Supporting Information

C–N coupling of (hetero)aryl bromides and chlorides for DNA-encoded chemical library synthesis

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1. General Information

Some of the general materials, equipment and procedures used in this study are adapted from those our group has reported previously[1-6] or other DNA-encoded library publications.[7,8]

1a. Materials and equipment used for the synthesis and analysis of oligonucleotides and DNA-encoded chemical libraries. The central dsDNA oligonucleotide with chemically-modified phosphates that end in an amine terminus (DEC-Tec Starting Unit/DTSU, **S1**, Figure S1) and encoding 5'-phosphorylated oligonucleotides were purchased from LGC Biosearch Technologies. All DNA oligonucleotides were assessed through the general analytical procedure for purity. DNA sequences were designed to maximize sequence-reads and minimize close similarity while sequencing. DNA oligomers in each codon duplexed pair was designed to feature divergent mass greater than 5 Da for efficient quality control analysis. A 10-mer DNA oligomer (spike-in), featured a cholesterol tag and amine terminus, was obtained from Sigma-Aldrich and charged in library pool to monitor chemical reactions. High-concentration T4 DNA ligase was obtained from Enzymatics (Qiagen). Oligomer ligation test with DTSU was incorporated to determine the ligase activity before use. DNA working solutions were prepared using DNAse/RNAse-free ultrapure water (Invitrogen), HPLC-grade acetonitrile (Fisher) or high-purity absolute ethanol (Koptec). LC/MS running solvents were made from Optima LC/MS grade water (Fisher), Optima LC/MS grade methanol (Fisher), hexafluoroisopropanol (99+% purity, Sigma-Aldrich) and HPLC-grade triethylamine (Fisher). All listed buffers and ionic solutions, including HEPES 10X ligation buffer (300 mM 2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid, 100 mM $MgCl_2$, 100 mM dithiothreitol, 10 mM adenosine triphosphate, pH 7.8), aq. NaOH, aq. NaCl (5 M) and basic borate buffer (250 mM sodium borate/boric acid, pH 9.5), were prepared in-house.

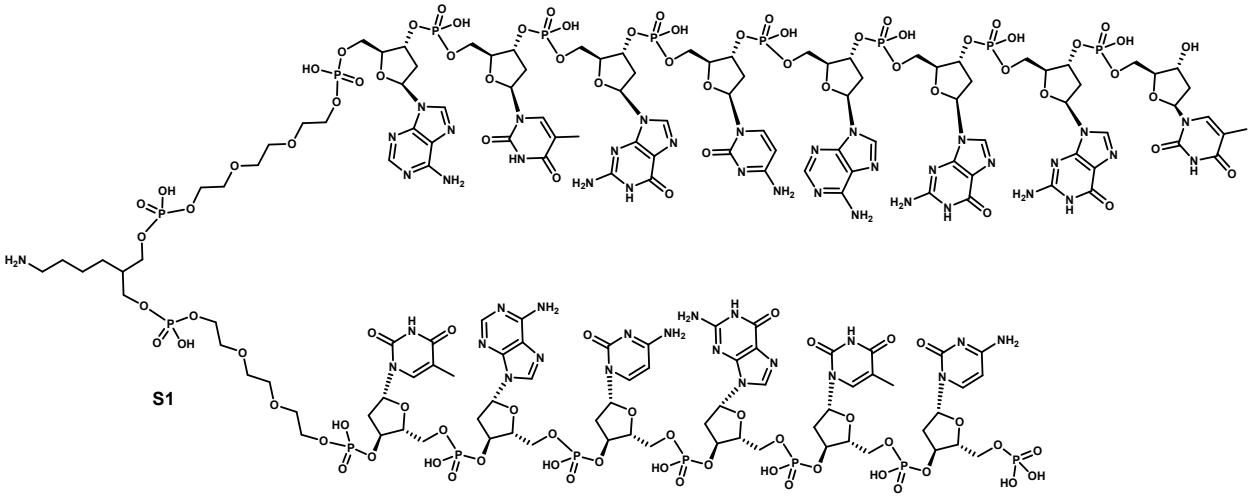


Figure S1. Structure of DTSU **S1** (5'-Phos-CTGCAT-Spacer 9-Amino C7-Spacer 9-ATGCAGGT 3').

Chemical building blocks and reagents were purchased from various vendor sources and used without further purification. Building blocks were generally used from aliquots dissolved in acetonitrile (MeCN), methoxyisopropanol (MIPO), dimethylacetamide (DMA) or mixed aqueous acetonitrile, and stored in 2D barcoded tubes (Phenix) with septa-caps at -80 °C. Barcoded tubes were read using a SampleScan 96 scanner (BiomicroLab) and decoded using Vortex software (Dotmatics). Solutions were transferred utilizing Biotix brand or Fisherbrand pipette tips and Biotix reservoirs. Reactions and library transformations were generally performed in polypropylene PCR tubes (Genemate), polypropylene tubes (Eppendorf), 96-well polypropylene PCR plates (Phenix or ThermoFisher), or 96-well, deep-well

plates (USA Scientific). Plates were sealed for incubation with AlumaSeal II sealing films (Excel Scientific) and large volume DNA precipitations were performed in polypropylene 250 mL screw-cap bottles (various vendors) or centrifuge tubes. Heated reactions were performed in benchtop heating blocks (ThermoFisher), Mastercycler nexus gradient (Eppendorf), or TS-DW deep well plate themoshaker (Grant), or laboratory ovens (Fisher). Solutions were centrifuged in 5424R centrifuges (Eppendorf), Allegra X-15R centrifuges (Beckman-Coulter) or Lynx 4000 centrifuges (ThermoFisher). Optical density measurements were made using a Biophotometer (Eppendorf). A Vanquish UHPLC system was integrated with LTQ XL ion trap mass spectrometer (ThermoFisher Scientific) for LC/MS analysis of oligonucleotides. DNA was visualized with Molecular Imager Gel Doc XR system (BIO-RAD) after staining in an ethidium bromide solution.

1b. General procedure for the analysis of oligonucleotide compositions. Diluted samples of DNA stocks or reaction mixtures were injected on a Vanquish/LTQ system in amounts of 5–10 µL containing 50–200 pmol DNA analyte.

LC/MS Parameters for Thermo Vanquish UHPLC with LTQ Ion Trap MS Instrument

(i) LC settings
Column: Thermo DNAPac RP (2.1 x 50 mm, 4µm)
Solvent A: 15mM triethylamine (TEA)/100mM hexafluoroisopropanol (HFIP) in water
Solvent B: 15mM TEA/100mM HFIP in 50% methanol
Solvent C: Methanol
Flow rate: 0.65 mL/min
Run time: 2 mins (gradient)
Column temperature: 100 °C (post column cooler at 40 °C)

(ii) MS settings
Source: ESI in negative mode
Spray voltage: 4100 V
Source heater temperature: 390 °C
Sheath Gas: 28 (instrument units)
Auxiliary Gas: 8 (instrument units)
Sweep Gas: 2 (instrument units)
Capillary temperature: 350 °C
Capillary voltage: -33.0 V
Tube lens: -92.0 V
MS Scan: 500 – 2000 *m/z*

Samples were analyzed on a Thermo Vanquish UHPLC system coupled to an electrospray LTQ ion trap mass spectrometer. An oligonucleotide column (Thermo DNAPac RP, 2.1 x 50 mm, 4 µm) was equipped with ion-pairing mobile phase (15 mM TEA/100 mM HFIP in a water/methanol solvent system) for all the separations. All mass spectra were acquired in the full scan negative-ion mode over the m/z range of 500–2000. The data analysis was performed by exporting the raw instrument data (.RAW) to an automated biomolecule deconvolution and reporting software (ProMass) which uses a novel algorithm (ZNova) to produce artifact-free mass spectra. Deconvoluted mass spectra were standardized against co-currently run samples of DTSU **S1** and HP **S2** to account for any drift from theoretical mass during deconvolution.

1c. General procedure for ethanol precipitation and DNA reconstitution. To a DNA reaction aqueous mixture was added 4% (*v/v*) 5 M NaCl solution and 3 times the reaction volume of absolute ethanol. The mixture was mixed thoroughly before stored at −20 °C overnight for DNA precipitation. The slurry was then centrifuged at 4000 x G for

an hour, followed by decanting the supernatant. The pellet was washed with 75% chilled ethanol and the pellet was centrifuged at 4000 x G for another hour. The DNA pellet was dried in air after supernatant was decanted. Water was added to reconstitute the DNA to the needed concentration. Ethanol precipitation was generally performed after each chemical reaction and ligation. Additional ethanol precipitation can be applied if residual reagents was observed after first purification. Dilution with 2-4 times the reaction volume of water may be added before purification while higher percentage of water miscible solvent was used, such as DMSO.

1d. Representative general procedure for DNA ligation (adopted procedure from DNA stability and ligation test)

To DNA conjugate **32** (2.7 nmol, 6 μL, 1.0 equiv) was added DNA_Forward (5'-ACACTTGCTGGT-3', 4 nmol, 4 μL, 1.5 equiv), DNA_Reverse (5'-CAGCAAGTGTGA-3', 4 nmol, 4 μL, 1.5 equiv), and DNase/RNase-free water (8.9 μL), followed by the addition of 10X HEPES buffer (2.7 μL) and T4 DNA ligase (1.0 μL). The final concentration of DNA oligomer was 0.24 mM. The reaction mixture was incubated at room temperature overnight. The ligation was assessed for completion by utilizing LC/MS and gel electrophoresis. The crude material **33** was purified by ethanol precipitation. Gel electrophoresis was performed with a 12-well 10% TBE acrylamide gel (Invitrogen) in 1X TBE buffer which was prepared in-house. The ligation mixture was diluted to the concentration of 12 ng/μL. The DNA loading sample was prepared by adding 10 μL of the diluted DNA sample and 2 μL of 6X DNA loading dye. The first lane of the gel was loaded with a DNA molecular weight ladder, and 5 μL of DNA-dye mixed samples was loaded into each lane. Gels were run at 160 V for 35 min and stained with 0.5 ng/mL ethidium bromide in 1X TBE buffer for 40 min. DNA fragments were visualized under a UV light device, and assessed for completed ligation. For smaller scale of ligation experiment, master-mix can be prepared by pre-mixing water, HEPES ligation buffer and DNA ligase before adding into the designated DNA starting material.

1e. Preparation of HP S2 from DTSU S1 for substrate preparation and library production.

All substrates were prepared with HP **S2** that was elaborated from DTSU **S1** through ligation of two duplexed 11-mer oligonucleotides (final sequence: 5' d TGA GTG AAT ACC TGC AT -Spacer 9-Amino C7-Spacer 9-ATG CAG GTA TTC ACT GAG G 3') and acylation of Fmoc-15-amino-4,7,10,13-tetraoxapentadecanoic acid with coupling reagent, DMTMM, and subsequent Fmoc deprotection with piperidine by the general procedures which yielded a longer linker with amine terminus. In the DNA stability and ligation test, two 39-mer duplexed oligonucleotides were used to prepare **31** through general ligation procedure (final sequence 5' d TAT GAT ACT AAA GTA AGT CAC ACA CAA TTG GAG CAG TCC TGA GTG AAT ACC TGC AT -Spacer 9-Amino C7- Spacer 9-ATG CAG GTA TTC ACT GAG GAC TGC TCC AAT TGT GTG TGA CTT ACT TTA GTA TCA TAT C 3').

1f. Representative chemical procedures for substrate preparation.

Acylation (DEPBT): To a 200 mM solution of carboxylic acid solution in MeCN (2.5 μL, 50 equiv) was added 50 equivalents of *N,N*-Diisopropyl-ethylamine (DIPEA, 2.5 μL, 200 mM in MeCN), and 50 equivalents of 3-(diethoxyphosphoryloxy)-1,2,3-benzotriazin-4(3H)-one (DEPBT, 2.5 μL, 200 mM in MeCN). The premixed mixture was allowed to stand at room temperature for 15 min before adding to a solution of on-DNA amine (10 μL, 1.0 mM in water) with 400 equivalents of pH 9.5 borate buffer (16 μL, 250 mM in water). The reaction was stirred at room temperature for 18 h, followed by being quenched by EtOH precipitation.

Acylation (HATU): A mixture of 100 equivalents of carboxylic acid solution (5 μL, 200 mM in MeCN), 100 equivalents of *N,N*-Diisopropyl-ethylamine (DIPEA, 5 μL, 200 mM in MeCN), and 100 equivalents of *O*-(7-Azabenzotriazol-1-yl)-*N,N,N',N'*-tetramethyluronium hexafluorophosphate (HATU, 5 μL, 200 mM in DMA) was allowed to stand at room temperature for 15 min. The premixed mixture was added to a solution of on-DNA amine (10 μL, 1.0 mM in water) with 500 equivalents of pH 8.2 borate buffer (20 μL, 250 mM in water). The reaction was shaken at room temperature for 18 h, followed by being quenched by EtOH precipitation.

Acylation (DMTMM): To a solution of on-DNA amine (10 μL, 1.0 mM in water) in 400 equivalents of pH 9.5 borate buffer (16 μL, 250 mM in water) was added 50 equivalents of carboxylic acid solution (2.5 μL, 200 mM in MeCN) and 50 equivalents of 4-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-methylmorpholinium chloride (DMTMM, 2.5 μL, 200 mM in water). The reaction was shaken at room temperature for 18 h and then quenched by EtOH precipitation.

Reductive amination ($NaBH_4$): To a solution of on-DNA amine (47.6 nmol, 50 μL, solution in water) in pH 9.5 borate buffer (23800 nmol, 95 μL, 500 equiv), additional acetonitrile (20 μL) and 100 equivalents of aldehyde building block (23.8 μL, 200 mM in MeCN) were added. The solution was allowed to sit at room temperature for 1 h. $NaBH_4$ (47.6 μL, 100 equiv, 100 mM in MeCN) was added and the reaction was incubated at room temperature for 18 h. The reactions were then assessed for completion and purified by EtOH precipitation.

Reductive Alkylation ($NaCNBH_3$): An aldehyde building block (1000 nmol, 5 μL, 200 mM in MeCN, 100 equiv) was added to a solution of on-DNA amine (10 μL, 1.0 mM in water) in H_2O with pH 5.5 phosphate buffer (4000 nmol, 16 μL, 250 mM, 400 equiv) followed by a solution of $NaCNBH_3$ (400 nmol, 2 μL, 200 mM in H_2O, 40 equiv) which was allowed to stir at 45 °C for 16 h before being quenched by EtOH precipitation.

Nucleophilic Aromatic Substitution: To a solution of on-DNA amine (10 μL, 1.0 mM in water) in 400 equivalents of pH 9.5 borate buffer (16 μL, 250 mM in water) was added 100 equivalents of aryl halide (5 μL, 200 mM in MeCN). The reaction was heated at 60 °C for 18 h before being quenched by EtOH precipitation.

***N*-Fmoc deprotection:** To a solution of *N*-Fmoc DNA (10 nmol, 10 μL, 1.0 mM, 1 equiv) in H_2O was added 500 equivalents of 10% (*v/v*) aq. piperidine (5 μL). The reaction was incubated at room temperature for 4 h. The solution was diluted with H_2O (40 μL) and then quenched by EtOH precipitation.

***N*-Boc deprotection**: To a solution of *N*-Boc DNA (10 nmol, 10 μL, 1.0 mM, 1 equiv) in H_2O with pH 9.5 borate buffer (4000 nmol, 16 μL, 250 mM, 400 equiv), additional H_2O (60 μL) was added and the reaction was heated at 80 °C for 36 h before being quenched by EtOH precipitation.

Nitro Reduction (sodium dithionite)[1]: To a solution of nitro-containing DNA conjugate (10 μL, 1.0 mM in water) was added sequentially 250 equivalents of pH 9.5 borate buffer (10 μL, 250 mM in water), 10 equivalents of methyl viologen (1 μL, 100 mM in water) and 100 equivalents of $Na_2S_2O_4$ (5 μL, 200 mM in water). The reaction mixture was heated at 80 °C for 15 minutes. The reaction mixture was then cooled to room temperature before being quenched and purified with EtOH precipitation.

Hydroxycarbonylation[6]: To a solution of aryl bromide DNA conjugate (10 μL, 1 mM in water) was added 400 equivalents of CsOH solution (10 μL, 400 mM in water) and 100 equivalents of molybdenum hexacarbonyl solution (5 μL, 200 mM in MIPO, sonicated for 20 minutes before using). The mixture was allowed to pipette mixed thoroughly before adding 12 equivalents of sSPhosPd G2 catalyst solution (6 μL, 20 mM in MIPO). The reaction was heated at 80 °C for 15 minutes and cooled to room temperature, followed by EtOH precipitation for quenching and purification.

2. C–N coupling

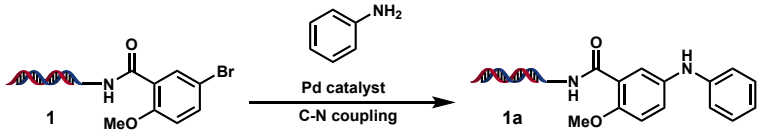
2a) Preparation of aryl halide substrates. From HP **S2**, compound **1, 5, 8, 12, 15, 16, 19, 27, 29** were prepared with the appropriate acid building block through the general acylation procedure with DEPBT; compound **3, 11, 20, 21, 22** were prepared with the appropriate acid building block through the general acylation procedure with HATU; compound **2, 4, 6, 9, 13, 14, 18, 30** were prepared with the appropriate acid building block through the general acylation procedure with DMTMM, where **30** underwent subsequent hydroxycarbonylation procedure; **17, 23, 24, 25, 26, 28** were prepared from the general nucleophilic aromatic substitution procedure, where **28** underwent

further nitro reduction with sodium dithionite; compound **7** was prepared using reductive alkylation with sodium borohydride, and **10** was prepared using reductive alkylation with sodium cyanoborohydride.

2b) General procedure for C–N coupling. To a solution of DNA-conjugated aryl halide substrate (10 μL, 10 nmol, 1.0 mM in water) was added DMA (3.5 μL), 1000 equivalents of CsOH (5 μL, 2000 mM in water), 500 equivalents of amines (12.5 μL, 400 mM in DMA) and 20 equivalents of freshly prepared sodium ascorbate (5 μL, 40 mM in water). The mixture was thoroughly pipette mixed before adding 2 equivalents of freshly prepared Pd-PEPPSI-iPent^{Cl}-pyr (4 μL, 5 mM in DMA). The reaction mixture was heated at 95 °C for 15 minutes, followed by the addition of 100 equivalents of scavenger, sodium L-cysteine (5 μL, 200 mM in water) and heated at 80 °C for another 15 minutes. The mixture was then cooled to room temperature before assessing with LC-MS or EtOH precipitation. PEPPSI catalysts used in this study were synthesized via known procedures[3] and/or purchased from either Total Synthesis Ltd. or Sigma-Aldrich and used without further purification. While conducting a subsequent ligation, insurance of maximum removal of residual building blocks or salts before ligation was necessary as large amount of residue may influence ligation efficiency. For best results, run reactions in a PCR plate and transfer to a preheated thermocycler at 95 °C immediately upon completion of pipette mixing and foil plate sealing.

3. Deconvoluted Mass Spectra of C–N coupling optimizing conditions

Table S1. The screening of palladium catalyst and solvent.[a]



Entry	condition	Conv.
1[b]	*t*BuXPhos Pd G1, CsOH	75%
2[c]	*t*BuXPhos Pd G3, NaOH	30%
3[d]	BrettPhos Pd G3, CsOH	33%
4[e]	BrettPhos Pd G3, CsOH	0%
5[f]	BrettPhos Pd G3, CsOH	6%
6[g]	Pd-PEPPSI-*i*Pent^{Cl}, CsOH	0%
7[h]	Pd-PEPPSI-*i*Pent^{Cl}, CsOH	14%
8[i]	Pd-PEPPSI-*i*Pent^{Cl}, CsOH, Na ascorbate	57%
9[j]	Pd-PEPPSI-*i*Pent^{Cl}, CsOH, Na ascorbate	63%

[a]The conversion was determined by LC-MS. [b]Condition was previously reported by GSK[10]. [c]Condition was previously reported by Eli Lilly[11]. [d]Condition was previously reported[4]. [e]Reaction condition: 5 nmol **1**, 250 equiv. of aniline (3.1 μL, 400 mM in MIPO), 2 equiv. of Pd catalyst (2 μL, 5 mM in MIPO), 500 equiv. of CsOH (2.5 μL, 1000 mM in water), H_2O (2.5 μL), MIPO (4.9 μL), 95 °C, 25 min. [f]Same reaction condition with e with alteration of solvent to DMA. [g]Reaction condition: 5 nmol **1**, 250 equiv. of aniline (3.1 μL, 400 mM in MIPO), 2 equiv. of Pd catalyst (2 μL, 5 mM in MIPO), 500 equiv. of CsOH (2.5 μL, 1000 mM in water), H_2O (2.5 μL), MIPO (4.9 μL) 95 °C, 25 min. [h]Same reaction condition with g with alteration of solvent to DMA. [i]Reaction condition: 5 nmol **1**, 250 equiv. of aniline (3.1 μL, 400 mM in DMA), 2 equiv. of Pd catalyst (2 μL, 5 mM in DMA), 500 equiv. of CsOH (2.5 μL, 1000 mM in water), 20 equiv. of sodium ascorbate (2.5 μL, 40 mM in water), DMA (4.9 μL) 95 °C, 25 min. [j]Same reaction condition with i with alteration of reaction time to 15 minutes. [k]DMA = dimethylacetamide. [l]MIPO = methoxyisopropanol.

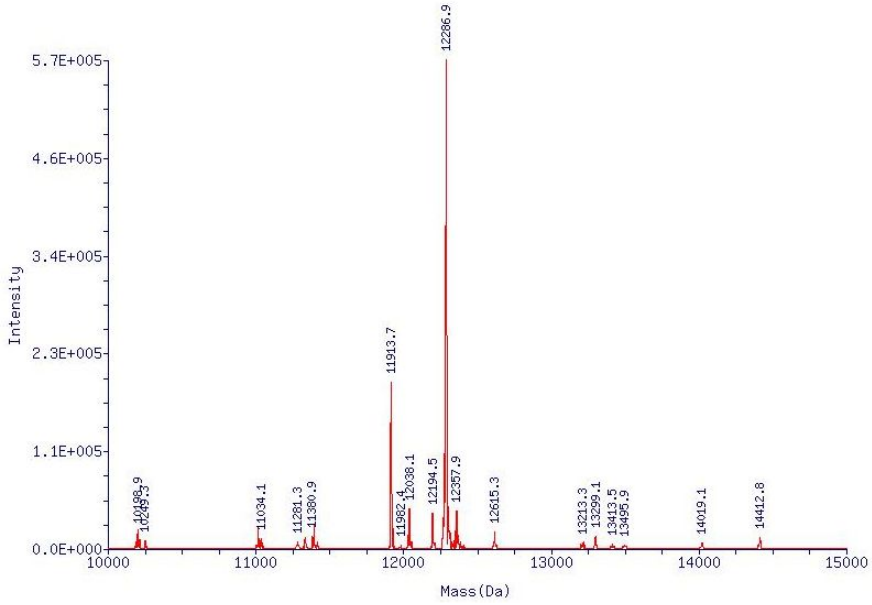


Figure S2. Deconvoluted mass spectrum of result in entry 1, table S1.

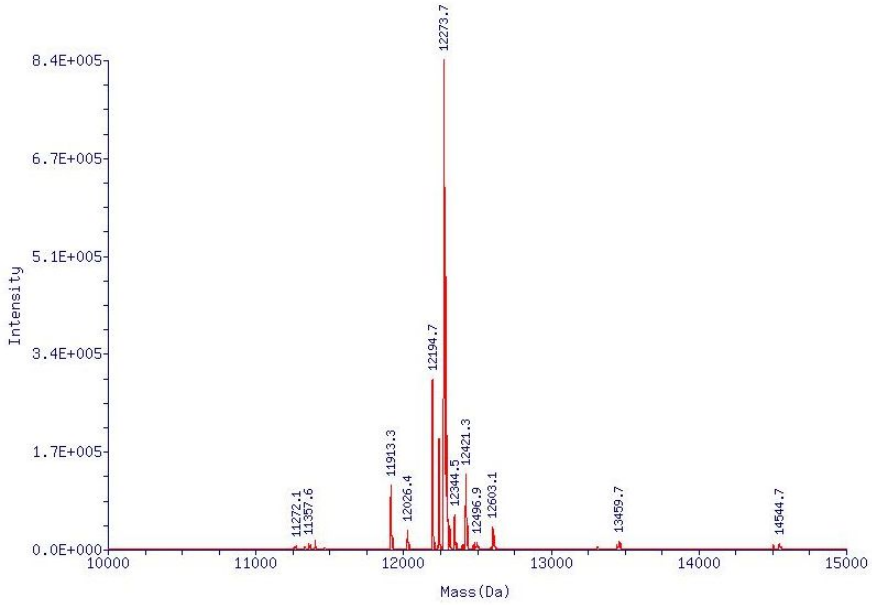


Figure S3. Deconvoluted mass spectrum of result in entry 2, table S1.

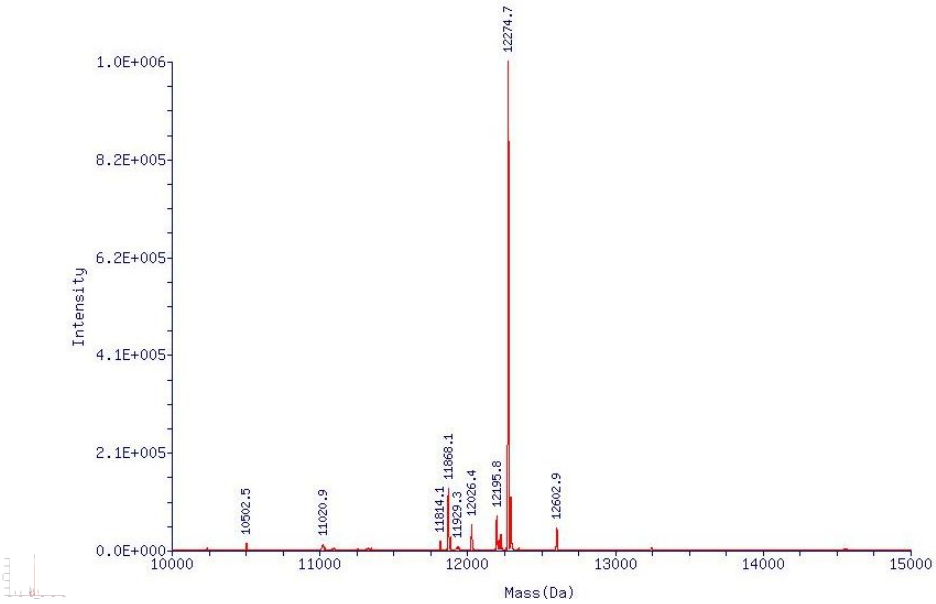


Figure S4. Deconvoluted mass spectrum of result in entry 4, table S1.

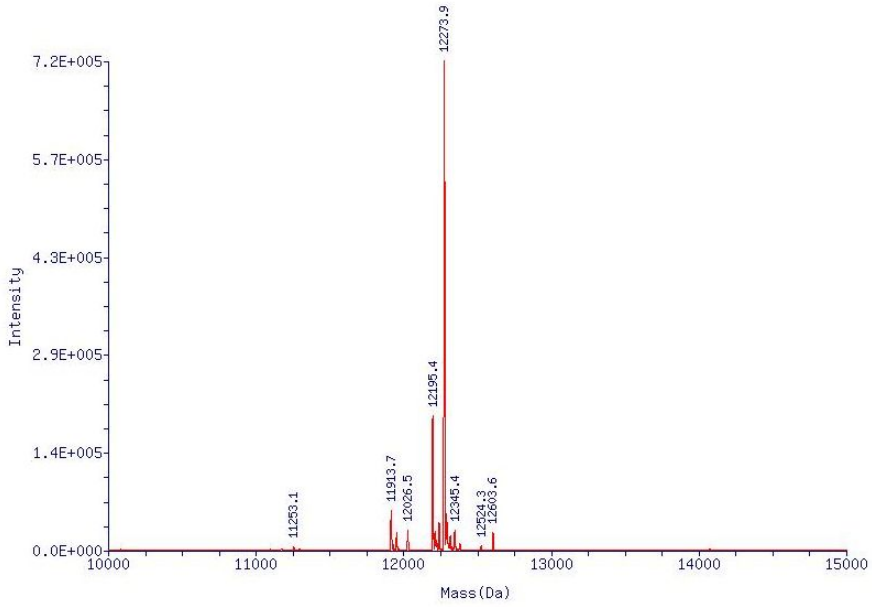


Figure S5. Deconvoluted mass spectrum of result in entry 5, table S1.

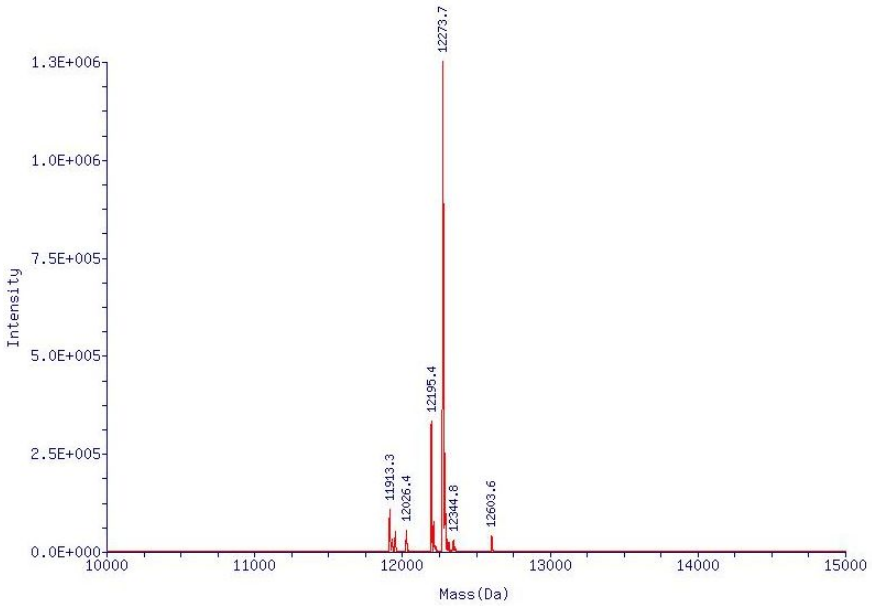


Figure S6. Deconvoluted mass spectrum of result in entry 6, table S1.

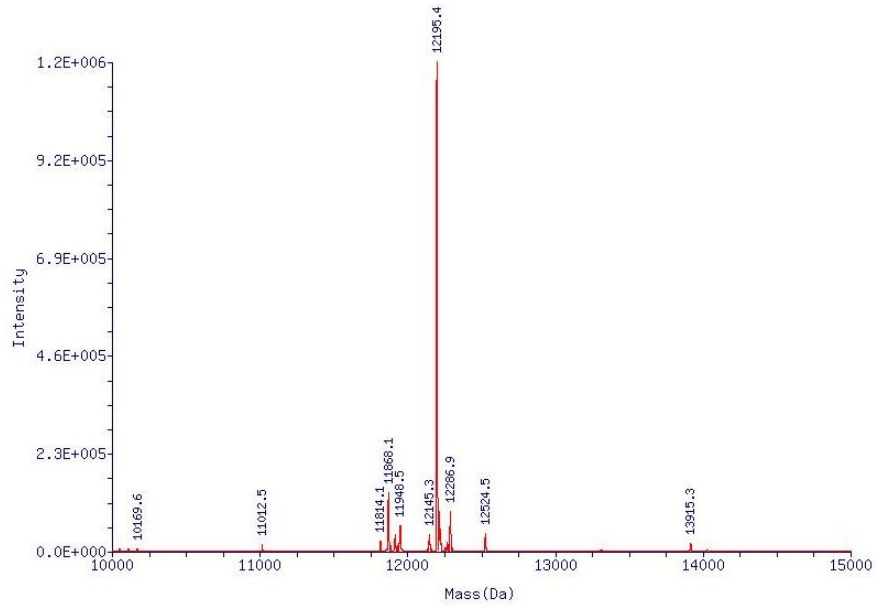


Figure S7. Deconvoluted mass spectrum of result in entry 7, table S1.

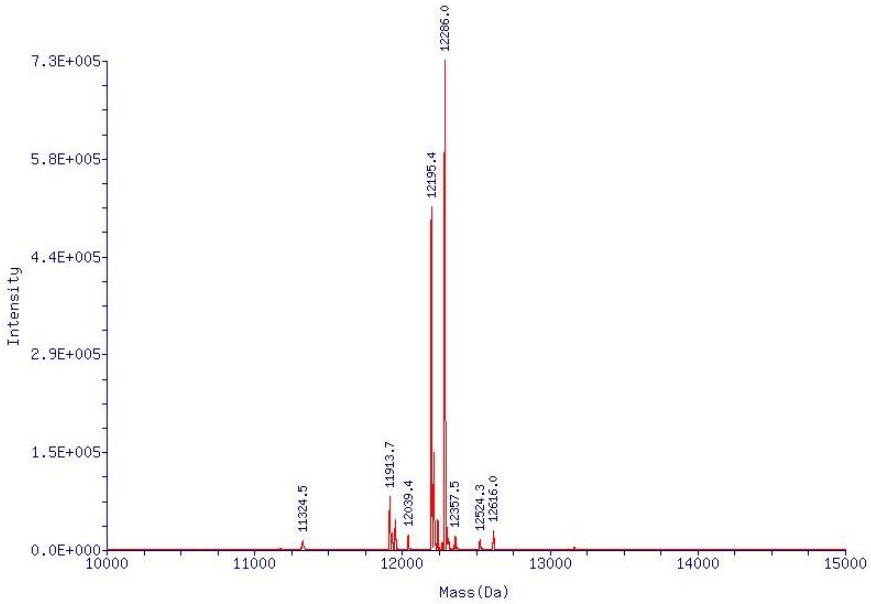


Figure S8. Deconvoluted mass spectrum of result in entry 8, table S1.

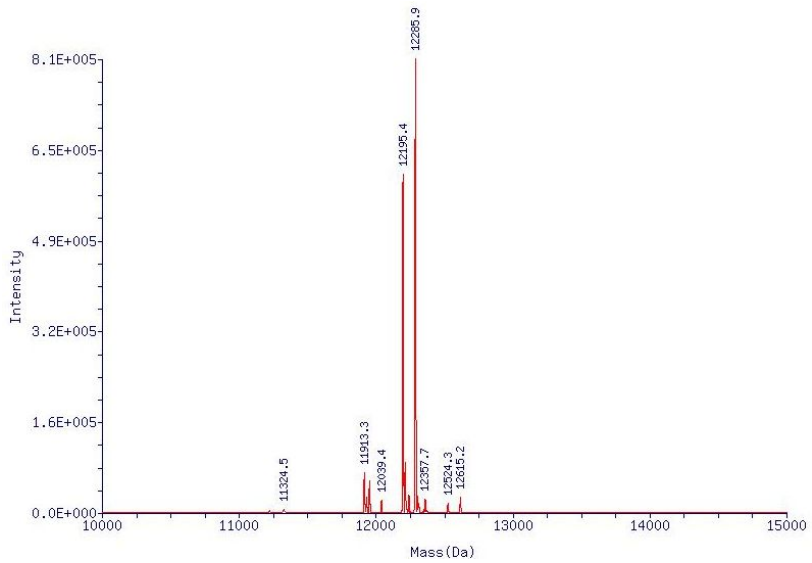
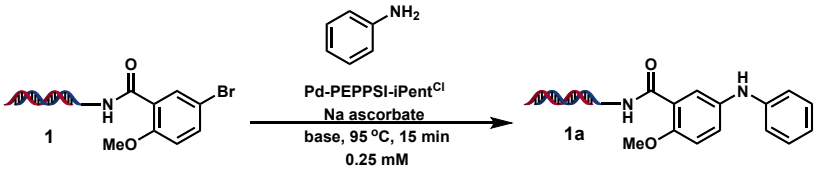


Figure S9. Deconvoluted mass spectrum of result in entry 9, table S1.

Table S2. Optimization of various parameters.[a]



Entry	Aniline (equiv)	Pd (equiv)	Na ascorbate (equiv)	Base (equiv)	Conv.
1	250	2	20	CsOH, 500	63%
2	250	2	40	CsOH, 500	63%
3	250	5	50	CsOH, 500	59%
4	250	1	5	CsOH, 500	0%
5	250	1	10	CsOH, 500	20
6	250	1	20	CsOH, 500	53%
7	250	2	20	Cs_2CO_3, 500	32%
8	250	2	20	pH 9.5 borate buffer, 500	0%
9[b]	250	2	20	CsOH, 500	0%
10[c]	250	2	20	CsOH, 500	63%
11[d]	250	2	20	CsOH, 500	56%
12[e]	250	2	20	CsOH, 500	0%
13	250	2	20	CsOH, 750	66%
14	250	2	20	CsOH, 1000	67%
15	**500**	**2**	**20**	**CsOH, 1000**	**80%**

[a]The conversion was determined by LC-MS. [b]The condition was carried out at 80 °C. [c]The reaction was run for 5 min. [d]The reaction was run for 60 min. [e]The reaction concentration was 0.05 mM.

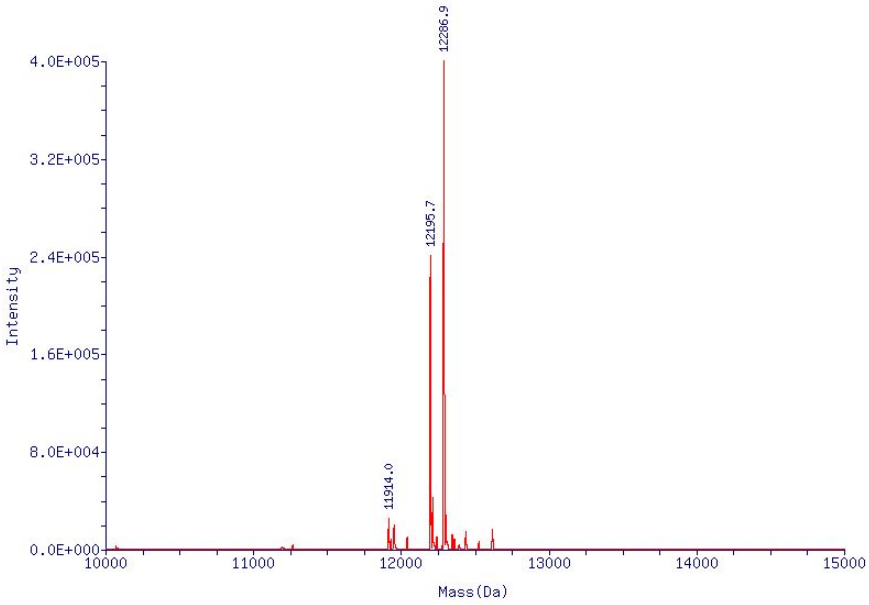


Figure S10. Deconvoluted mass spectrum of result in entry 1, table S2.

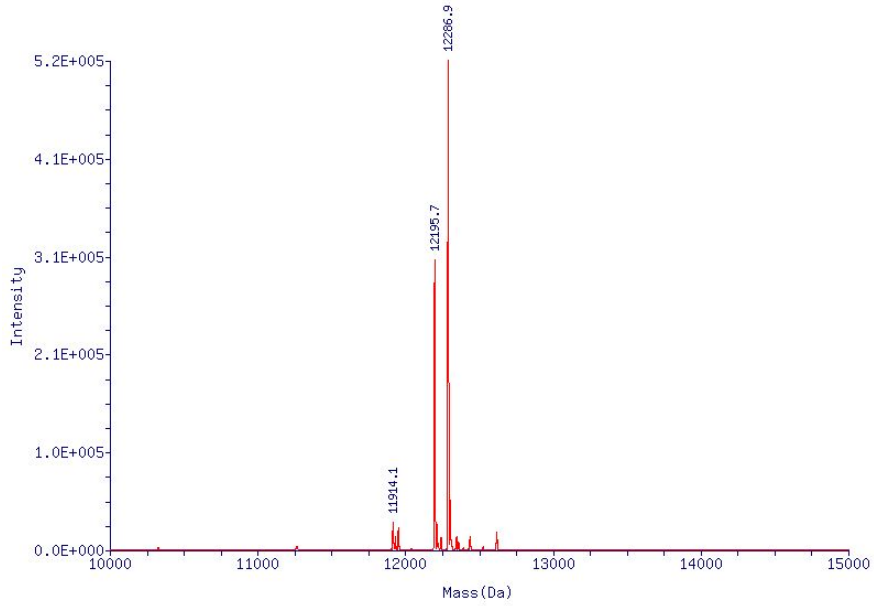


Figure S11. Deconvoluted mass spectrum of result in entry 2, table S2.

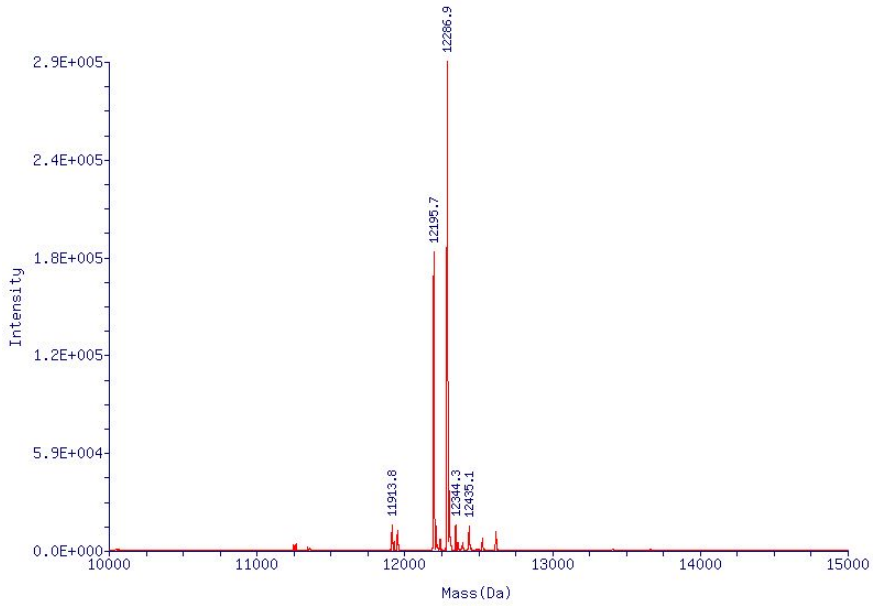


Figure S12. Deconvoluted mass spectrum of result in entry 3, table S2.

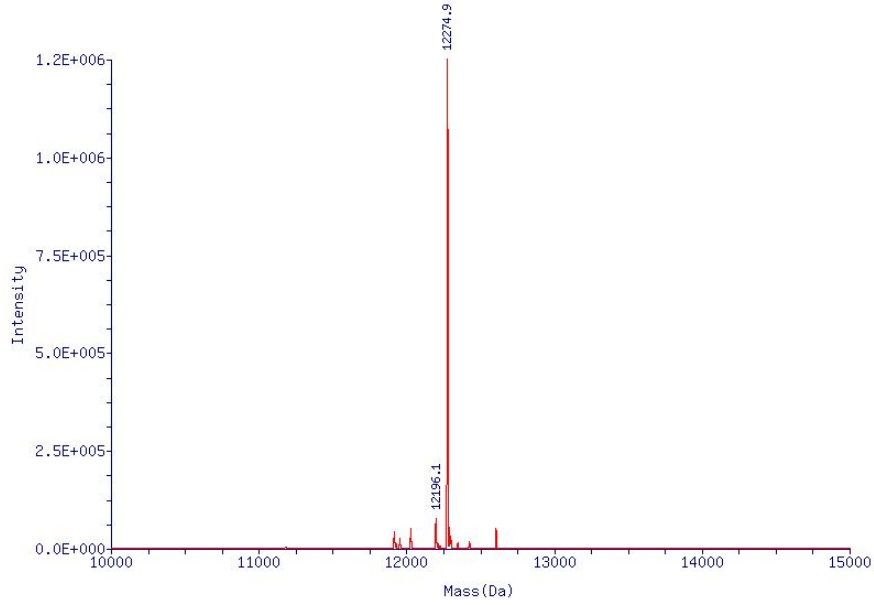


Figure S13. Deconvoluted mass spectrum of result in entry 4, table S2.

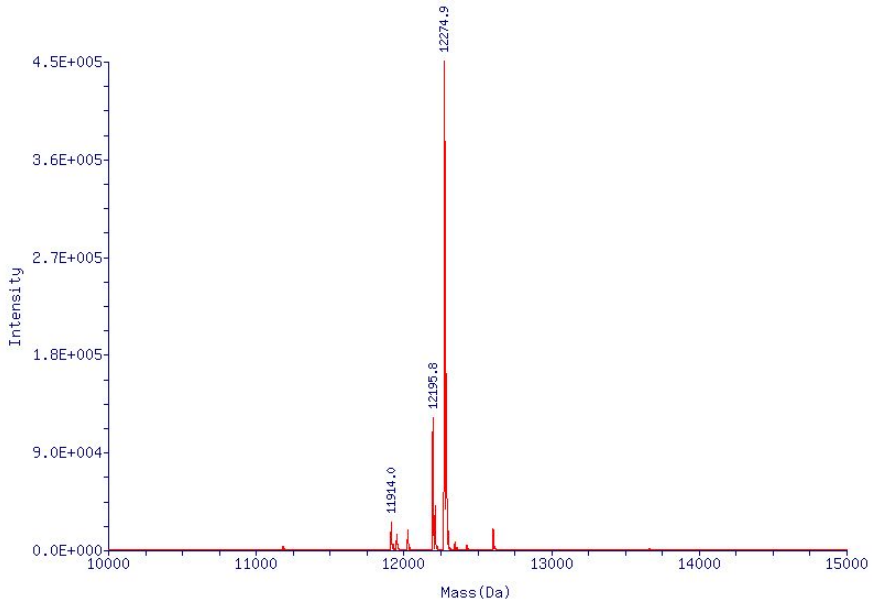


Figure S14. Deconvoluted mass spectrum of result in entry 5, table S2.

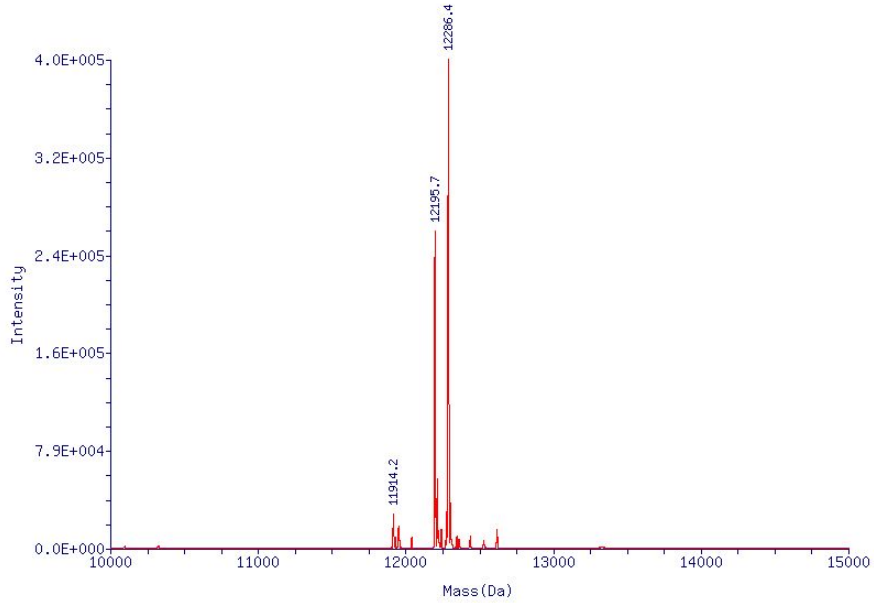


Figure S15. Deconvoluted mass spectrum of result in entry 6, table S2.

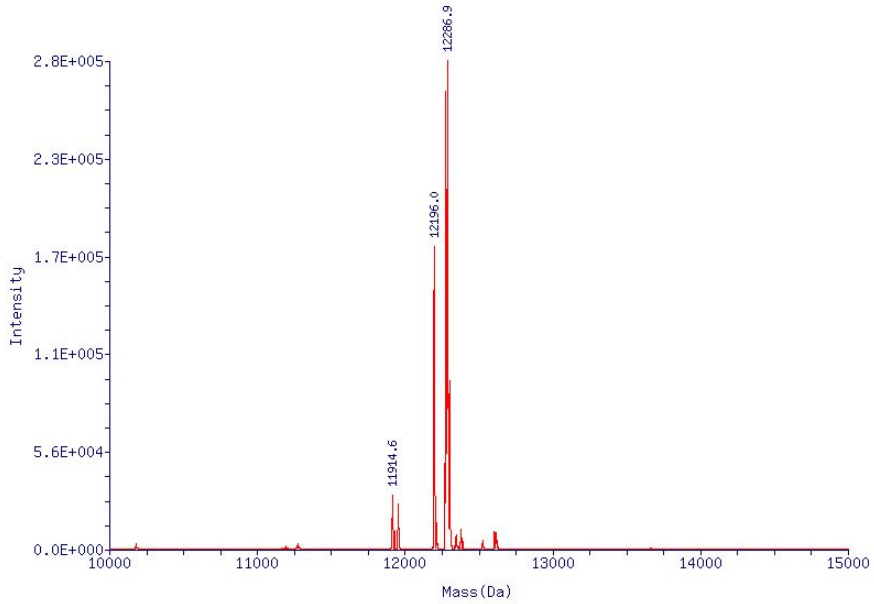


Figure S16. Deconvoluted mass spectrum of result in entry 7, table S2.

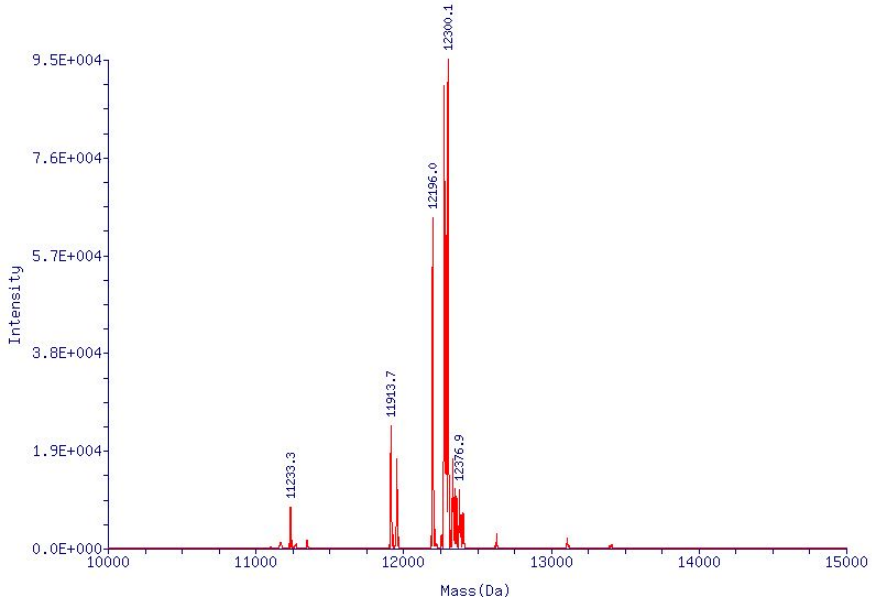


Figure S17. Deconvoluted mass spectrum of result in entry 8, table S2.

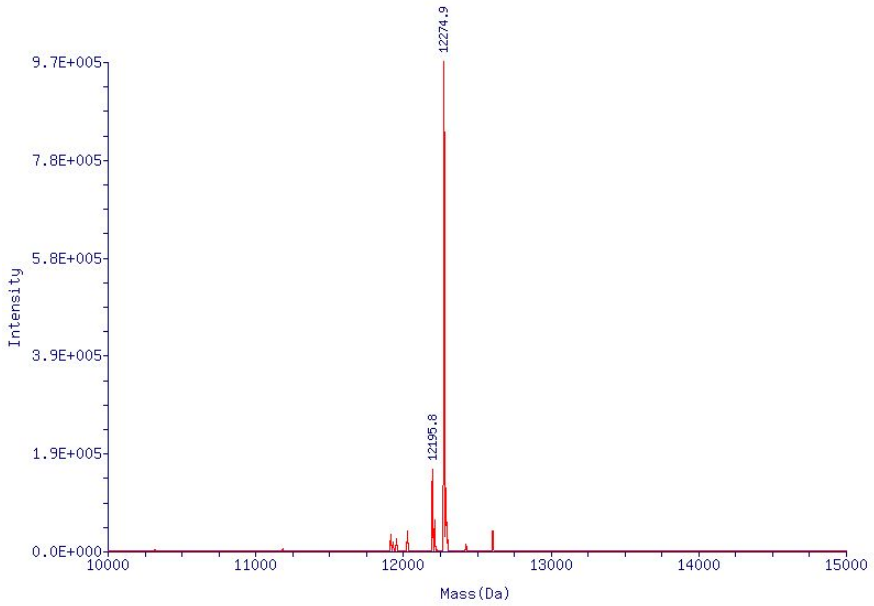


Figure S18. Deconvoluted mass spectrum of result in entry 9, table S2.

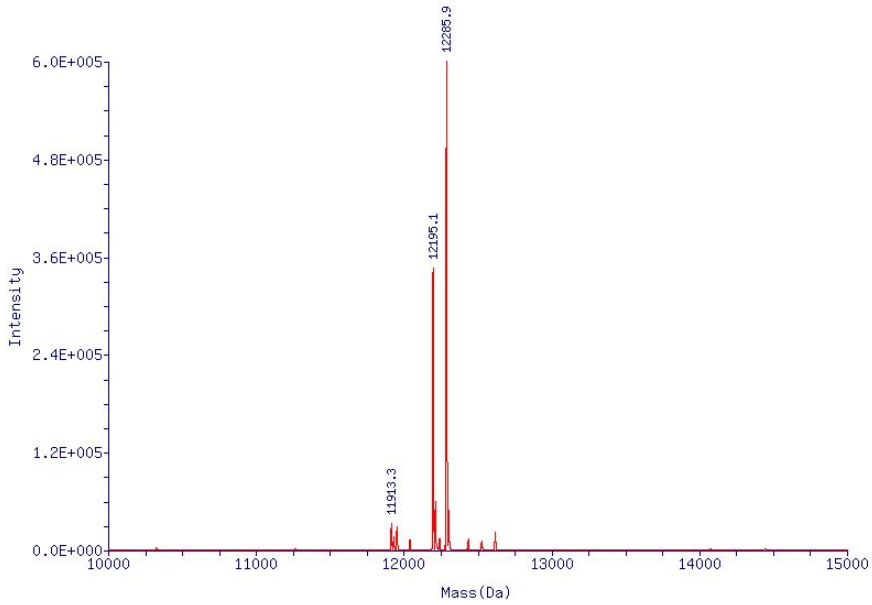


Figure S19. Deconvoluted mass spectrum of result in entry 10, table S2.

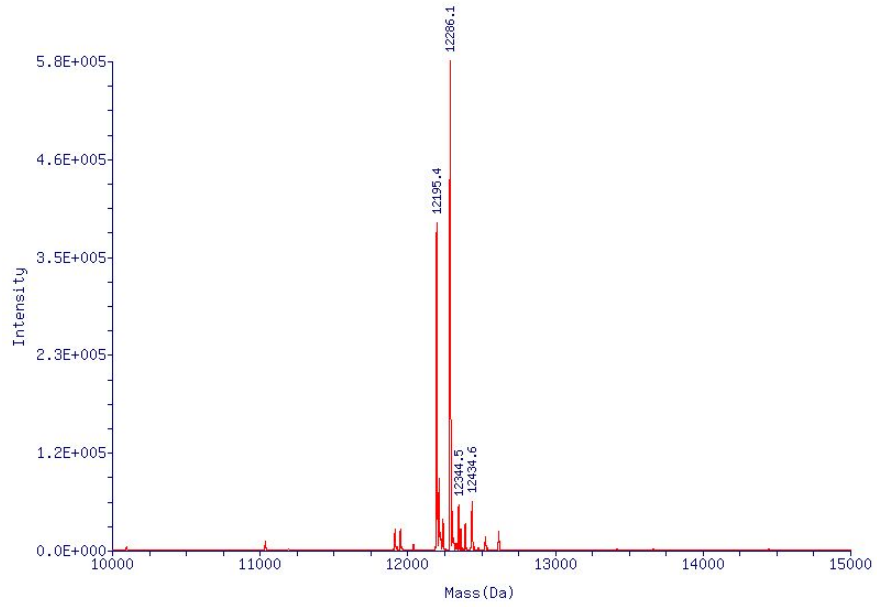


Figure S20. Deconvoluted mass spectrum of result in entry 11, table S2.

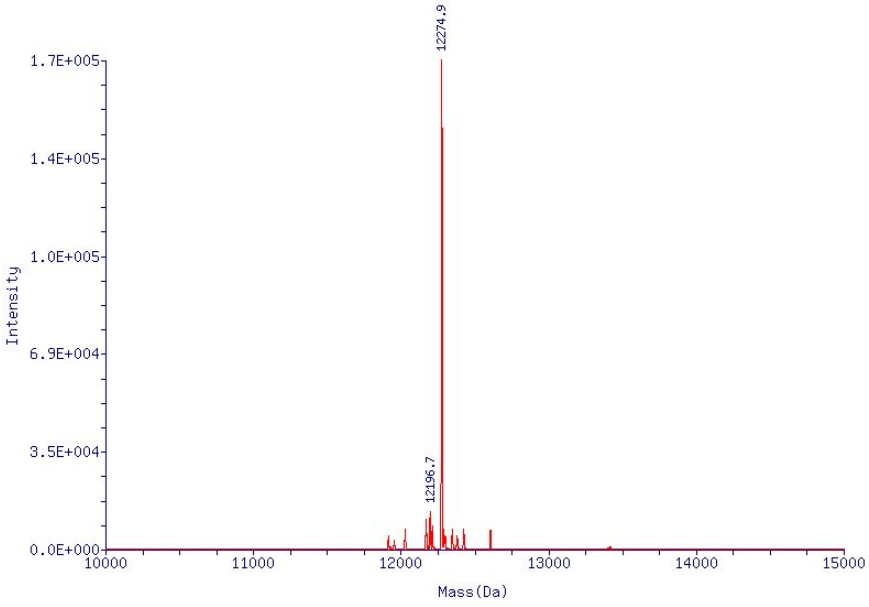


Figure S21. Deconvoluted mass spectrum of result in entry 12, table S2.

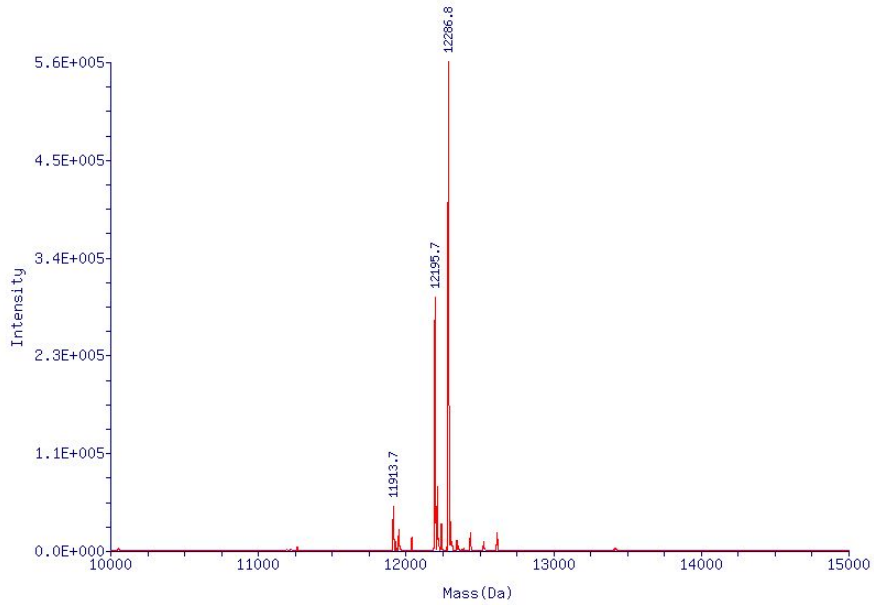


Figure S22. Deconvoluted mass spectrum of result in entry 13, table S2.

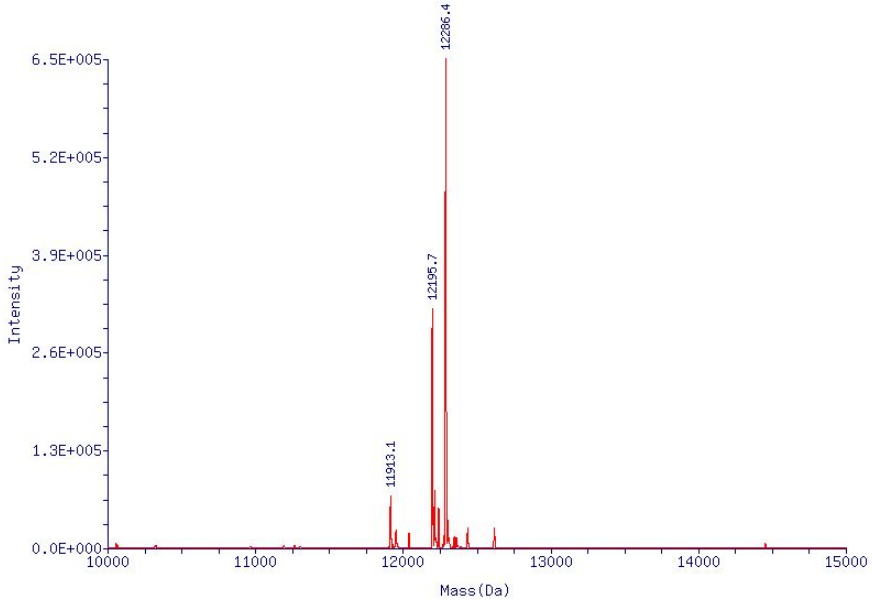


Figure S23. Deconvoluted mass spectrum of result in entry 14, table S2.

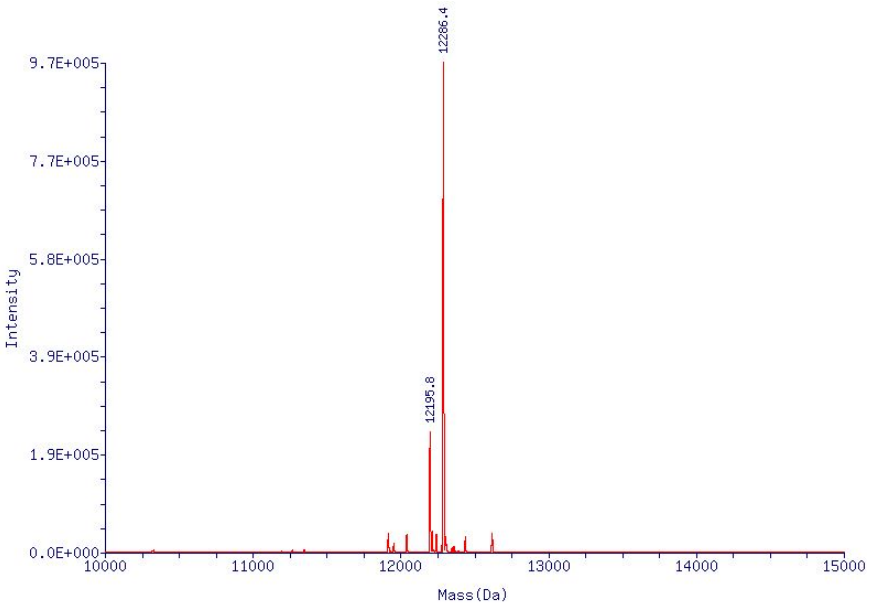
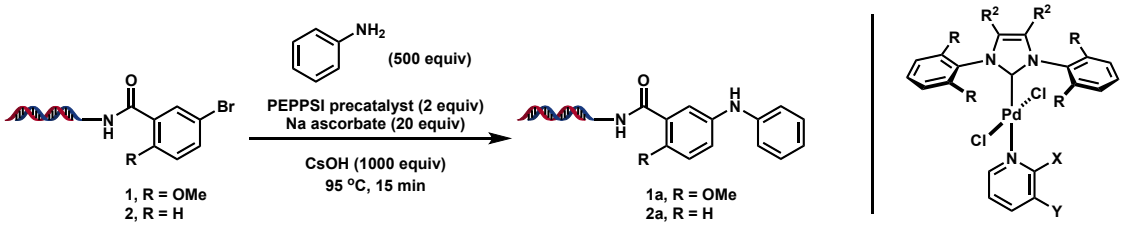


Figure S24. Deconvoluted mass spectrum of result in entry 15, table S2.

Table S3. Screening PEPPSI analogues for C–N coupling.[a]



Entry	NHC catalyst	R^1	R^2	X	Y	**1a**	**2a**
1	Pd-PEPPSI-iPr	*i*-Pr	H	H	Cl	0%	0%
2	Pd-PEPPSI-iPent	*i*-Pent	H	H	Cl	0%	0%
3	Pd-PEPPSI-iHept	*i*-Hept	H	H	Cl	0%	0%
4	Pd-PEPPSI-SIPr	*i*-Pr	H[b]	H	Cl	0%	0%
5	Pd-PEPPSI-iPr^{Cl}	*i*-Pr	Cl	H	Cl	0%	0%
6	Pd-PEPPSI-iPent^{Cl}	*i*-Pent	Cl	H	Cl	80%	92%
7	Pd-PEPPSI-iPent^{Cl}-*o*-picoline	*i*-Pent	Cl	Me	H	69%	91%
8	Pd-PEPPSI-iPent^{Cl}-pyr	*i*-Pent	Cl	H	H	78%	91%
9	Pd-PEPPSI-iHept^{Cl}	*i*-Hept	Cl	H	Cl	80%	90%

[a]The conversion was determined by LC-MS. [b]PEPPSI-SIPr has saturated NHC ring.

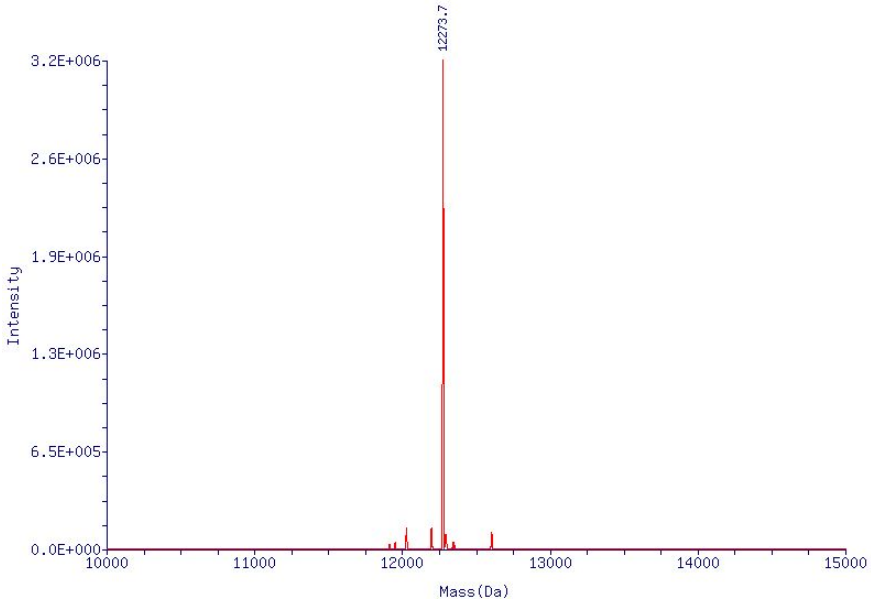


Figure S25. Deconvoluted mass spectrum of result for **1a** in entry 1, table S3.

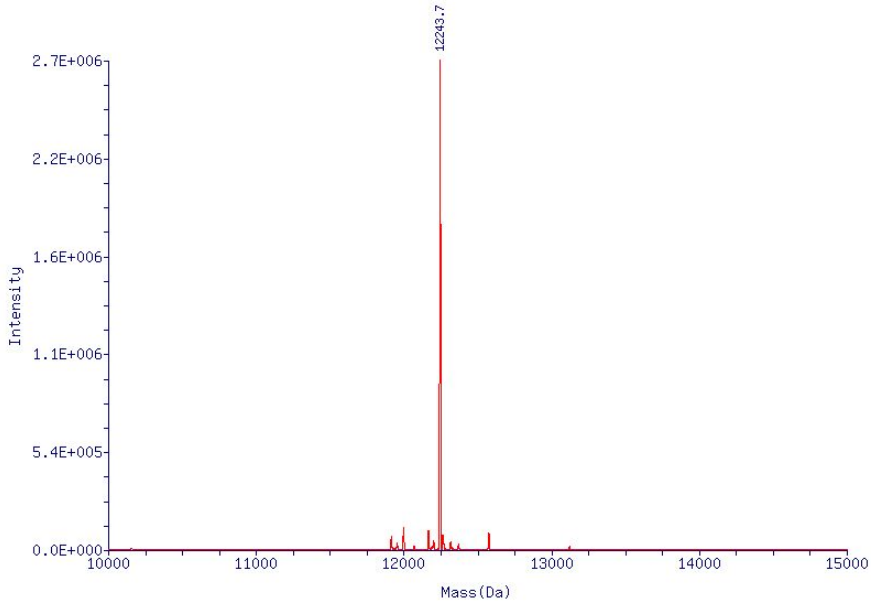


Figure S26. Deconvoluted mass spectrum of result for **2a** in entry 1, table S3.

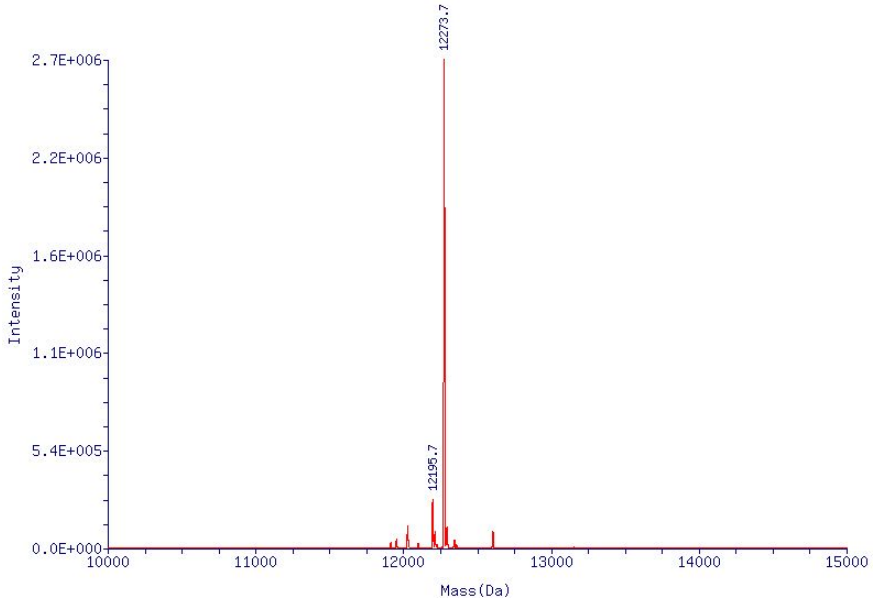


Figure S27. Deconvoluted mass spectrum of result for **1a** in entry 2, table S3.

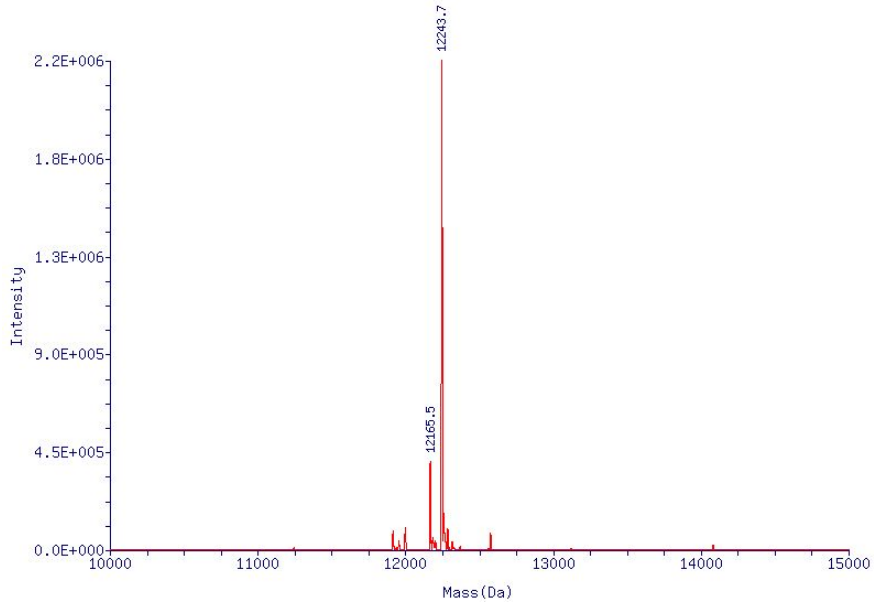


Figure S28. Deconvoluted mass spectrum of result for **2a** in entry 2, table S3.

