

Supporting Information

A Simple Reaction for DNA Sensing and Chemical Delivery

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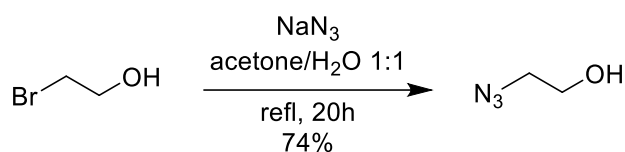
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1. General methods

Unless otherwise indicated, all reagents were obtained from commercial suppliers (Aldrich or TCI) and were used without further purification. Analytical thin layer chromatography was performed on Kieselgel F-254 pre-coated aluminum sheets TLC plates from Merck. Visualization was performed with a 254 nm UV lamp and/or a KMnO₄ solution. Flash column chromatography (FC) was carried out using Brunschwig silica gel (60 Å, 32-63 mesh). ¹H NMR and ¹³C RMN spectra were recorded on a Bruker Avance III 300 MHz spectrometer in CD₃CN obtained from Cambridge Isotope Laboratory. Chemical shifts are expressed in parts per million (δ) using residual solvent protons as internal standards. Coupling constant (*J*) are reported in Hz. Splitting patterns are designated as s (singlet), d (doublet), dd (double doublet), t (triplet), dt (double triplet), q (quartet), br. s. (broad singlet), m (multiplet). A Perkin Elmer Lambda 40 UV/VIS spectrometer was employed for the optical spectra. Mass spectra at high resolution were recorded on a Bruker 4.7T BioApex II mass spectrometer. A Bruker Tensor 27 spectrometer equipped with a golden gate was used to record IR spectra. MALDI-TOF analyses were performed on a Bruker Ultraflex extreme mass spectrometer. Method details: matrix: 3-HPA sat. with DAC 10 mg/ml in MeCN/ddH₂O 1:1. Sample: 50 pmol/μl of DNA solution in ddH₂O. 0.5 μl of matrix and 0.5 μl of sample solution are mixed together and then poured on the target. The mixture is let to dry for 15 min, then analyzed in linear positive or reflective mode. All the oligonucleotides were synthesized by Microsynth AG Balgach.

3. Synthesis of the 2-azidoacyl 4-(*N*-Boc-2-aminoethyl)-imidazole

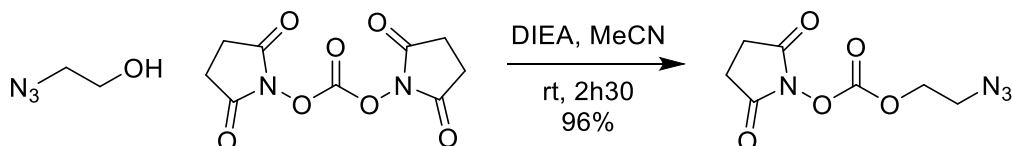


Scheme S-1: Preparation of 2-azidoethan-1-ol.

Sodium azide (154 mmol, 10 g) was added to a solution of 2-bromoethanol (70.5 mmol, 5 ml) in 15 ml of a 1:1 mixture of acetone and water. The mixture was heated at reflux for 20h (GC-MS control), then it was extracted 5x with DCM. The collected organic layers were dried over Na_2SO_4 and concentrated under vacuum to afford 4.532 g (52 mmol, 73.8% yield) of a colorless oil.¹²

^1H NMR (400 MHz, CD_3CN) δ 3.66 (q, J = 5.4 Hz, 2 H), 3.29 (t, J = 5.0 Hz, 2 H), 3.01 (t, J = 5.6 Hz, 1 H).

FT-IR (golden gate, 600-4000 cm^{-1}) 2093, 1288, 1064.



Scheme S-2: Preparation of 2-azidoethyl (2,5-dioxopyrrolidin-1-yl) carbonate.

A solution of 2-azidoethanol (4.59 mmol, 400 mg), bis(2,5-dioxopyrrolidin-1-yl) carbonate (5.97 mmol, 1.530 g) and dry DIEA (9.19 mmol, 1.604 mL) in 25 ml of dry MeCN was stirred at rt for 2h30. The acetonitrile was evaporated, then EtOAc was added and the solution was washed with sat. NaHCO_3 . The organic layer was dried over Na_2SO_4 , concentrated under vacuum and purified by FC ($\text{MeOH}/\text{CHCl}_3$ 0% --> 5%) to afford the final product (970 mg, 4.08 mmol, 96% yield) as a colorless oil.²

¹ Chen, S.; Zhao, X.; Chen, J.; Chen, J.; Kuznetsova, L.; Wong, S. S.; Ojima, I. Mechanism-Based Tumor-Targeting Drug Delivery System. Validation of Efficient Vitamin Receptor-Mediated Endocytosis and Drug Release. *Bioconjugate Chem.* **2010**, *21*, 979-987.

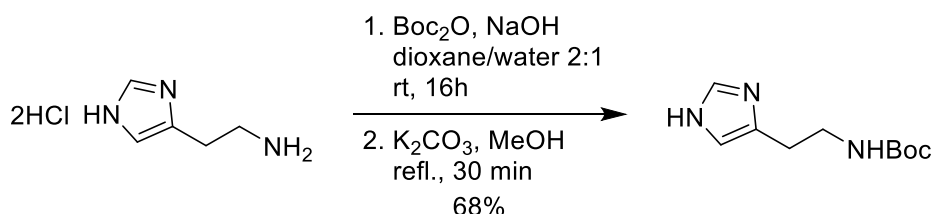
² Fujishima, S.-h.; Yasui, R.; Miki, T.; Ojida, A.; Hamachi, I. Ligand-Directed Acyl Imidazole Chemistry for Labeling of Membrane-Bound Proteins on Live Cells. *J. Am. Chem. Soc.* **2012**, *134*, 3961-3964.

¹H NMR (400MHz, CD₃CN) δ 4.45 (t, *J* = 4.9 Hz, 2 H), 3.63 (t, *J* = 4.9 Hz, 2 H), 2.77 (s, 4 H).

¹³C NMR (101MHz, CD₃CN) δ 170.7, 152.6, 70.7, 50.3, 26.4.

FT-IR (golden gate, 600-4000 cm⁻¹) 2110, 1789, 1737, 1205.

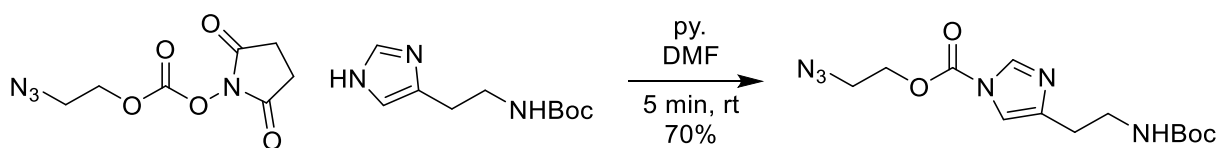
HR-MS (ESI) for (M+Na⁺): calcd 251.03869, found 251.03869.



Scheme S-3: Preparation of tert-butyl (2-(1H-imidazol-4-yl)ethyl)carbamate.

A mixture of 2-(1H-imidazol-5-yl)ethan-1-amine dihydrochloride (0.272 mmol, 50 mg) in 0.9 ml of dioxane/water 2:1 was basified with NaOH 4 N at pH 12. Di-tert-butyl dicarbonate (0.679 mmol, 0.148 g) was added and the mixture was stirred at rt for 16 hours, then diluted with water and extracted with DCM. The collected organic layers were dried over Na₂SO₄, filtered and concentrated under vacuum. The product was dissolved in 2 ml of MeOH. 20 mg of K₂CO₃ were added and the mixture was heated at reflux for 30 min, then diluted with water and extracted with EtOAc. The collected organic layers were dried over Na₂SO₄, filtered and concentrated under vacuum to afford 39 mg of a yellowish oil (0.272 mmol, 68% yield).³

¹H NMR (400MHz, CD₃OD) δ 7.57 (s, 1 H), 6.82 (s, 1 H), 3.28 (t, *J* = 7.1 Hz, 2 H), 2.73 (t, *J* = 7.2 Hz, 2 H), 1.42 (s, 9 H).



Scheme S-4: Preparation of 2-azidoethyl 4-(2-(((tert-butoxycarbonyl)amino)ethyl)-1H-imidazole-1-carboxylate.

³ Dubey, R. K.; Kumar, N.; Jain, R. Facile Syntheses of Histamine- and Imidazole-4-propionic Acid-Derived Room-Temperature Ionic Liquids. *Synth. Commun.* **2012**, 42, 2207.

A mixture of 2-azidoethyl (2,5-dioxopyrrolidin-1-yl) carbonate (0.408 mmol, 93 mg), tert-butyl (2-(1H-imidazol-4-yl)ethyl)carbamate (0.408 mmol, 0.086 g) and dry pyridine (1.223 mmol, 0.099 mL) in 5 mL of dry DMF was stirred at rt for 5 min, then diluted with water and extracted with DCM. The collected organic layers were dried over Na₂SO₄, filtered and concentrated under vacuum. FC (EtOAc/pentane 50% → 100%) gave 92 mg (0.408 mmol, 70% yield) of a white solid.²

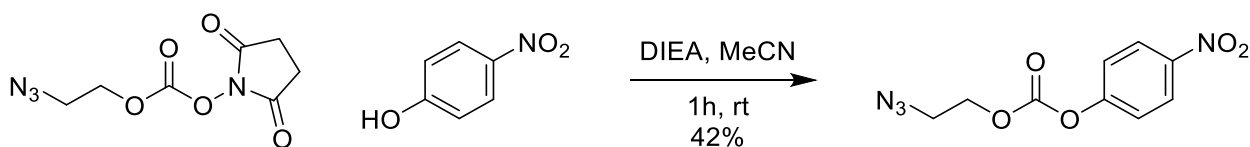
¹H NMR (400 MHz, CD₃CN) δ 8.05 (s, 1 H), 7.24 (s, 1 H), 5.49 (br. s., 1 H), 4.50 (t, *J* = 4.9 Hz, 2 H), 3.64 (t, *J* = 4.9 Hz, 2 H), 3.28 (q, *J* = 6.6 Hz, 2 H), 2.65 (t, *J* = 6.7 Hz, 2 H), 1.39 (s, 9 H).

¹³C NMR (75 MHz, CD₃CN) δ 156.8, 149.5, 142.8, 138.0, 114.7, 79.2, 67.5, 50.4, 40.5, 29.2, 28.7.

FT-IR (golden gate, 600–4000 cm⁻¹) 3307, 3129, 2982, 2937, 2142, 2110, 1750, 1703, 1529, 1491, 1456, 1409, 1367, 1263, 1225, 1161, 978, 856, 766, 754, 641.

HR-MS (ESI) for (M+H⁺): calcd 347.14382, found 347.14305.

4. Synthesis of the 2-azidoethyl 4-nitrophenyl carbonate



Scheme S-5: Preparation of 2-azidoethyl (4-nitrophenyl) carbonate.

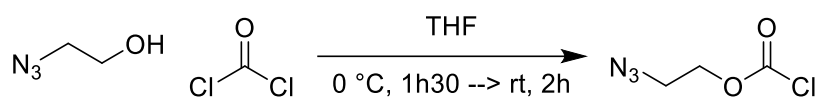
A solution of 4-nitrophenol (0.263 mmol, 0.037 g), 2-azidoethyl (2,5-dioxopyrrolidin-1-yl) carbonate (0.219 mmol, 50 mg) and dry DIEA (0.329 mmol, 0.057 mL) in 1 mL of dry MeCN was stirred at rt for 1h, then it was diluted with sat. NaHCO₃ and extracted with DCM. The collected organic layers were dried over Na₂SO₄ and concentrated under vacuum. FC (EtOAc/pentane 20% → 100%) gave 23 mg of a colorless oil (0.22 mmol, 41.6% yield).

¹H NMR (300 MHz, CD₃CN) δ 8.30 - 8.30 (m, 1 H), 8.28 (d, *J* = 9.3 Hz, 2 H), 7.45 (d, *J* = 9.3 Hz, 2 H), 4.39 (t, *J* = 5.0 Hz, 2 H), 3.63 (t, *J* = 5.0 Hz, 2 H).

¹³C NMR (75 MHz, CD₃CN) δ 156.6, 153.3, 146.8, 126.4, 123.3, 68.6, 50.4.

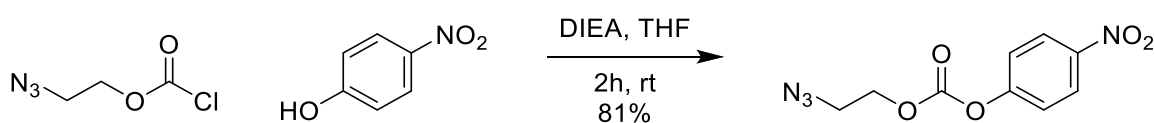
FT-IR (golden gate, 600–4000 cm⁻¹) 2103, 1764, 1522, 1347, 1164, 859.

HR-MS (ESI) for (M+Na⁺): calcd 275.03869, found 275.03948.



Scheme S-6: Preparation of 2-azidoethyl chloroformate.

To a solution of phosgene (5.74 mmol, 4.1 ml, 15 wt. % in toluene) in 10 ml of dry THF at 0 °C was added dropwise the 2-azidoethanol (5.74 mmol , 500 mg). The mixture was stirred at 0°C for 1h30 and at rt for 2h, then bubbled with argon for 1h and used with no further treatment.



Scheme S-7: Preparation of 2-azidoethyl (4-nitrophenyl) carbonate.

To a solution of 4-nitrophenol (0.36 mmol, 50 mg,) in 1.5 ml of dry THF at -15 °C were added dry DIEA (0.40 mmol, 51 mg, 69 μ l) and 0.8 ml of a 0.5 M solution of 2-azidoethyl chloroformate (0.40 mmol, 59 mg, 0.8 ml) in dry THF. The reaction was stirred at -15 °C for 20 min, then it was let warm up to rt and it was stirred for 2h. The mixture was then diluted with HCl 0.1N and extracted with EtOAc. The collected organic layers were dried over Na₂SO₄, filtered and concentrated under vacuum to give 73 mg of a colorless oil (0.29 mmol, 81% yield).

5. 2-strand system

Probes design

Hexynyl-5'-ODN

5-hexynyl-5'- AAT GAT AAA GTG TGG CGC ATG C -3' 22 mer

MALDI-TOF calcd 6981, found 7002.

Probe 2a

5'- GCA TGC GCC ACA CTT TAT CAT T -3'-hexylamine 22 mer

MALDI-TOF calcd 6822, found 6841.

Control Probe

3'- AAT GAT AAA GTG TGG CGC ATG C -5'-hexylamine 22 mer

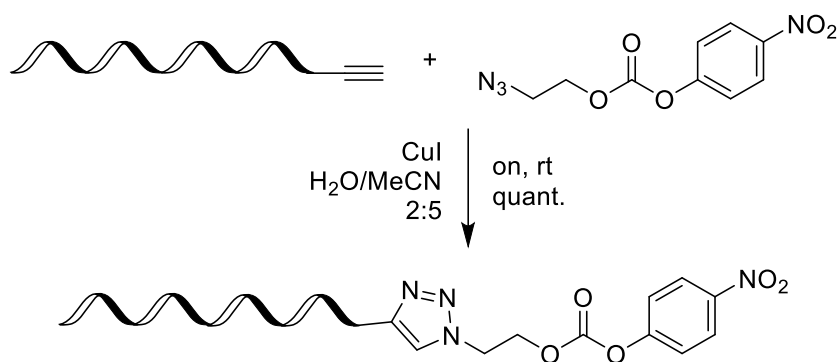
MALDI-TOF calcd 7000, found 7022.

PTO-3'ODN

5'- GCA TGC GCC ACA CTT TAT CAT T -3'-phosphorothioate 22 mer

MALDI-TOF calcd 6740, found 6750.

Synthesis of Probe 1a



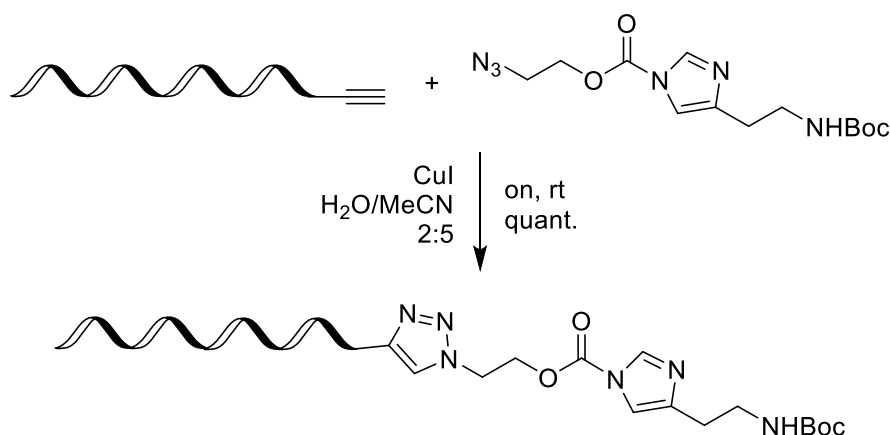
Scheme S-8: Preparation of Probe 1a.

A mixture of 22mer-5'-hexynyl (10 nmol, 1 mM in H₂O, 10 μ l), 2-azidoethyl 4-nitrophenyl carbonate (500 nmol, 100 mM in MeCN, 5 μ l) and CuI (100 nmol, 10 mM in MeCN, 10 μ l) (final volume 25 μ l, final concentration 400 μ M) was let at rt for 16h. The reaction mixture was diluted with 200 μ l of MeCN, let at -20 $^{\circ}$ C for 20 min and then centrifuged at 12'100 G

for 15 min. The supernatant was removed. The residue was diluted with 200 μ l of MeCN, let at -20 $^{\circ}$ C for 20 min and centrifuged at 12'100 G for 15 min. The procedure was repeated three more times. The residue was dried under vacuum and then redissolved in 50 μ l of MeCN/ddH₂O 1:1. The OD260 showed a quantitative ON recovery and the MALDI-TOF spectrum a full conversion.

