

Novel peptide foldameric motifs: a step forward in our understanding of  
the fully-extended conformation /  $3_{10}$ -helix coexistence

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**SUPPORTING INFORMATION**

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NMR spectra.....	S8-S17
Mass spectra.....	S17-S20

Table S1. Selected torsion angles (°) for PyrAc-(Deg)<sub>2</sub>-O-(*p*NO<sub>2</sub>)Bzl

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C02-C01-C17-C0	123.5(6)
C06-C01-C17-C0	-55.8(12)
C06'-C01'-C17'-C0	-65(2)
C02'-C01'-C17'-C0	119.7(10)
C01-C17-C0-N1	146.7(6)
C01'-C17'-C0-N1	155.9(10)
C17-C0-N1-C1A	176.6(4)
C17'-C0-N1-C1A	176.4(6)
C0-N1-C1A-C1	-171.32(14)
N1-C1A-C1B1-C1G1	-53.3(2)
N1-C1A-C1B2-C1G2	63.65(18)
N1-C1A-C1-N2	-169.49(12)
C1A-C1-N2-C2A	-174.55(12)
C1-N2-C2A-C2	-42.95(18)
N2-C2A-C2B1-C2G1	175.58(17)
N2-C2A-C2B2-C2G2	55.7(2)
N2-C2A-C2-OT1	-45.31(17)
C2A-C2-OT1-CT1	172.55(15)
C2-OT1-CT1-CT2	-159.89(15)
OT1-CT1-CT2-CT7	90.6(2)
OT1-CT1-CT2-CT3	-89.24(19)
CT6-CT5-NT1-OT2	5.5(3)
CT4-CT5-NT1-OT3	4.9(3)

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Table S2. Selected torsion angles (°) for PyrAc-(Deg)<sub>5</sub>-O-(pNO<sub>2</sub>)Bzl

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C06-C01-C17-C0	80.3(4)
C02-C01-C17-C0	-96.9(4)
C01-C17-C0-N1	-154.8(3)
C17-C0-N1-C1A	-173.7(2)
C0-N1-C1A-C1	-53.8(3)
N1-C1A-C1B1-C1G1	177.8(3)
N1-C1A-C1B2-C1G2	58.4(4)
N1-C1A-C1-N2	-41.7(3)
C1A-C1-N2-C2A	-174.6(3)
C1-N2-C2A-C2	-55.0(4)
N2-C2A-C2B1-C2G1	179.5(4)
N2-C2A-C2B2-C2G2	58.8(4)
N2-C2A-C2-N3	-31.5(3)
C2A-C2-N3-C3A	-173.1(2)
C2-N3-C3A-C3	-53.4(3)
N3-C3A-C3B1-C3G1	-179.4(4)
N3-C3A-C3B2-C3G2	60.9(5)
N3-C3A-C3-N4	-34.8(3)
C3A-C3-N4-C4A	-175.9(2)
C3-N4-C4A-C4	-59.2(3)
N4-C4A-C4B1-C4G1	-169.4(3)
N4-C4A-C4B2-C4G2	59.8(4)
N4-C4A-C4-N5	-31.5(3)
C4A-C4-N5-C5A	175.2(2)
C4-N5-C5A-C5	49.9(3)
N5-C5A-C5B1-C5G1	-69.9(3)
N5-C5A-C5B2-C5G2	-175.1(3)
N5-C5A-C5-OT1	54.8(3)
C5A-C5-OT1-CT1	159.6(3)
C5-OT1-CT1-CT2	140.9(3)
OT1-CT1-CT2-CT7	-14.9(6)
OT1-CT1-CT2-CT3	166.0(3)

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Table S3. Selected torsion angles (°) for PyrAc-(Aib)<sub>5</sub>-OtBu

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C02-C01-C17-C0	-96.82(15)
C06-C01-C17-C0	78.99(15)
C01-C17-C0-N1	107.95(13)
C17-C0-N1-C1A	-176.03(12)
C0-N1-C1A-C1	55.39(16)
N1-C1A-C1-N2	31.35(16)
C1A-C1-N2-C2A	173.84(11)
C1-N2-C2A-C2	54.97(16)
N2-C2A-C2-N3	30.43(16)
C2A-C2-N3-C3A	178.43(12)
C2-N3-C3A-C3	52.05(19)
N3-C3A-C3-N4	35.79(19)
C3A-C3-N4-C4A	175.23(12)
C3-N4-C4A-C4	57.90(15)
N4-C4A-C4-N5	37.55(16)
C4A-C4-N5-C5A	170.16(12)
C4-N5-C5A-C5	-49.30(17)
N5-C5A-C5-OT	-43.22(15)
C5A-C5-OT-CT1	-174.68(12)
C5-OT-CT1-CT2	-60.5(2)
C5-OT-CT1-CT4	-178.6(2)
C5-OT-CT1-CT3	62.1(2)

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Table S4. Hydrogen bonds for PyrAc-(Deg)<sub>2</sub>-O-(*p*NO<sub>2</sub>)Bzl [ $\text{\AA}$  and  $^\circ$ ].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1...O1	0.86	2.13	2.5669(17)	110.8
N2-H2...O0#1	0.86	2.25	3.0845(15)	165.3

Symmetry transformations used to generate equivalent atoms:

#1  $-x+1/2, y-1/2, -z+3/2$

Table S5. Hydrogen bonds for PyrAc-(Deg)<sub>5</sub>-O-(*p*NO<sub>2</sub>)Bzl [ $\text{\AA}$  and  $^\circ$ ].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N3-H3...O0	0.86	2.20	2.996(3)	154.7
N4-H4...O1	0.86	2.40	3.218(3)	158.2
N5-H5...O2	0.86	2.22	2.951(3)	143.2
N1-H1...O4#1	0.86	2.00	2.862(3)	174.0

Symmetry transformations used to generate equivalent atoms:

#1  $x, y, z+1$

Table S6. Hydrogen bonds for PyrAc-(Aib)<sub>5</sub>-O*t*Bu

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N3-H3...O0	0.86	2.32	3.1407(14)	159.2
N4-H4...O1	0.86	2.19	2.9973(13)	156.4
N5-H5...O2	0.86	2.26	3.0335(14)	149.8
N1-H1...O4#1	0.86	2.09	2.9212(14)	161.9

Symmetry transformations used to generate equivalent atoms:

#1  $x+1, y, z$

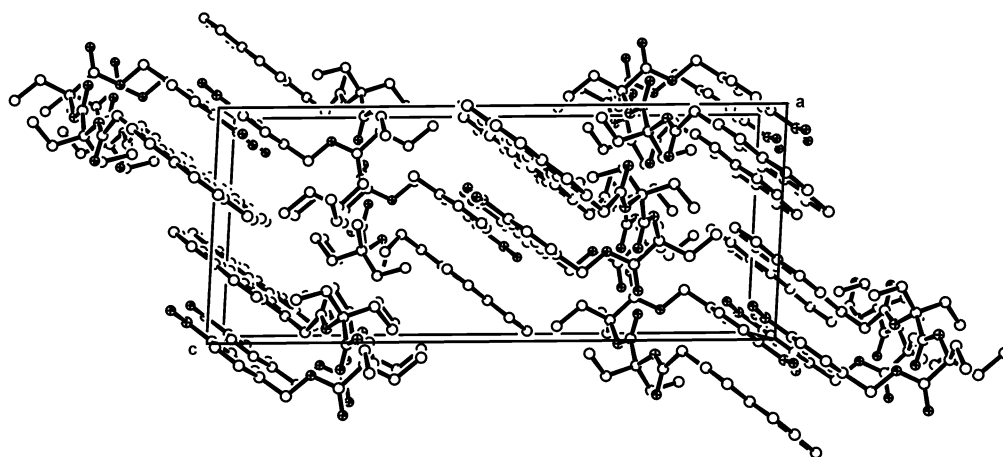


Figure S1 – Packing mode of PyrAc-(Deg)<sub>2</sub>-O-(pNO<sub>2</sub>)Bzl as viewed down the *b* axis.

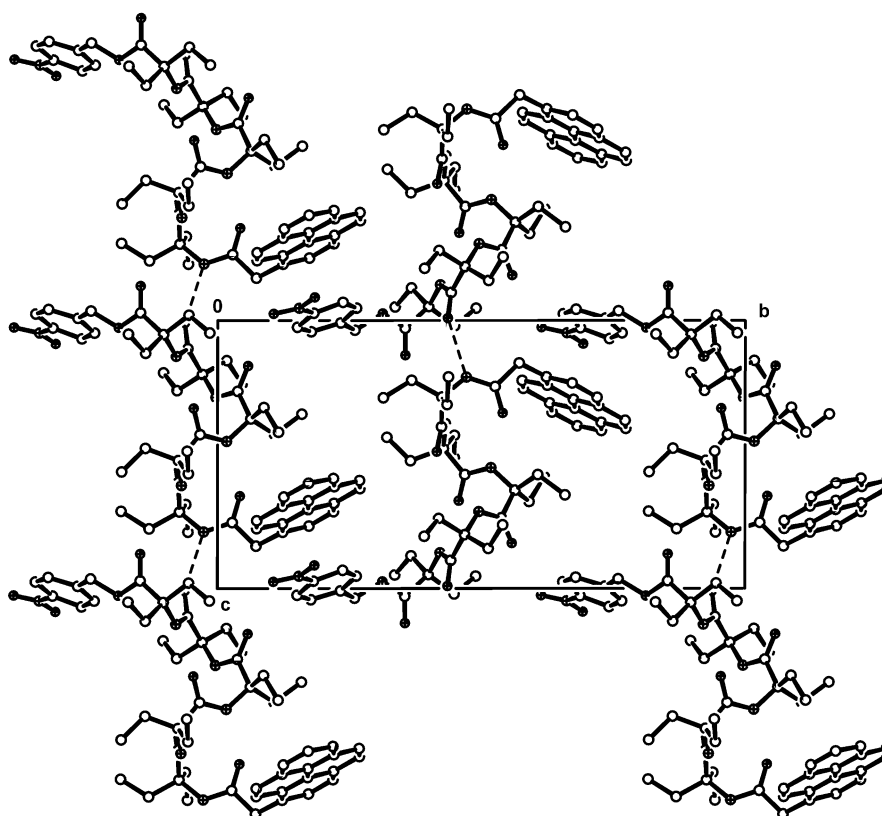


Figure S2 – Packing mode of PyrAc-(Deg)<sub>5</sub>-O-(pNO<sub>2</sub>)Bzl as viewed down the *a* axis. The intermolecular H-bonds are indicated by dashed lines.