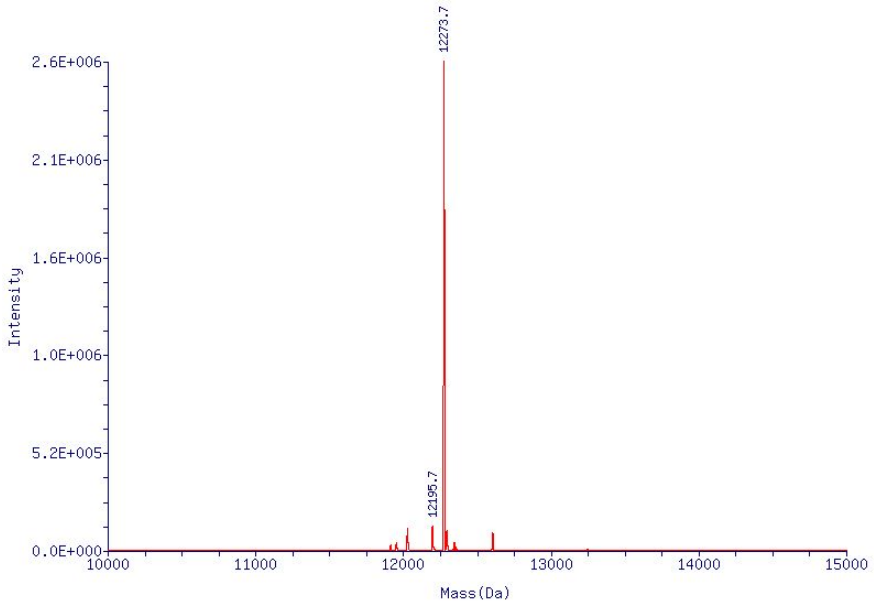


Figure S29. Deconvoluted mass spectrum of result for **1a** in entry 4, table S3.

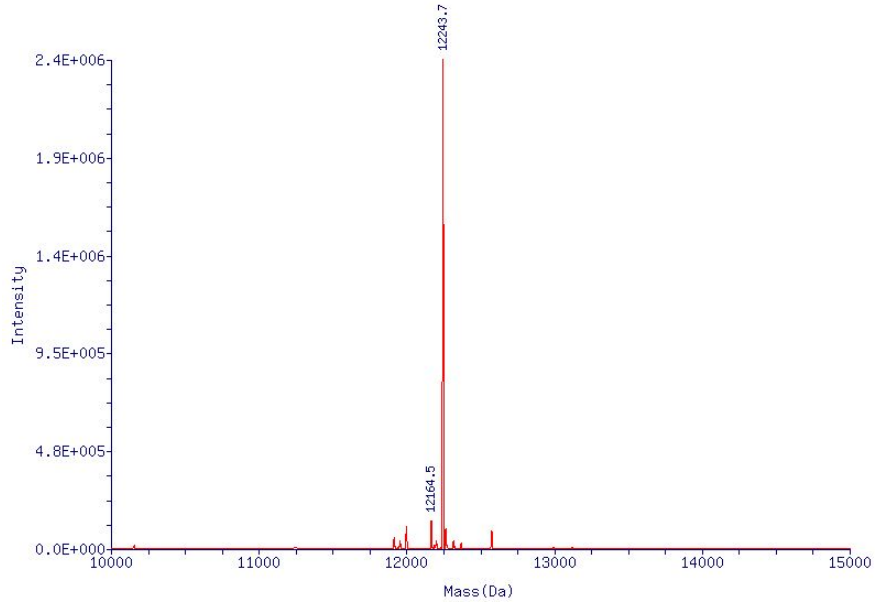


Figure S30. Deconvoluted mass spectrum of result for **2a** in entry 4, table S3.

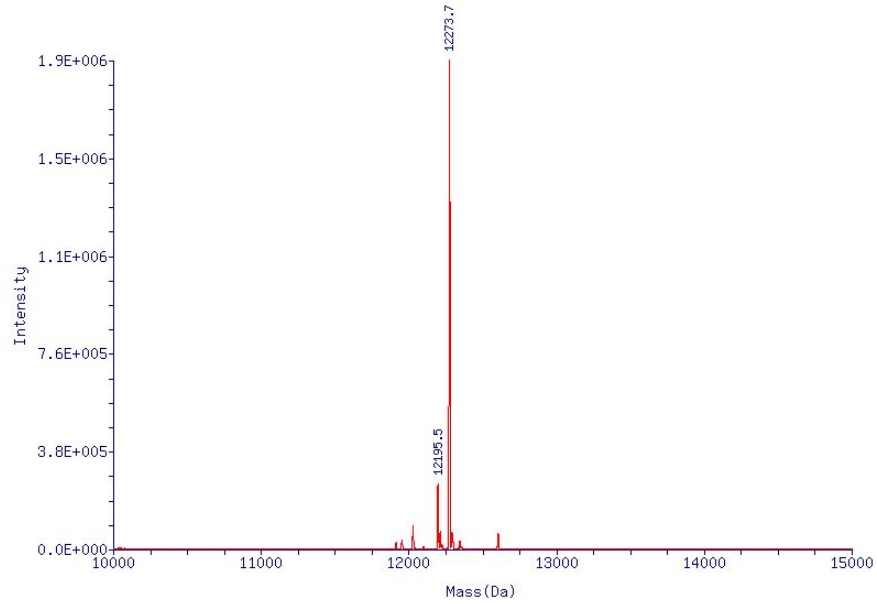


Figure S31. Deconvoluted mass spectrum of result for **1a** in entry 5, table S3.

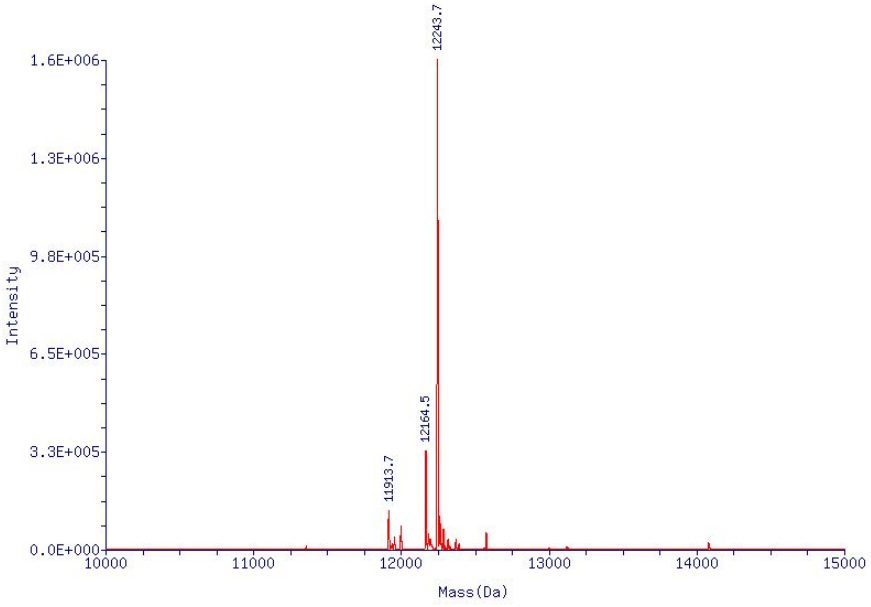


Figure S32. Deconvoluted mass spectrum of result for **2a** in entry 5, table S3.

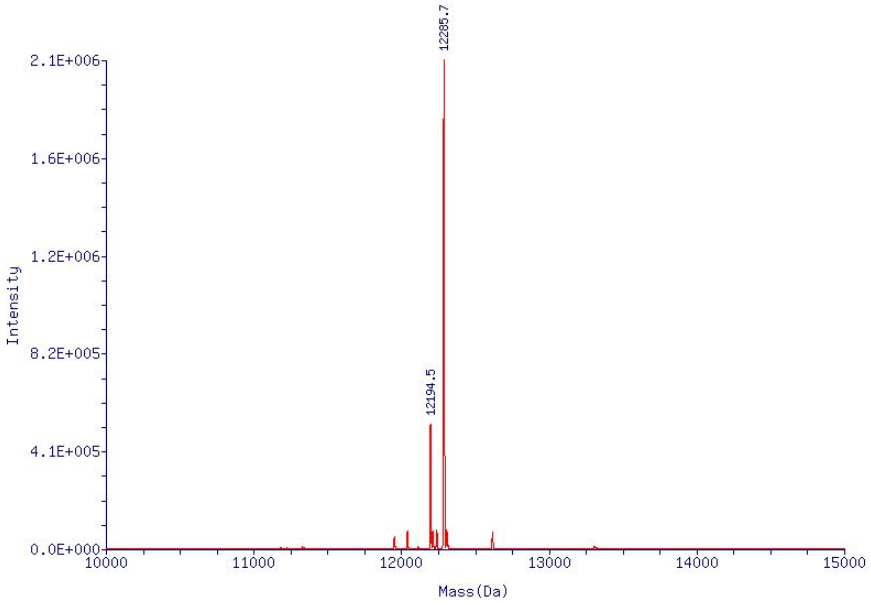


Figure S33. Deconvoluted mass spectrum of result for **1a** in entry 6, table S3.

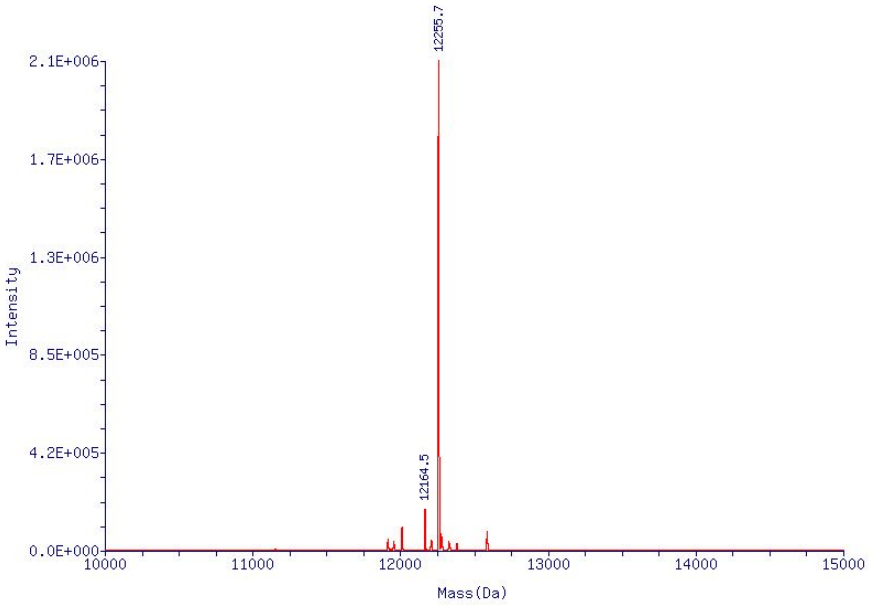


Figure S34. Deconvoluted mass spectrum of result for **2a** in entry 6, table S3.

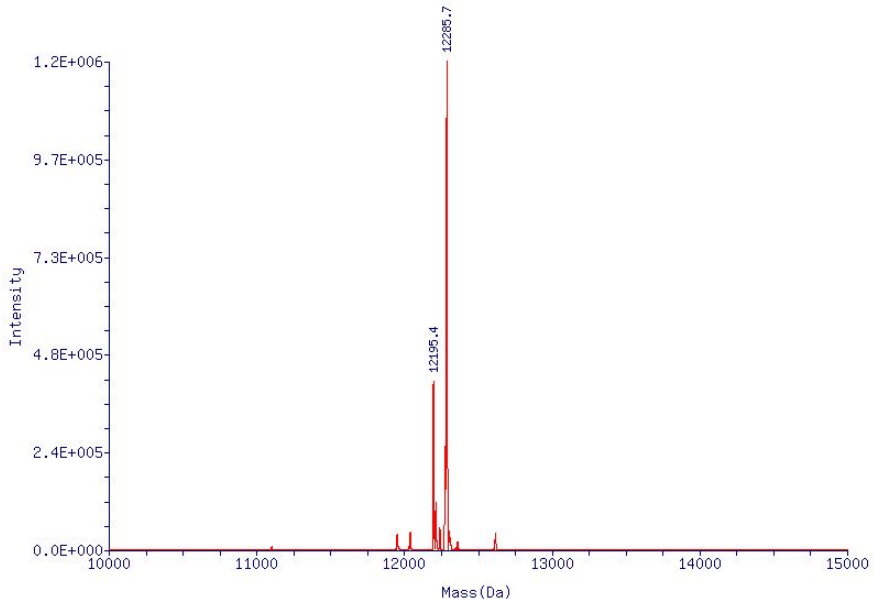


Figure S35. Deconvoluted mass spectrum of result for **1a** in entry 7, table S3.

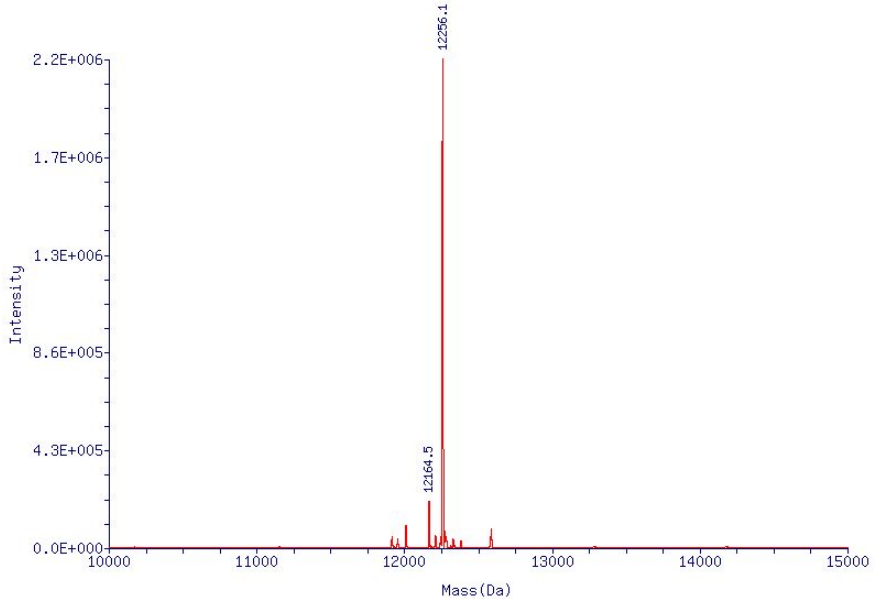


Figure S36. Deconvoluted mass spectrum of result for **2a** in entry 7, table S3.

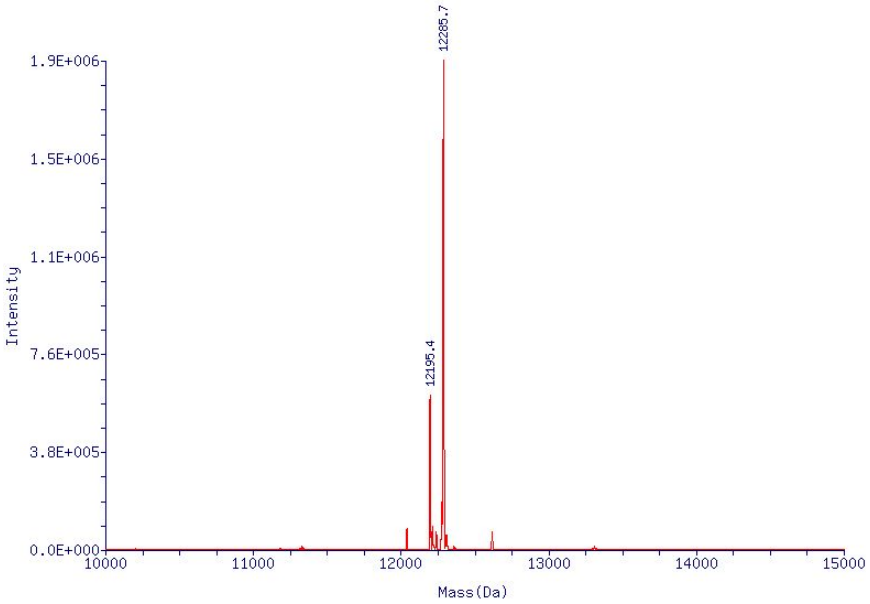


Figure S37. Deconvoluted mass spectrum of result for **1a** in entry 8, table S3.

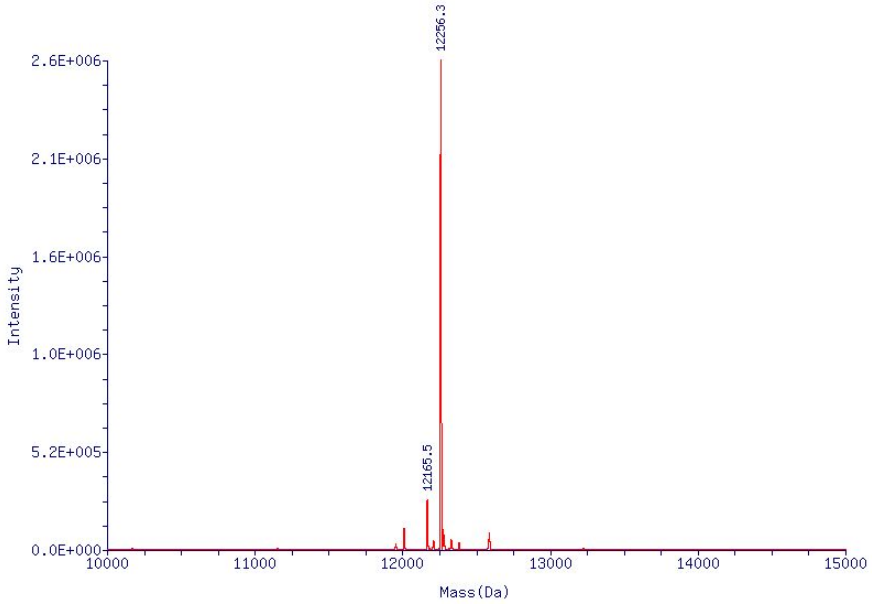


Figure S38. Deconvoluted mass spectrum of result for **2a** in entry 8, table S3.

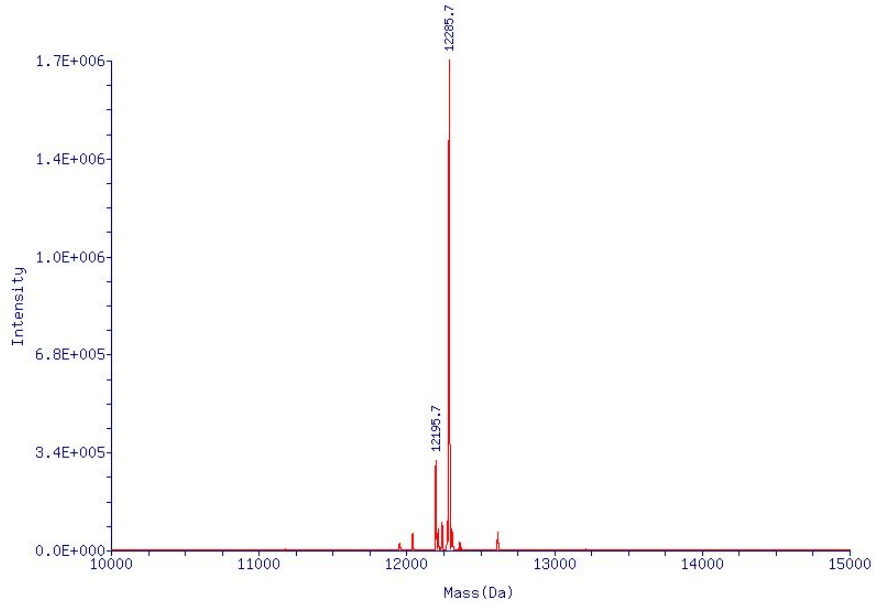


Figure S39. Deconvoluted mass spectrum of result for **1a** in entry 9, table S3.

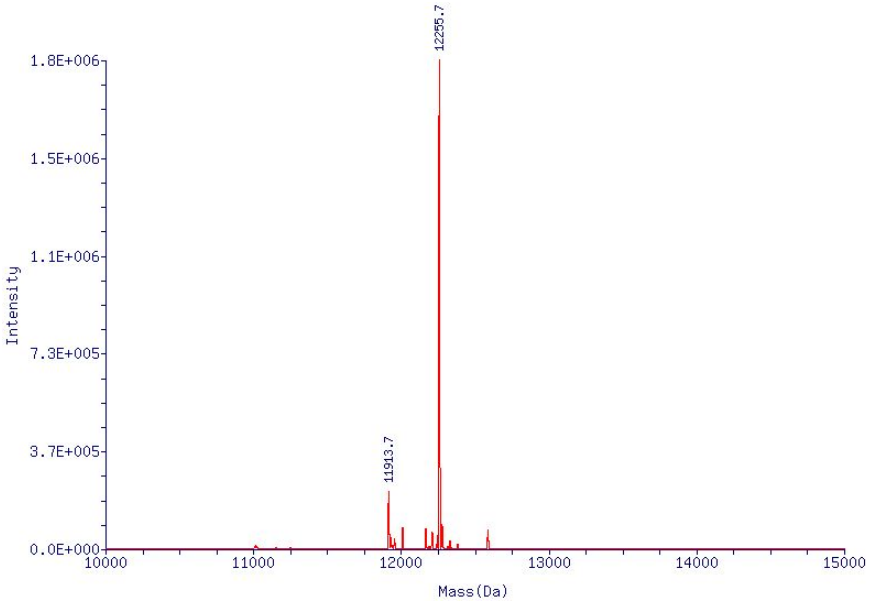


Figure S40. Deconvoluted mass spectrum of result for **2a** in entry 9, table S3.

4. Deconvoluted Mass Spectra of DNA-conjugated aryl halide substrates

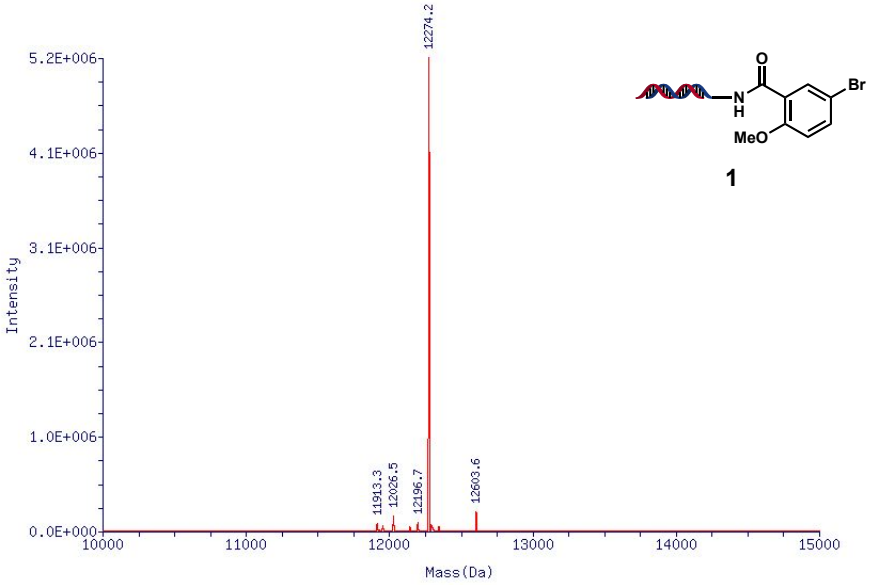


Figure S41. Deconvoluted mass spectrum of DNA **1**, expected: 12273; observed 12274.2.

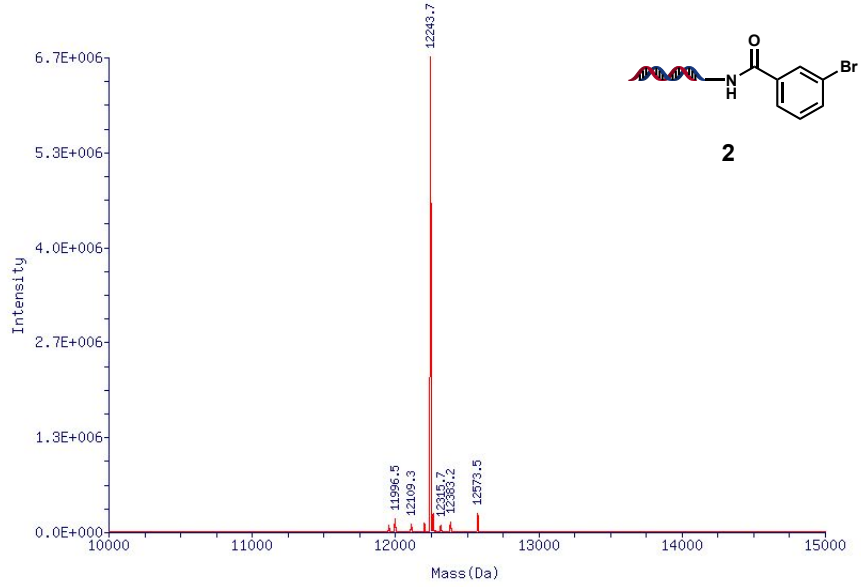


Figure S42. Deconvoluted mass spectrum of DNA **2**, expected: 12243; observed 12243.7.

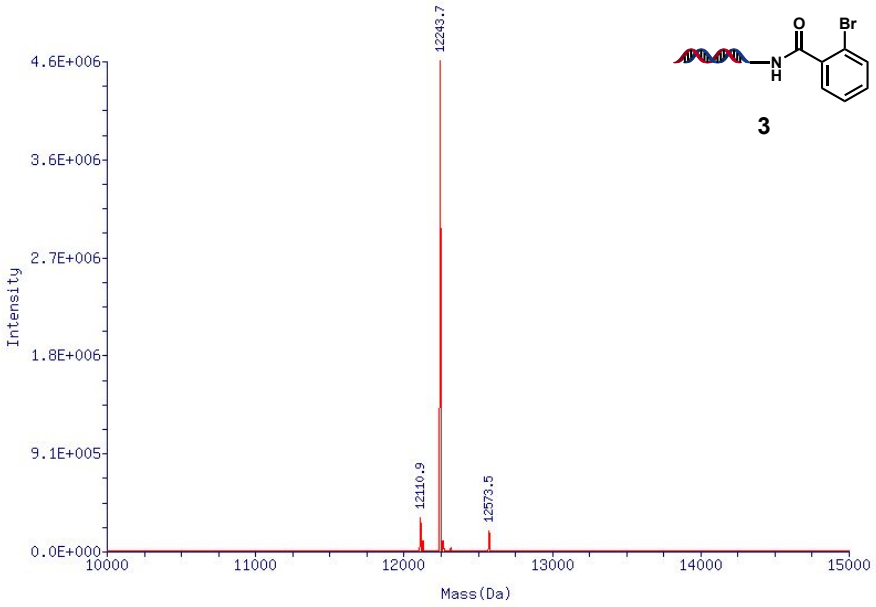


Figure S43. Deconvoluted mass spectrum of DNA **3**, expected: 12243; observed 12243.7.

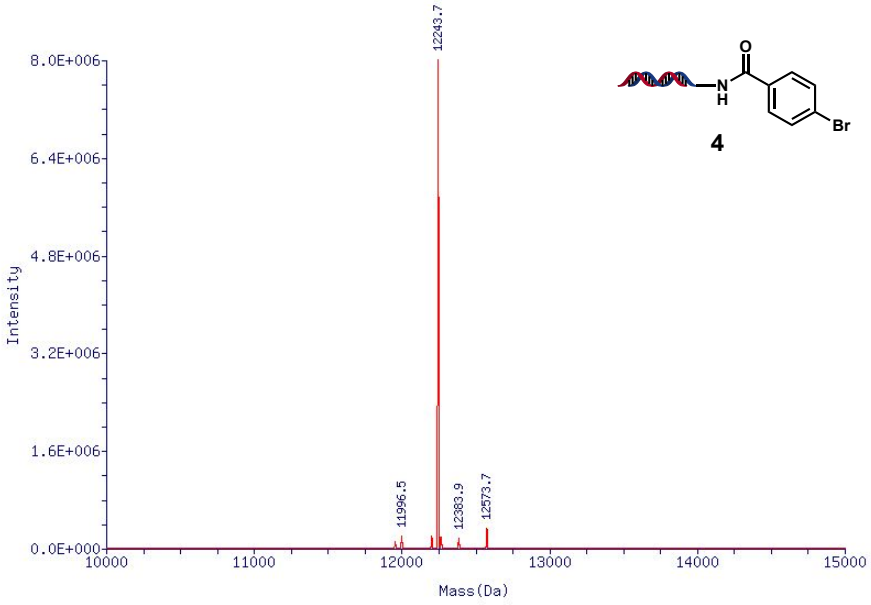


Figure S44. Deconvoluted mass spectrum of DNA **4**, expected: 12243; observed 12243.7.

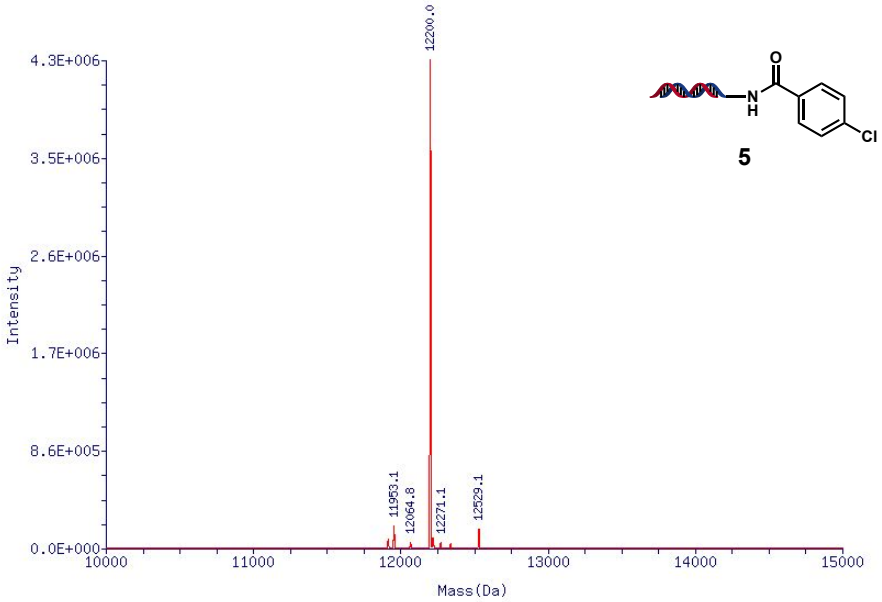


Figure S45. Deconvoluted mass spectrum of DNA **5**, expected: 12198.6; observed 12200.

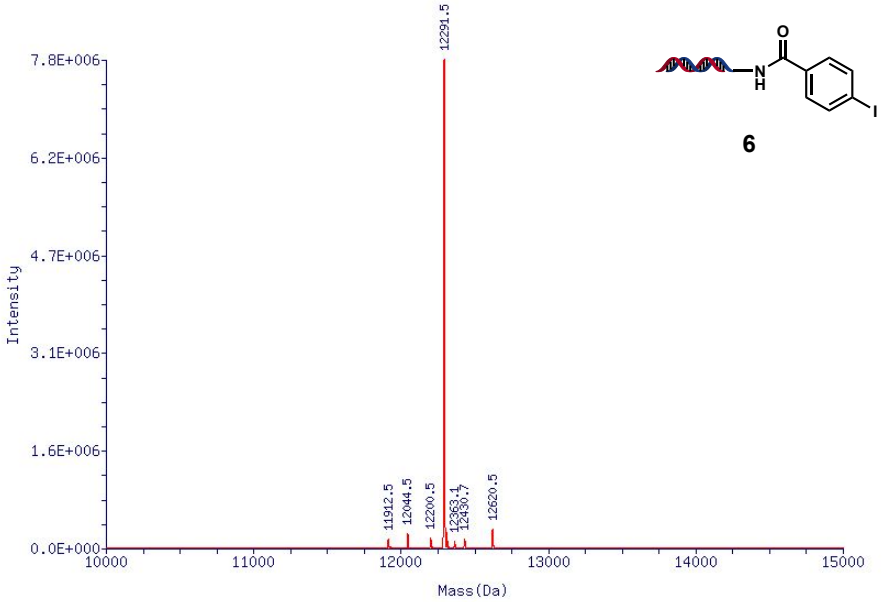


Figure S46. Deconvoluted mass spectrum of DNA **6**, expected: 12290; observed 12291.5.

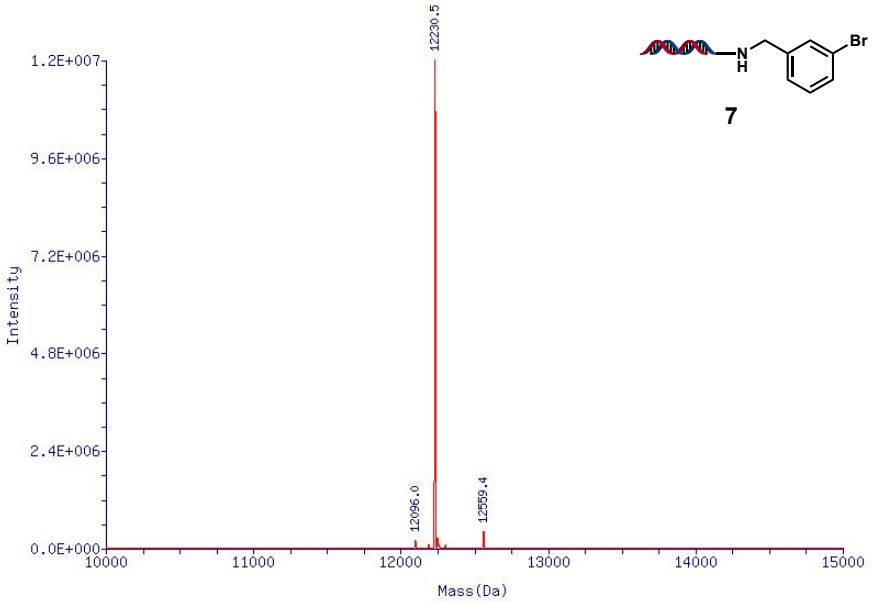


Figure S47. Deconvoluted mass spectrum of DNA **7**, expected: 12229; observed 12230.5.

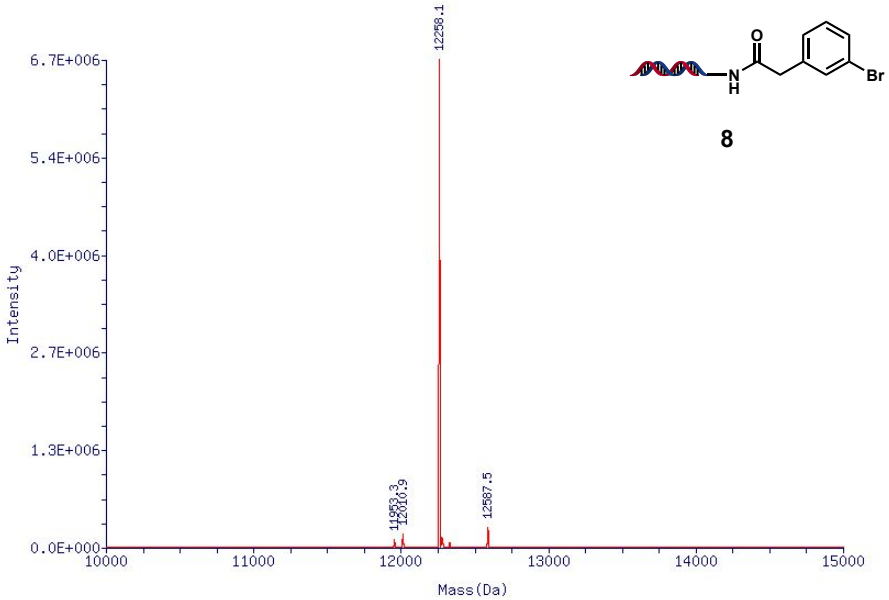


Figure S48. Deconvoluted mass spectrum of DNA **8**, expected: 12257; observed 12258.1.

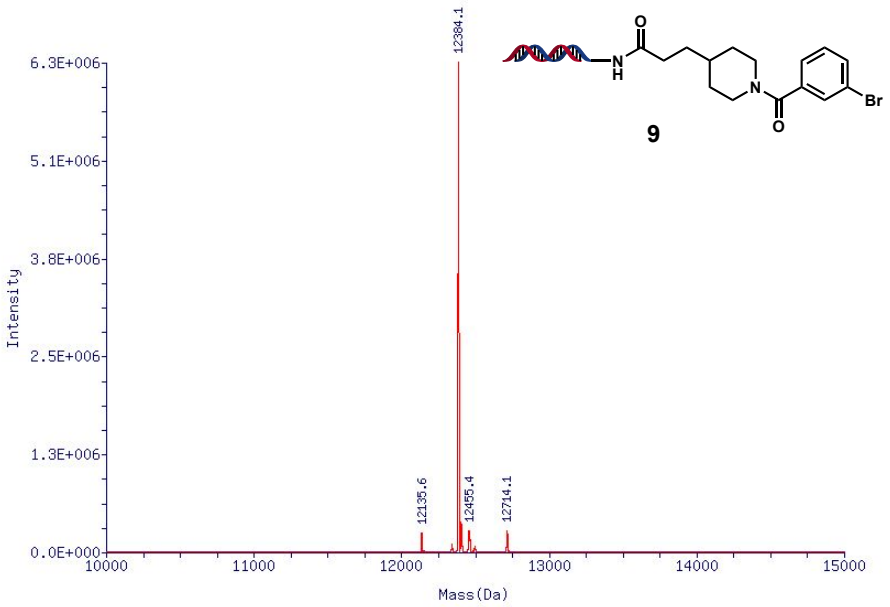


Figure S49. Deconvoluted mass spectrum of DNA **9**, expected: 12382.2; observed 12384.1.

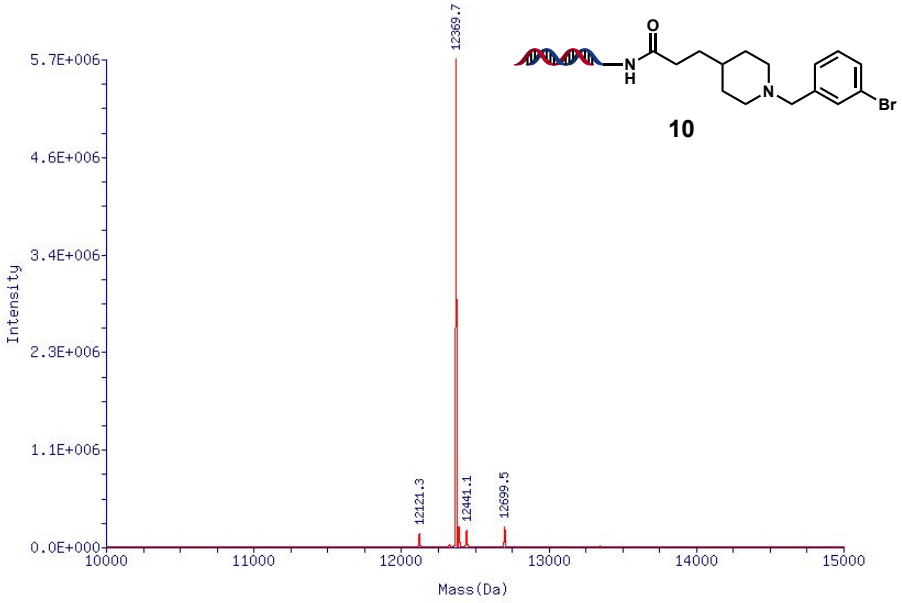


Figure S50. Deconvoluted mass spectrum of DNA **10**, expected: 12368.2; observed 12369.7.

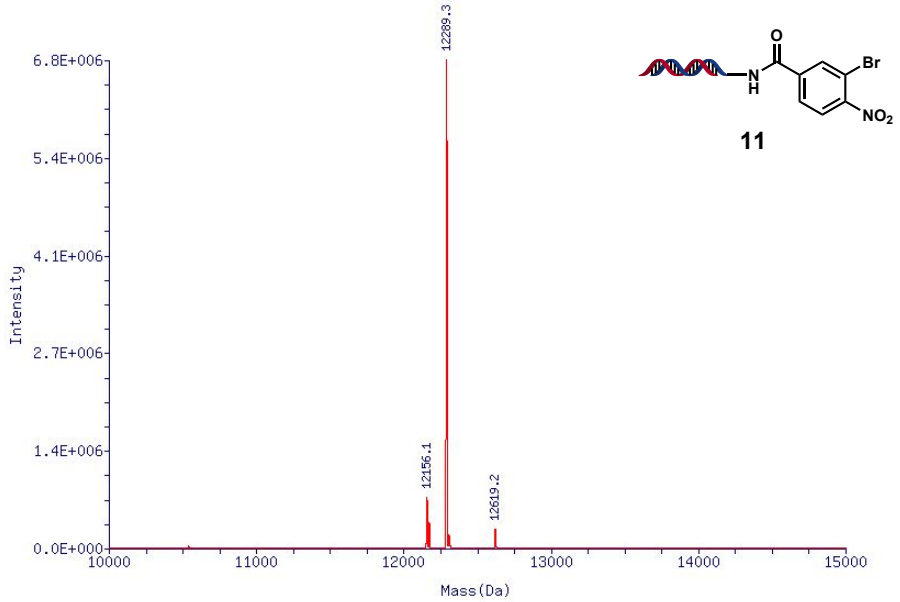


Figure S51. Deconvoluted mass spectrum of DNA **11**, expected: 12288; observed 12289.3.

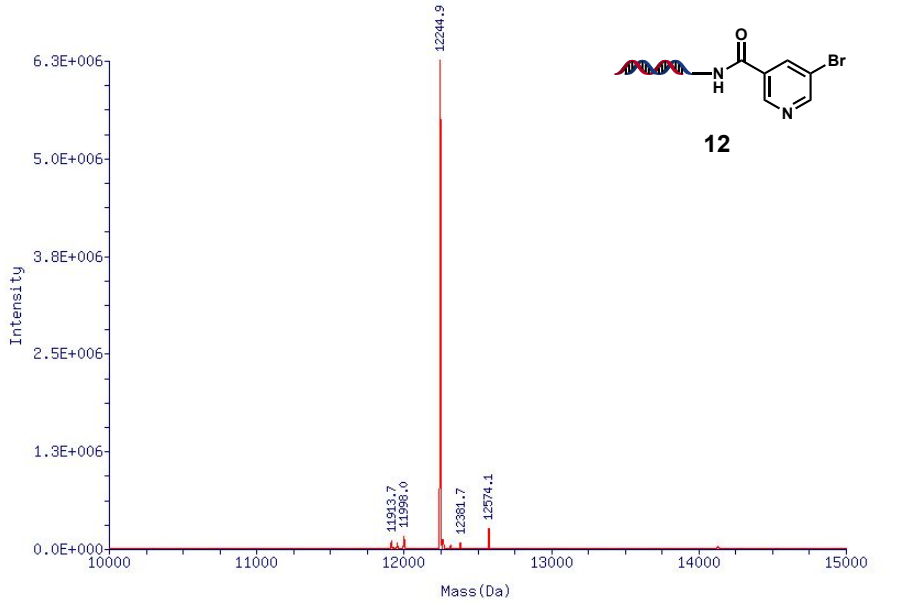


Figure S52. Deconvoluted mass spectrum of DNA **12**, expected: 12244; observed 12244.9.

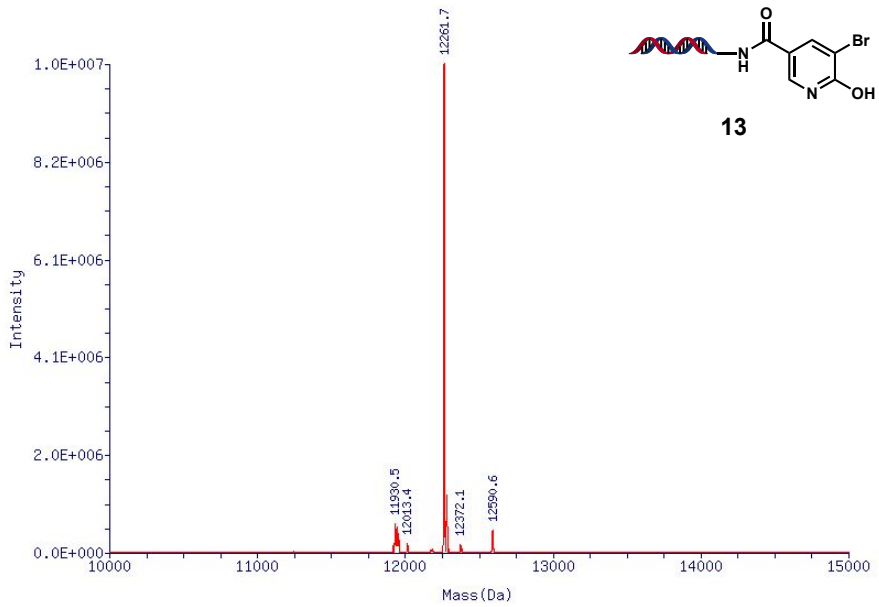


Figure S53. Deconvoluted mass spectrum of DNA **13**, expected: 12260; observed 12261.7.

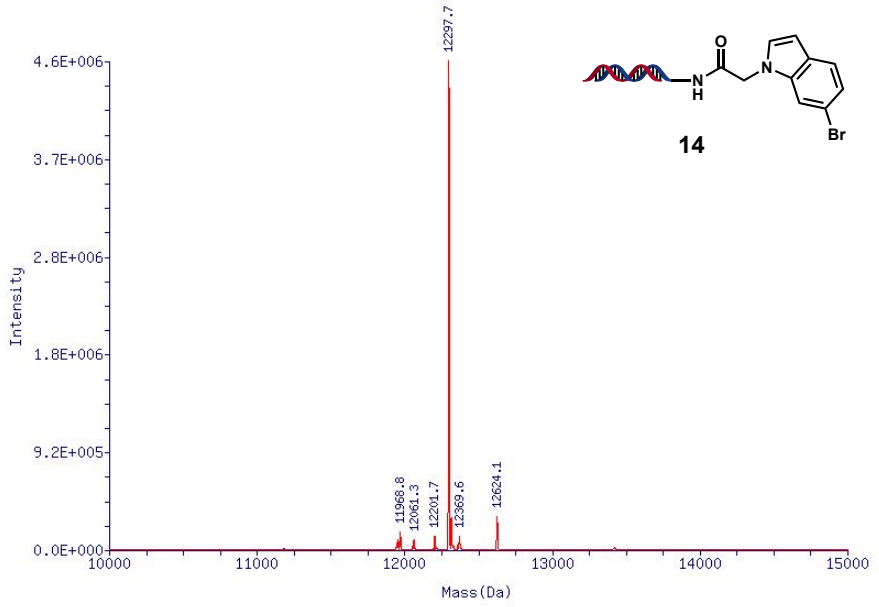


Figure S54. Deconvoluted mass spectrum of DNA **14**, expected: 12296.1; observed 12297.7.

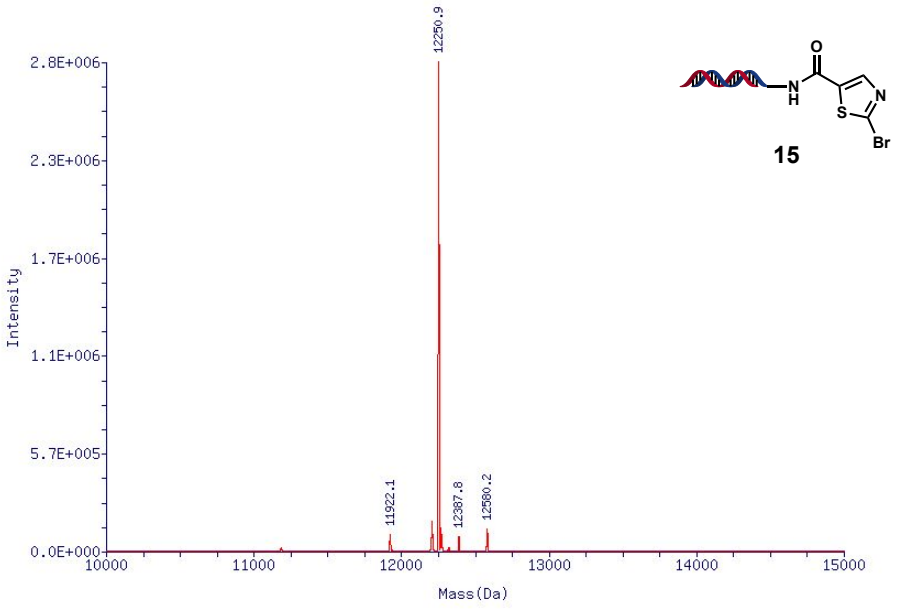


Figure S55. Deconvoluted mass spectrum of DNA **15**, expected: 12250; observed 12250.9.

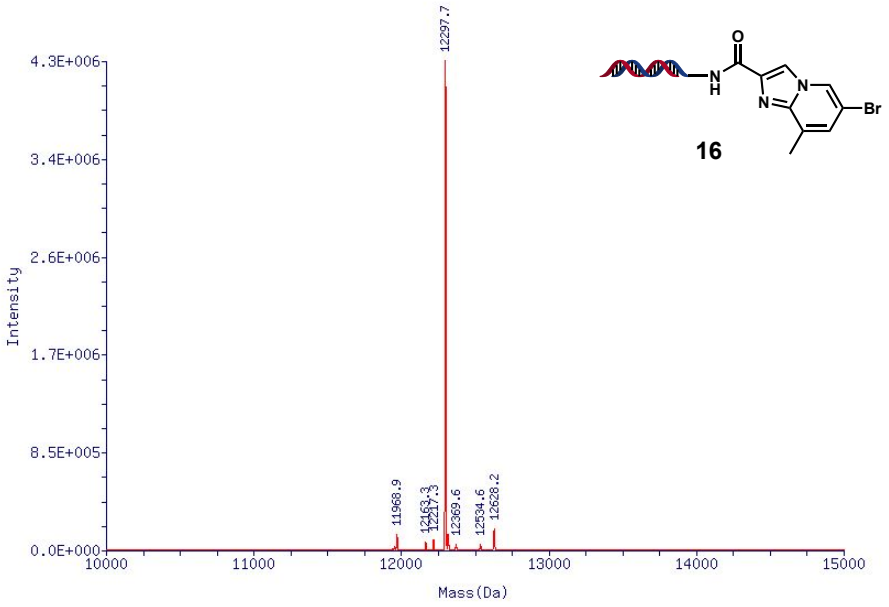


Figure S56. Deconvoluted mass spectrum of DNA **16**, expected: 12297.1; observed 12297.7.

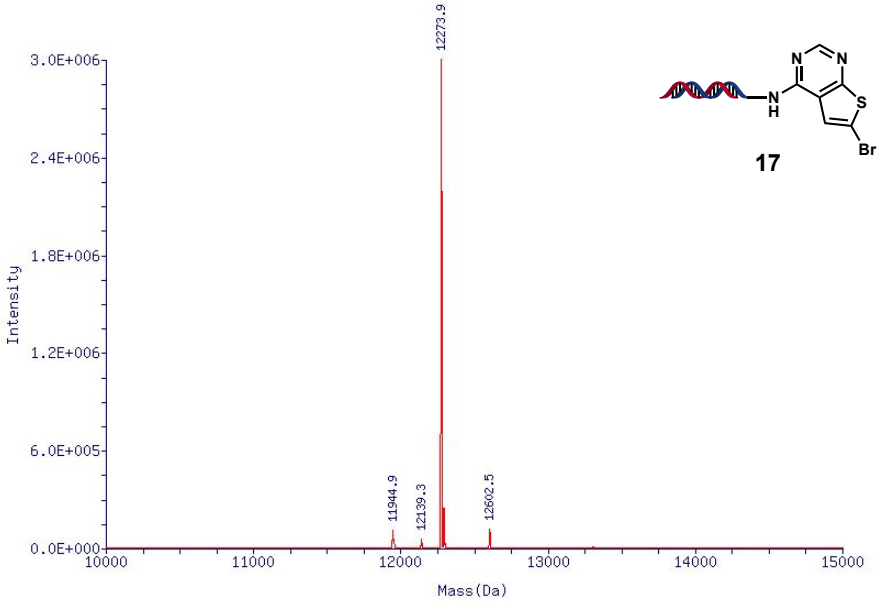


Figure S57. Deconvoluted mass spectrum of DNA **17**, expected: 12273.1; observed 12273.9.

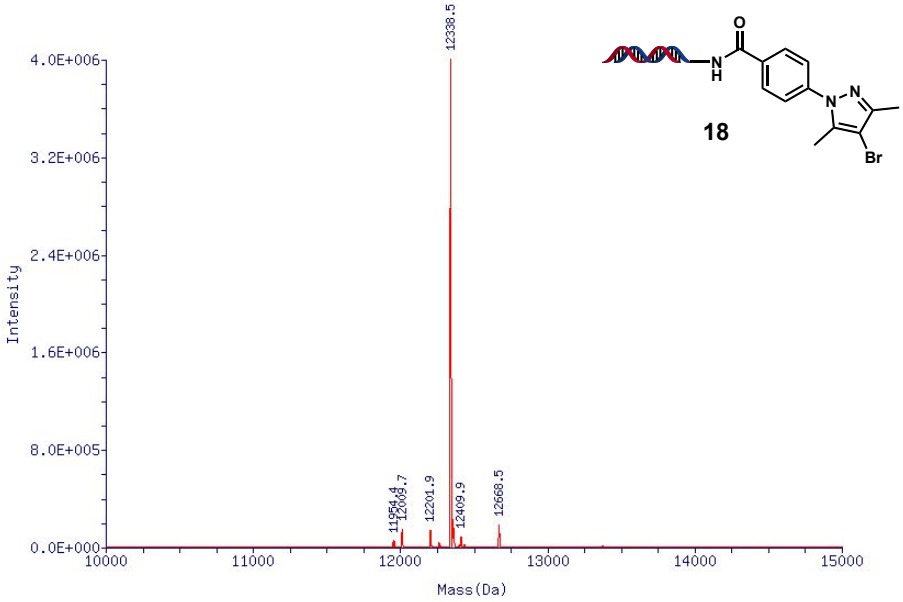


Figure S58. Deconvoluted mass spectrum of DNA **18**, expected: 12337.1; observed 12338.5.

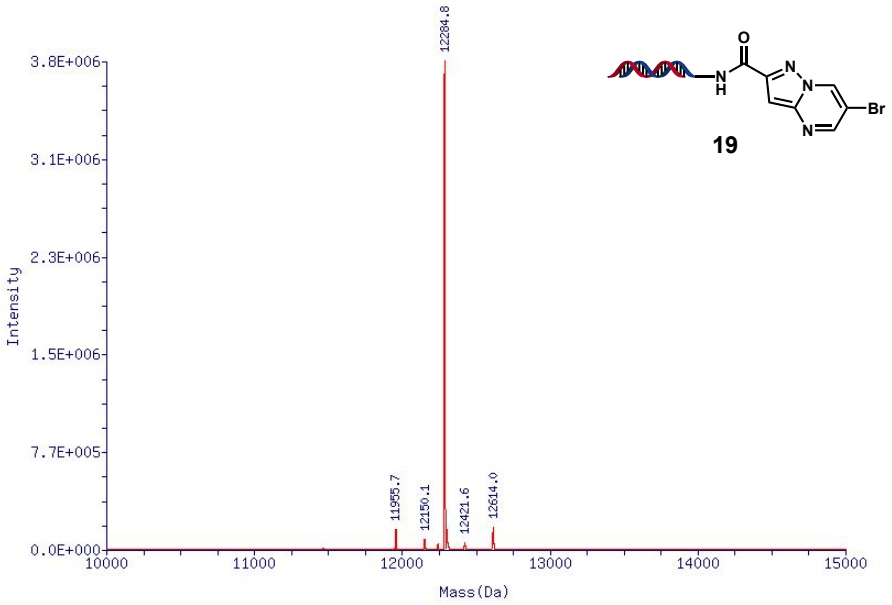


Figure S59. Deconvoluted mass spectrum of DNA **19**, expected: 12284; observed 12284.8.

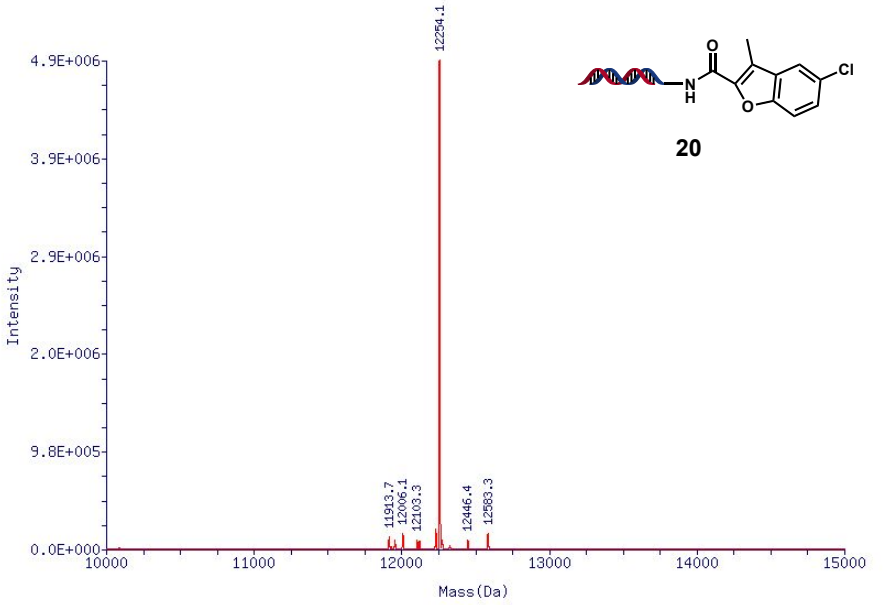


Figure S60. Deconvoluted mass spectrum of DNA **20**, expected: 12252.6; observed 12254.1.

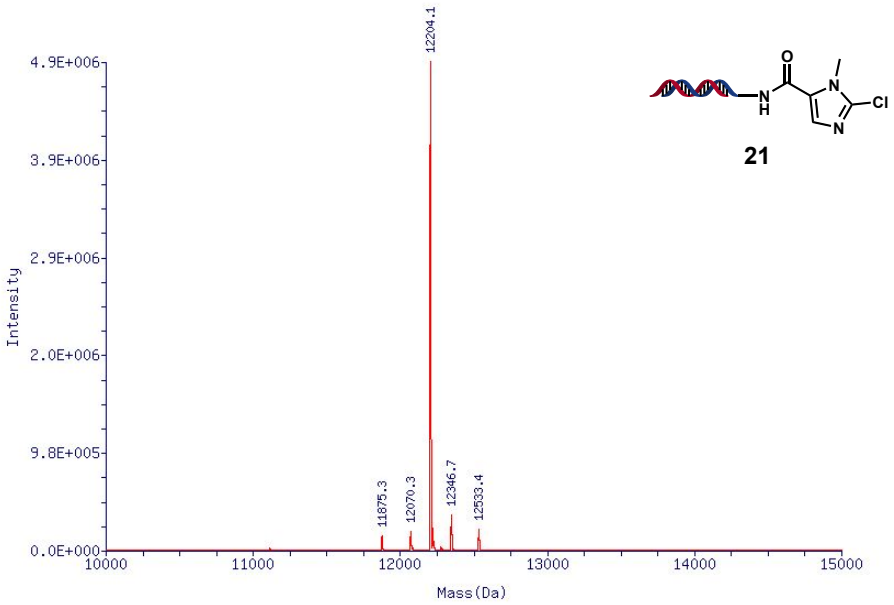


Figure S61. Deconvoluted mass spectrum of DNA **21**, expected: 12202.5; observed 12204.1.

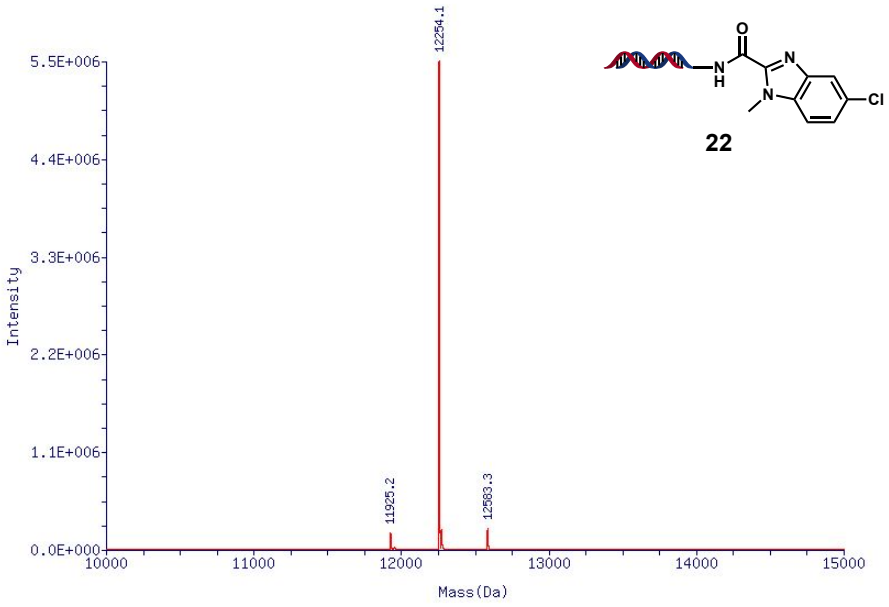


Figure S62. Deconvoluted mass spectrum of DNA **22**, expected: 12252.6; observed 12254.1.

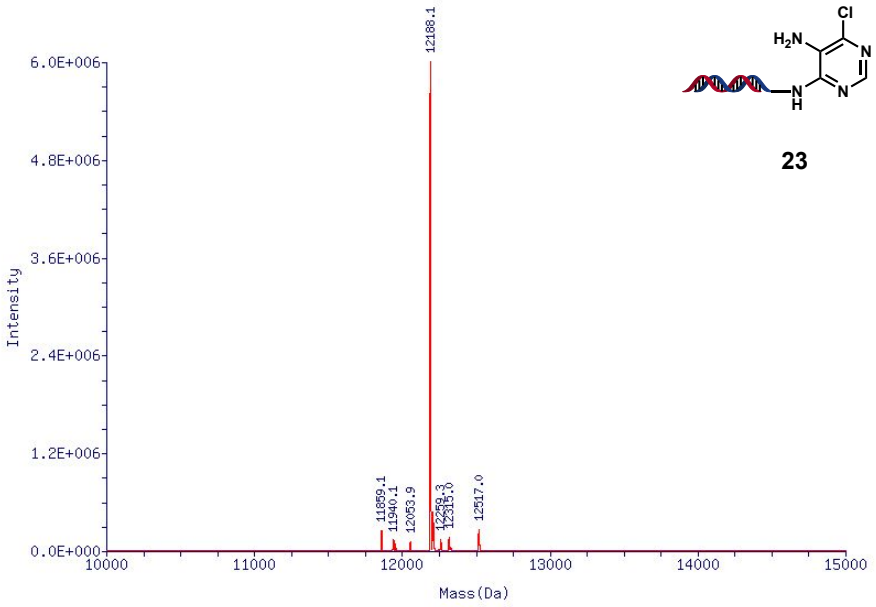


Figure S63. Deconvoluted mass spectrum of DNA **23**, expected: 12187.5; observed 12188.1.

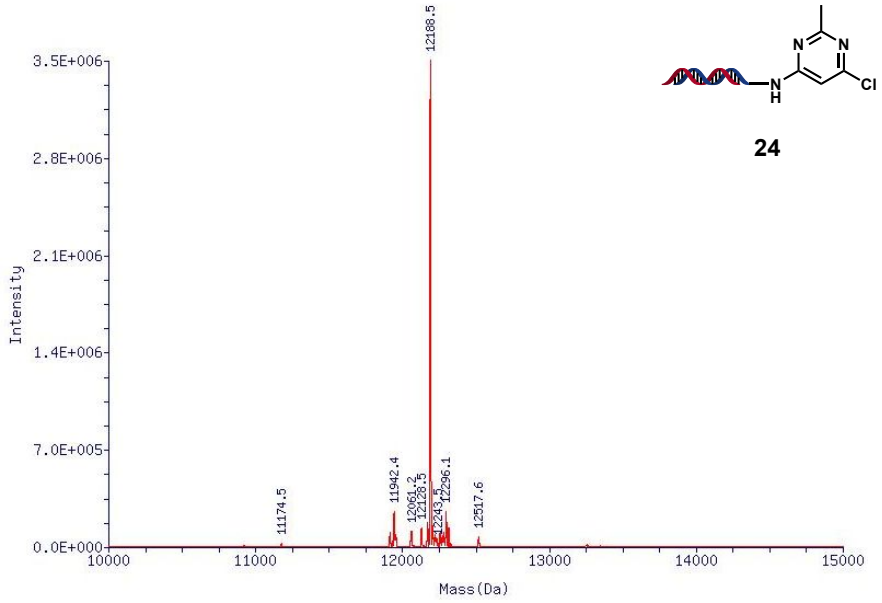


Figure S64. Deconvoluted mass spectrum of DNA **24**, expected: 12186.5; observed 12288.5.

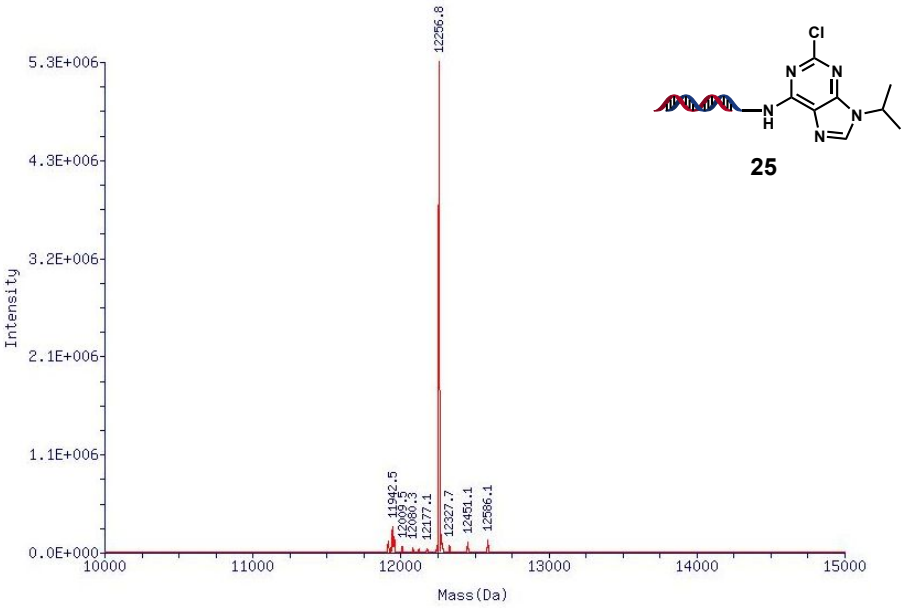


Figure S65. Deconvoluted mass spectrum of DNA **25**, expected: 12254.6; observed 12256.8.

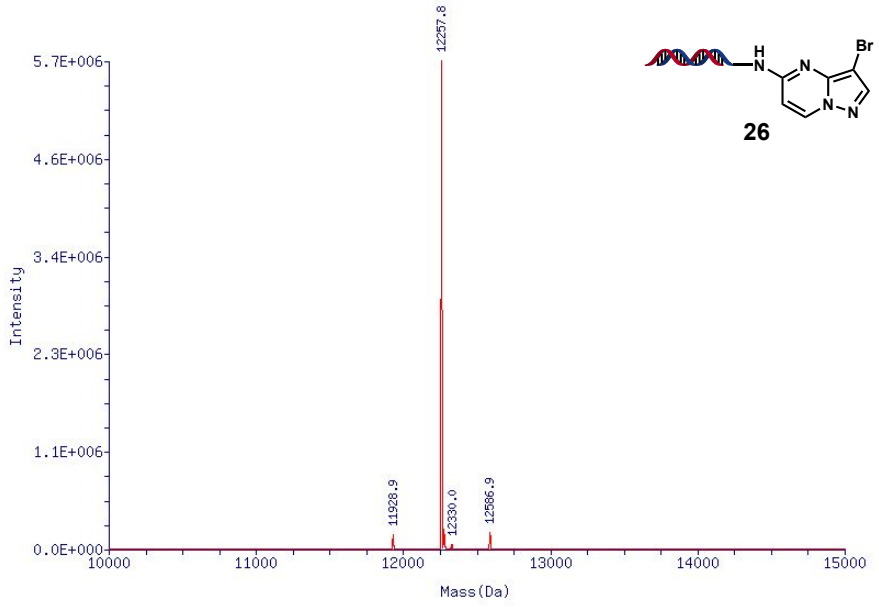


Figure S66. Deconvoluted mass spectrum of DNA **26**, expected: 12256; observed 12257.8.

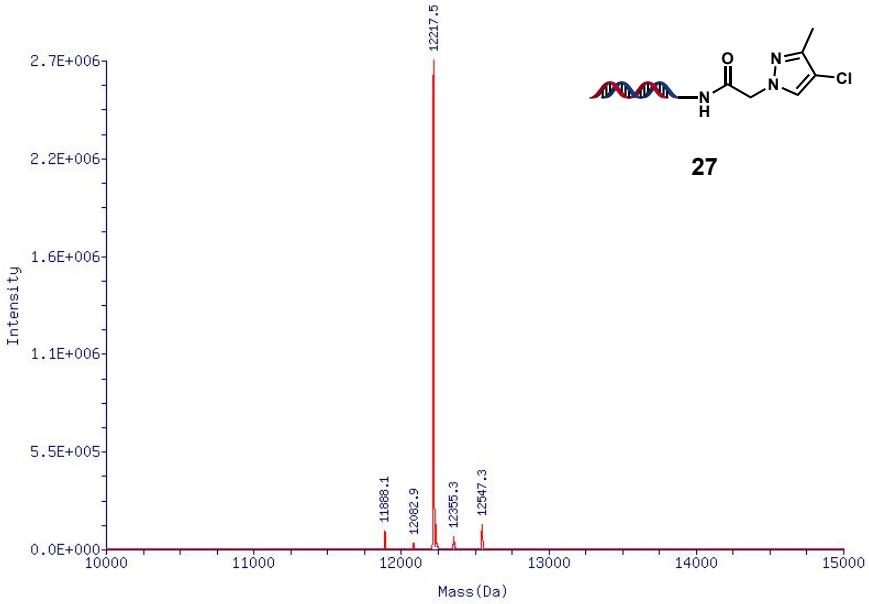


Figure S67. Deconvoluted mass spectrum of DNA **27**, expected: 12216.6; observed 12217.5.

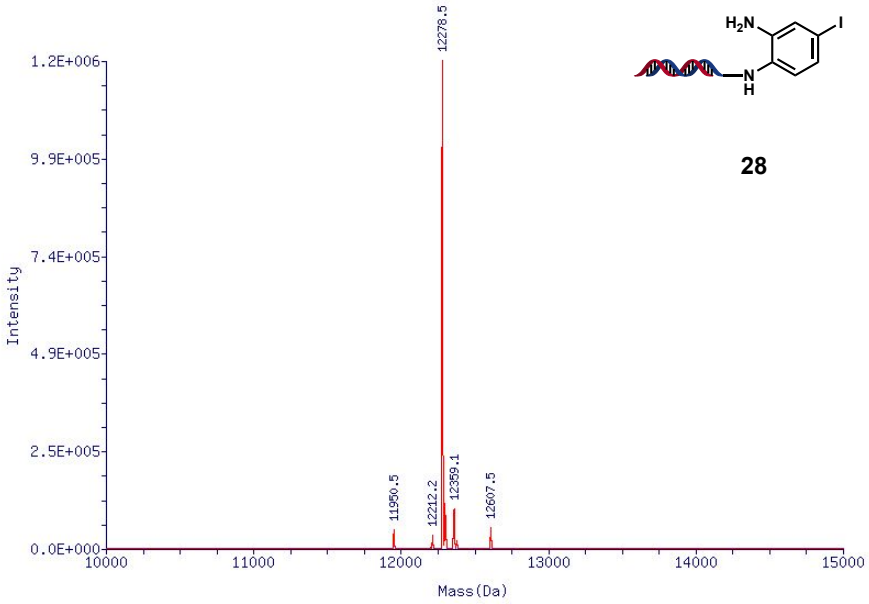


Figure S68. Deconvoluted mass spectrum of DNA **28**, expected: 12277; observed 12278.5.