MALDI-TOF calcd 7233, found 7243.

Synthesis of acyl imidazole probe



Scheme S-9: Preparation of the acyl imidazole probe.

A mixture of 22mer-5'-hexynyl (10 nmol, 1 mM in H₂O, 10 μ l), 2-azidoacetyl 4-(*N*-Boc-2-aminoethyl)-imidazole (500 nmol, 100 mM in MeCN, 5 μ l) and CuI (100 nmol, 10 mM in MeCN, 10 μ l) (final volume 25 μ l, final concentration 400 μ M) was let at rt for 16h. The reaction mixture was diluted with 200 μ l of MeCN, let at -20 $^{\circ}$ C for 20 min and then centrifuged at 12'100 G for 15 min. The supernatant was removed. The residue was diluted with 200 μ l of MeCN, let at -20 $^{\circ}$ C for 20 min and centrifuged at 12'100 G for 15 min. The procedure was repeated three more times. The residue was dried under vacuum and then redissolved in 50 μ l of MeCN/ddH₂O 1:1. The OD260 showed a quantitative ON recovery and the MALDI-TOF spectrum a full conversion.

MALDI-TOF calcd 7328, found 7324.

Reaction with Probe 2a

10 μ M mixtures of Probe 1 and Probe 2 and of acyl imidazole probe and Probe 2 in PBS buffer (150 mM NaCl, 4 mM phosphate, 10 mM MgCl₂) at pH 7.4 were let react at room temperature for a given time, then analyzed by PAGE. A quick hybridization was confirmed by the decrease of ~30% of the absorbance at 260 nm.

PAGE: The mixture of ODNs (100 pmol) was mixed with 2 μ l of denaturing tracking dye buffer (90% formamide, 10 mM NaOH, 1 mM EDTA and trace amounts of bromophenol blue and xylene cyanol FF). Gel: 20% denaturing, 10x10.5 cm, 0.75 mm width, 10 wells, 8.3 M urea. Running buffer: 89 mM Tris, 89 mM boric acid and 2 mM EDTA. Run: Hoefer SE 260 electrophoresis unit at room temperature (no cooling, 200 V, constant voltage) for 3h.

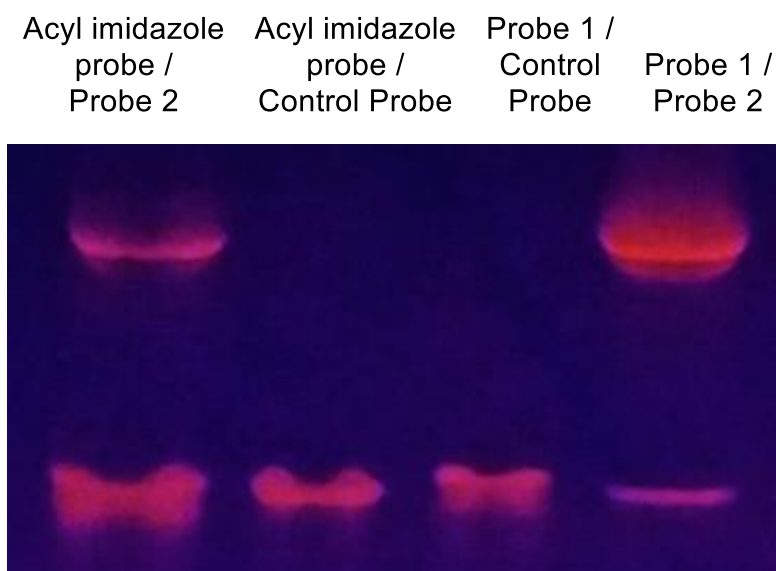


Figure S-1: Determination of the best electrophile.

10 μ M mixtures of Probe 1 and Probe 2 in PBS buffer (150 mM NaCl, 4 mM phosphate, 10 mM MgCl₂) at pH 7.4, 8.0, 8.5 and 9.0 were let react at room temperature for a given time, then analyzed by PAGE and UV/Vis. A quick hybridization was confirmed by the decrease of ~30% of the absorbance at 260 nm.

PAGE: The mixture of ODNs (100 pmol) was mixed with 2 μ l of denaturing tracking dye buffer (90% formamide, 10 mM NaOH, 1 mM EDTA and trace amounts of bromophenol blue and xylene cyanol FF). Gel: 20% denaturing, 10x10.5 cm, 0.75 mm width, 10 wells, 8.3 M urea. Running buffer: 89 mM Tris, 89 mM boric acid and 2 mM EDTA. Run: Hoefer SE 260 electrophoresis unit at room temperature (no cooling, 200 V, constant voltage) for 3h.

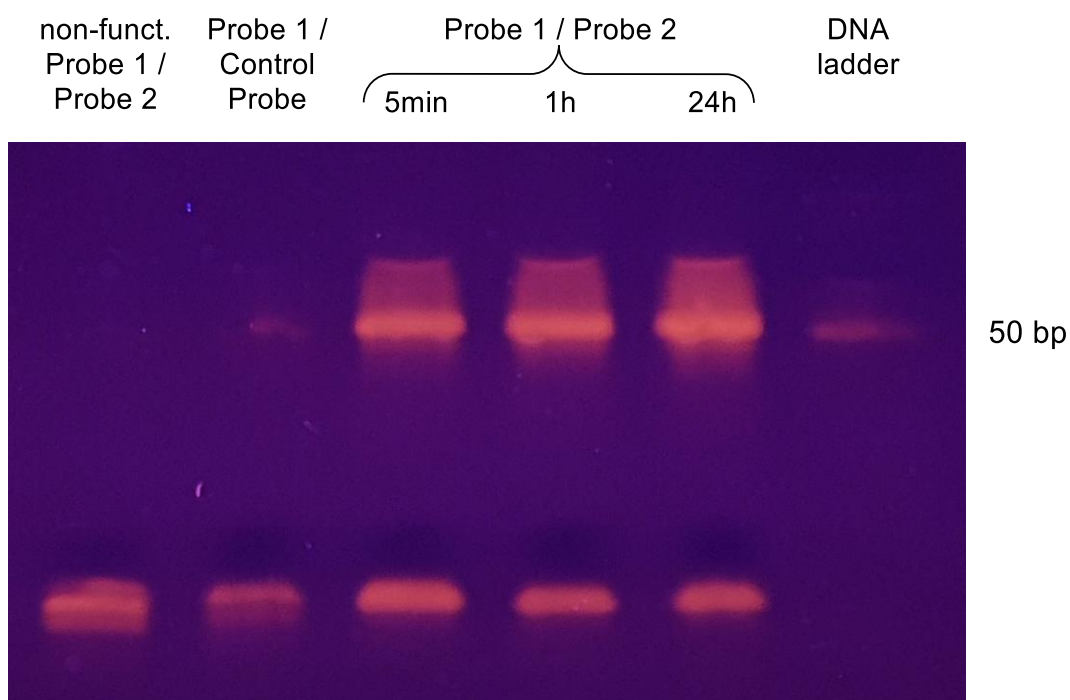


Figure S-2: Reactivity of the carbonate Probe 1.

The PAGE shows that there is reaction only with the matched probes. The lane corresponding to the ligated product was cut from the gel, the DNA was extracted by letting the gel piece in an elution buffer (500 mM ammonium acetate, 10 mM magnesium acetate, 2 mM EDTA) overnight and the salts were removed prior to the analysis using 3k Amicon spin filters.

MALDI-TOF calcd 13916, found 13929.

UV/Vis: The absorbance at 405 nm was monitored and the conversion plotted as a function of the time. The half-life time of the reaction and the first order kinetic constant were extrapolated. The reactivity of the non-templated system (control) comes from the general base-catalyzed hydrolysis of **Probe 1a**, however without precluding its use in a colorimetric sensing system.

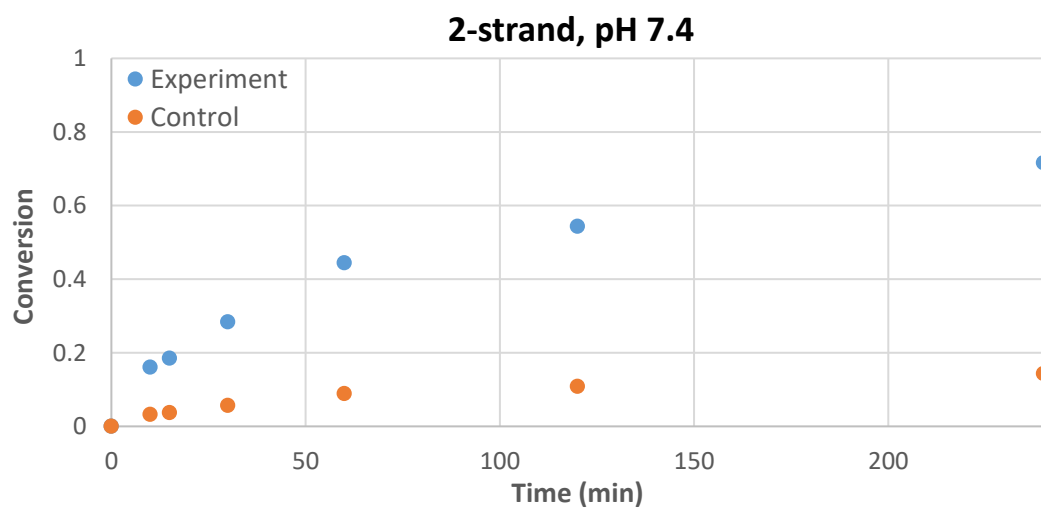


Chart S-1: Reactivity of Probe 1a at pH 7.4.

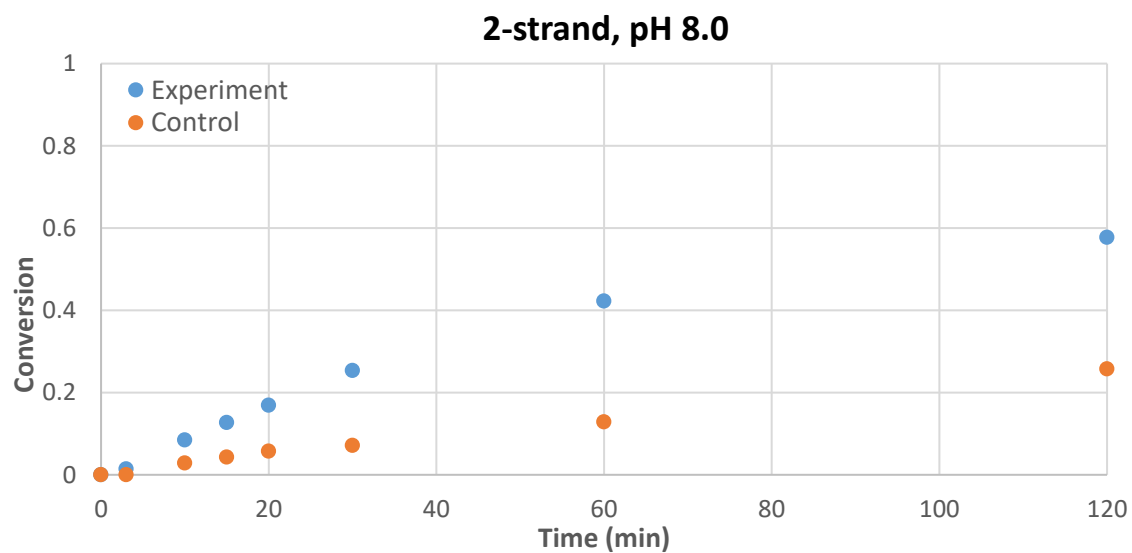


Chart S-2: Reactivity of Probe 1a at pH 8.0.

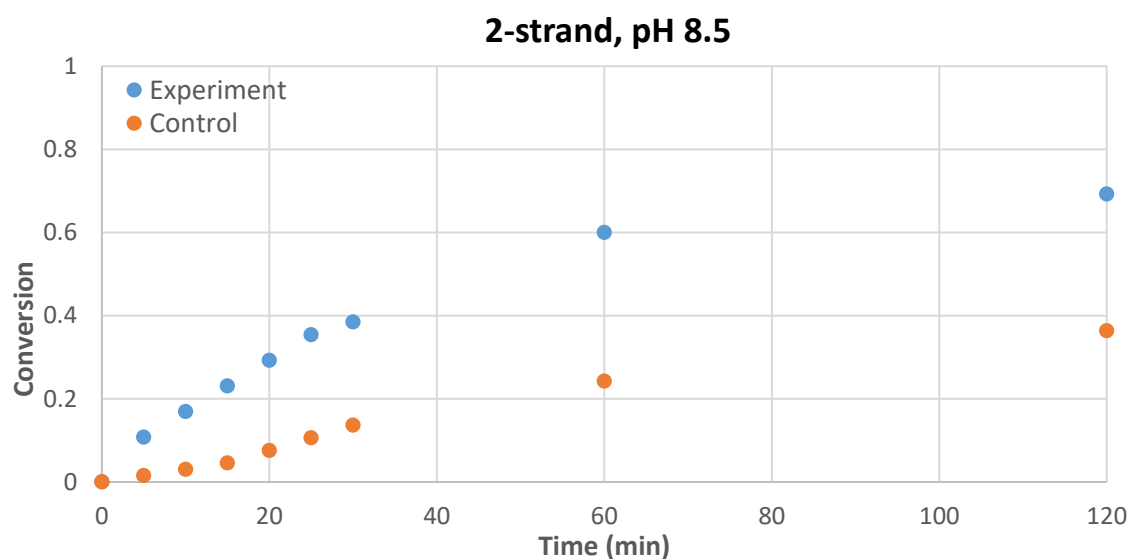


Chart S-3: Reactivity of Probe 1a at pH 8.5.

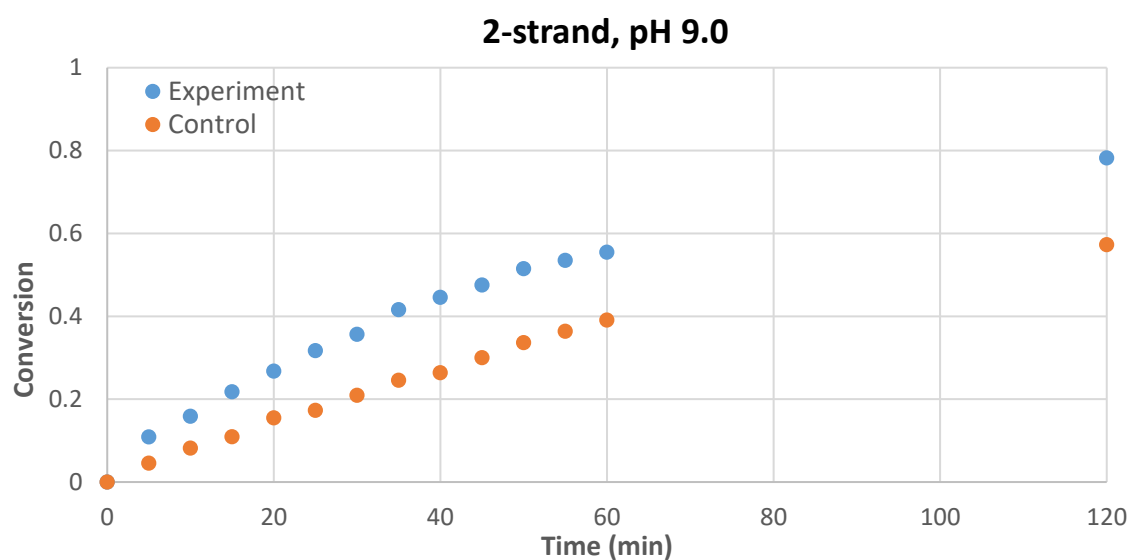


Chart S-4: Reactivity of Probe 1a at pH 9.0.

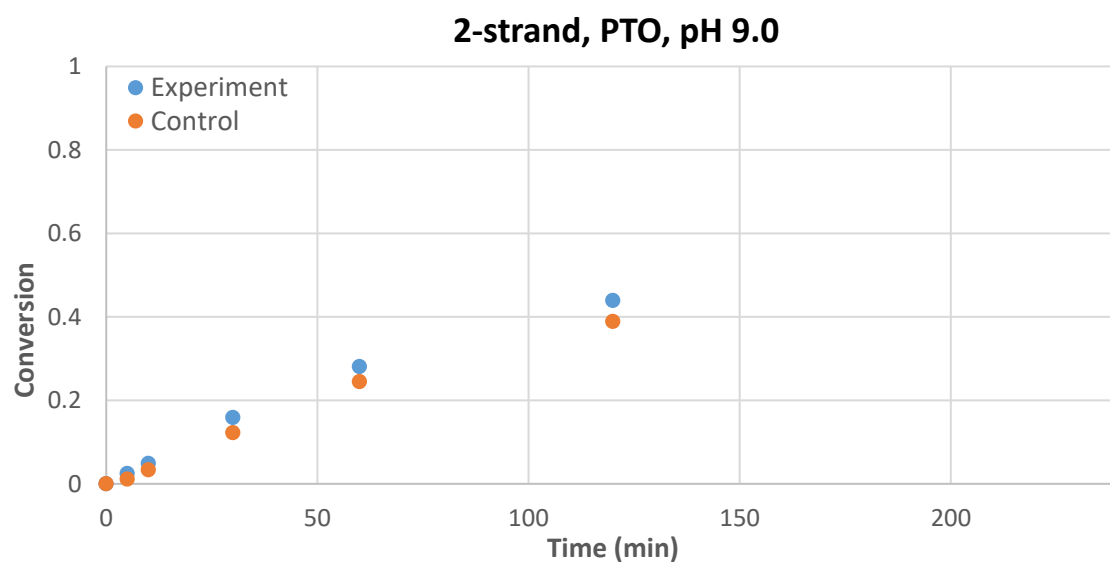


Chart S-5: Reactivity of Probe 1a with a PTO nucleophile at pH 9.0.

6. 3-strand system

Probes design

Hexynyl-5'-ODN

5-hexynyl-5'- AAT GTG CC -3' 8 mer

MALDI-TOF calcd 2569, found 2570.

Probe 2b

5'- GAG ATG AG -3'-hexylamine 8 mer

MALDI-TOF calcd 2677, found 2678.