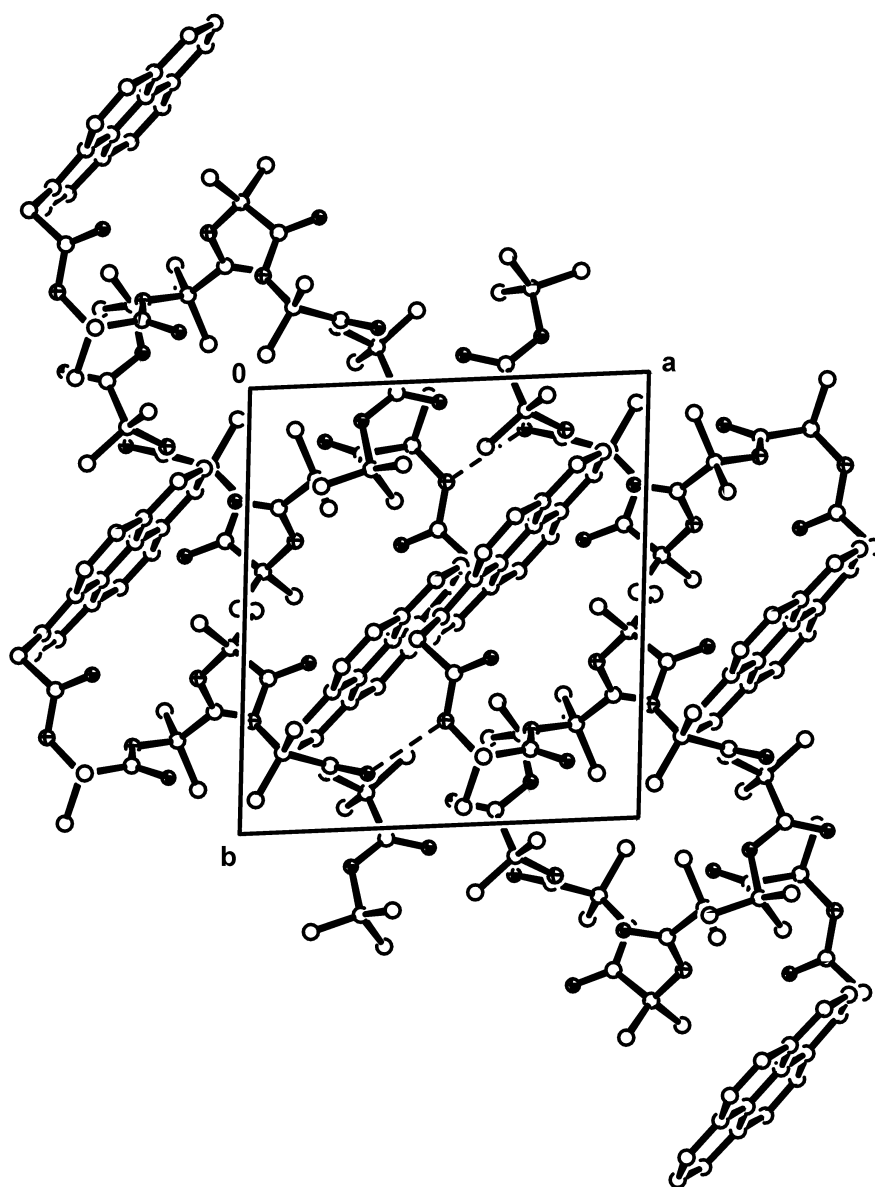
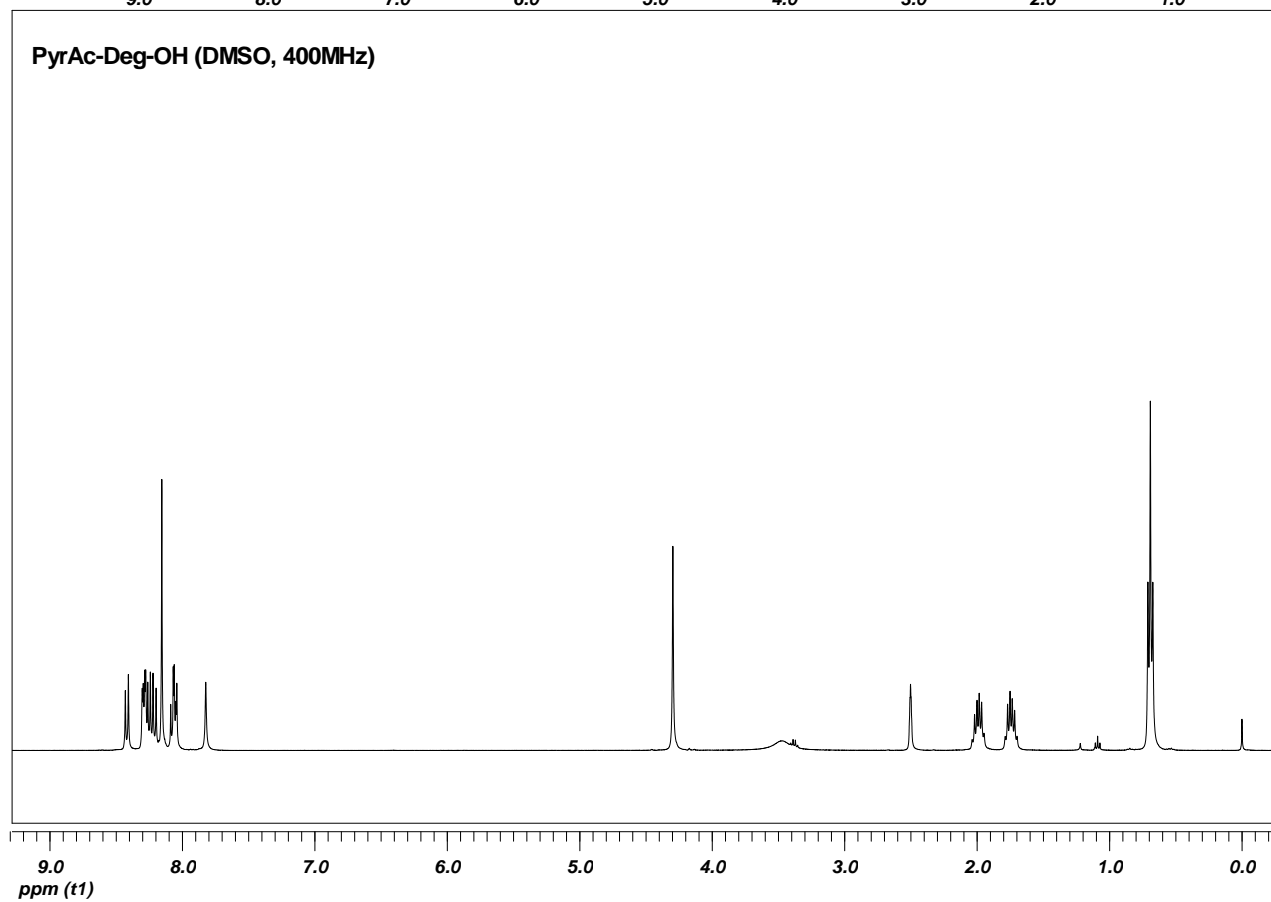
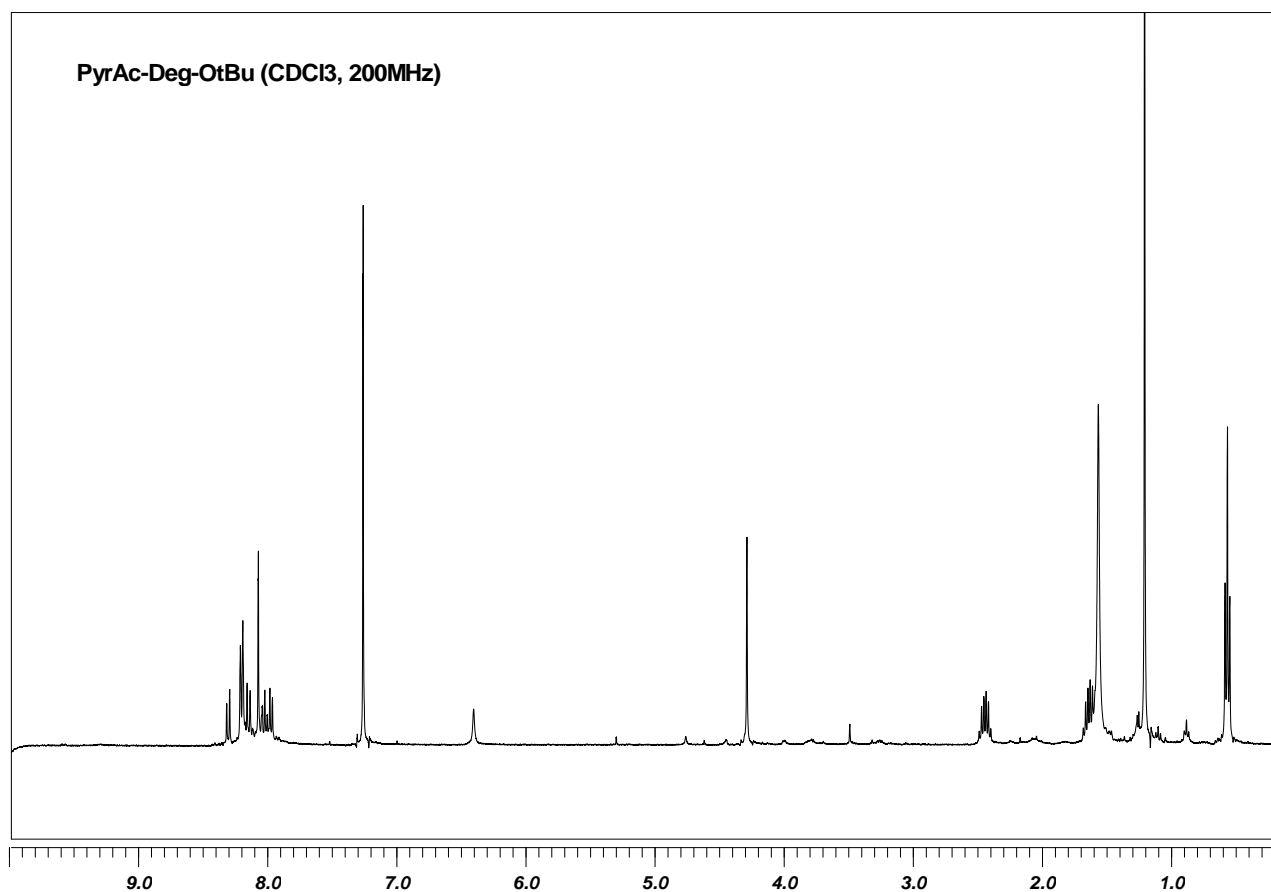
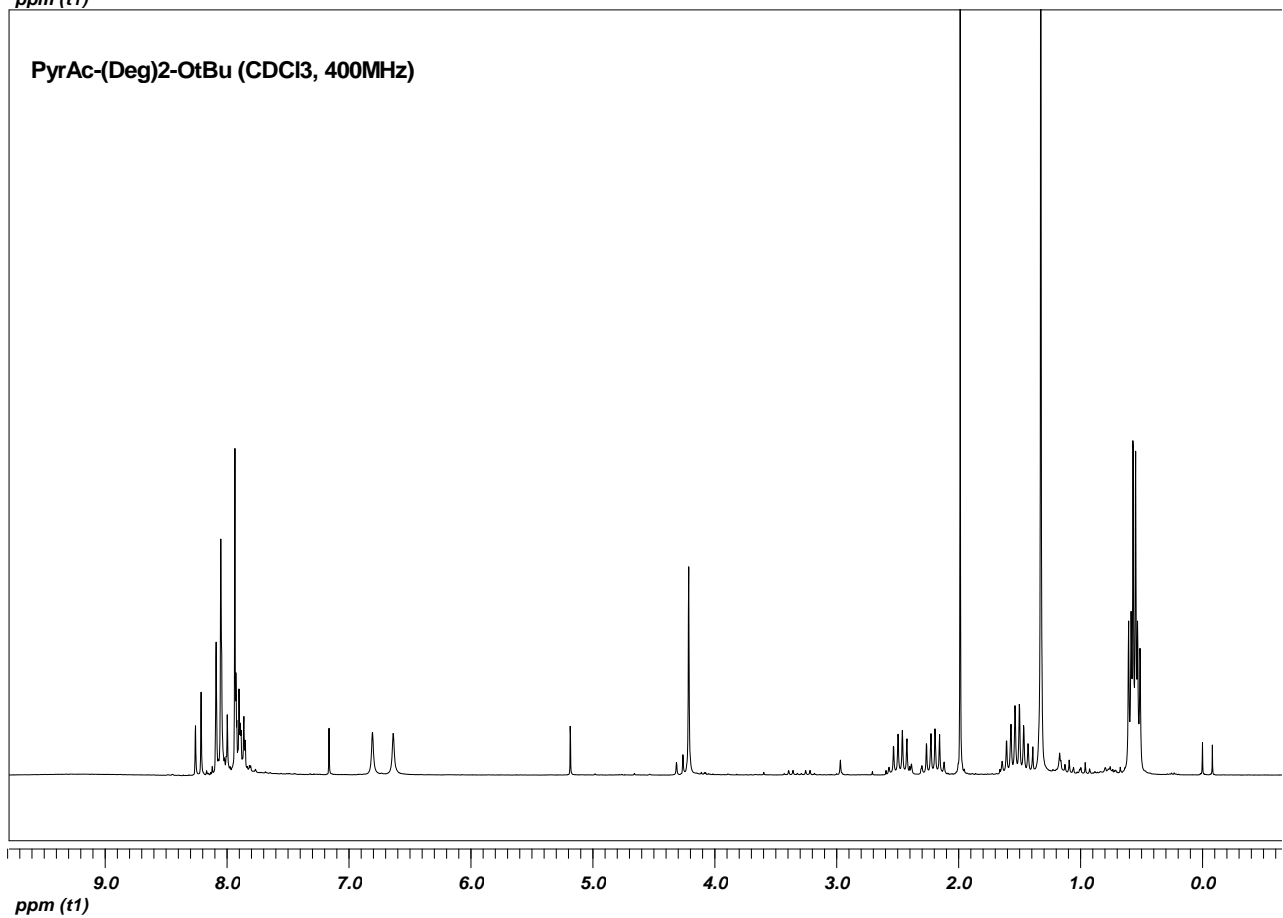
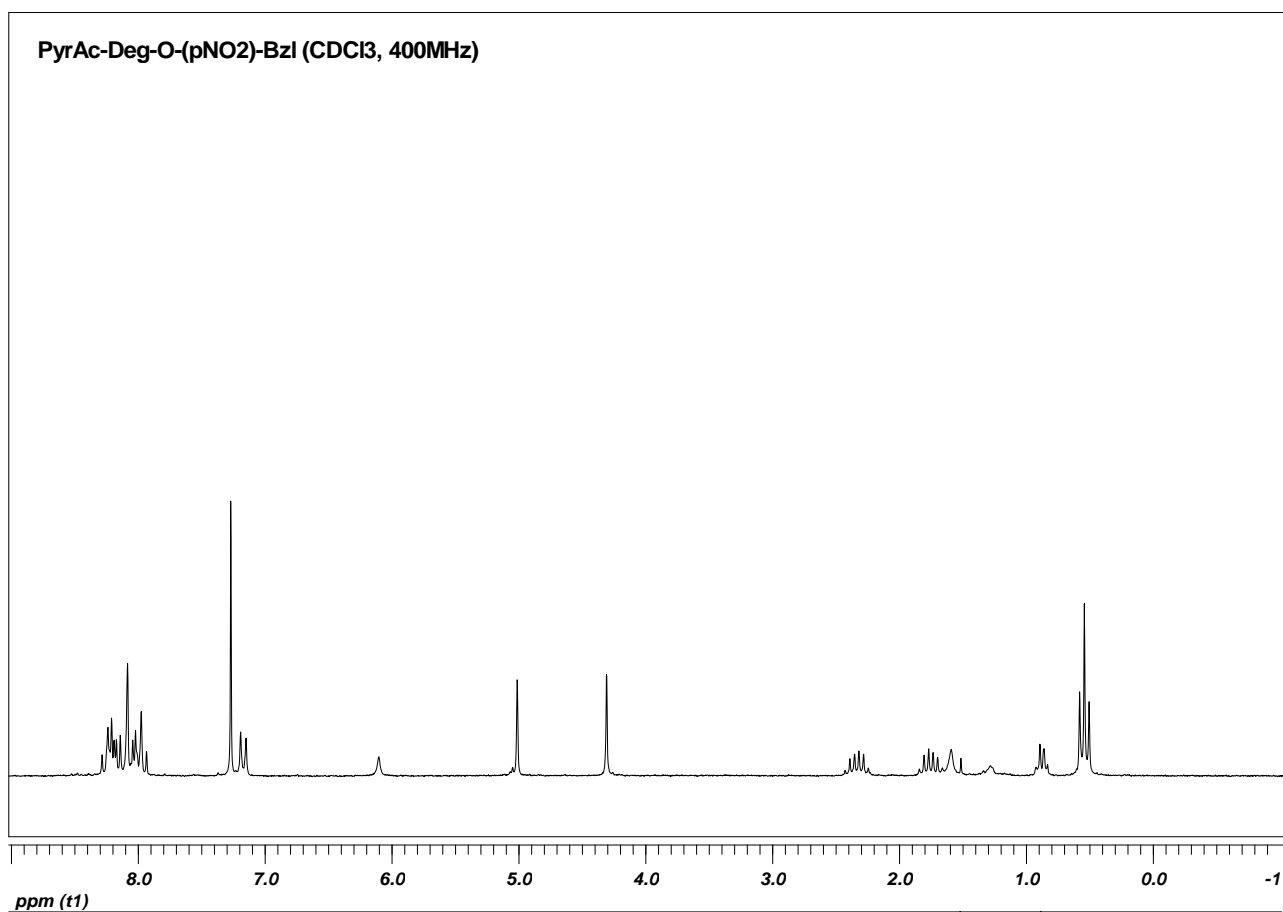
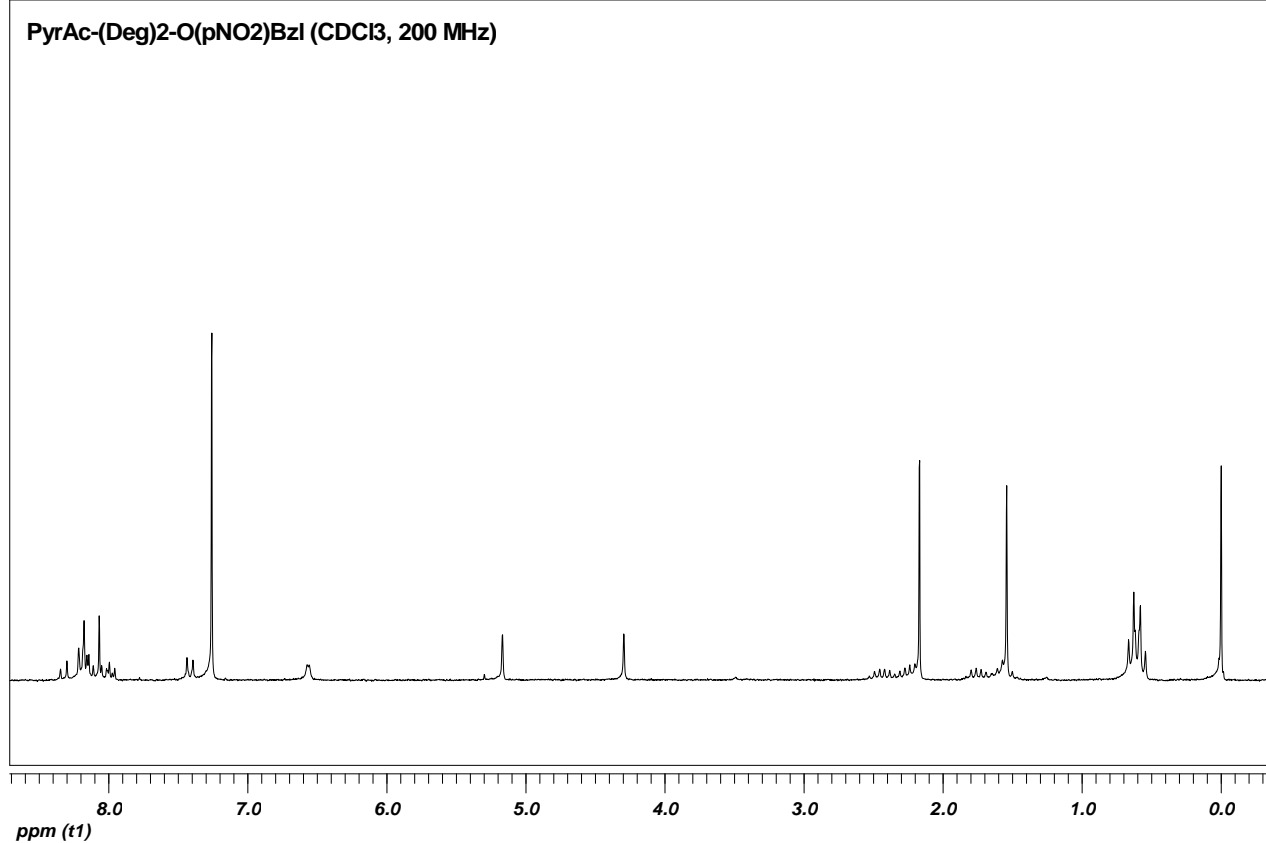
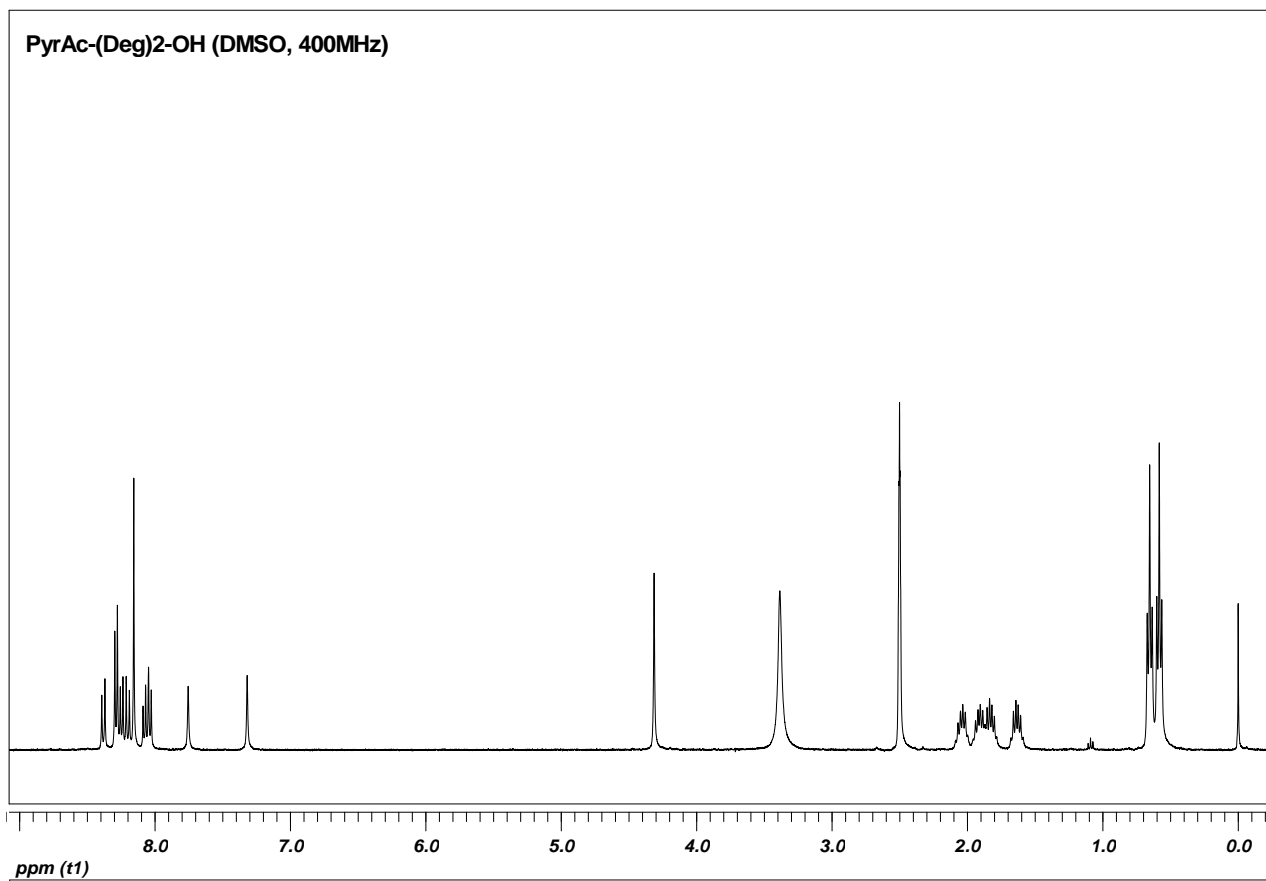