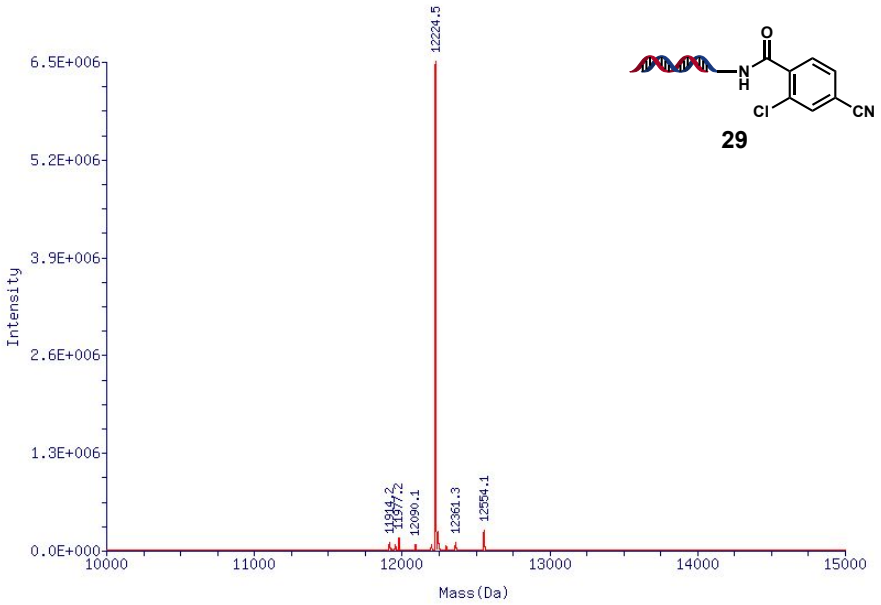


Figure S69. Deconvoluted mass spectrum of DNA **29**, expected: 12223.6; observed 12224.5.

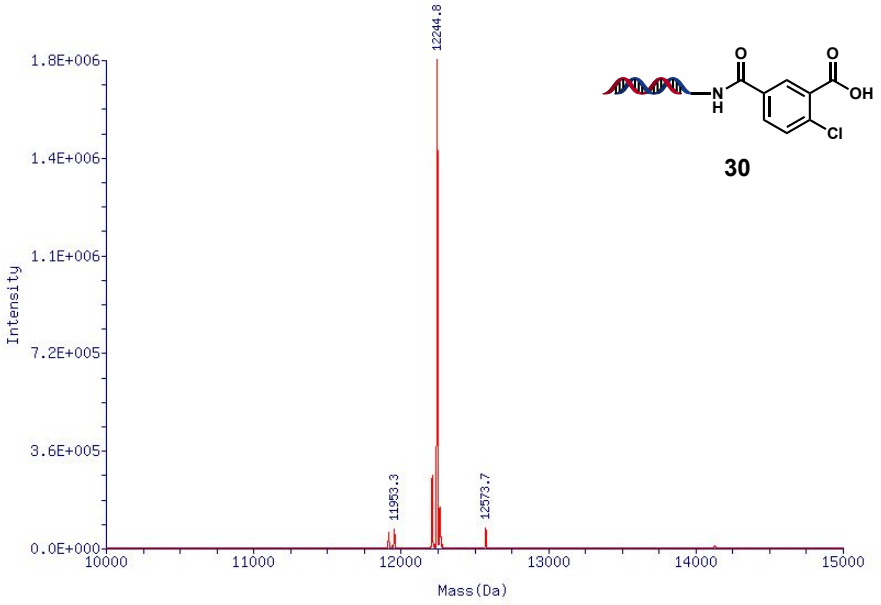


Figure S70. Deconvoluted mass spectrum of DNA **30**, expected: 12242.6; observed 12244.8.

5. Deconvoluted Mass Spectra of C–N cross coupling screening results

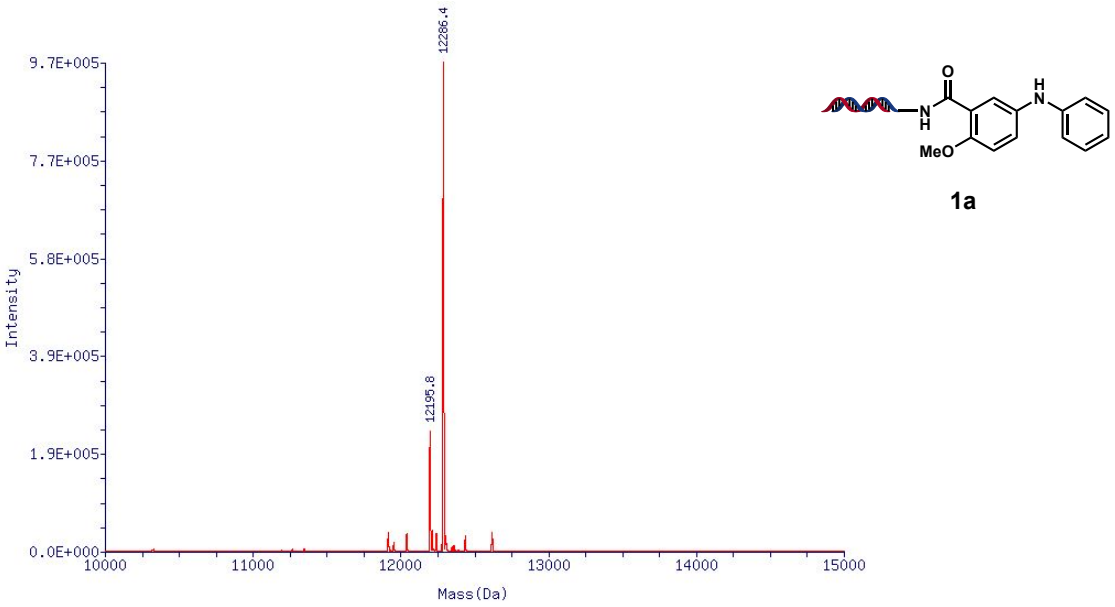


Figure S71. Deconvoluted mass spectrum of DNA **1a**, expected: 12285.3; observed 12286.4.

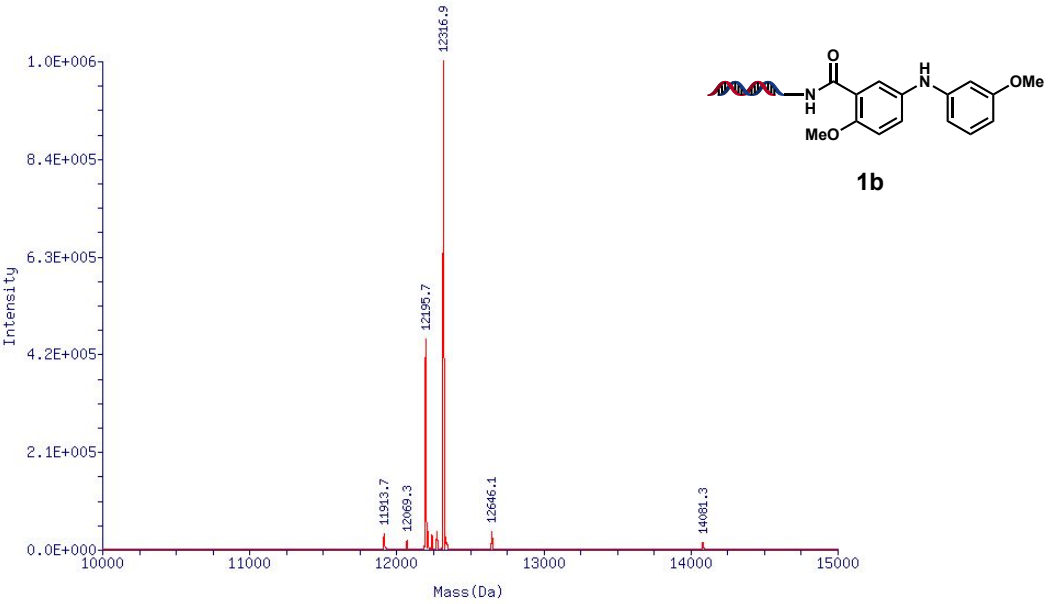


Figure S72. Deconvoluted mass spectrum of DNA **1b**, expected: 12315.3; observed 12316.9.

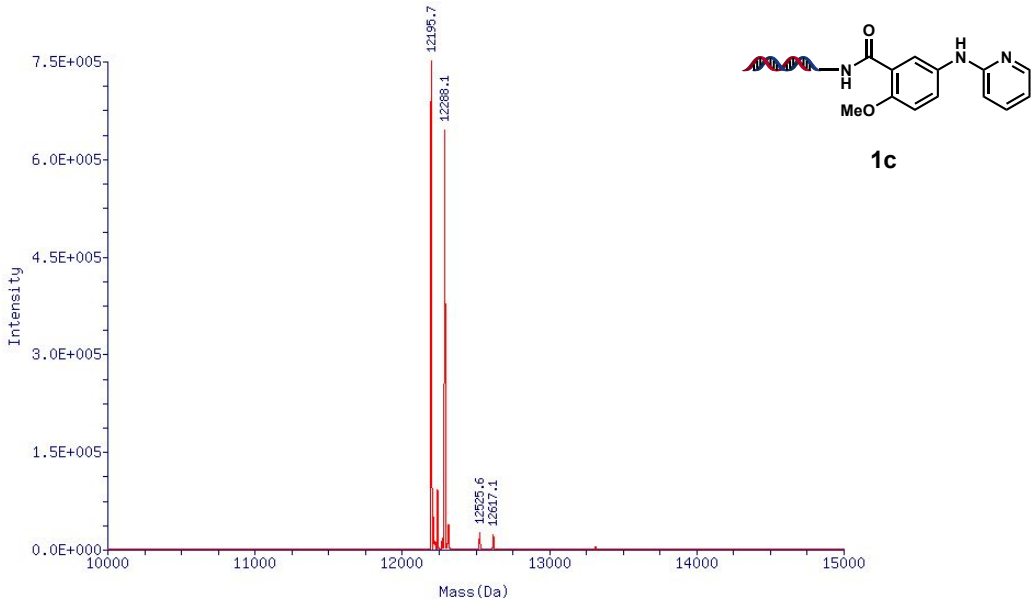


Figure S73. Deconvoluted mass spectrum of DNA **1c**, expected: 12286.2; observed 12288.1.

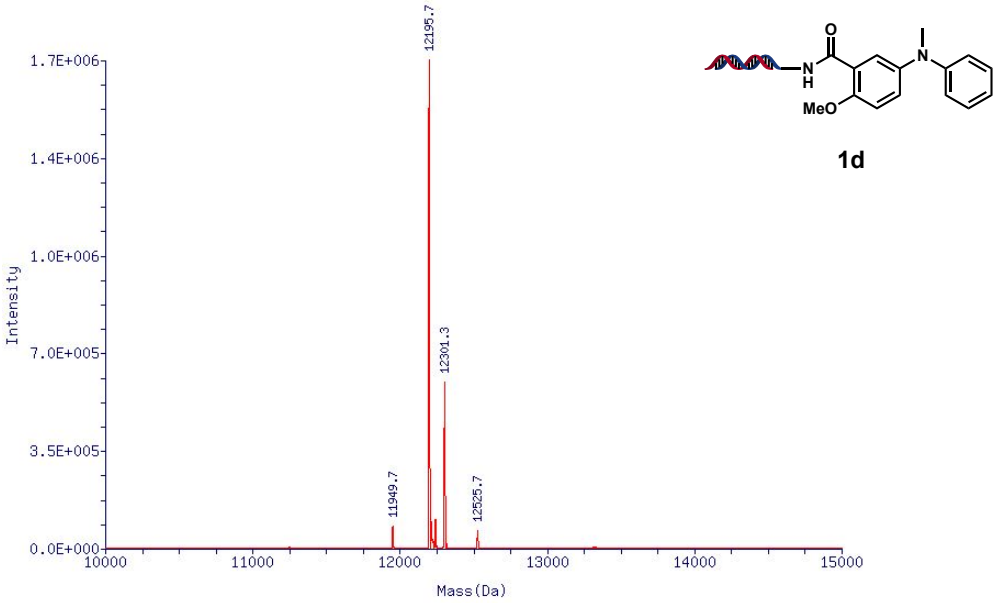


Figure S74. Deconvoluted mass spectrum of DNA **1d**, expected: 12299.3; observed 12301.3.

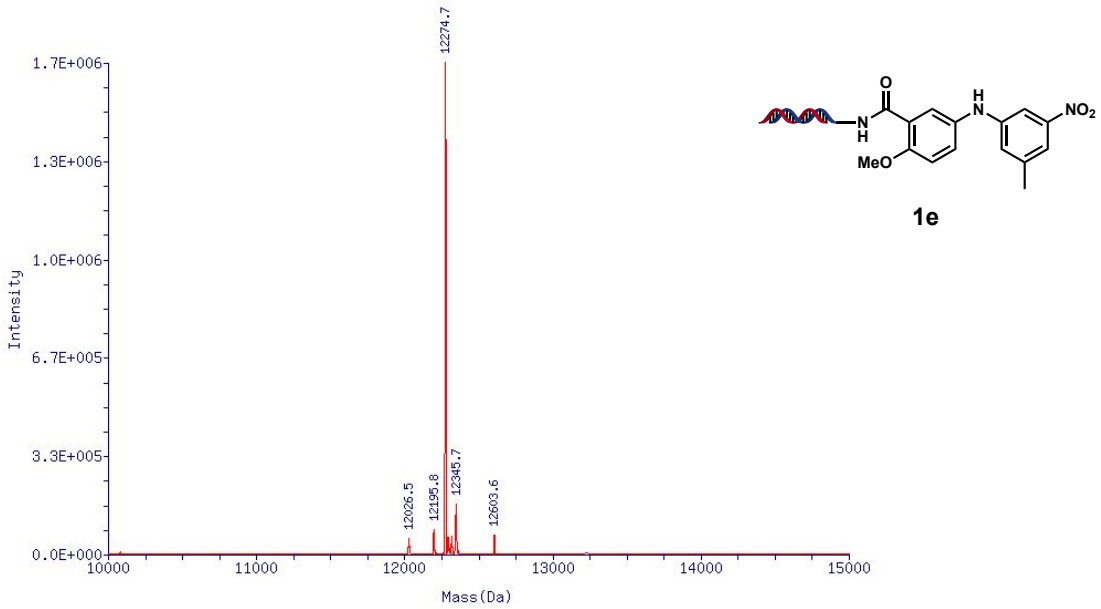


Figure S75. Deconvoluted mass spectrum of DNA **1e**, expected: 12344.3; observed 12345.7.

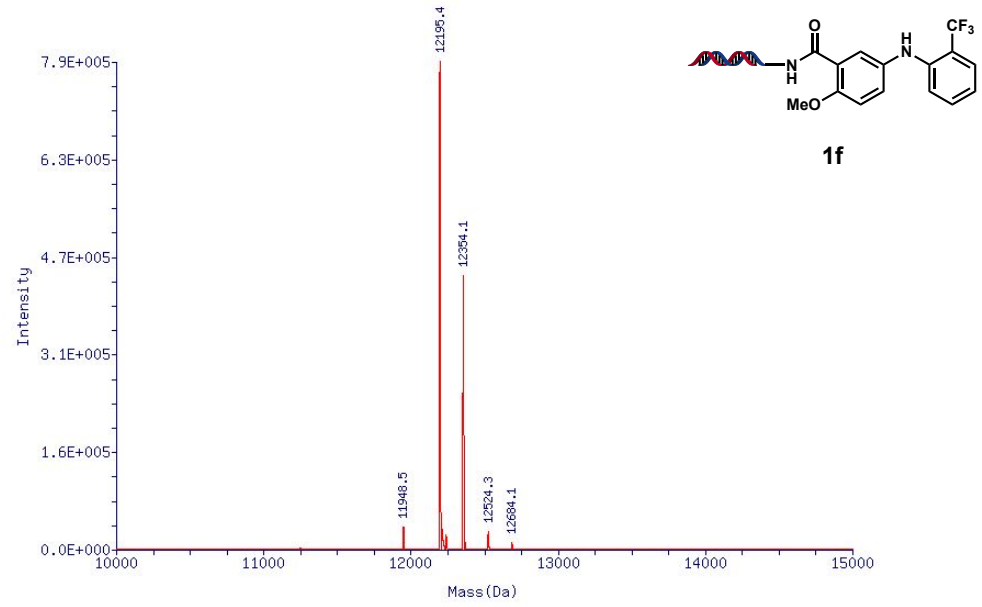


Figure S76. Deconvoluted mass spectrum of DNA **1f**, expected: 12353.3; observed 12354.1.

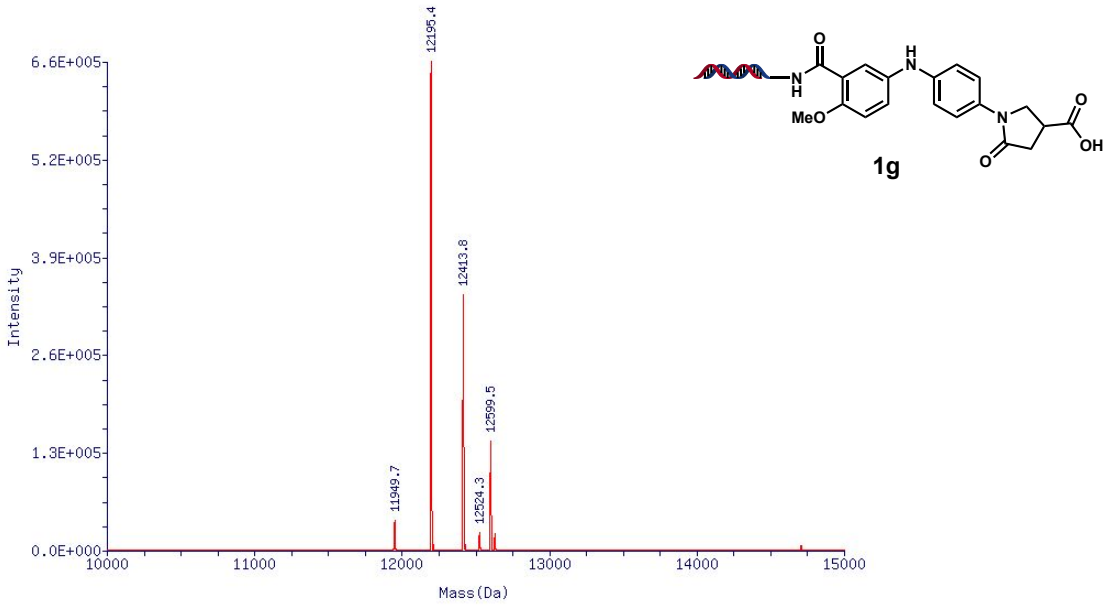


Figure S77. Deconvoluted mass spectrum of DNA **1g**, expected: 12413.3; observed 12413.8.

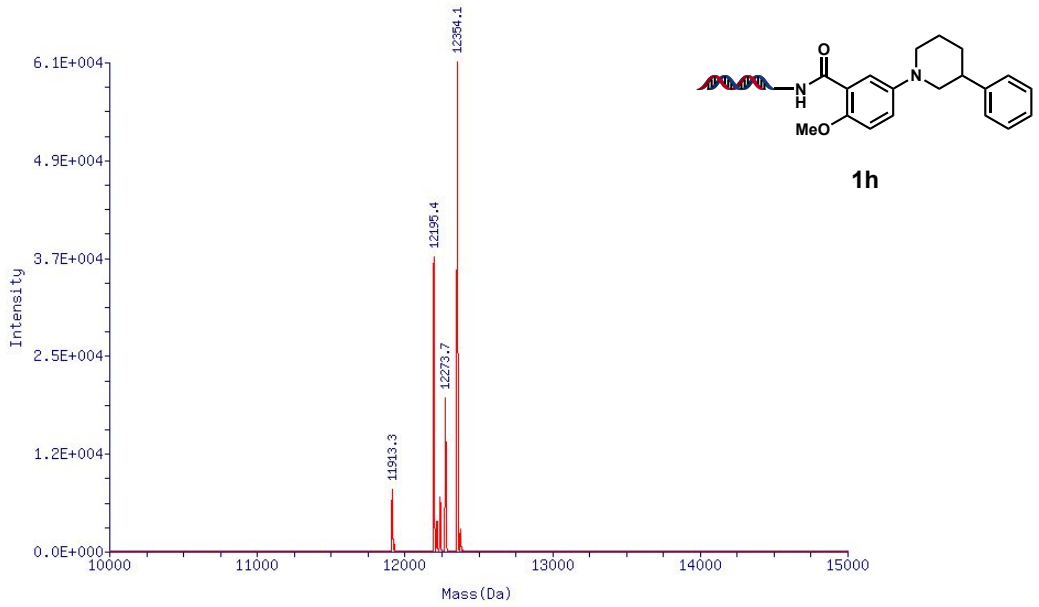
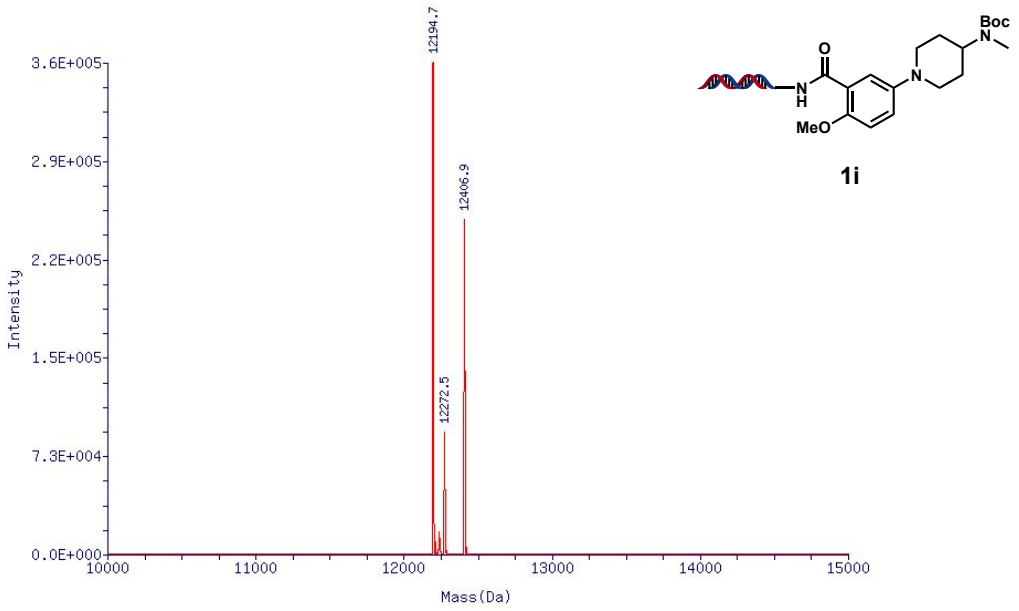
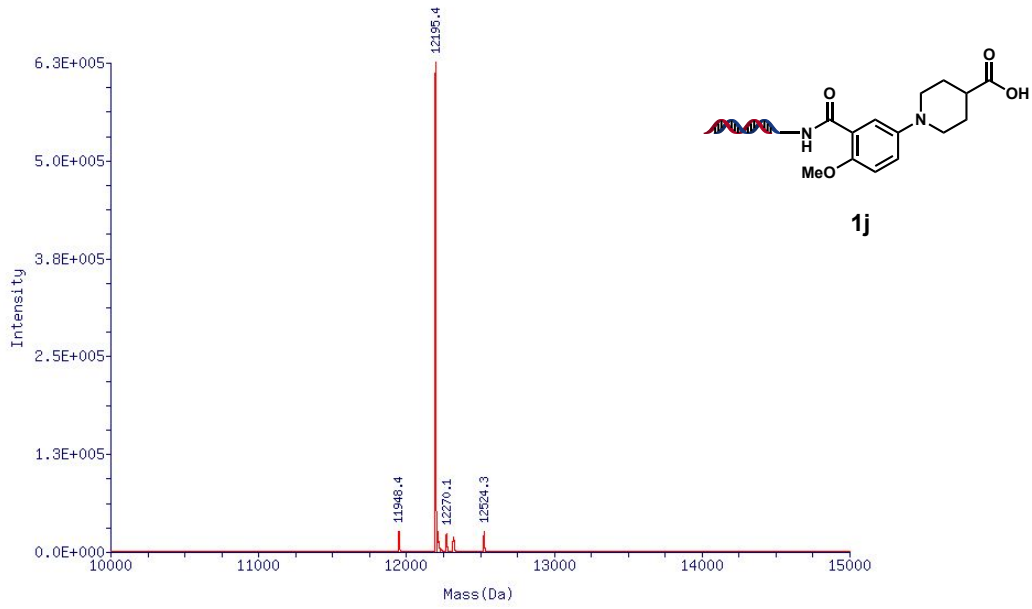


Figure S78. Deconvoluted mass spectrum of DNA **1h**, expected: 12353.4; observed 12354.1.



1i

Figure S79. Deconvoluted mass spectrum of DNA **1i**, expected: 12406.4; observed 12406.9.



1j

Figure S80. Deconvoluted mass spectrum of DNA **1j**, expected: 12321.3; no product observed.

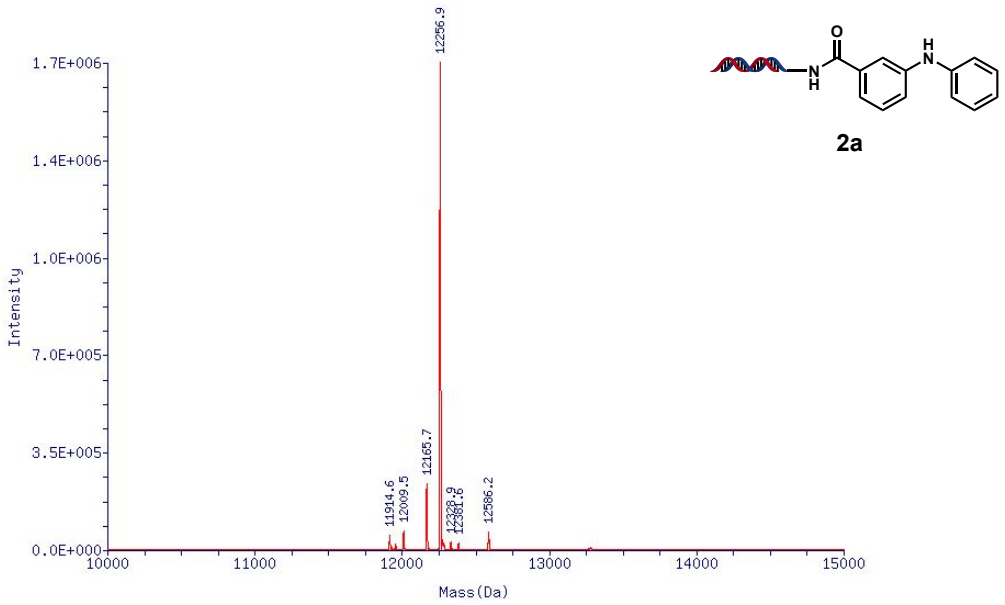


Figure S81. Deconvoluted mass spectrum of DNA **2a**, expected: 12255.2; observed 12256.9.

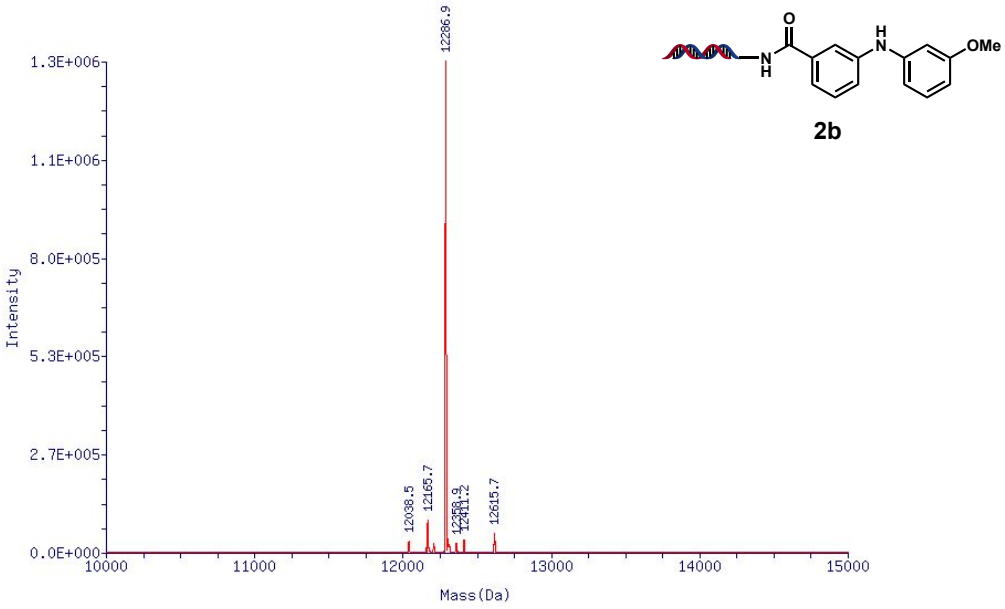


Figure S82. Deconvoluted mass spectrum of DNA **2b**, expected: 12285.3; observed 12286.9.

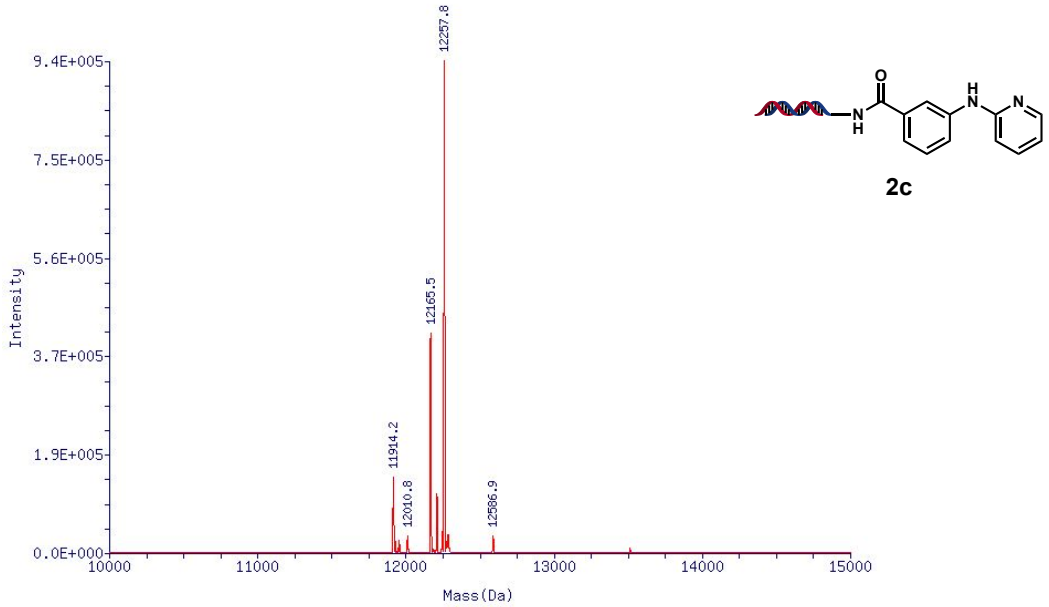


Figure S83. Deconvoluted mass spectrum of DNA **2c**, expected: 12256.2; observed 12257.8.

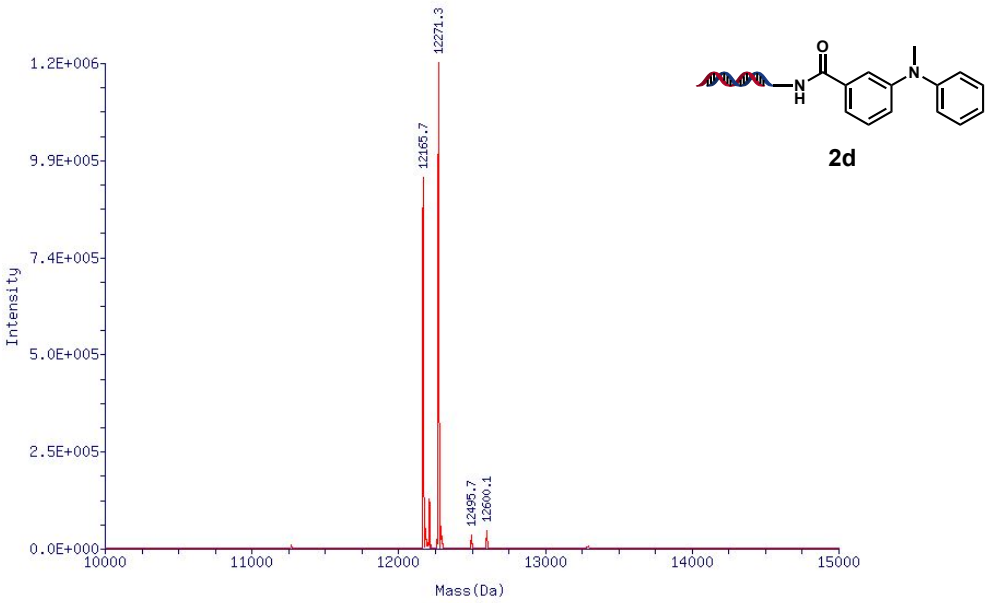


Figure S84. Deconvoluted mass spectrum of DNA **2d**, expected: 12269.3; observed 12271.3.

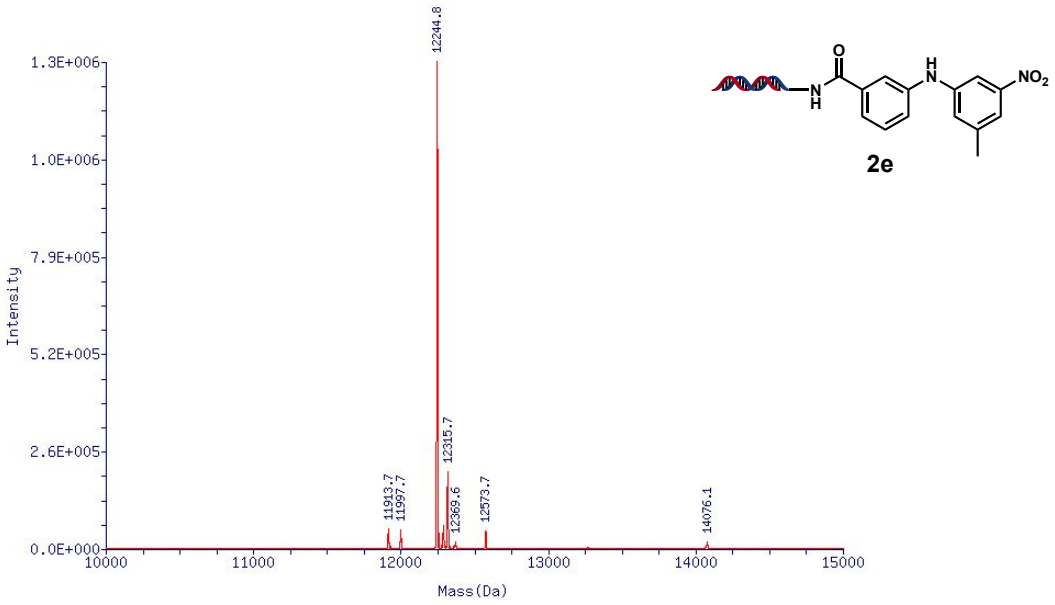


Figure S85. Deconvoluted mass spectrum of DNA **2e**, expected: 12314.2; observed 12315.7.

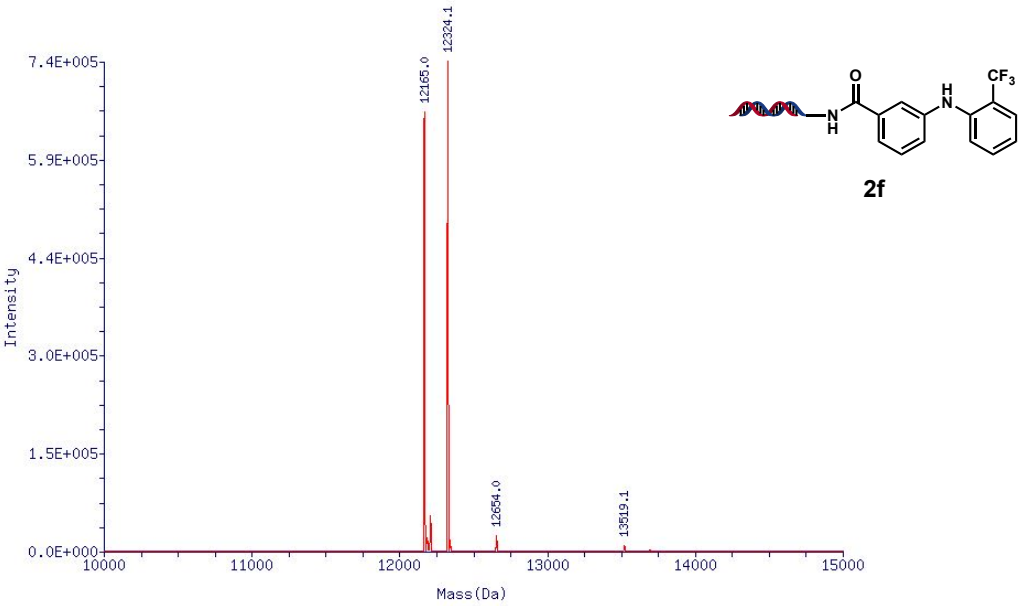


Figure S86. Deconvoluted mass spectrum of DNA **2f**, expected: 12323.2; observed 12324.1.

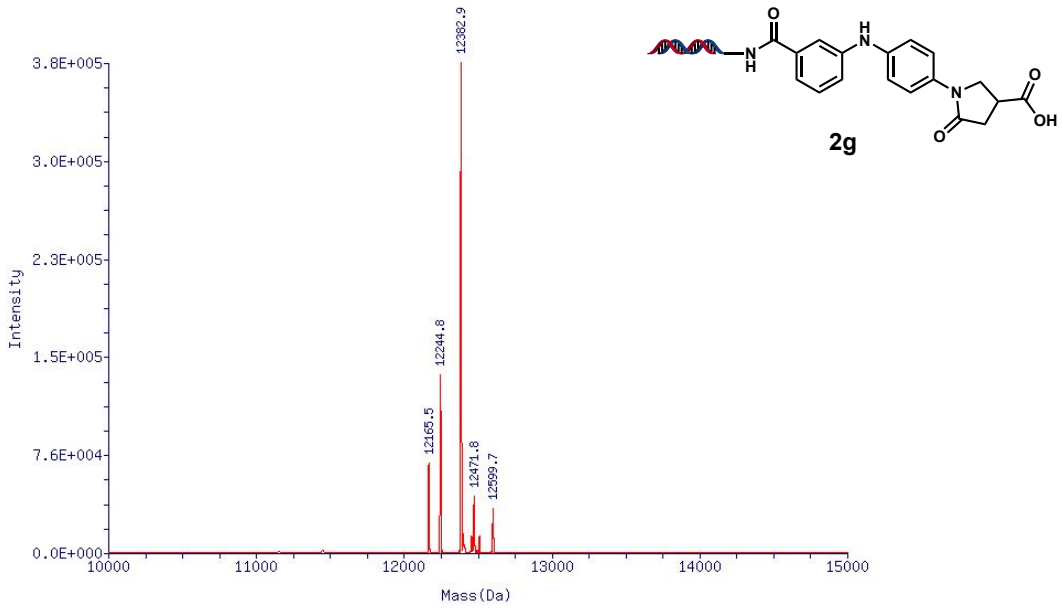


Figure S87. Deconvoluted mass spectrum of DNA **2g**, expected: 12382.2; observed 12382.9.

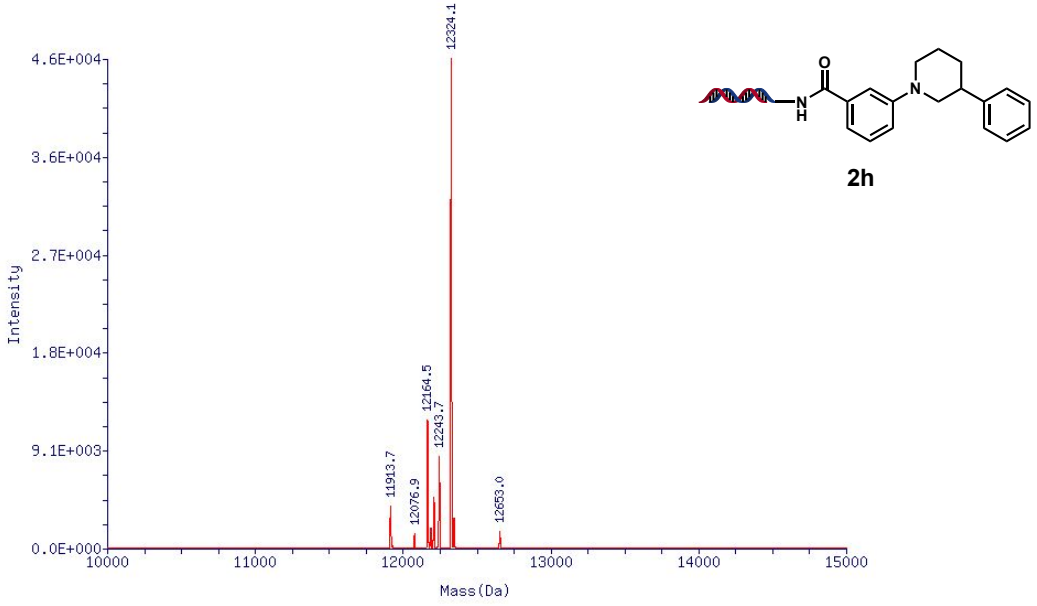


Figure S88. Deconvoluted mass spectrum of DNA **2h**, expected: 12323.3; observed 12324.1.

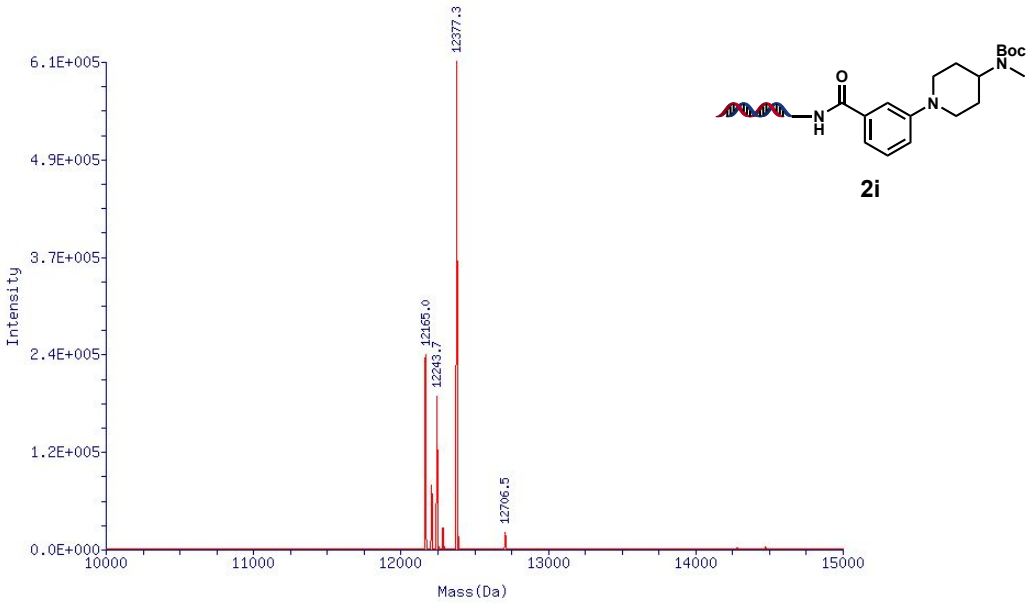


Figure S89. Deconvoluted mass spectrum of DNA **2i**, expected: 12376.4; observed 12377.3.

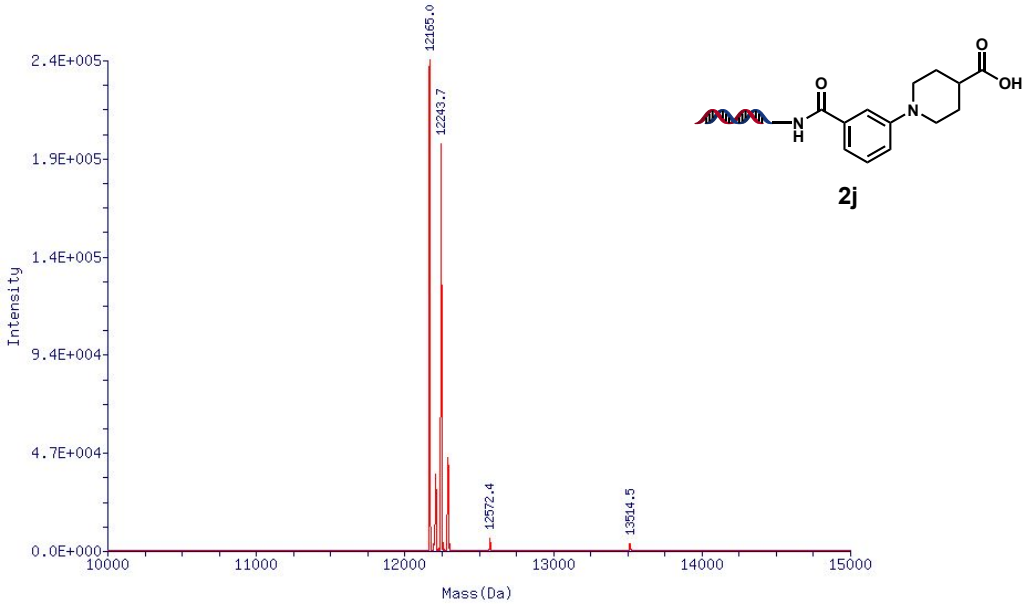


Figure S90. Deconvoluted mass spectrum of DNA **2j**, expected: 12291.3; observed 12291.

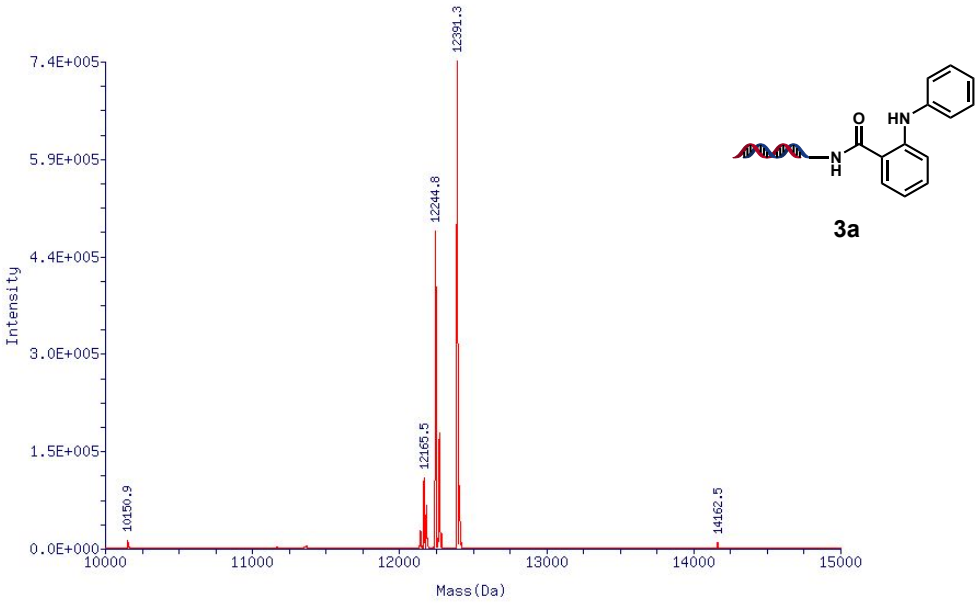


Figure S90. Deconvoluted mass spectrum of DNA **3a**, expected: 12255.2; no product observed.

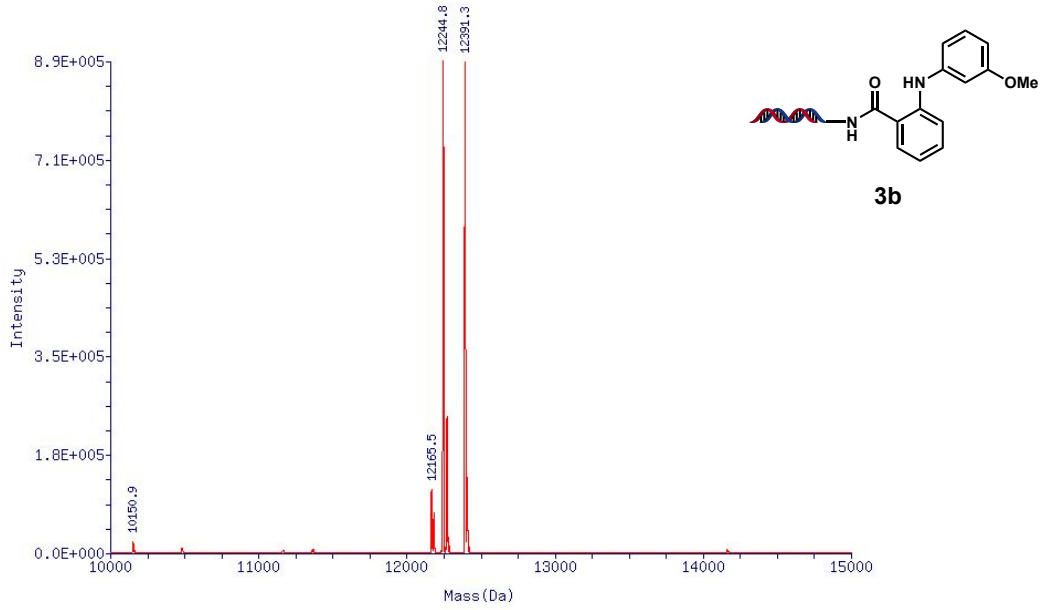


Figure S91. Deconvoluted mass spectrum of DNA **3b**, expected: 12285.3; no product observed.

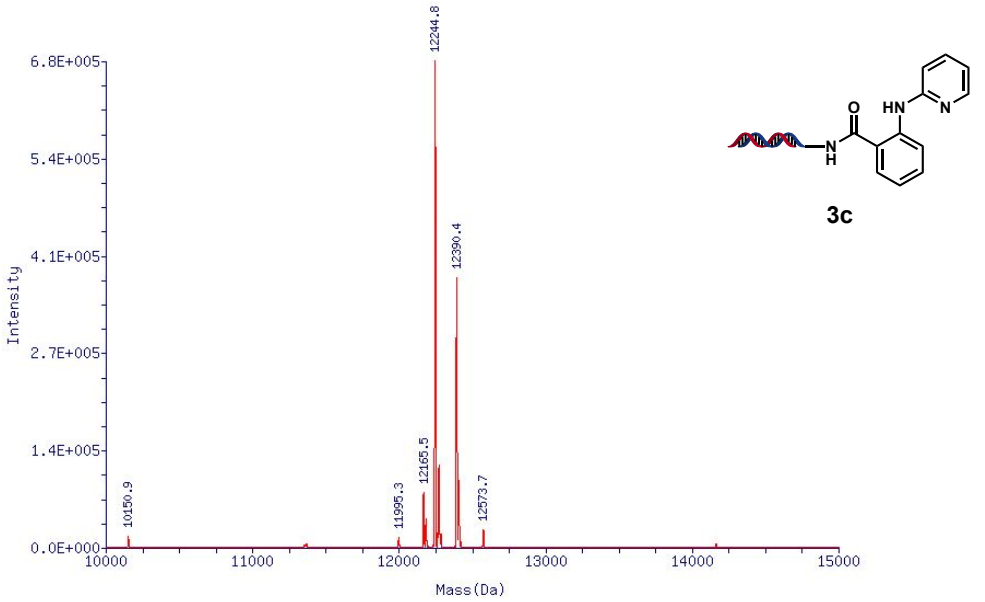


Figure S92. Deconvoluted mass spectrum of DNA **3c**, expected: 12256.2; no product observed.

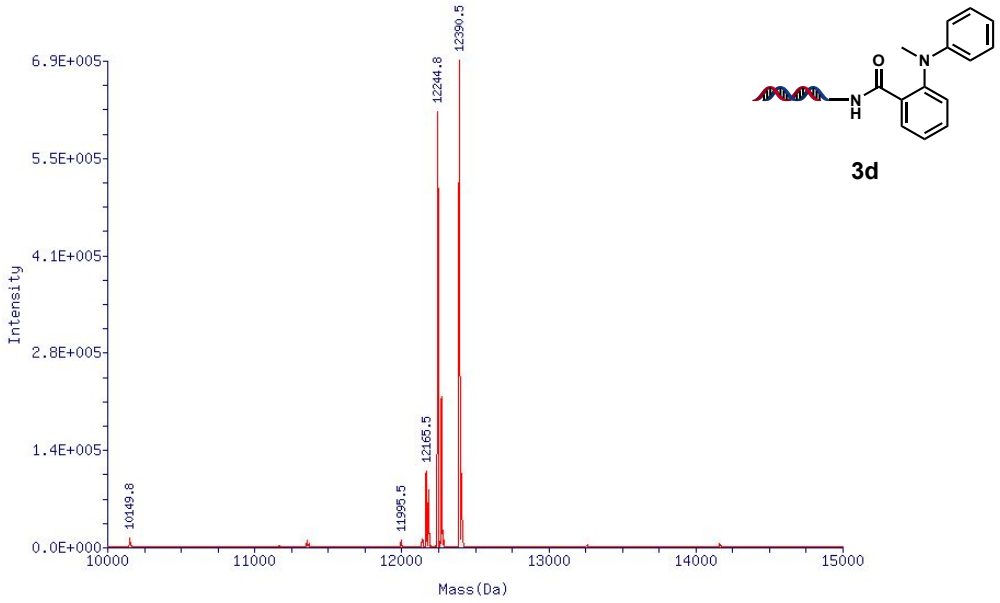


Figure S93. Deconvoluted mass spectrum of DNA **3d**, expected: 12269.3; no product observed.

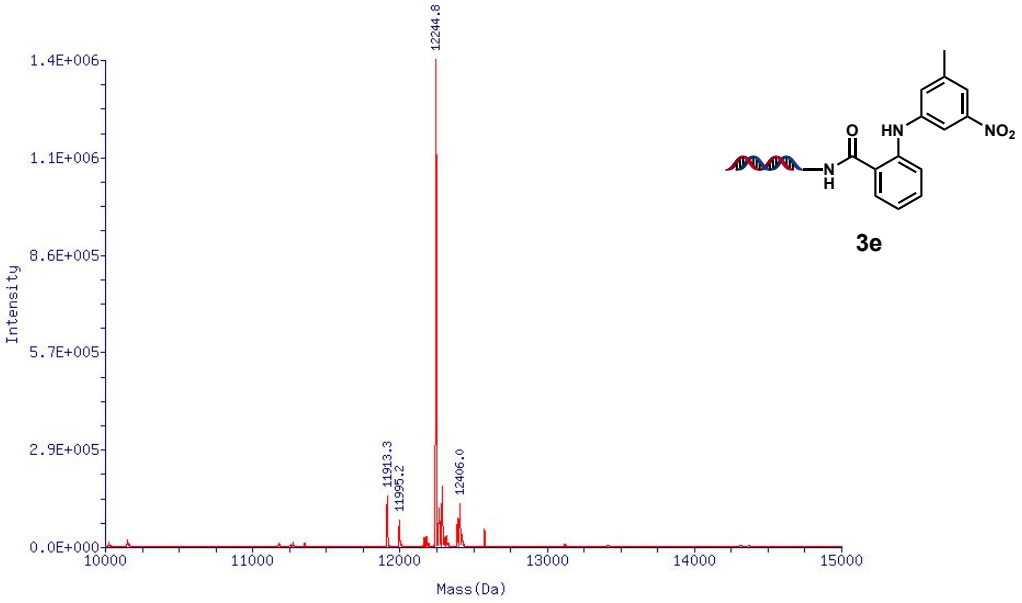


Figure S94. Deconvoluted mass spectrum of DNA **3e**, expected: 12314.2; no product observed.

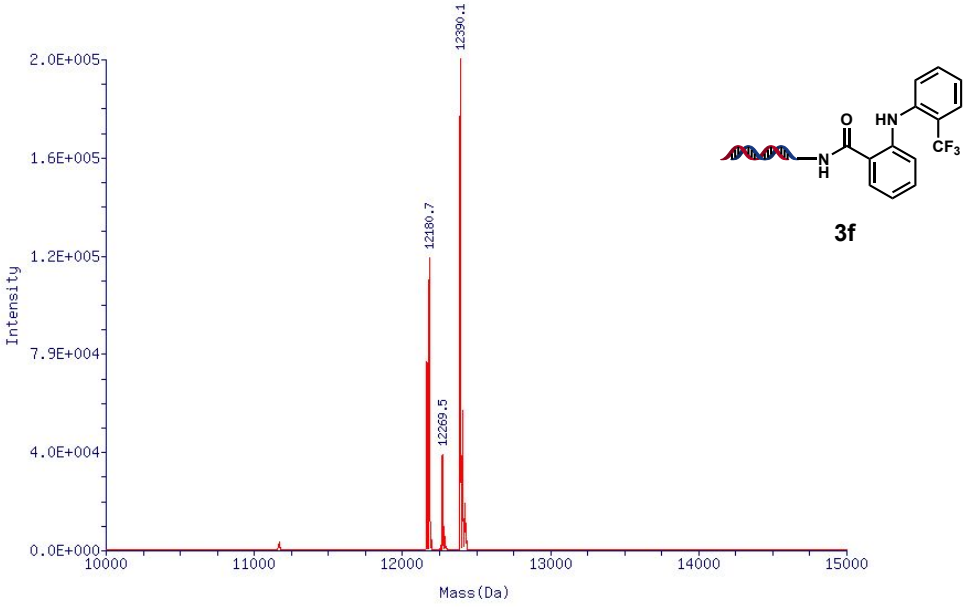


Figure S95. Deconvoluted mass spectrum of DNA **3f**, expected: 12323.2; no product observed.

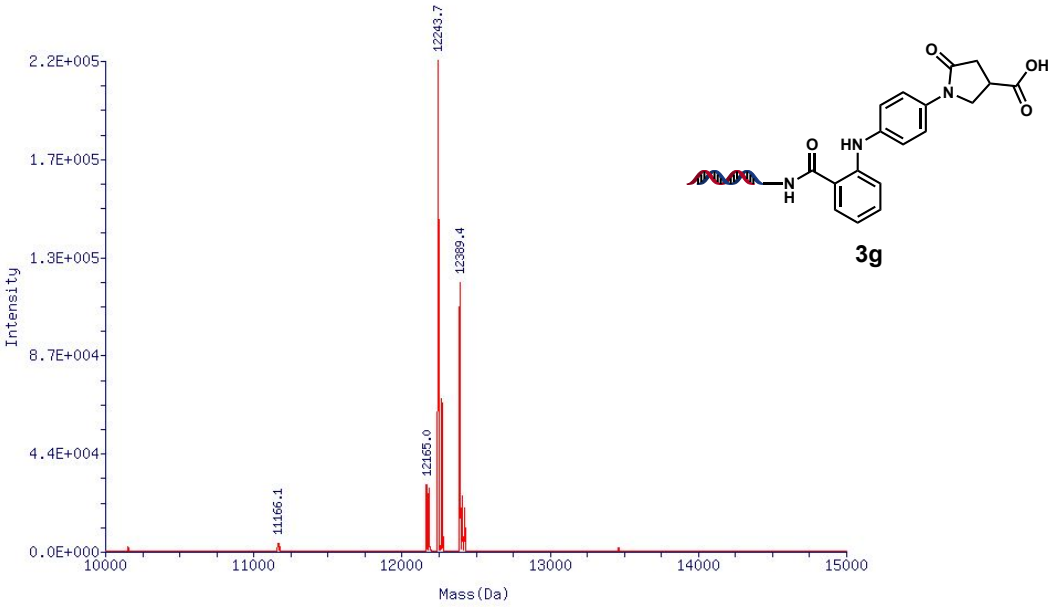


Figure S96. Deconvoluted mass spectrum of DNA **3g**, expected: 12382.2; no product observed.

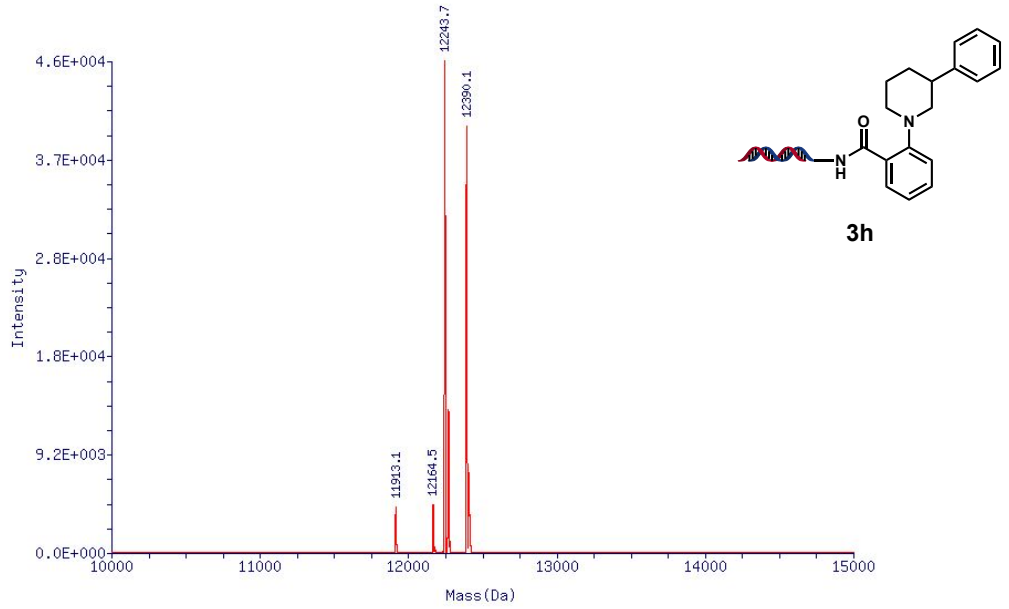


Figure S97. Deconvoluted mass spectrum of DNA **3h**, expected: 12323.3; no product observed.

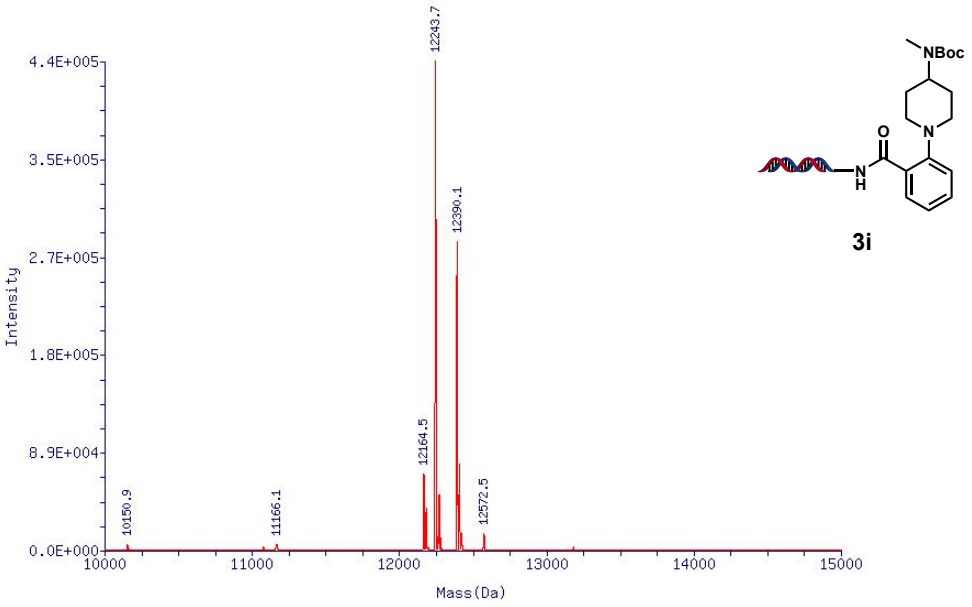


Figure S98. Deconvoluted mass spectrum of DNA **3i**, expected: 12376.4; no product observed.

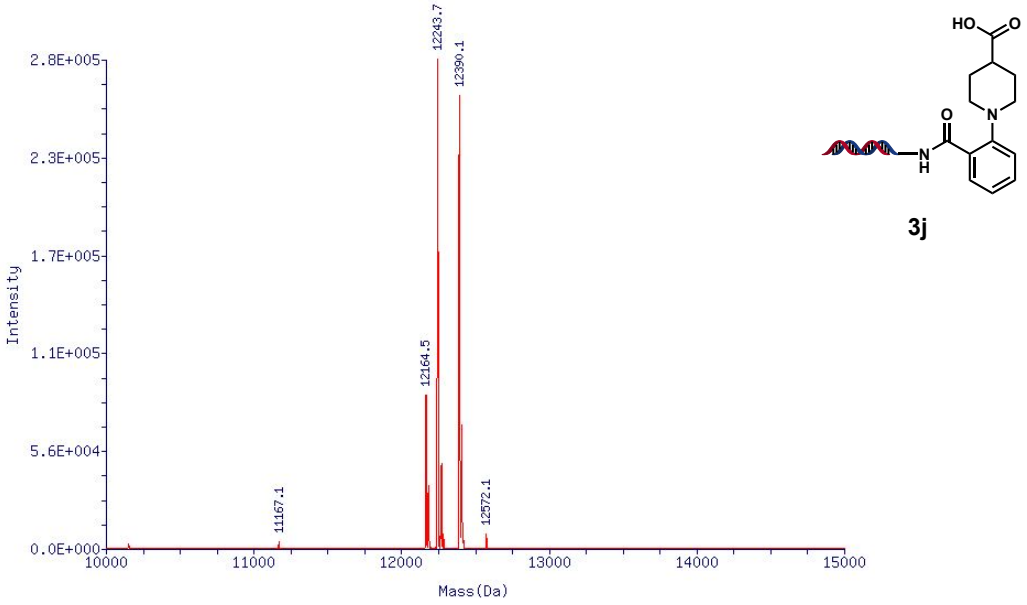


Figure S99. Deconvoluted mass spectrum of DNA **3j**, expected: 12291.3; no product observed.

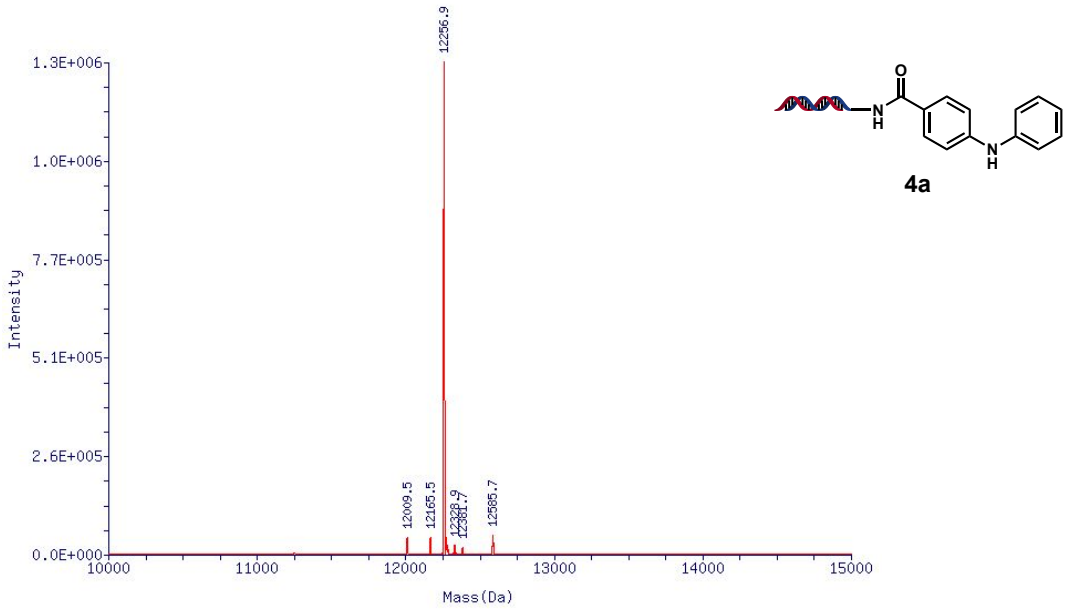


Figure S100. Deconvoluted mass spectrum of DNA **4a**, expected: 12255.2; observed 12256.9.

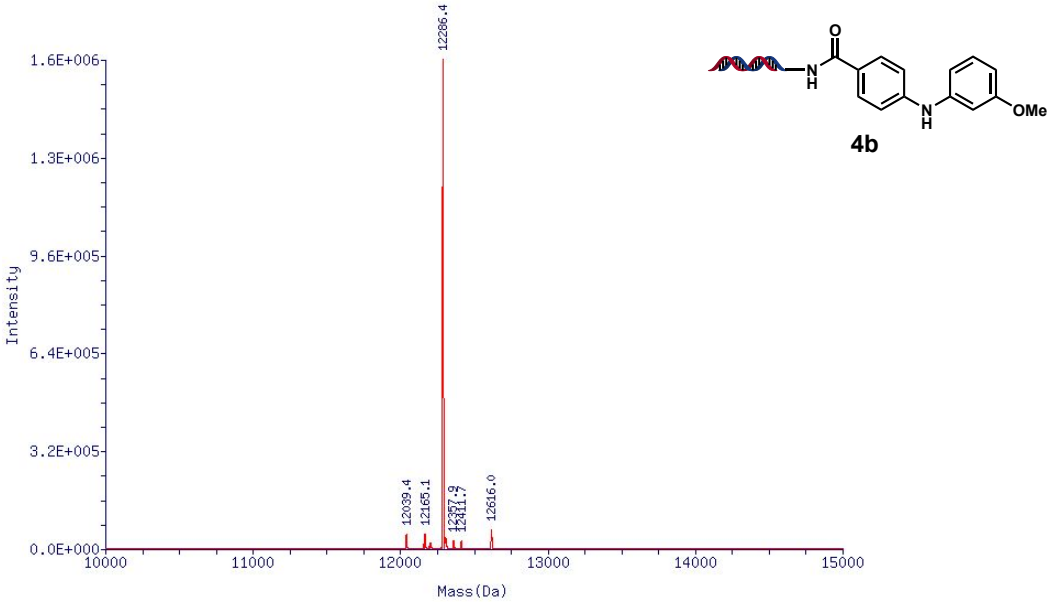


Figure S101. Deconvoluted mass spectrum of DNA **4b**, expected: 12285.3; observed 12286.4.

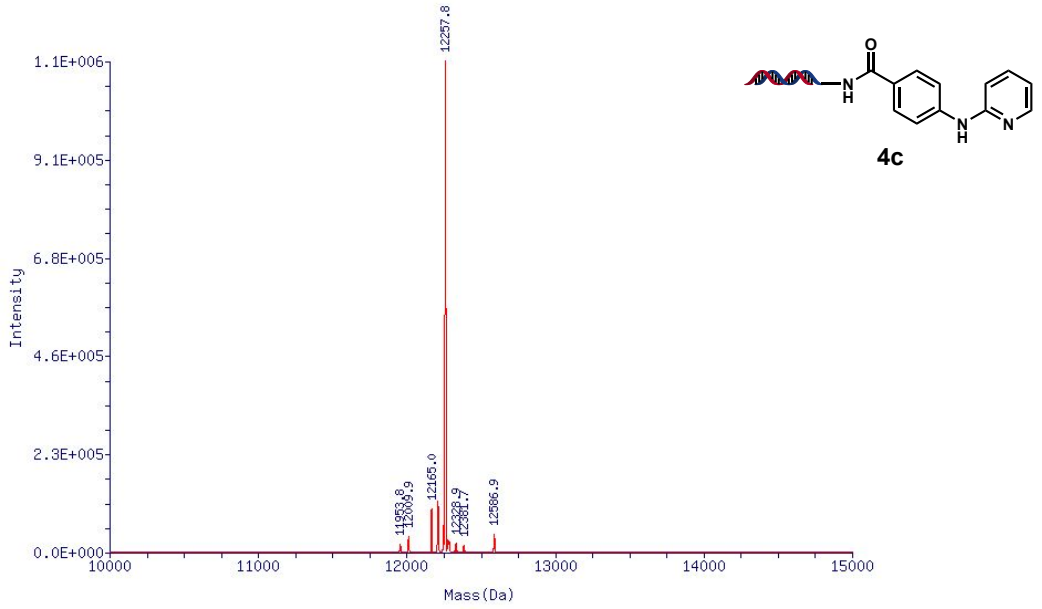


Figure S102. Deconvoluted mass spectrum of DNA **4c**, expected: 12256.2; observed 12257.8.

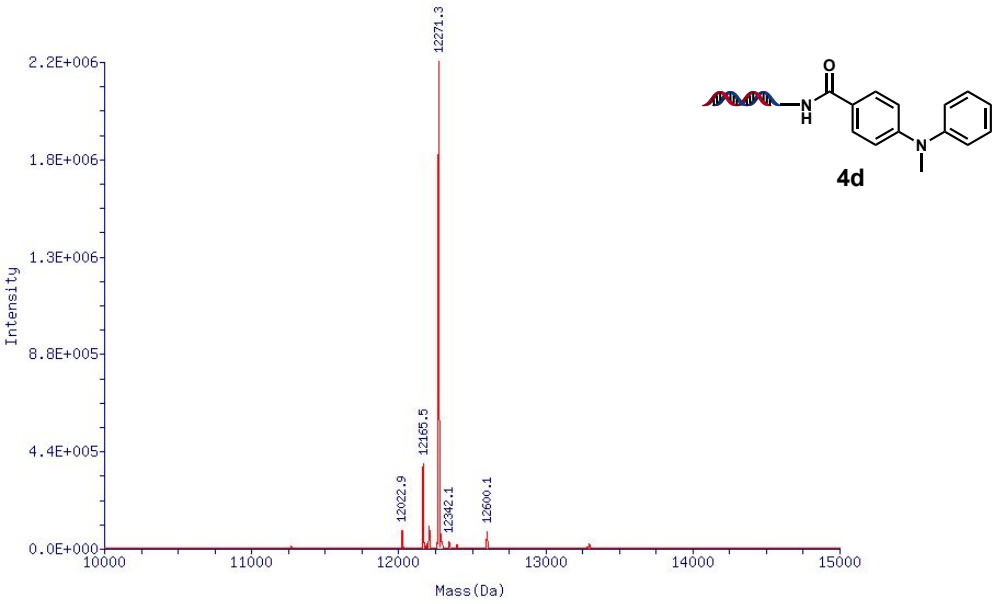


Figure S103. Deconvoluted mass spectrum of DNA **4d**, expected: 12269.3; observed 12271.3.