Template 1

5'- GGC ACA TTC TCA TCT C -3' 16 mer

MALDI-TOF calcd 4791, found 4800.

Template 2

5'- GGC ACA TTA CTC ATC TC -3' 17 mer 1 additional nucleotide

MALDI-TOF calcd 5104, found 5115.

Template 3

5'- GGC ACA GTC TCA TCT C -3' 16 mer 1 mismatch

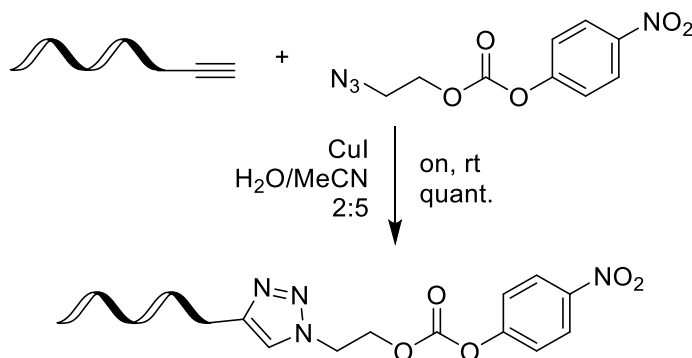
Template 4

5'- GGA ACA TTC TCA GCT C -3' 16 mer 2 mismatch

Template 5

5'- GGC ACA UUC UCA UCU C -3' 16 mer RNA

Synthesis of Probe 1b



Scheme S-10: Preparation of Probe 1b.

A mixture of 8mer-5'-hexynyl (10 nmol, 1 mM in H₂O, 10 μ l), 2-azidoethyl 4-nitrophenyl carbonate (500 nmol, 100 mM in MeCN, 5 μ l) and CuI (100 nmol, 10 mM in MeCN, 10 μ l) (final volume 25 μ l, final concentration 400 μ M) was let at rt for 16h. The reaction mixture was diluted with 200 μ l of MeCN, let at -20 $^{\circ}$ C for 20 min and then centrifuged at 12'100 G for 15 min. The supernatant was removed. The residue was diluted with 200 μ l of MeCN, let at -20 $^{\circ}$ C for 20 min and centrifuged at 12'100 G for 15 min. The procedure was repeated three more times. The residue was dried under vacuum and then redissolved in 50 μ l of MeCN/ddH₂O 1:1. The OD₂₆₀ showed a quantitative ON recovery and the MALDI-TOF spectrum a full conversion.

MALDI-TOF calcd 2821, found 2822.

Templated reactions

10 μ M mixtures of Probe 1, Probe 2 and Template in PBS buffer (150 mM NaCl, 4 mM phosphate, 10 mM MgCl₂) at pH 7.4, 8.0, 8.5 and 9.0 were let react at room temperature for a given time, then analyzed by UV/Vis. A quick hybridization was confirmed by the decrease of ~30% of the absorbance at 260 nm.

UV/Vis: The absorbance at 405 nm was monitored and the conversion plotted as a function of the time. The half-life time of the reaction and the first order kinetic constant were extrapolated.

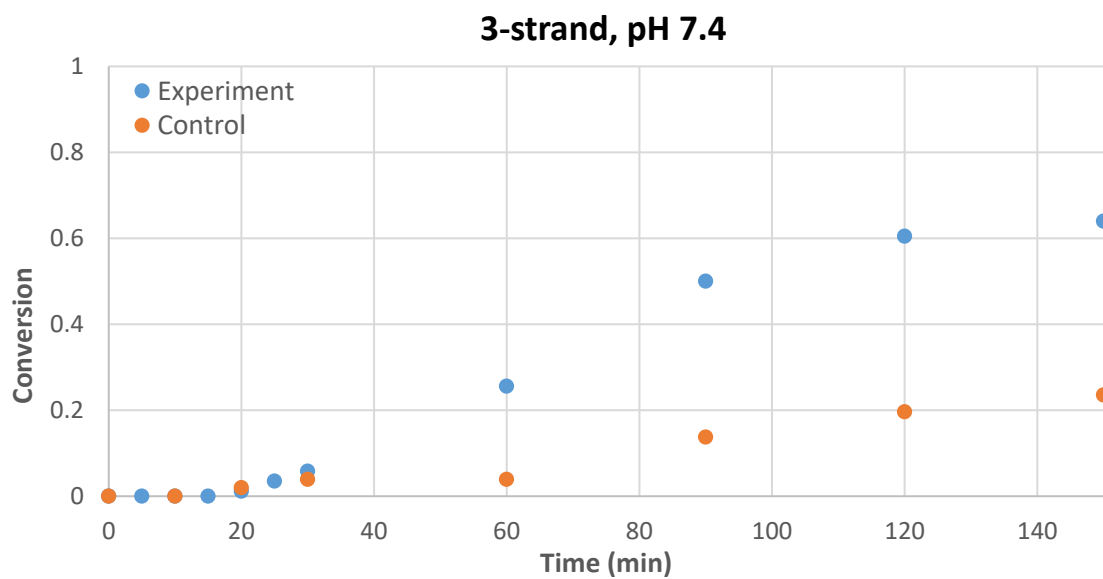


Chart S-6: Reactivity of Probe 1b, Probe 2b and Template 1 at pH 7.4.

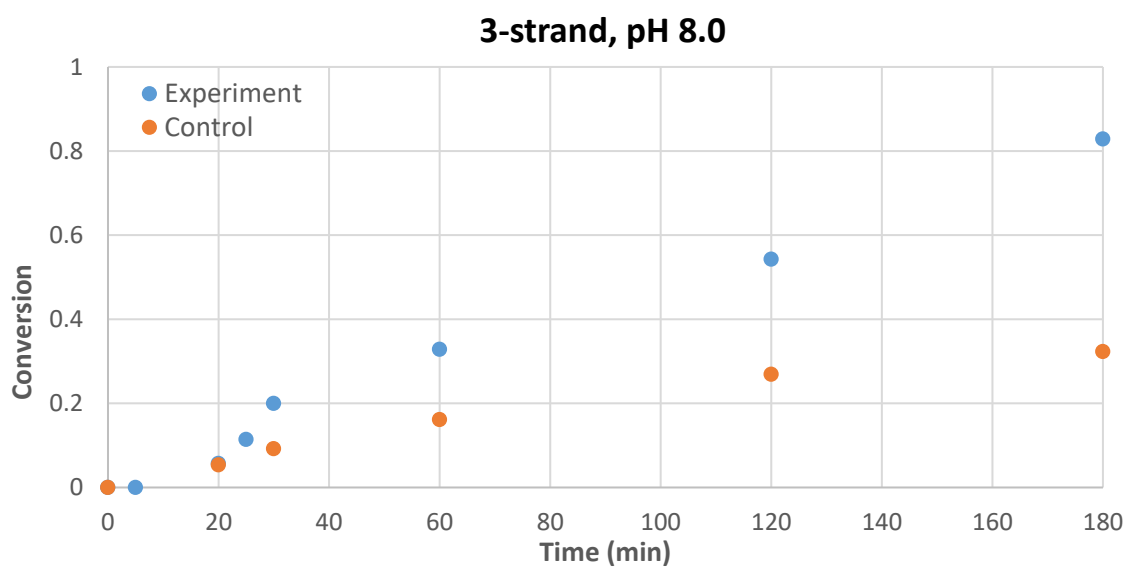


Chart S-7: Reactivity of Probe 1b, Probe 2b and Template 1 at pH 8.0.

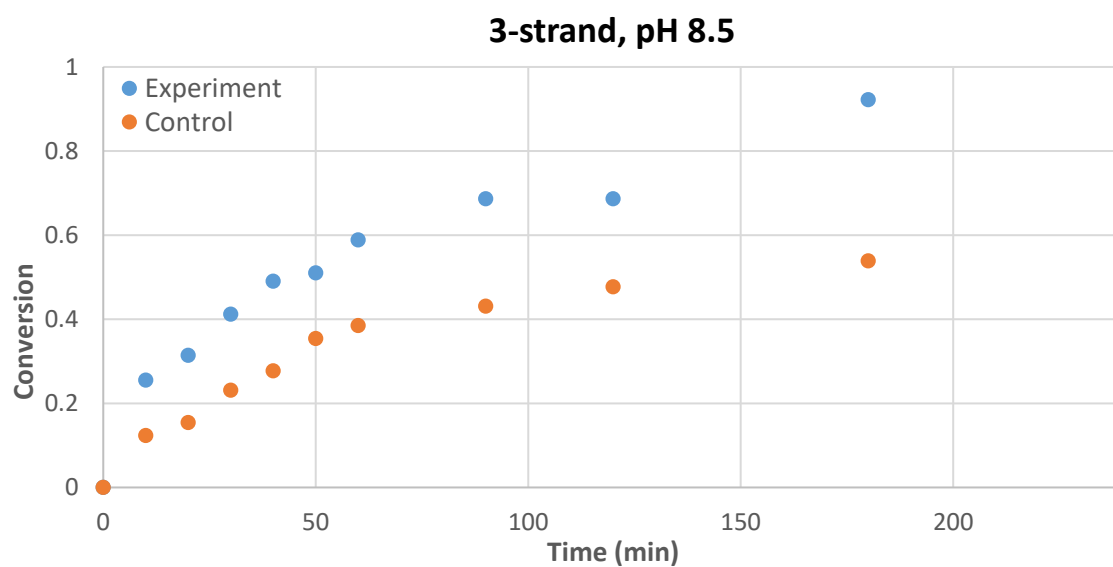


Chart S-8: Reactivity of Probe 1b, Probe 2b and Template 1 at pH 8.5.

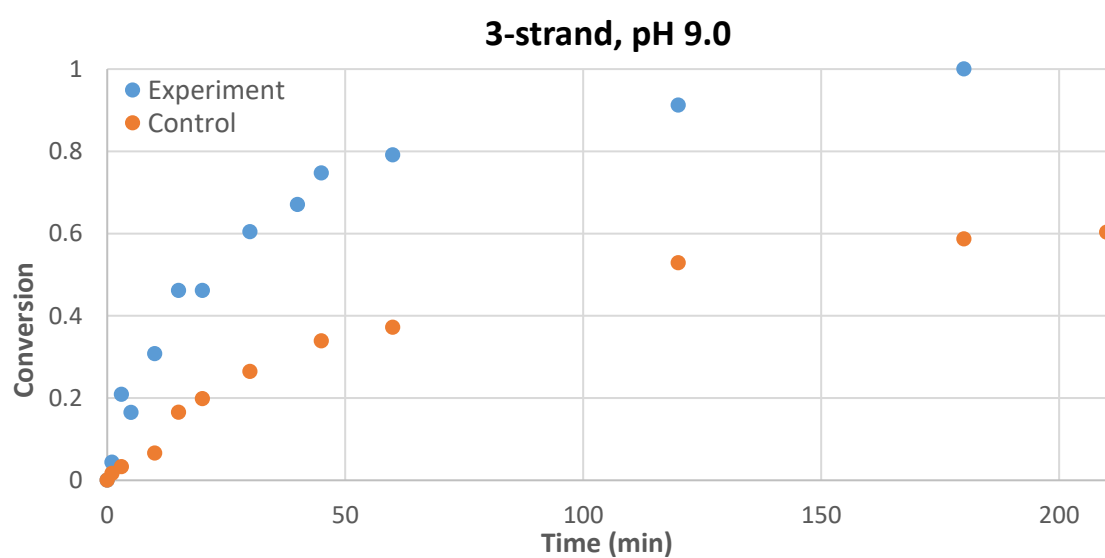


Chart S-9: Reactivity of Probe 1b, Probe 2b and Template 1 at pH 9.0.

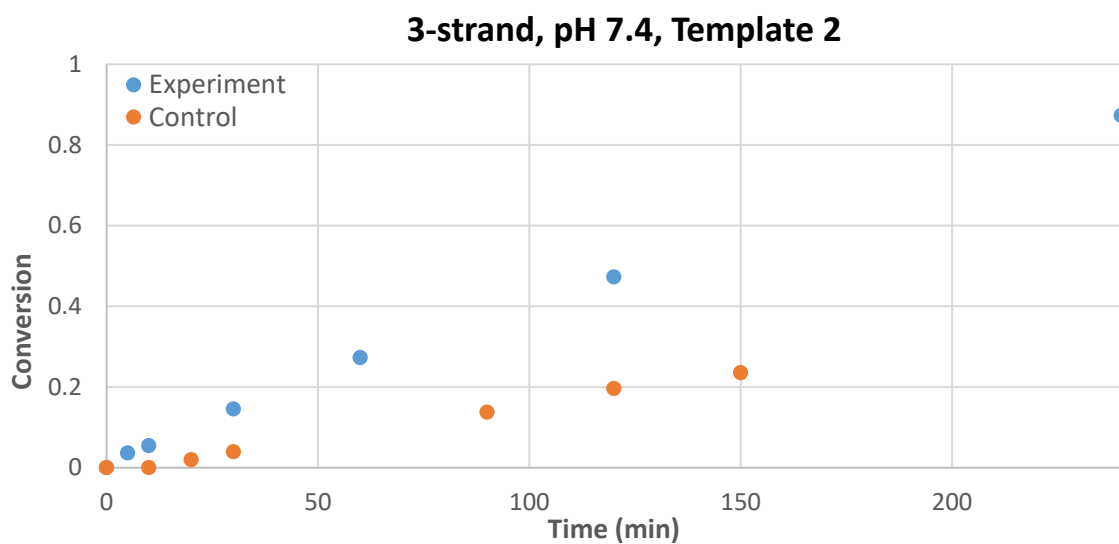


Chart S-10: Reactivity of Probe 1b, Probe 2b and Template 2 at pH 7.4.

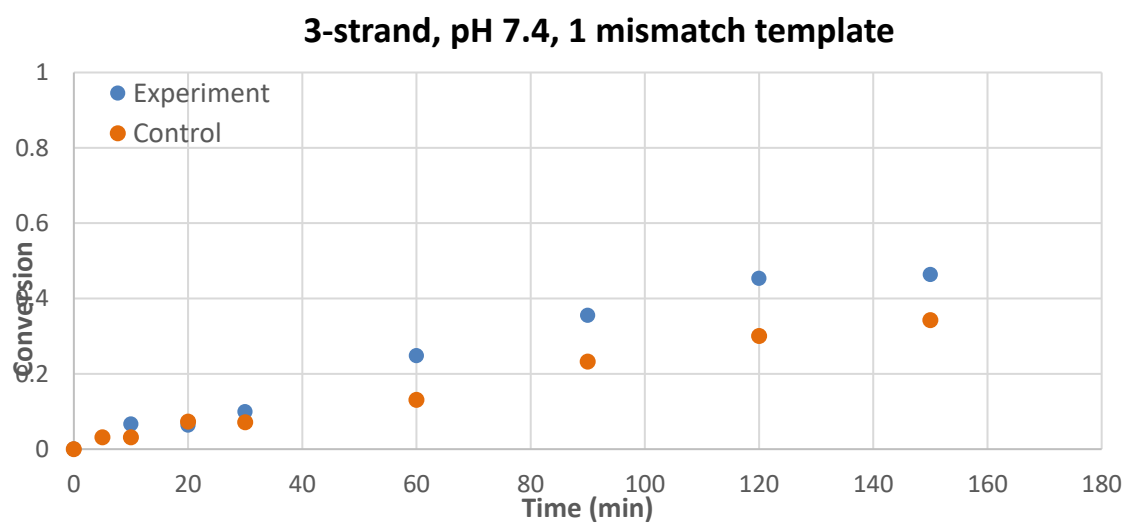


Chart S-11: Reactivity of Probe 1b, Probe 2b and Template 3 at pH 7.4.

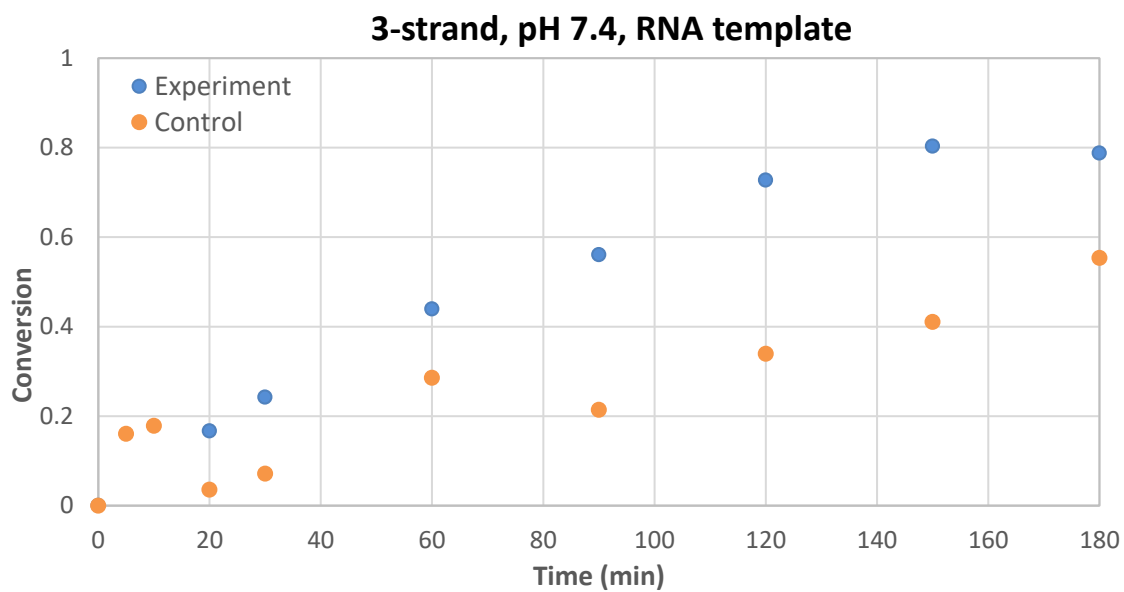


Chart S-12: Reactivity of Probe 1b, Probe 2b and Template 5 at pH 7.4.