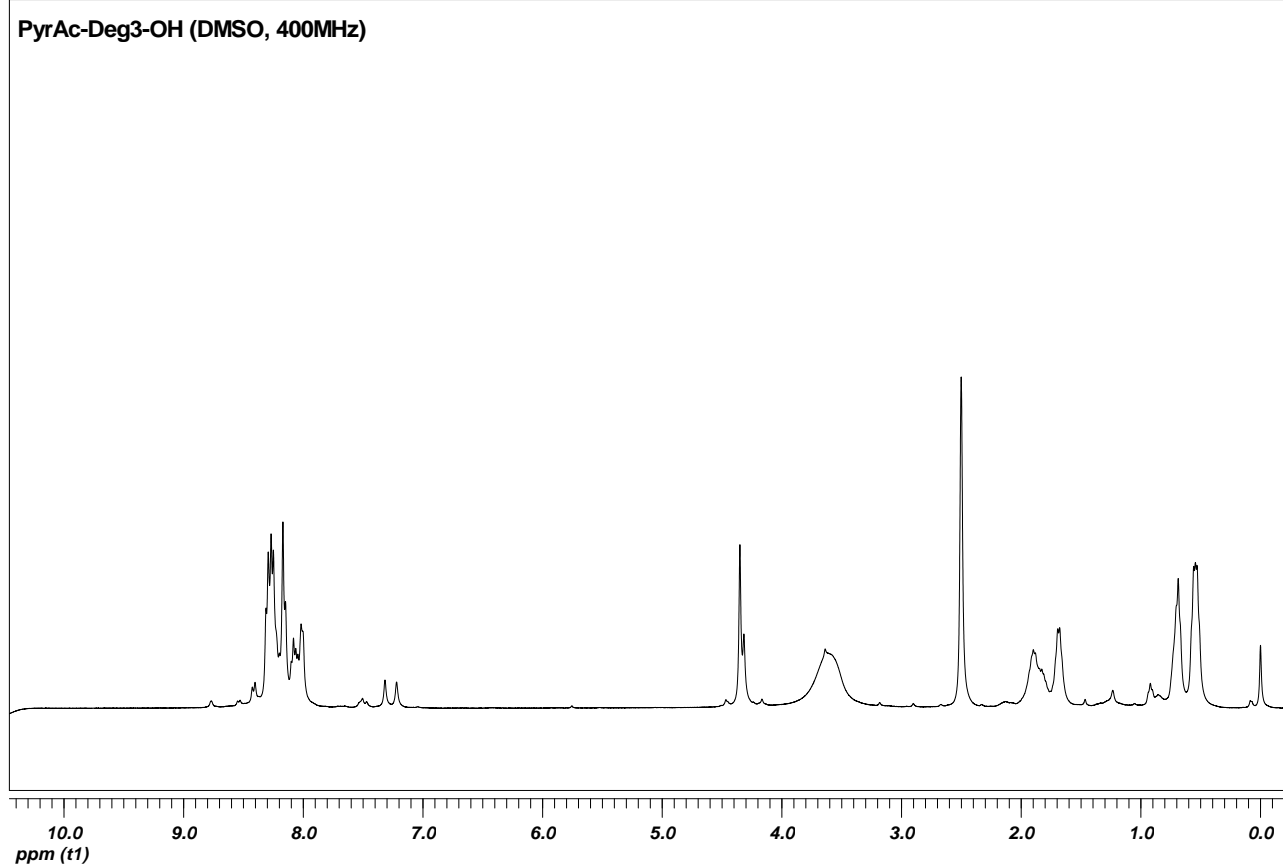
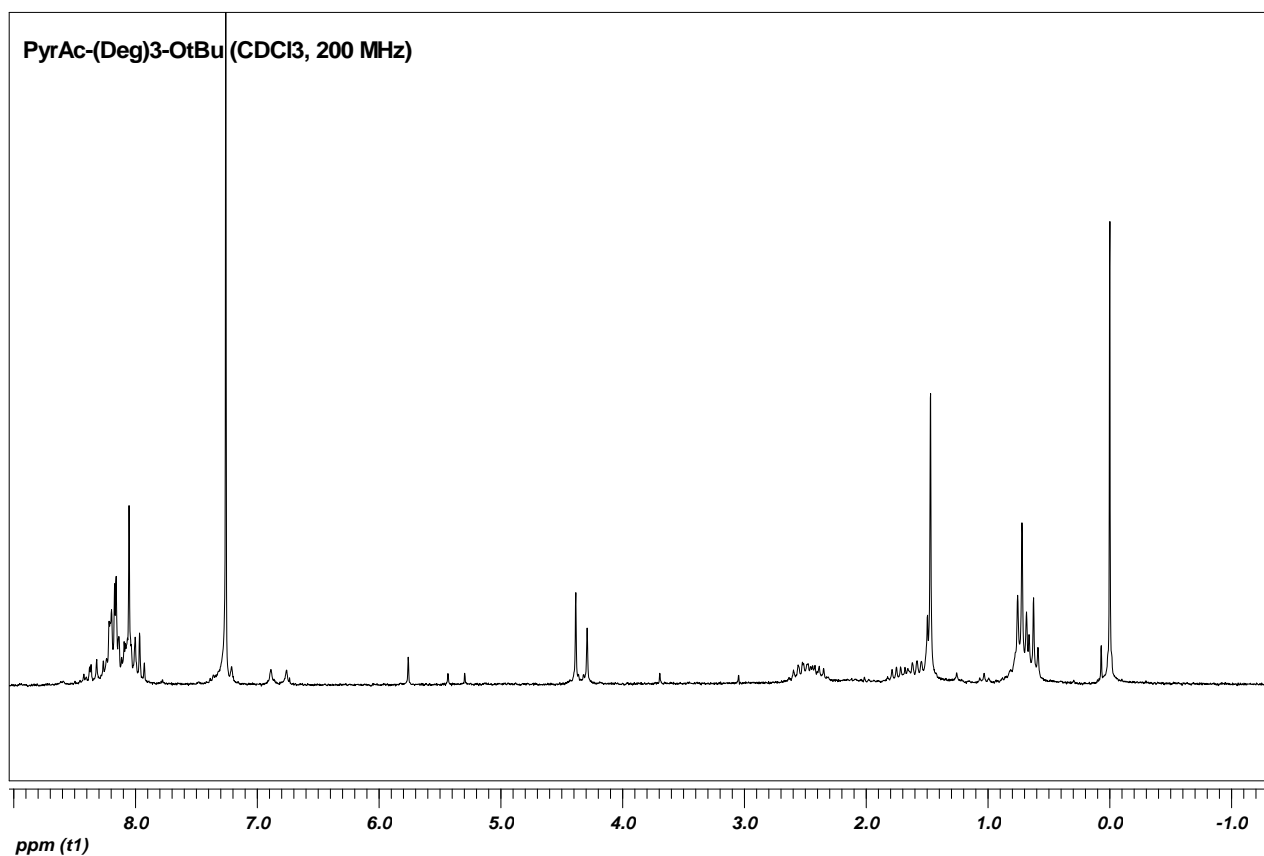
Figure S3 – Packing mode of PyrAc-(Aib)<sub>5</sub>-OtBu as viewed down the *c* axis. The intermolecular H-bonds are indicated by dashed lines.