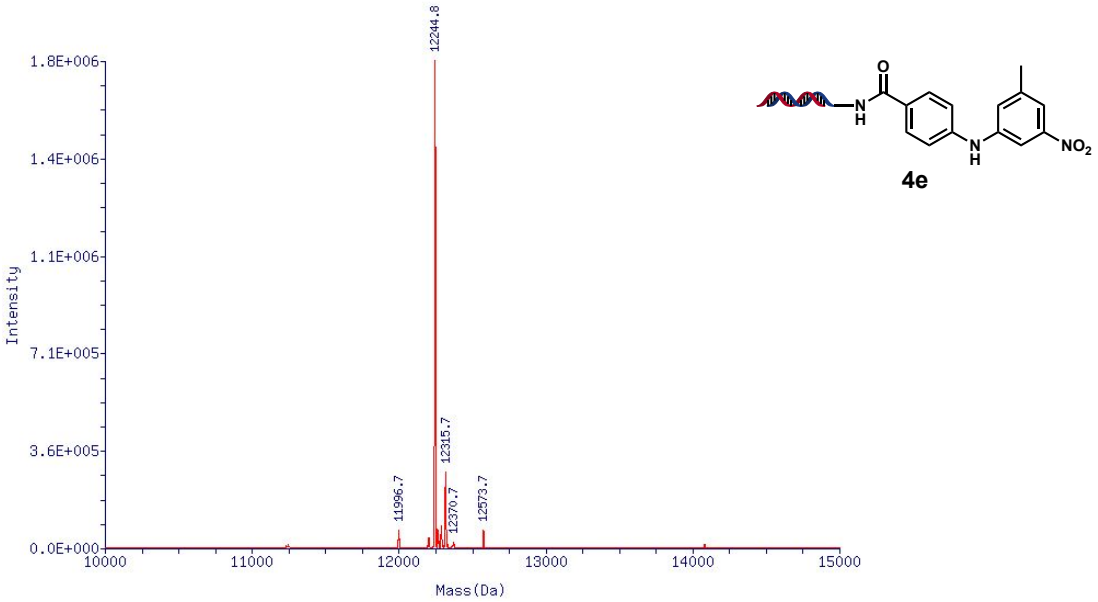


Figure S104. Deconvoluted mass spectrum of DNA **4e**, expected: 12314.2; observed 12315.7.

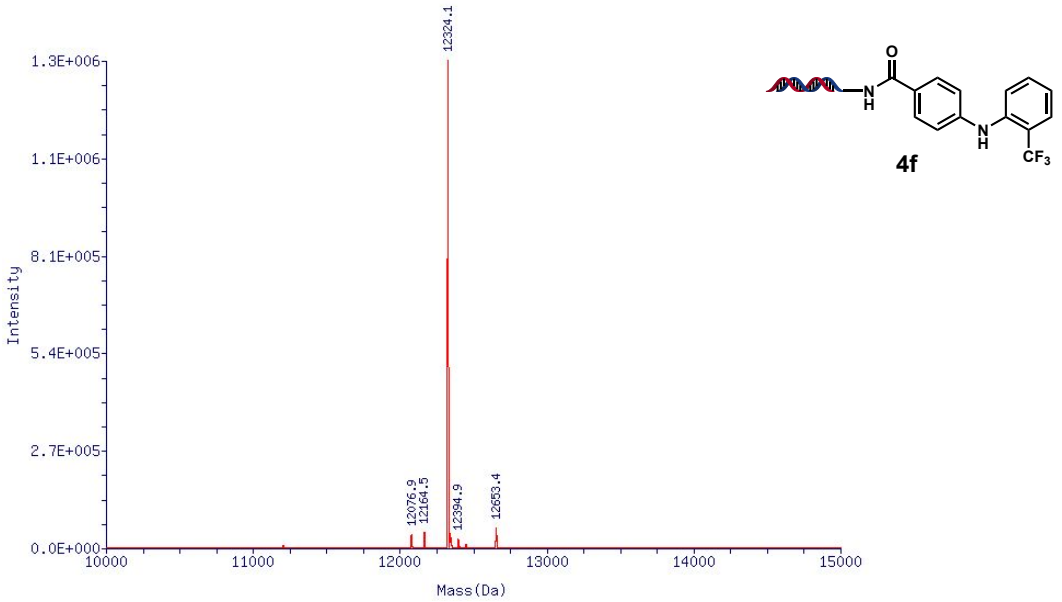


Figure S105. Deconvoluted mass spectrum of DNA **4f**, expected: 12323.2; observed 12324.1.

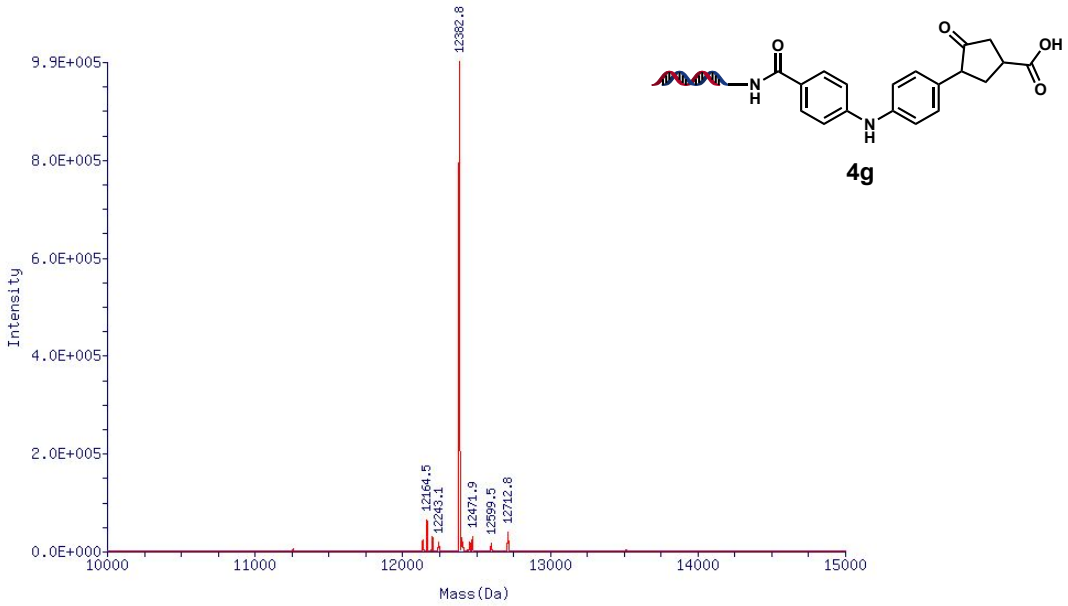


Figure S106. Deconvoluted mass spectrum of DNA **4g**, expected: 12382.2; observed 12382.8.

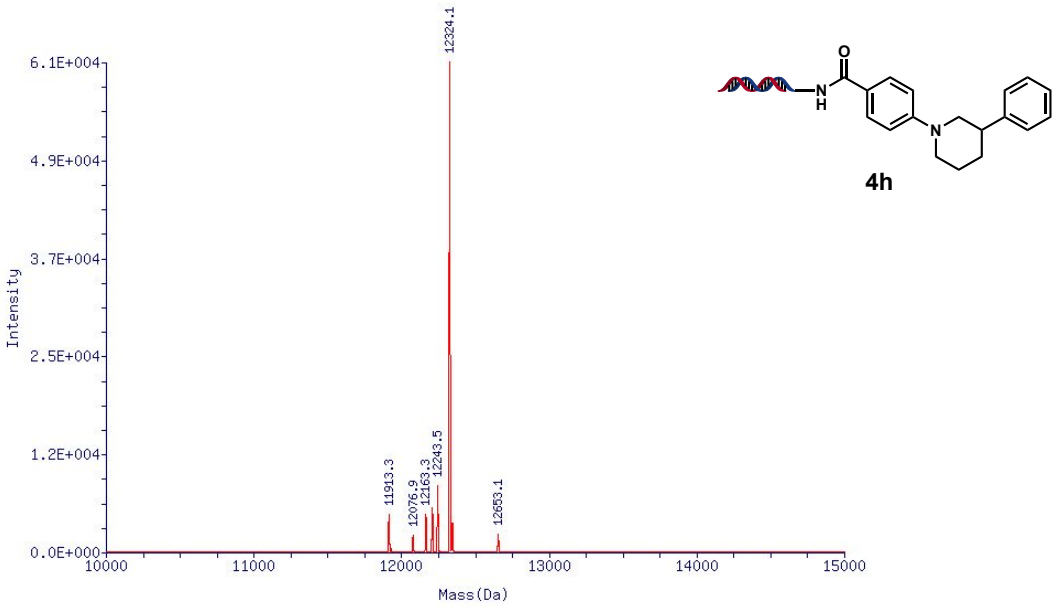


Figure S107. Deconvoluted mass spectrum of DNA **4h**, expected: 12323.3; observed 12324.1.

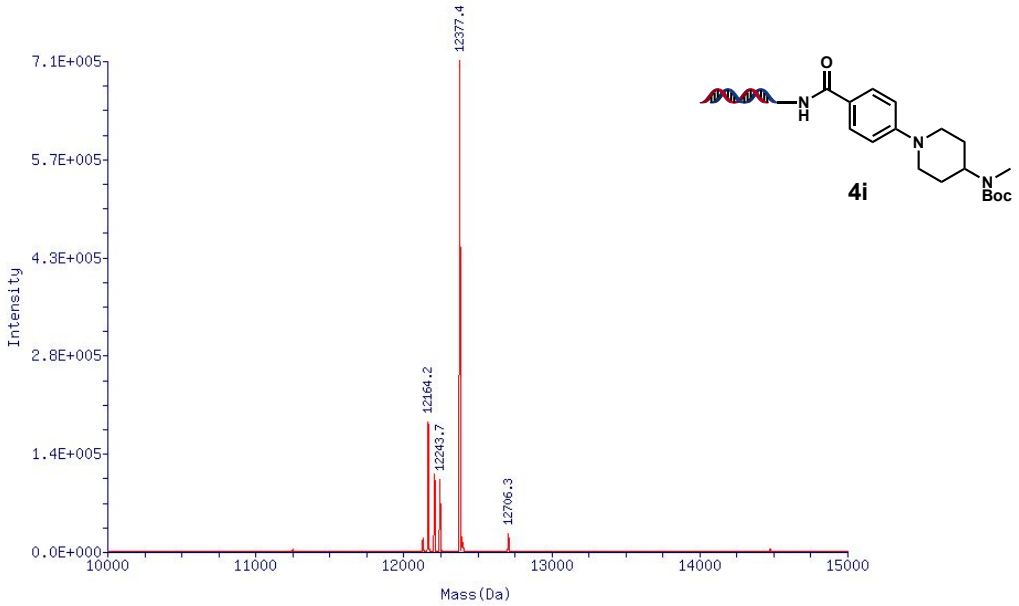


Figure S108. Deconvoluted mass spectrum of DNA **4i**, expected: 12376.4; observed 12377.4.

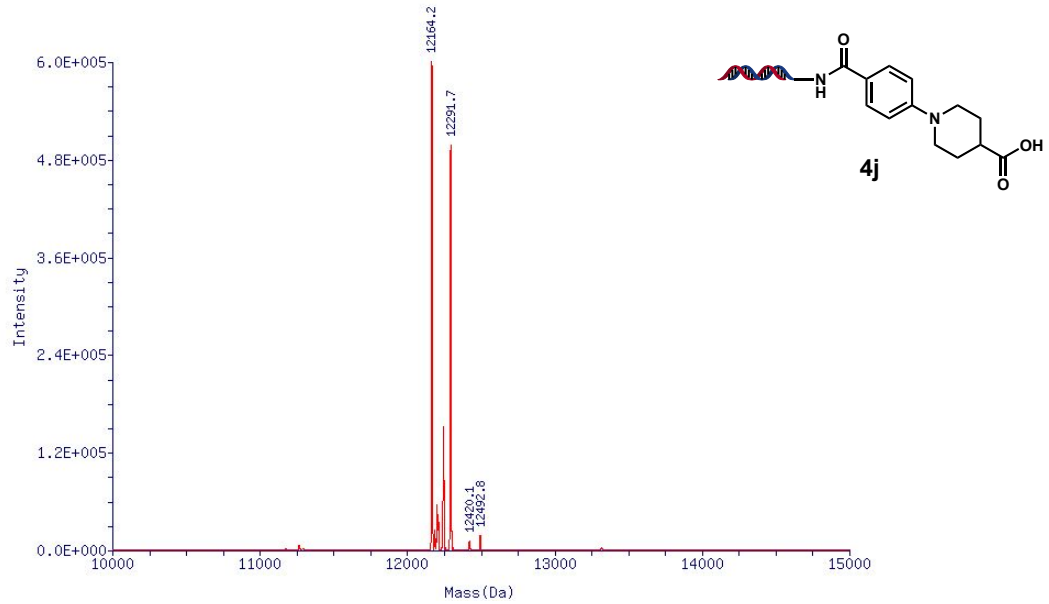


Figure S109. Deconvoluted mass spectrum of DNA **4j**, expected: 12291.3; observed 12291.7.

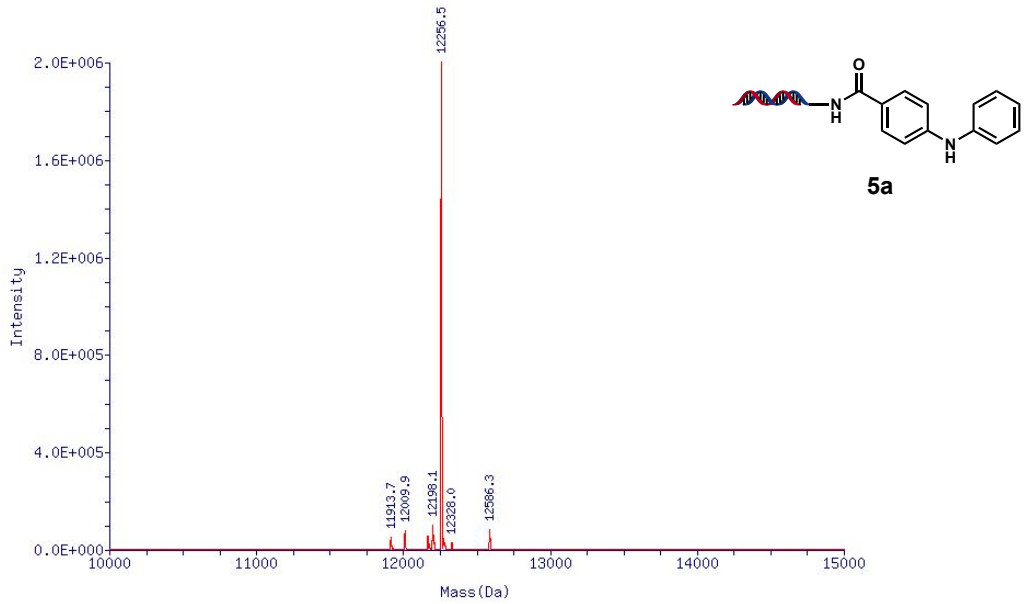


Figure S110. Deconvoluted mass spectrum of DNA **5a**, expected: 12255.2; observed 12256.5.

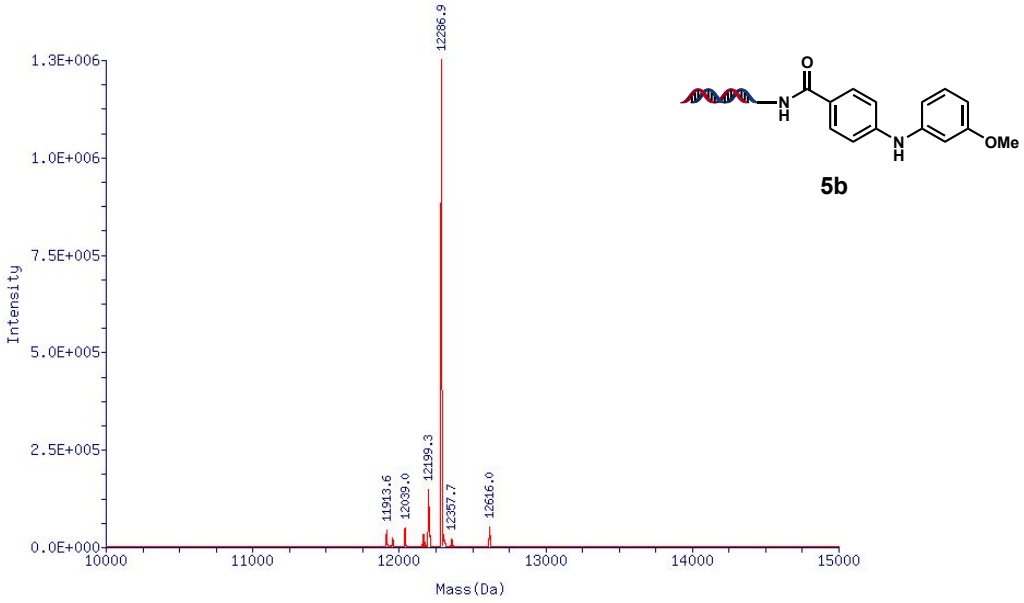


Figure S111. Deconvoluted mass spectrum of DNA **5b**, expected: 12285.3; observed 12286.9.

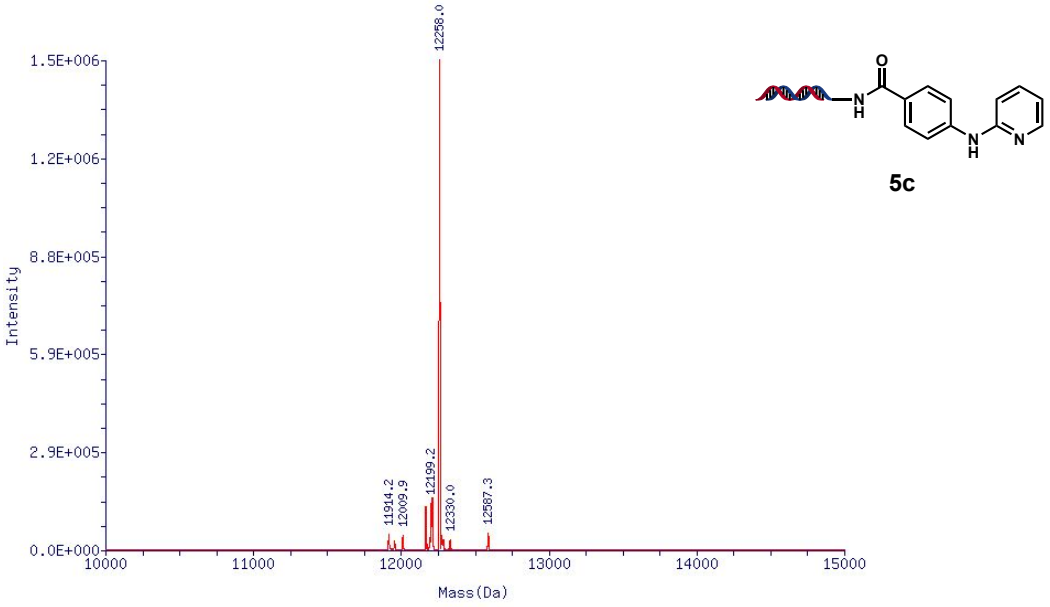


Figure S112. Deconvoluted mass spectrum of DNA **5c**, expected: 12256.2; observed 12258.

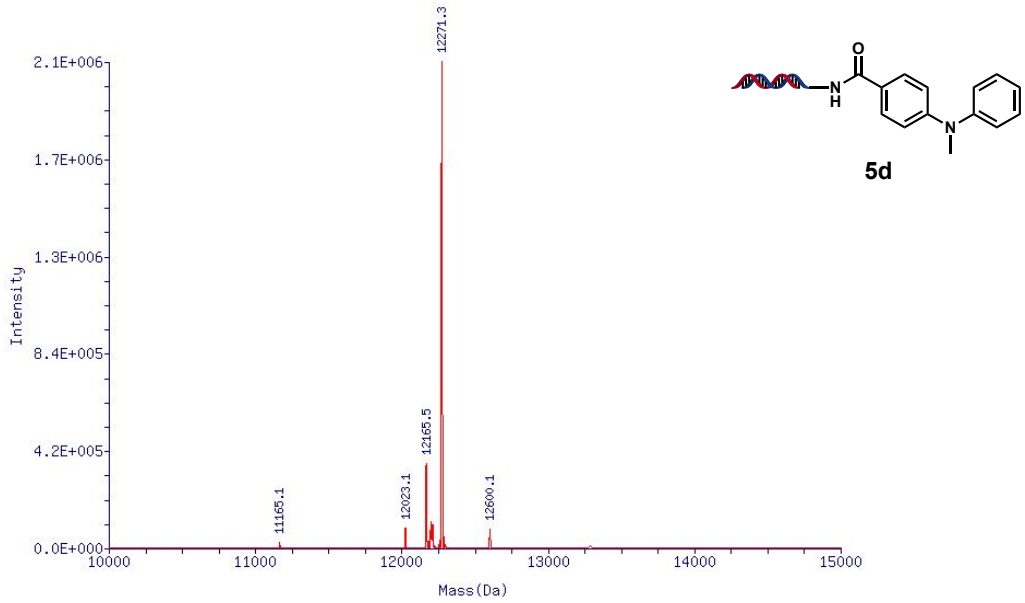


Figure S113. Deconvoluted mass spectrum of DNA **5d**, expected: 12269.3; observed 12271.3.

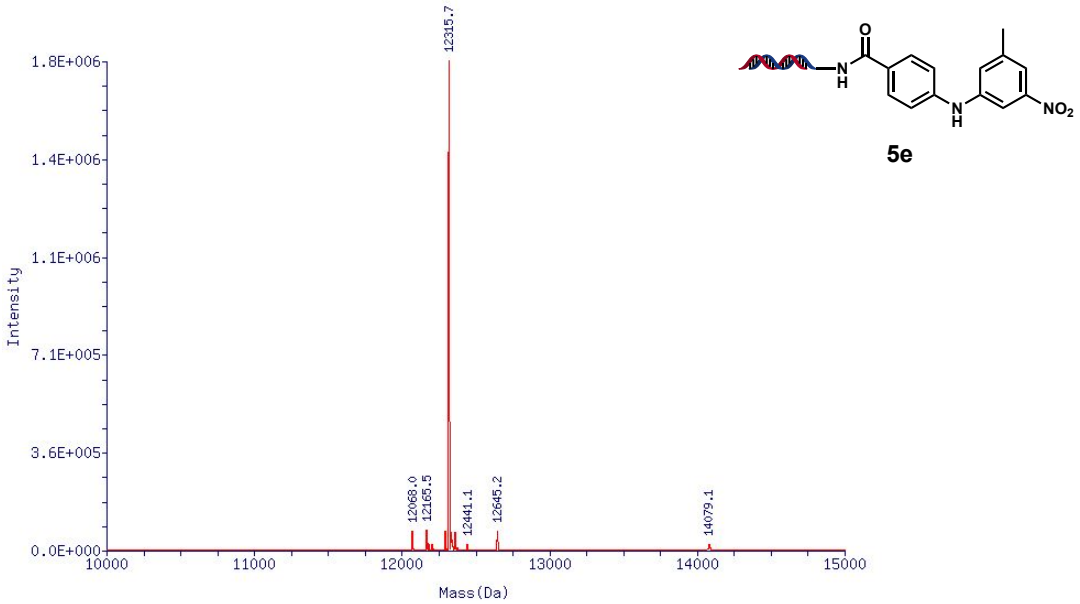


Figure S114. Deconvoluted mass spectrum of DNA **5e**, expected: 12314.2; observed 12315.7.

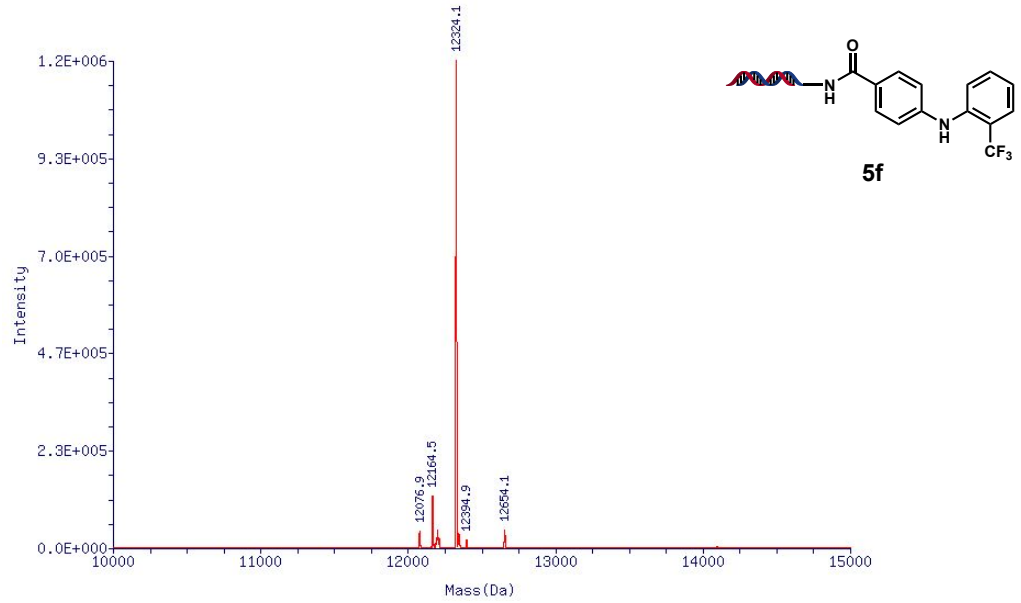


Figure S115. Deconvoluted mass spectrum of DNA **5f**, expected: 12323.2; observed 12324.1.

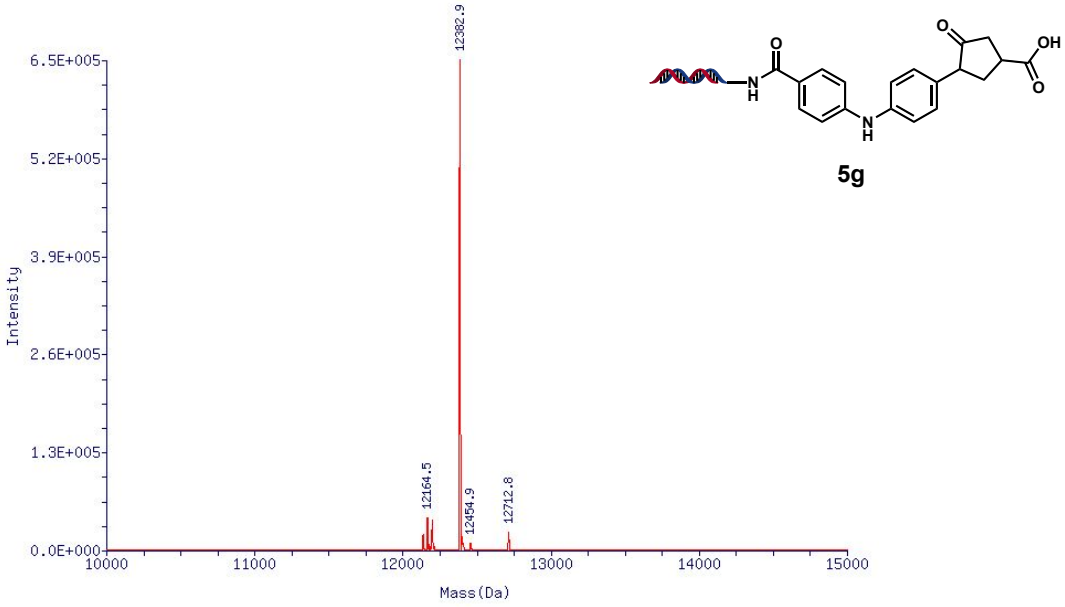


Figure S116. Deconvoluted mass spectrum of DNA **5g**, expected: 12382.2; observed 12382.9.

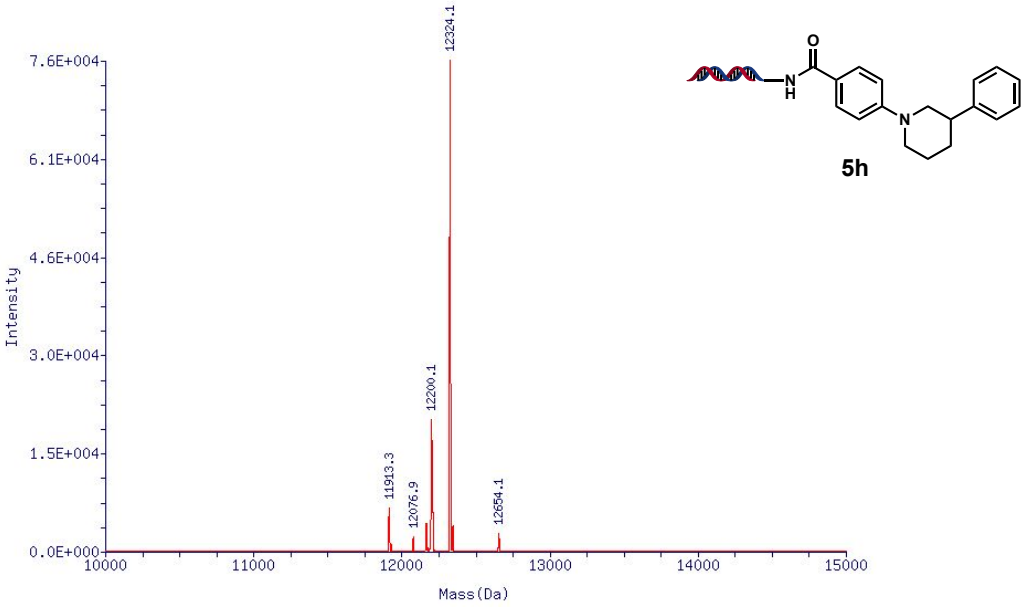


Figure S117. Deconvoluted mass spectrum of DNA **5h**, expected: 12323.3; observed 12324.1.

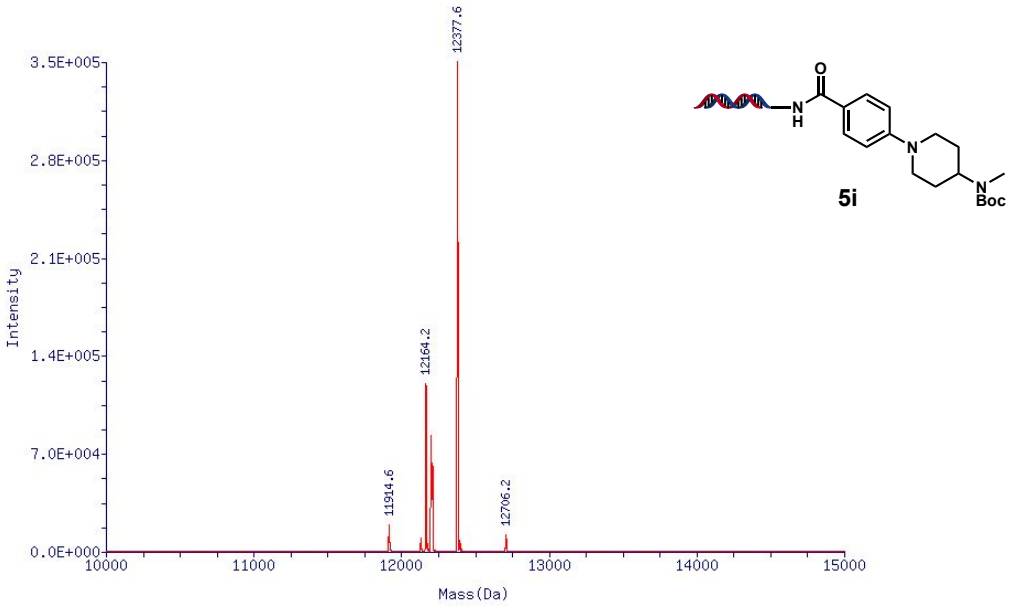


Figure S118. Deconvoluted mass spectrum of DNA **5i**, expected: 12376.4; observed 12377.6.

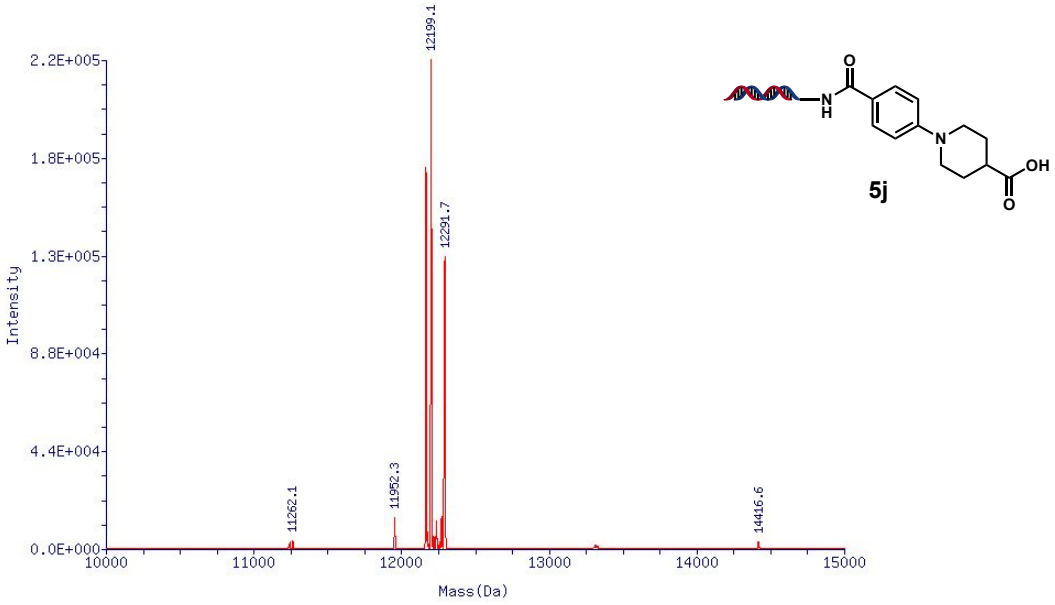


Figure S119. Deconvoluted mass spectrum of DNA **5j**, expected: 12291.3; observed 12291.7.

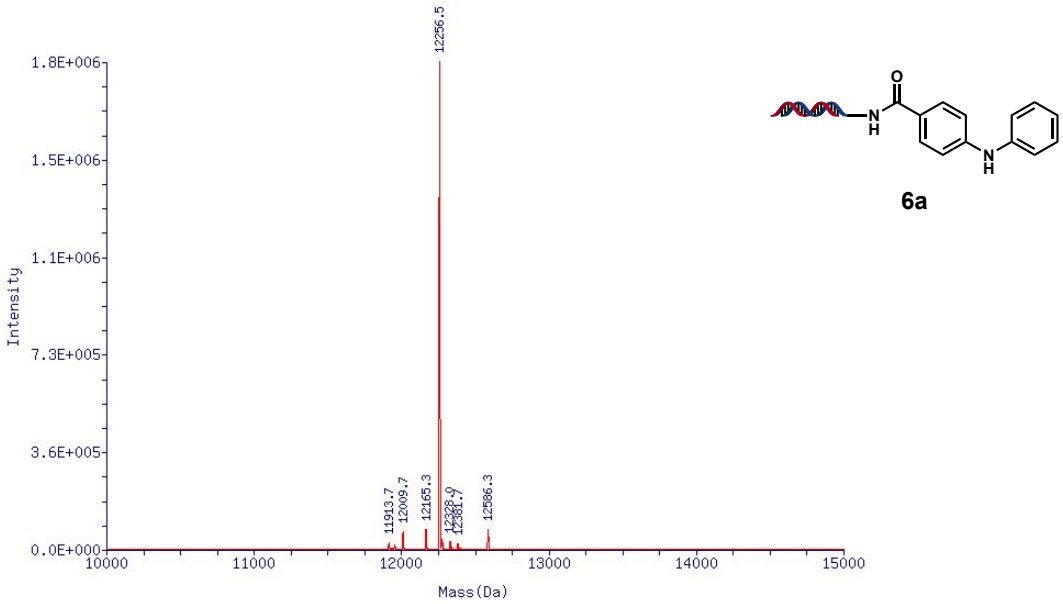


Figure S120. Deconvoluted mass spectrum of DNA **6a**, expected: 12255.1; observed 12256.5.

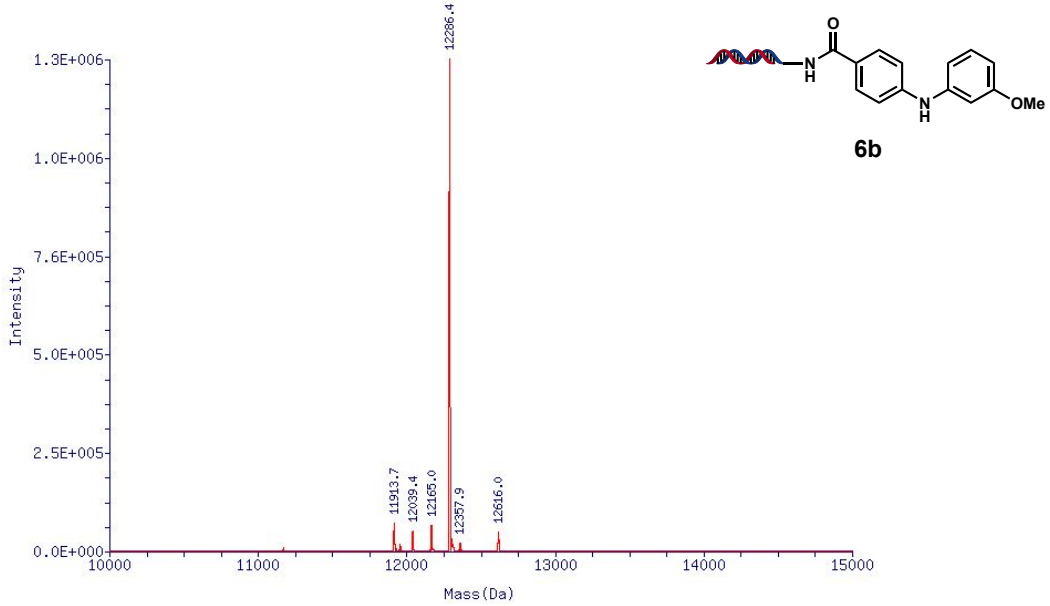


Figure S121. Deconvoluted mass spectrum of DNA **6b**, expected: 12285.1; observed 12286.4.

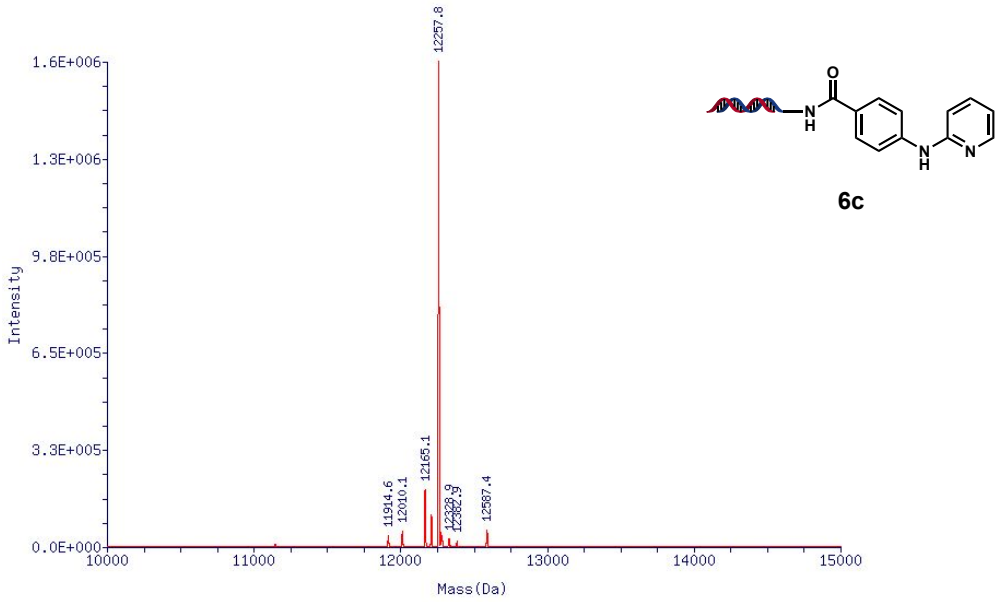


Figure S122. Deconvoluted mass spectrum of DNA **6c**, expected: 12256.1; observed 12257.8.

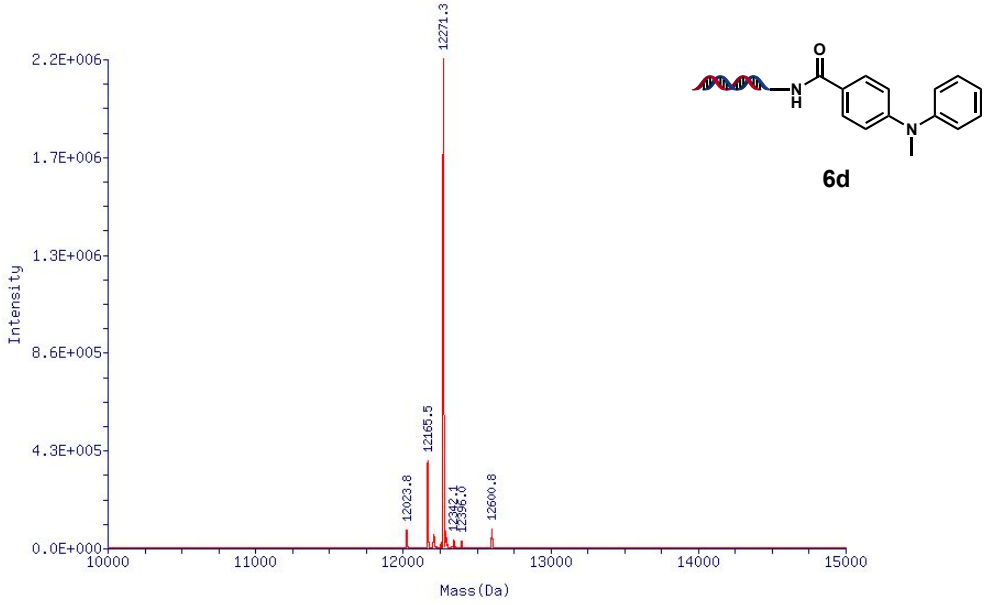


Figure S123. Deconvoluted mass spectrum of DNA **6d**, expected: 12269.1; observed 12271.3.

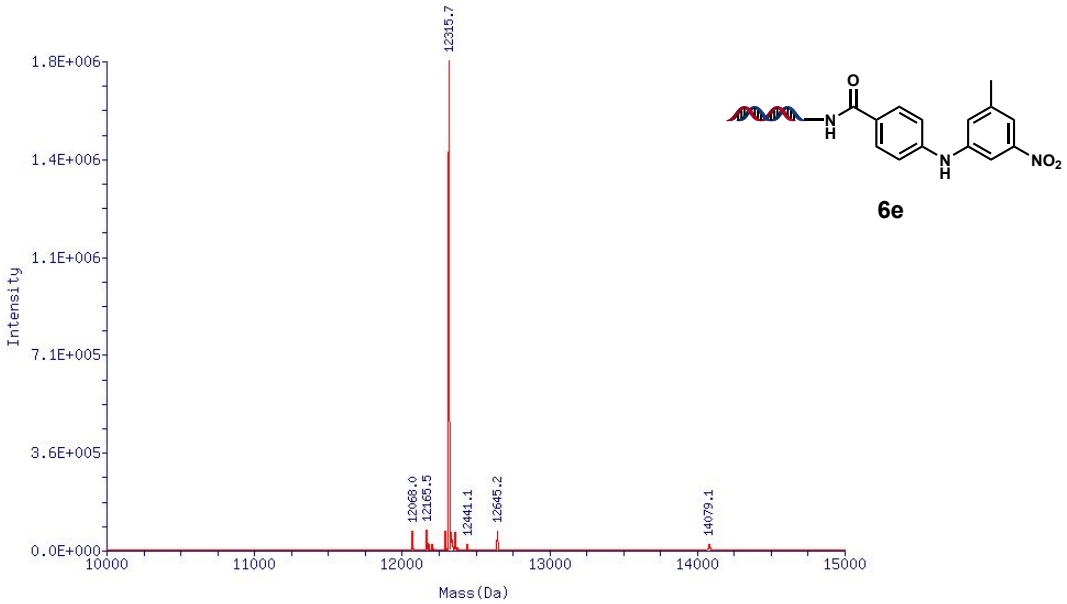


Figure S124. Deconvoluted mass spectrum of DNA **6e**, expected: 12314.1; observed 12315.7.

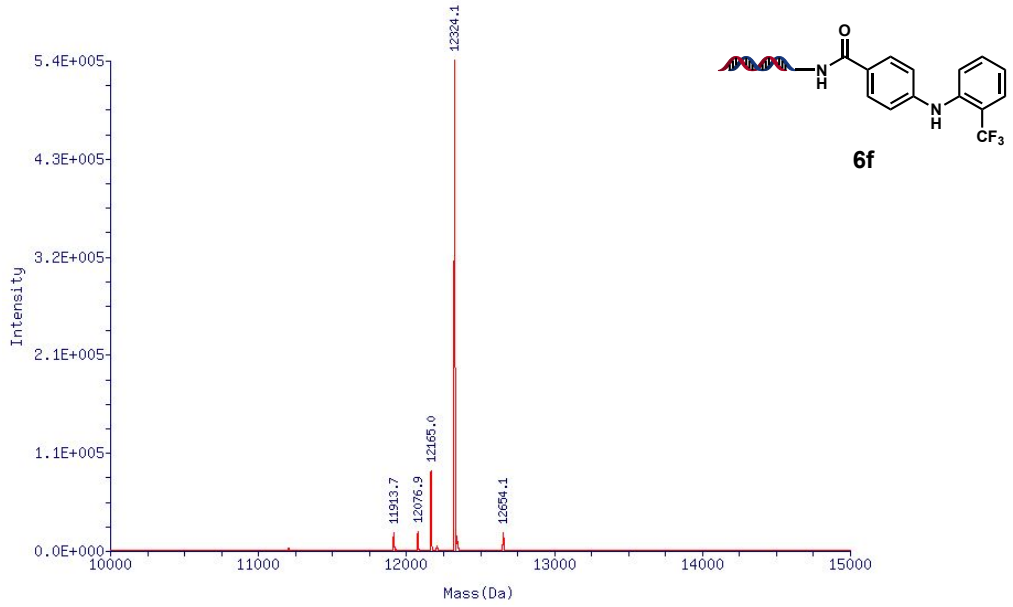


Figure S125. Deconvoluted mass spectrum of DNA **6f**, expected: 12323.1; observed 12324.1.

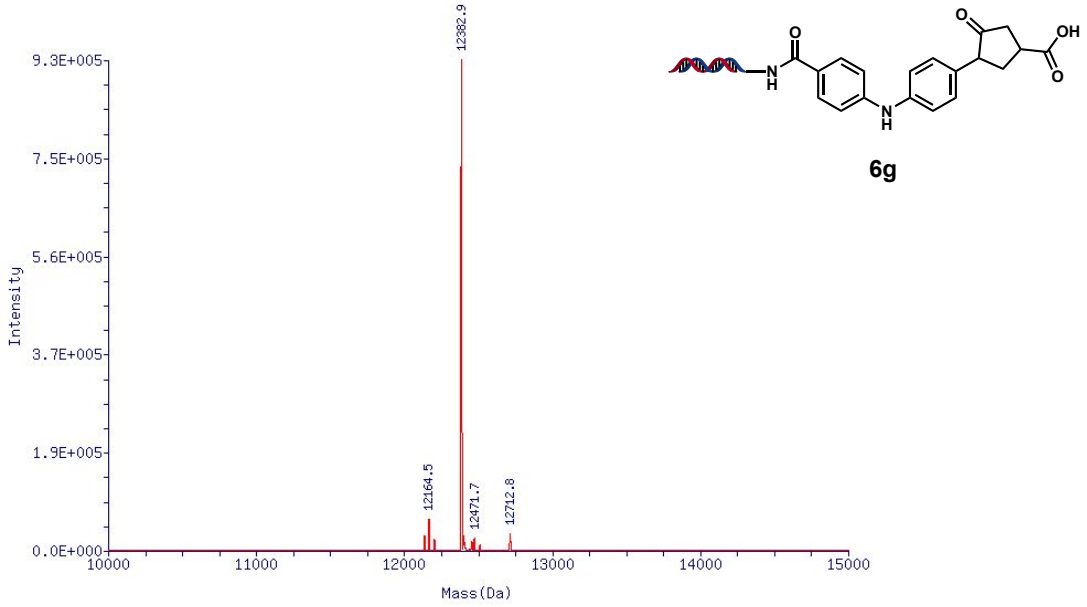


Figure S126. Deconvoluted mass spectrum of DNA **6g**, expected: 12382.1; observed 12382.9.

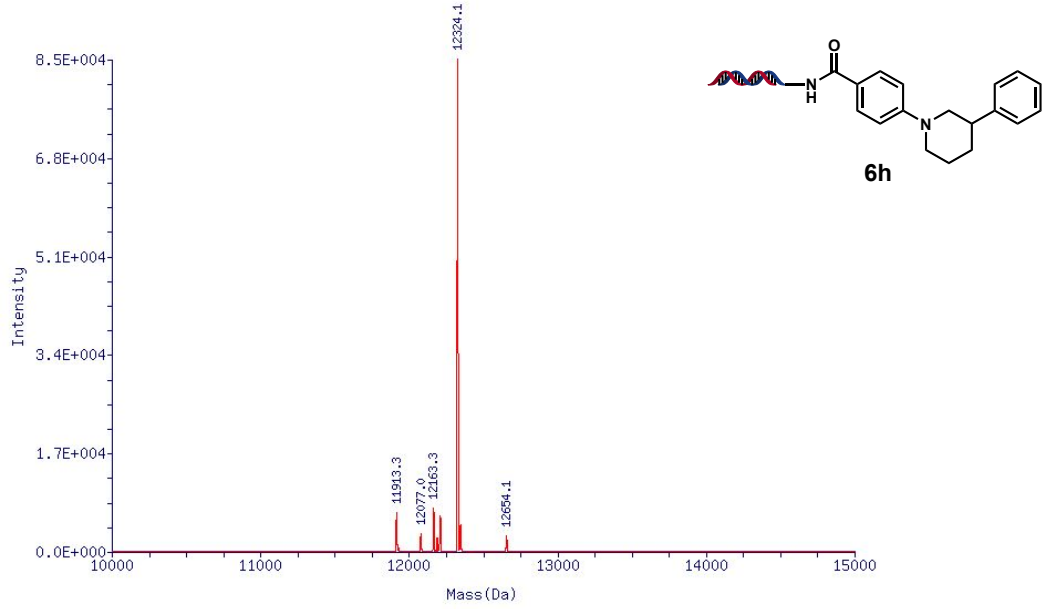


Figure S127. Deconvoluted mass spectrum of DNA **6h**, expected: 12323.3; observed 12324.1.

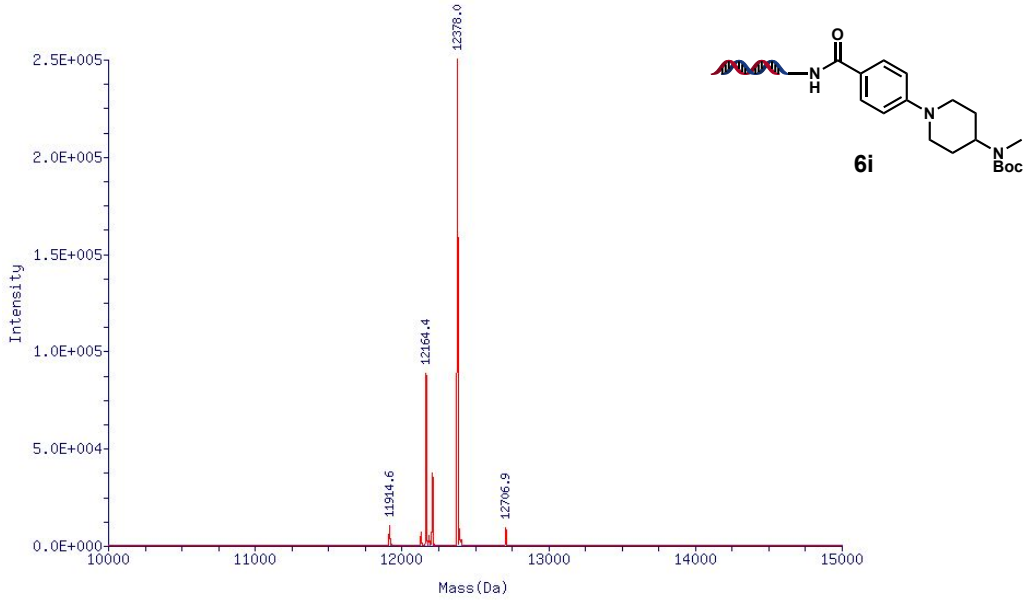


Figure S128. Deconvoluted mass spectrum of DNA **6i**, expected: 12376.3; observed 12378.

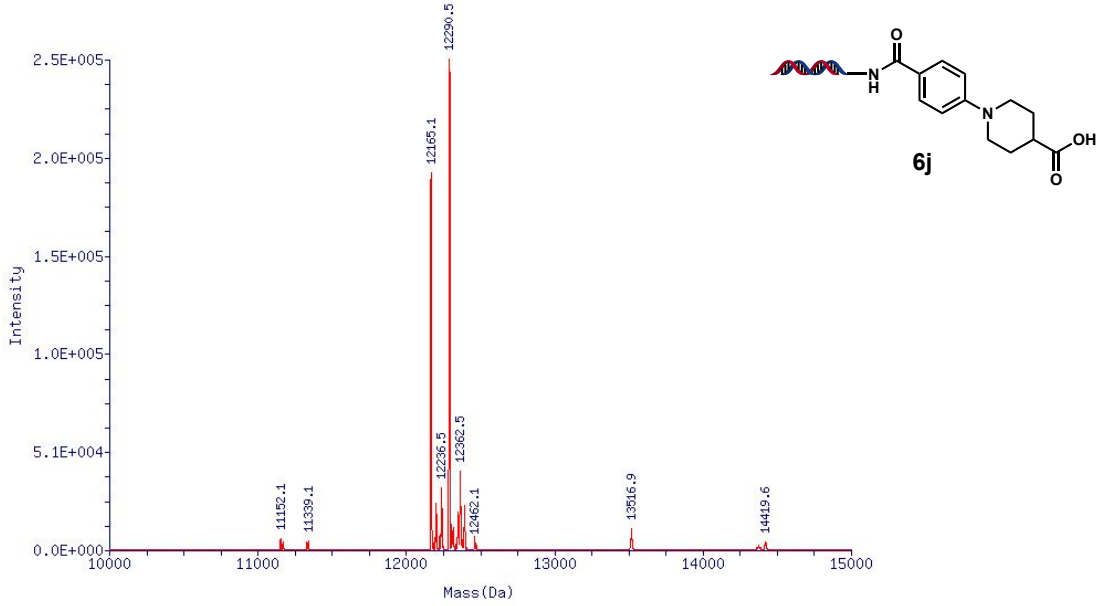


Figure S129. Deconvoluted mass spectrum of DNA **6j**, expected: 12291.1; observed 12290.5.

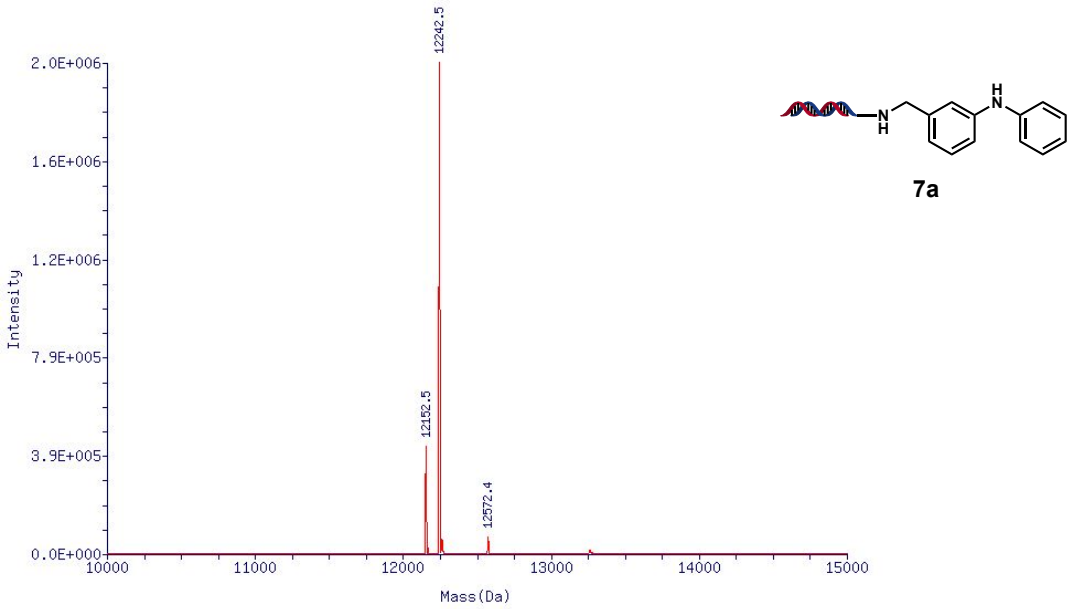


Figure S130. Deconvoluted mass spectrum of DNA **7a**, expected: 12241.2; observed 12242.5.

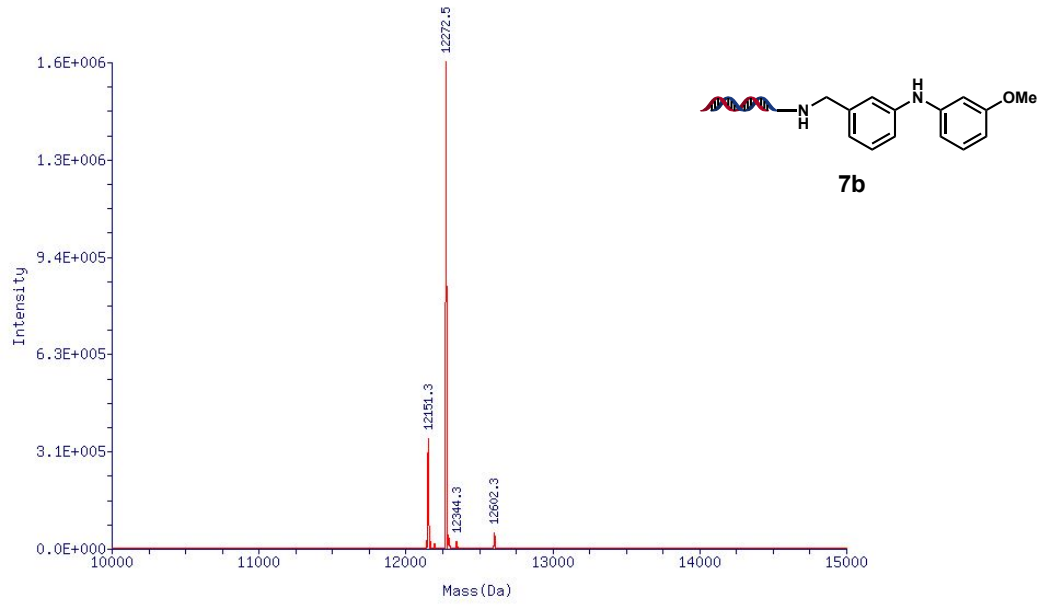


Figure S131. Deconvoluted mass spectrum of DNA **7b**, expected: 12271.3; observed 12272.5.

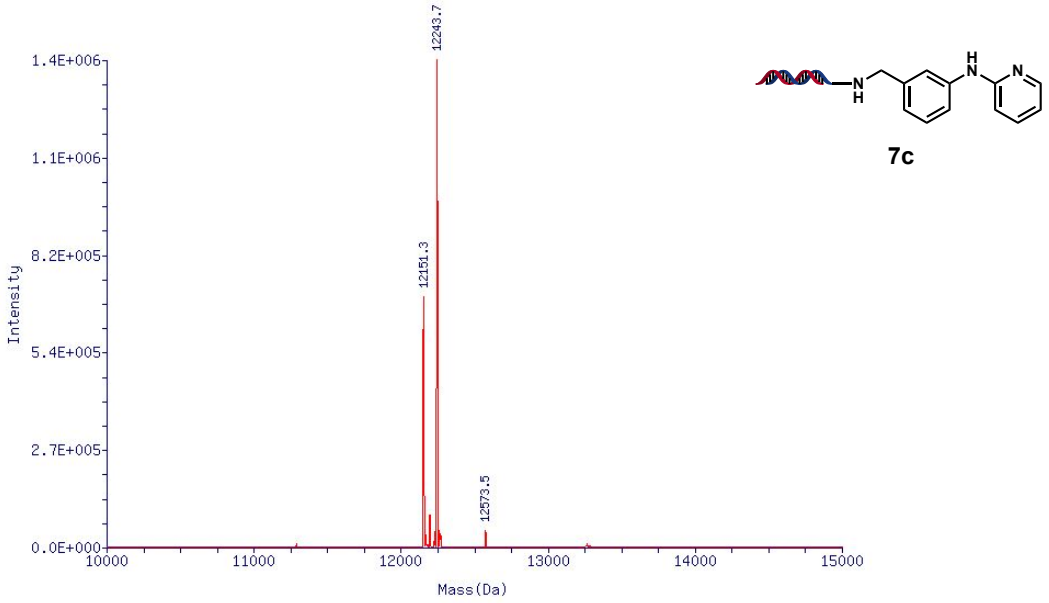


Figure S132. Deconvoluted mass spectrum of DNA **7c**, expected: 12242.2; observed 12243.7.

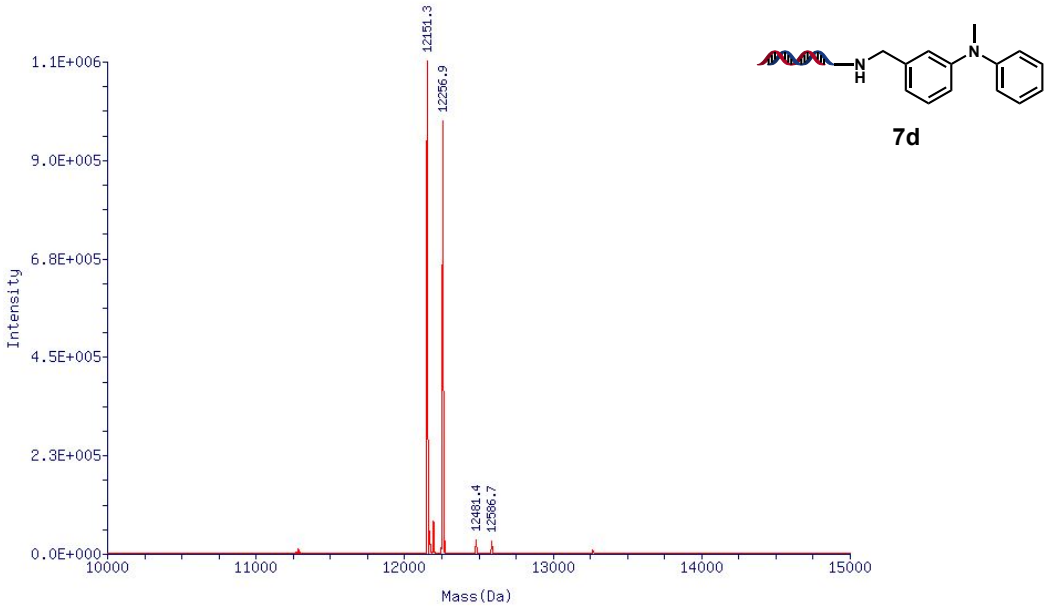


Figure S133. Deconvoluted mass spectrum of DNA **7d**, expected: 12255.3; observed 12256.9.

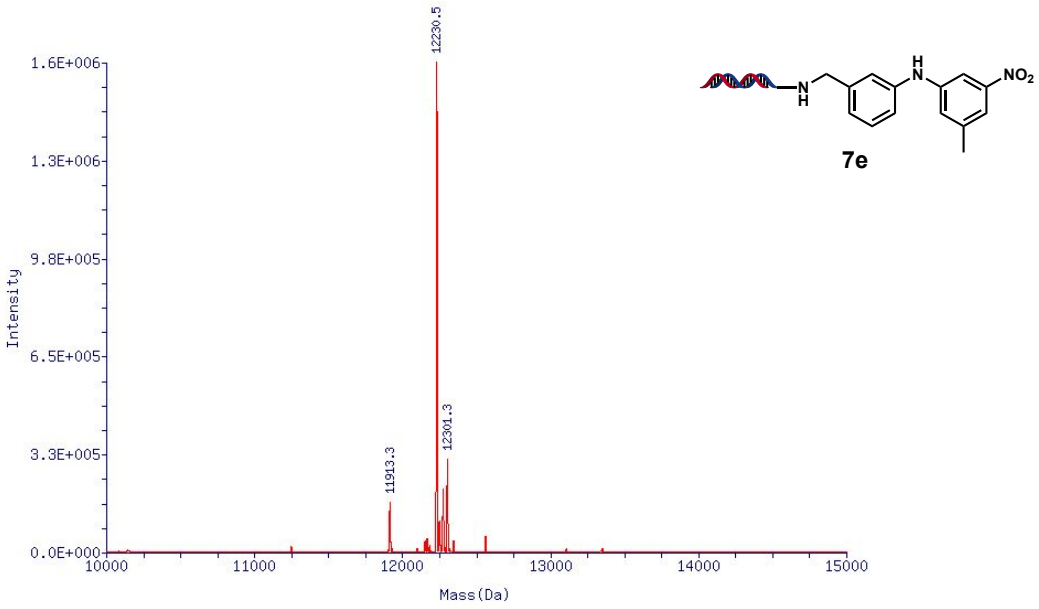


Figure S134. Deconvoluted mass spectrum of DNA **7e**, expected: 12300.3; observed 12301.3.

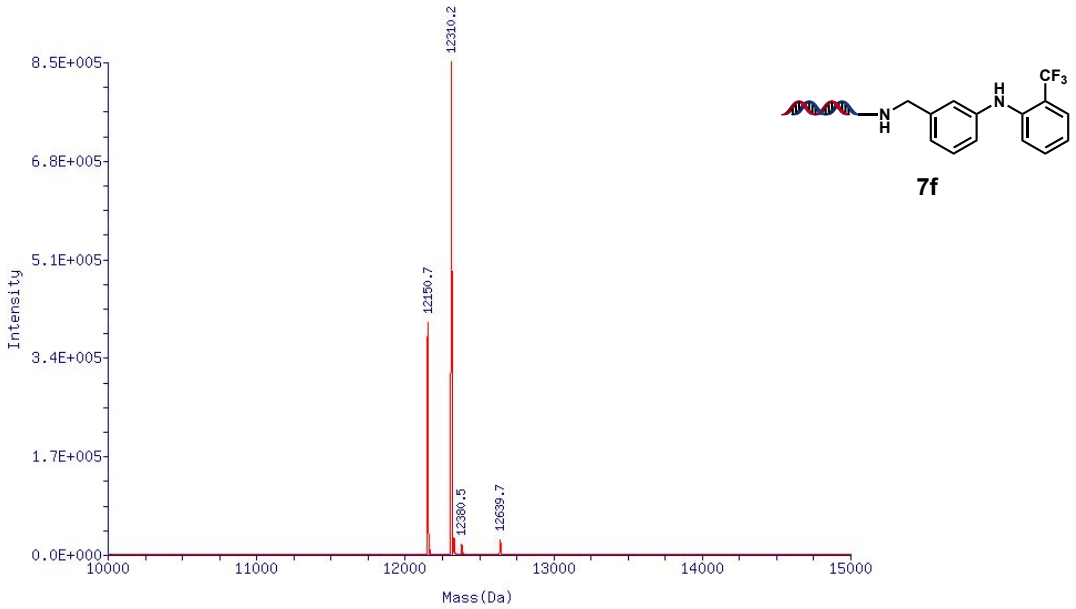


Figure S135. Deconvoluted mass spectrum of DNA **7f**, expected: 12309.2; observed 12310.2.

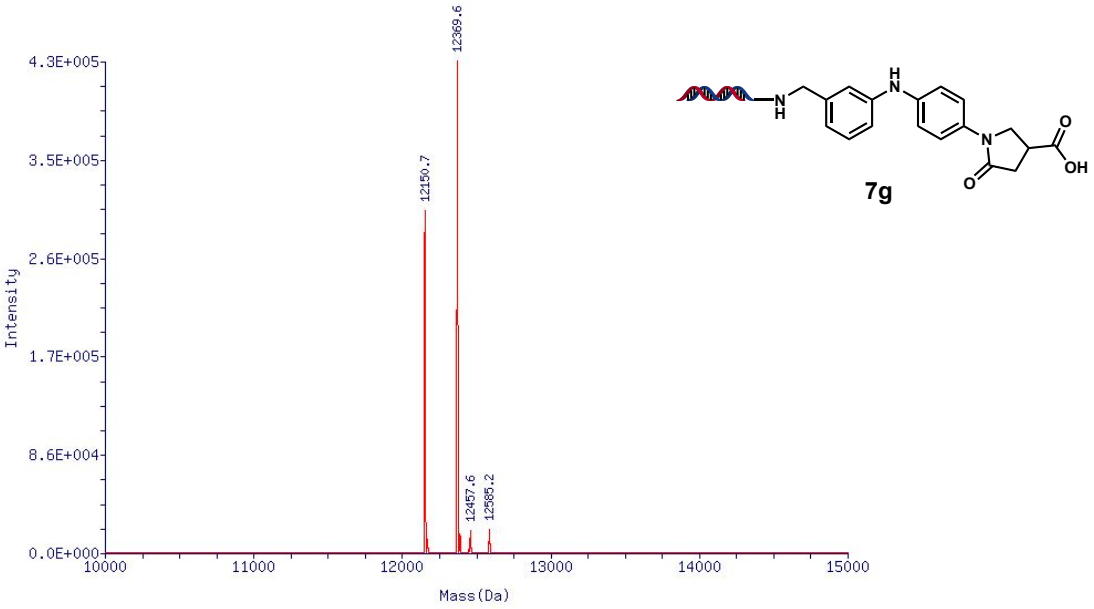


Figure S136. Deconvoluted mass spectrum of DNA **7g**, expected: 12368.3; observed 12369.6.

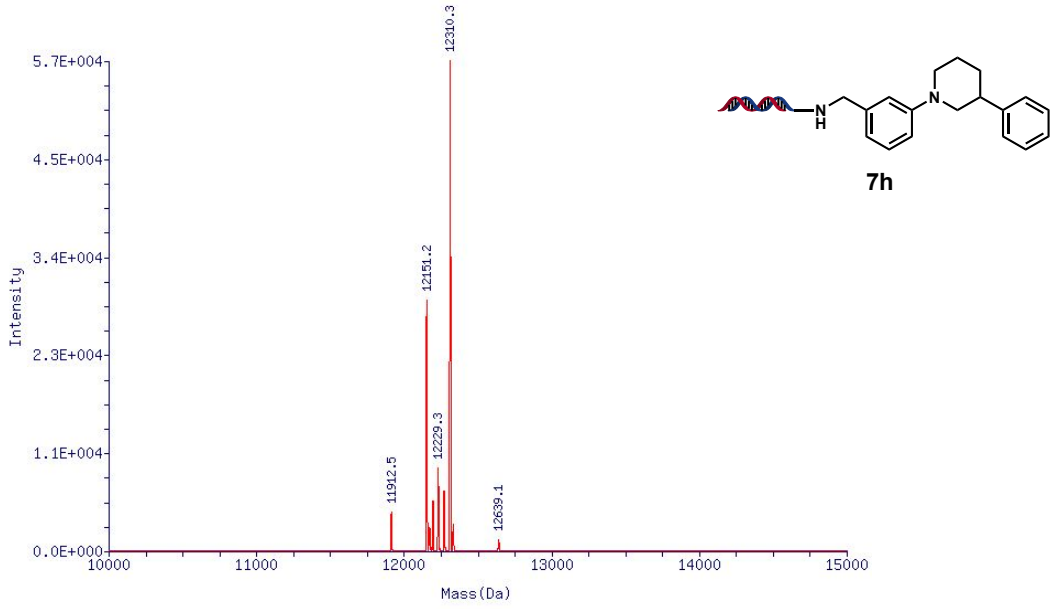


Figure S137. Deconvoluted mass spectrum of DNA **7h**, expected: 12309.4; observed 12310.3.