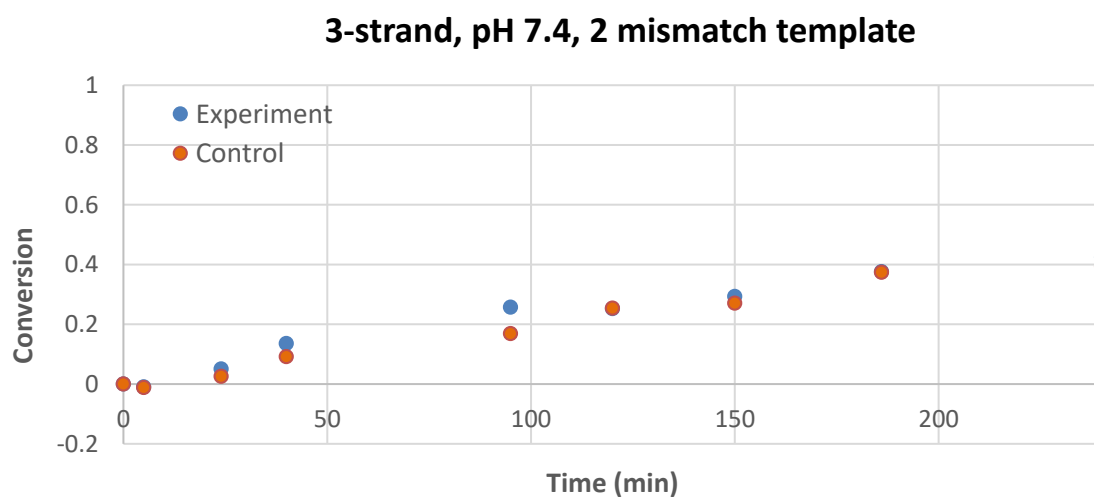


Chart S-13: Reactivity of Probe 1b, Probe 2b and Template 4 at pH 7.4.

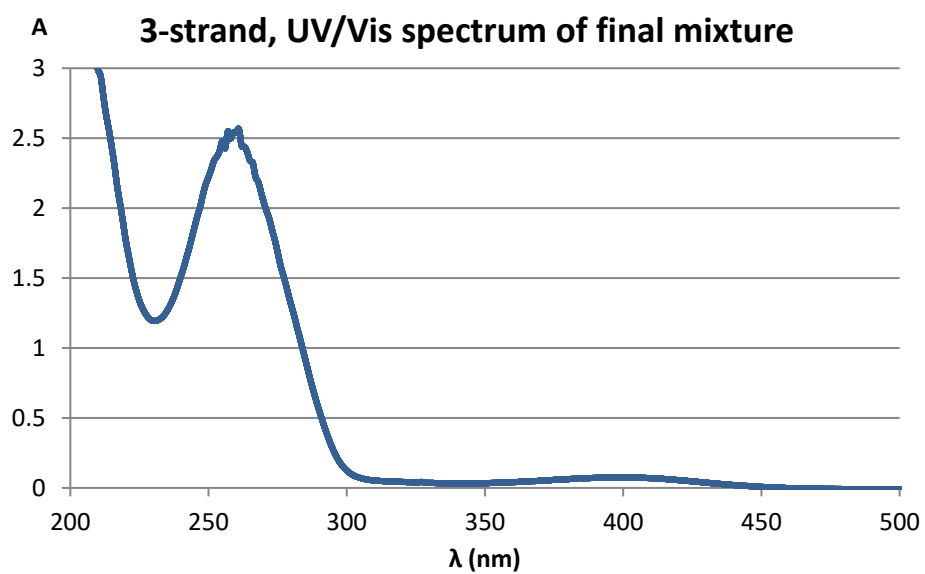


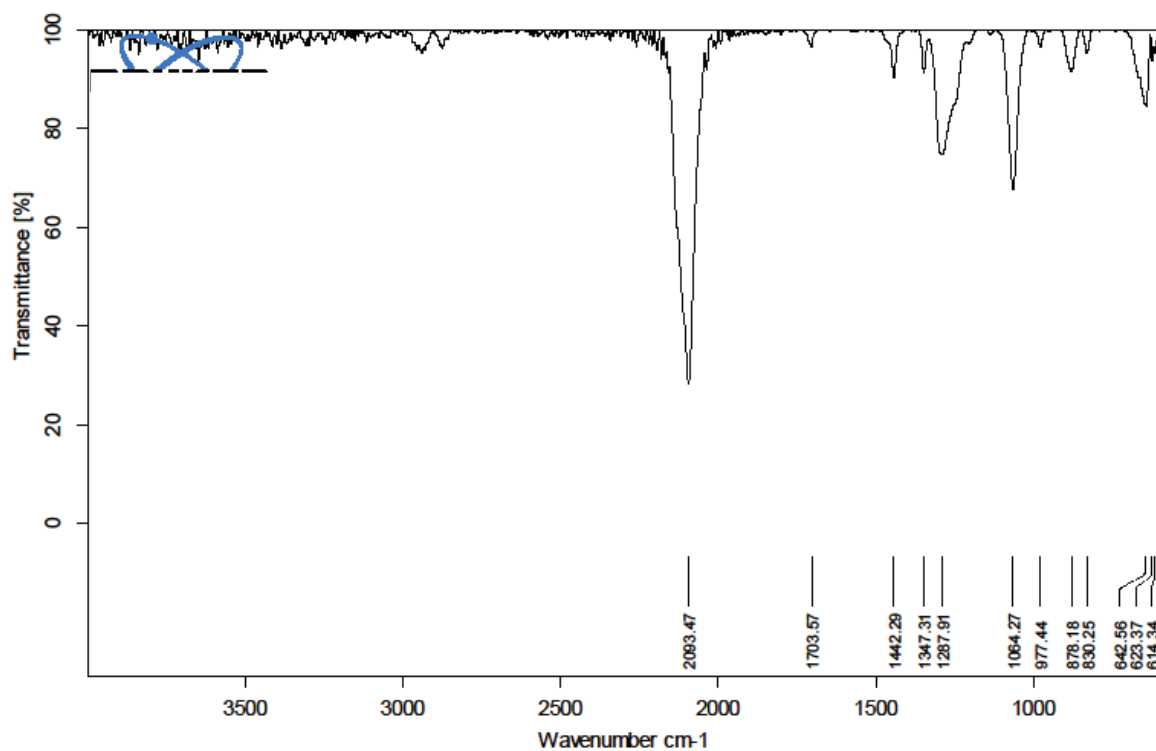
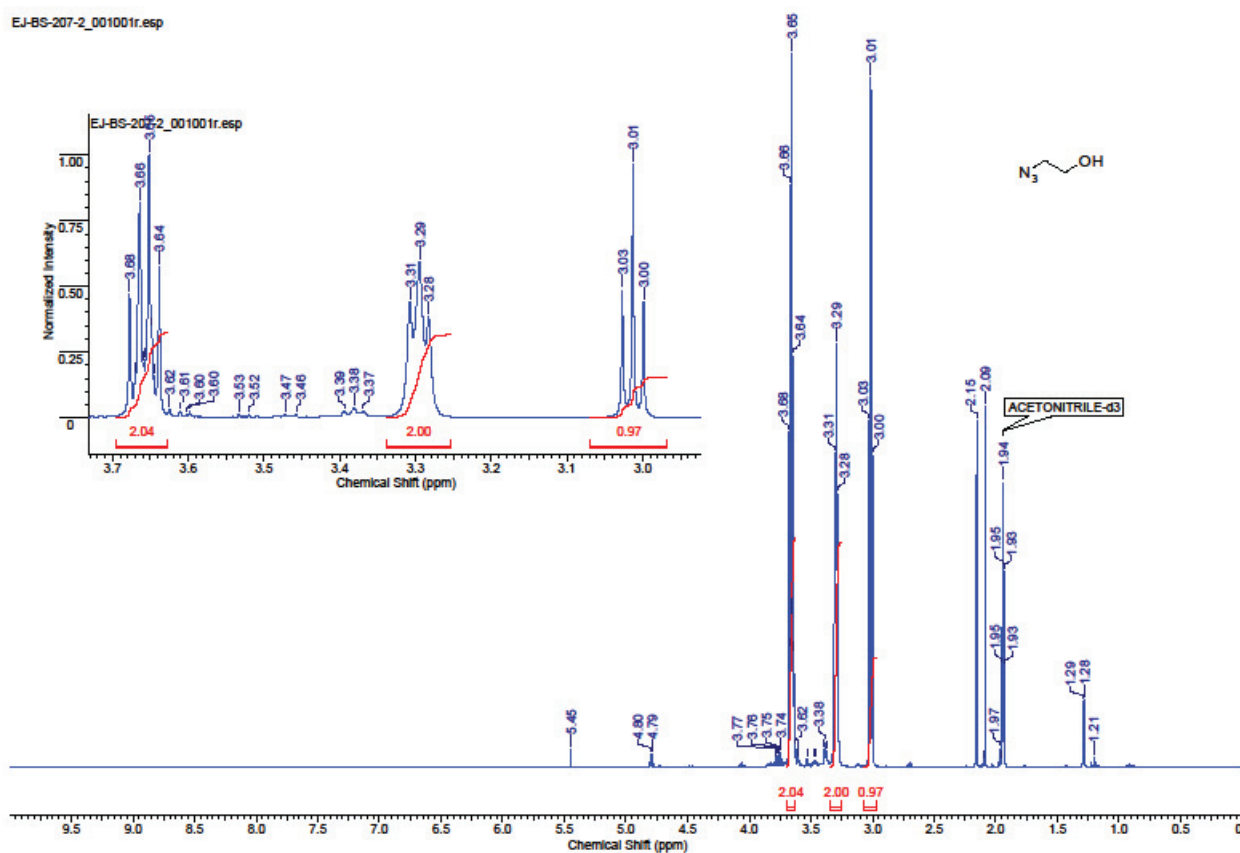
Chart S-14: UV/Vis spectrum of an equilibrated mixture of Probe 1b, Probe 2b and Template 1.

7. References

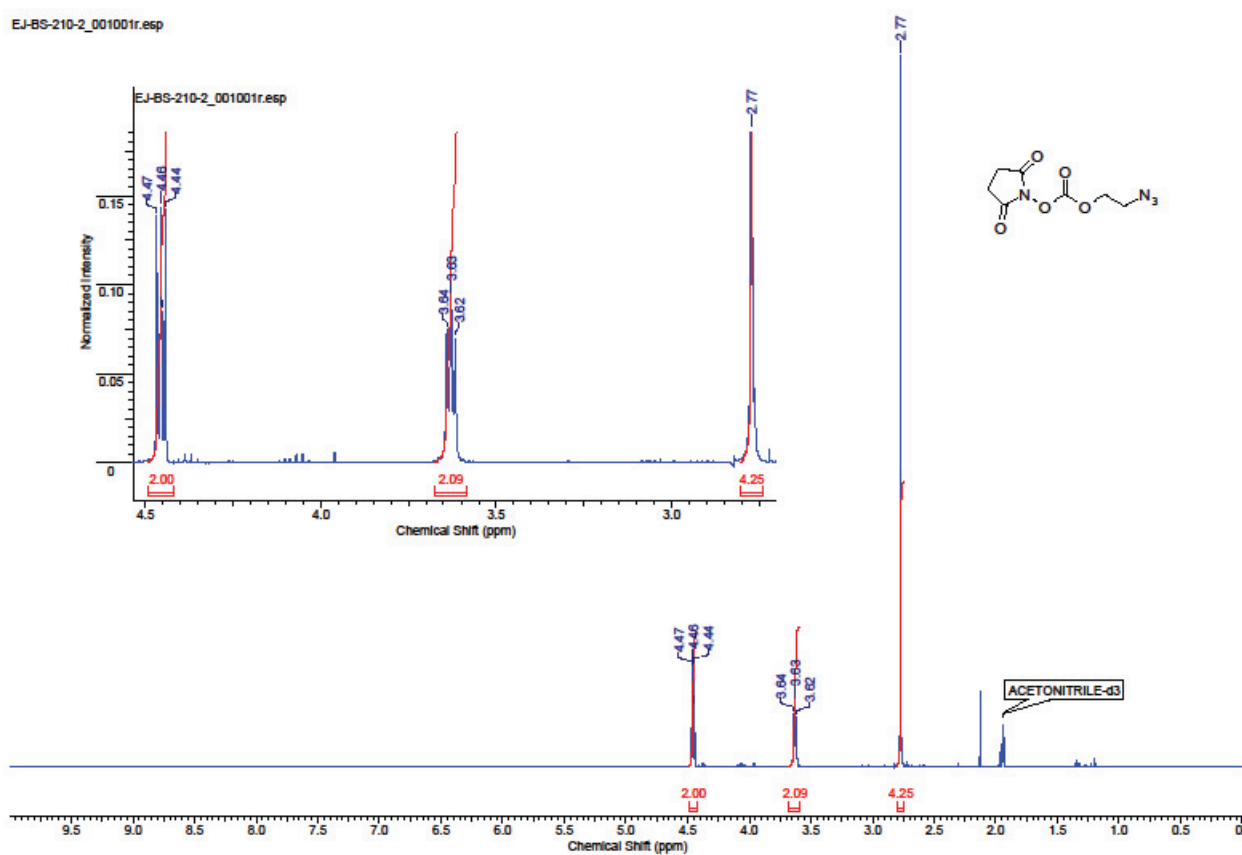
- [1] Chen, S.; Zhao, X.; Chen, J.; Chen, J.; Kuznetsova, L.; Wong, S. S.; Ojima, I. Mechanism-Based Tumor-Targeting Drug Delivery System. Validation of Efficient Vitamin Receptor-Mediated Endocytosis and Drug Release. *Bioconjugate Chem.* **2010**, *21*, 979-987.
- [2] Fujishima, S.-h.; Yasui, R.; Miki, T.; Ojida, A.; Hamachi, I. Ligand-Directed Acyl Imidazole Chemistry for Labeling of Membrane-Bound Proteins on Live Cells. *J. Am. Chem. Soc.* **2012**, *134*, 3961-3964.
- [3] Dubey, R. K.; Kumar, N.; Jain, R. Facile Syntheses of Histamine- and Imidazole-4-propionic Acid-Derived Room-Temperature Ionic Liquids. *Synth. Commun.* **2012**, *42*, 2207.

8. Spectra

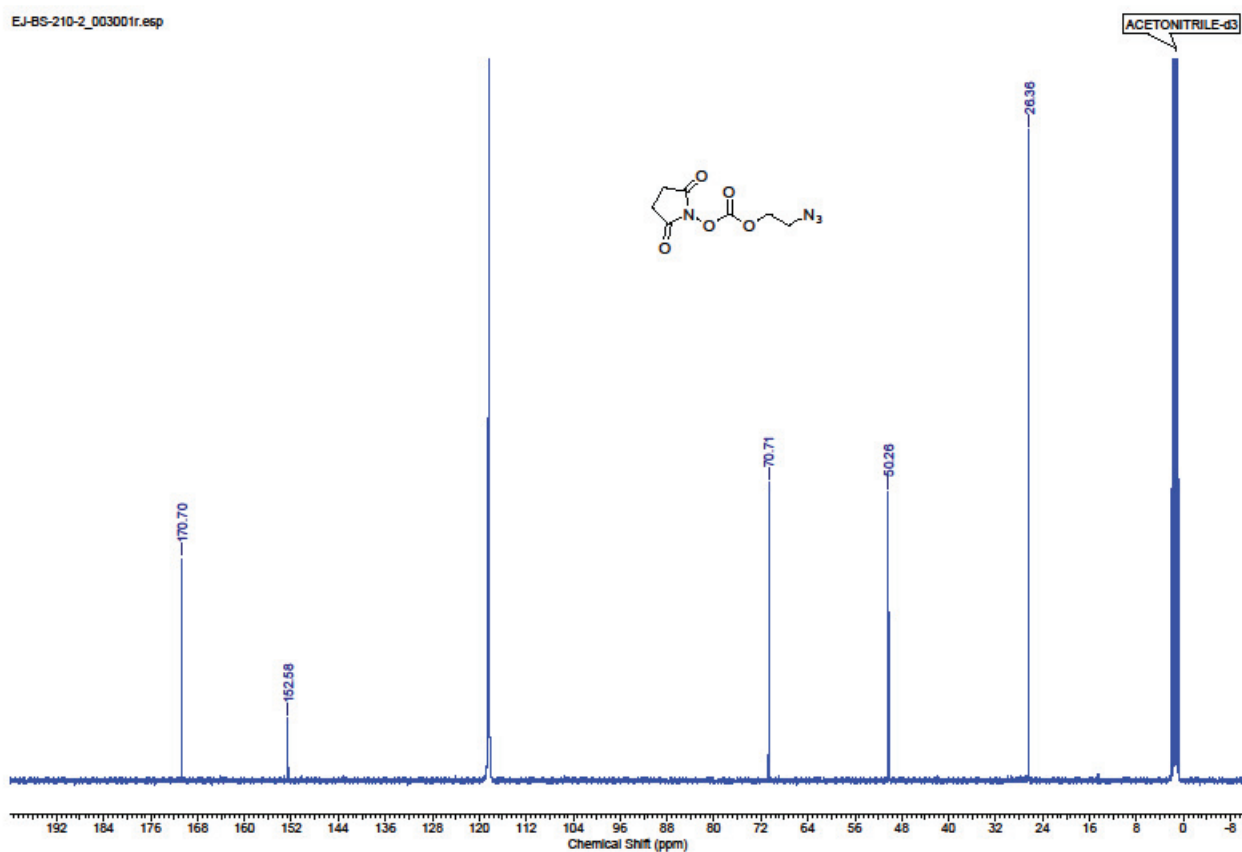
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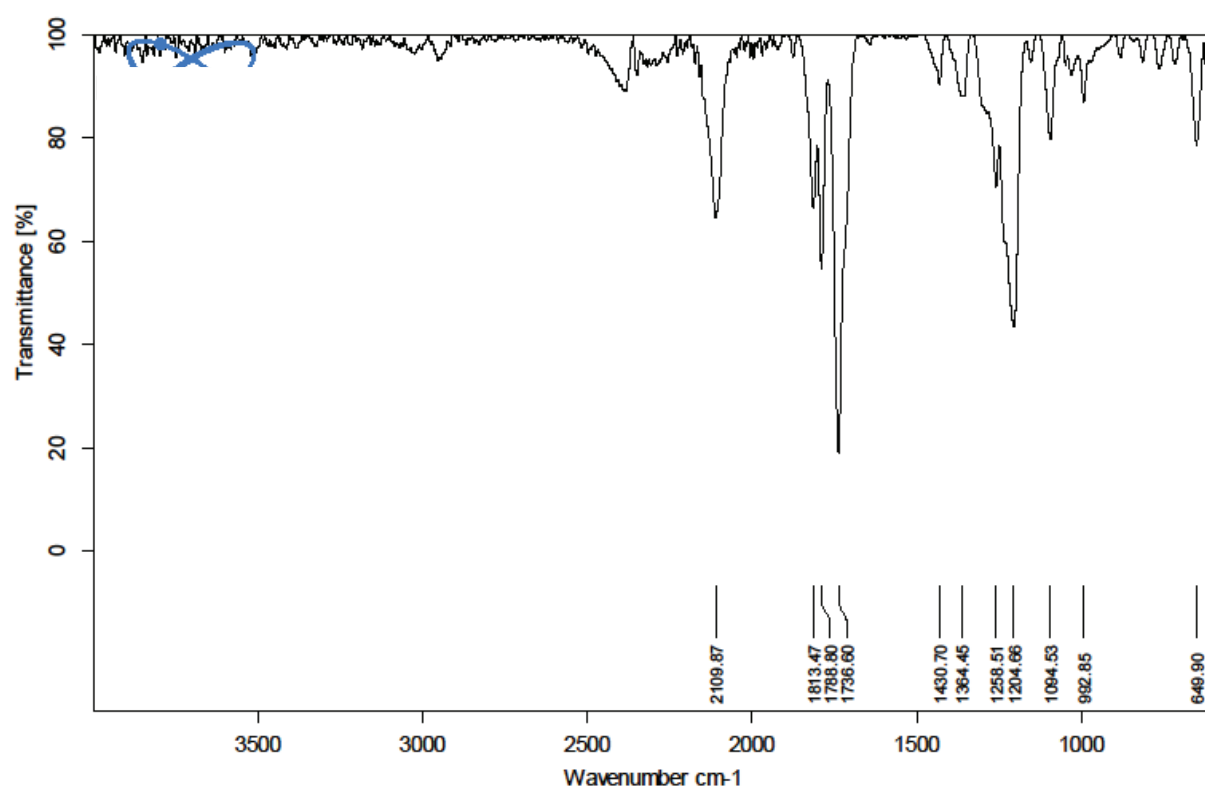


