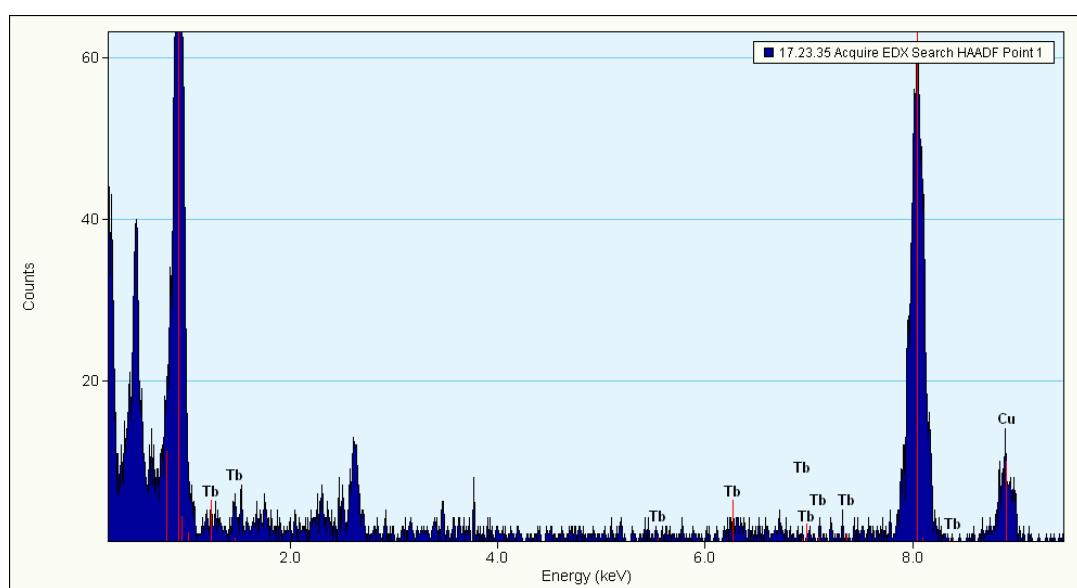
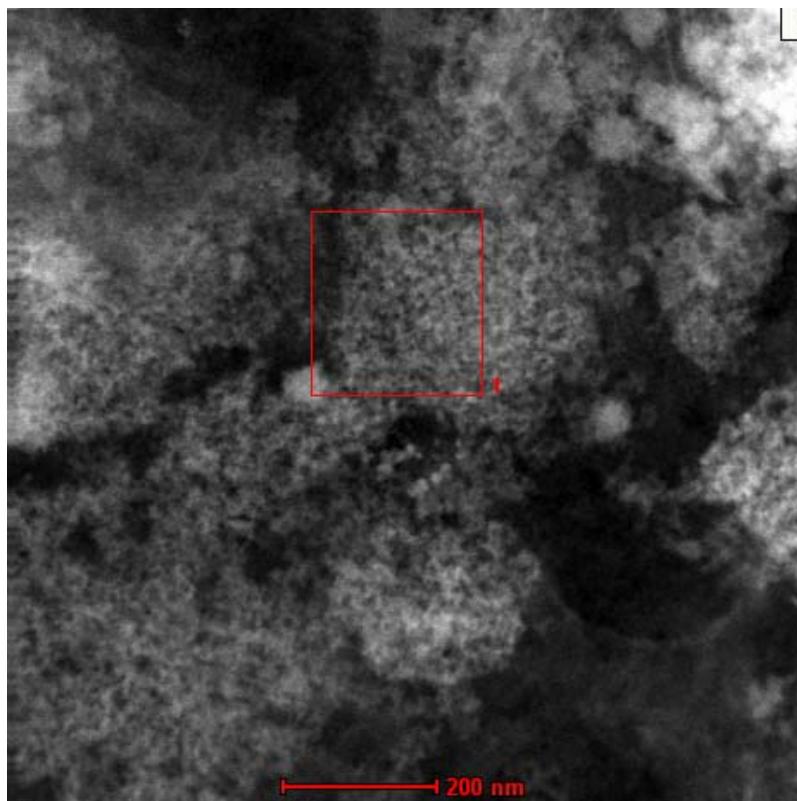


Figure 11S. STEM images of SWNTs bundles decorated by complex **1** (top). The EDX spectrum of the **1***SWNT hybrids at area 1. The blue curve is the experimental spectrum; the red lines show the energy of bands (down).