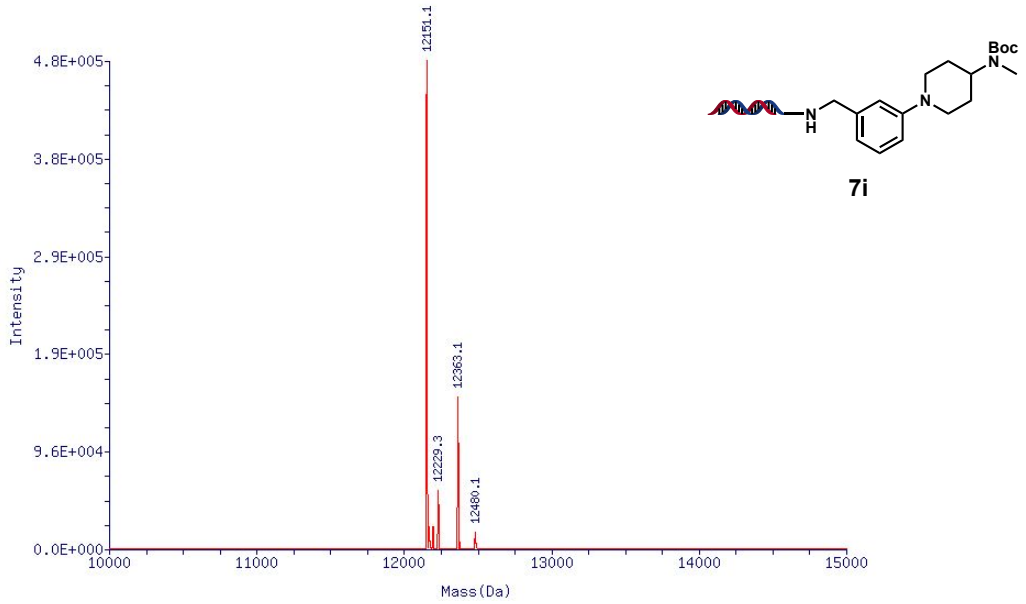


Figure S138. Deconvoluted mass spectrum of DNA **7i**, expected: 12362.4; observed 12363.1.

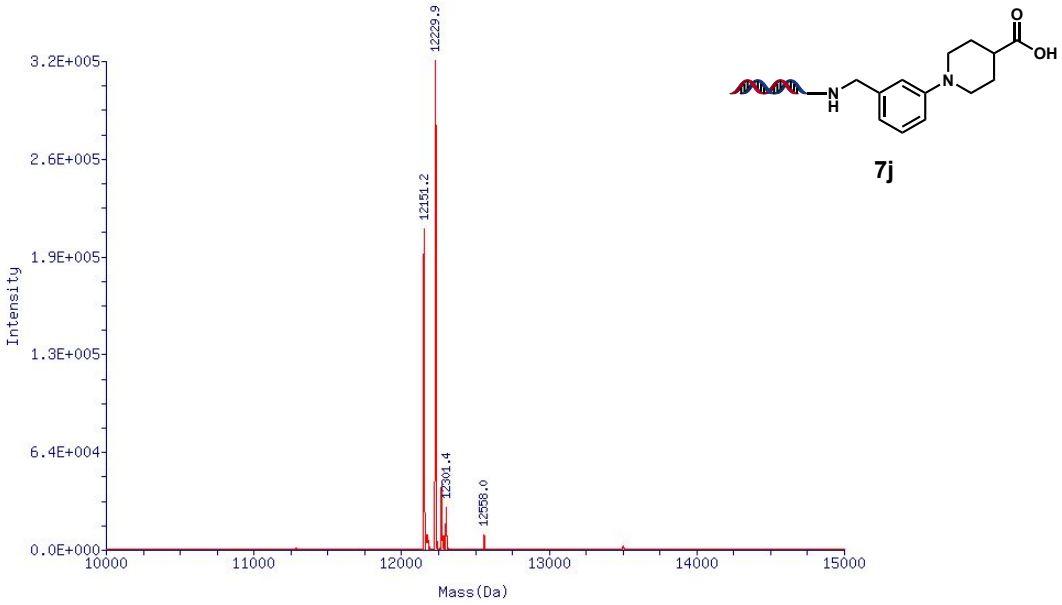


Figure S139. Deconvoluted mass spectrum of DNA **7j**, expected: 12277.3; no product observed.

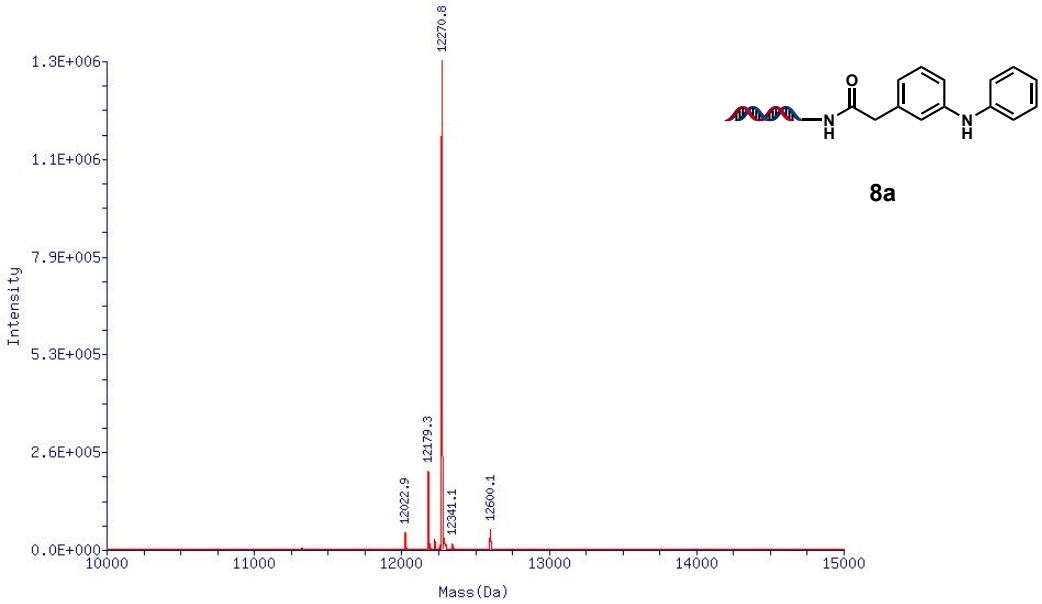


Figure S140. Deconvoluted mass spectrum of DNA **8a**, expected: 12269.3; observed 12270.8.

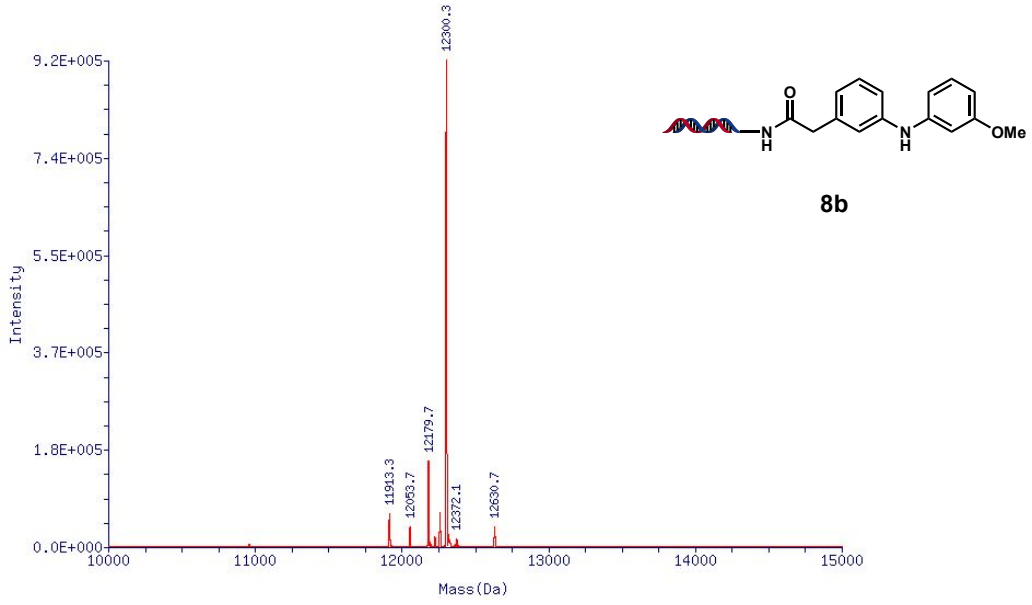


Figure S141. Deconvoluted mass spectrum of DNA **8b**, expected: 12299.3; observed 12300.3.

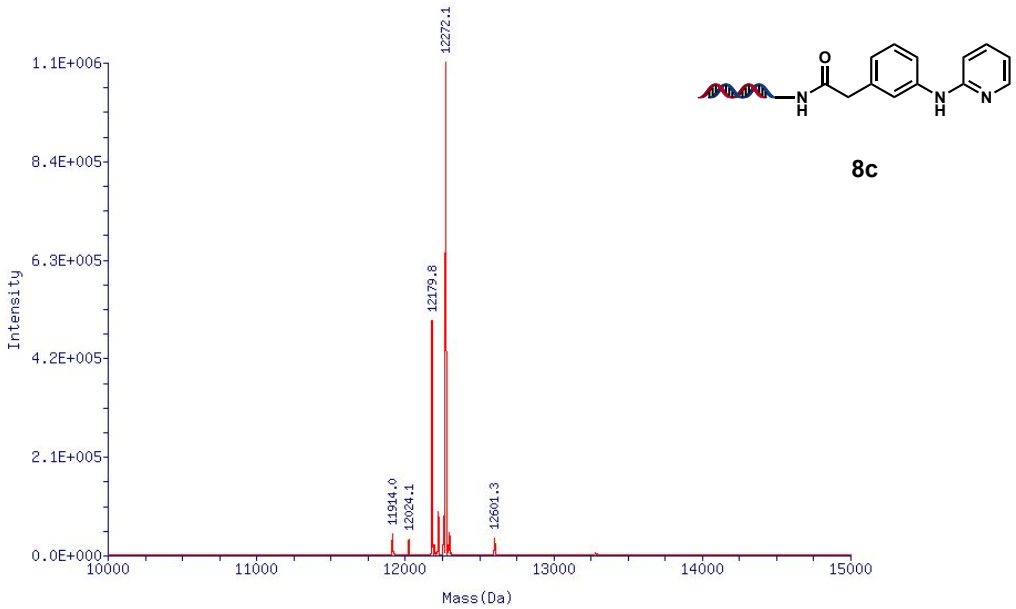


Figure S142. Deconvoluted mass spectrum of DNA **8c**, expected: 12270.2; observed 12272.1.

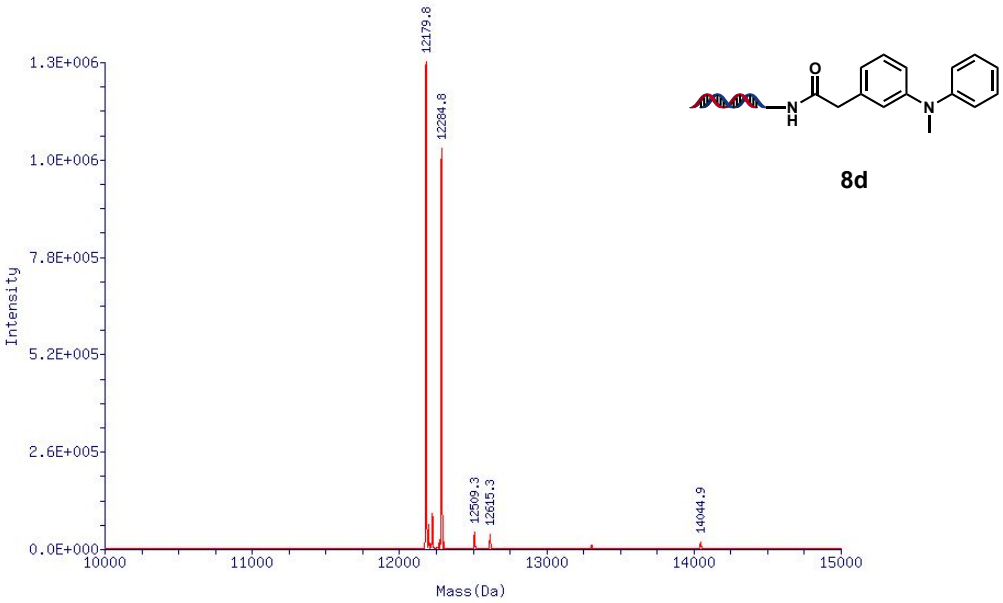


Figure S143. Deconvoluted mass spectrum of DNA **8d**, expected: 12283.3; observed 12284.8.

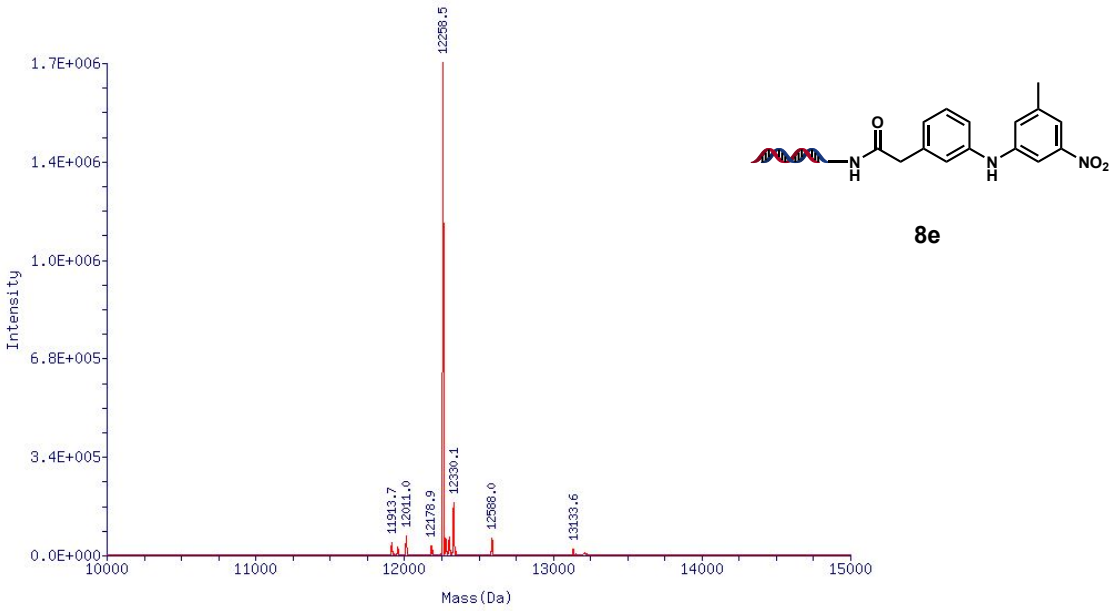


Figure S144. Deconvoluted mass spectrum of DNA **8e**, expected: 12328.3; observed 12330.1.

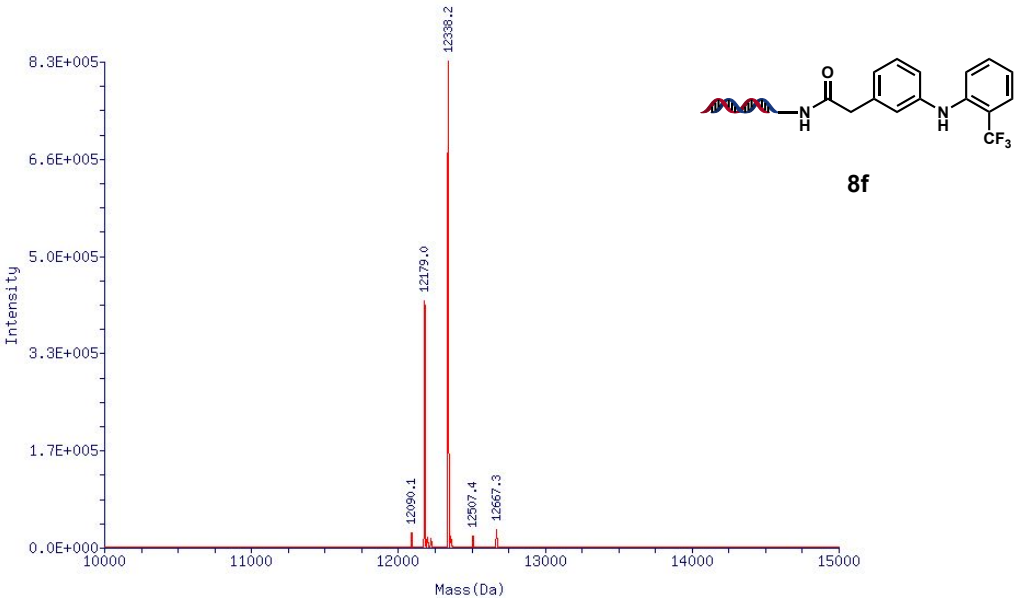


Figure S145. Deconvoluted mass spectrum of DNA **8f**, expected: 12337.3; observed 12338.2.

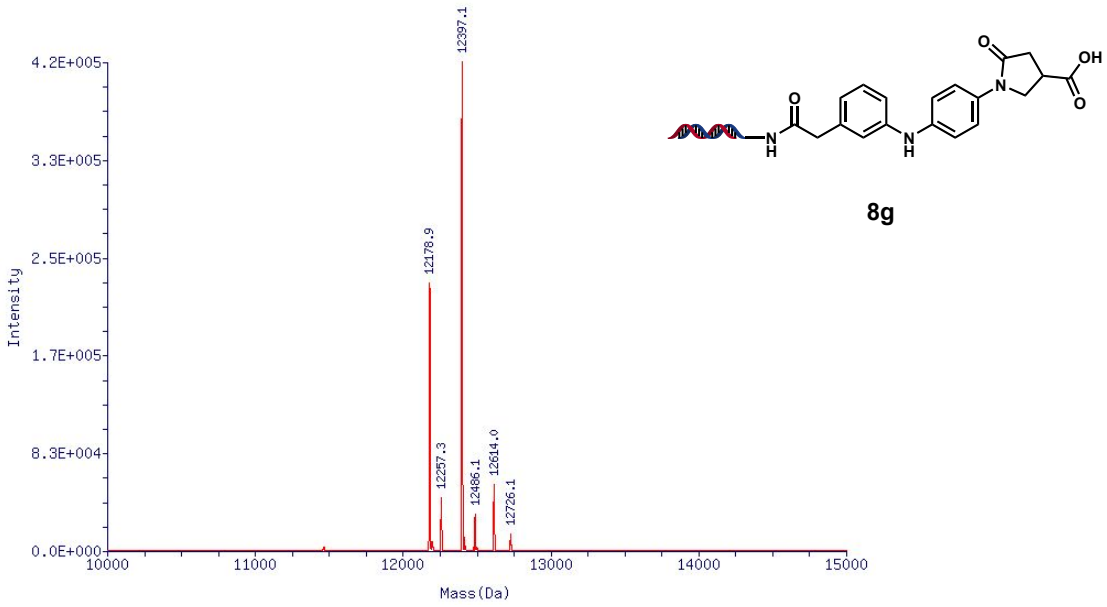


Figure S146. Deconvoluted mass spectrum of DNA **8g**, expected: 12396.3; observed 12397.1.

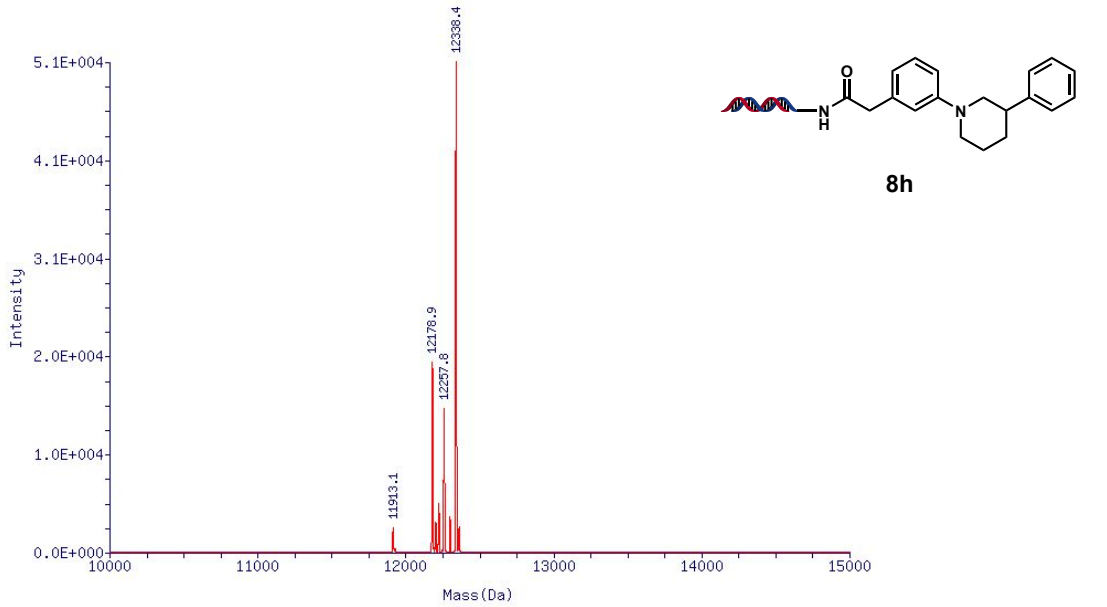


Figure S147. Deconvoluted mass spectrum of DNA **8h**, expected: 12337.4; observed 12338.4.

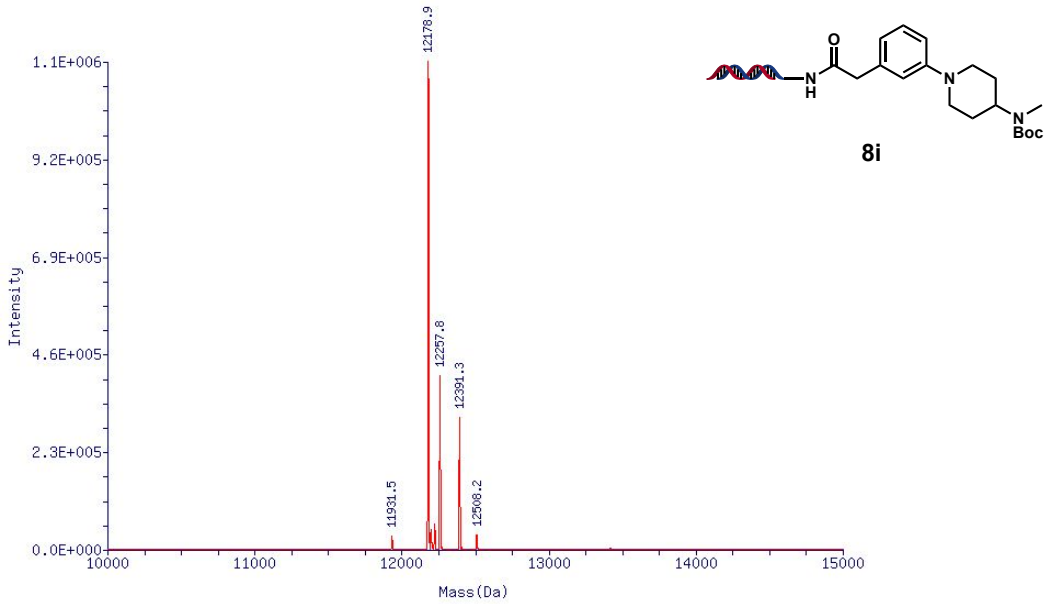


Figure S148. Deconvoluted mass spectrum of DNA **8i**, expected: 12390.4; observed 12391.3.

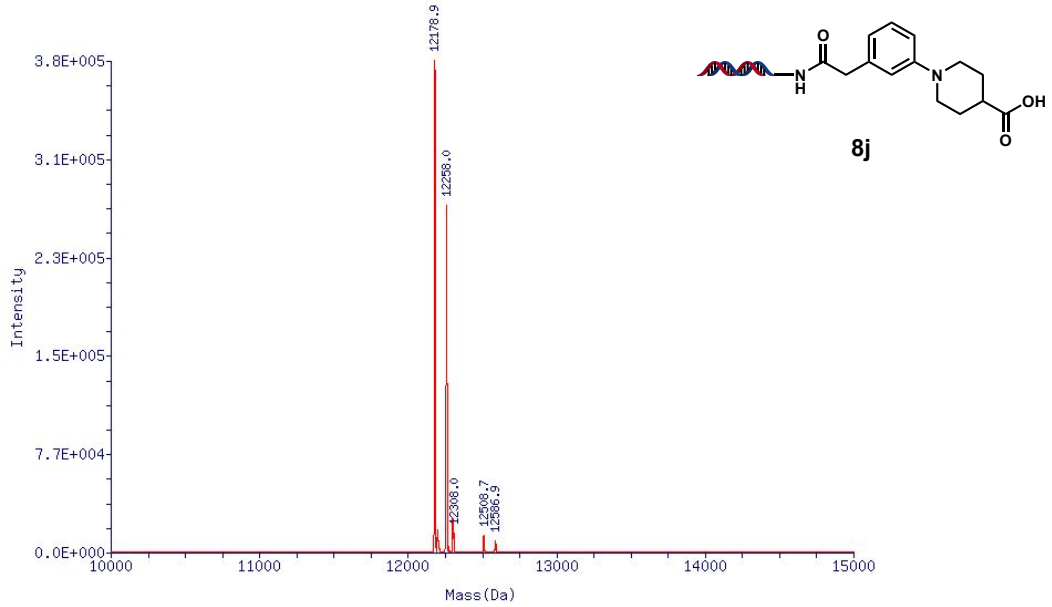


Figure S149. Deconvoluted mass spectrum of DNA **8j**, expected: 12305.3; no product observed.

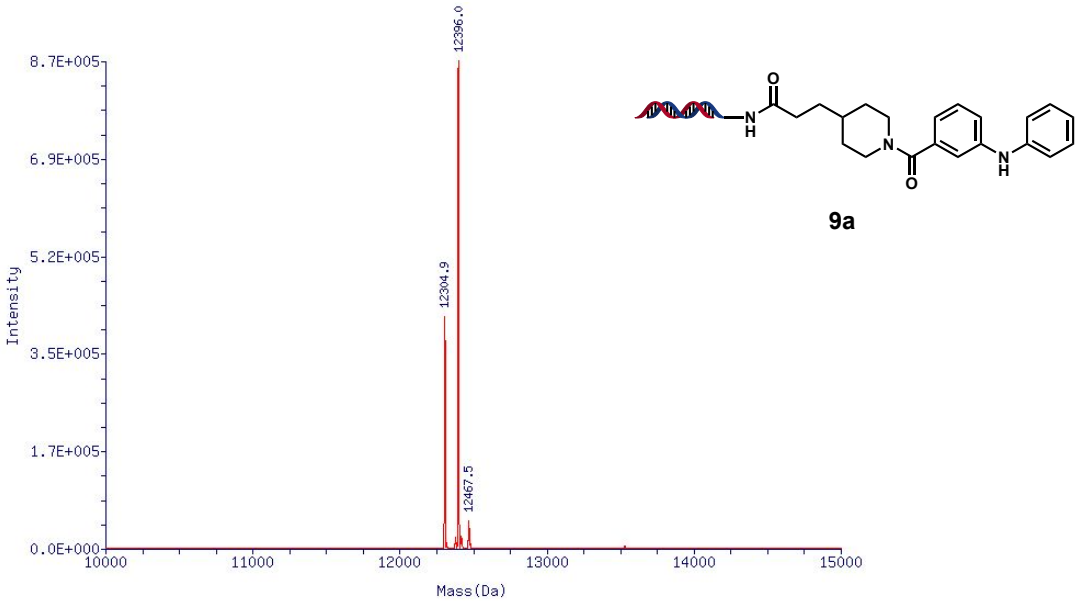


Figure S150. Deconvoluted mass spectrum of DNA **9a**, expected: 12394.4; observed 12396.

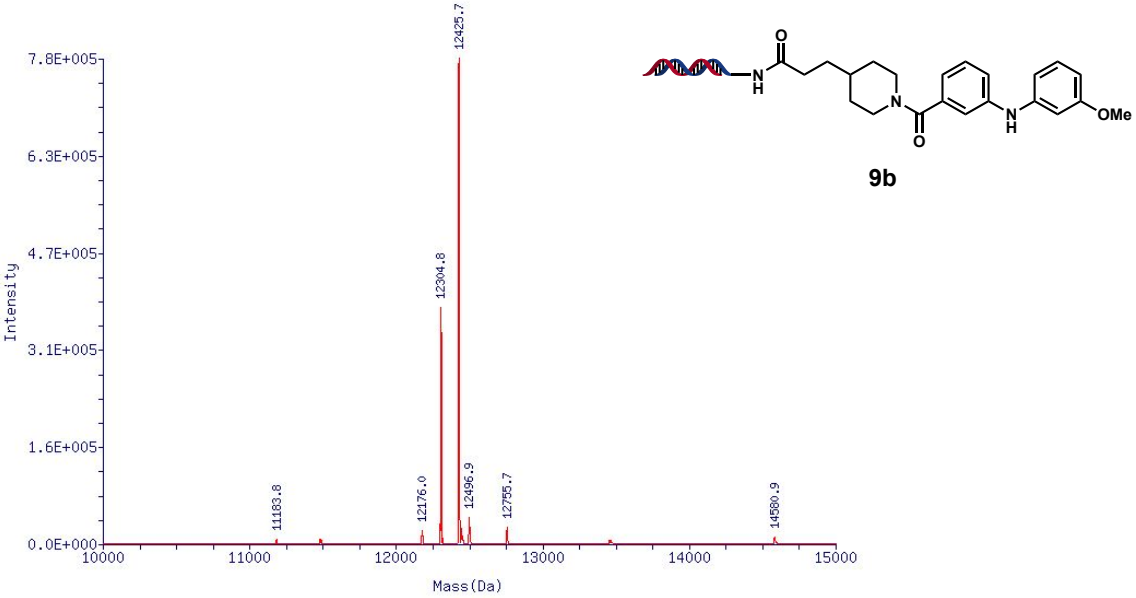


Figure S151. Deconvoluted mass spectrum of DNA **9b**, expected: 12424.5; observed 12425.7.

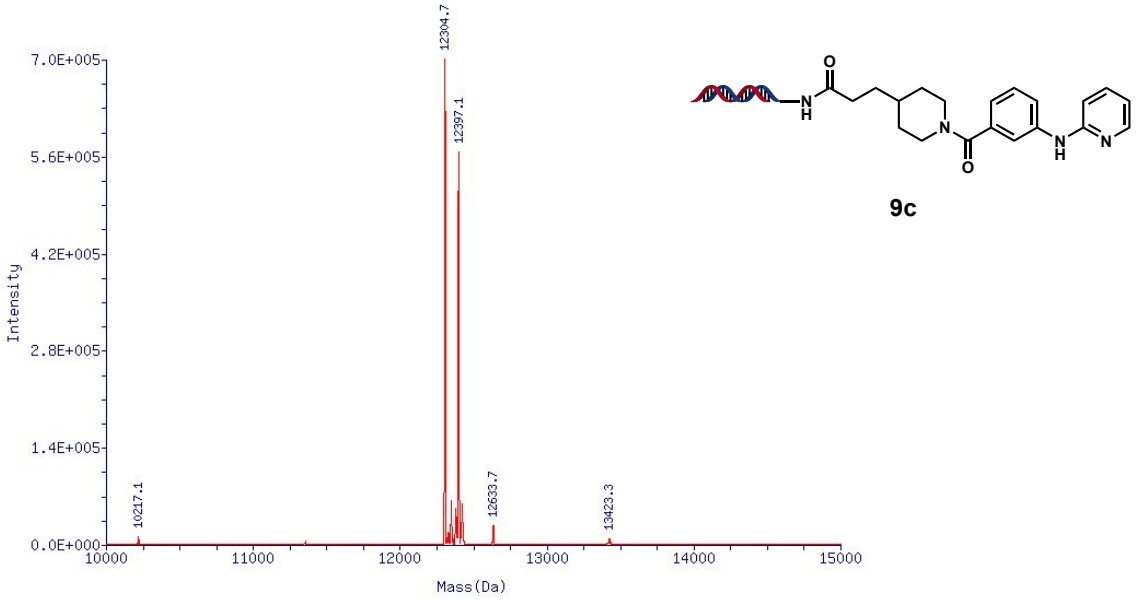


Figure S152. Deconvoluted mass spectrum of DNA **9c**, expected: 12395.4; observed 12397.1.

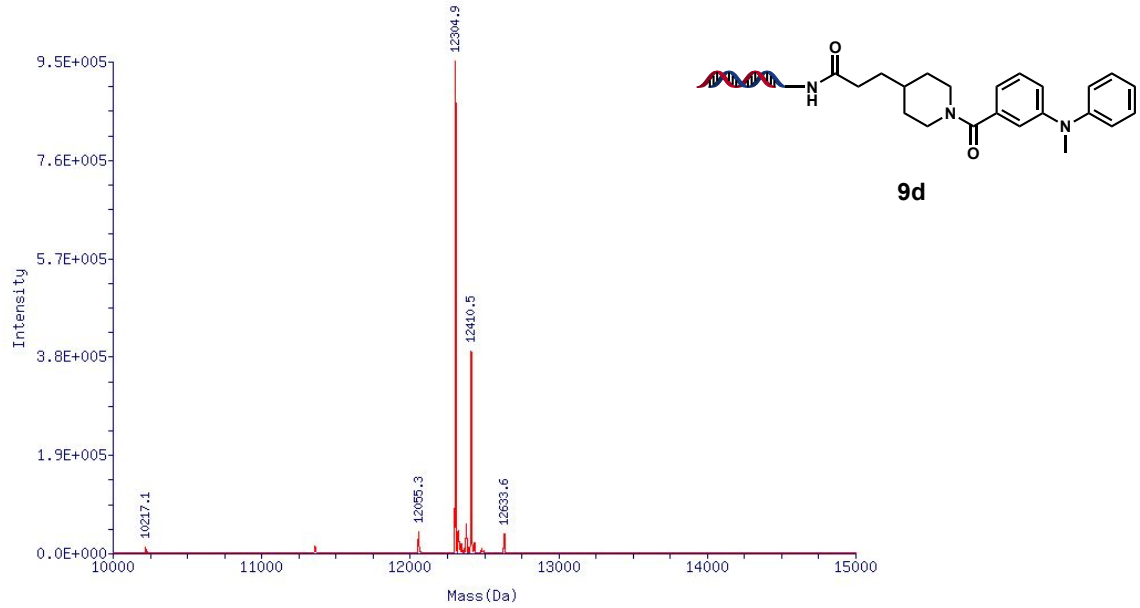


Figure S153. Deconvoluted mass spectrum of DNA **9d**, expected: 12408.5; observed 12410.5.

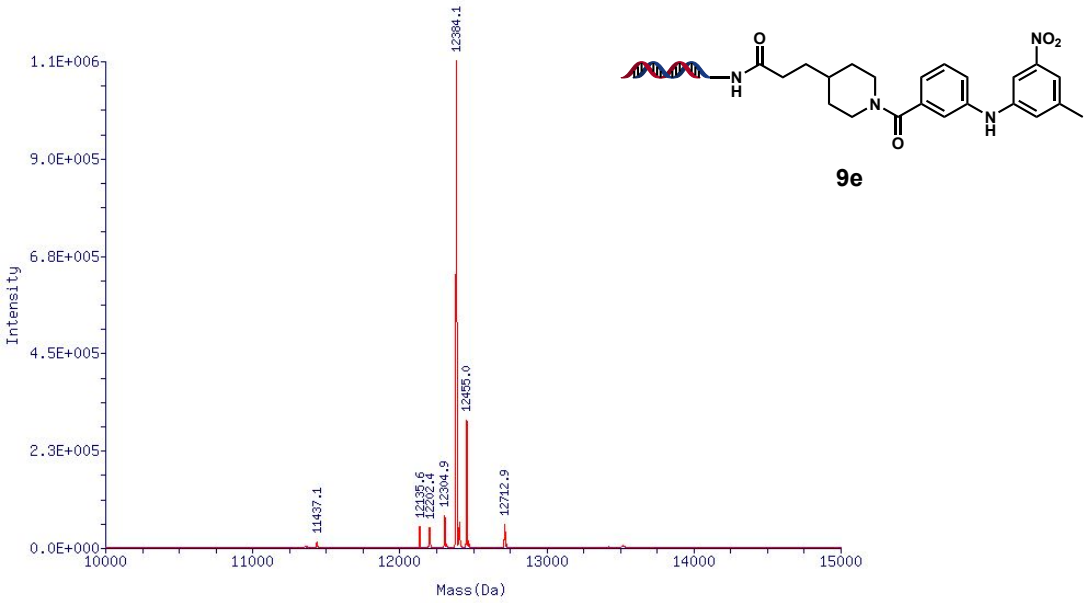


Figure S154. Deconvoluted mass spectrum of DNA **9e**, expected: 12453.4; observed 12455.

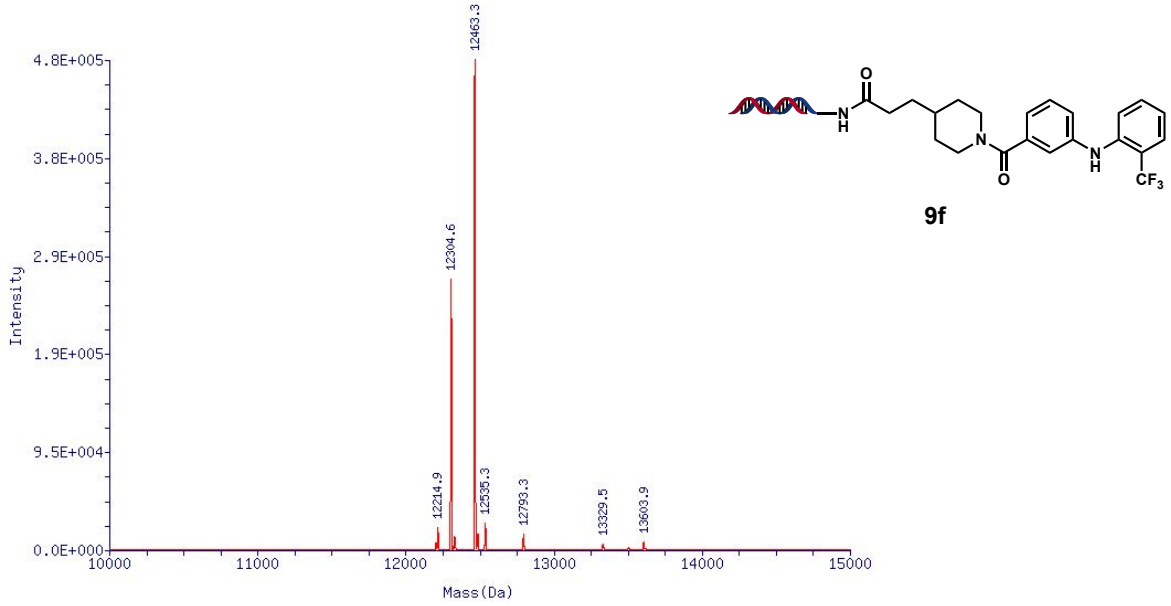


Figure S155. Deconvoluted mass spectrum of DNA **9f**, expected: 12462.4; observed 12463.3.

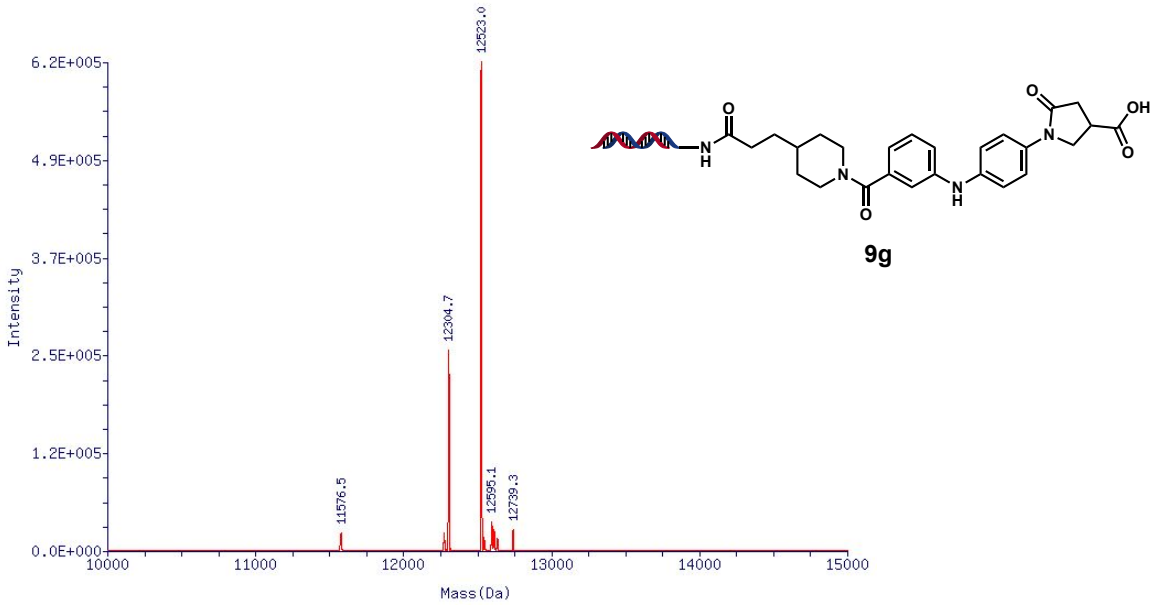


Figure S156. Deconvoluted mass spectrum of DNA **9g**, expected: 12521.4; observed 12523.

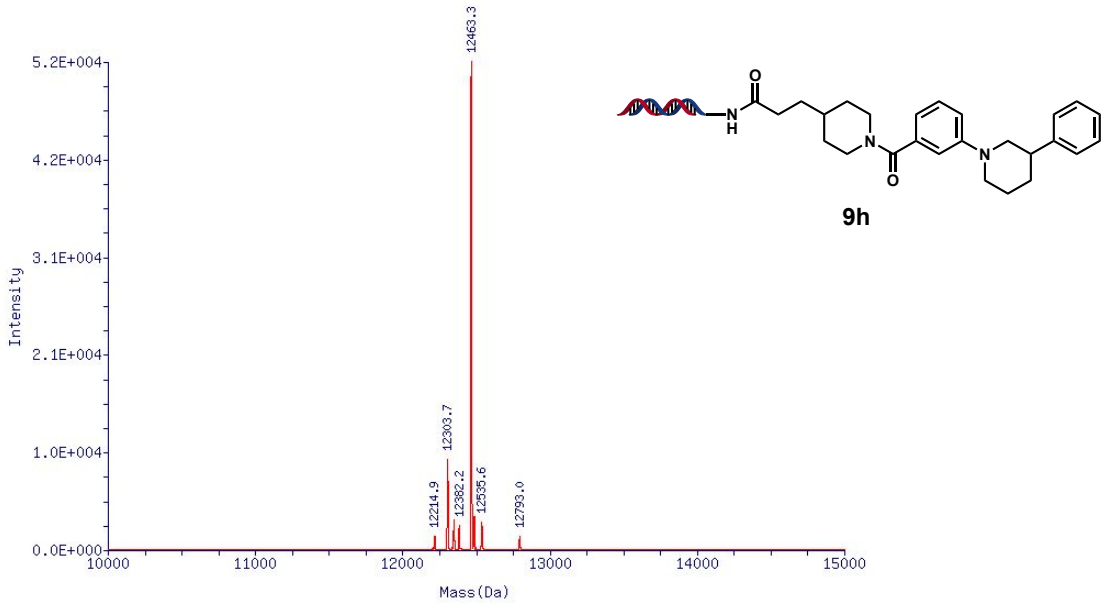


Figure S157. Deconvoluted mass spectrum of DNA **9h**, expected: 12462.5; observed 12463.3.

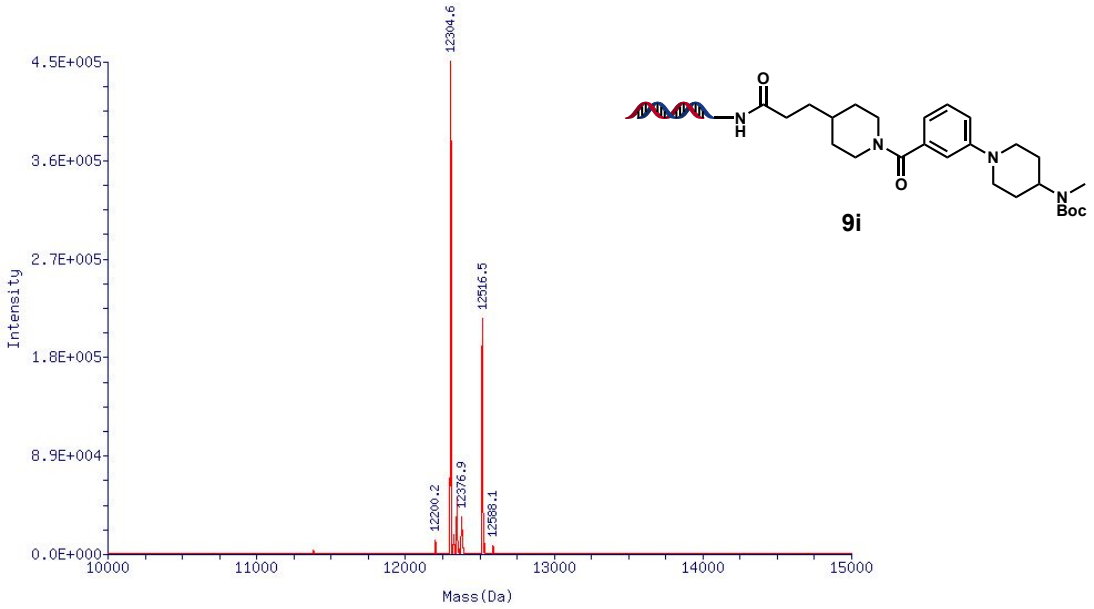


Figure S158. Deconvoluted mass spectrum of DNA **9i**, expected: 12515.6; observed 12516.5.

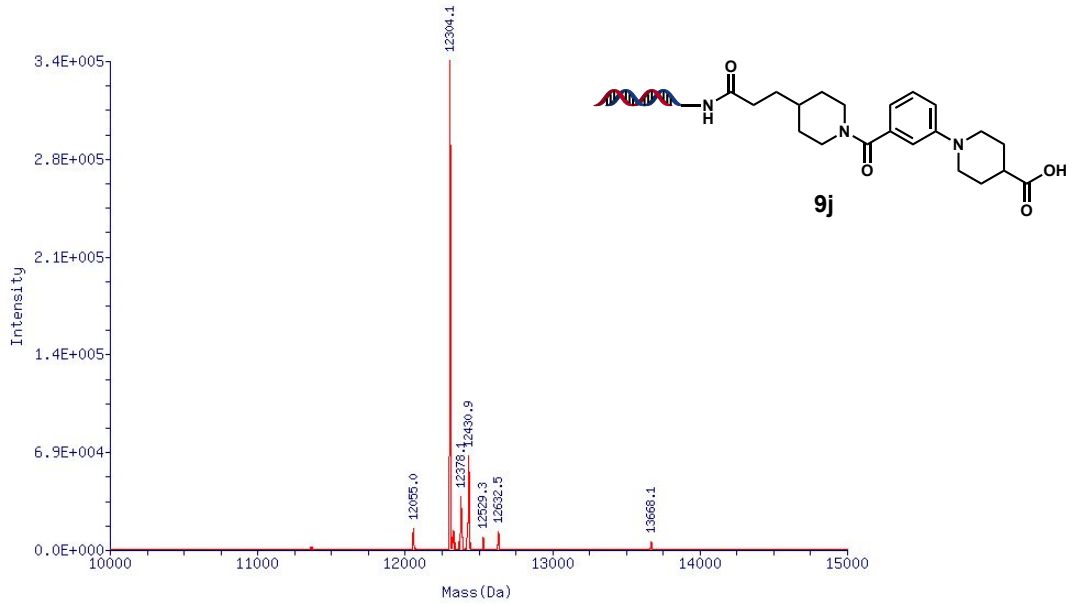


Figure S159. Deconvoluted mass spectrum of DNA **9j**, expected: 12430.5; observed 12430.9.

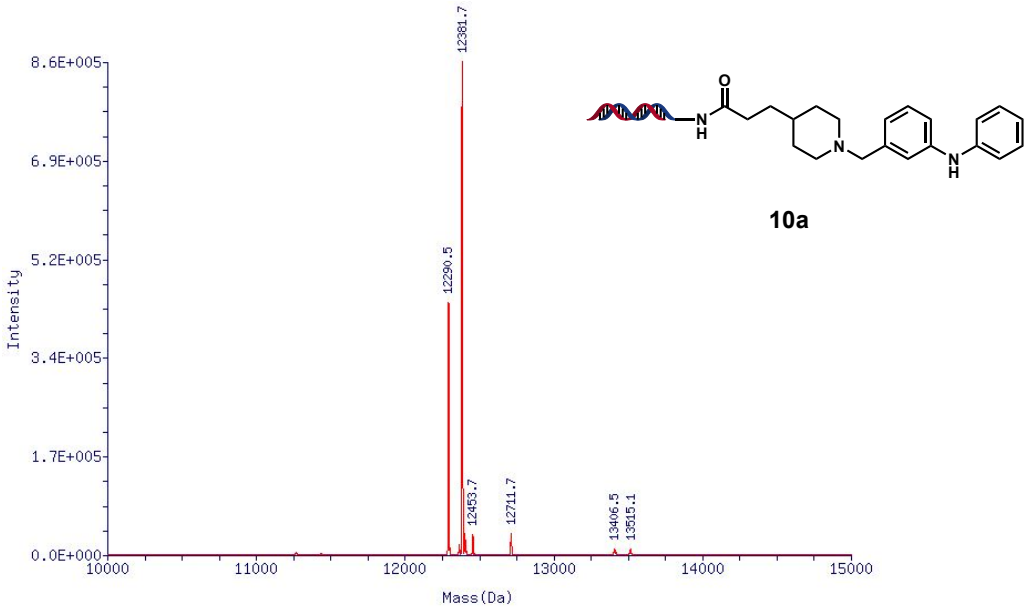


Figure S160. Deconvoluted mass spectrum of DNA **10a**, expected: 12380.4; observed 12381.7.

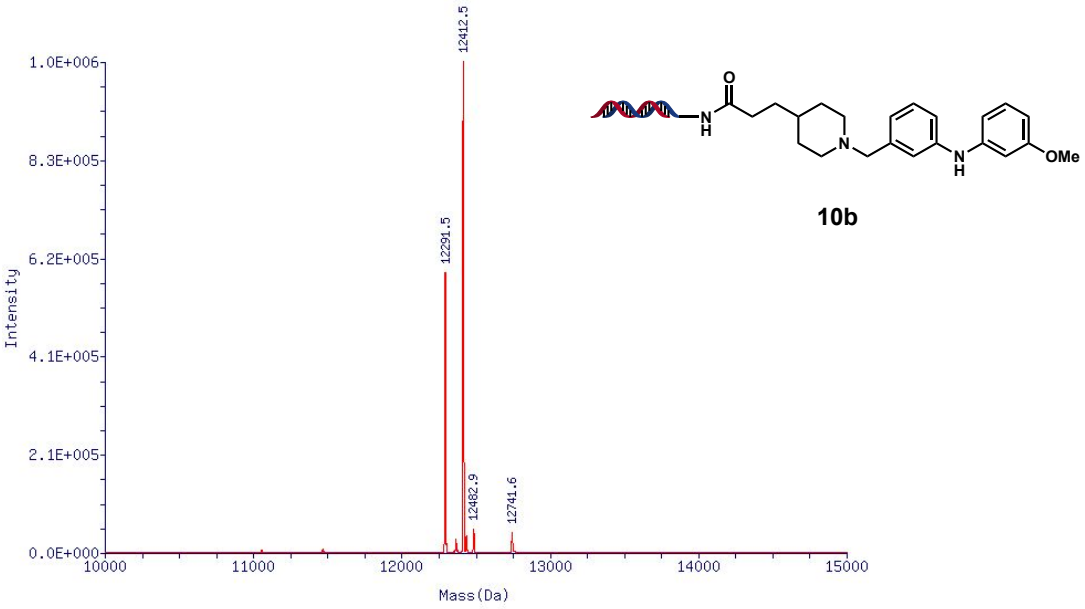


Figure S161. Deconvoluted mass spectrum of DNA **10b**, expected: 12410.5; observed 12412.5.

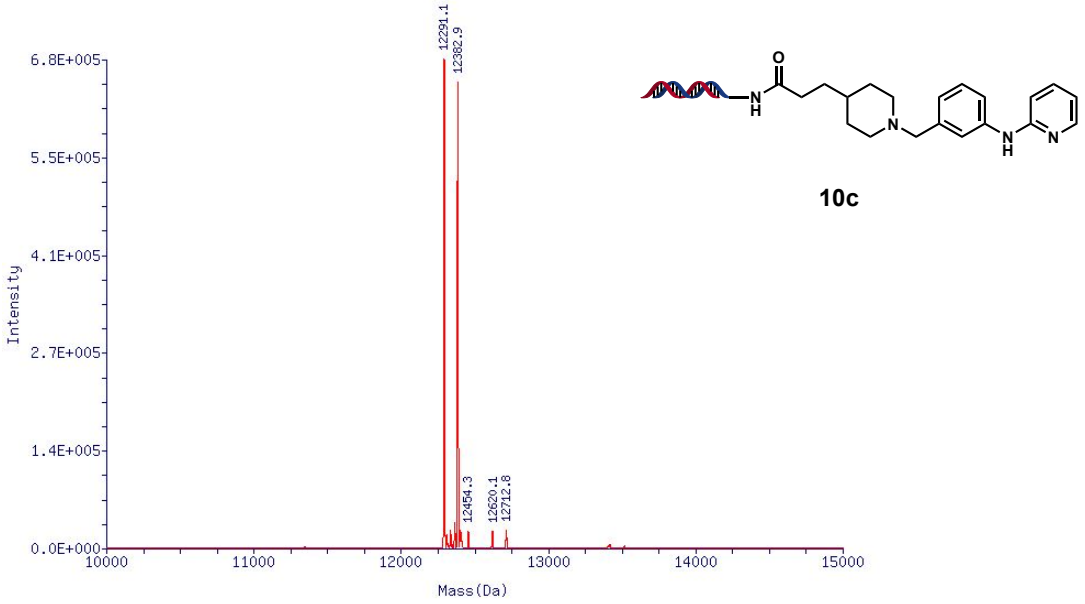


Figure S162. Deconvoluted mass spectrum of DNA **10c**, expected: 12381.4; observed 12382.9.

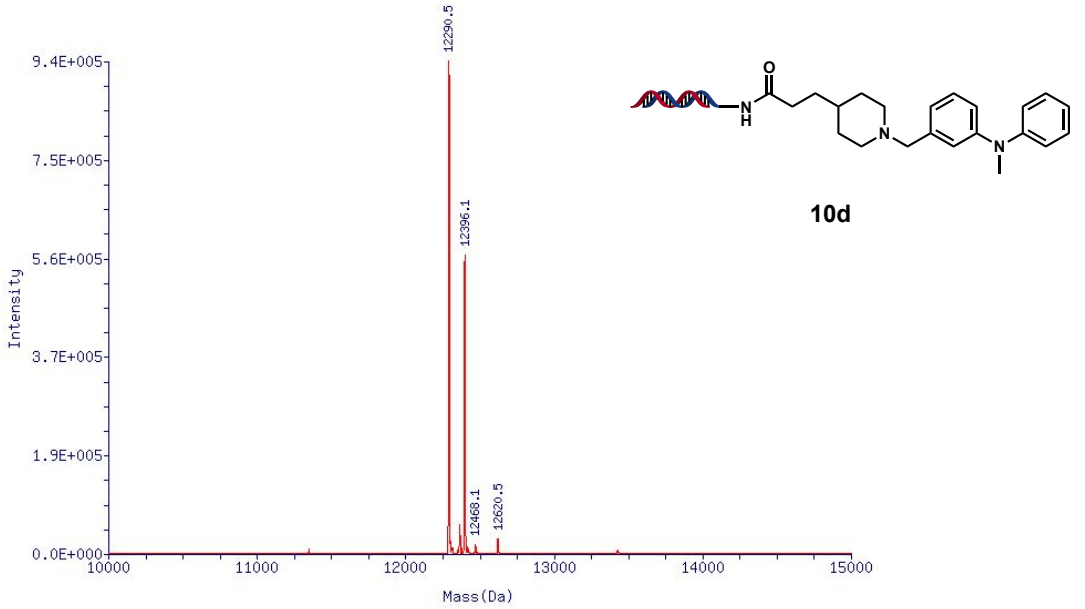


Figure S163. Deconvoluted mass spectrum of DNA **10d**, expected: 12394.5; observed 12396.1.

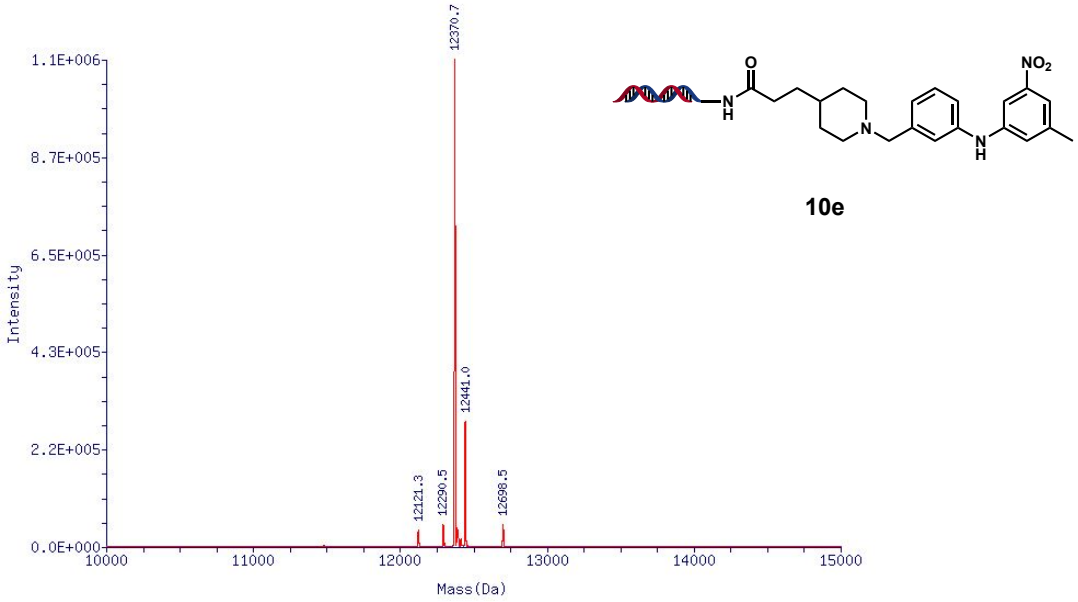


Figure S164. Deconvoluted mass spectrum of DNA **10e**, expected: 12439.5; observed 12441.

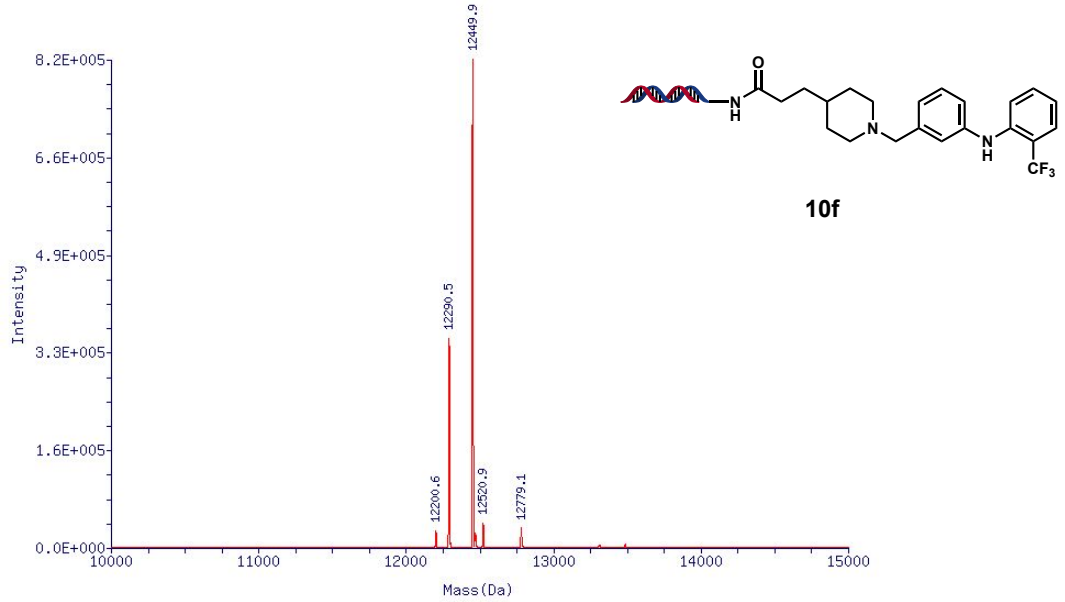


Figure S165. Deconvoluted mass spectrum of DNA **10f**, expected: 12448.4; observed 12449.9.

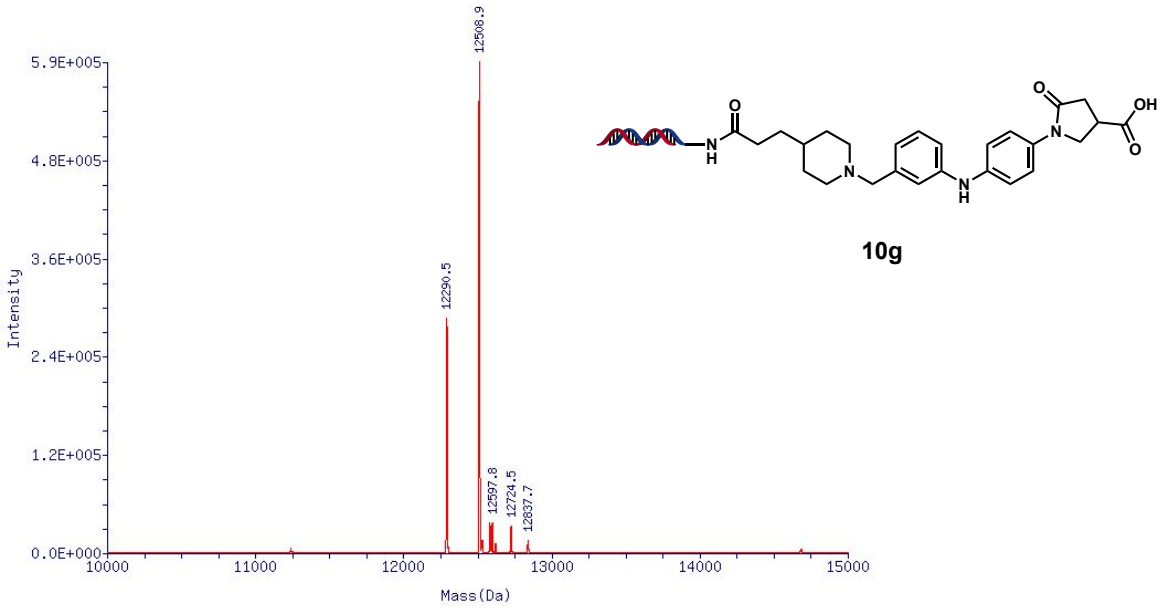


Figure S166. Deconvoluted mass spectrum of DNA **10g**, expected: 12507.5; observed 12508.9.

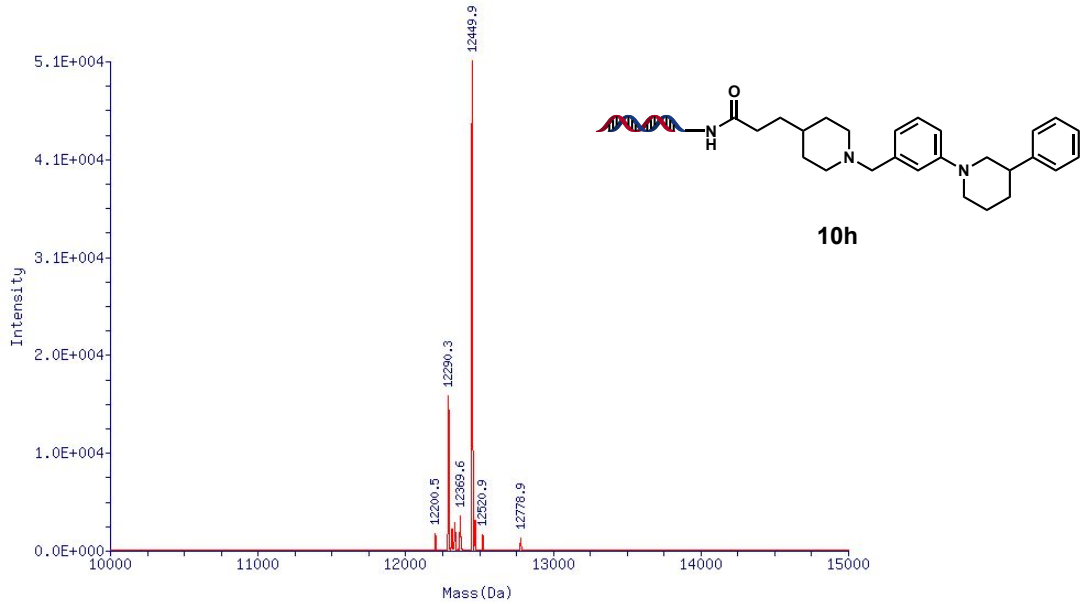


Figure S167. Deconvoluted mass spectrum of DNA **10h**, expected: 12448.6; observed 12449.9.

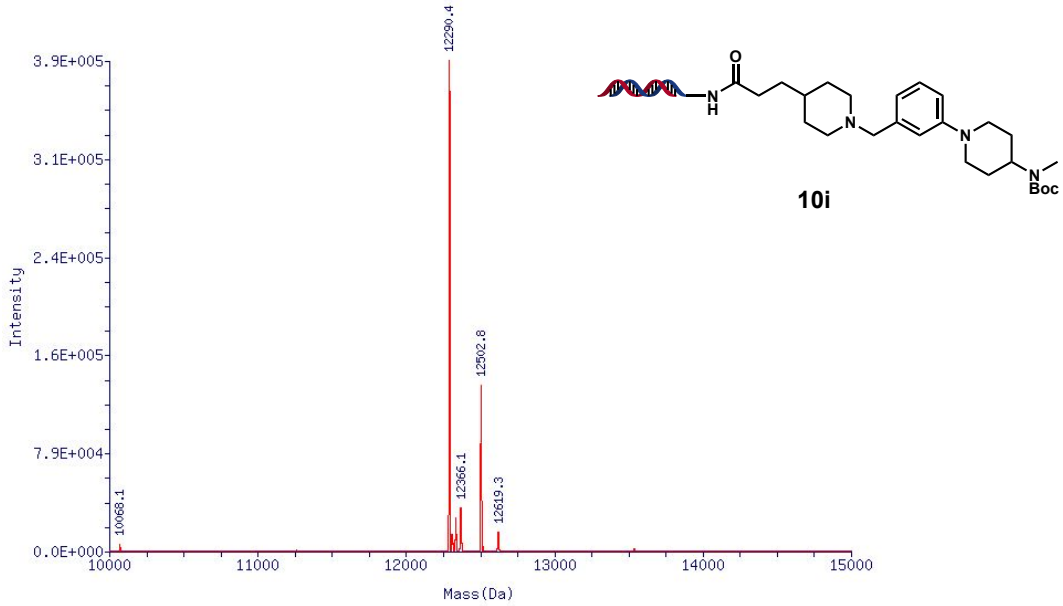


Figure S168. Deconvoluted mass spectrum of DNA **10i**, expected: 12501.6; observed 12502.8.

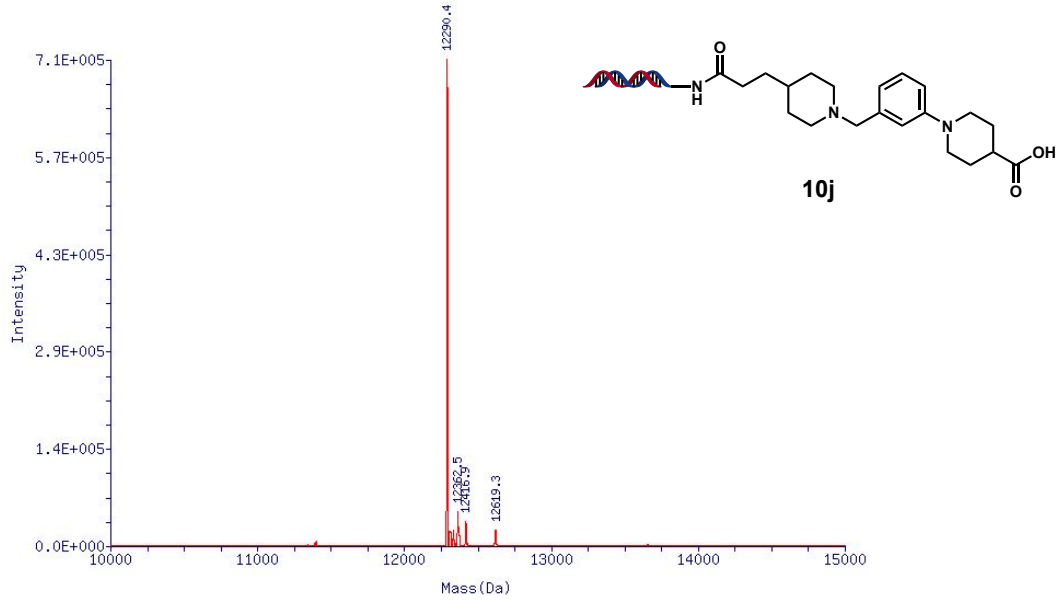
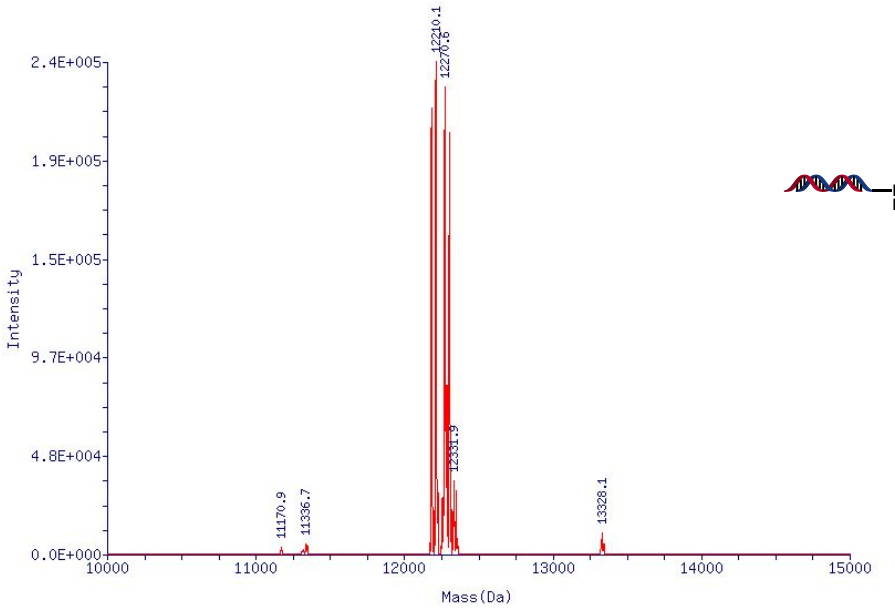
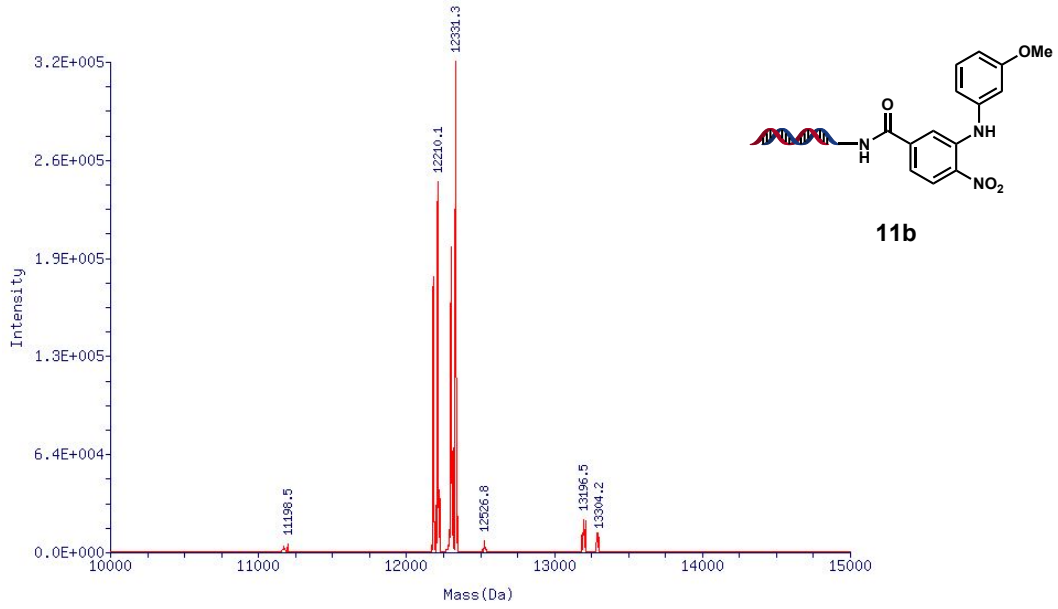


Figure S169. Deconvoluted mass spectrum of DNA **10j**, expected: 12416.5; no product observed.