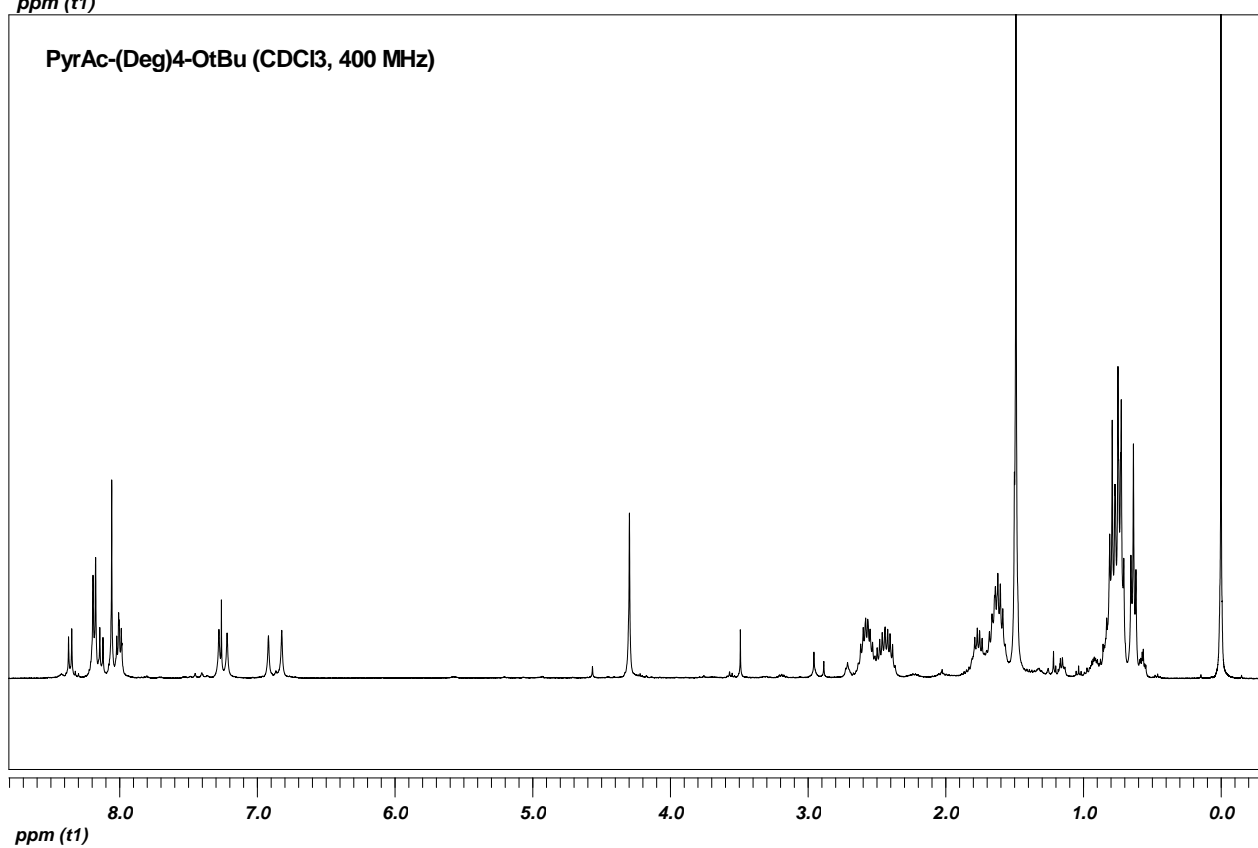
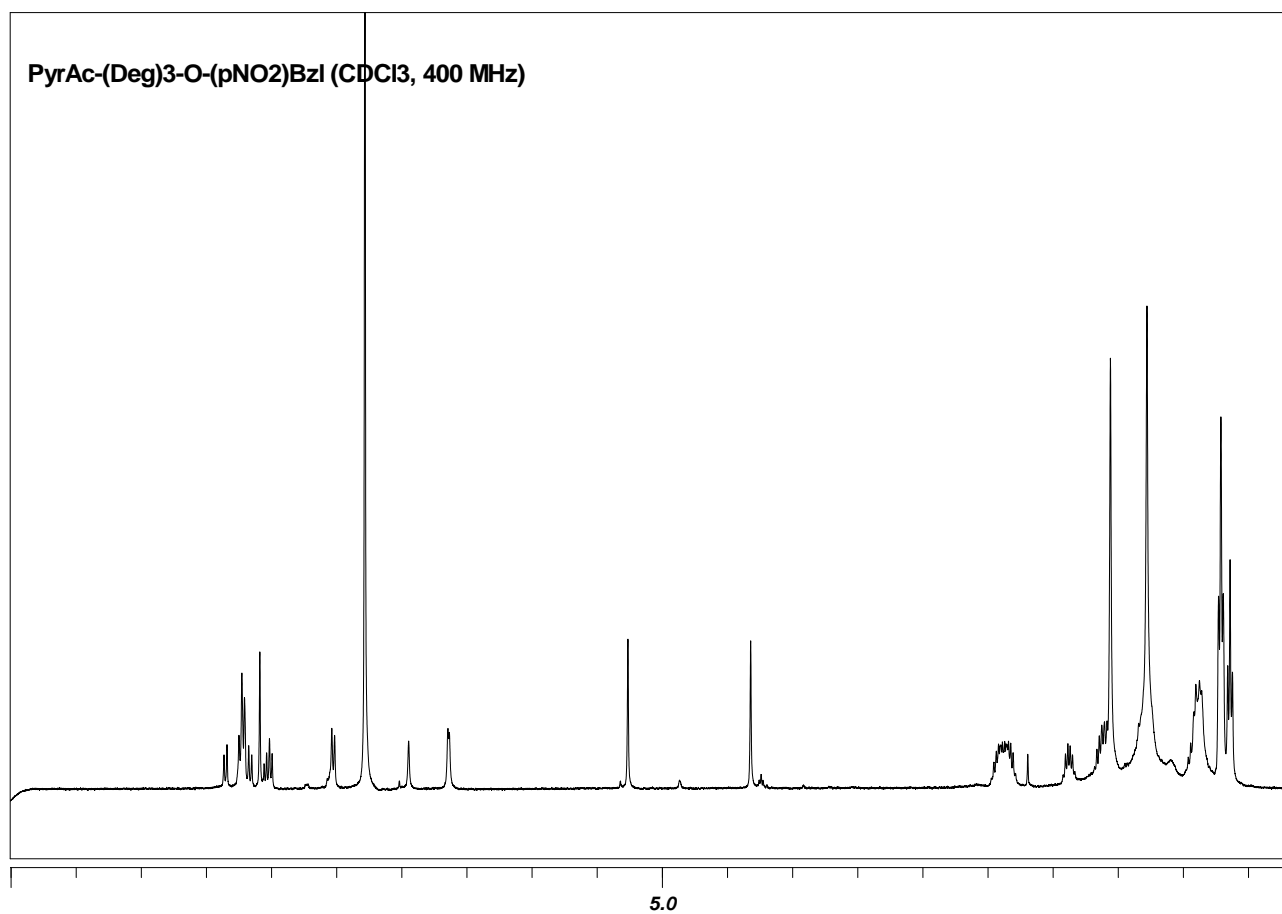