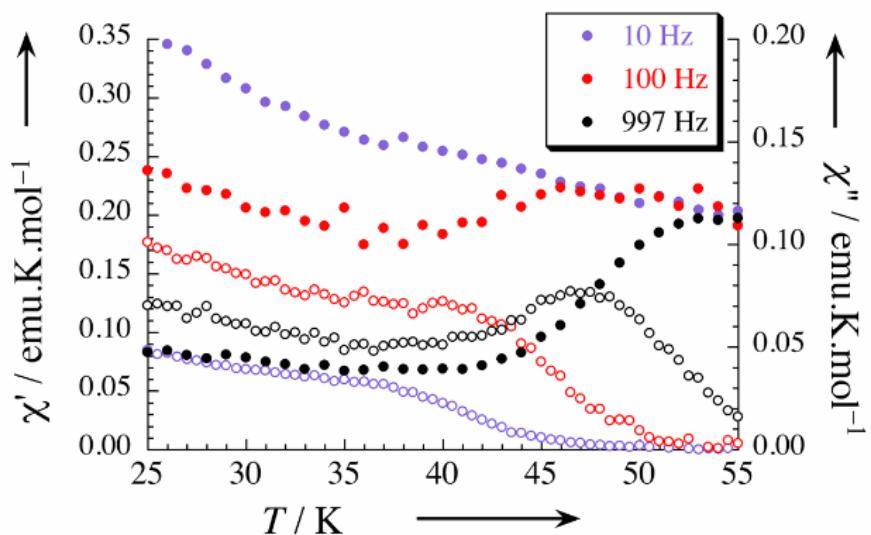
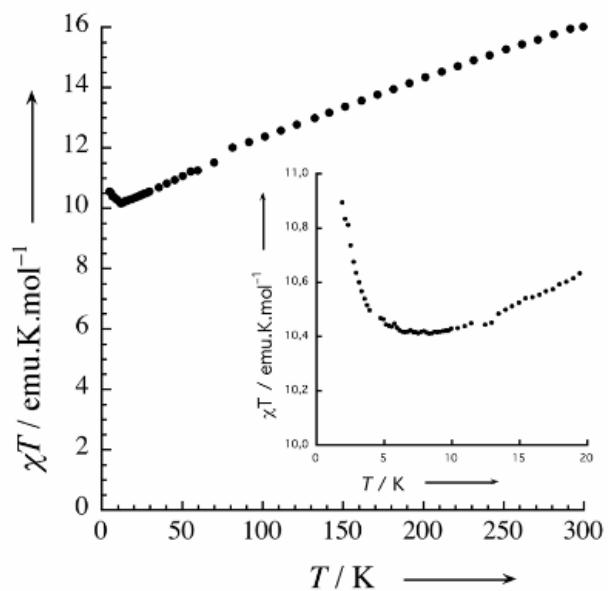


Figure 12S. Plot of χT against temperature for the powder sample of **1** (top). Temperature dependence of the in-phase (χ'_M , filled marks) and out-of-phase (χ''_M , open marks) components of the ac molar magnetic susceptibility of bulk **1** (down).

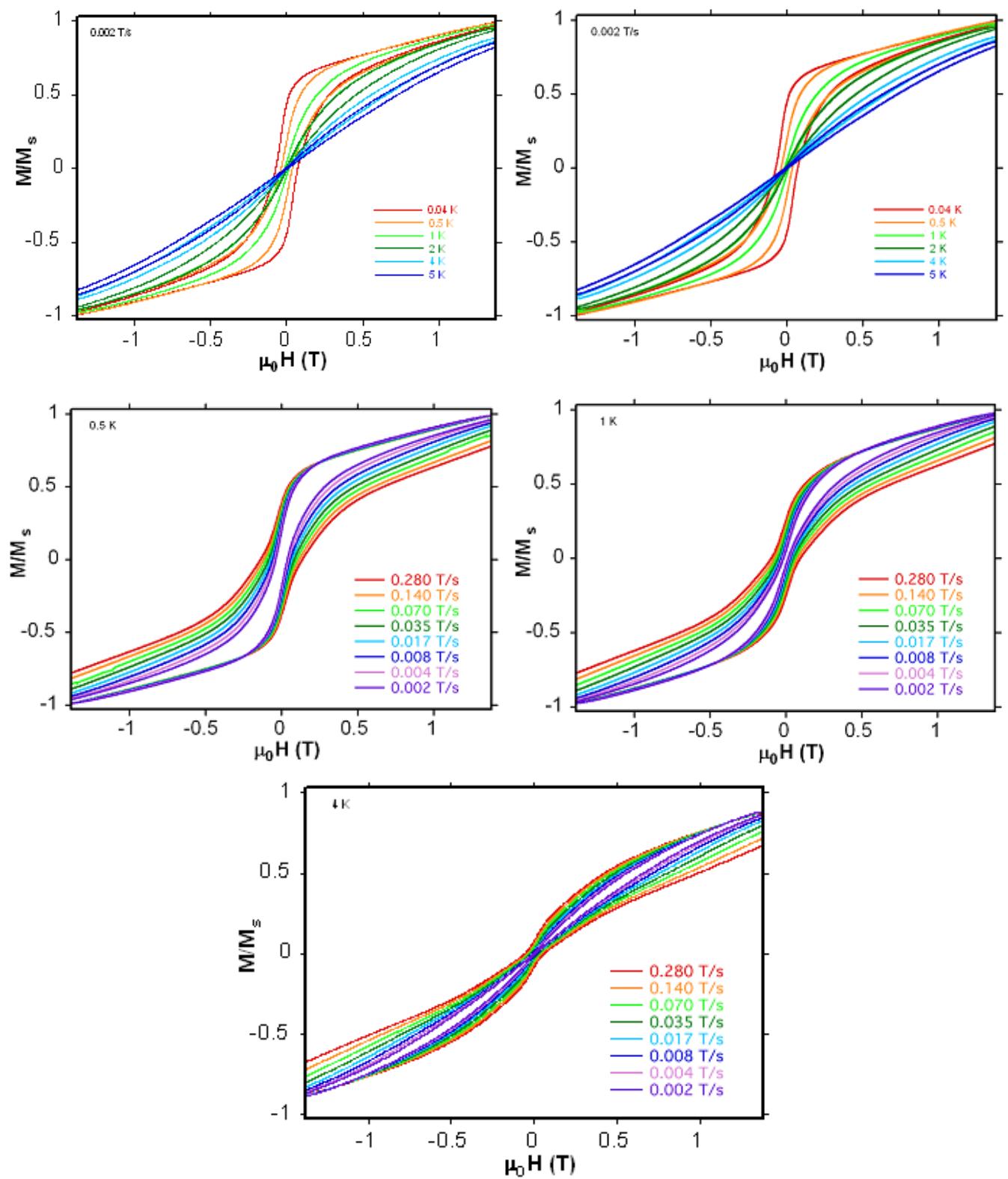


Figure 13S. Micro-SQUID hysteresis cycles of the 1^*SWNT conjugate recorded for different temperature and scan rates.