11a

Figure S170. Deconvoluted mass spectrum of DNA **11a**, expected: 12300.2 and 12270.2 (for nitro reduced); observed 12301.3 and 12270.6 (for nitro reduced).



11b

Figure S171. Deconvoluted mass spectrum of DNA **11b**, expected: 12330.3 and 12300.3 (for nitro reduced); observed 12331.3 and 12300.7 (for nitro reduced).

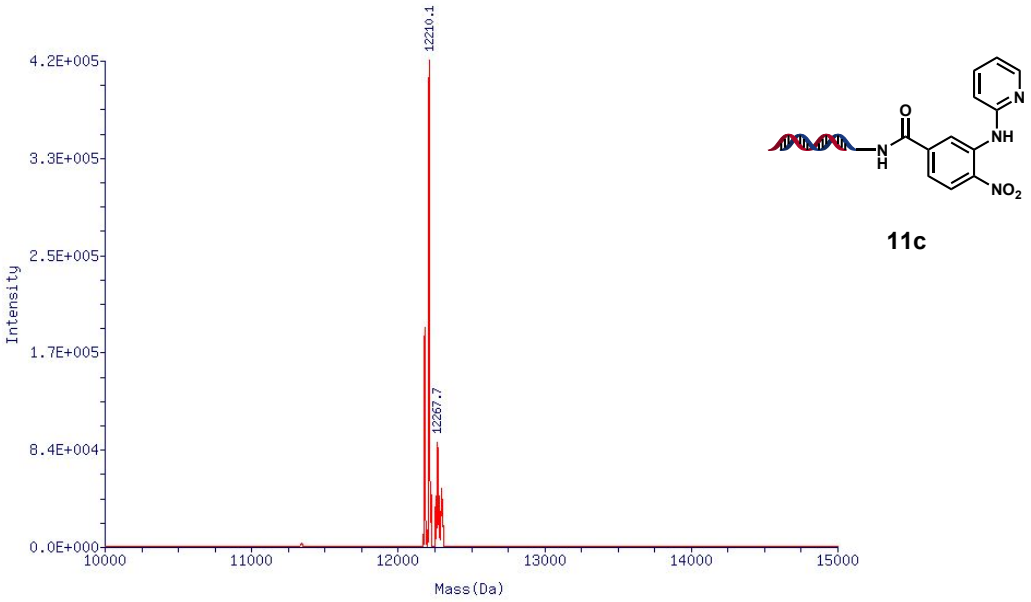


Figure S172. Deconvoluted mass spectrum of DNA **11c**, expected: 12301.2 and 12271.2 (for nitro reduced); no product observed.

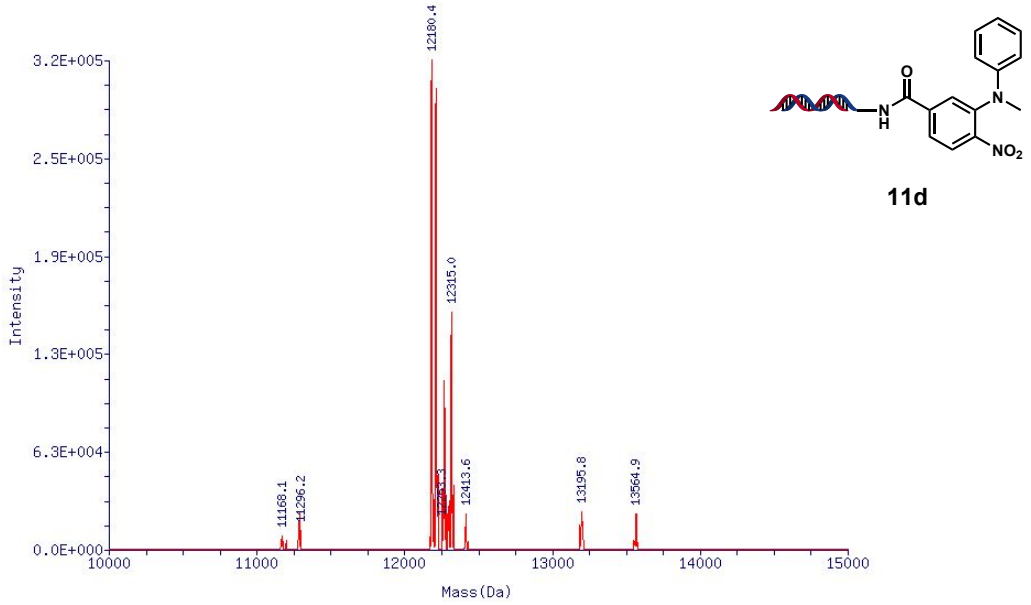


Figure S173. Deconvoluted mass spectrum of DNA **11d**, expected: 12314.3 and 12284.3 (for nitro reduced); observed 12315.

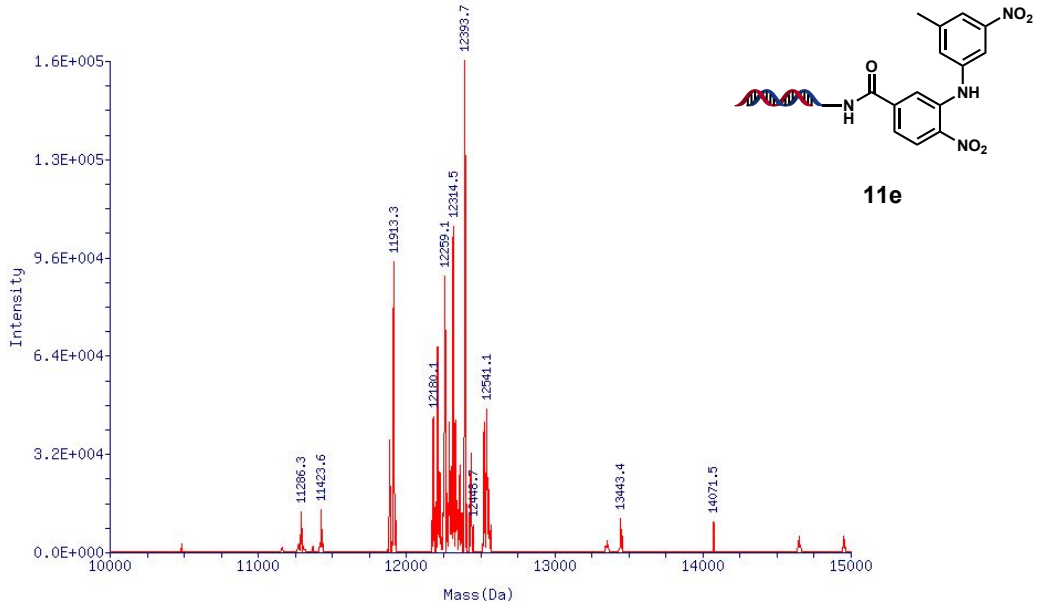


Figure S174. Deconvoluted mass spectrum of DNA **11e**, expected: 12359.2 and 12329.3 (for nitro reduced); no product observed.

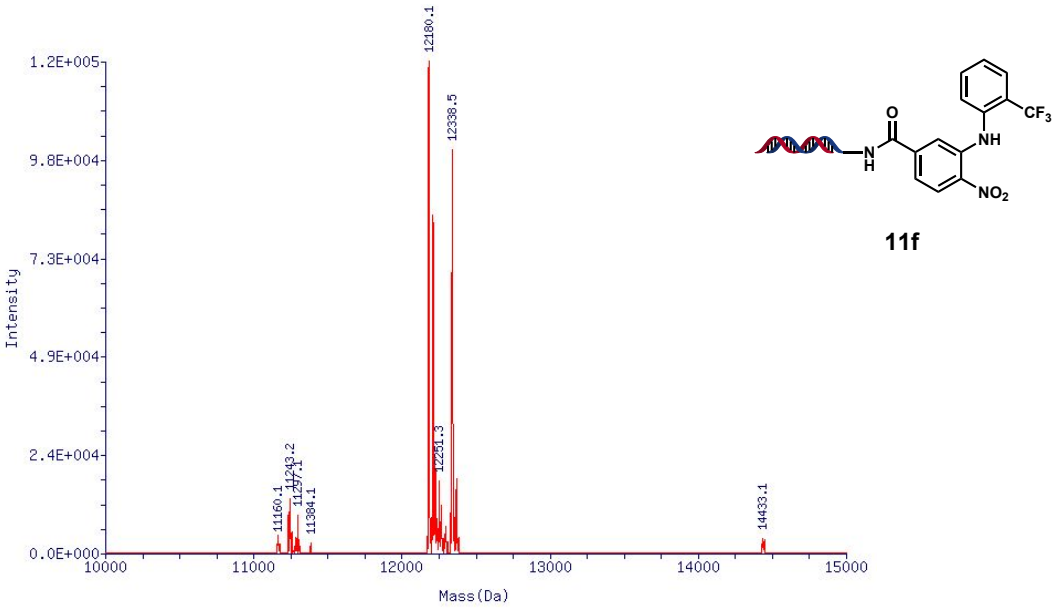


Figure S175. Deconvoluted mass spectrum of DNA **11f**, expected: 12368.2 and 12338.2 (for nitro reduced); observed 12338.5 (for nitro reduced).

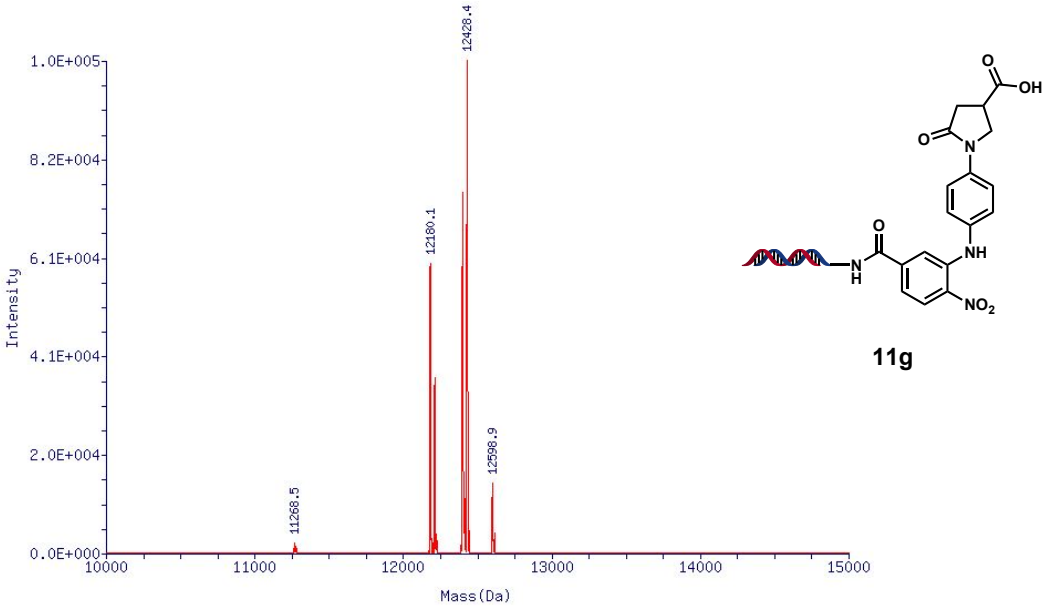


Figure S176. Deconvoluted mass spectrum of DNA **11g**, expected: 12427.2 and 12397.3 (for nitro reduced); observed 12428.4 and 12398.1 (for nitro reduced).

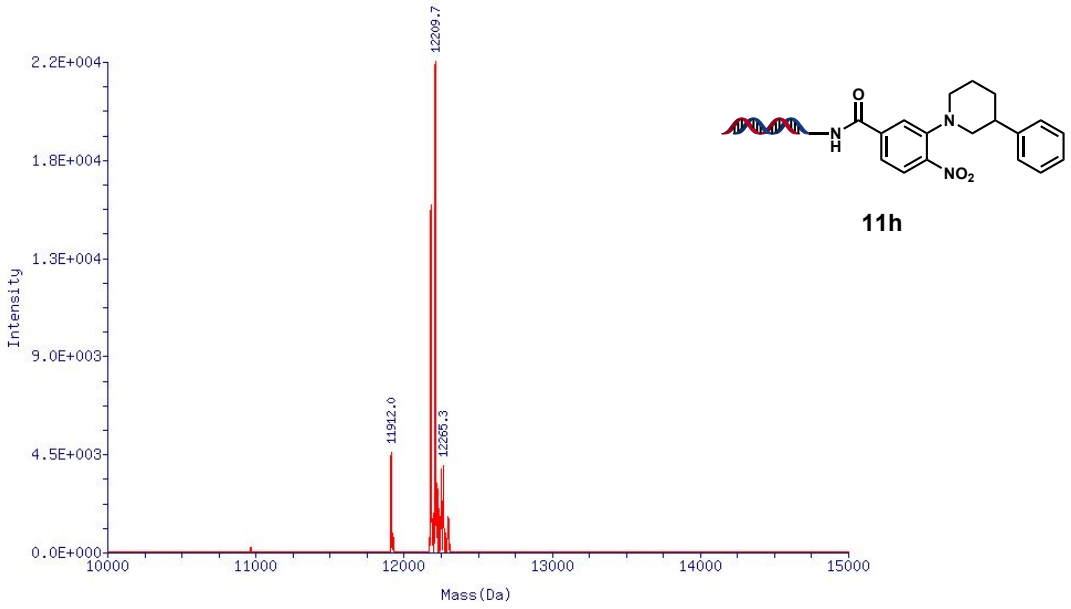


Figure S177. Deconvoluted mass spectrum of DNA **11h**, expected: 12368.3 and 12338.4 (for nitro reduced); no product observed.

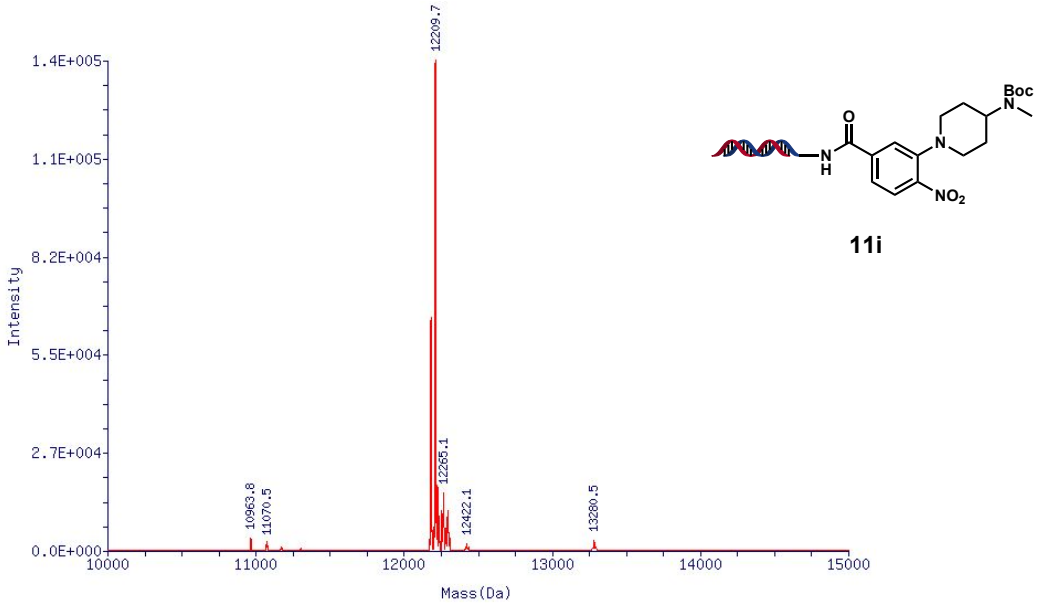


Figure S178. Deconvoluted mass spectrum of DNA **11i**, expected: 12421.4 and 12391.4 (for nitro reduced); no product observed.

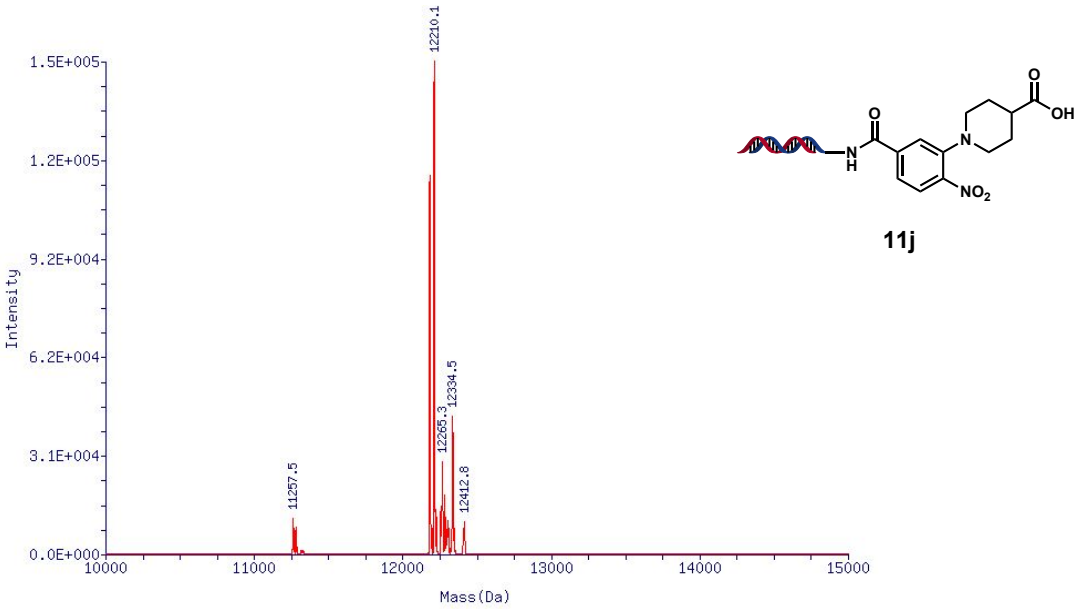


Figure S179. Deconvoluted mass spectrum of DNA **11j**, expected: 12336.3 and 12306.3 (for nitro reduced); observed 12334.5.

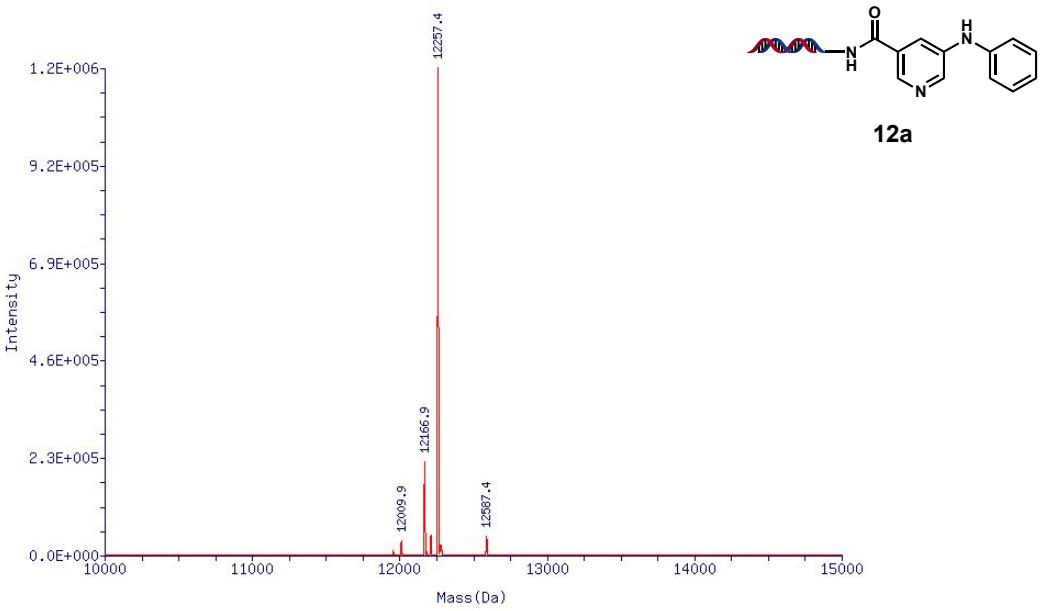


Figure S180. Deconvoluted mass spectrum of DNA **12a**, expected: 12256.2; observed 12257.4.

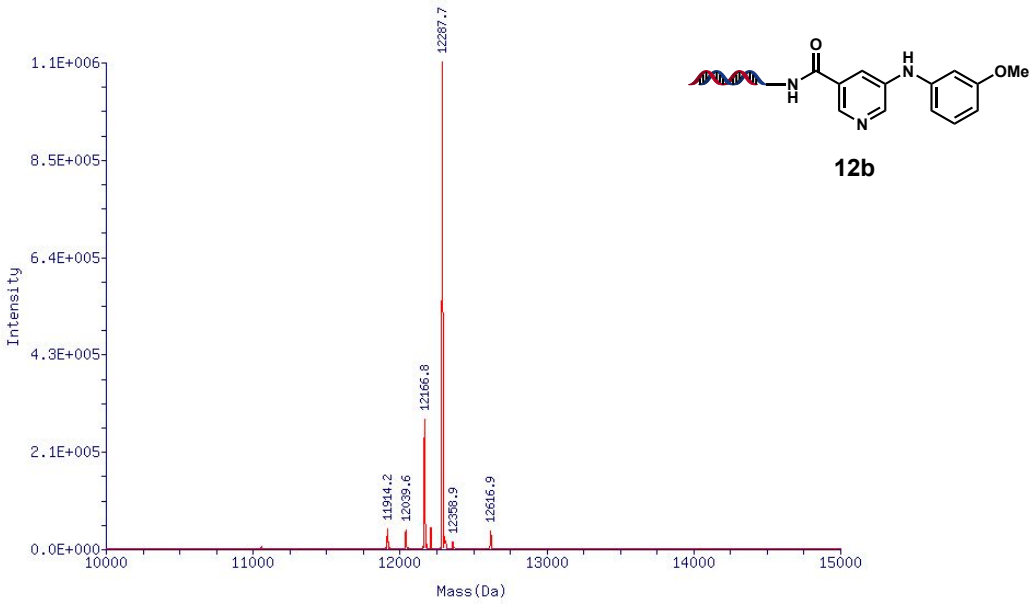


Figure S181. Deconvoluted mass spectrum of DNA **12b**, expected: 12286.2; observed 12287.7.

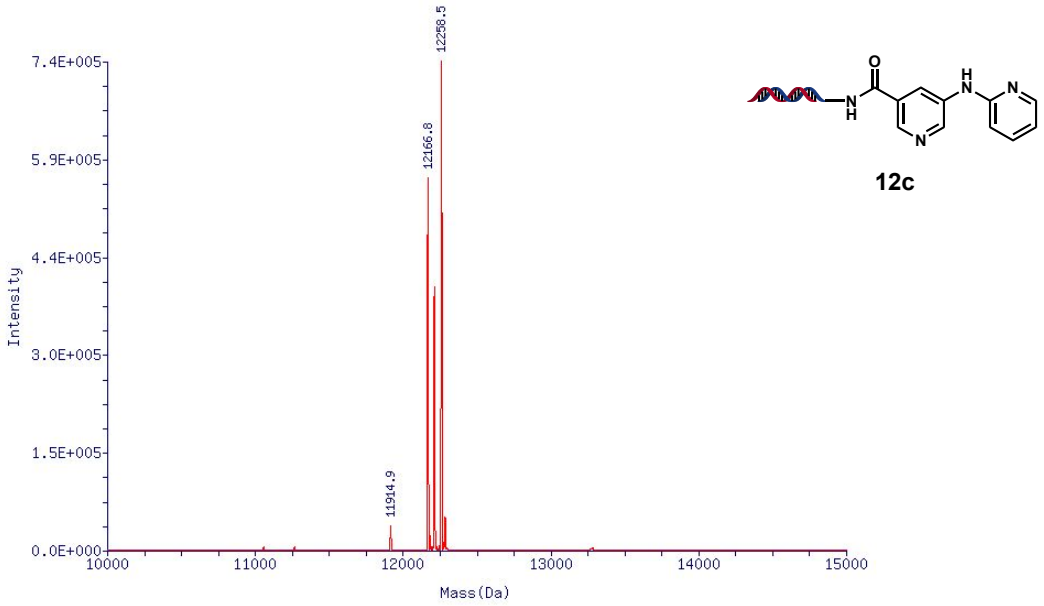


Figure S182. Deconvoluted mass spectrum of DNA **12c**, expected: 12257.2; observed 12258.5.

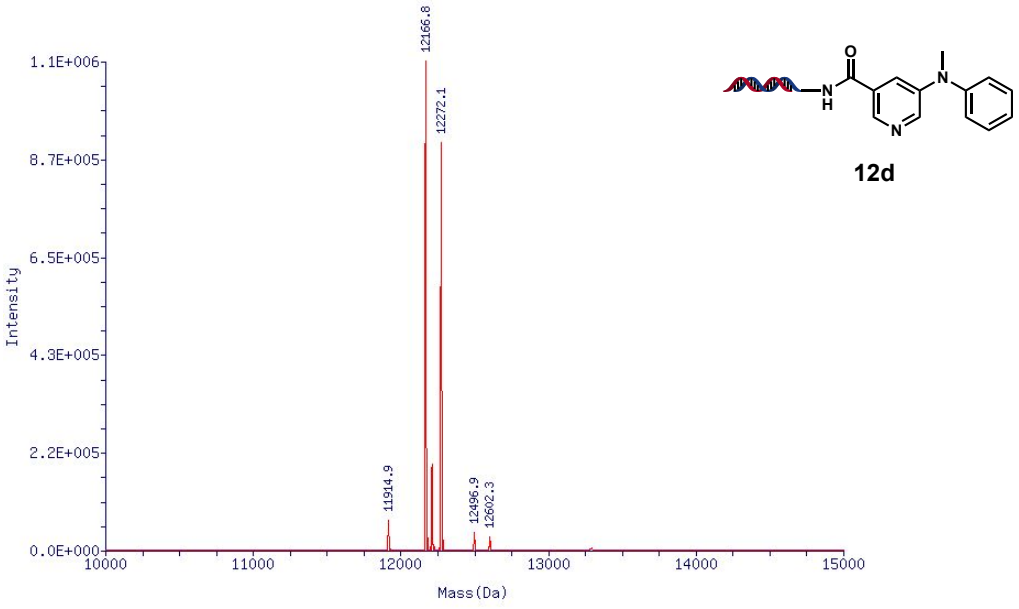


Figure S183. Deconvoluted mass spectrum of DNA **12d**, expected: 12270.4; observed 12272.1.

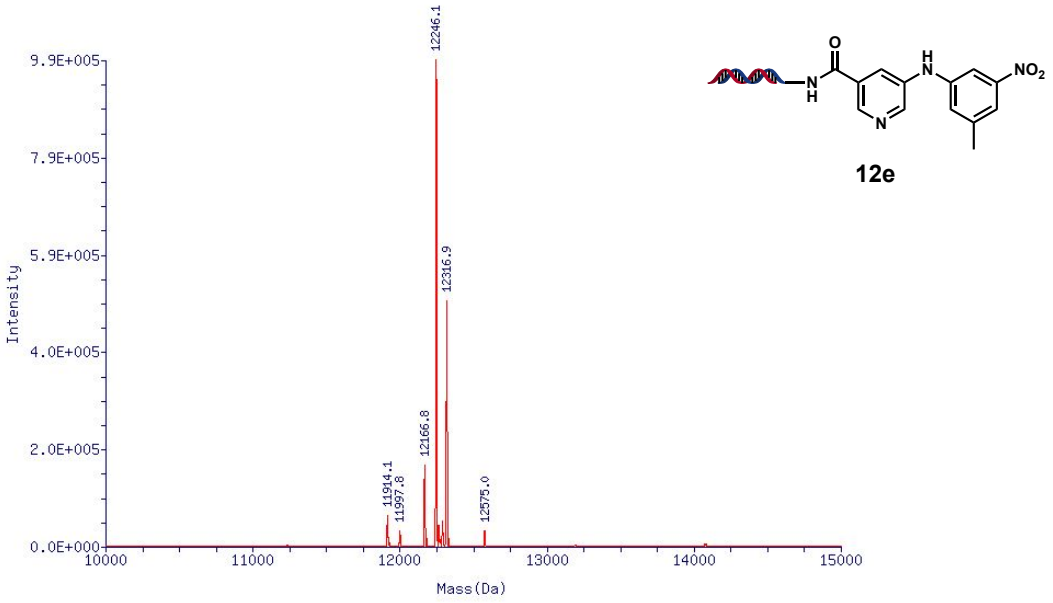


Figure S184. Deconvoluted mass spectrum of DNA **12e**, expected: 12315.2; observed 12316.9.

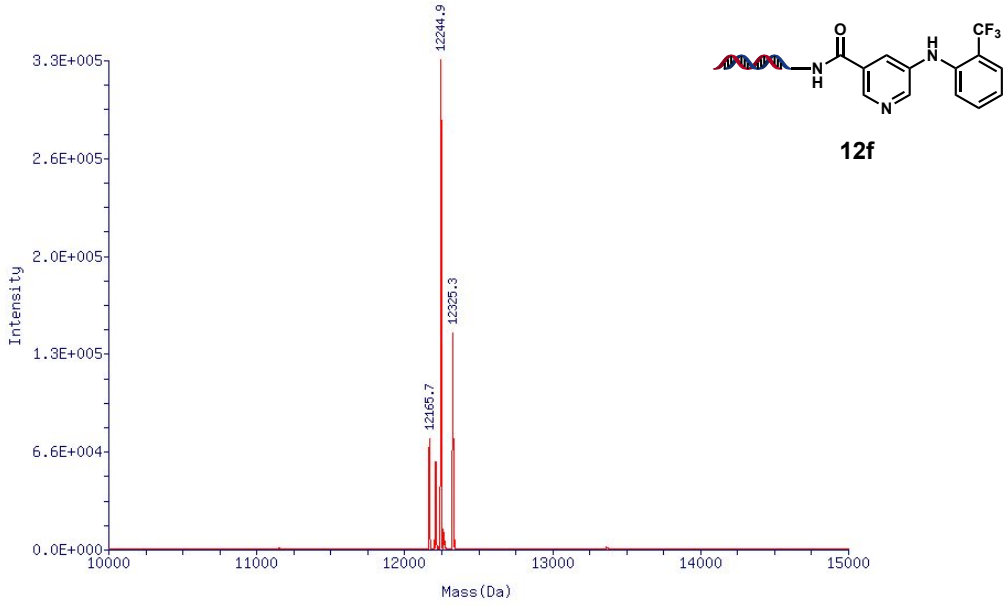


Figure S185. Deconvoluted mass spectrum of DNA **12f**, expected: 12324.2; observed 12325.3.

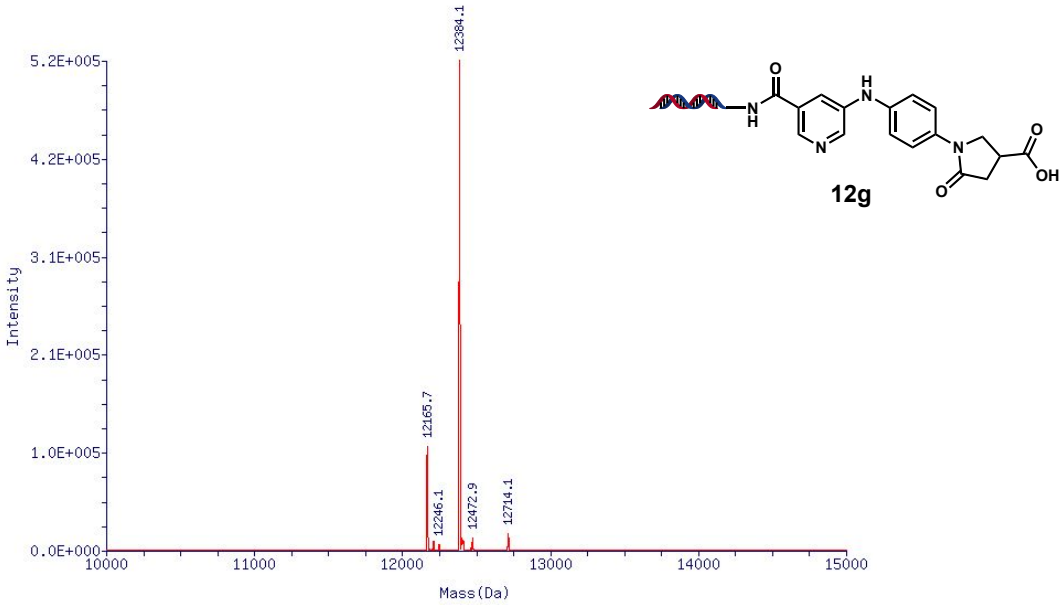


Figure S186. Deconvoluted mass spectrum of DNA **12g**, expected: 12383.2; observed 12384.1.

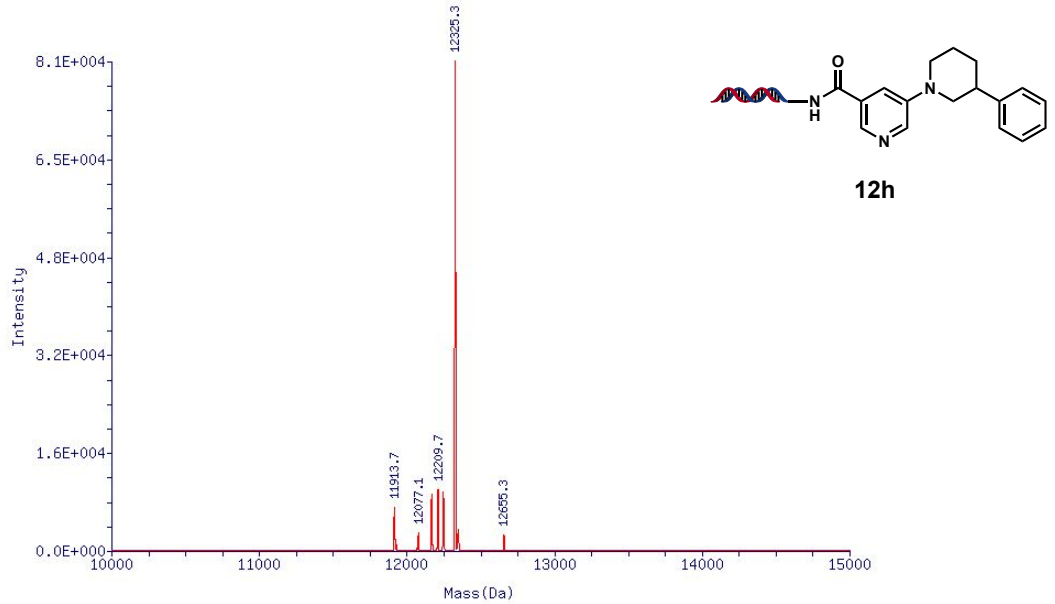


Figure S187. Deconvoluted mass spectrum of DNA **12h**, expected: 12324.3; observed 12325.3.

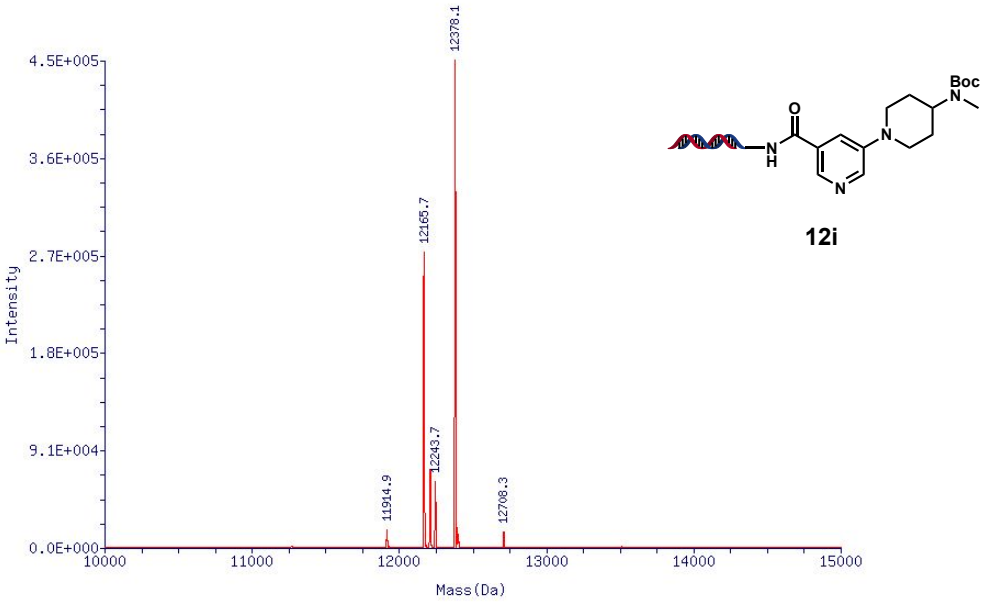


Figure S188. Deconvoluted mass spectrum of DNA **12i**, expected: 12377.4; observed 12378.1.

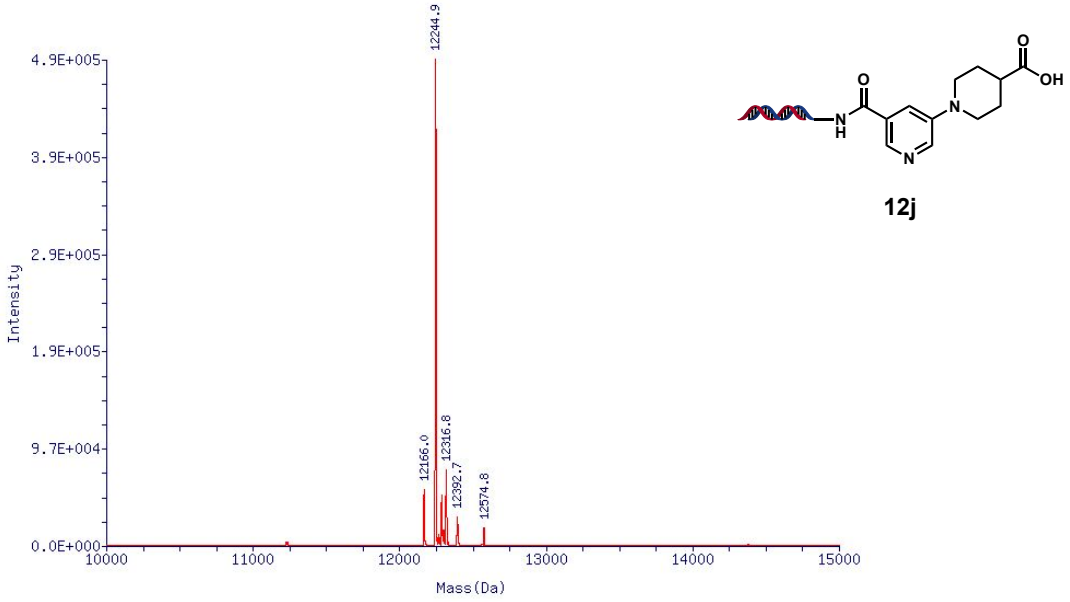


Figure S189. Deconvoluted mass spectrum of DNA **12j**, expected: 12292.2; no product observed.

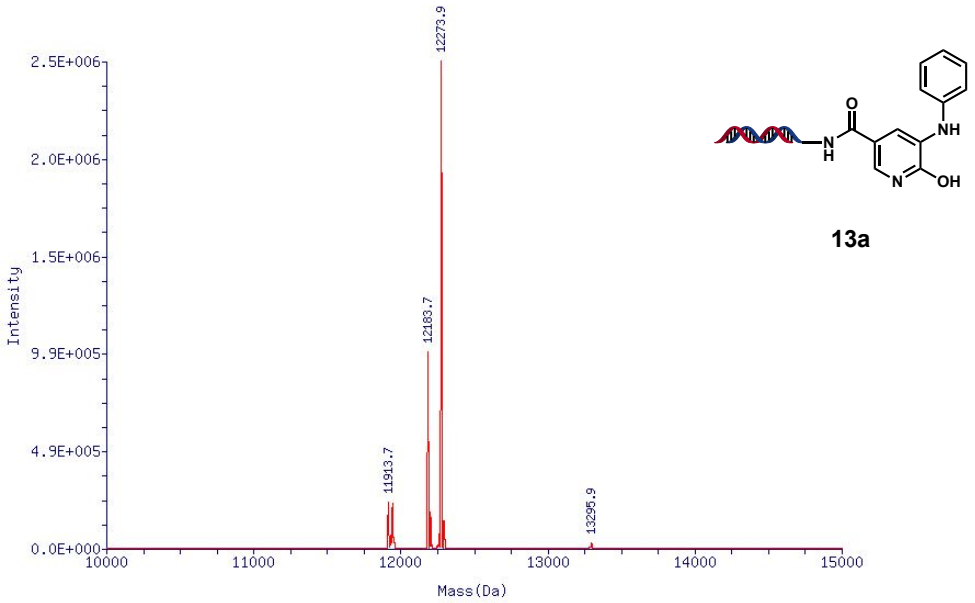


Figure S190. Deconvoluted mass spectrum of DNA **13a**, expected: 12272.2; observed 12273.9.

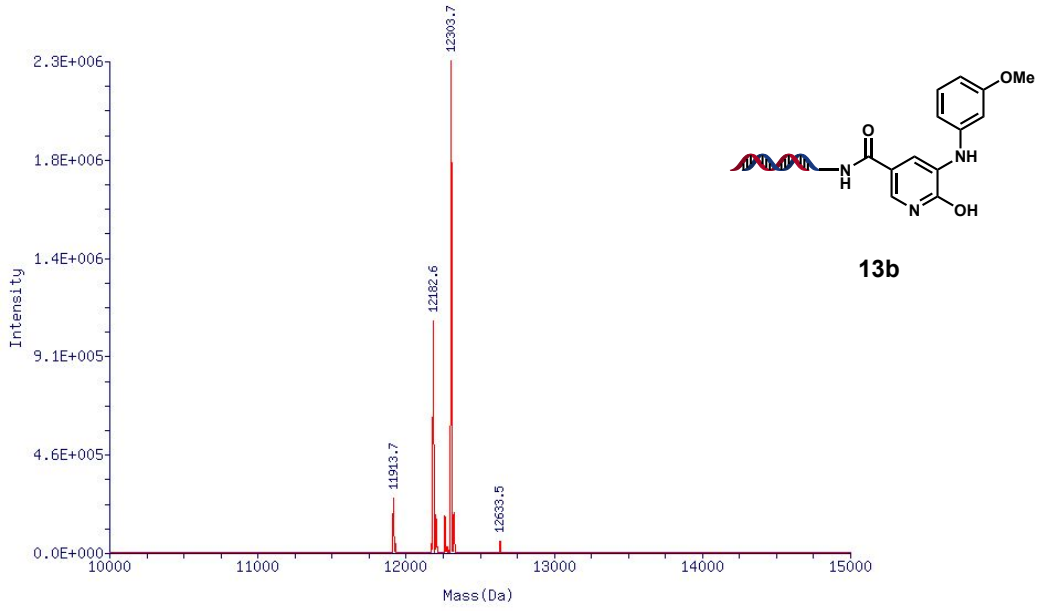


Figure S191. Deconvoluted mass spectrum of DNA **13b**, expected: 12302.2; observed 12303.7.

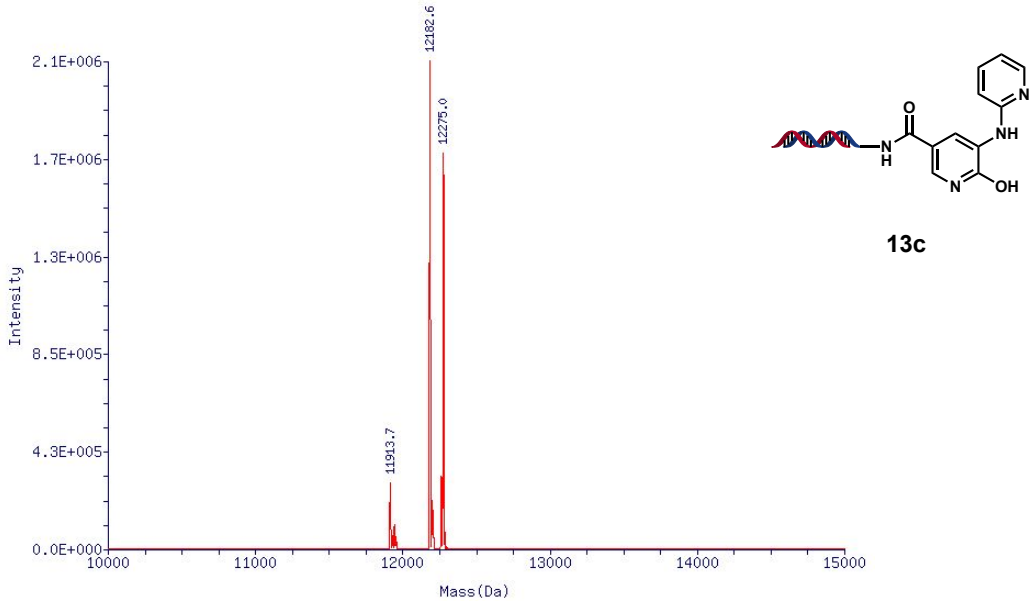


Figure S192. Deconvoluted mass spectrum of DNA **13c**, expected: 12273.2; observed 12275.

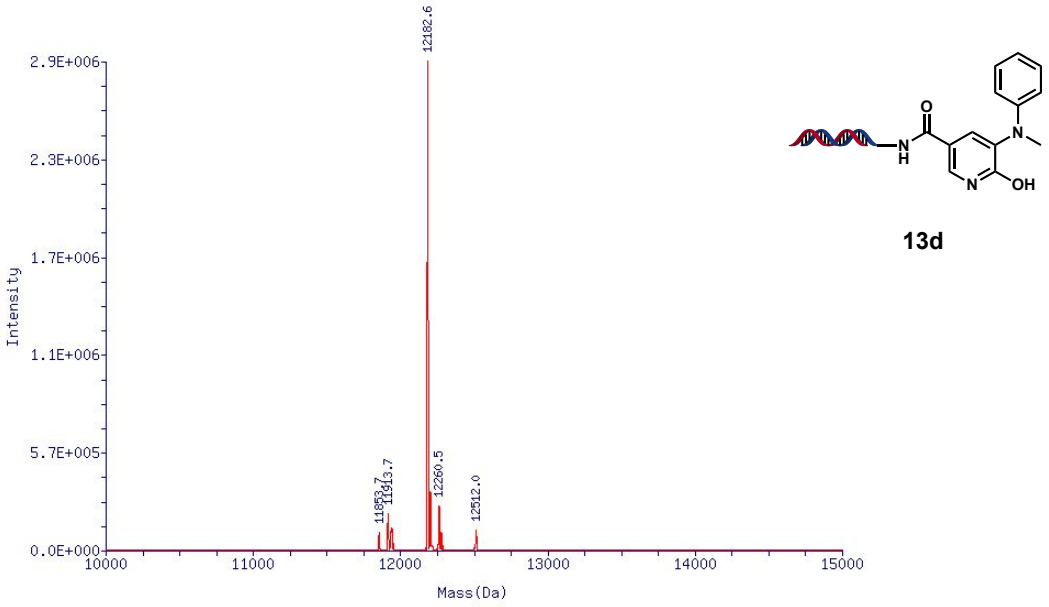


Figure S193. Deconvoluted mass spectrum of DNA **13d**, expected: 12286.2; no product observed.

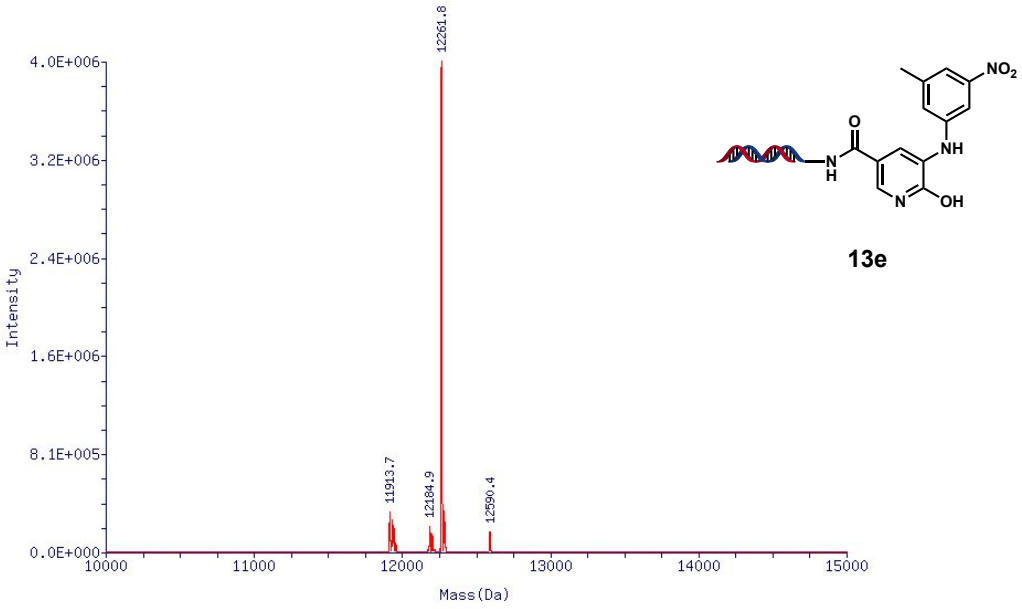


Figure S194. Deconvoluted mass spectrum of DNA **13e**, expected: 12331.2; observed 12333.3.

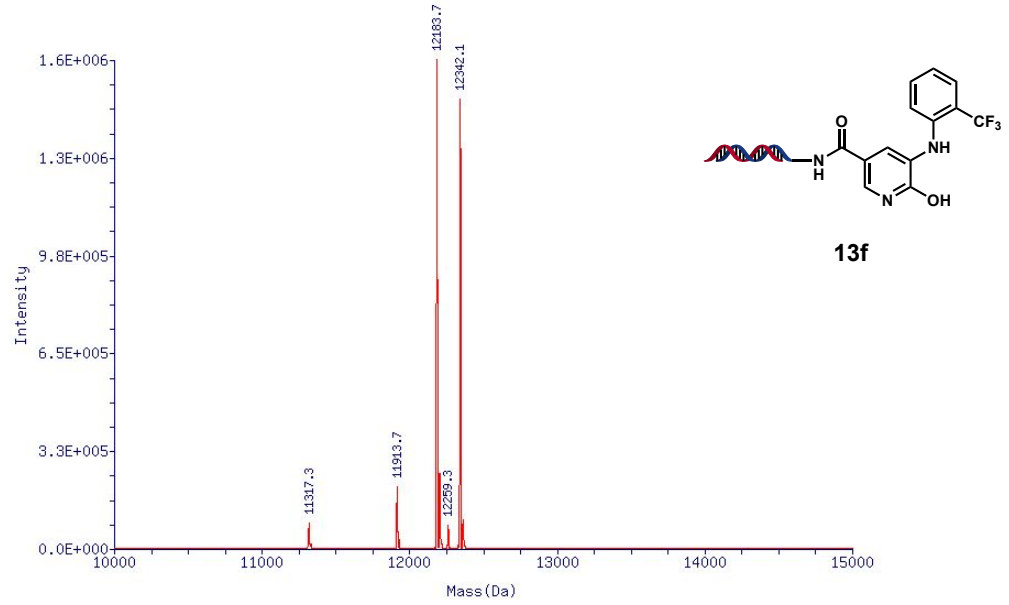


Figure S195. Deconvoluted mass spectrum of DNA **13f**, expected: 12340.2; observed 12342.1.

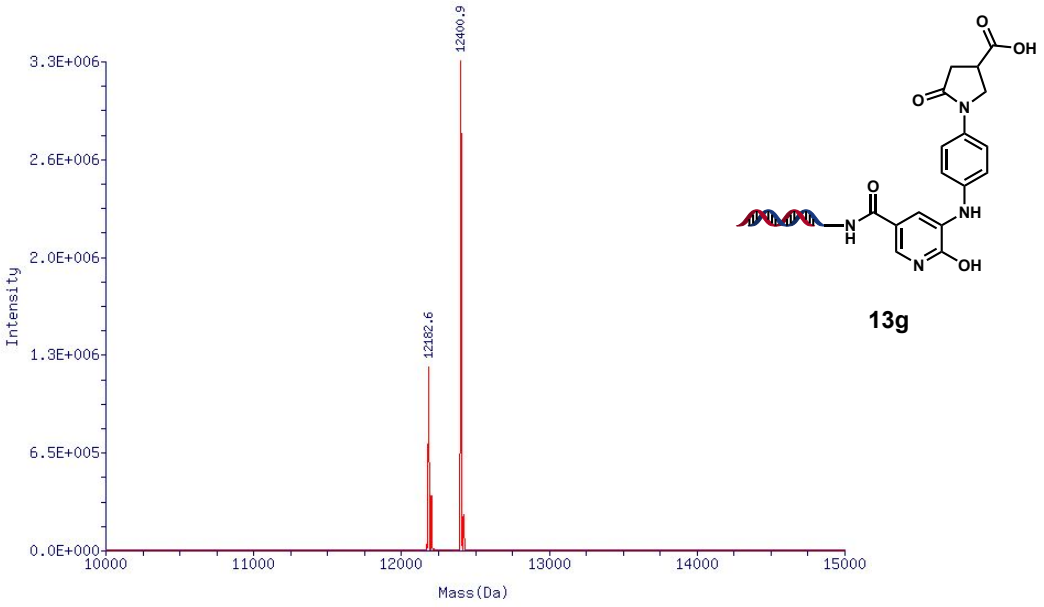


Figure S196. Deconvoluted mass spectrum of DNA **13g**, expected: 12399.2; observed 12400.9.

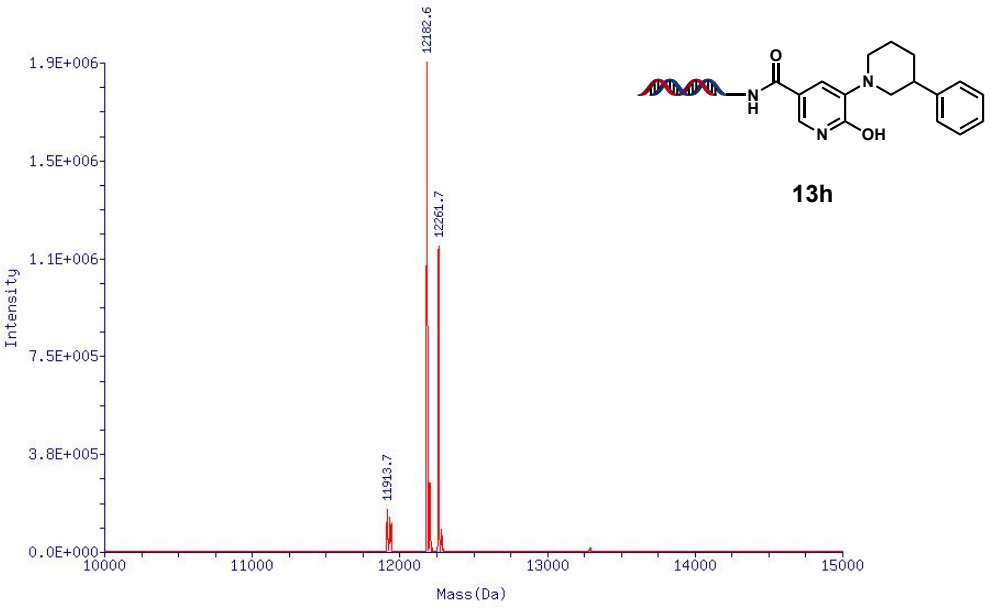
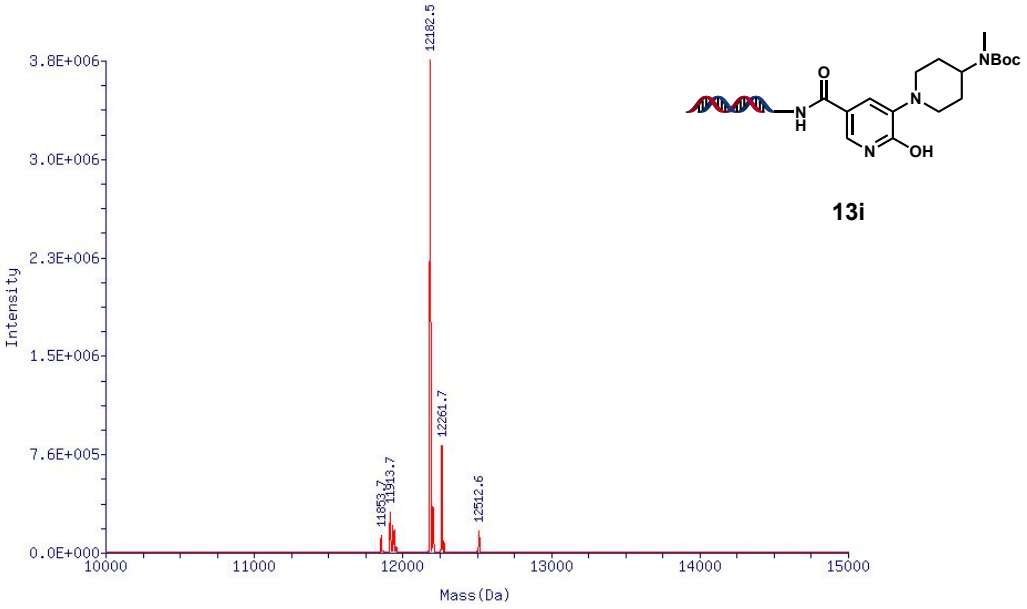
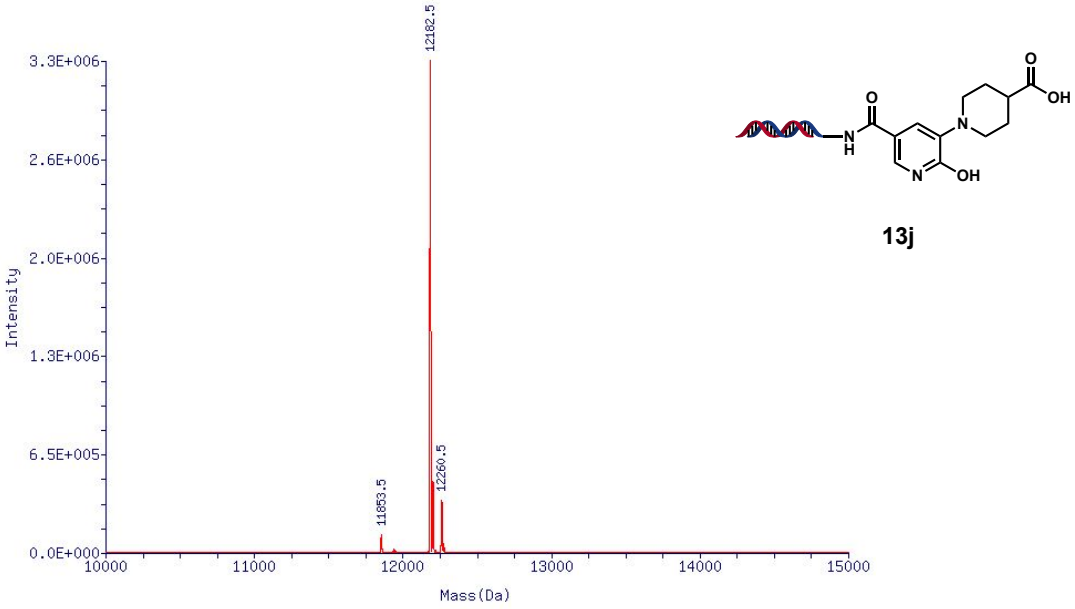


Figure S197. Deconvoluted mass spectrum of DNA **13h**, expected: 12340.3; no product observed.



13i

Figure S198. Deconvoluted mass spectrum of DNA **13i**, expected: 12393.4; no product observed.



13j

Figure S199. Deconvoluted mass spectrum of DNA **13j**, expected: 12308.2; no product observed.

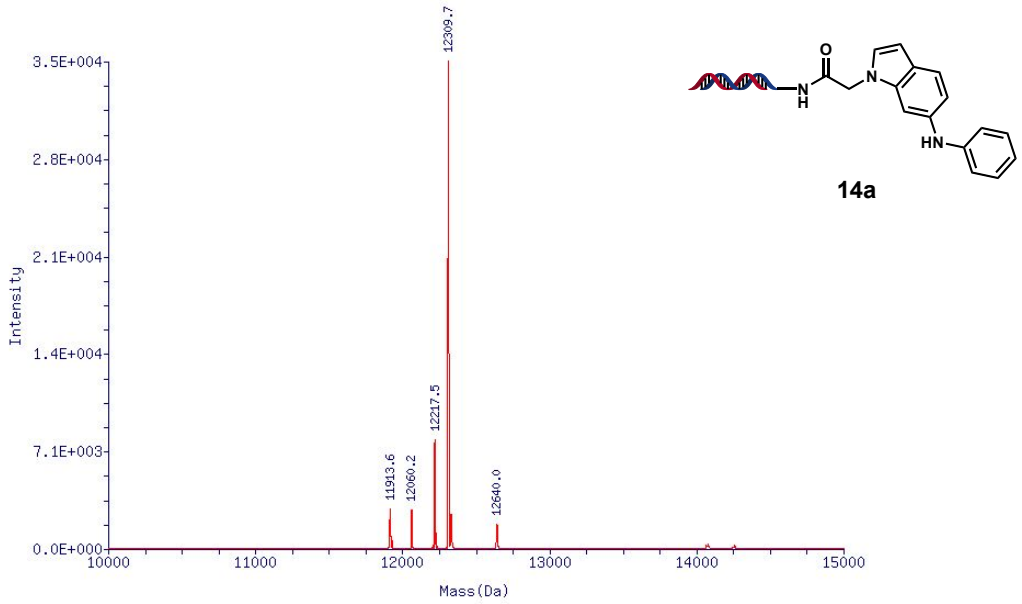


Figure S200. Deconvoluted mass spectrum of DNA **14a**, expected: 12308.3; observed 12309.7.

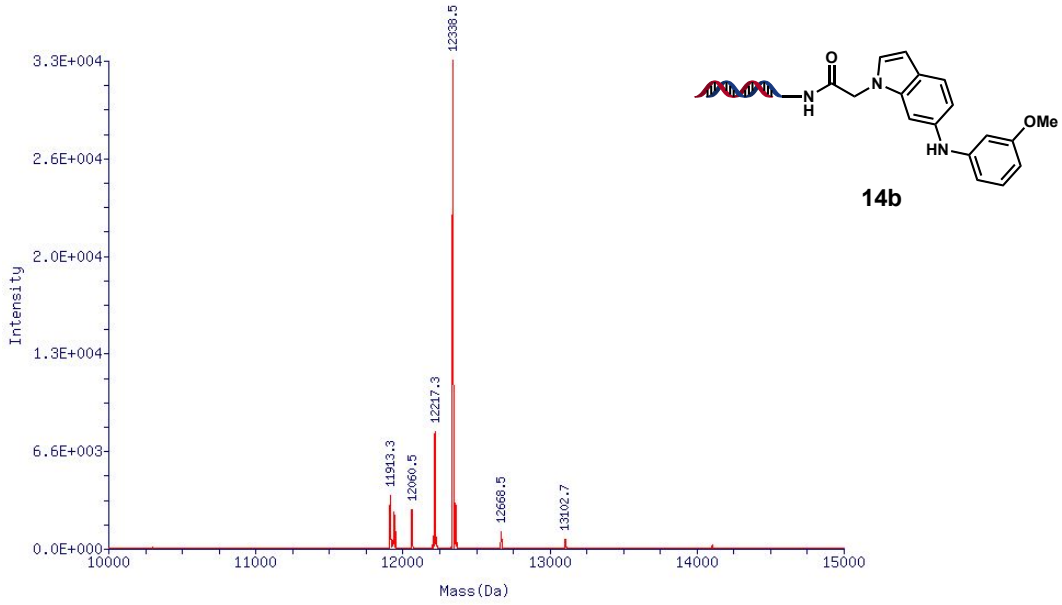


Figure S201. Deconvoluted mass spectrum of DNA **14b**, expected: 12338.3; observed 12338.5.

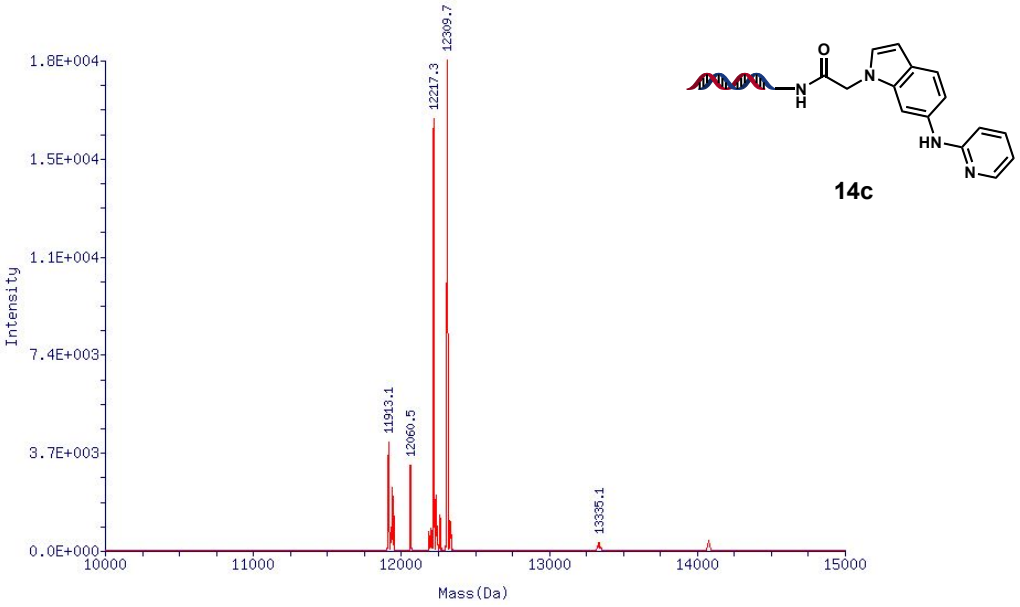


Figure S202. Deconvoluted mass spectrum of DNA **14c**, expected: 12309.3; observed 12309.7.

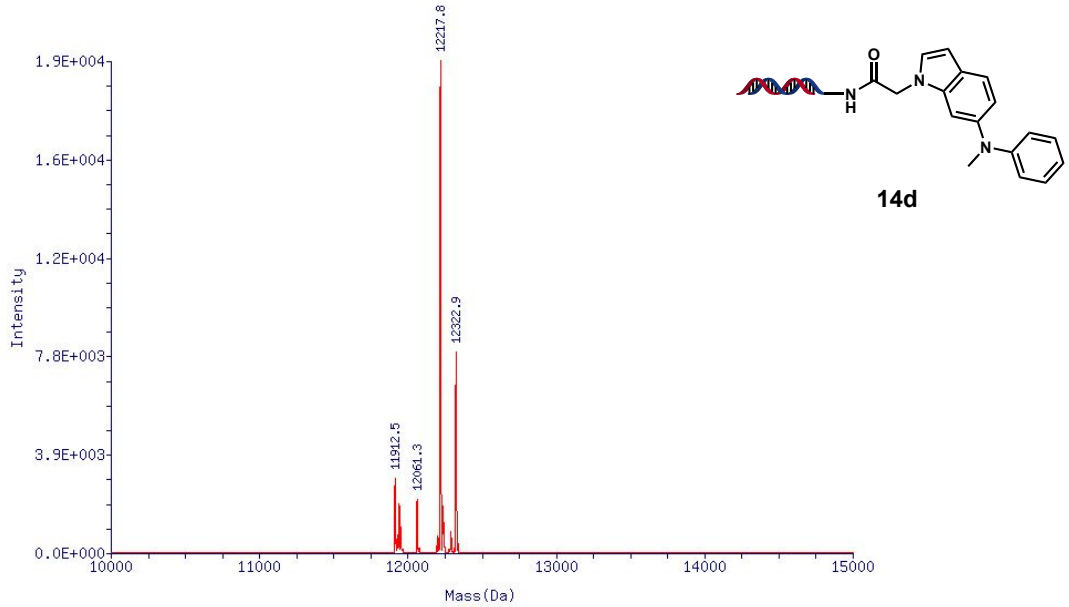


Figure S203. Deconvoluted mass spectrum of DNA **14d**, expected: 12322.3; observed 12322.9.

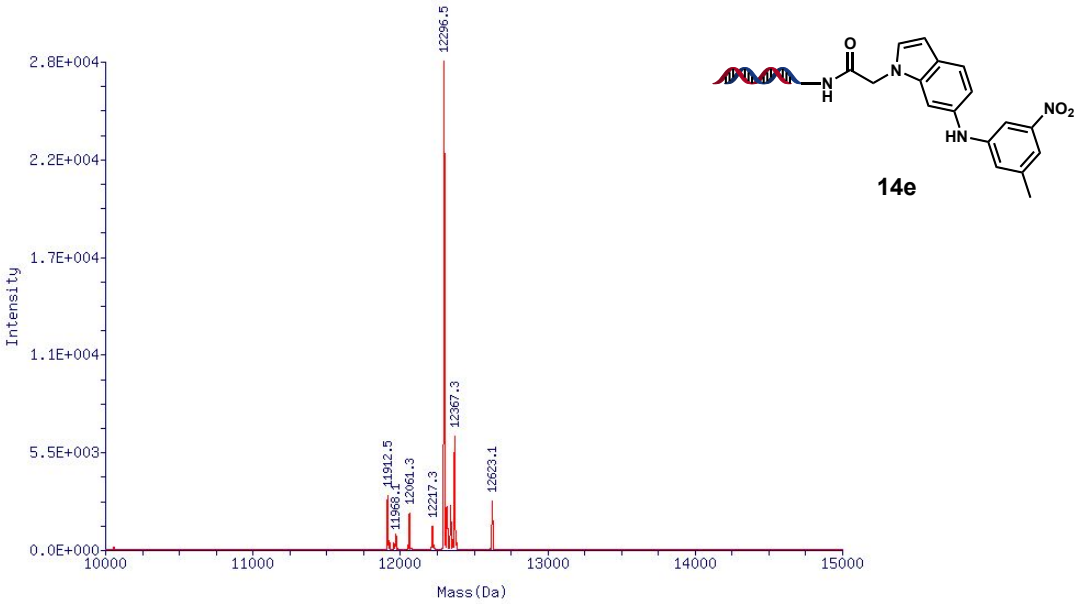


Figure S204. Deconvoluted mass spectrum of DNA **14e**, expected: 12367.3; observed 12367.3.

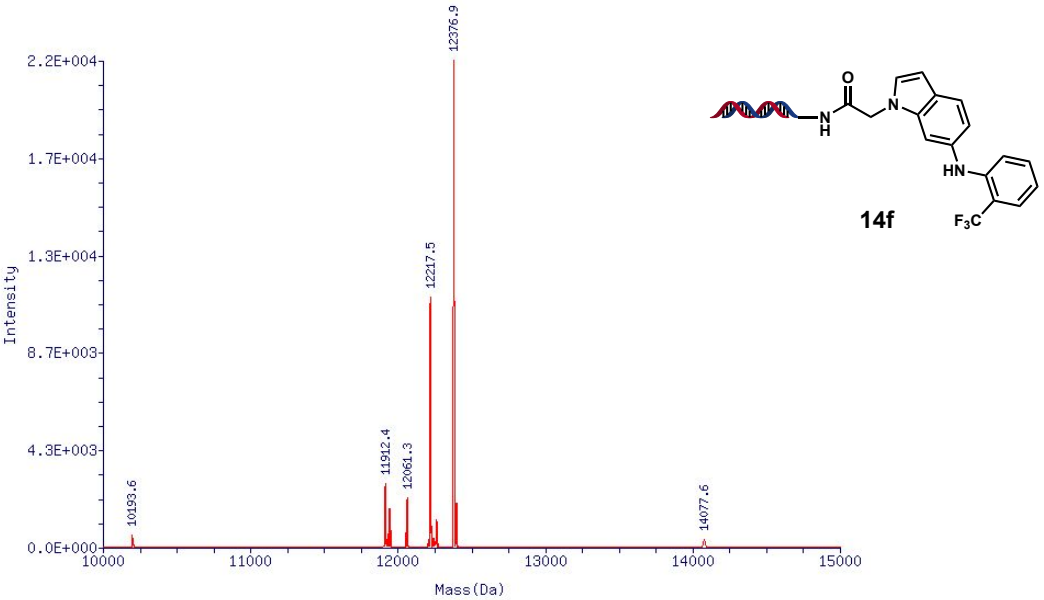


Figure S205. Deconvoluted mass spectrum of DNA **14f**, expected: 12376.3; observed 12376.9.