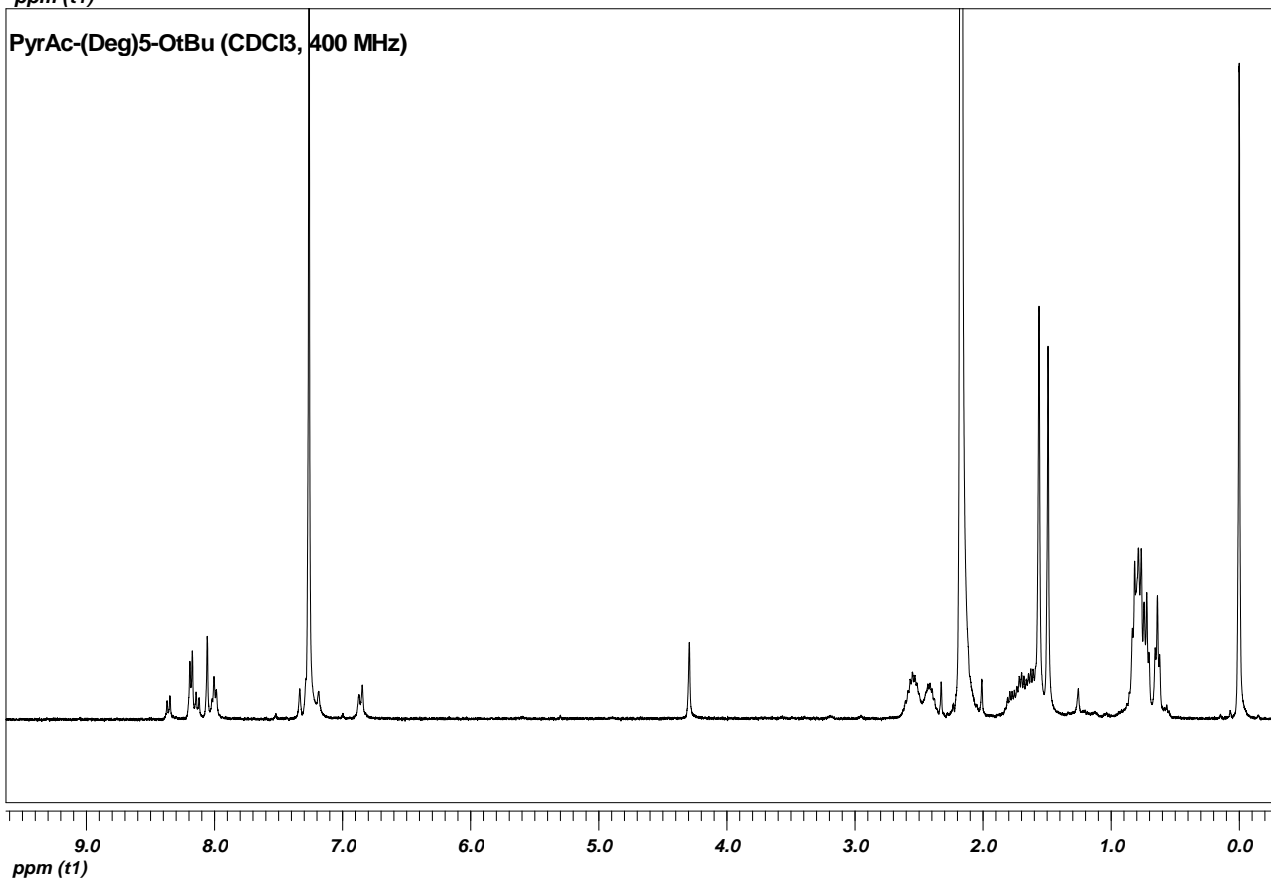
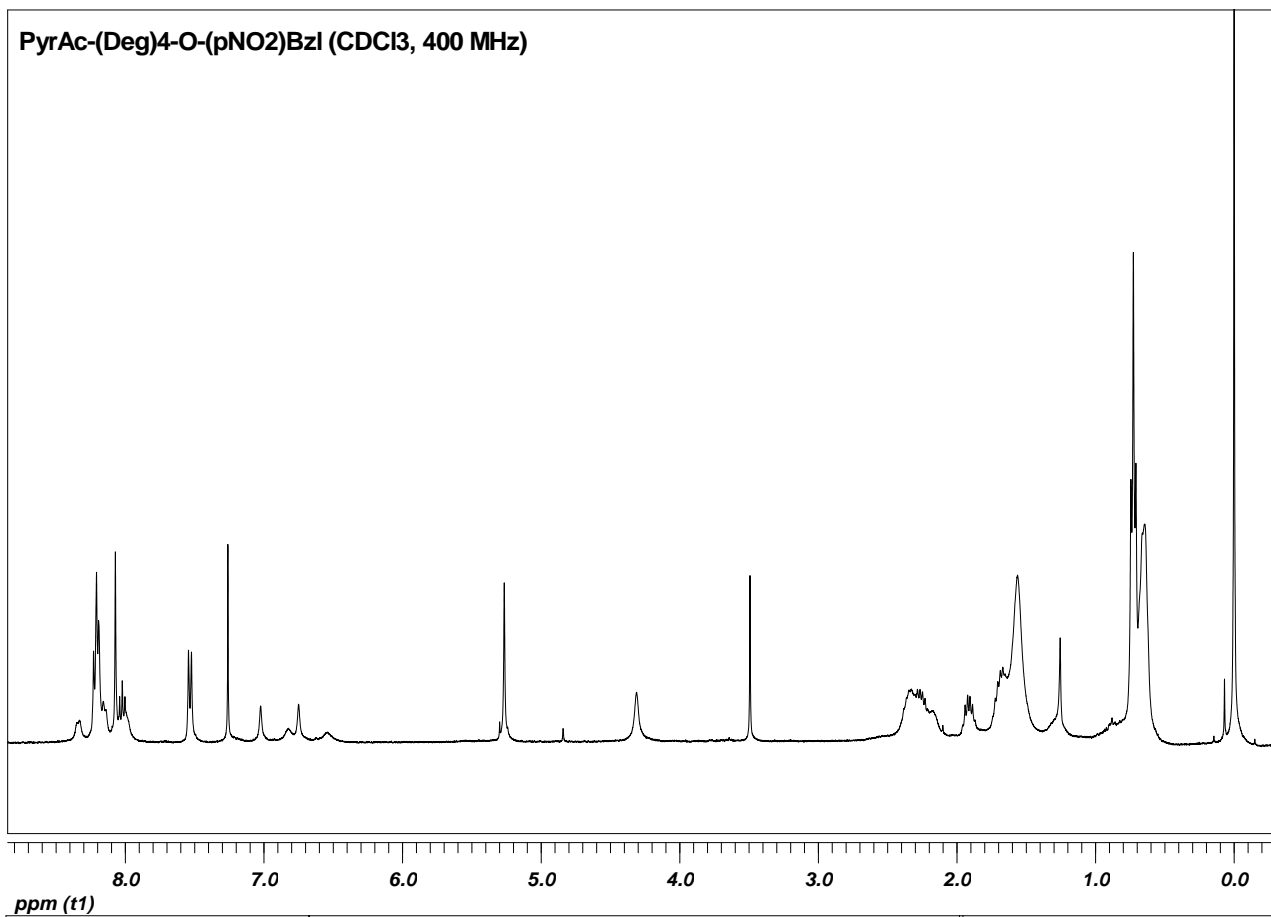


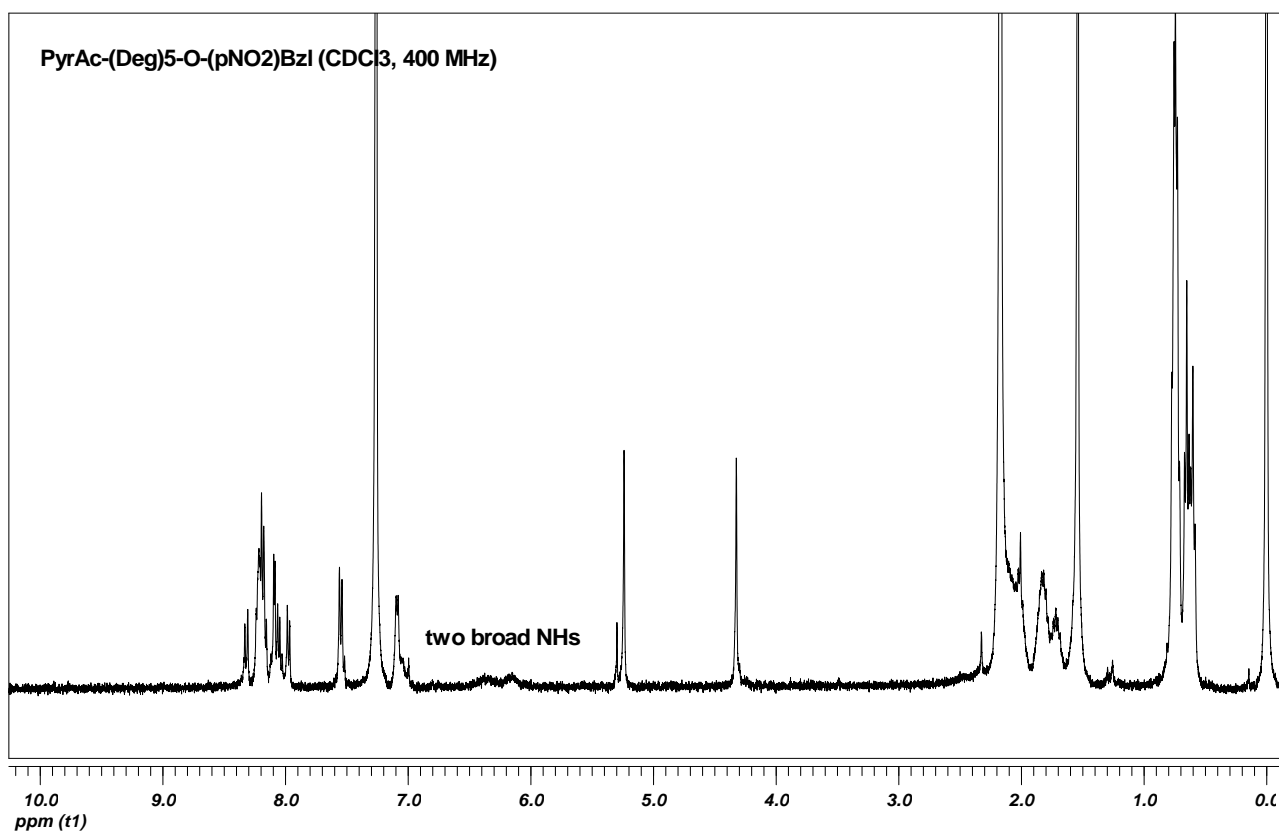
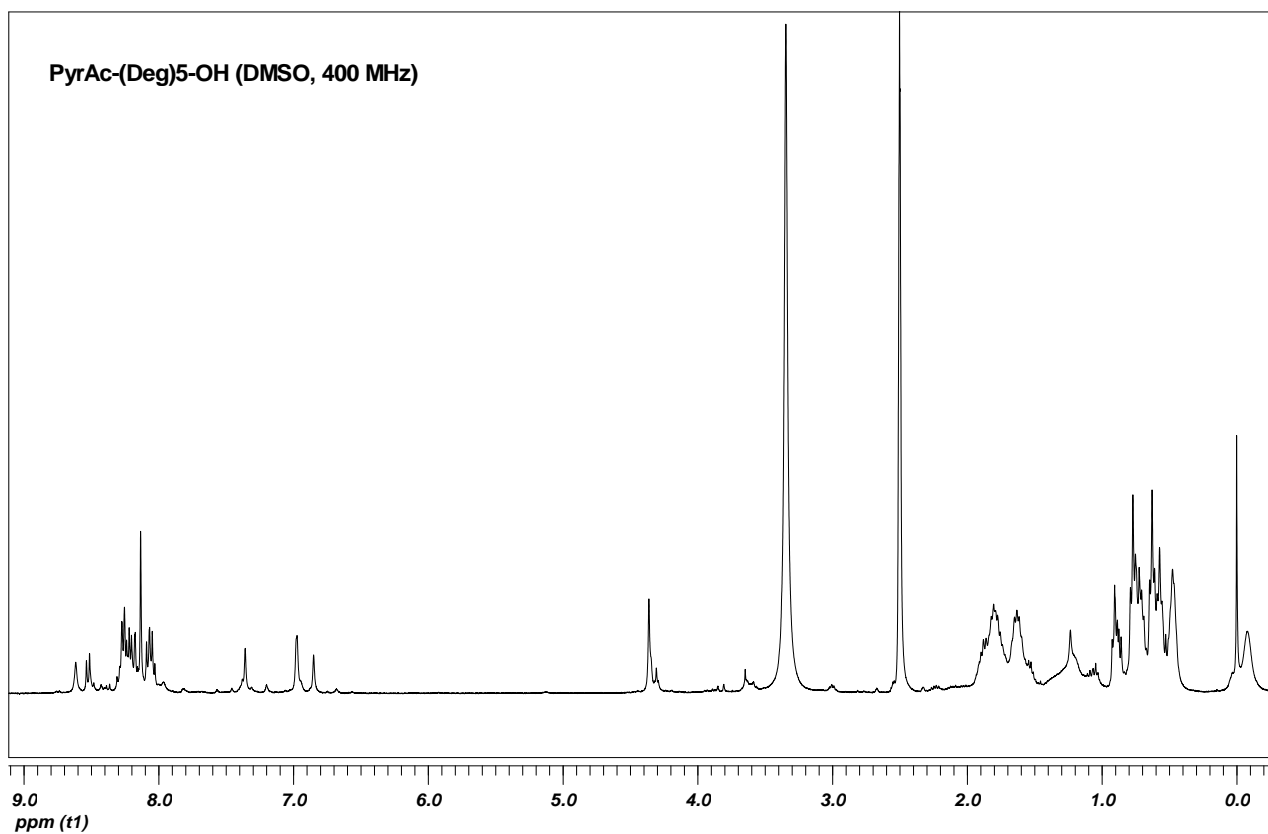