EJ-BS-210-2_001001r.esp



EJ-BS-210-2_003001r.esp





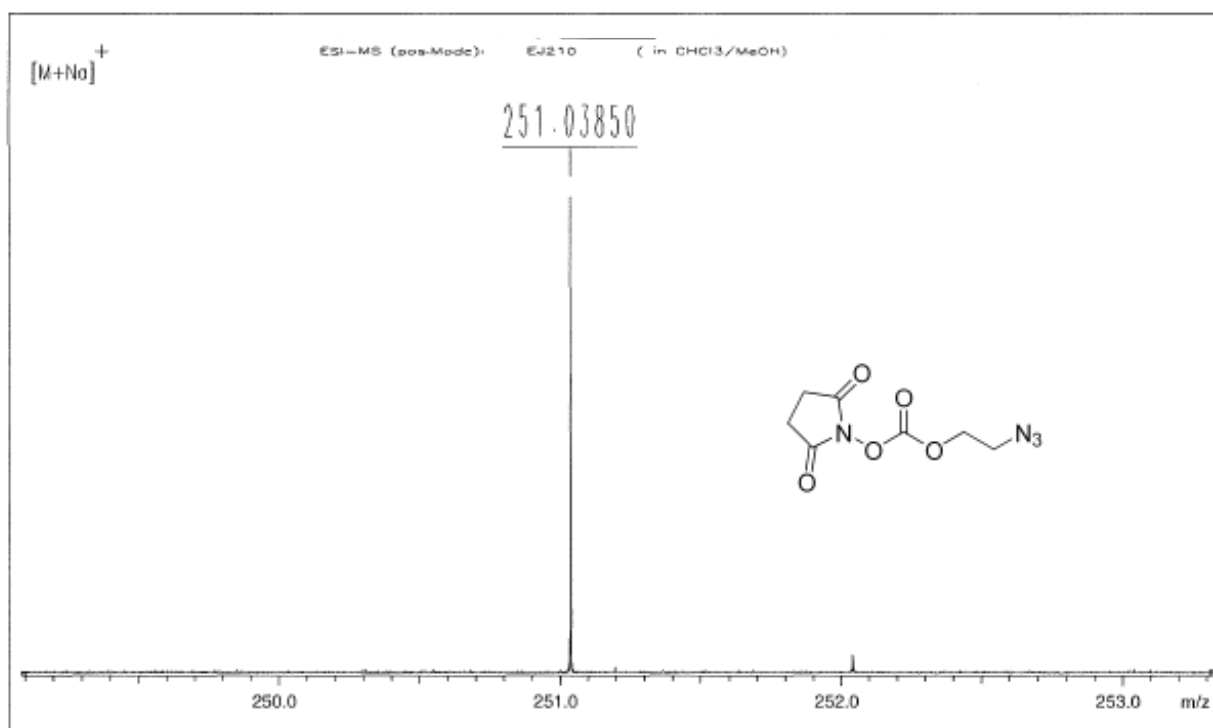
ESI-MS: EJ210

XMASS Mass Analysis for /Data/UNI_FR/JANE1690_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 251.0385020

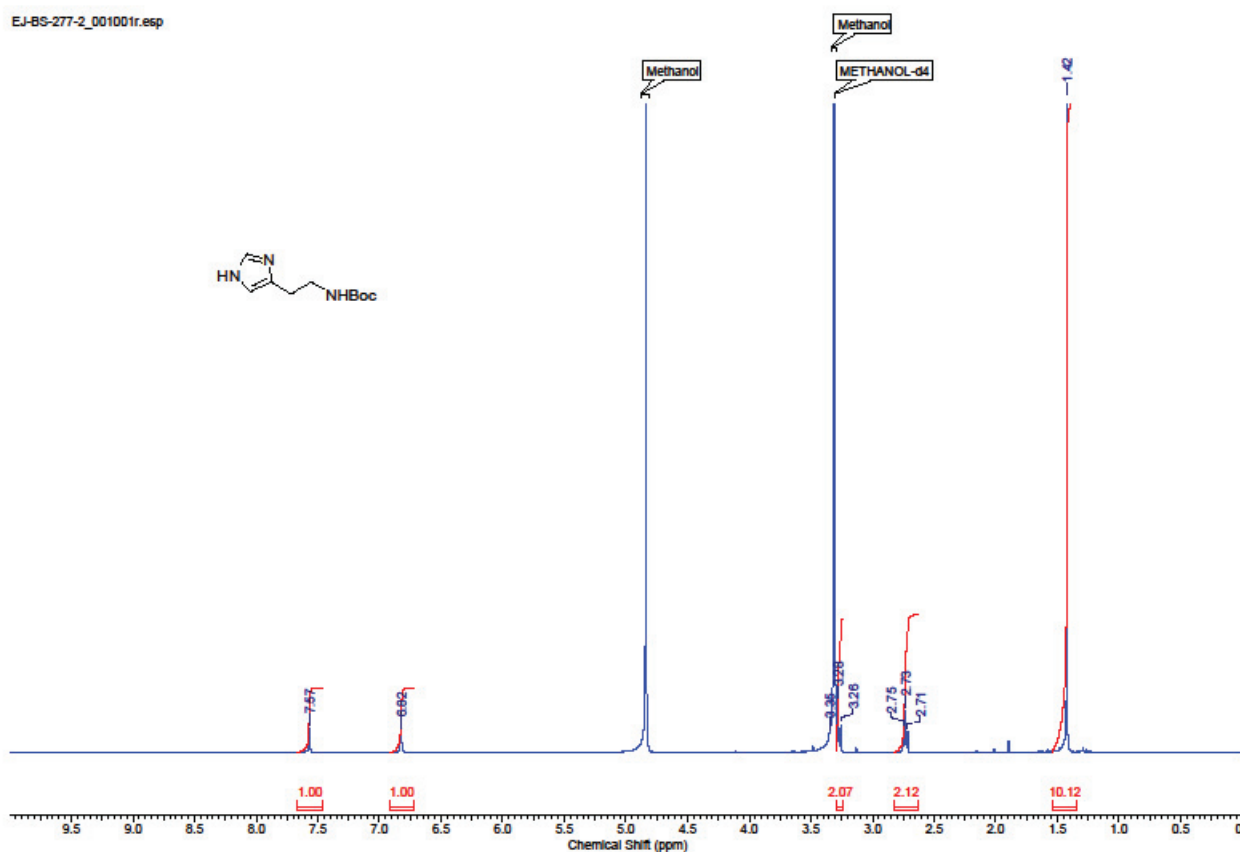
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 251.0385020								
1	7	8	4	5	1	251.0386905	5.5	1.885e-04
2	5	6	7	4	1	251.0373478	6.0	1.154e-03
3	7	5	7	4	0	251.0397531	9.0	1.251e-03
4	9	10	1	6	1	251.0400331	5.0	1.531e-03
5	18	5	1	1	0	251.0365652	17.0	1.937e-03
6	9	7	4	5	0	251.0410958	8.5	2.594e-03
7	10	6	5	2	1	251.0413706	10.0	2.869e-03
8	11	9	1	6	0	251.0424384	8.0	3.936e-03
9	12	8	2	3	1	251.0427132	9.5	4.211e-03
10	16	6	1	1	1	251.0341599	14.0	4.342e-03