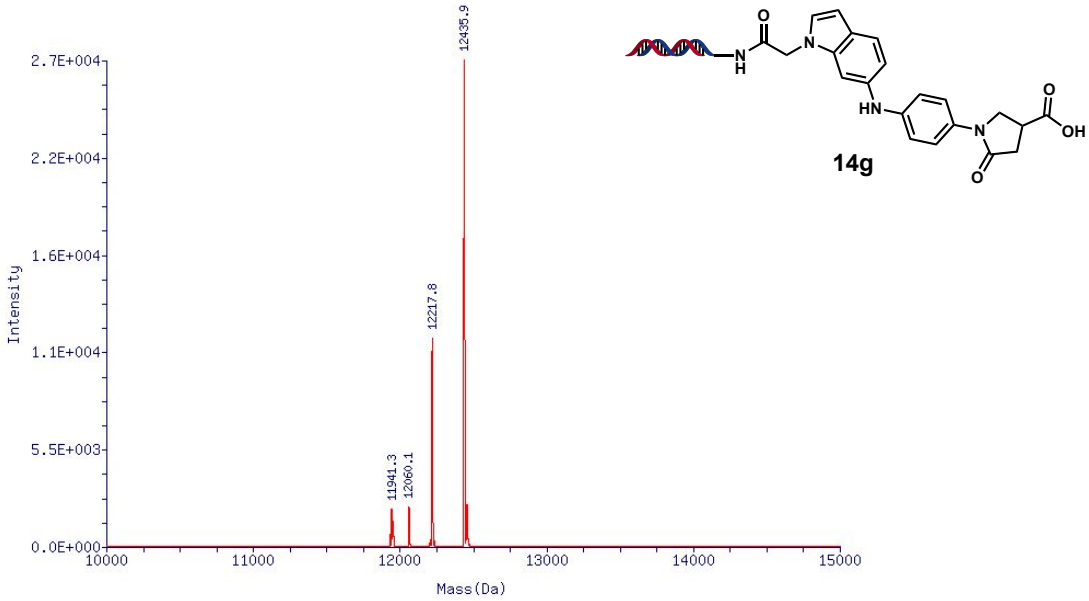


Figure S206. Deconvoluted mass spectrum of DNA **14g**, expected: 12435.3; observed 12435.9.

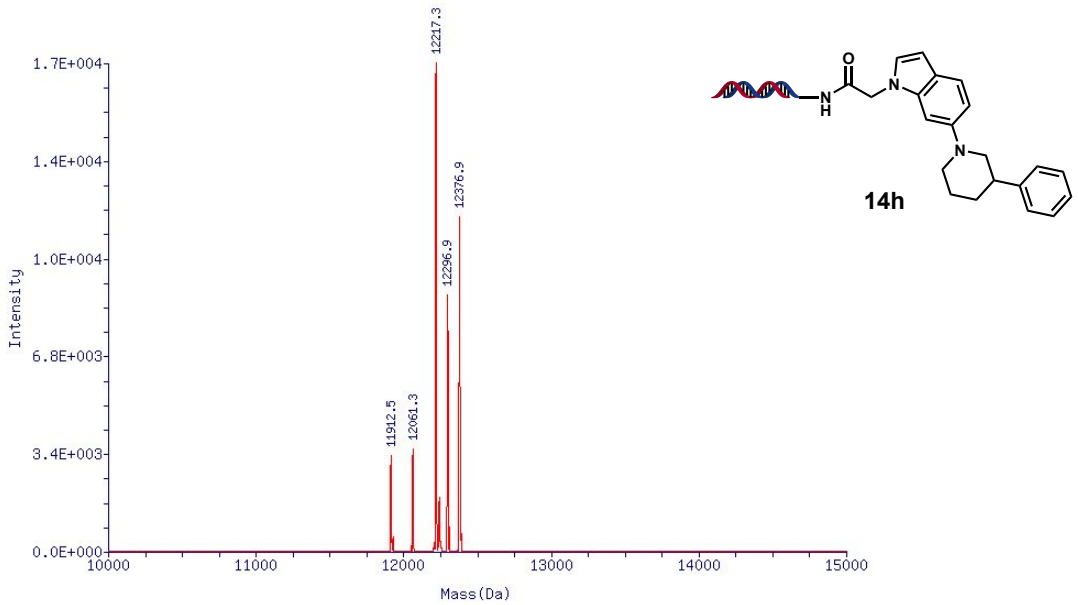


Figure S207. Deconvoluted mass spectrum of DNA **14h**, expected: 12376.4; observed 12376.9.

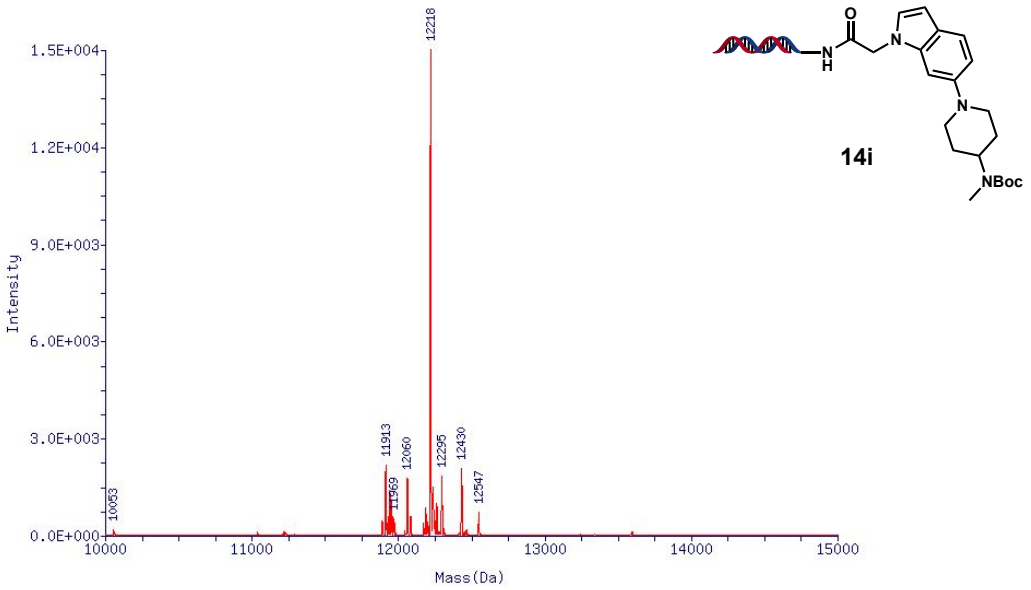


Figure S208. Deconvoluted mass spectrum of DNA **14i**, expected: 12429.5; observed 12430.

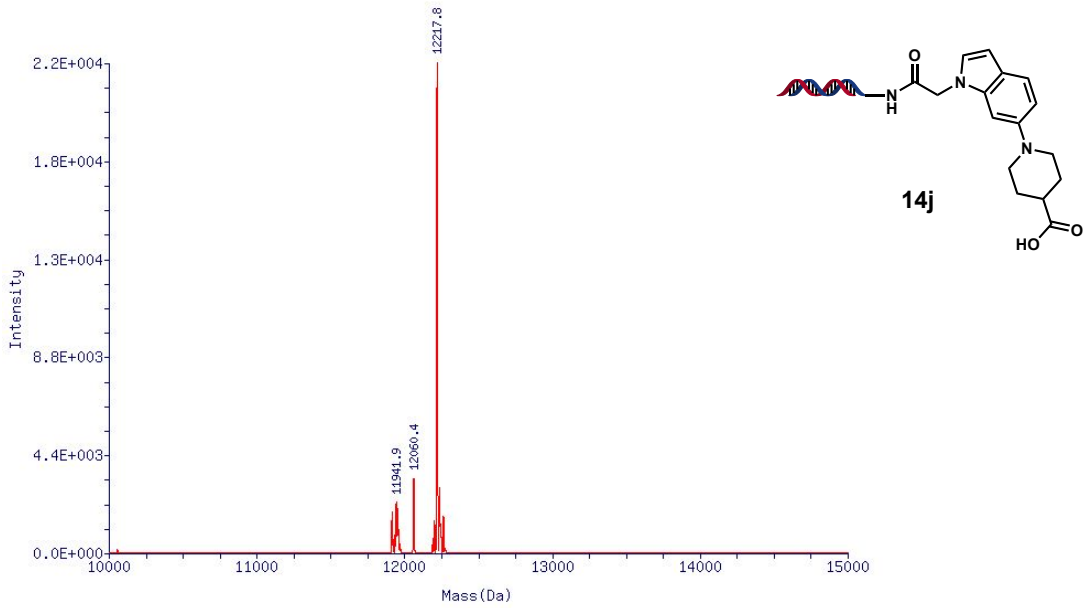


Figure S209. Deconvoluted mass spectrum of DNA **14j**, expected: 12344.3; no product observed.

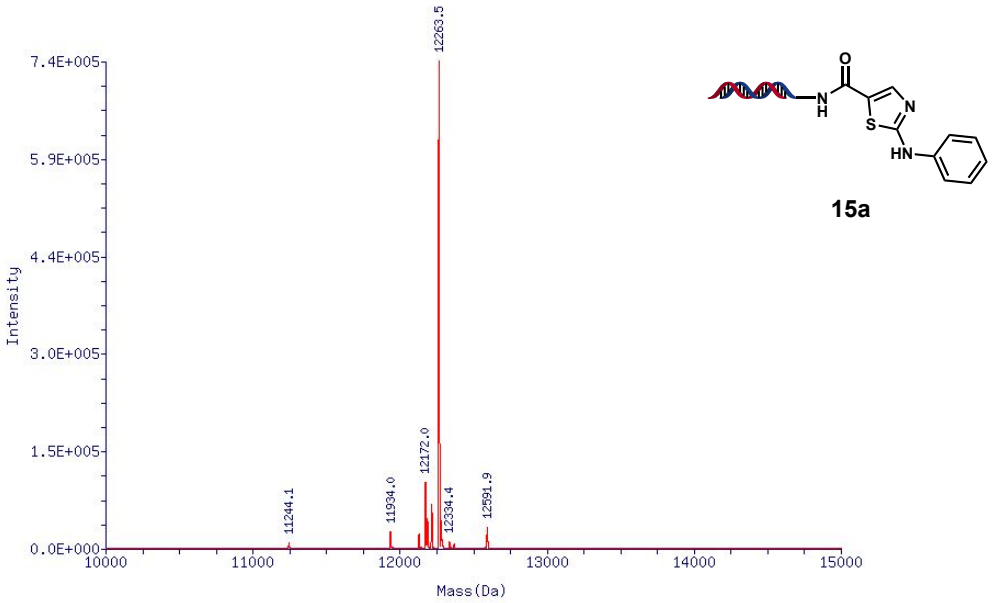


Figure S210. Deconvoluted mass spectrum of DNA **15a**, expected: 12262.2; observed 12263.5.

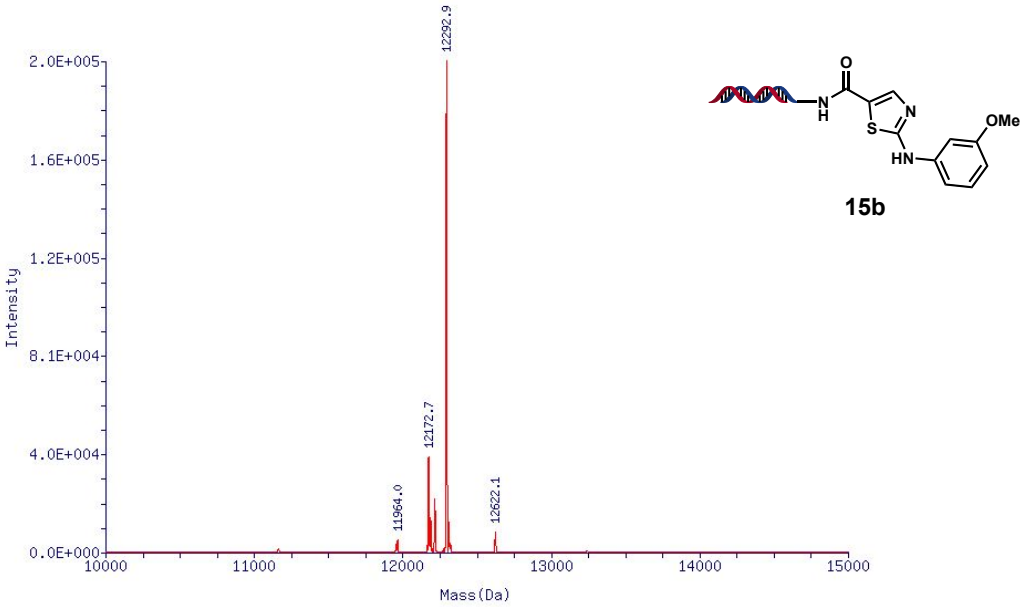


Figure S211. Deconvoluted mass spectrum of DNA **15b**, expected: 12292.3; observed 12292.9.

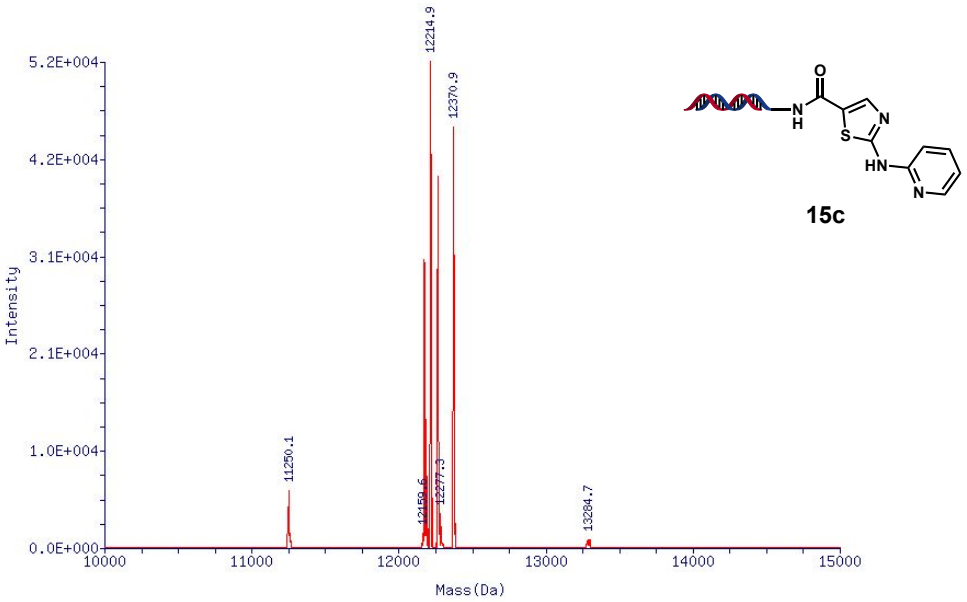


Figure S212. Deconvoluted mass spectrum of DNA **15c**, expected: 12263.2; no product observed.

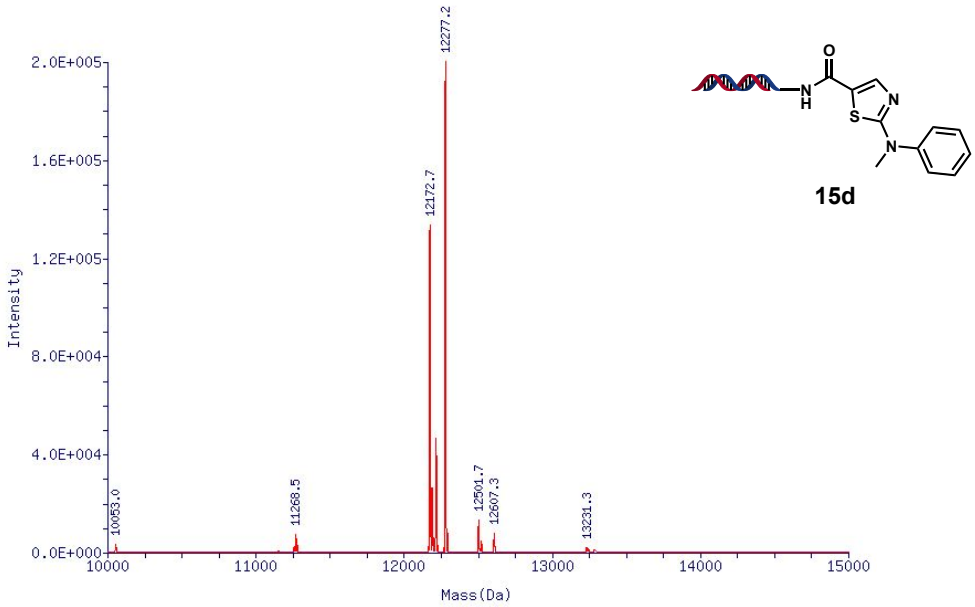


Figure S213. Deconvoluted mass spectrum of DNA **15d**, expected: 12276.3; observed 12277.2.

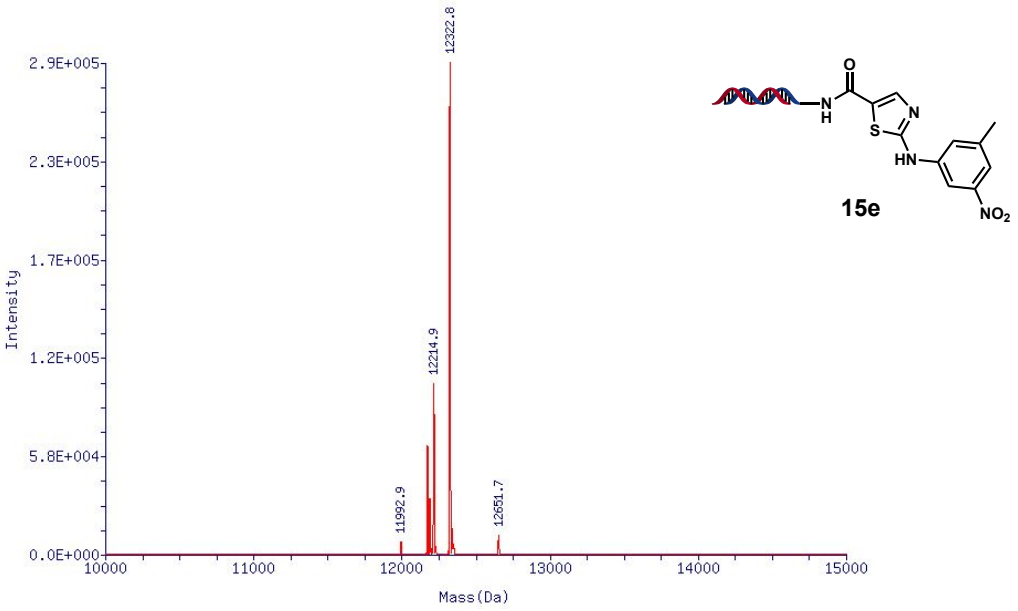


Figure S214. Deconvoluted mass spectrum of DNA **15e**, expected: 12321.3; observed 12322.8.

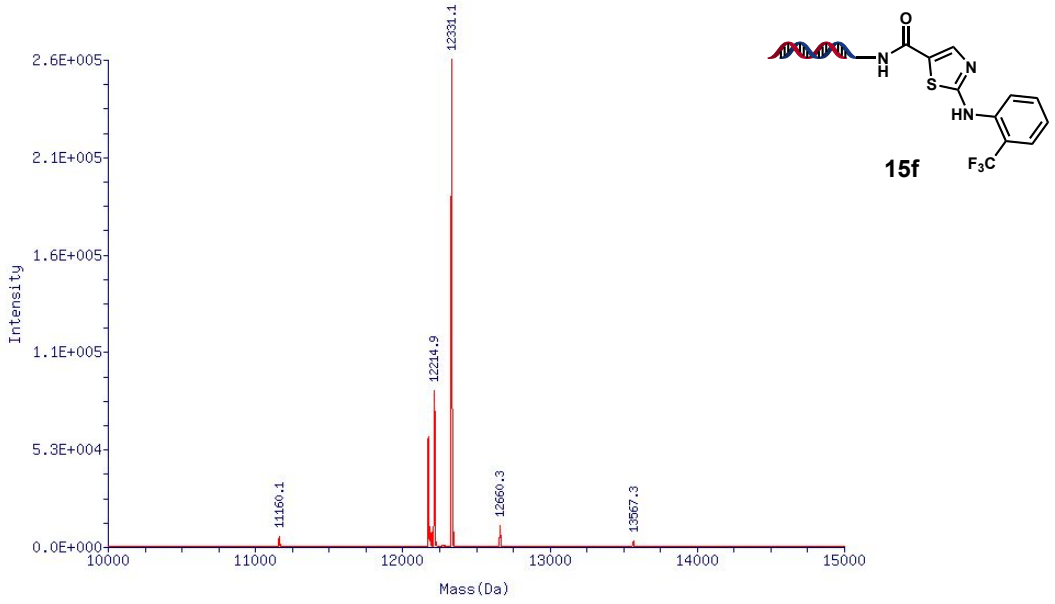


Figure S215. Deconvoluted mass spectrum of DNA **15f**, expected: 12330.2; observed 12331.1.

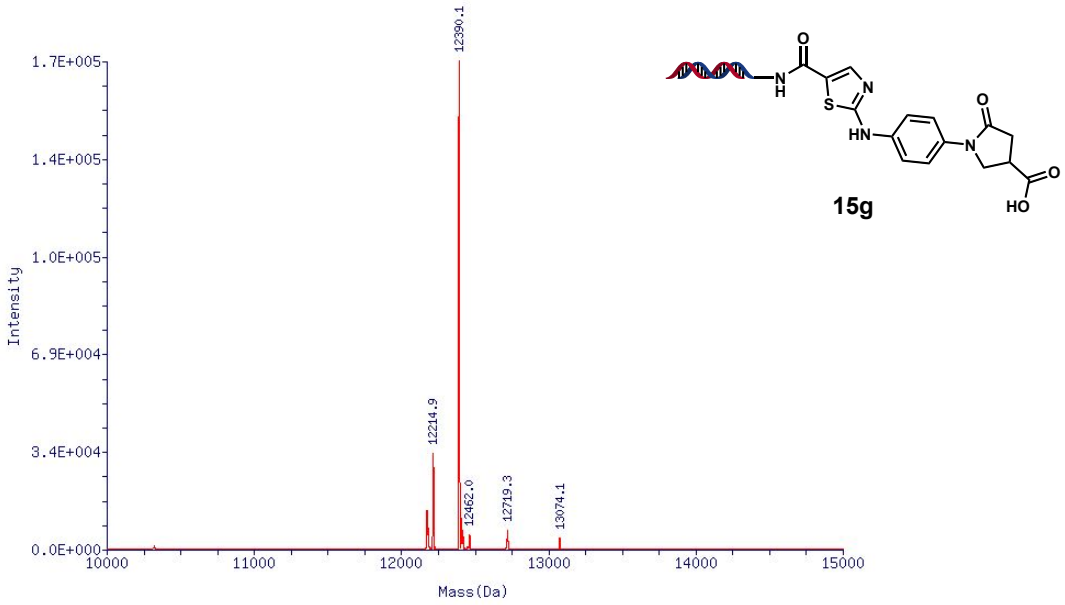


Figure S216. Deconvoluted mass spectrum of DNA **15g**, expected: 12389.2; observed 12390.1.

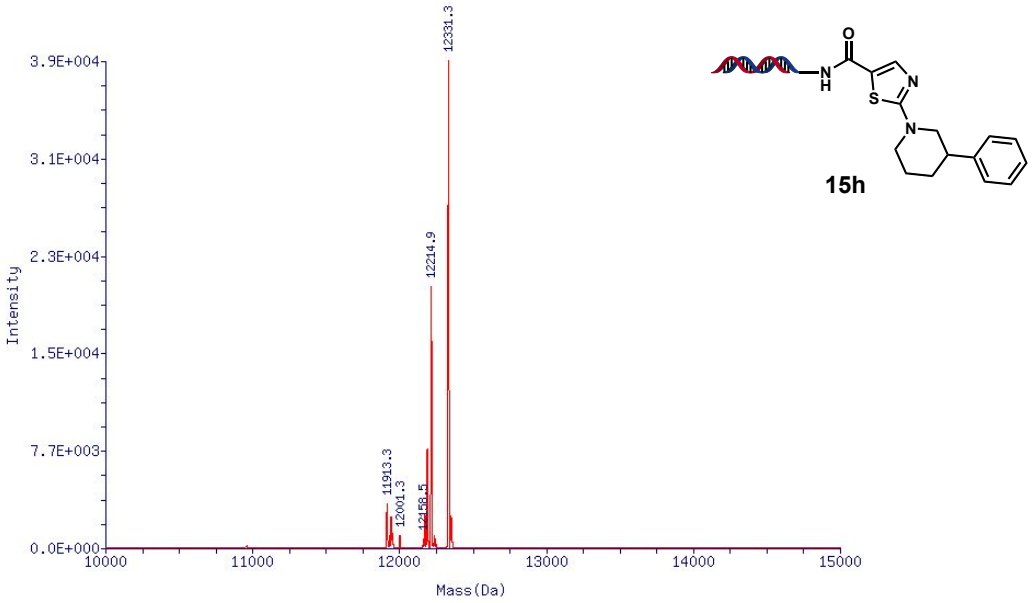


Figure S217. Deconvoluted mass spectrum of DNA **15h**, expected: 12330.4; observed 12331.3.

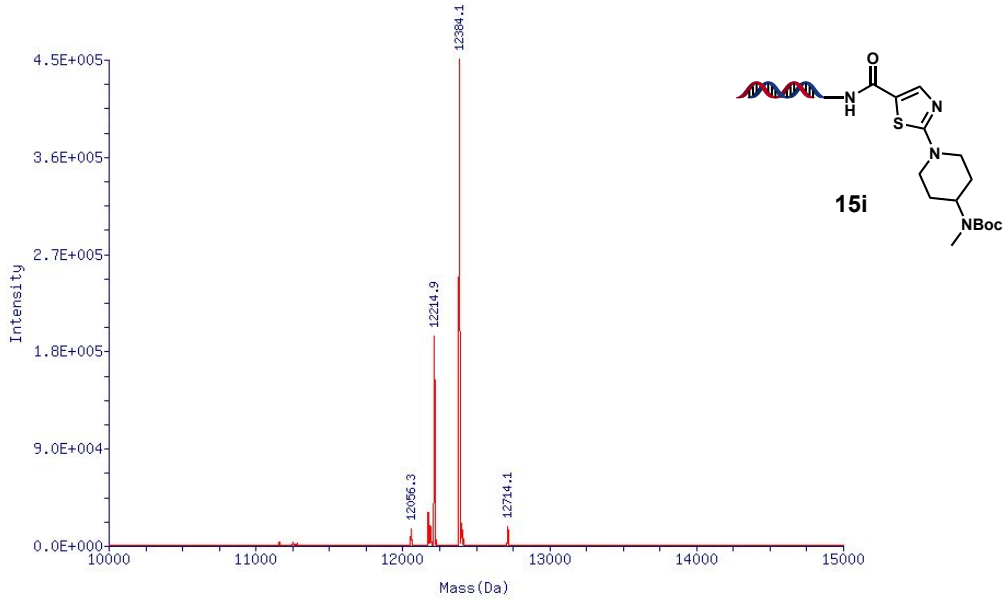


Figure S218. Deconvoluted mass spectrum of DNA **15i**, expected: 12383.4; observed 12384.1.

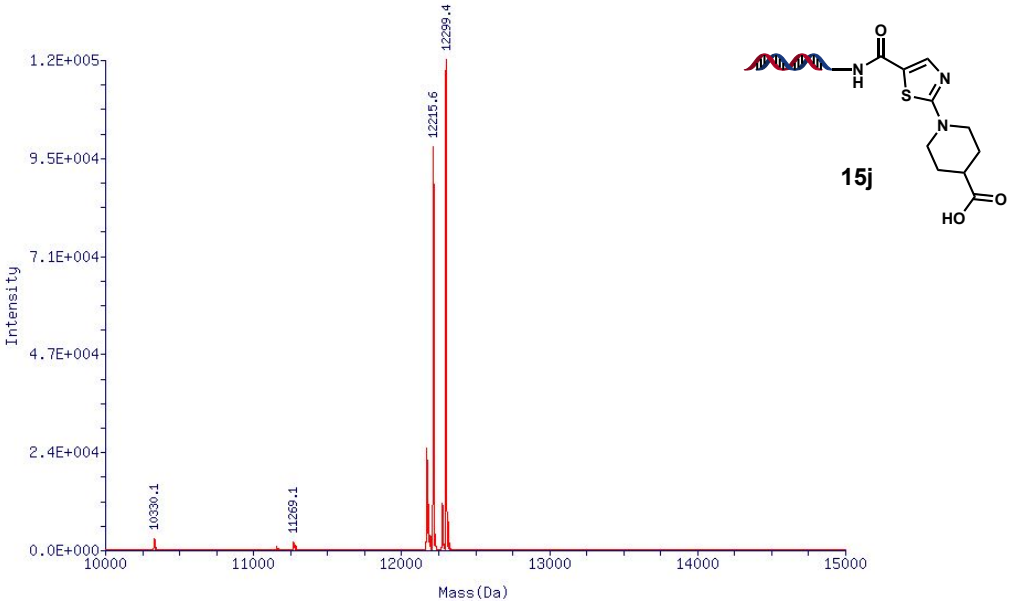


Figure S219. Deconvoluted mass spectrum of DNA **15j**, expected: 12298.3; observed 12299.4.

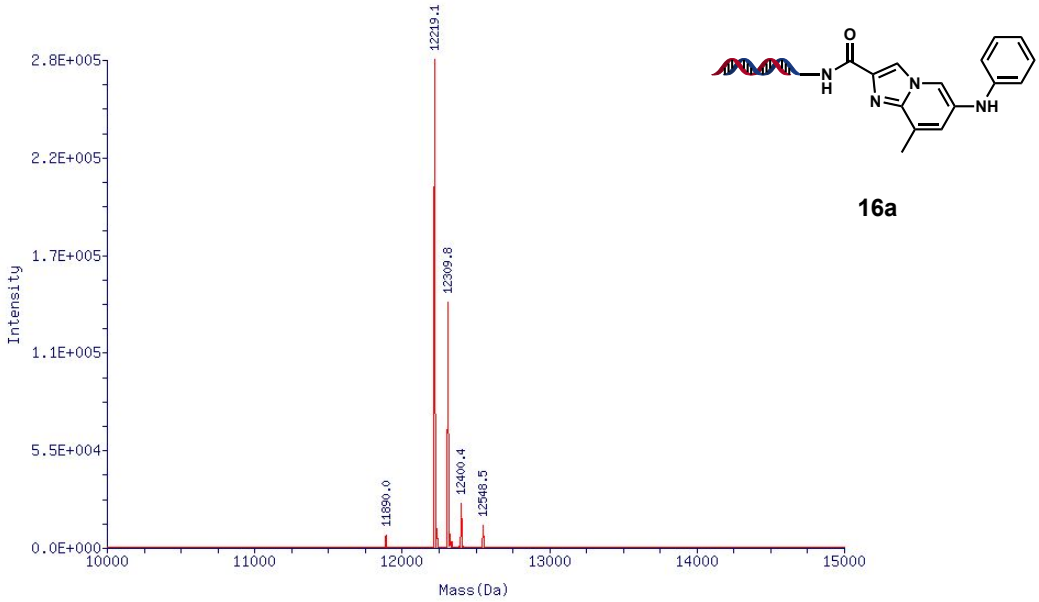


Figure S220. Deconvoluted mass spectrum of DNA **16a**, expected: 12309.3; observed 12309.8

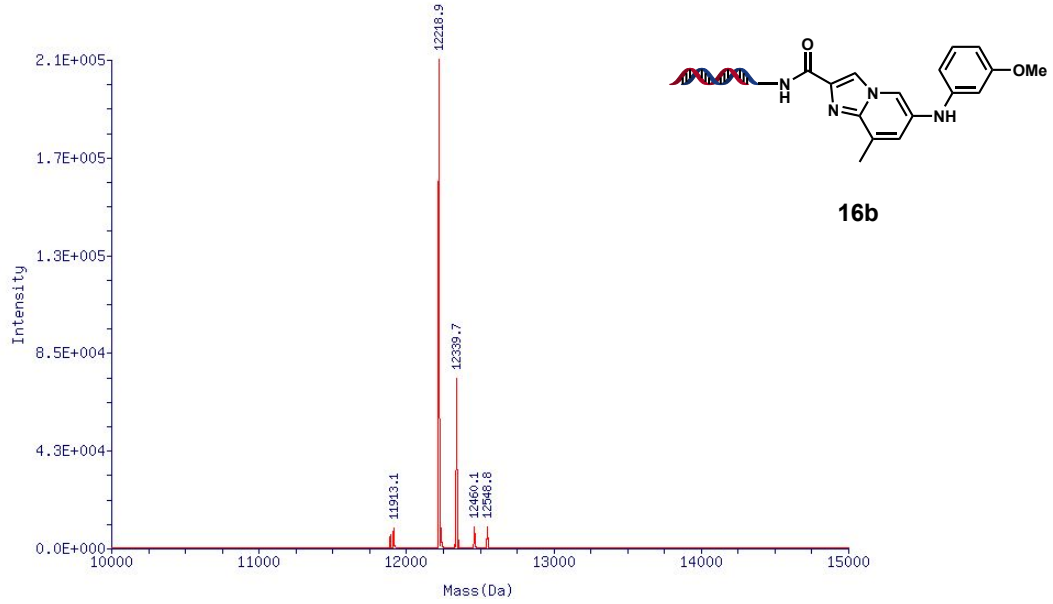


Figure S221. Deconvoluted mass spectrum of DNA **16b**, expected: 12339.3; observed 12339.7.

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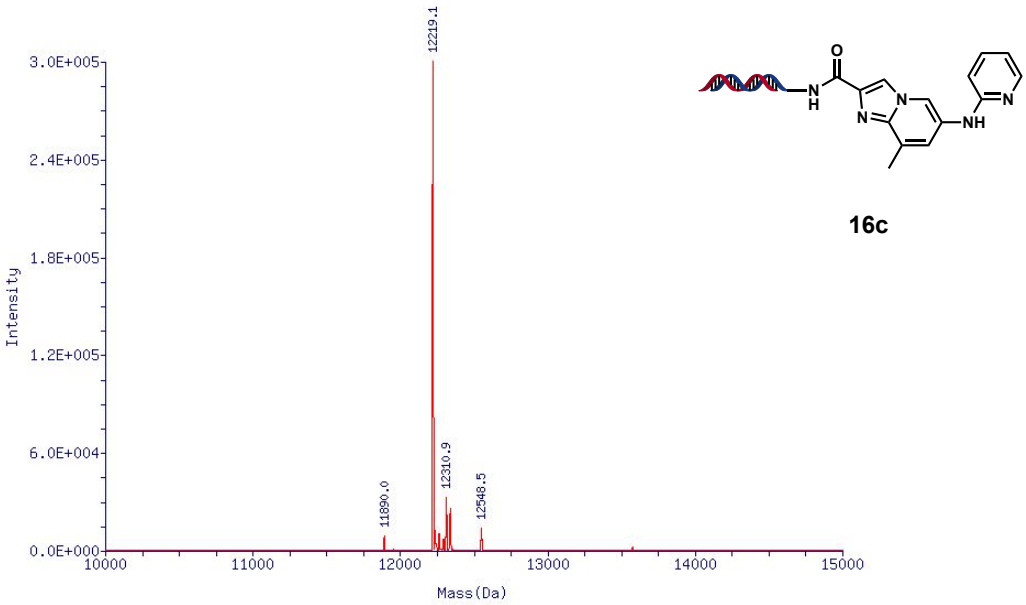
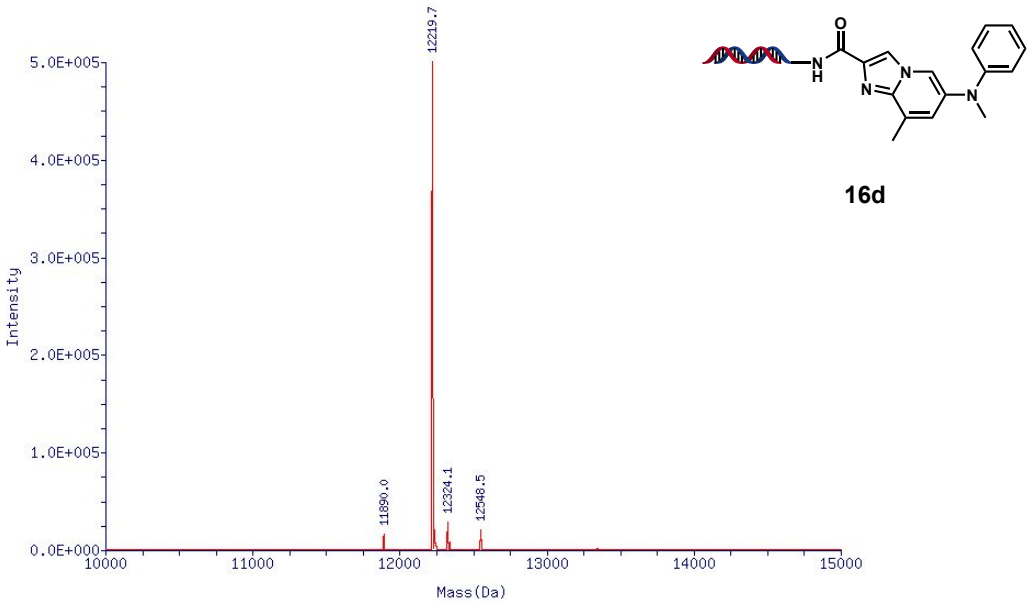


16c

Figure S222. Deconvoluted mass spectrum of DNA **16c**, expected: 12310.3; observed 12310.9.



16d

Figure S223. Deconvoluted mass spectrum of DNA **16d**, expected: 12323.3; observed 12324.1.

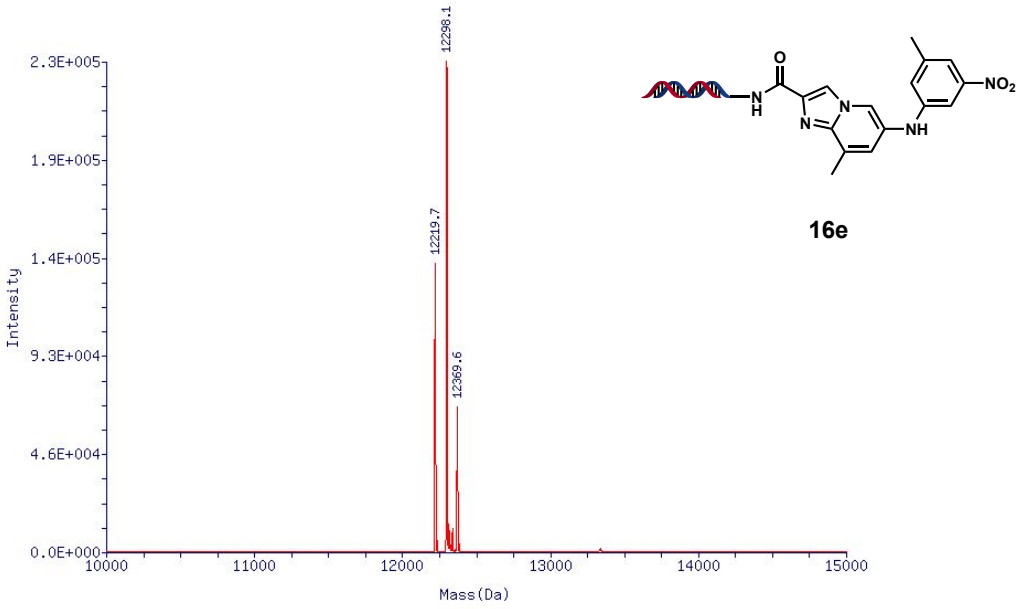


Figure S224. Deconvoluted mass spectrum of DNA **16e**, expected: 12368.3; observed 12369.6.

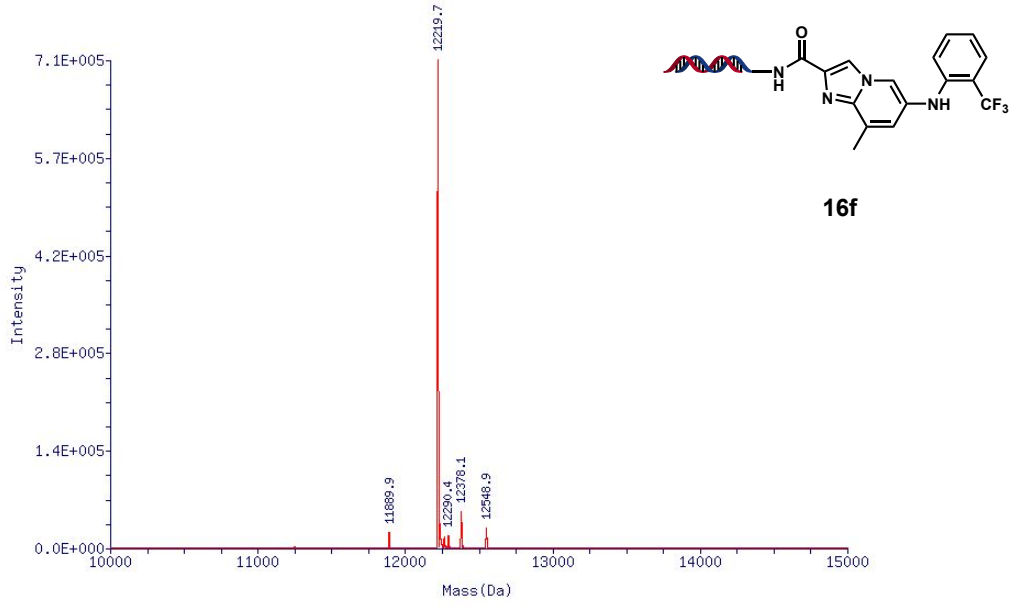


Figure S225. Deconvoluted mass spectrum of DNA **16f**, expected: 12377.3; observed 12378.1.

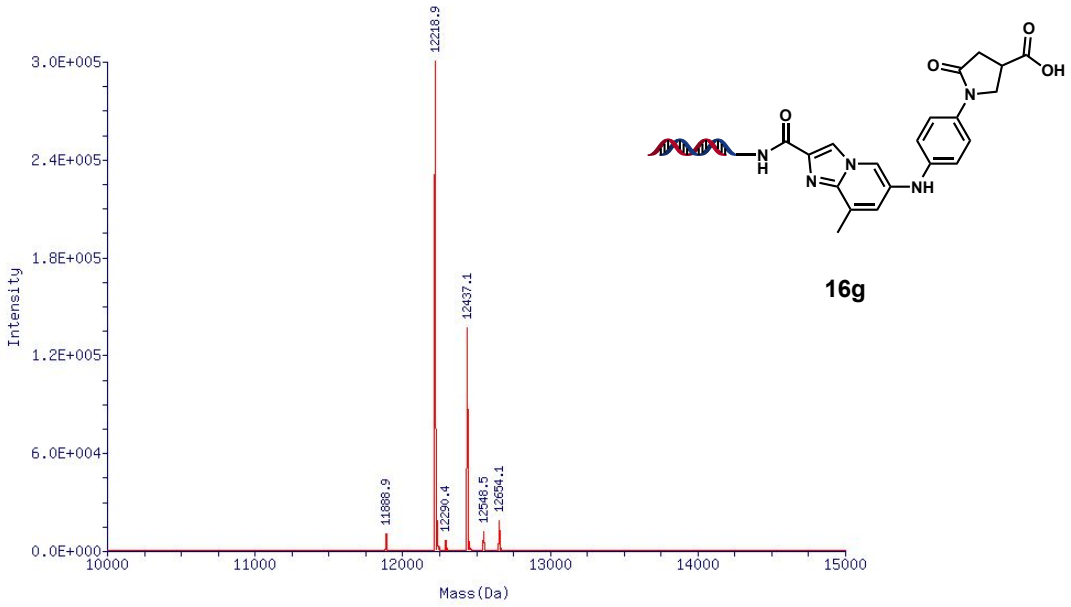


Figure S226. Deconvoluted mass spectrum of DNA **16g**, expected: 12436.3; observed 12437.1.

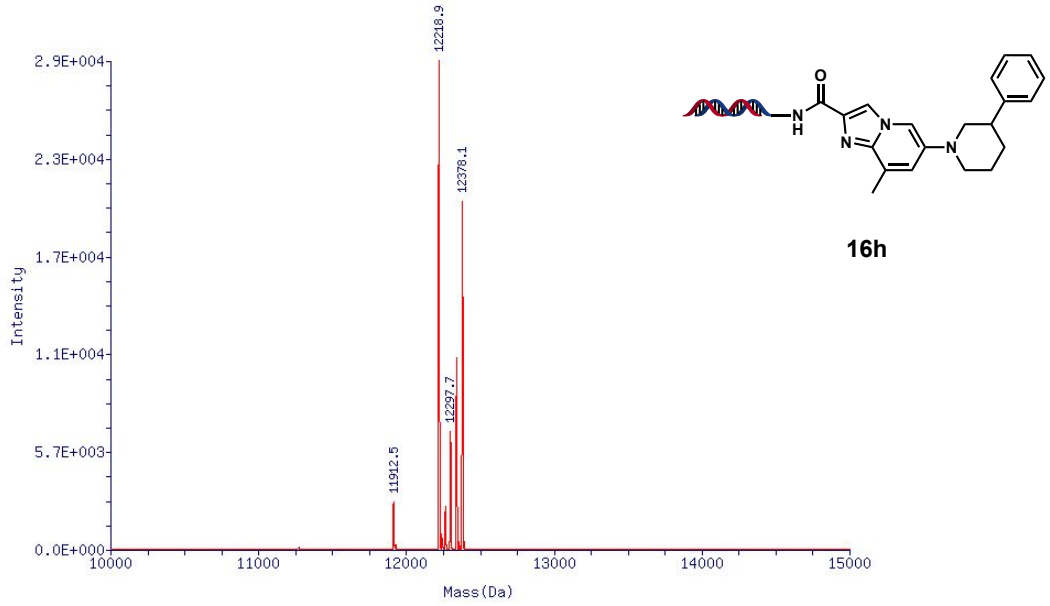


Figure S227. Deconvoluted mass spectrum of DNA **16h**, expected: 12377.4; observed 12378.1.

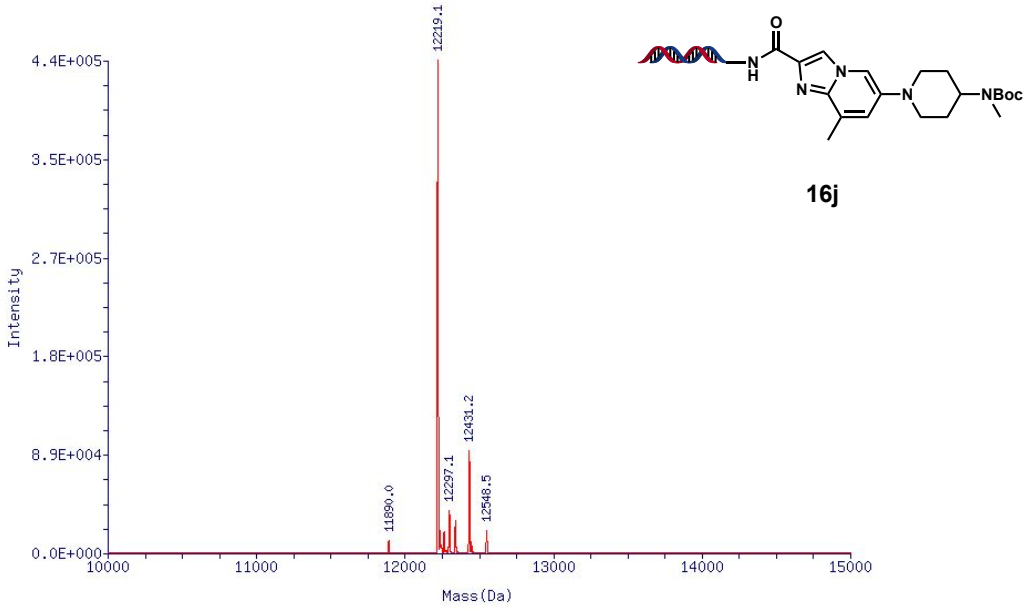


Figure S228. Deconvoluted mass spectrum of DNA **16i**, expected: 12430.5; observed 12431.2.

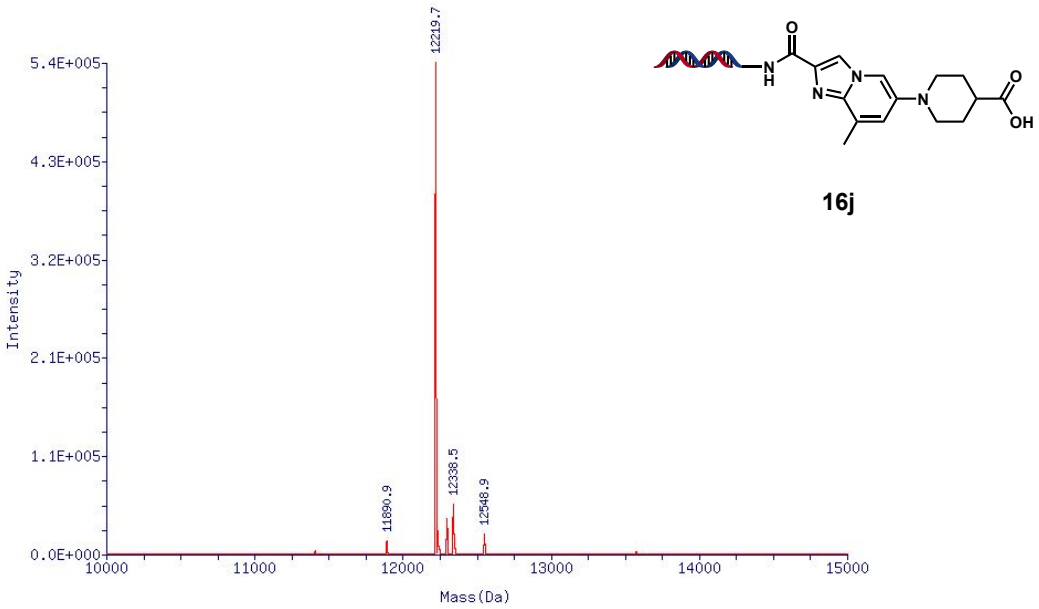


Figure S229. Deconvoluted mass spectrum of DNA **16j**, expected: 12345.3; no product observed.

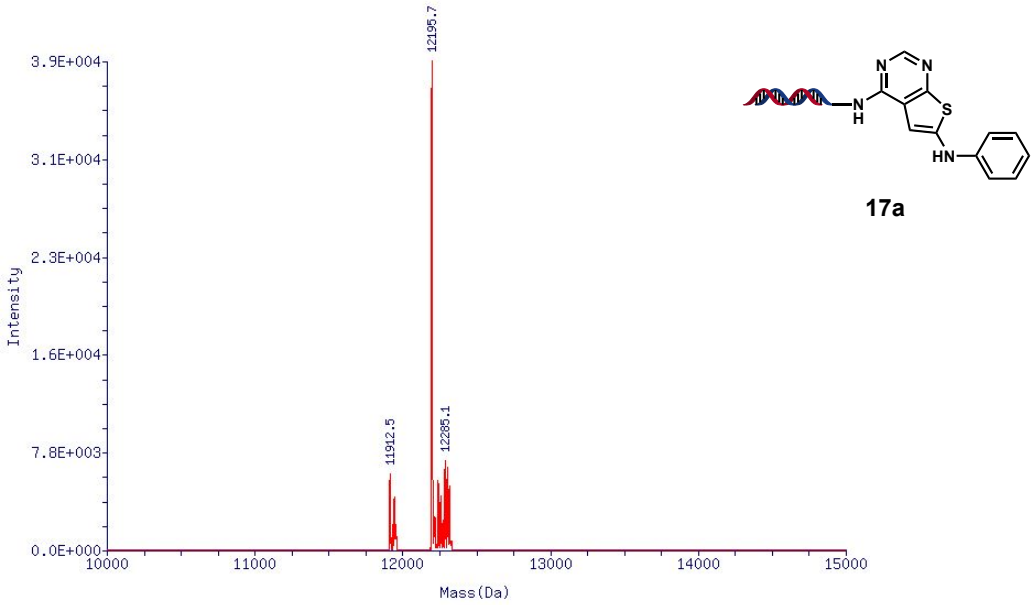


Figure S230. Deconvoluted mass spectrum of DNA **17a**, expected: 12285.3; observed 12285.2.

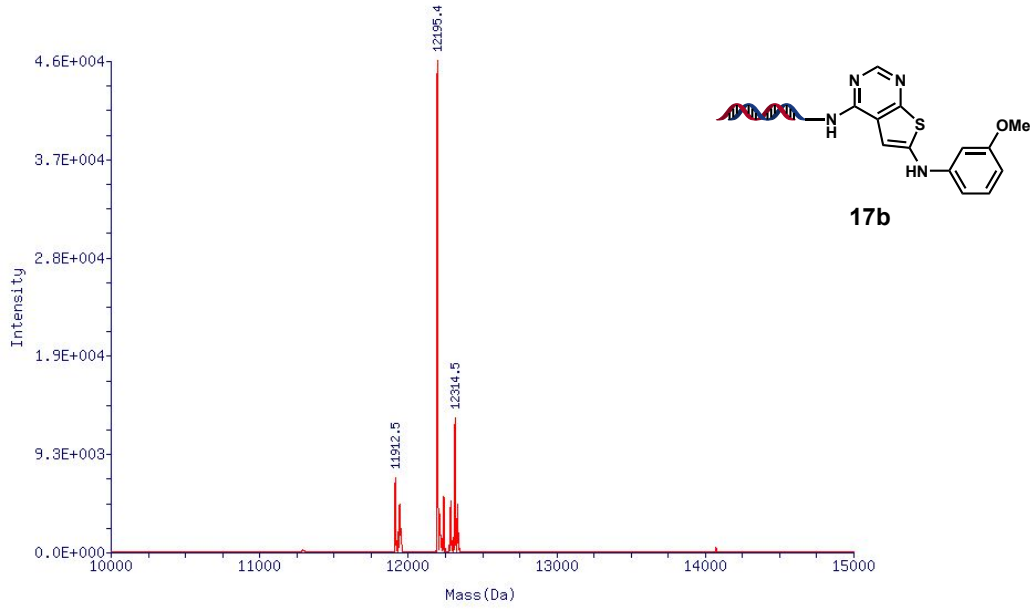


Figure S231. Deconvoluted mass spectrum of DNA **17b**, expected: 12315.3; observed 12314.4.

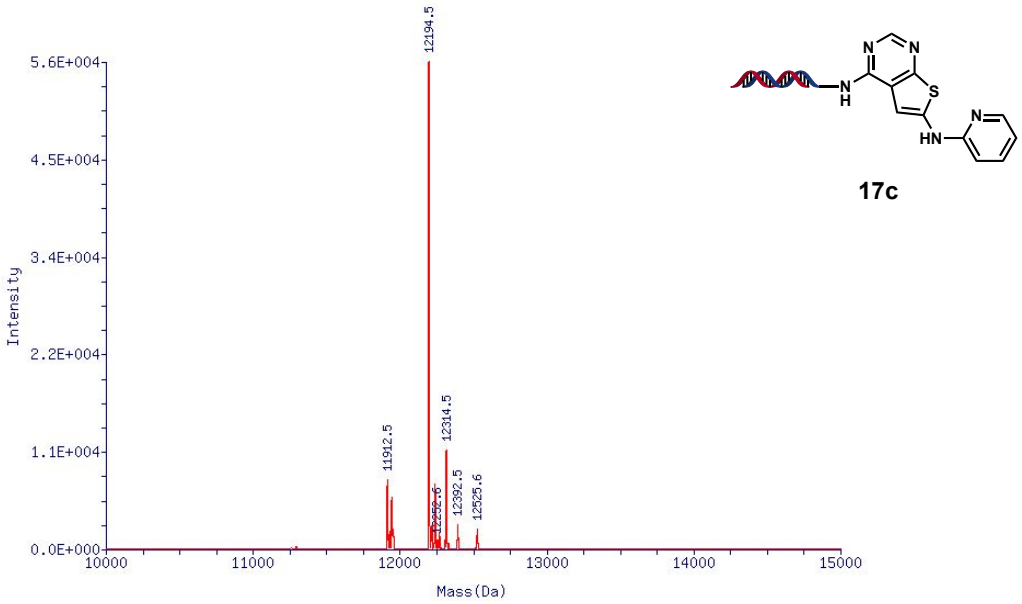


Figure S232. Deconvoluted mass spectrum of DNA **17c**, expected: 12286.3; no product observed.

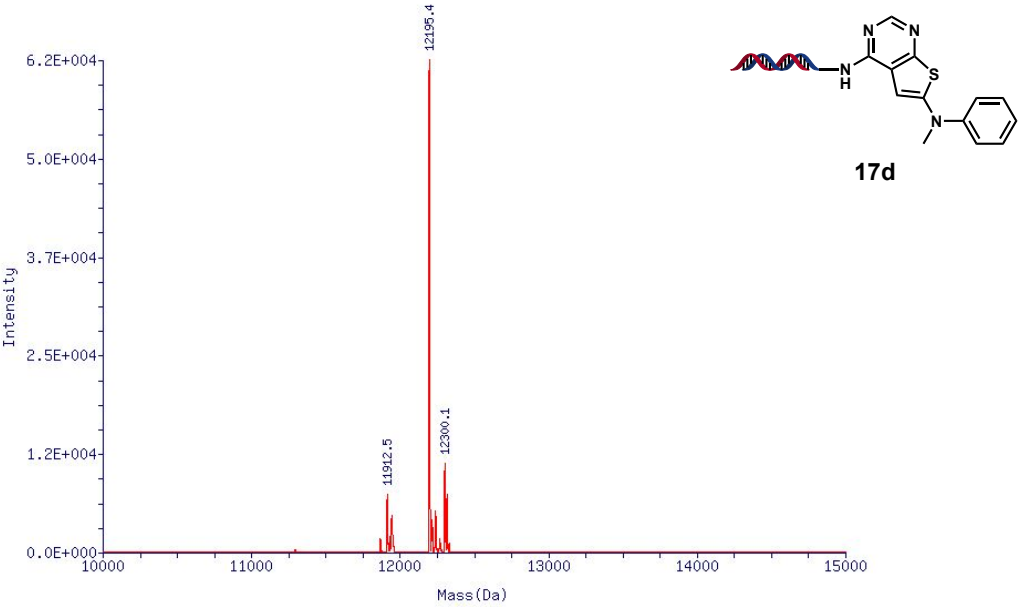


Figure S233. Deconvoluted mass spectrum of DNA **17d**, expected: 12299.3; observed 12300.1.

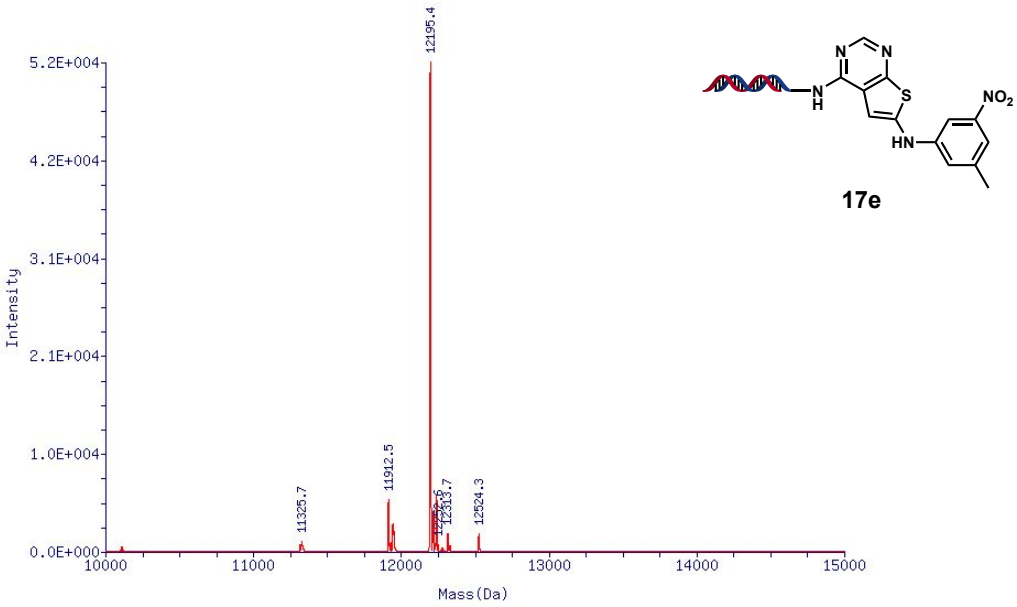


Figure S234. Deconvoluted mass spectrum of DNA **17e**, expected: 12344.3; no product observed.

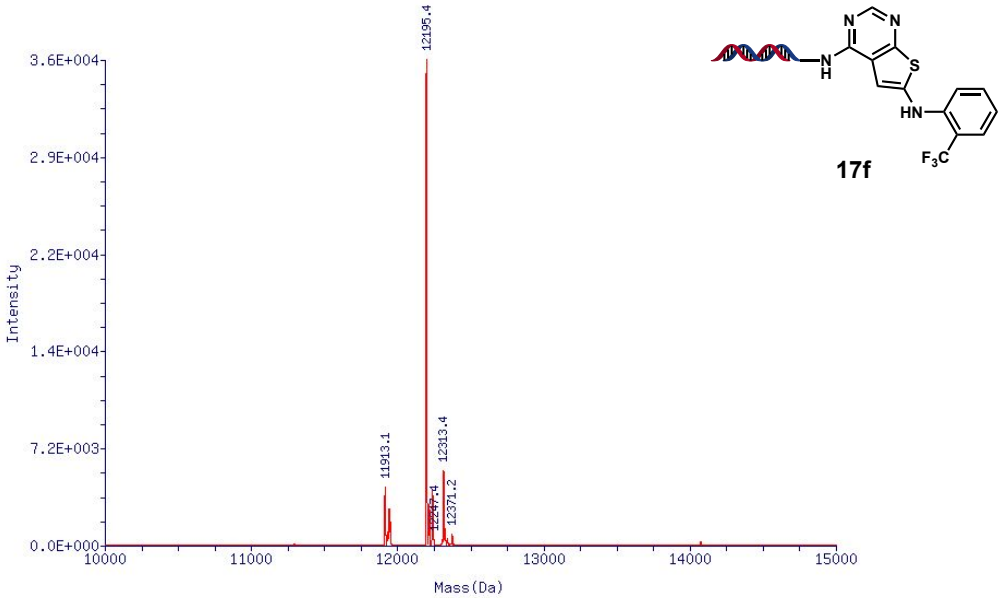


Figure S235. Deconvoluted mass spectrum of DNA **17f**, expected: 12353.3; no product observed.

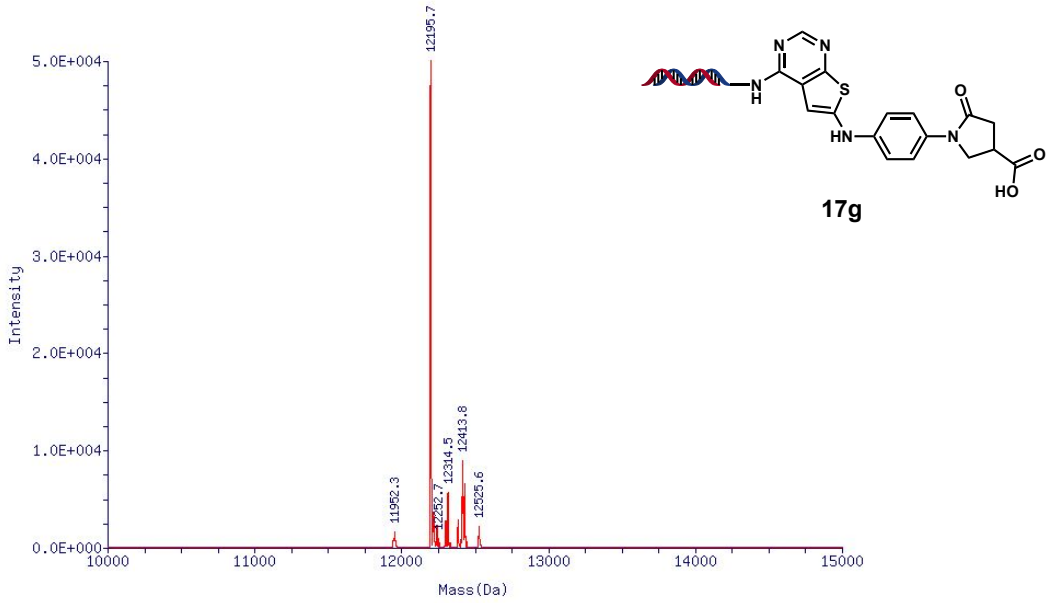


Figure S236. Deconvoluted mass spectrum of DNA **17g**, expected: 12412.3; observed 12413.8.

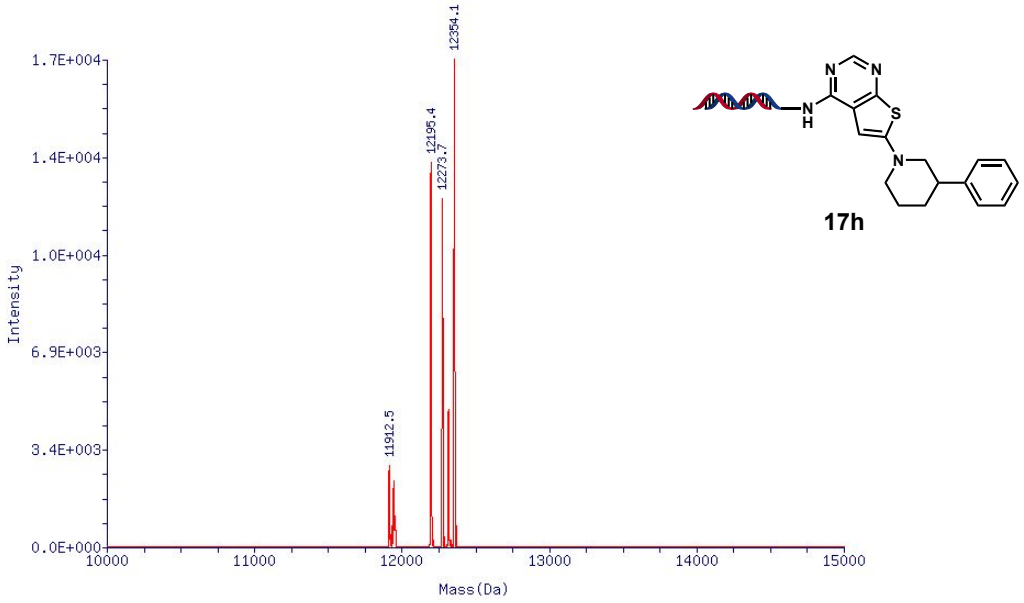


Figure S237. Deconvoluted mass spectrum of DNA **17h**, expected: 12353.4; observed 12354.1.

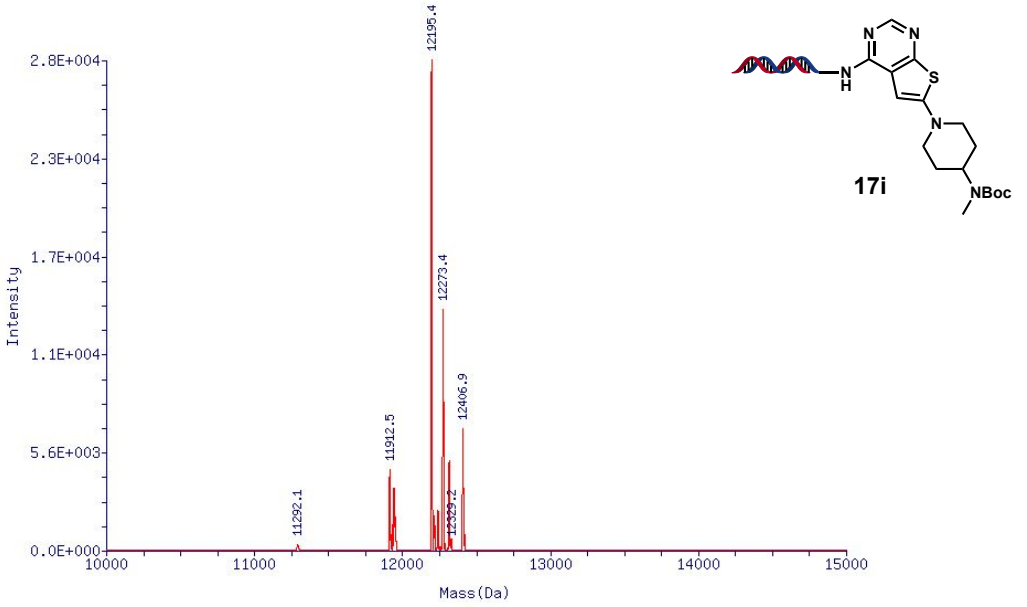


Figure S238. Deconvoluted mass spectrum of DNA **17i**, expected: 12406.5; observed 12406.9.

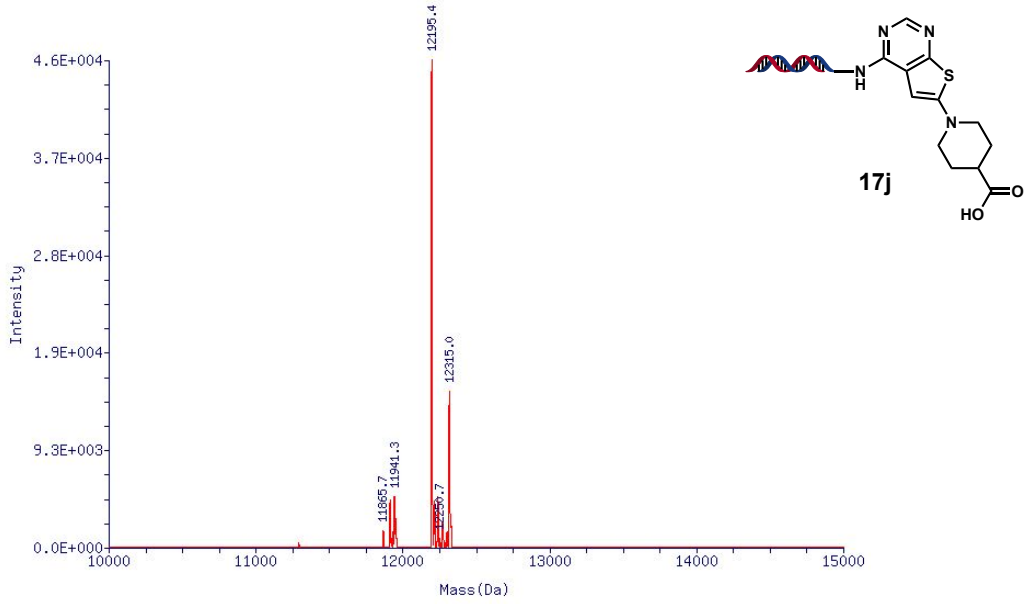


Figure S239. Deconvoluted mass spectrum of DNA **17j**, expected: 12321.3; no product observed.

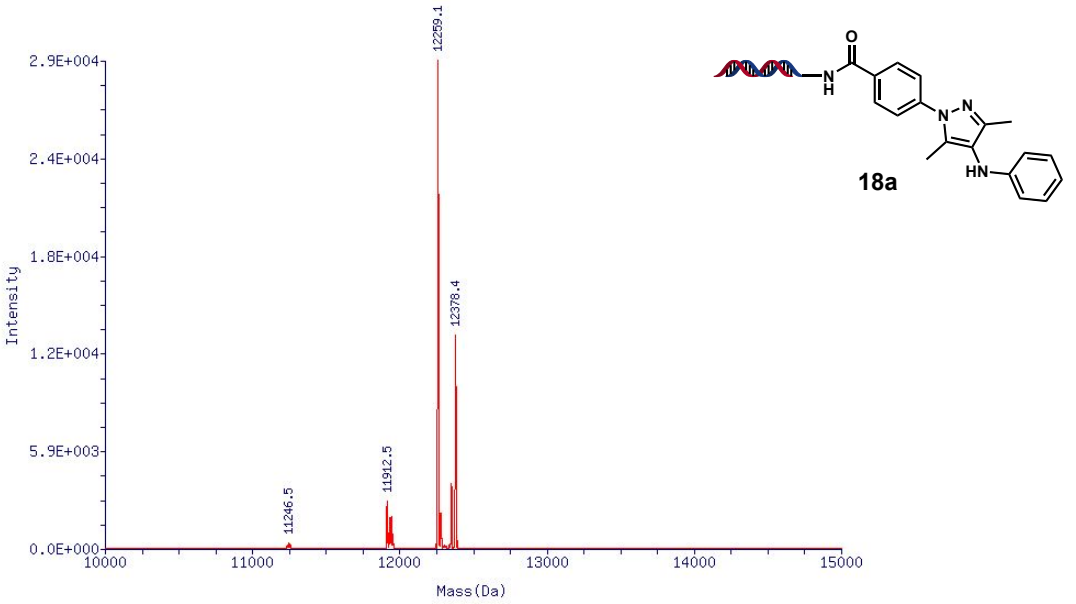


Figure S240. Deconvoluted mass spectrum of DNA **18a**, expected: 12349.3; observed 12350.1.