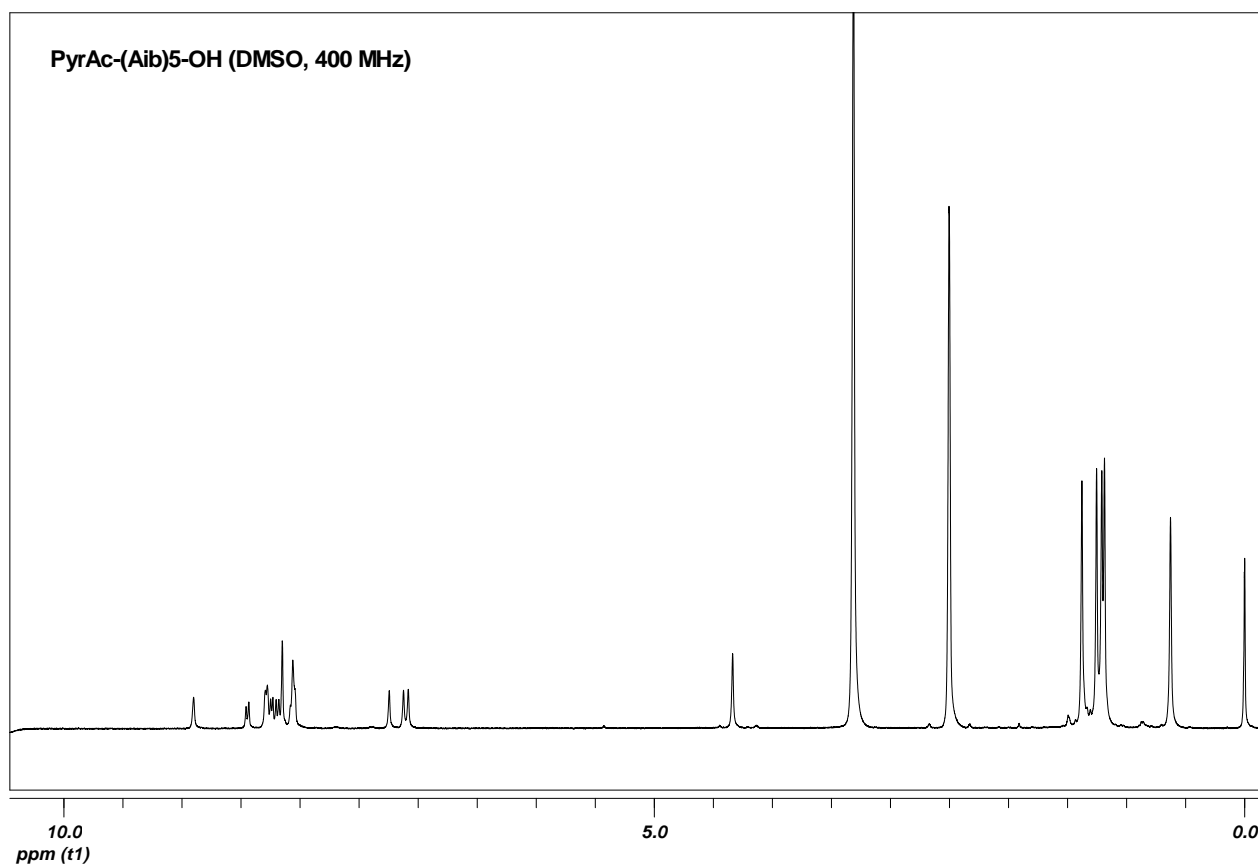
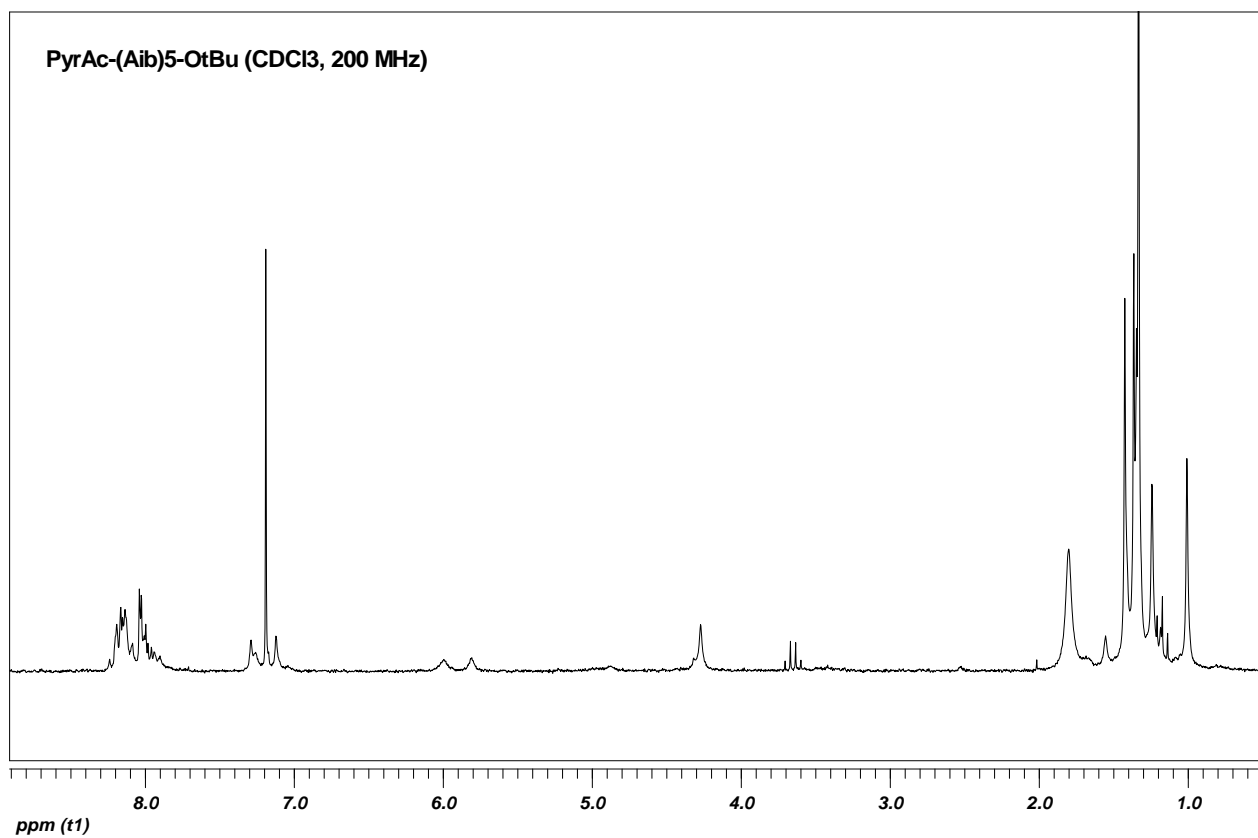


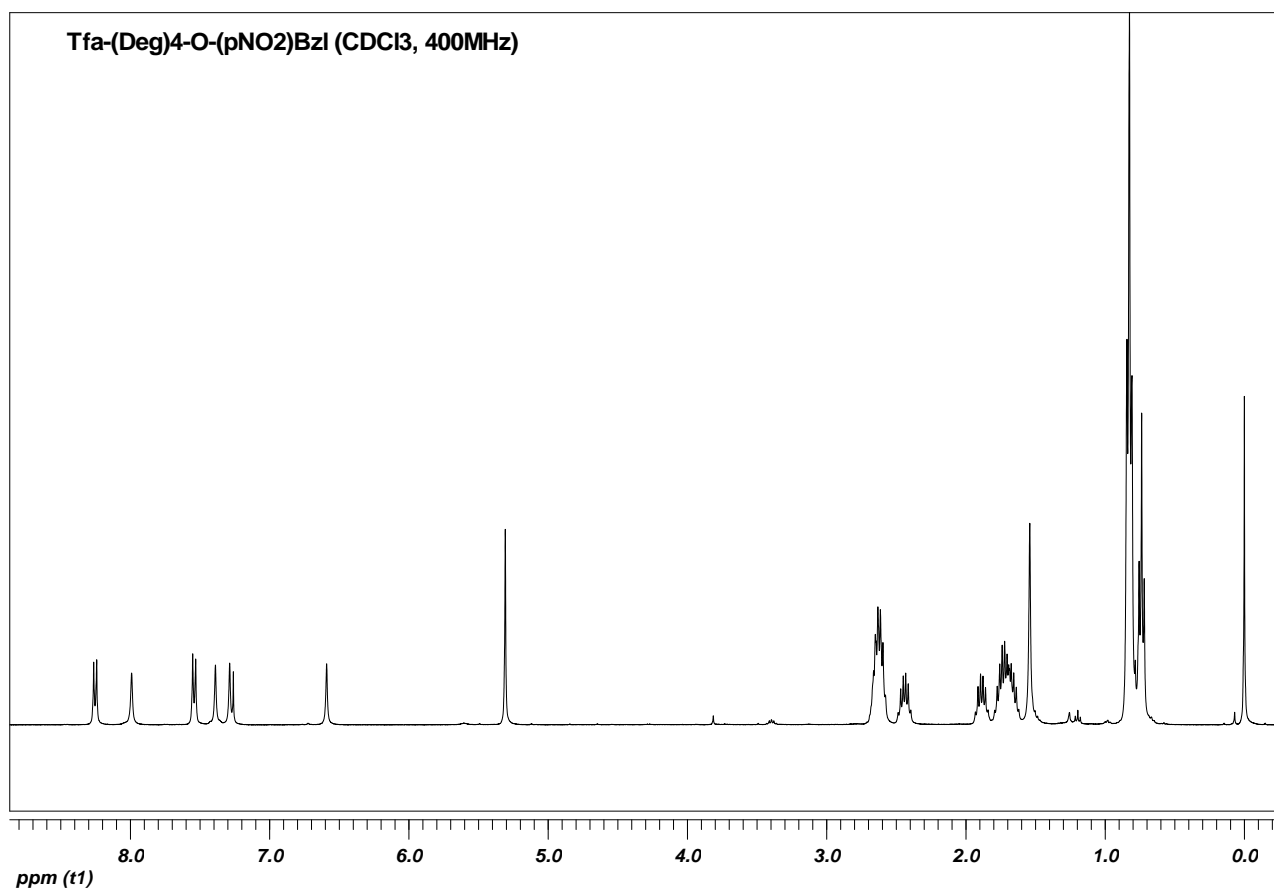
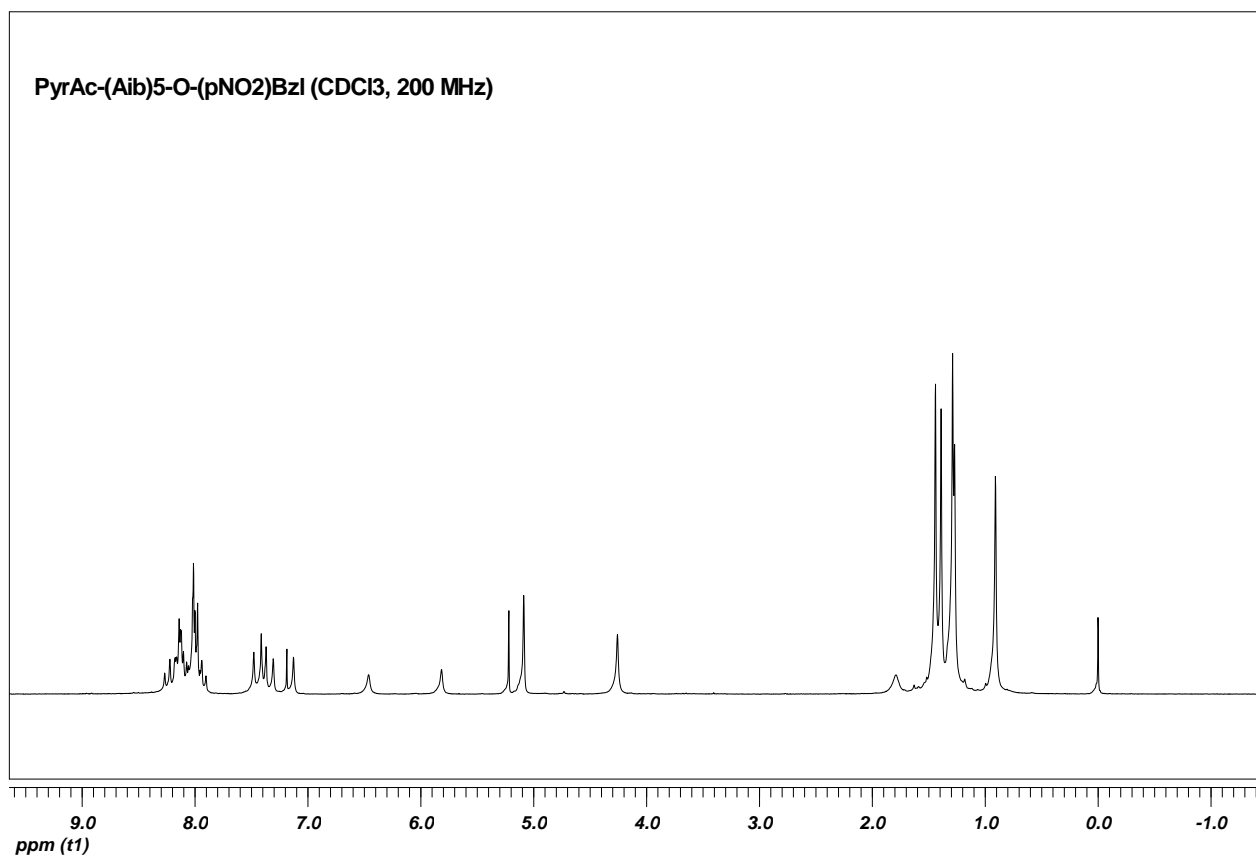