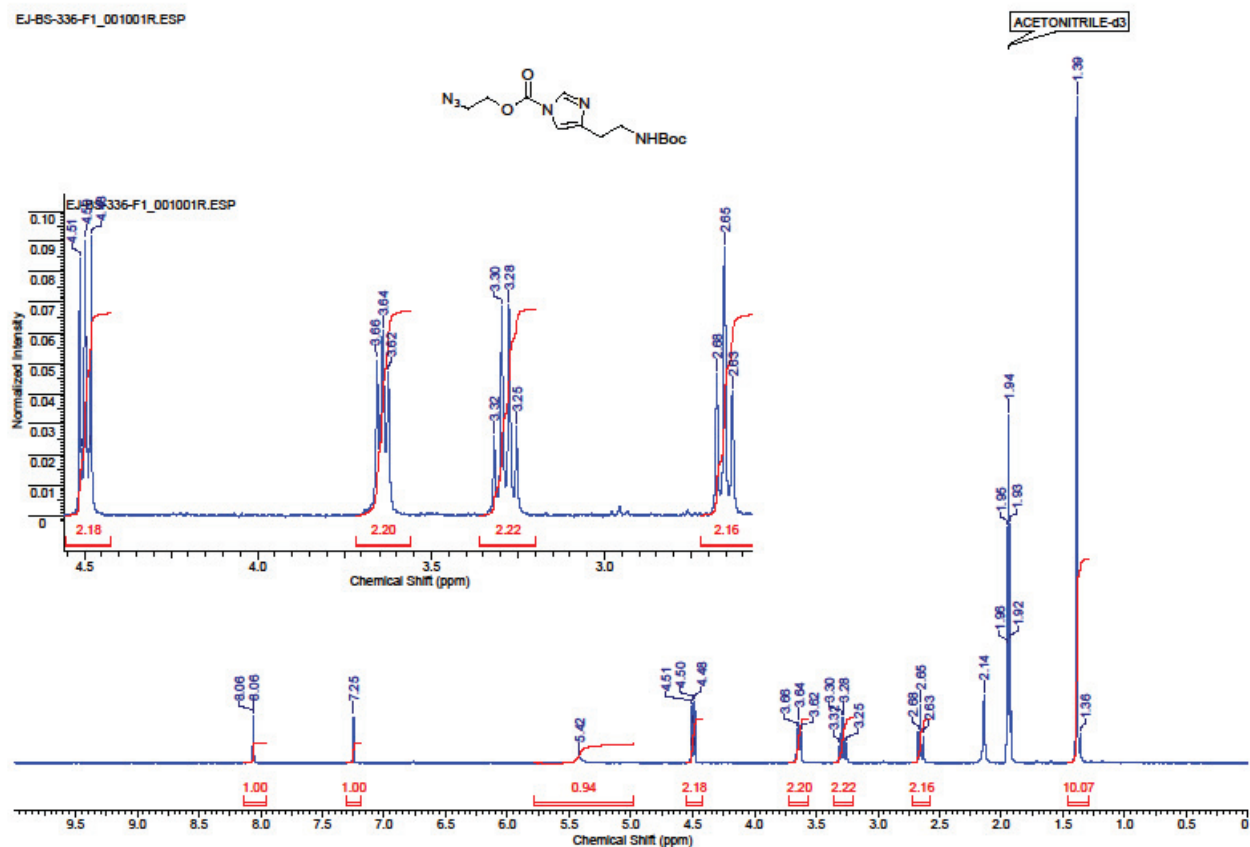


/Data/UNI_FR/JANE1690_ESI/1/pdata/1 FTMS USER Tue May 31 18:20:25 2016

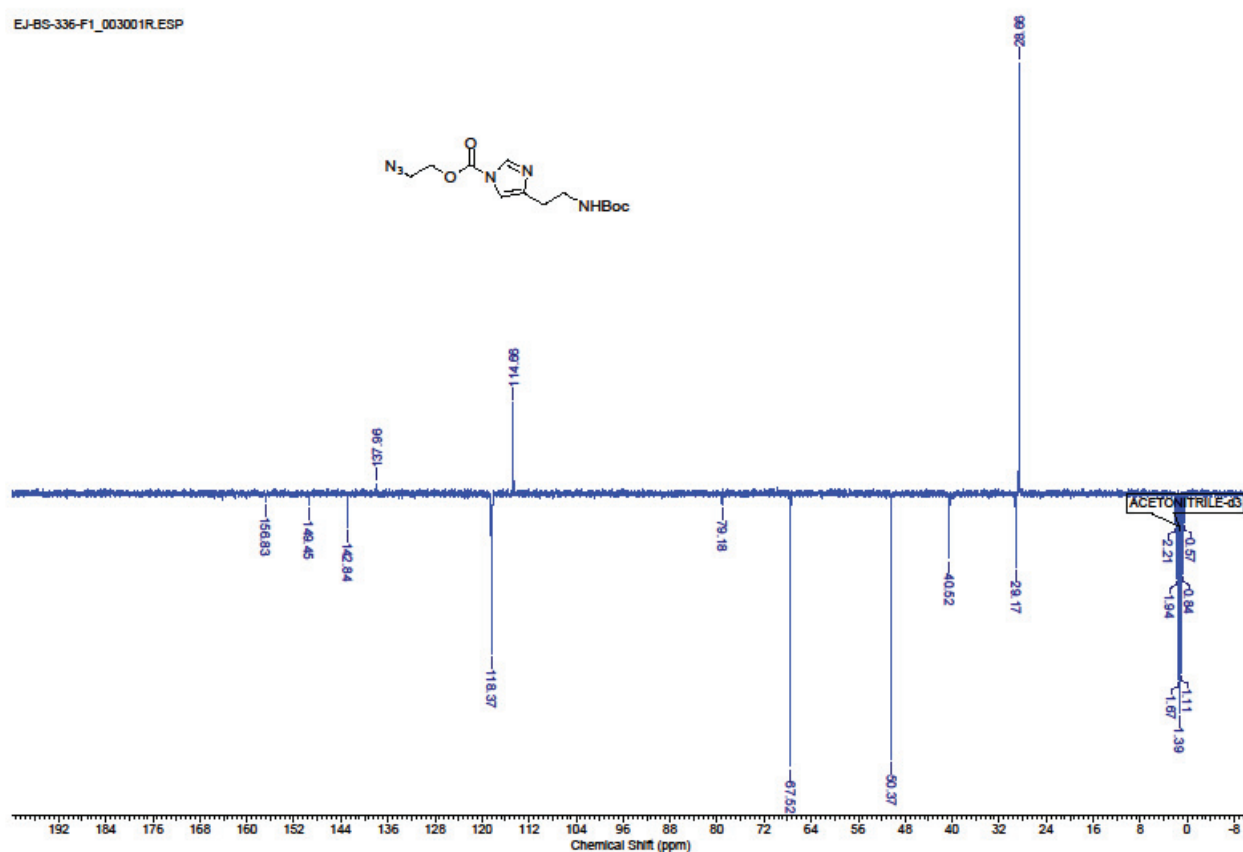
EJ-BS-277-2_001001r.esp



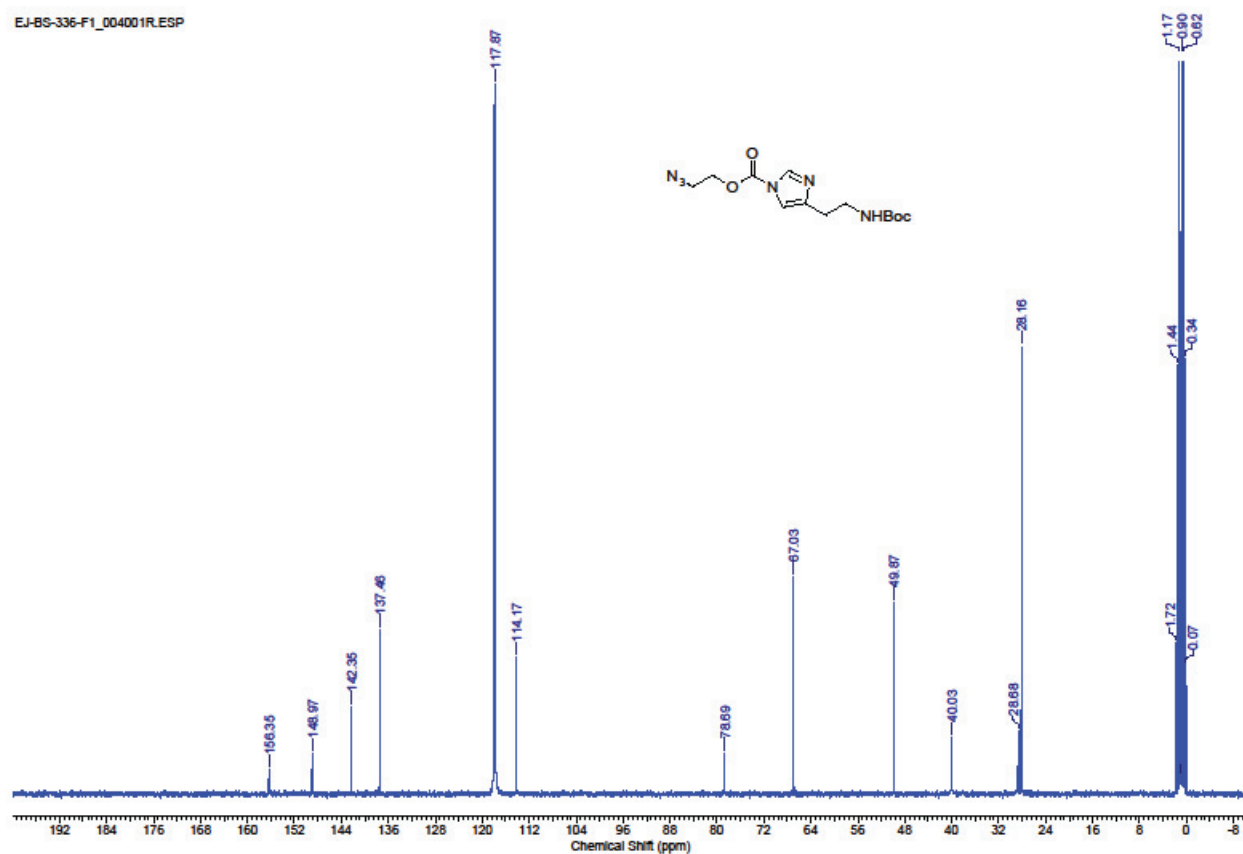
EJ-BS-336-F1_001001R.ESP

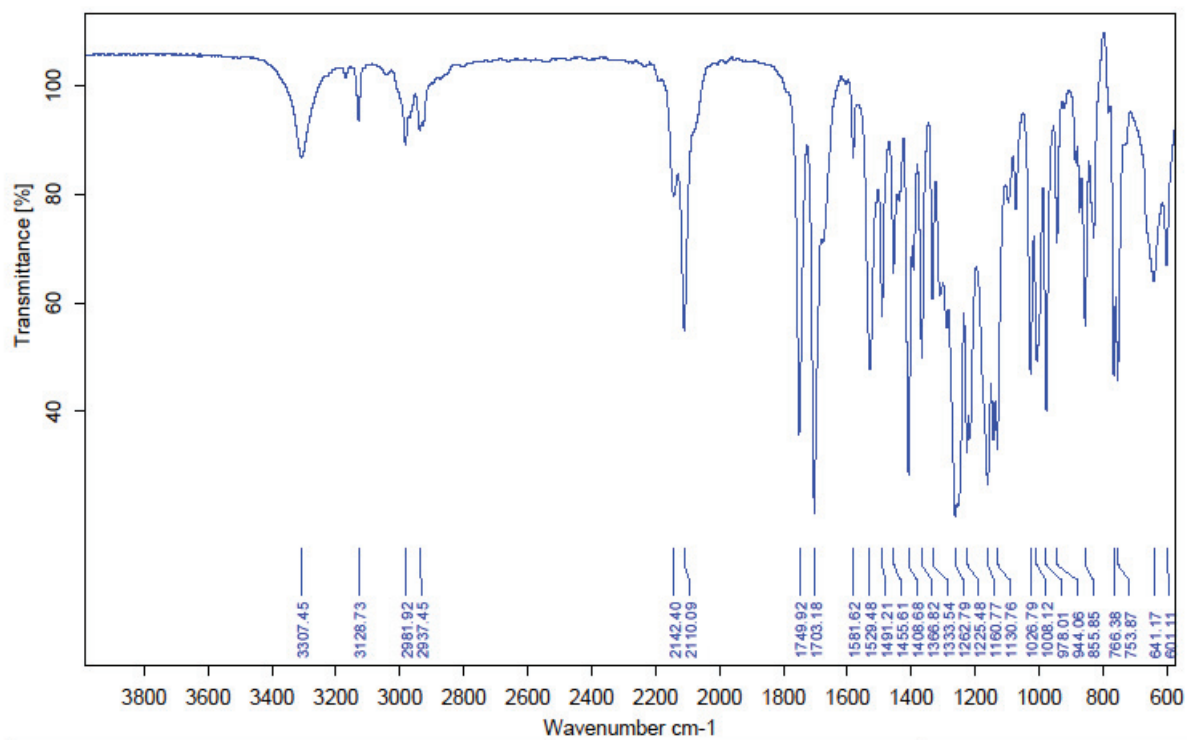


EJ-BS-336-F1_003001R.ESP



EJ-BS-336-F1_004001R.ESP





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EJ-BS-312.1

Date: 20.02.2017, 11:14:54

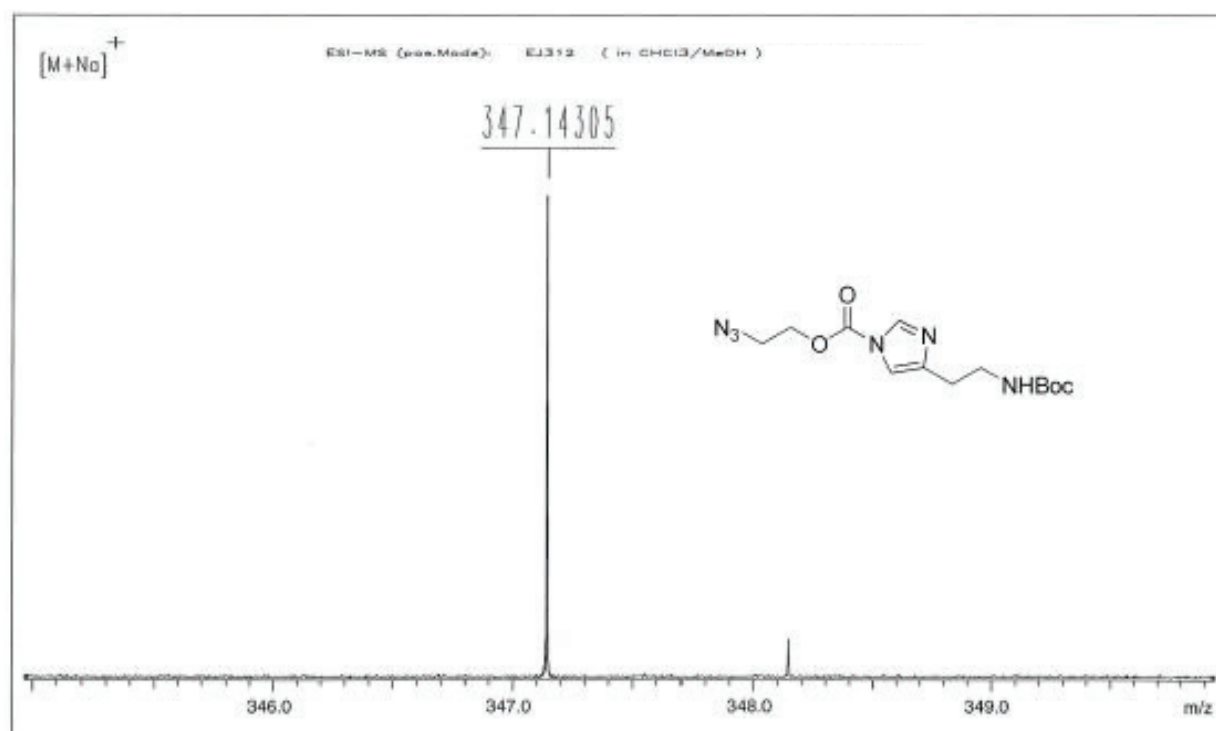
ESI-MS: EJ312

XMASS Mass Analysis for /Data/UNI_FR/JANE2638_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 347.1430540

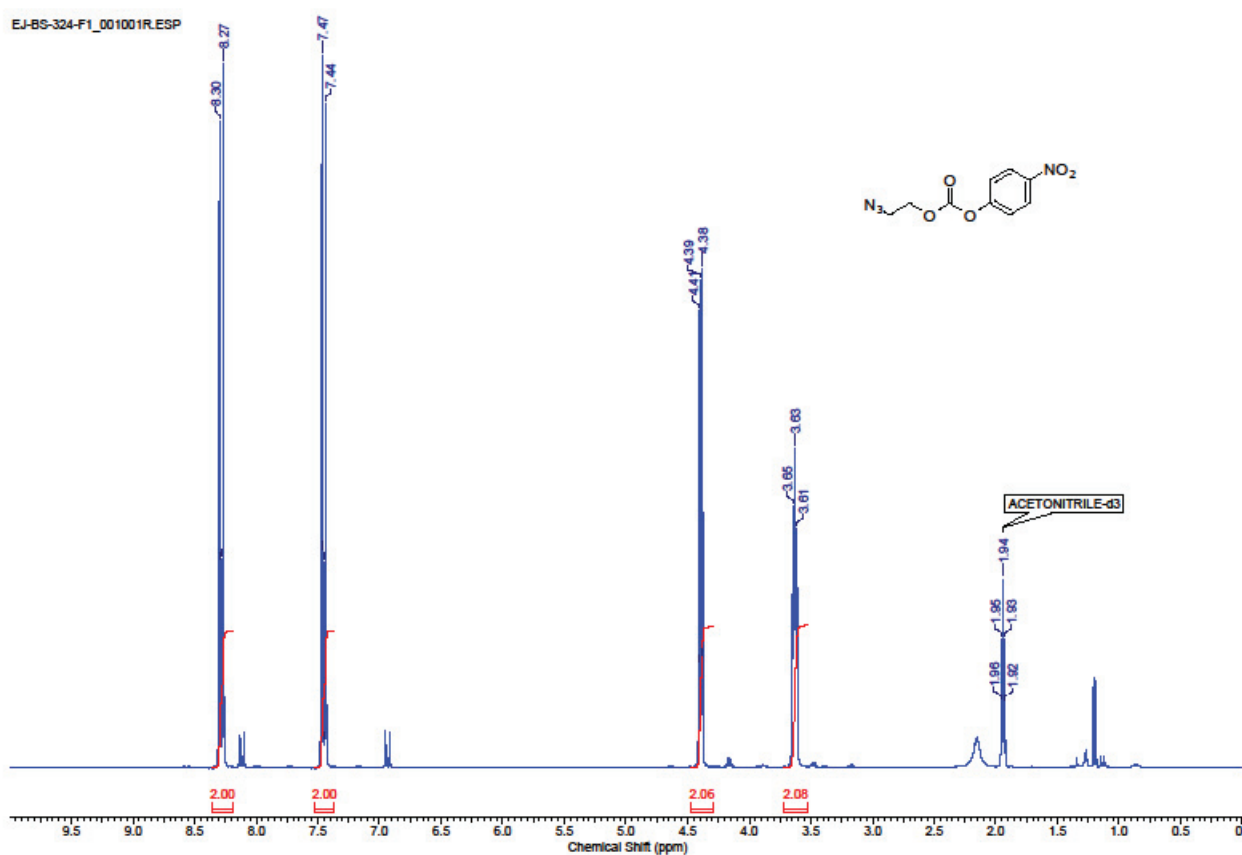
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 347.1430540								
1	13	20	6	4	1	347.1438243	6.5	7.703e-04
2	10	19	8	6	0	347.1422068	5.5	8.472e-04
3	15	22	3	5	1	347.1451669	6.0	2.113e-03
4	15	19	6	4	0	347.1462295	9.5	3.176e-03
5	8	20	8	6	1	347.1398015	2.5	3.252e-03
6	21	19	2	3	0	347.1390189	13.5	4.035e-03
7	17	21	3	5	0	347.1475722	9.0	4.518e-03
8	18	20	4	2	1	347.1478470	10.5	4.793e-03
9	19	17	5	2	0	347.1376762	14.0	5.378e-03
10	19	20	2	3	1	347.1366136	10.5	6.440e-03