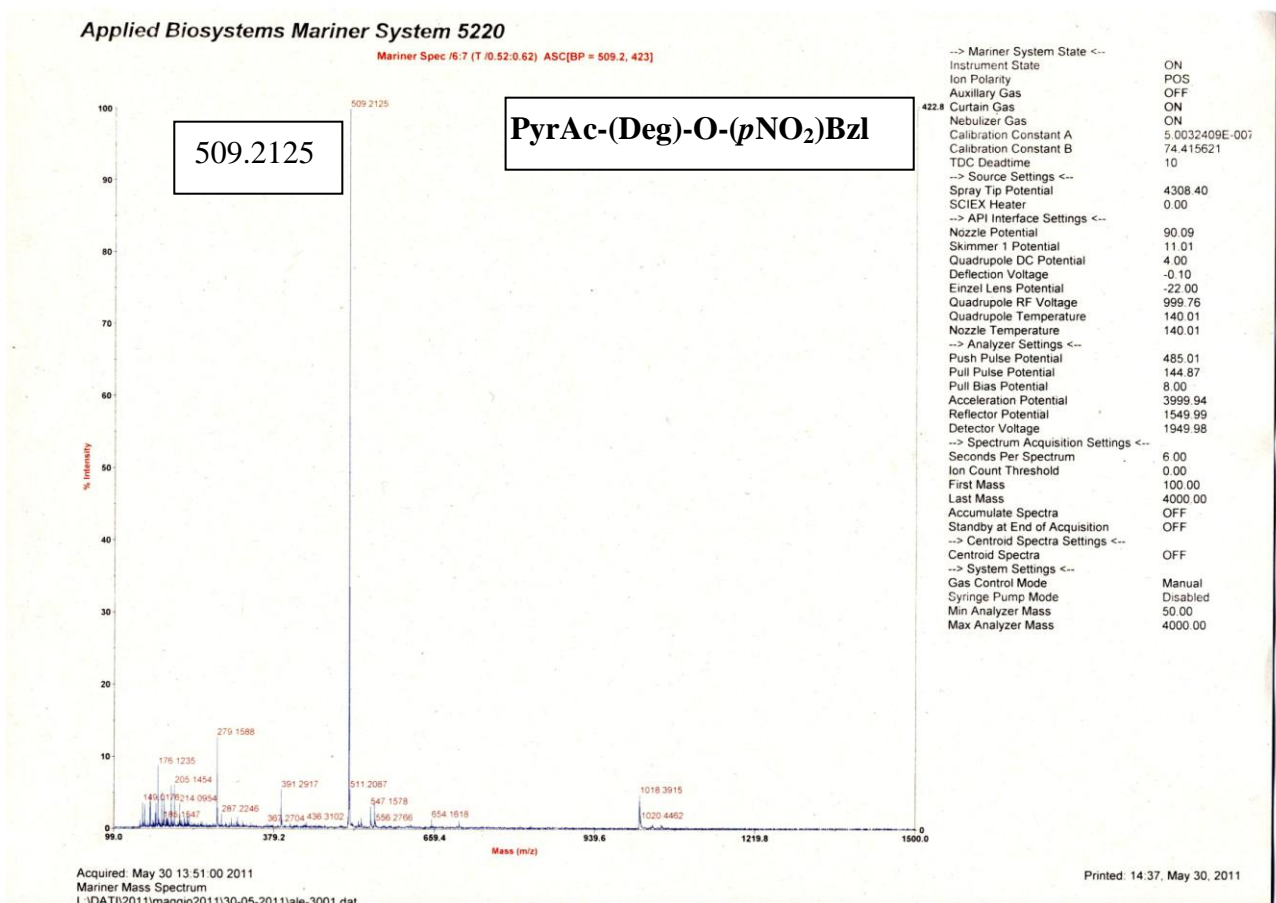
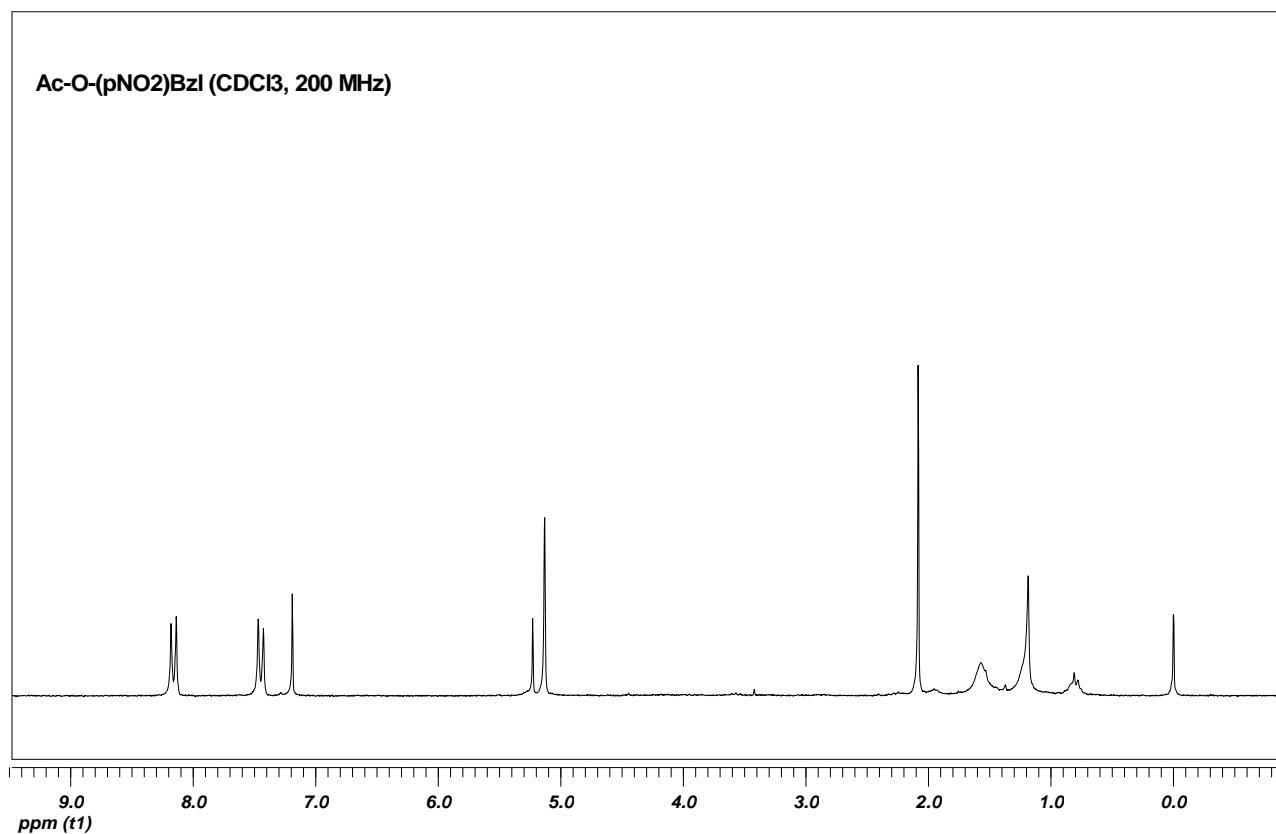






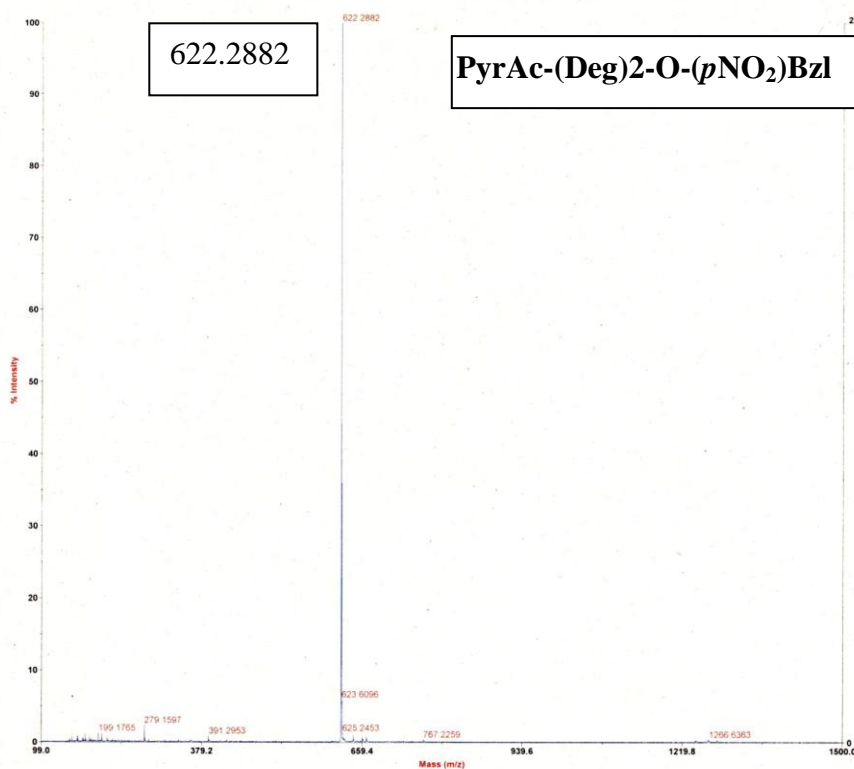






Applied Biosystems Mariner System 5220

Mariner Spec 7:8 (T /0.62:0.73) ASC[BP = 622.3, 2311]



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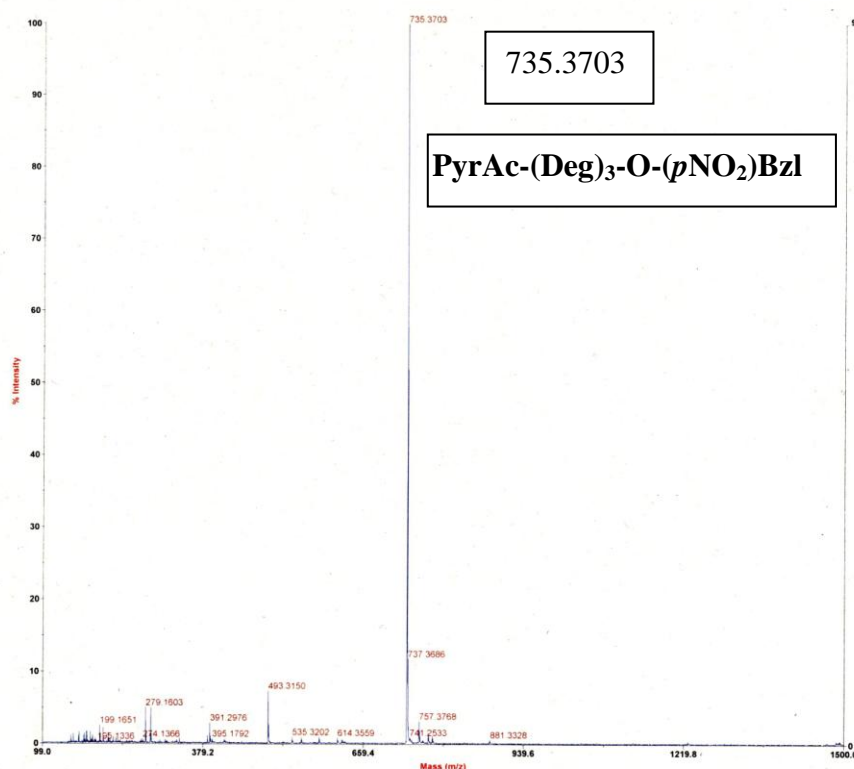
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Ion Polarity         OFF
Auxiliary Gas        ON
Curtain Gas          ON
Nebulizer Gas        ON
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Calibration Constant B 74.415621
TDC Deadtime         10
--> Source Settings <--
Spray Tip Potential   4308.40
SCIEX Heater         0.00
--> API Interface Settings <--
Nozzle Potential     90.09
Skimmer 1 Potential  11.01
Quadrupole DC Potential 4.00
Deflection Voltage   -0.10
Einzel Lens Potential -22.00
Quadrupole RF Voltage 999.76
Quadrupole Temperature 140.01
Nozzle Temperature   140.01
--> Analyzer Settings <--
Push Pulse Potential 485.01
Pull Pulse Potential 144.87
Pull Bias Potential   8.00
Acceleration Potential 3999.94
Reflector Potential   1549.99
Detector Voltage      1949.98
--> Spectrum Acquisition Settings <--
Seconds Per Spectrum 6.00
Ion Count Threshold   0.00
First Mass            100.00
Last Mass             4000.00
Accumulate Spectra   OFF
Standby at End of Acquisition OFF
--> Centroid Spectra Settings <--
Centroid Spectra     OFF
--> System Settings <--
Gas Control Mode     Manual
Syringe Pump Mode    Disabled
Min Analyzer Mass     50.00
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Applied Biosystems Mariner System 5220

Mariner Spec 7:8 (T /0.62:0.73) ASC[BP = 735.4, 977]