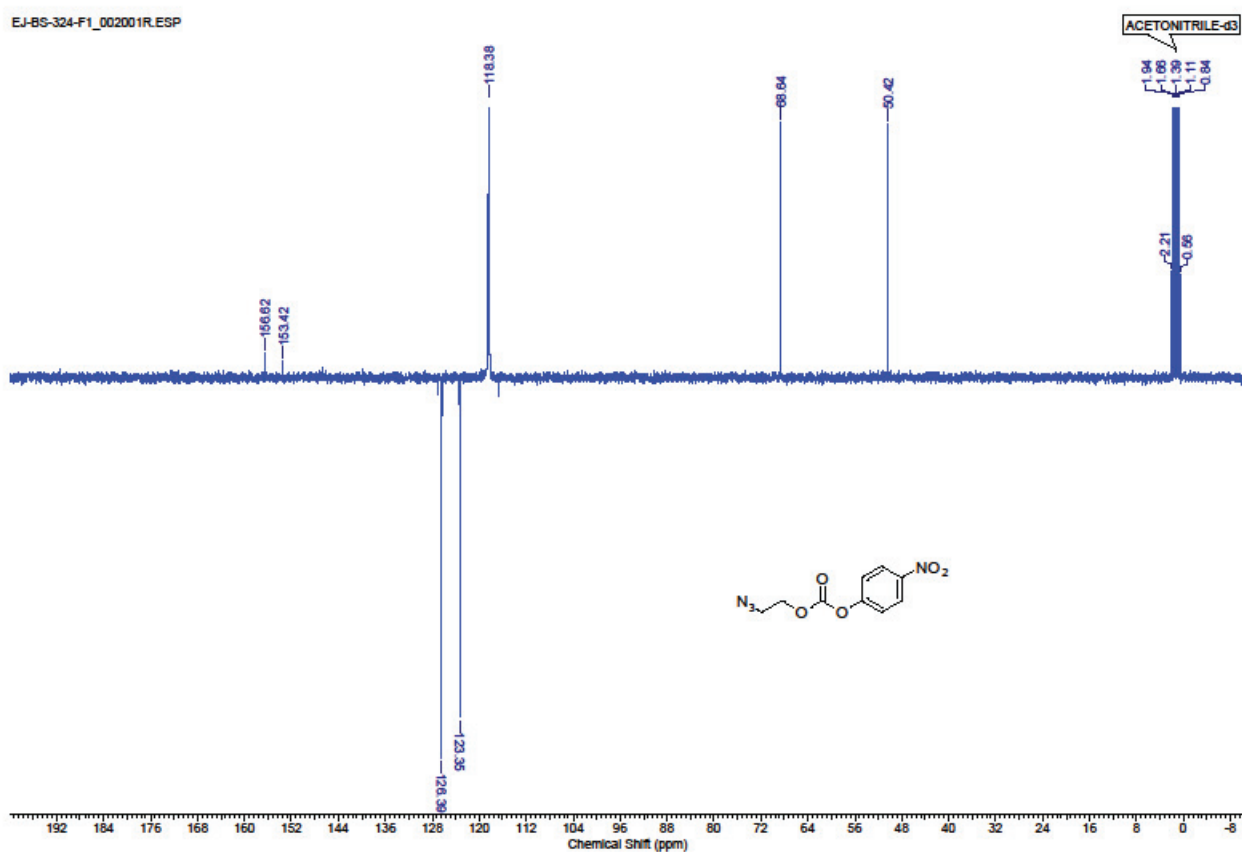


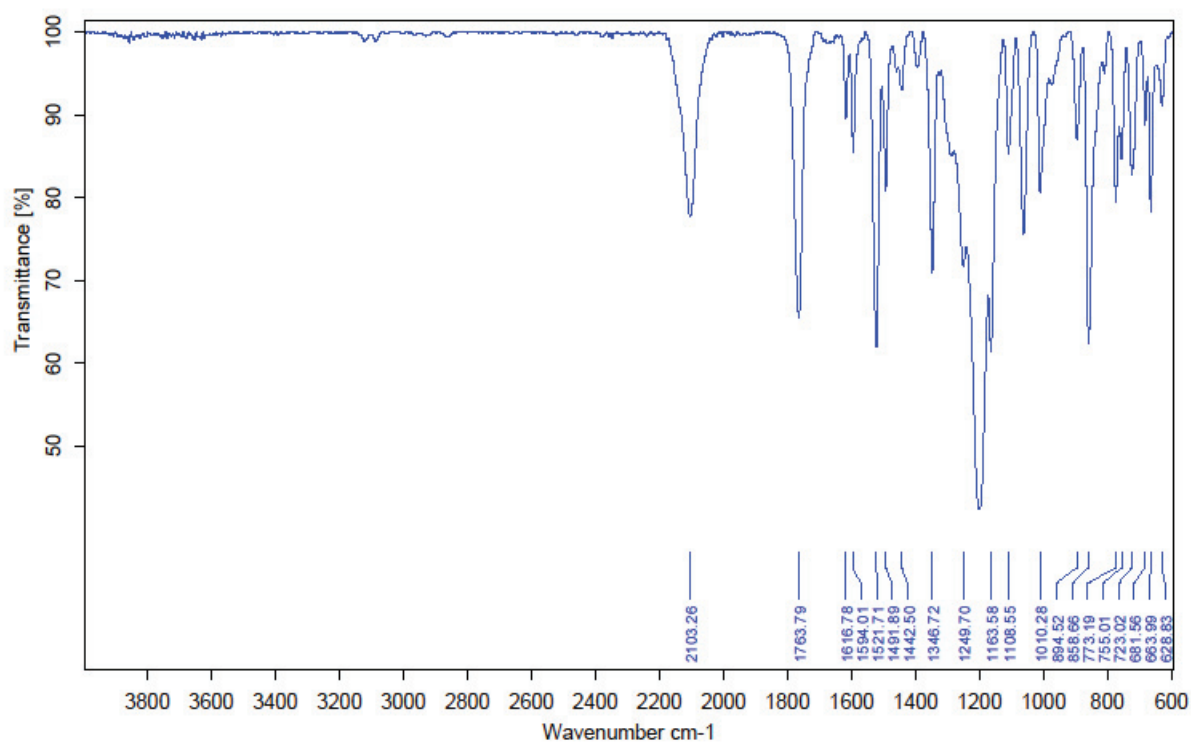
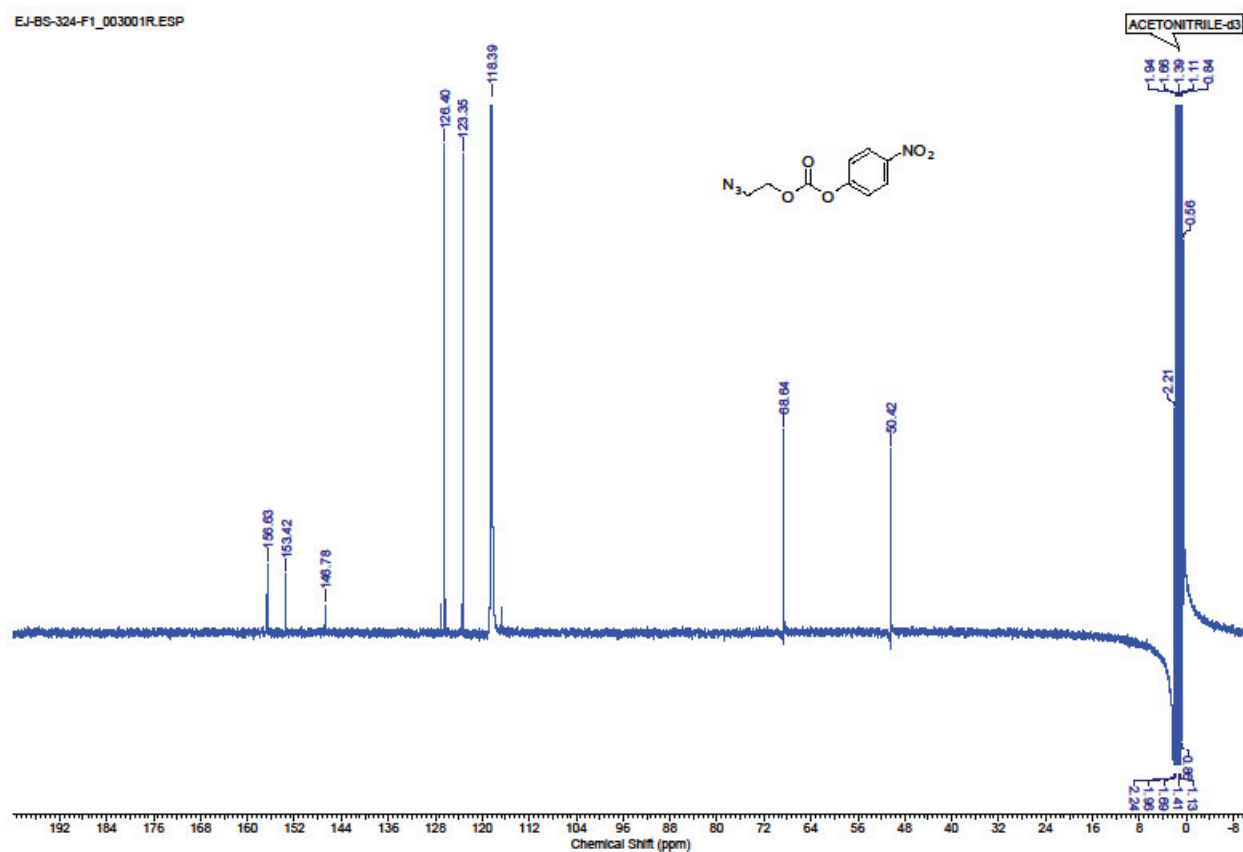
/Data/UNI_FR/JANE2638_ESI/2/pdata/1 FTMS USER Mon Feb 20 15:25:13 2017

EJ-BS-324-F1_001001R.ESP



EJ-BS-324-F1_002001R.ESP





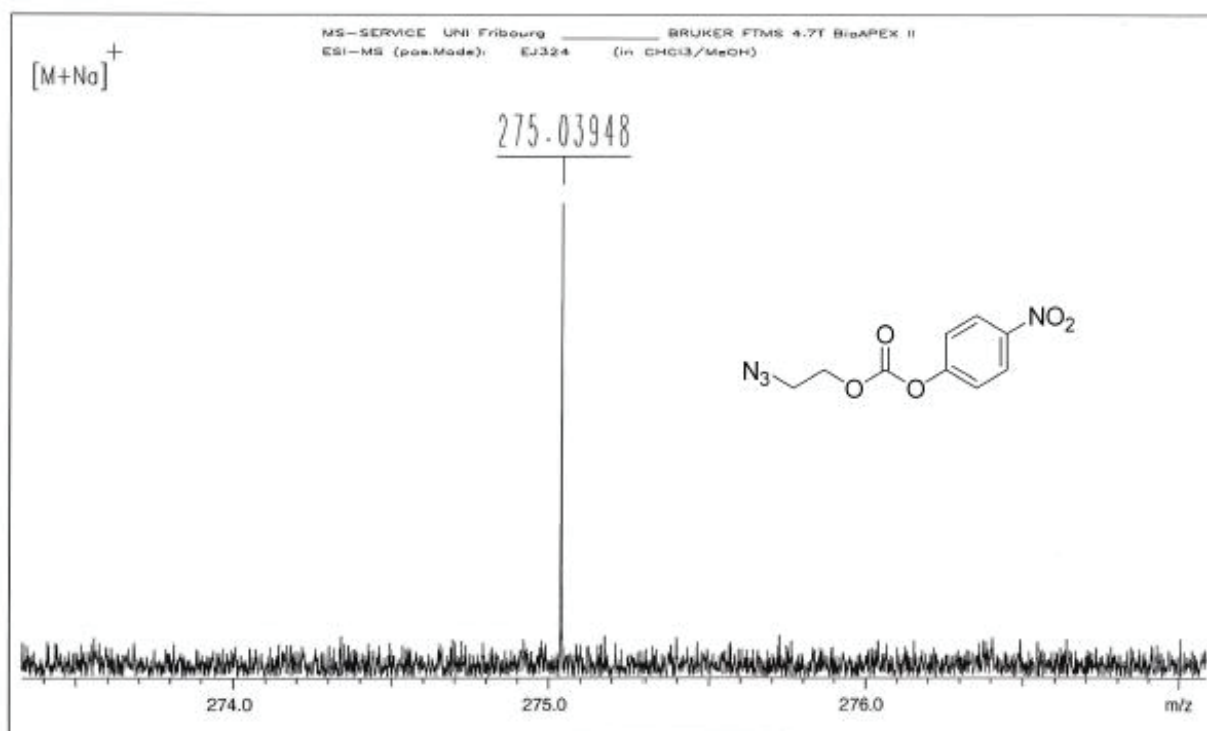
ESI-MS: EJ324

XMASS Mass Analysis for /Data/UNI_FR/JANE2935_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 275.0394760

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 275.0394760								
1	9	8	4	5	1	275.0386905	7.5	7.855e-04
2	8	9	3	8	0	275.0384157	6.0	1.060e-03
3	11	7	4	5	0	275.0410958	10.5	1.620e-03
4	12	6	5	2	1	275.0413706	12.0	1.895e-03
5	6	7	6	7	0	275.0370730	6.5	2.403e-03
6	14	8	2	3	1	275.0427132	11.5	3.237e-03
7	6	10	3	8	1	275.0360104	3.0	3.466e-03
8	14	5	5	2	0	275.0437759	15.0	4.300e-03
9	16	7	2	3	0	275.0451185	14.5	5.643e-03
10	15	5	3	3	0	275.0325425	15.0	6.934e-03

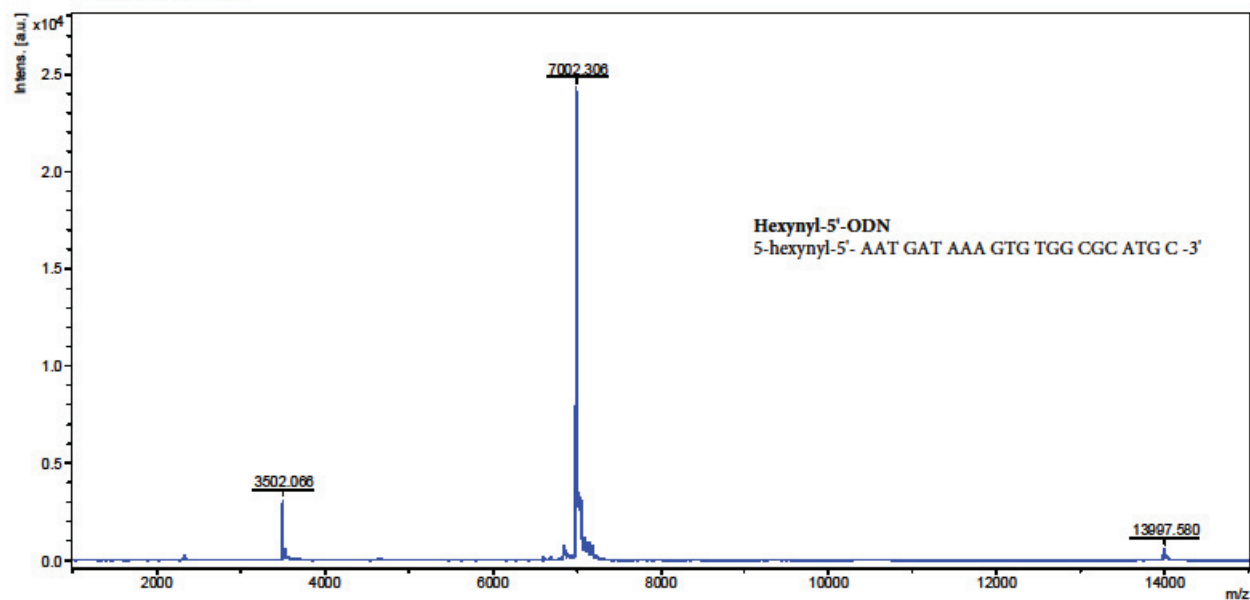


/Data/UNI_FR/JANE2935_ESI/5/pdata/1 FTMS USER Mon Apr 24 13:29:56 2017

Comment 1

Comment 2

Instrument type: MALDI-TOF

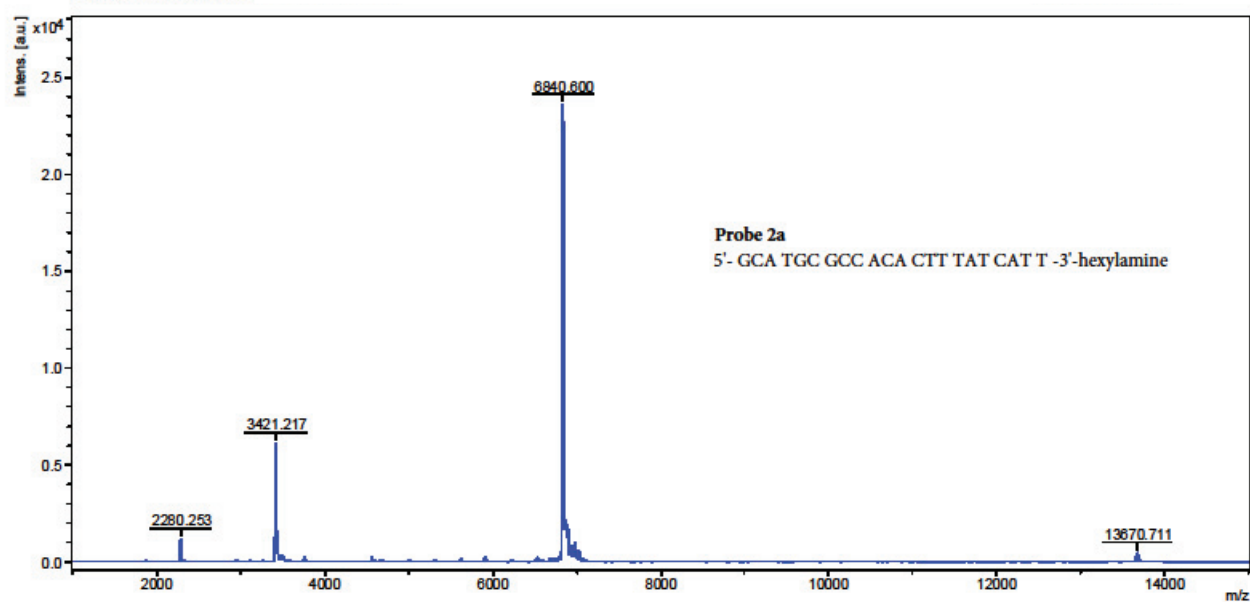


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Comment 1

Comment 2

Instrument type: MALDI-TOF

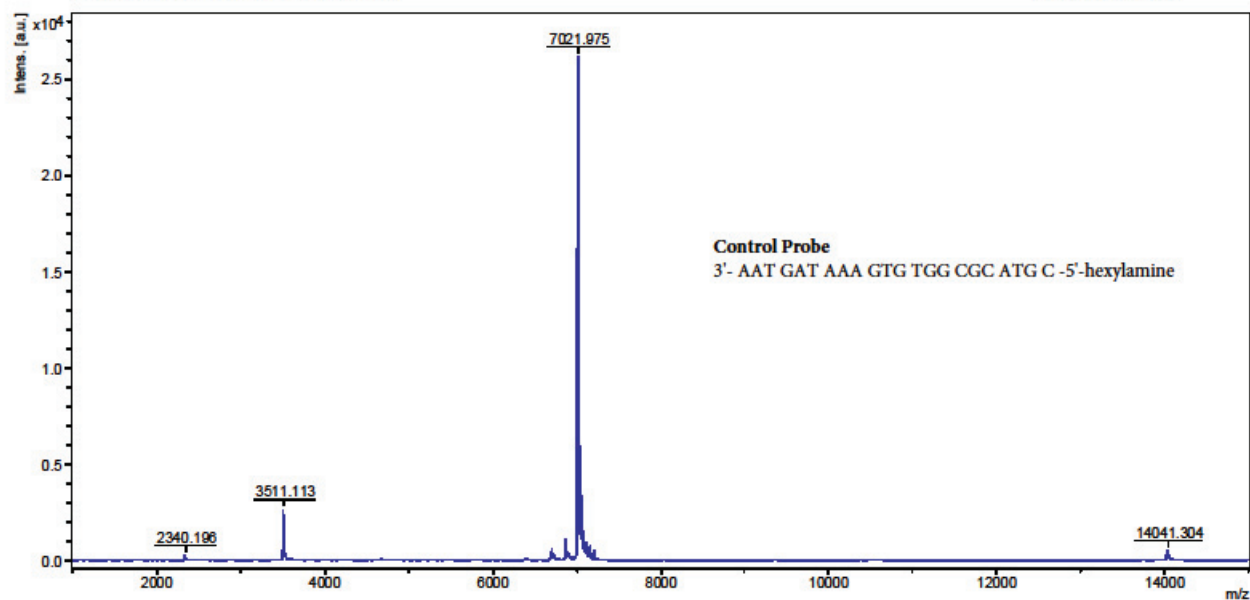


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Comment 1

Comment 2

Instrument type: MALDI-TOF

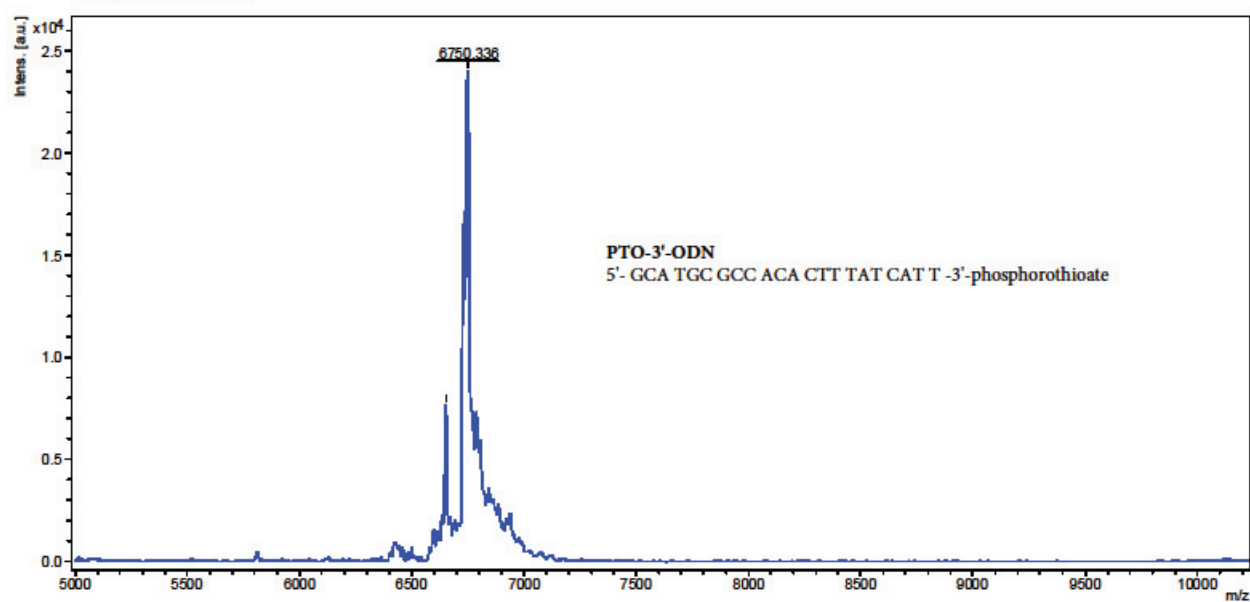


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Comment 1

Comment 2

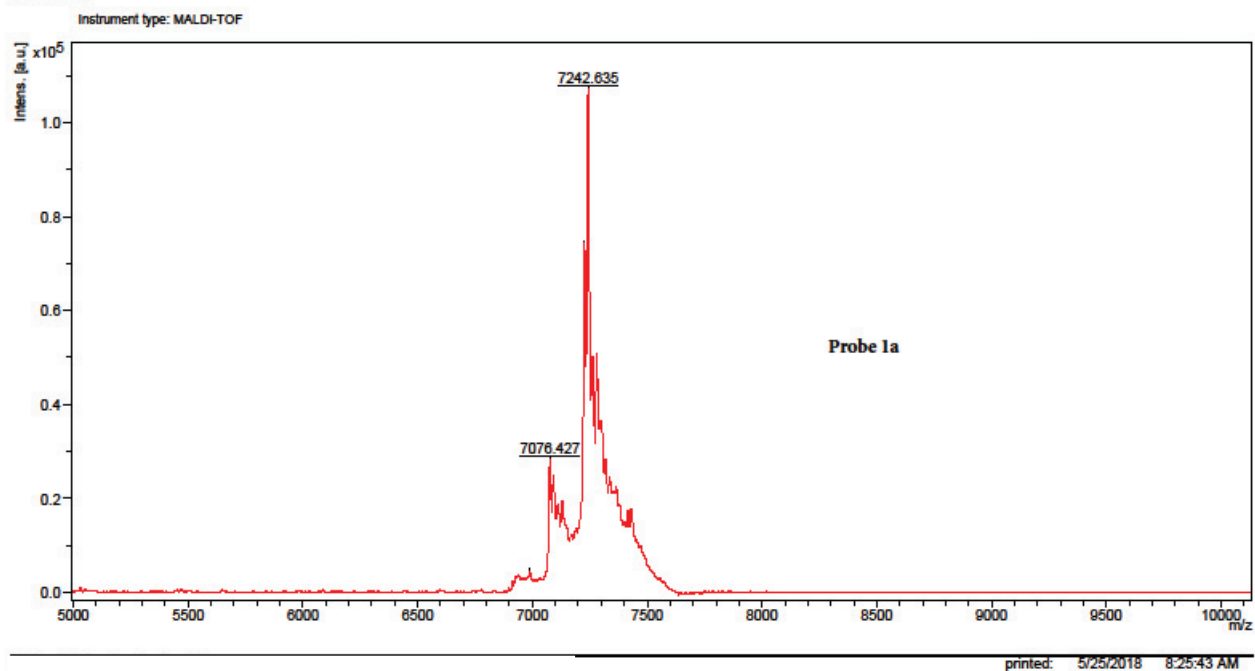
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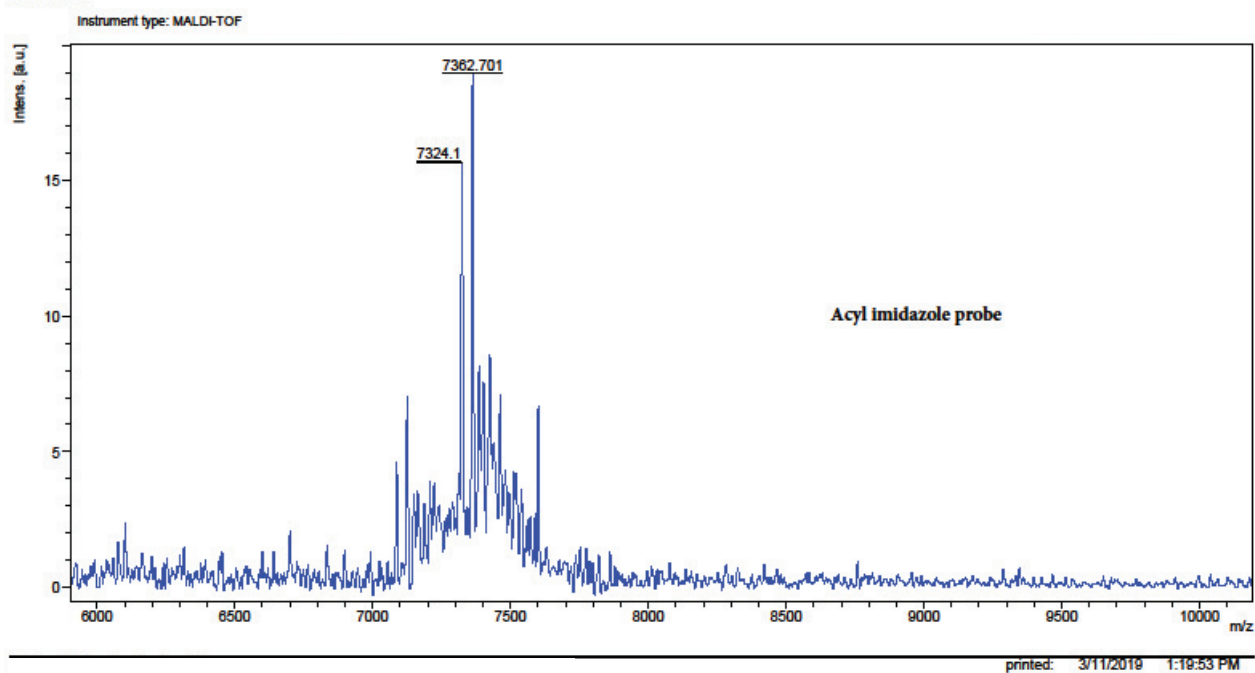
Comment 1

Comment 2



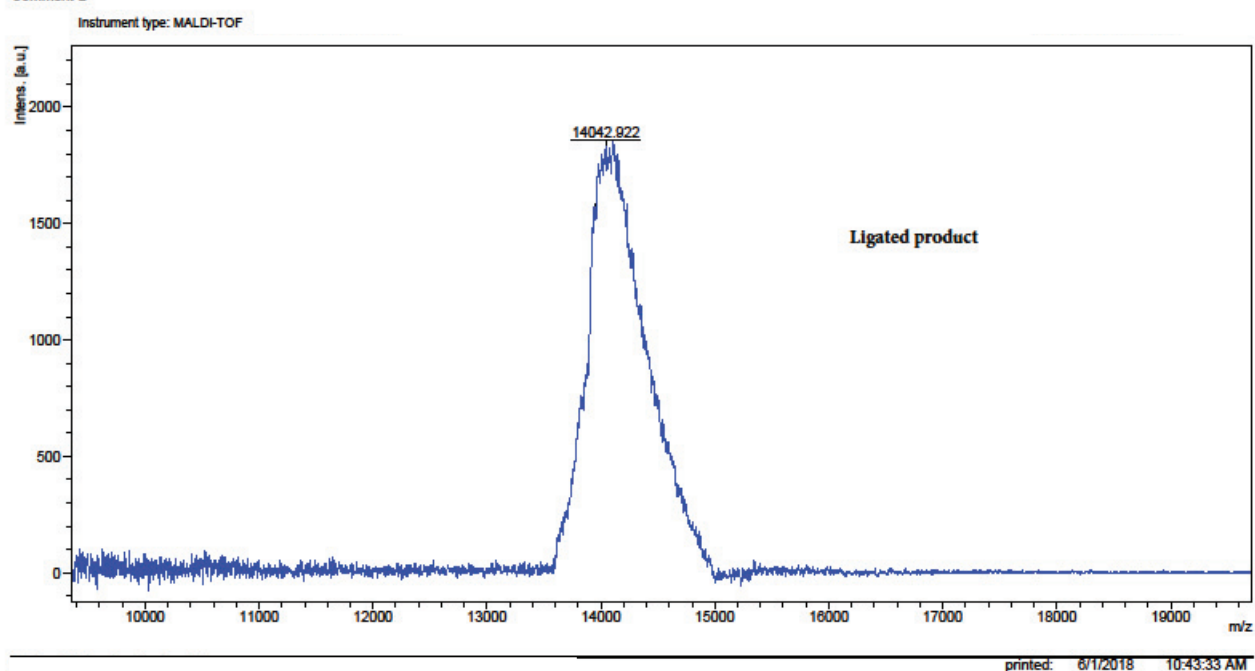
Comment 1

Comment 2



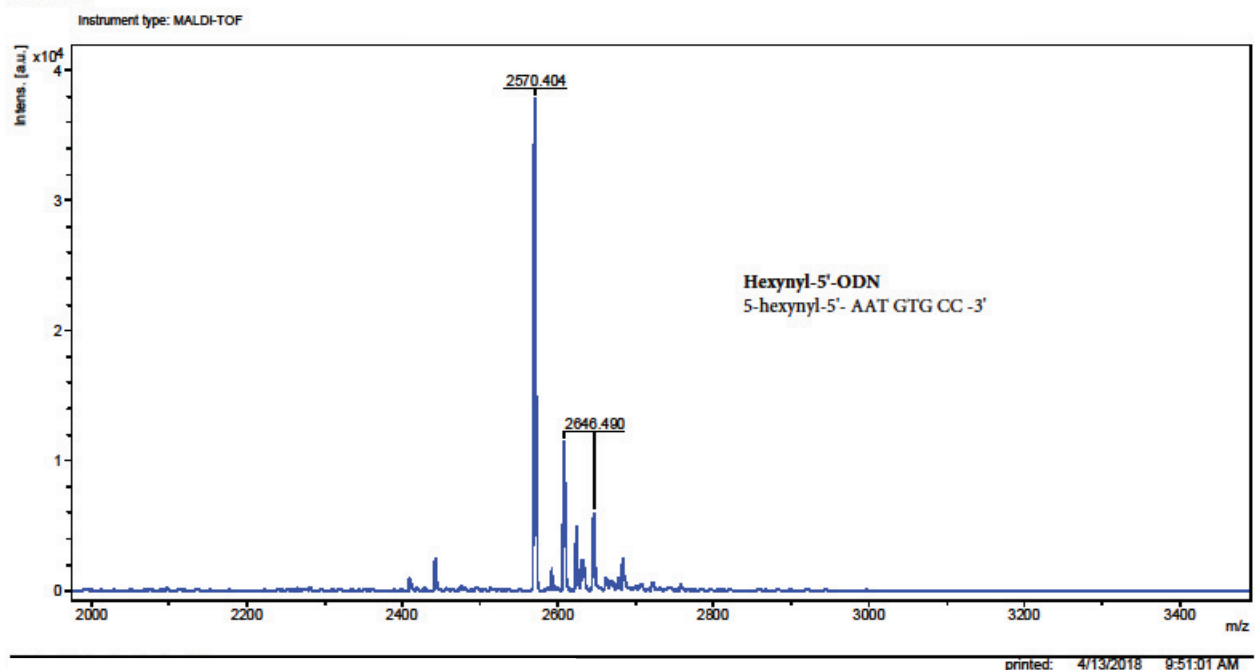
Comment 1

Comment 2



Comment 1

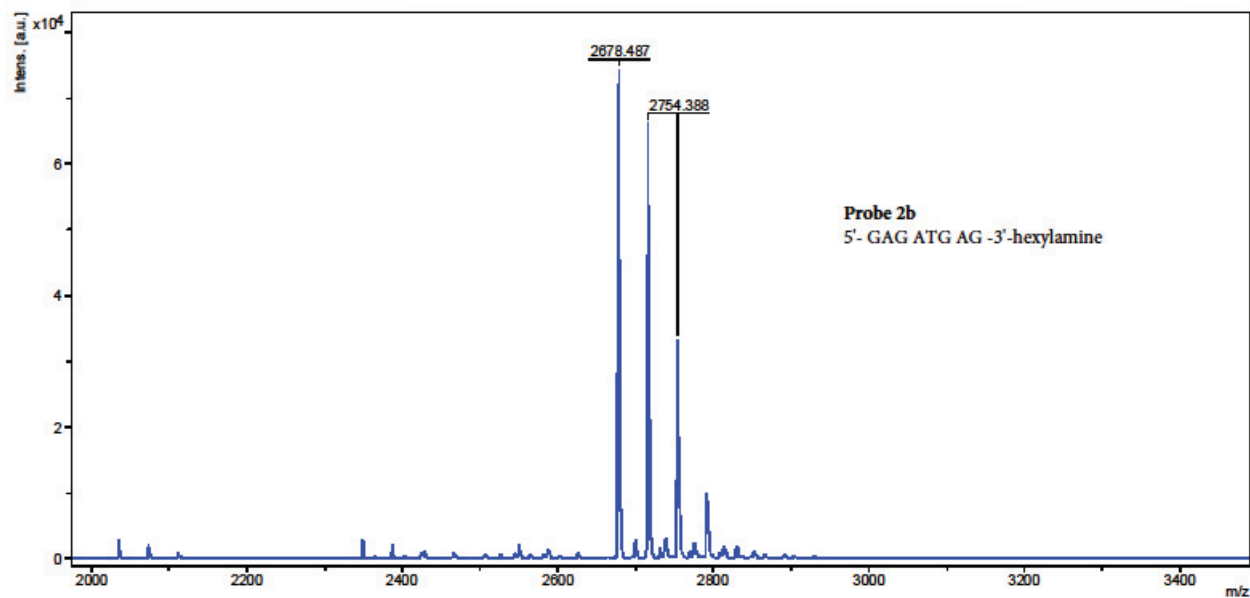
Comment 2



Comment 1

Comment 2

Instrument type: MALDI-TOF

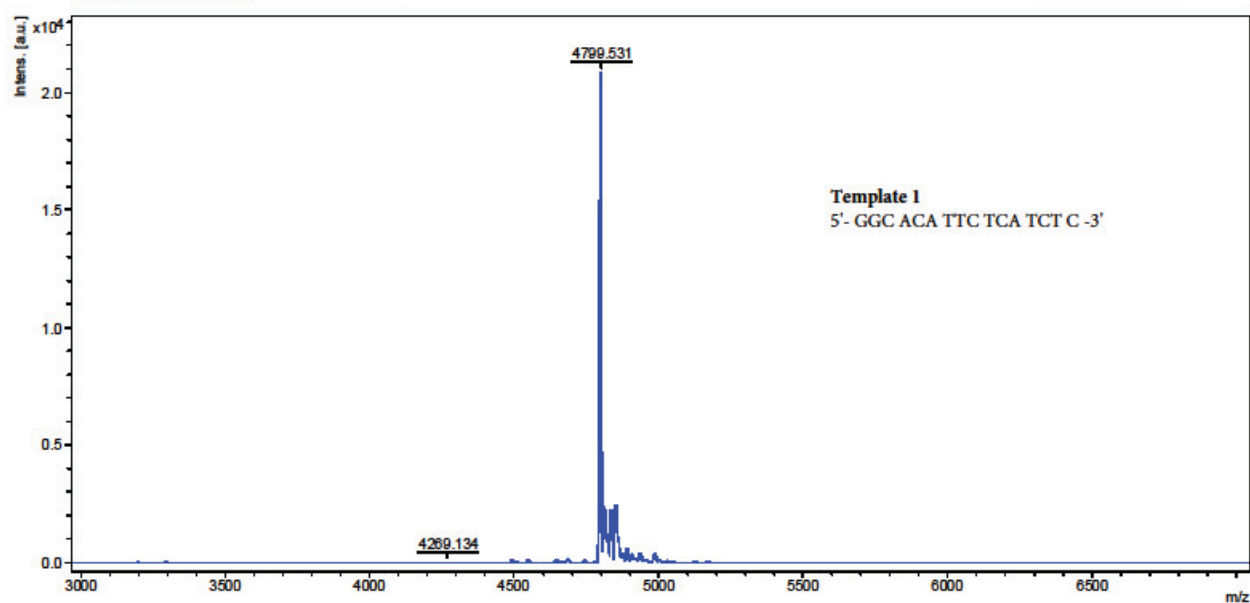


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Comment 1

Comment 2

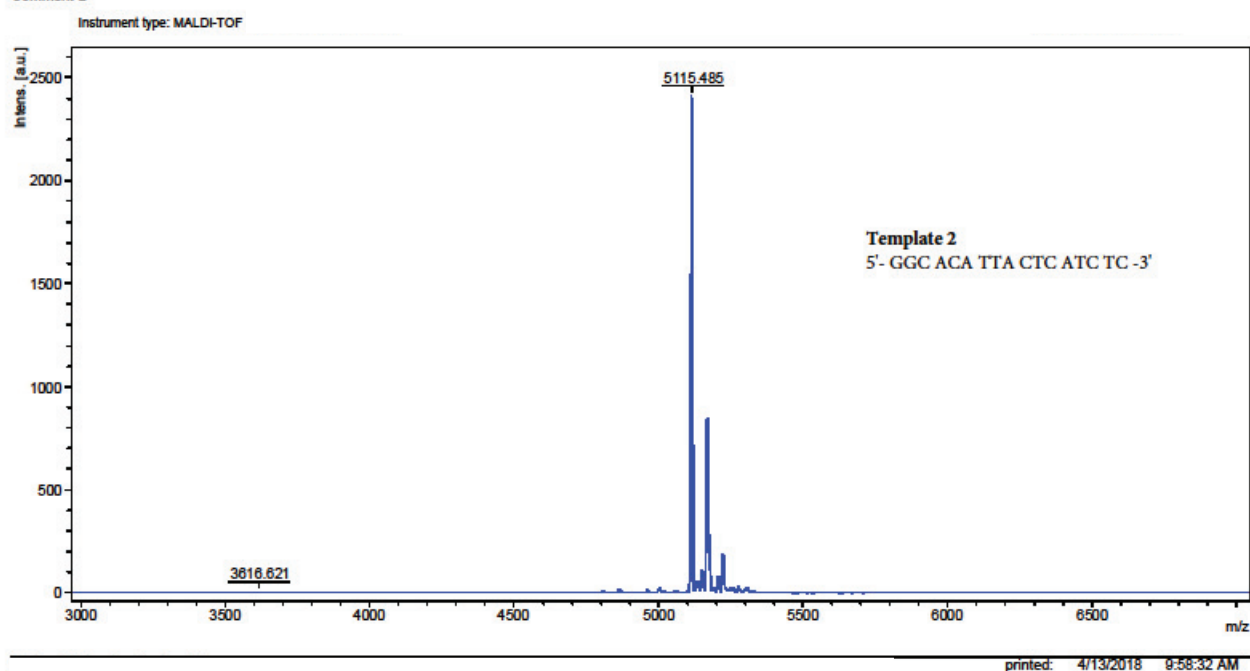
Instrument type: MALDI-TOF



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Comment 1

Comment 2



Comment 1

Comment 2