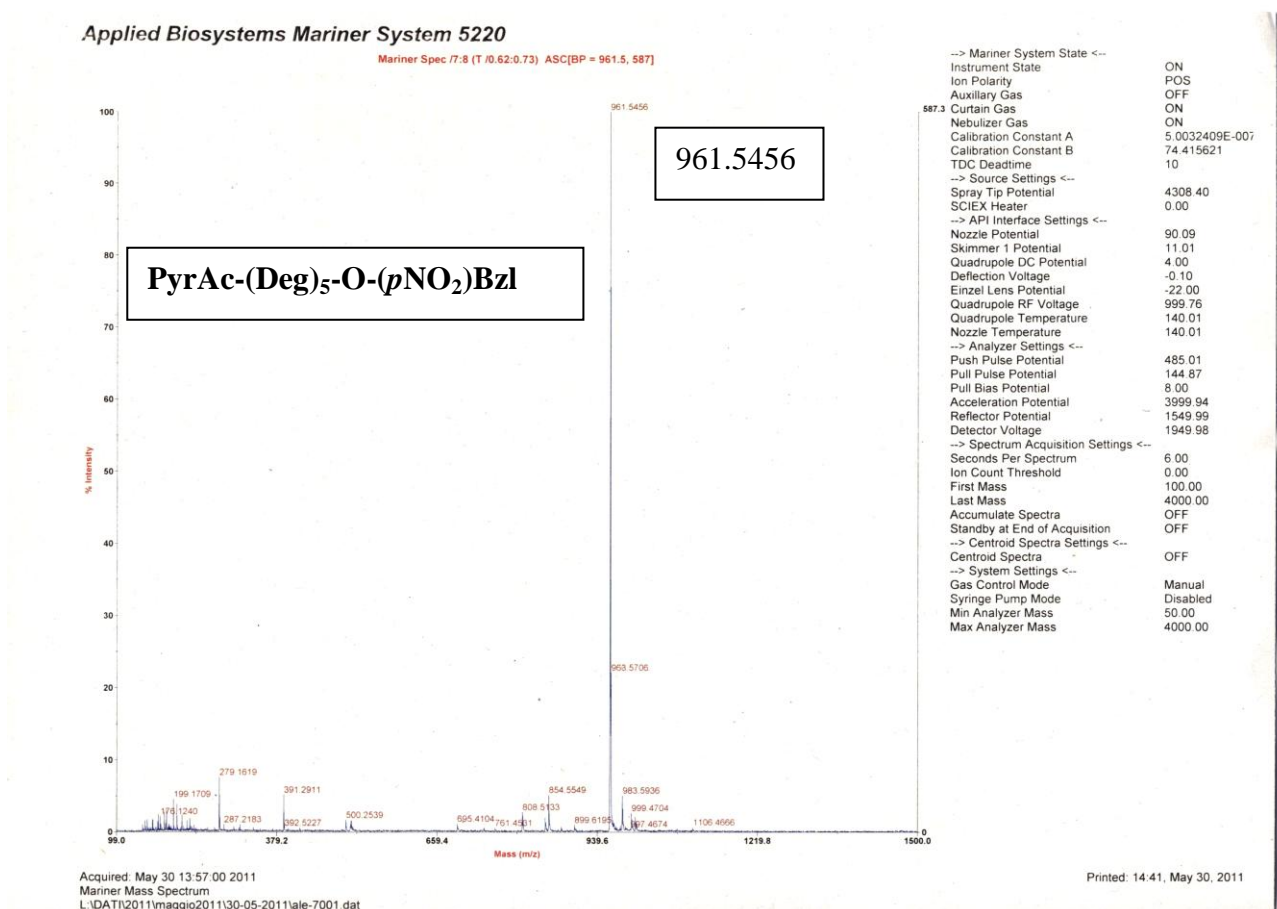
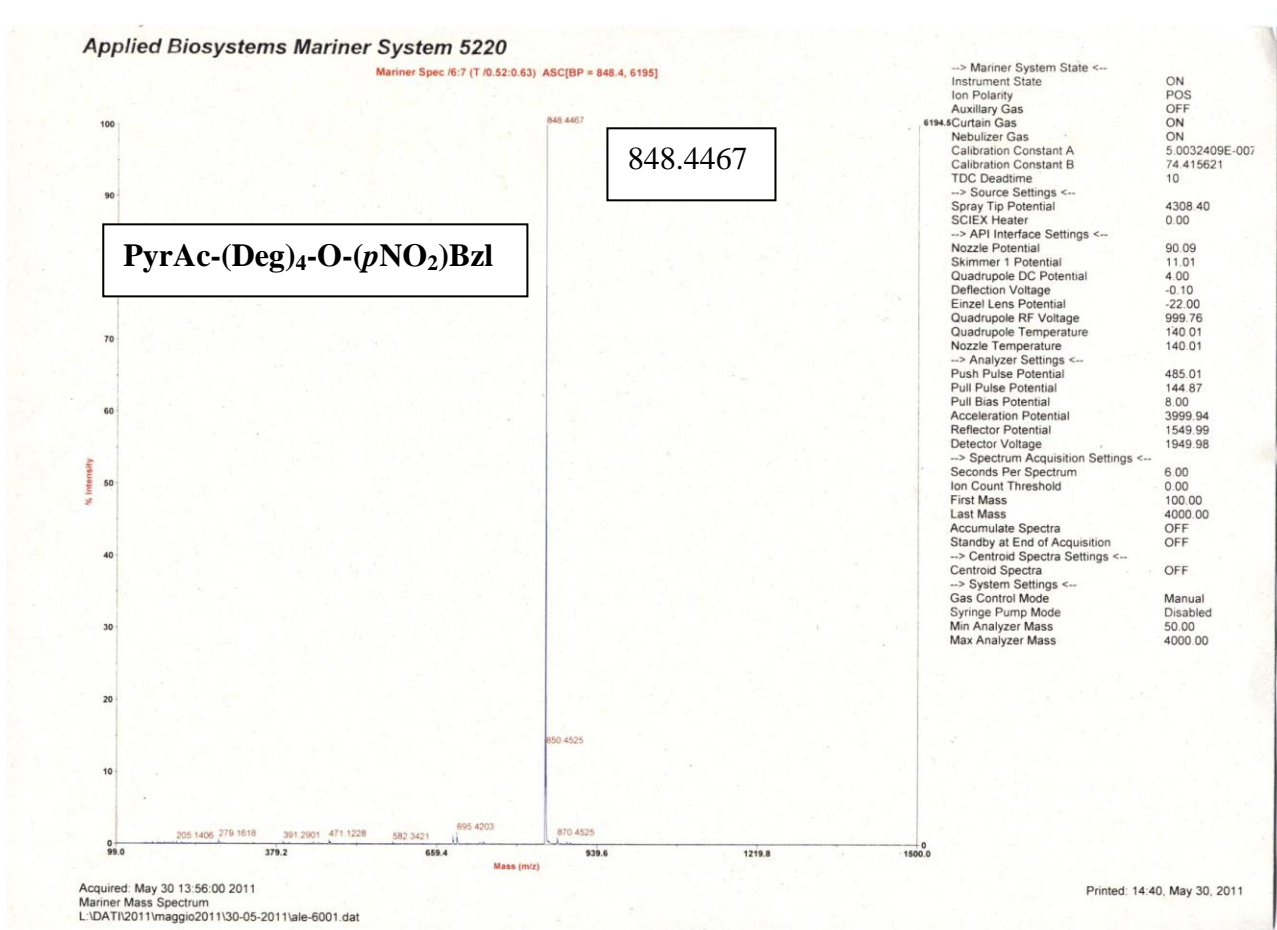


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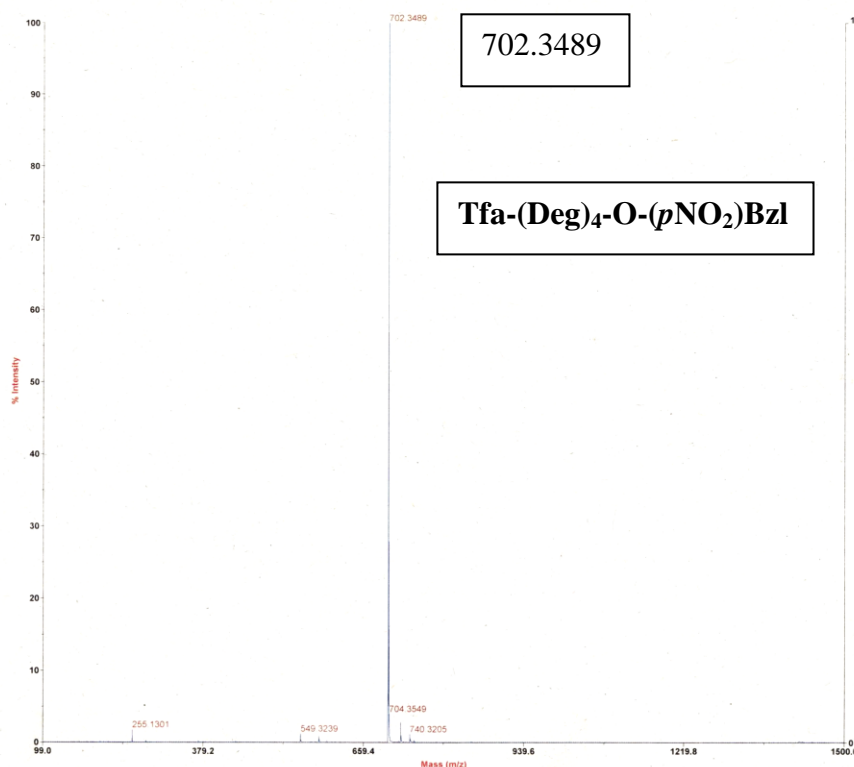
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Auxiliary Gas        ON
Curtain Gas          ON
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Calibration Constant B 74.415621
TDC Deadtime         10
--> Source Settings <--
Spray Tip Potential   4308.40
SCIEX Heater         0.00
--> API Interface Settings <--
Nozzle Potential     90.09
Skimmer 1 Potential  11.01
Quadrupole DC Potential 4.00
Deflection Voltage   -0.10
Einzel Lens Potential -22.00
Quadrupole RF Voltage 999.76
Quadrupole Temperature 140.01
Nozzle Temperature   140.01
--> Analyzer Settings <--
Push Pulse Potential 485.01
Pull Pulse Potential 144.87
Pull Bias Potential   8.00
Acceleration Potential 3999.94
Reflector Potential   1549.99
Detector Voltage      1949.98
--> Spectrum Acquisition Settings <--
Seconds Per Spectrum 6.00
Ion Count Threshold   0.00
First Mass            100.00
Last Mass             4000.00
Accumulate Spectra   OFF
Standby at End of Acquisition OFF
--> Centroid Spectra Settings <--
Centroid Spectra     OFF
--> System Settings <--
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Syringe Pump Mode    Disabled
Min Analyzer Mass     50.00
Max Analyzer Mass     4000.00
    
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Applied Biosystems Mariner System 5220

Mariner Spec /6.8 (T /0.52:0.73) ASC[BP = 702.4, 19220]



702.3489

Tfa-(Deg)<sub>4</sub>-O-(pNO<sub>2</sub>)Bzl

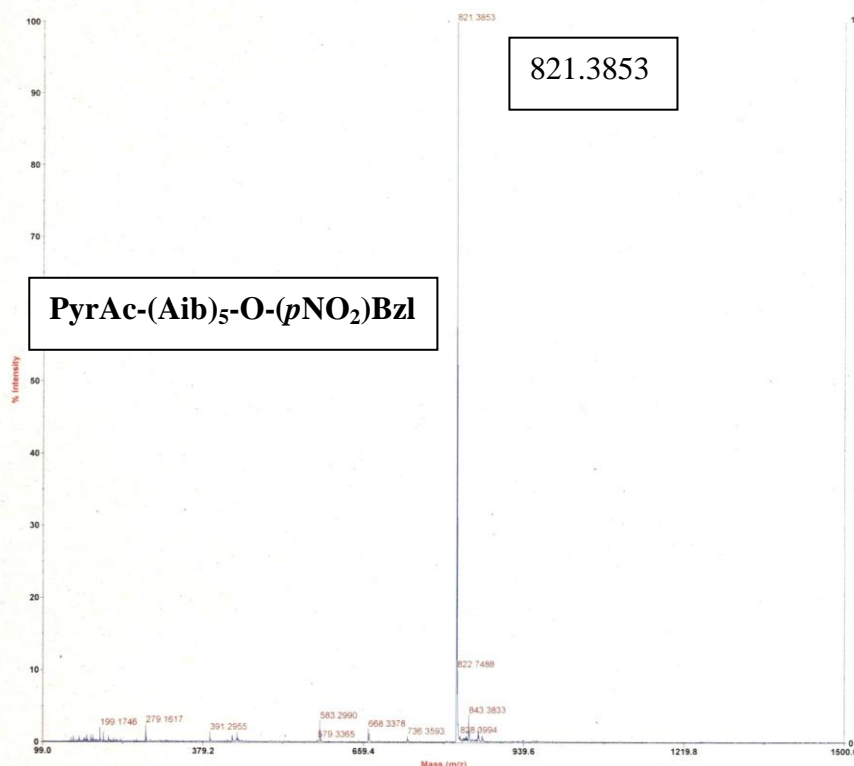
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TDC Deadtime	10
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Skimmer 1 Potential	11.01
Quadrupole DC Potential	4.00
Deflection Voltage	-0.10
Einzel Lens Potential	-22.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
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Pull Pulse Potential	144.87
Pull Bias Potential	8.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1949.98
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Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
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Syringe Pump Mode	Disabled
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Max Analyzer Mass	4000.00

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Applied Biosystems Mariner System 5220

Mariner Spec /6.7 (T /0.52:0.63) ASC[BP = 821.4, 1551]



821.3853

PyrAc-(Aib)<sub>5</sub>-O-(pNO<sub>2</sub>)Bzl

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Nebulizer Gas	ON
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Skimmer 1 Potential	11.01
Quadrupole DC Potential	4.00
Deflection Voltage	-0.10
Einzel Lens Potential	-22.00
Quadrupole RF Voltage	999.76
Quadrupole Temperature	140.01
Nozzle Temperature	140.01
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Pull Pulse Potential	144.87
Pull Bias Potential	8.00
Acceleration Potential	3999.94
Reflector Potential	1549.99
Detector Voltage	1949.98
--> Spectrum Acquisition Settings <--	
Seconds Per Spectrum	6.00
Ion Count Threshold	0.00
First Mass	100.00
Last Mass	4000.00
Accumulate Spectra	OFF
Standby at End of Acquisition	OFF
--> Centroid Spectra Settings <--	
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--> System Settings <--	
Gas Control Mode	Manual
Syringe Pump Mode	Disabled
Min Analyzer Mass	50.00
Max Analyzer Mass	4000.00

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