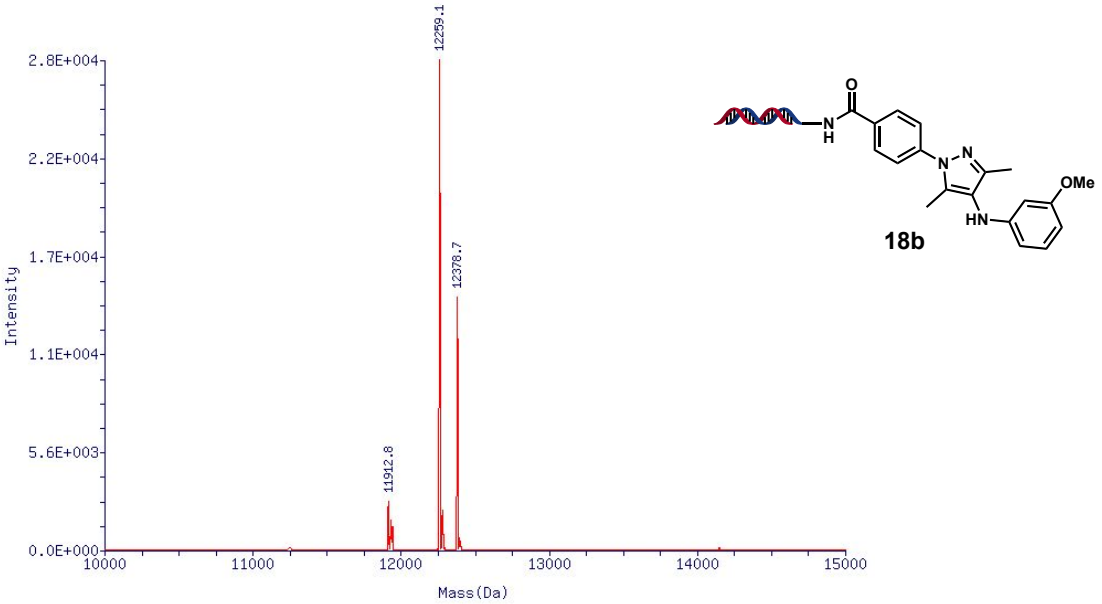


Figure S241. Deconvoluted mass spectrum of DNA **18b**, expected: 12379.4; observed 12378.7.

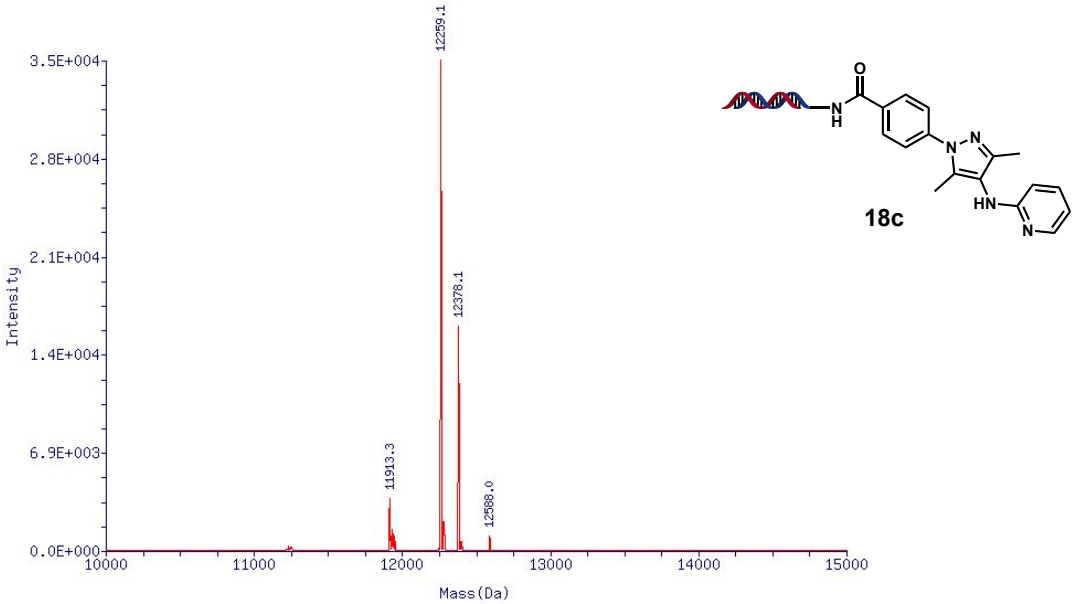


Figure S242. Deconvoluted mass spectrum of DNA **18c**, expected: 12350.3; no product observed.

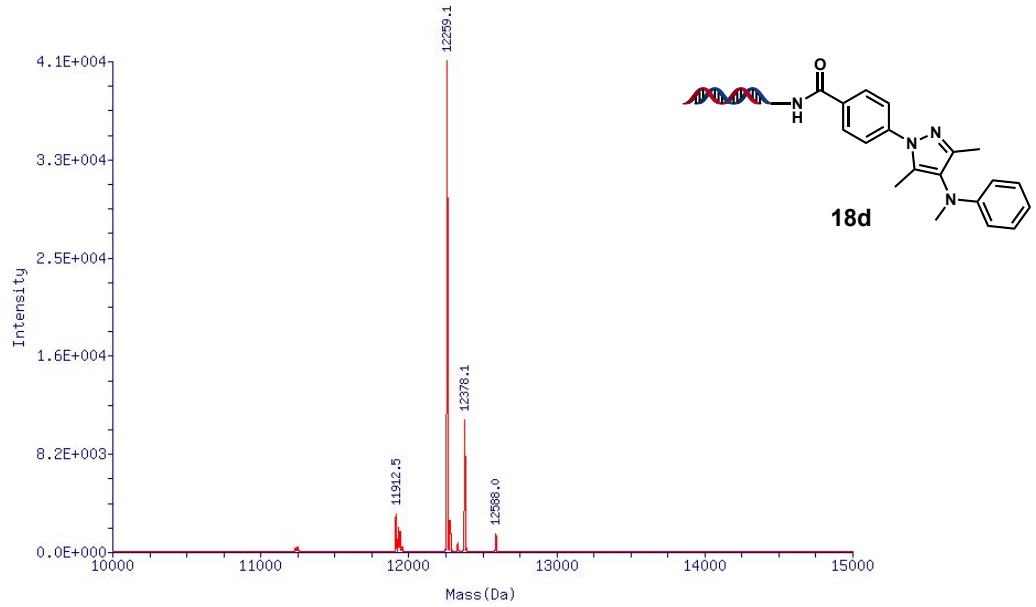


Figure S243. Deconvoluted mass spectrum of DNA **18d**, expected: 12363.4; no product observed.

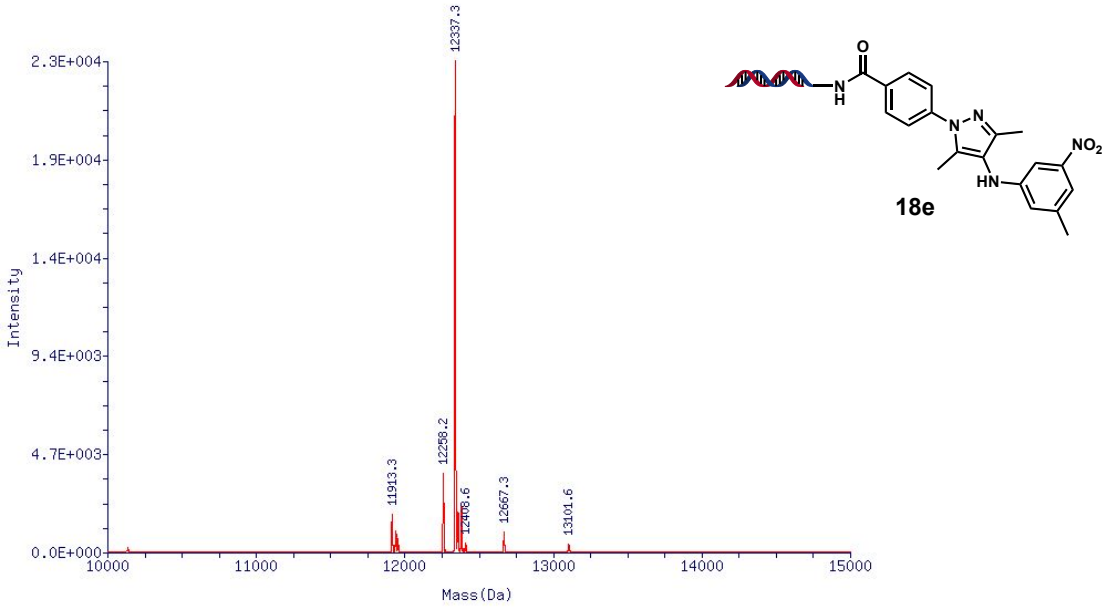


Figure S244. Deconvoluted mass spectrum of DNA **18e**, expected: 12408.4; no product observed.

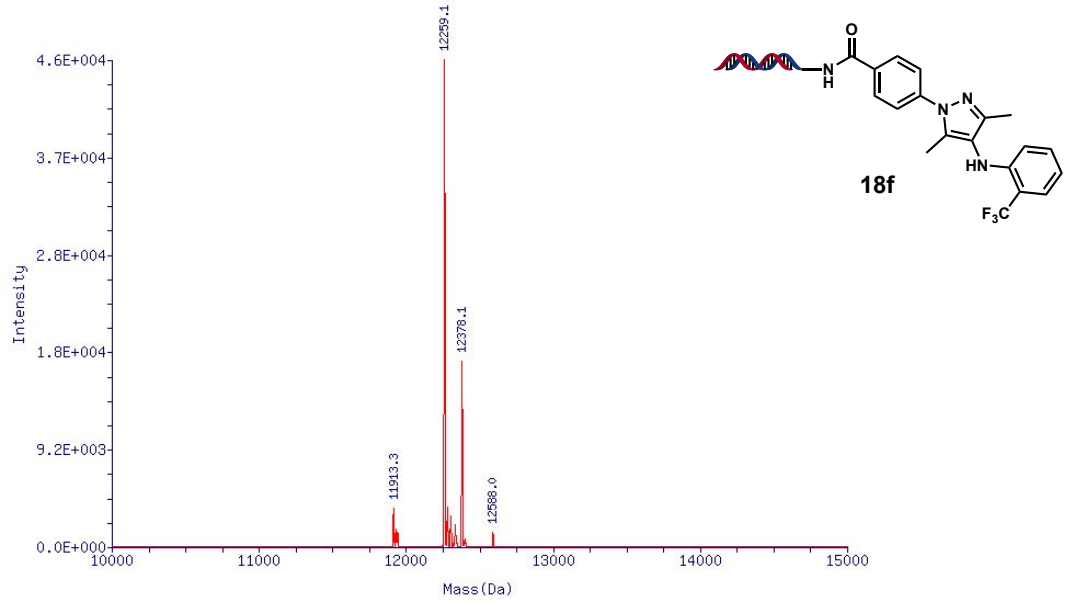


Figure S245. Deconvoluted mass spectrum of DNA **18f**, expected: 12417.3; no product observed.

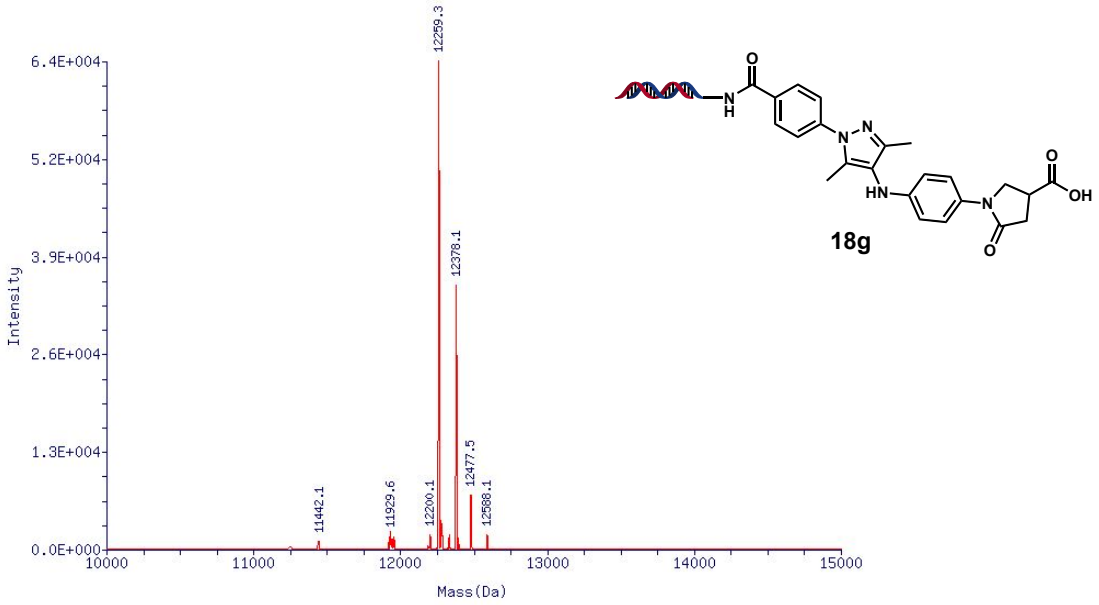


Figure S246. Deconvoluted mass spectrum of DNA **18g**, expected: 12476.4; observed 12477.5.

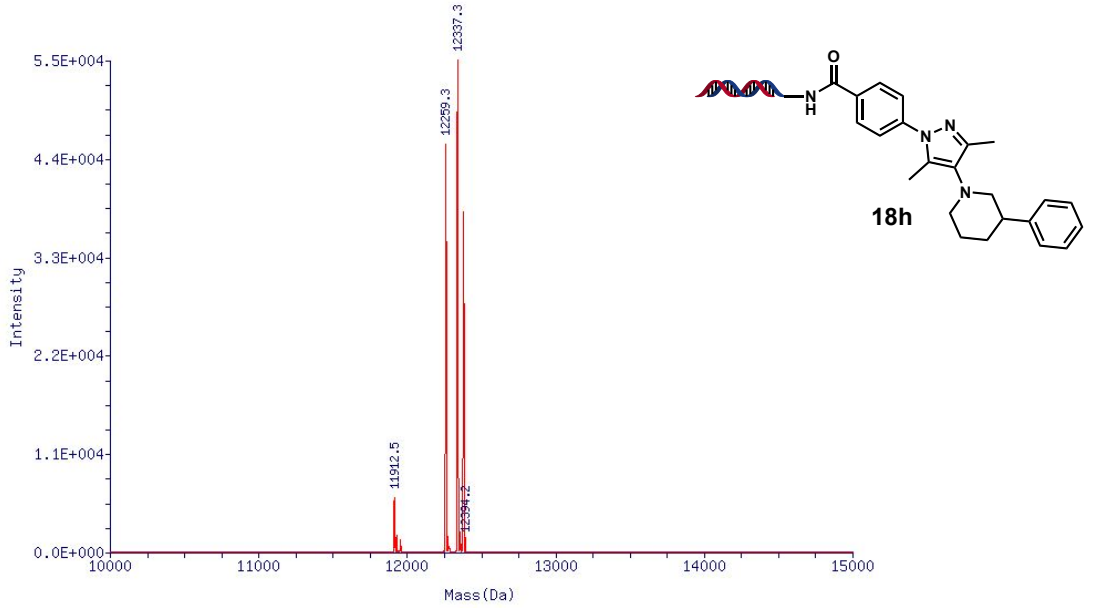


Figure S247. Deconvoluted mass spectrum of DNA **18h**, expected: 12417.5; no product observed.

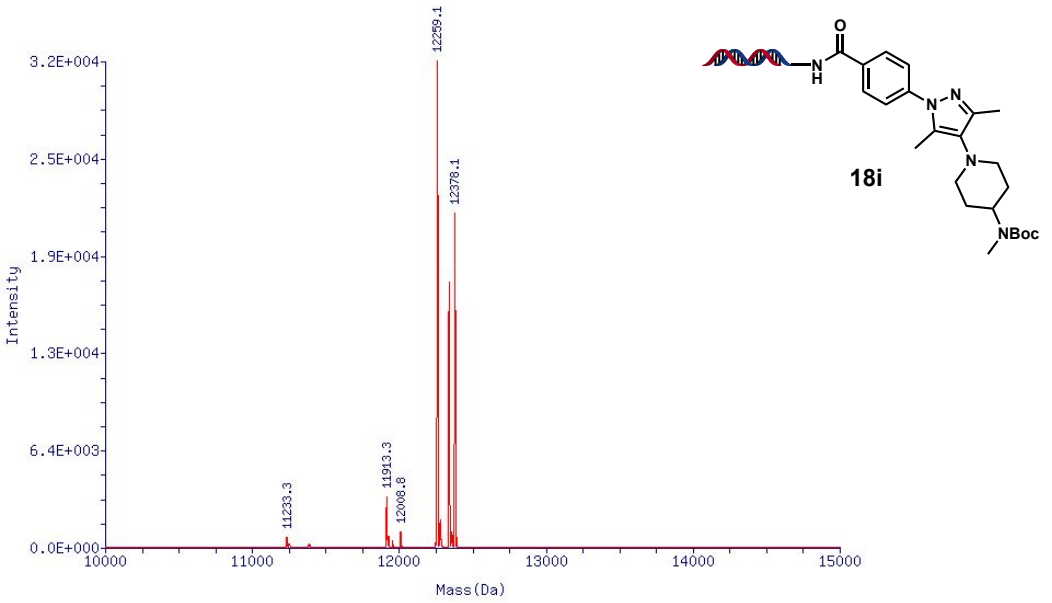


Figure S248. Deconvoluted mass spectrum of DNA **18i**, expected: 12470.5; no product observed.

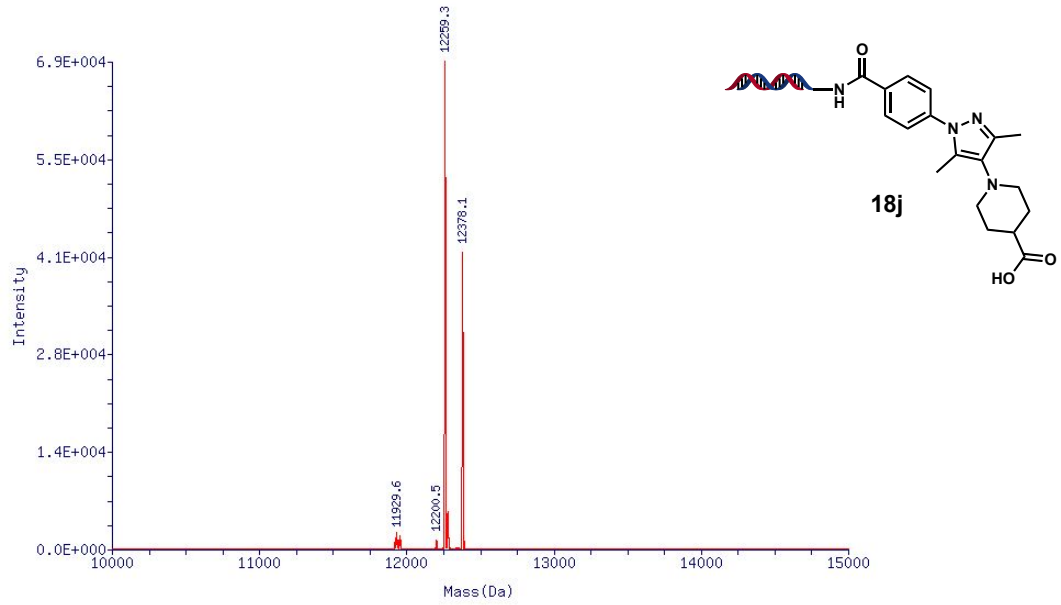


Figure S249. Deconvoluted mass spectrum of DNA **18j**, expected: 12385.4; no product observed.

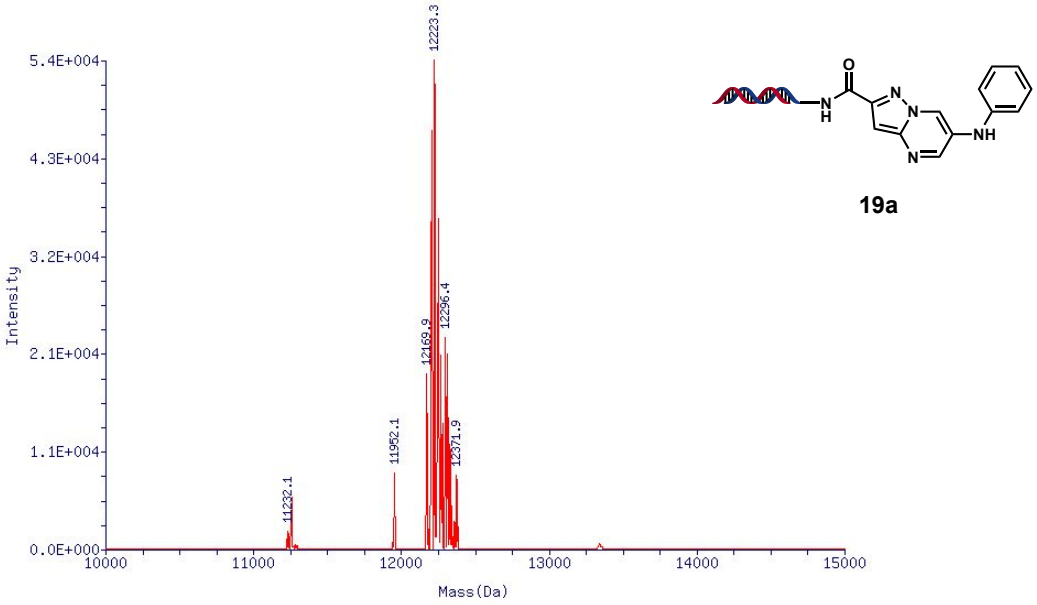


Figure S250. Deconvoluted mass spectrum of DNA **19a**, expected: 12296.2; observed 12296.4.

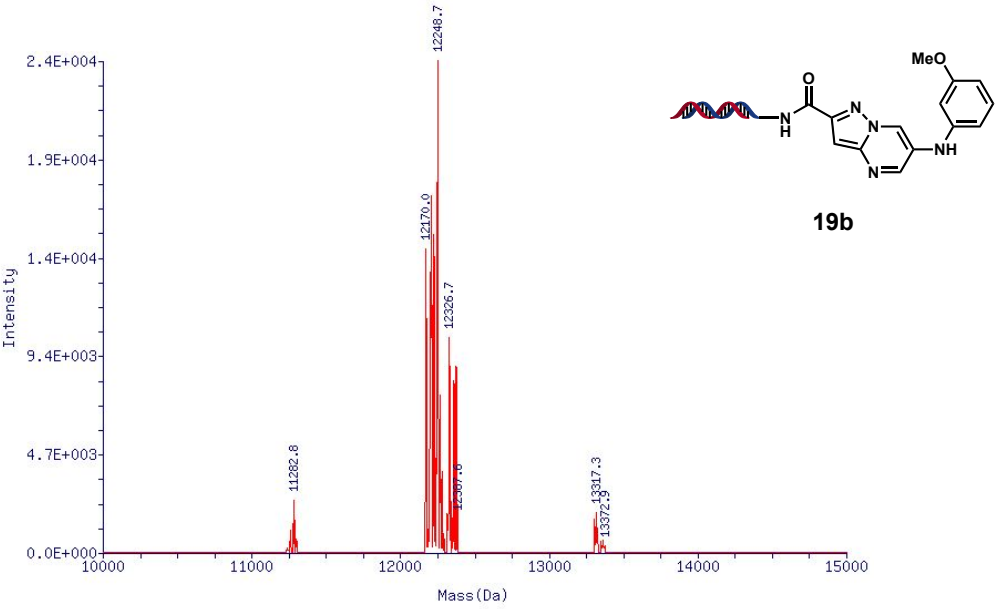


Figure S251. Deconvoluted mass spectrum of DNA **19b**, expected: 12326.3; observed 12326.7.

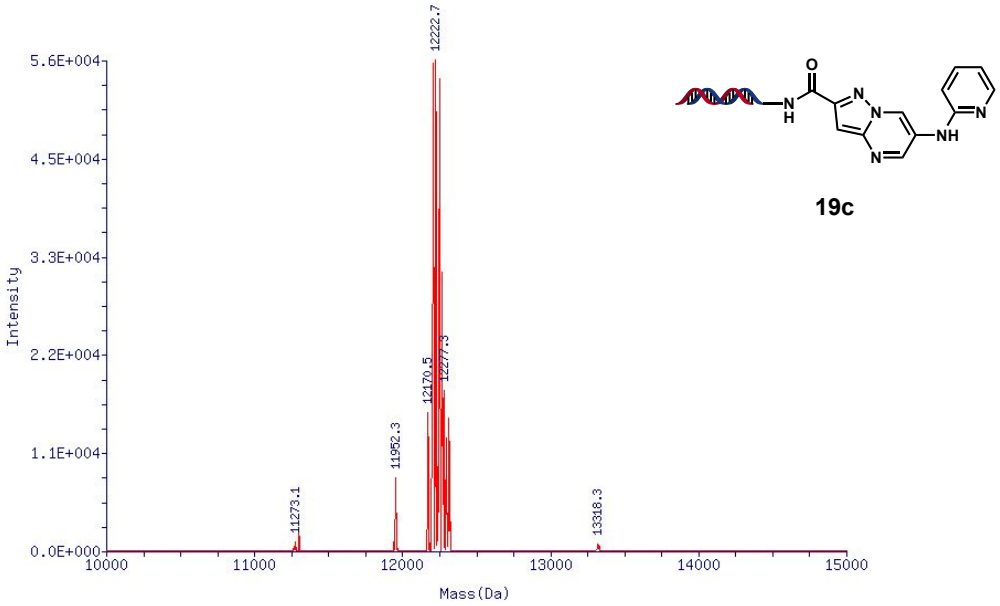


Figure S252. Deconvoluted mass spectrum of DNA **19c**, expected: 12297.2; no product observed.

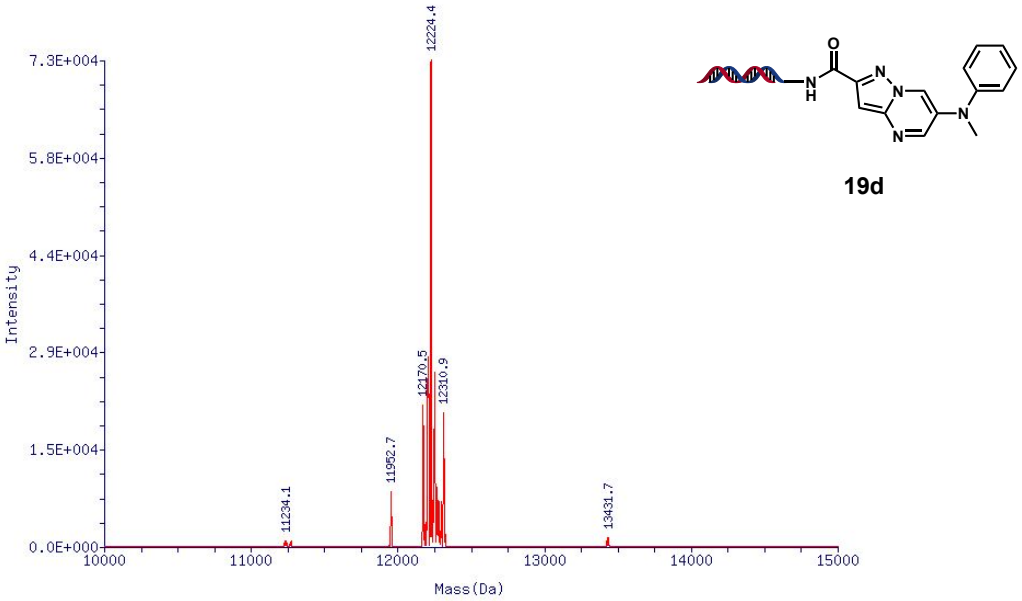


Figure S253. Deconvoluted mass spectrum of DNA **19d**, expected: 12310.3; observed 12310.9.

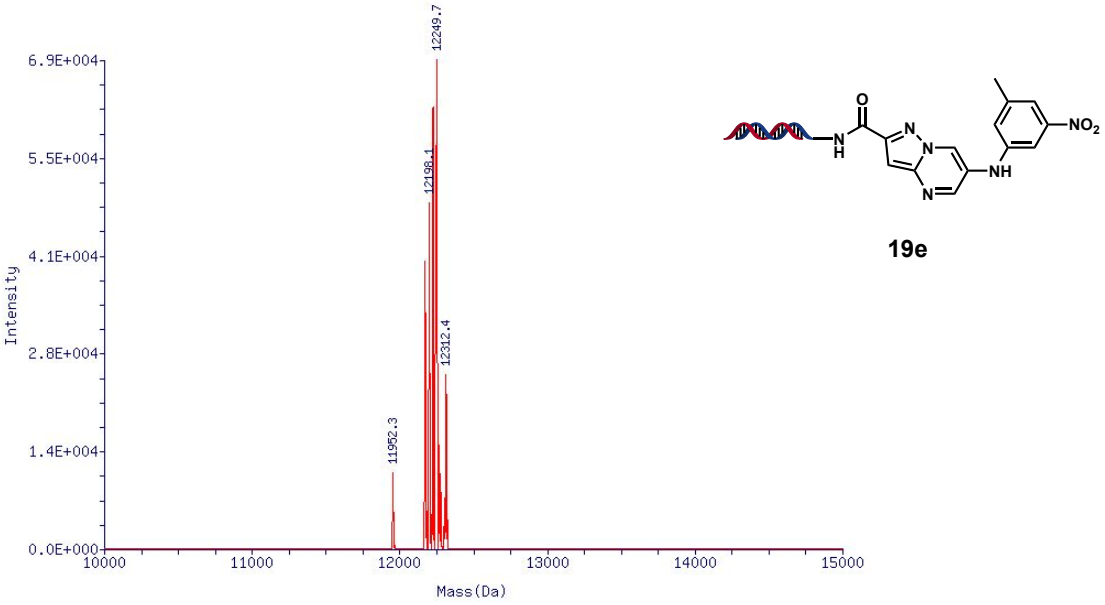


Figure S254. Deconvoluted mass spectrum of DNA **19e**, expected: 12355.3; no product observed.

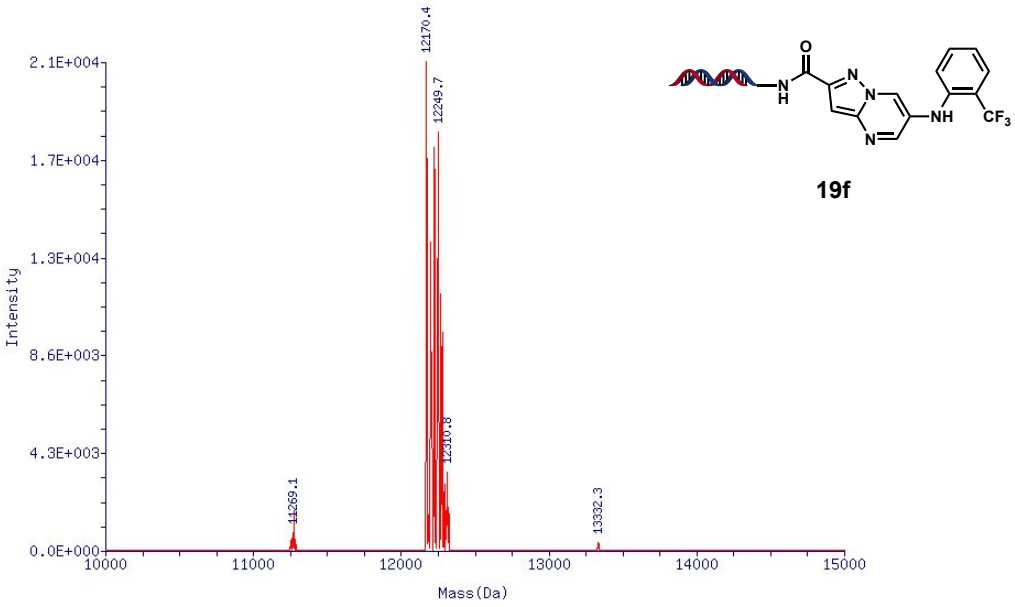


Figure S255. Deconvoluted mass spectrum of DNA **19f**, expected: 12364.2; no product observed.

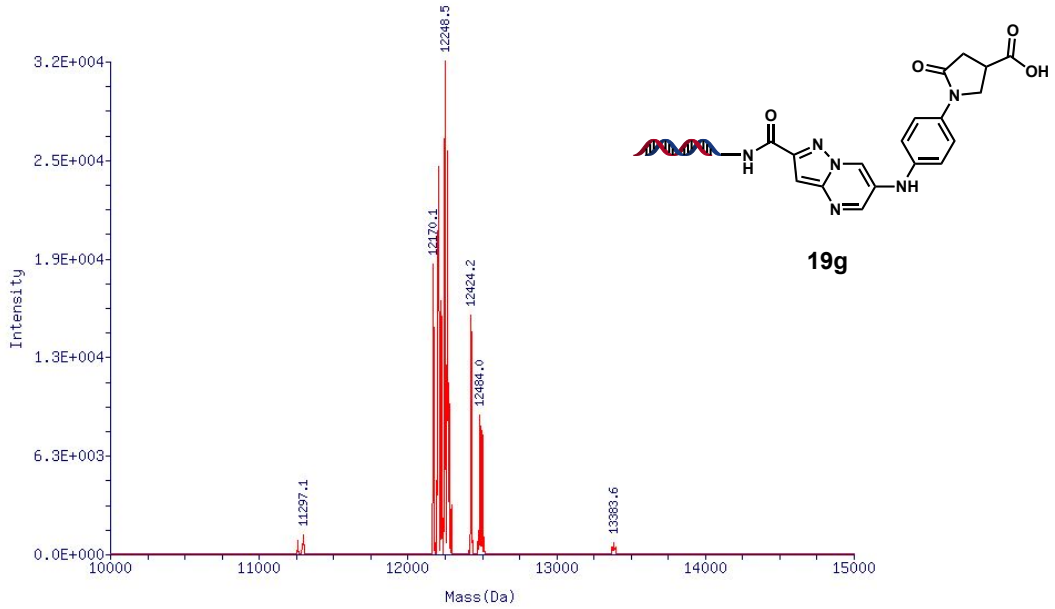


Figure S256. Deconvoluted mass spectrum of DNA **19g**, expected: 12423.3; observed 12424.2.

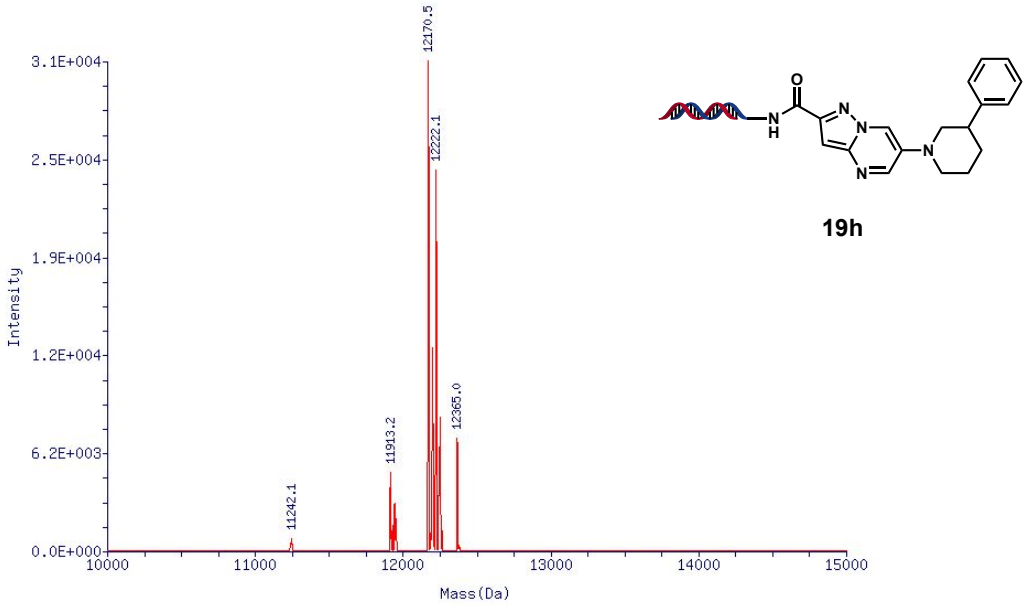
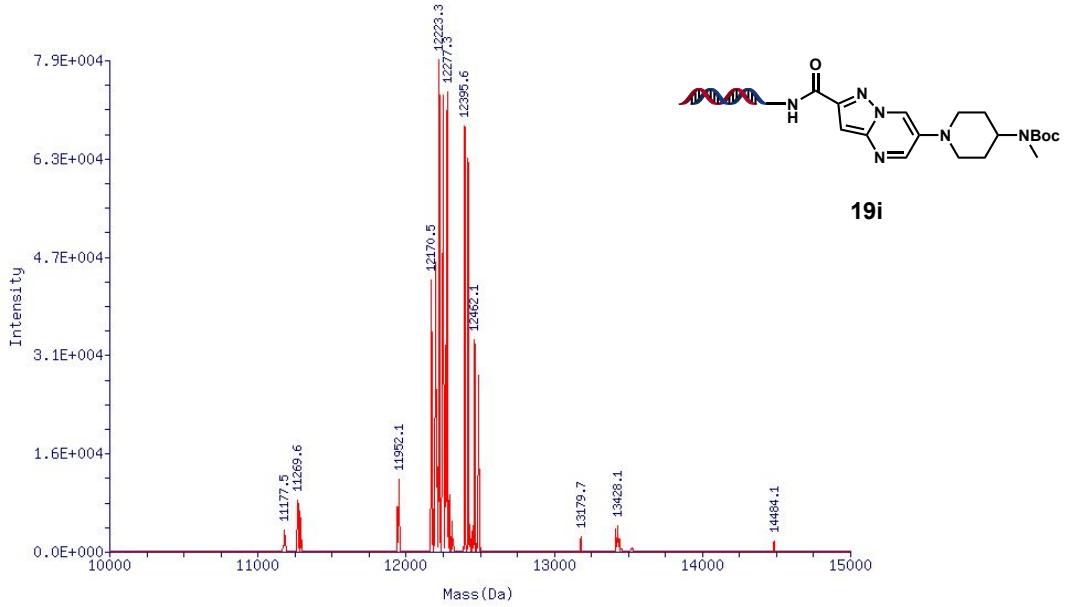
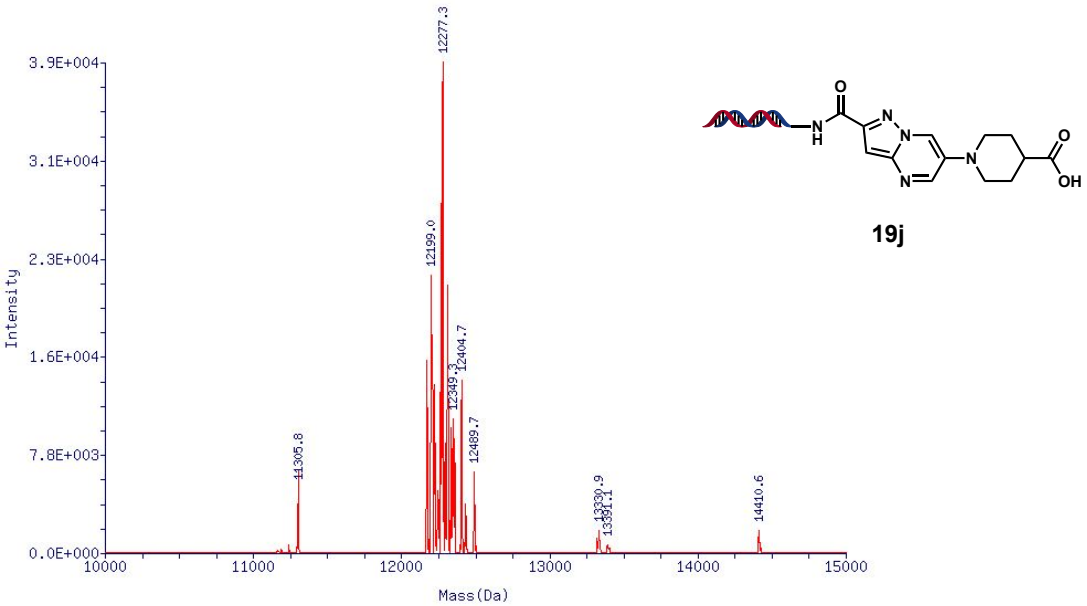


Figure S257. Deconvoluted mass spectrum of DNA **19h**, expected: 12364.4; observed 12365.



19i

Figure S258. Deconvoluted mass spectrum of DNA **19i**, expected: 12417.4; observed 12417.8.



19j

Figure S259. Deconvoluted mass spectrum of DNA **19j**, expected: 12332.3; no product observed.

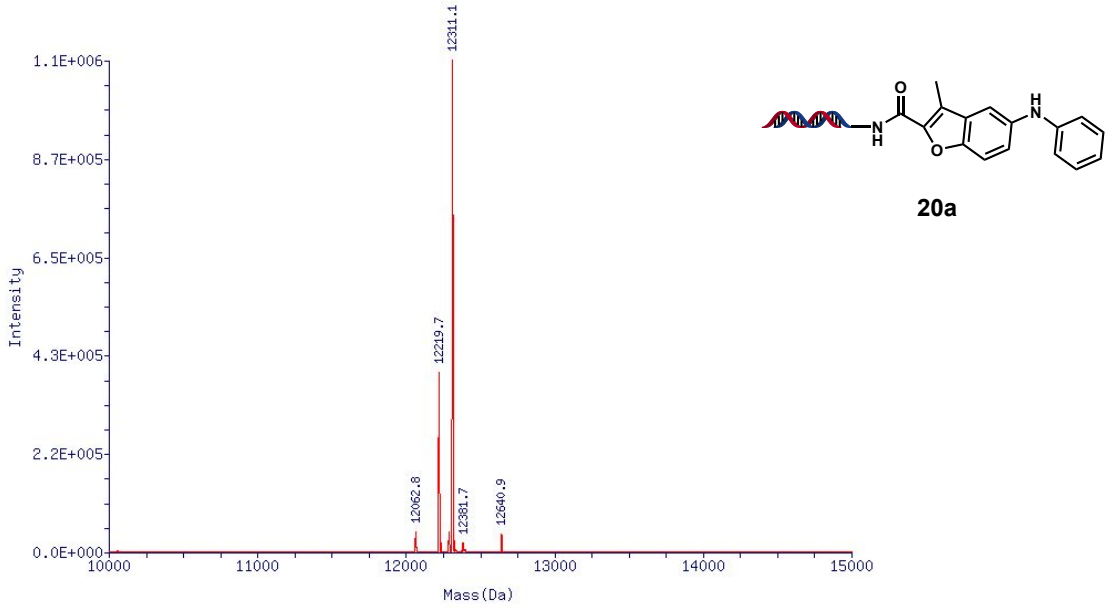


Figure S260. Deconvoluted mass spectrum of DNA **20a**, expected: 12309.3; observed 12311.1.

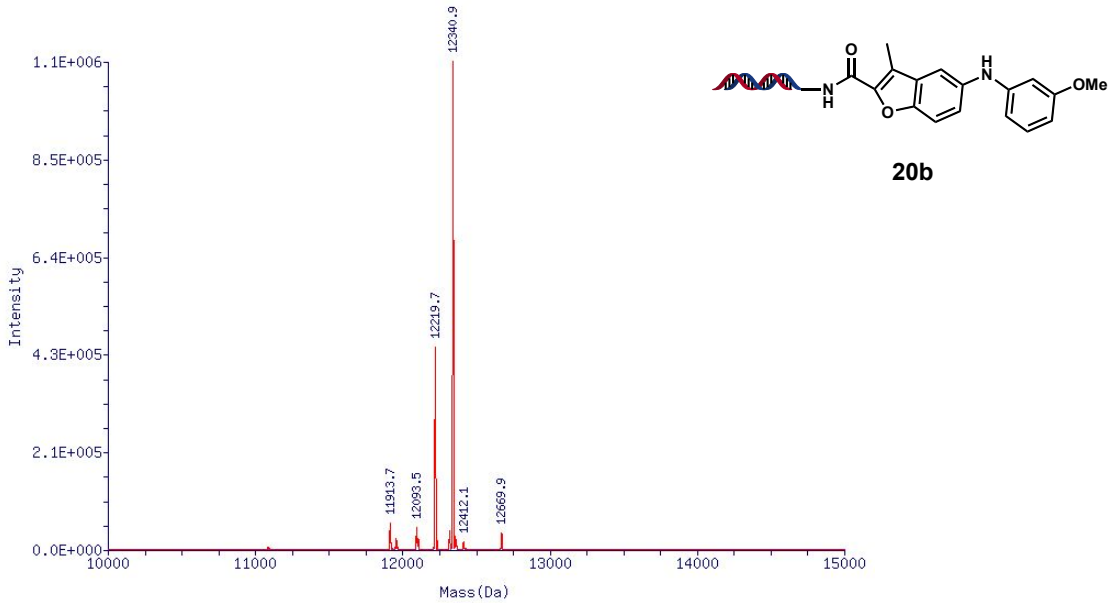


Figure S261. Deconvoluted mass spectrum of DNA **20b**, expected: 12339.3; observed 12340.9.

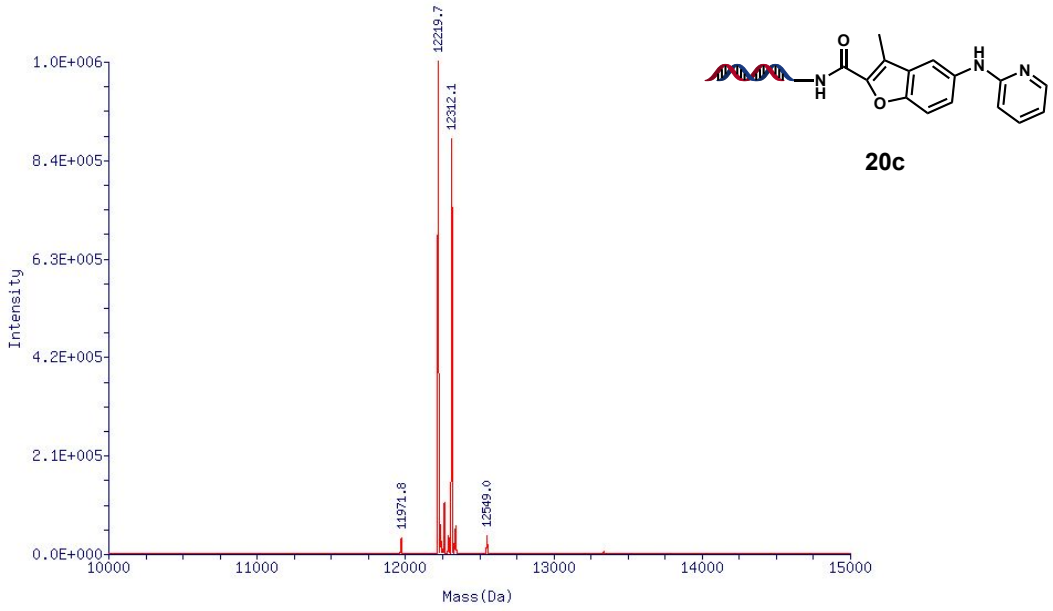


Figure S262. Deconvoluted mass spectrum of DNA **20c**, expected: 12310.3; observed 12312.1.

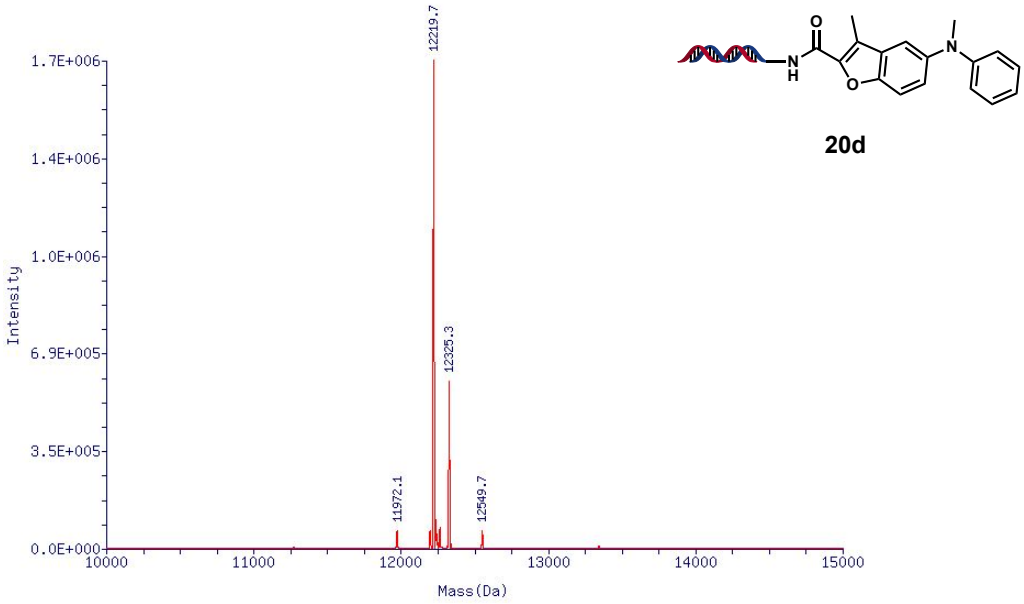


Figure S263. Deconvoluted mass spectrum of DNA **20d**, expected: 12323.3; observed 12325.3.

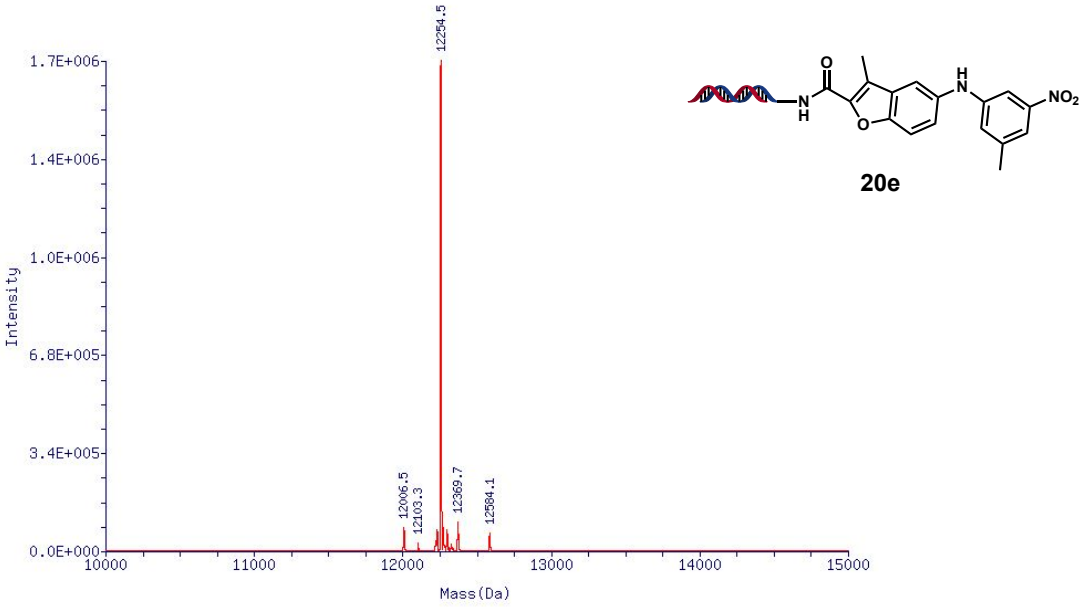


Figure S264. Deconvoluted mass spectrum of DNA **20e**, expected: 12368.3; observed 12369.7.

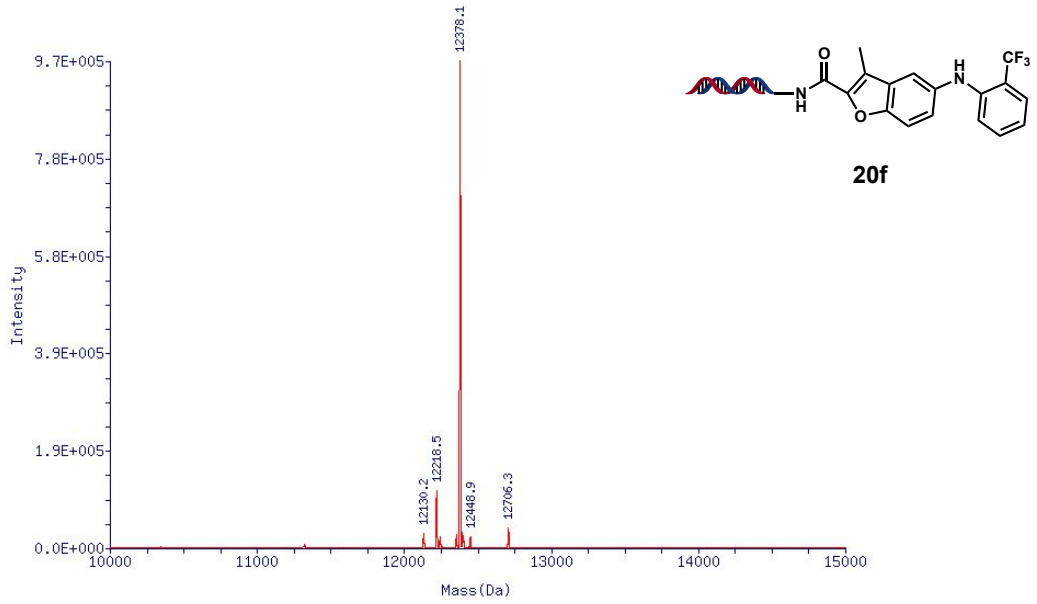


Figure S265. Deconvoluted mass spectrum of DNA **20f**, expected: 12377.3; observed 12378.1.

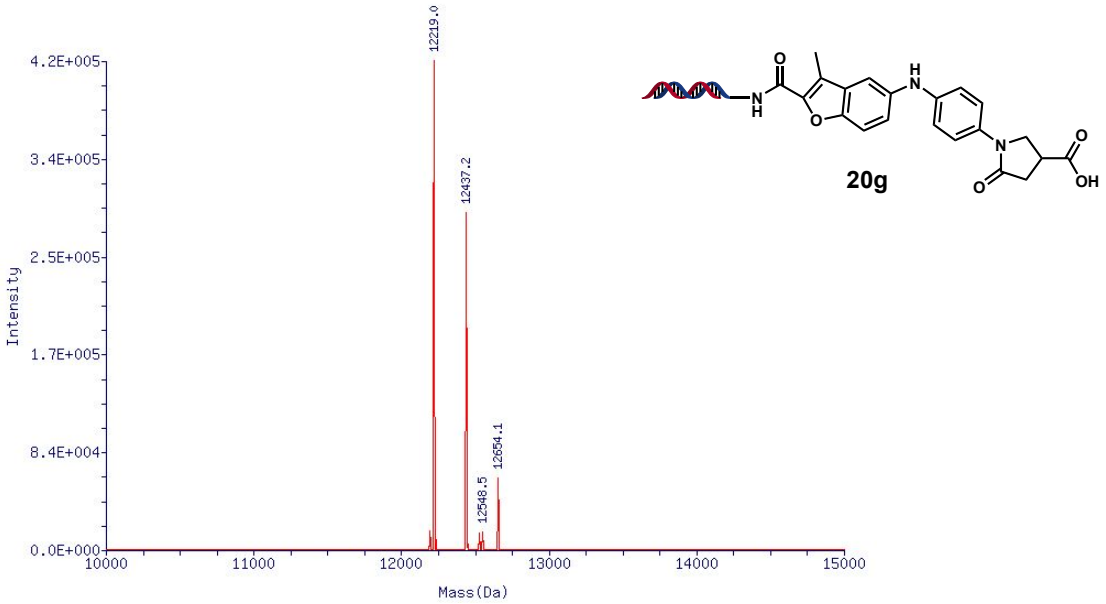


Figure S266. Deconvoluted mass spectrum of DNA **20g**, expected: 12436.3; observed 12437.2.

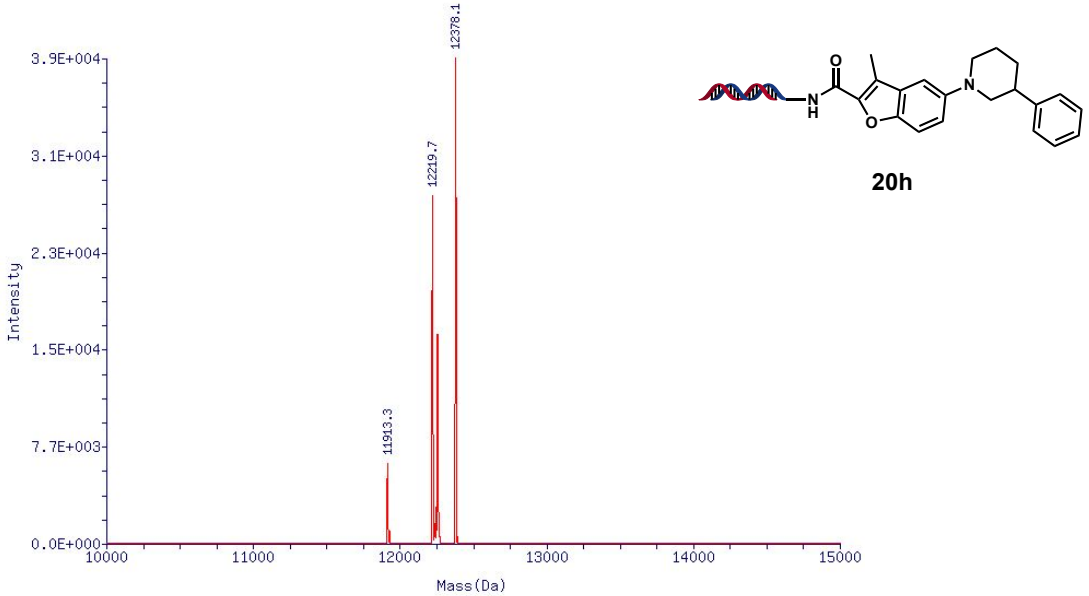


Figure S267. Deconvoluted mass spectrum of DNA **20h**, expected: 12377.4; observed 12378.1.

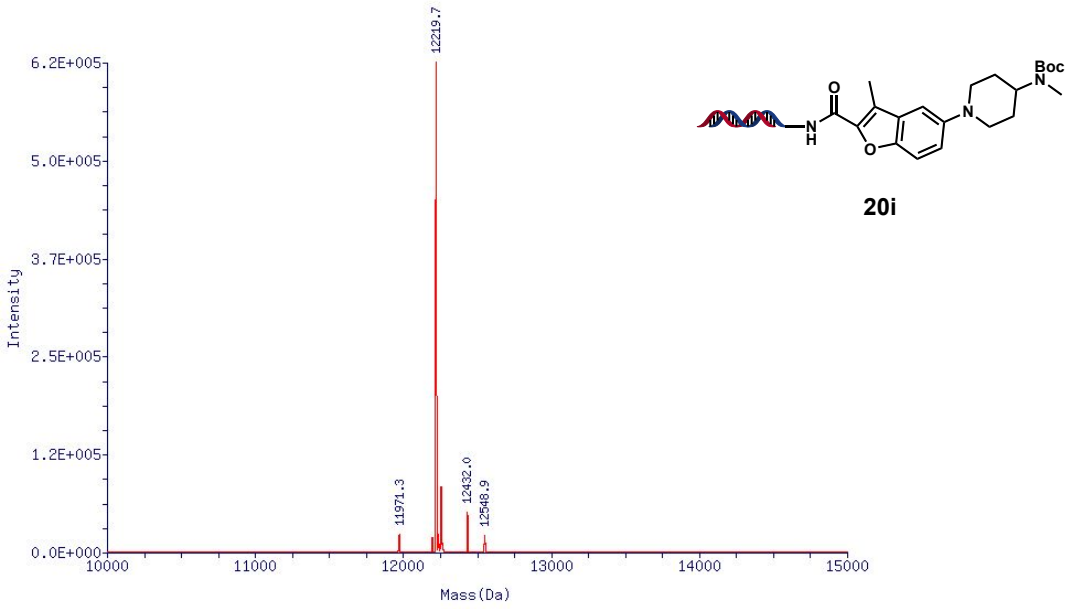


Figure S268. Deconvoluted mass spectrum of DNA **20i**, expected: 12430.5; observed 12432.

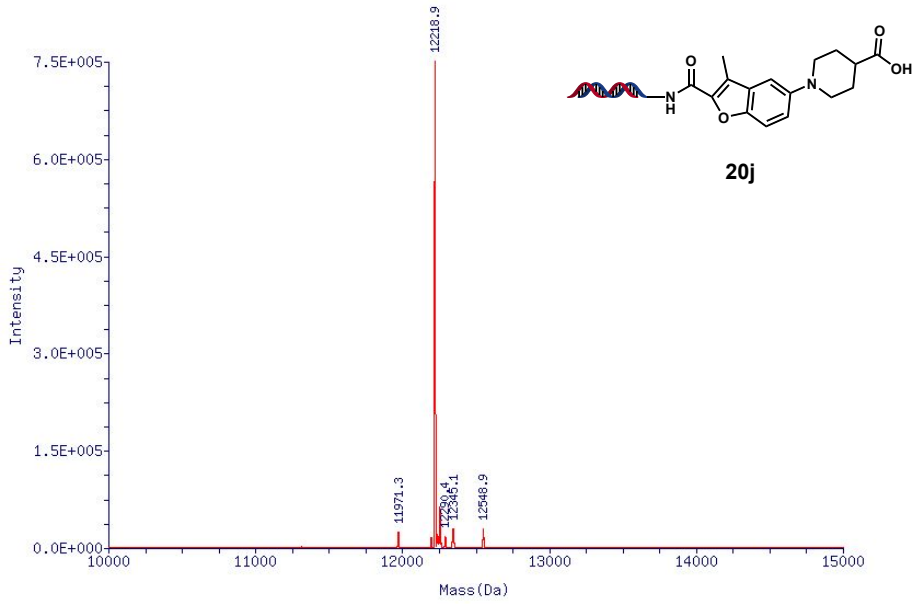


Figure S269. Deconvoluted mass spectrum of DNA **20j**, expected: 12345.3; no product observed.

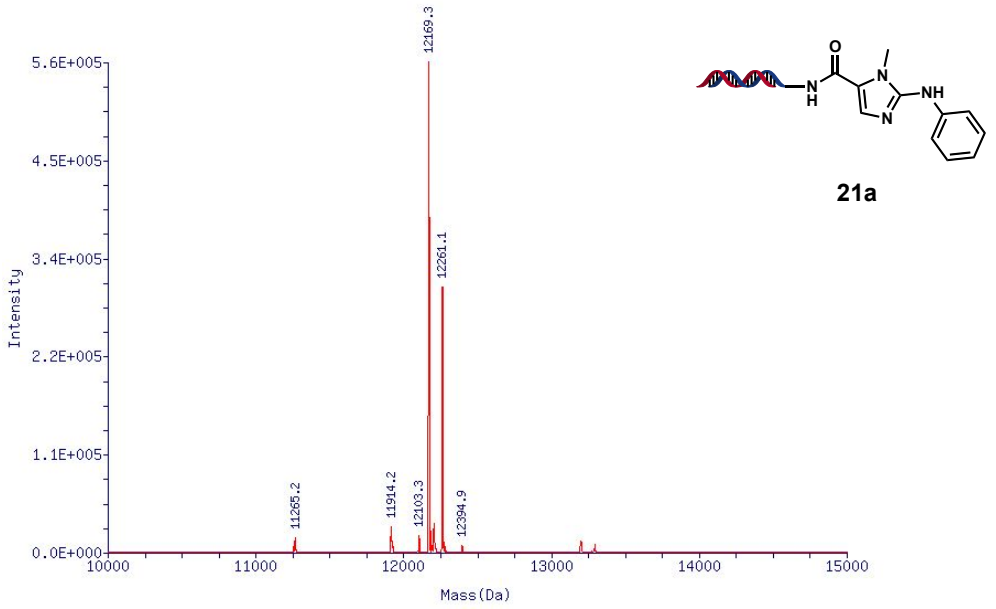


Figure S270. Deconvoluted mass spectrum of DNA **21a**, expected: 12259.2; observed 12261.1.

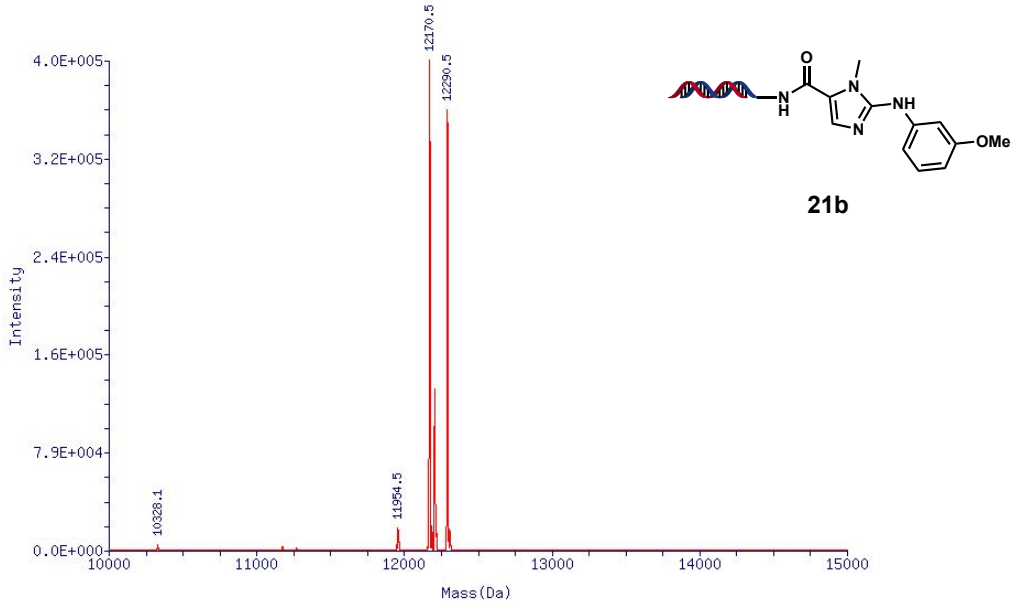


Figure S271. Deconvoluted mass spectrum of DNA **21b**, expected: 12289.2; observed 12290.5.

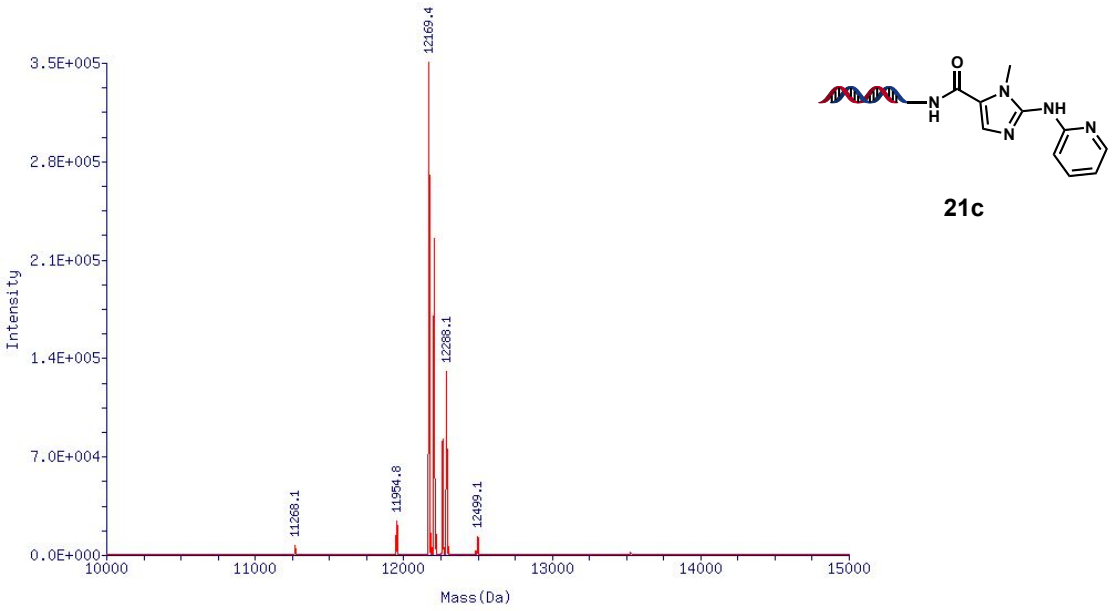


Figure S272. Deconvoluted mass spectrum of DNA **21c**, expected: 12260.2; observed 12261.8.

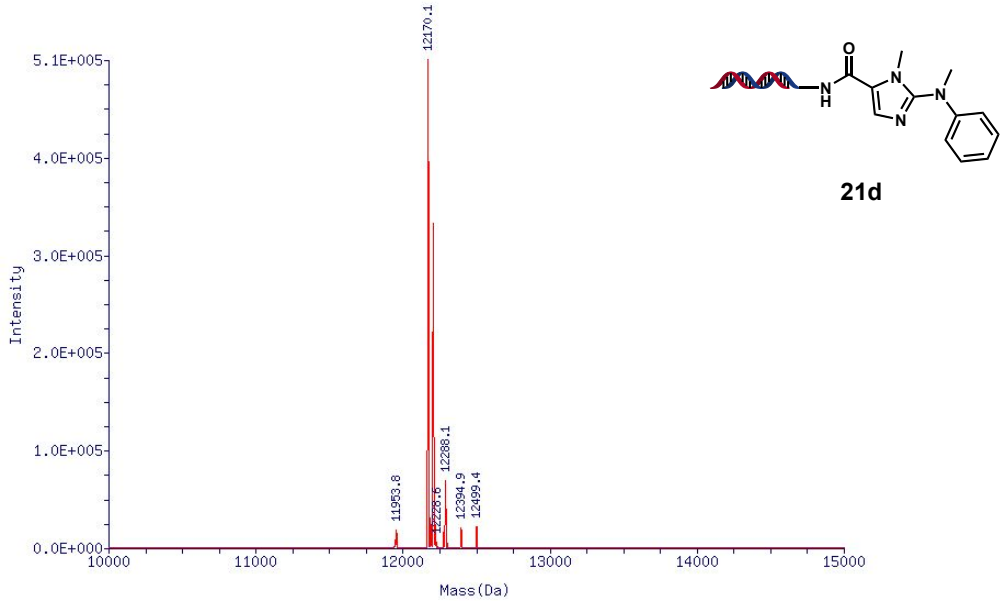


Figure S273. Deconvoluted mass spectrum of DNA **21d**, expected: 12273.2; no product observed.

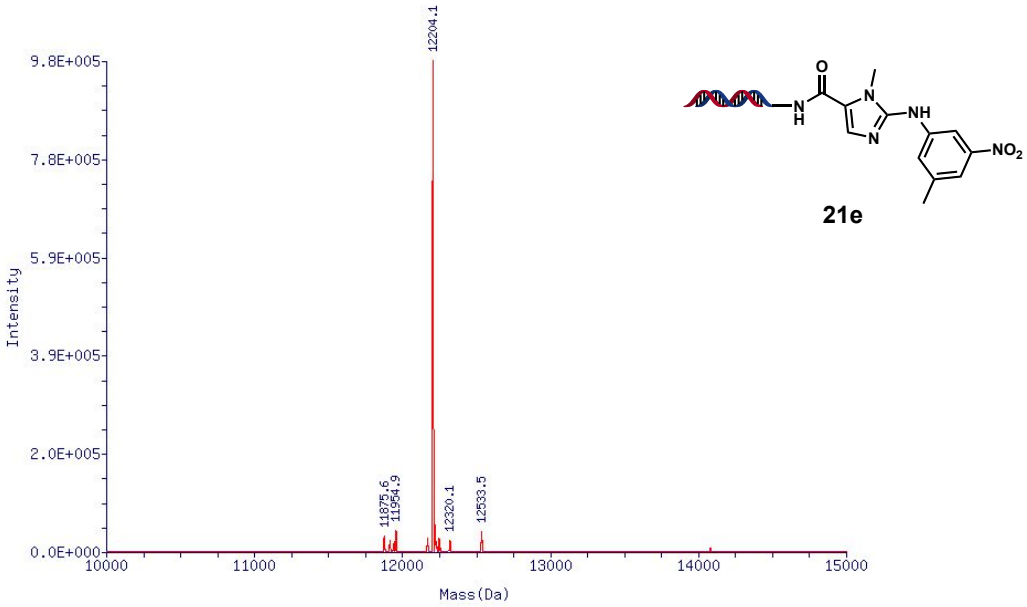


Figure S274. Deconvoluted mass spectrum of DNA **21e**, expected: 12318.2; no product observed.

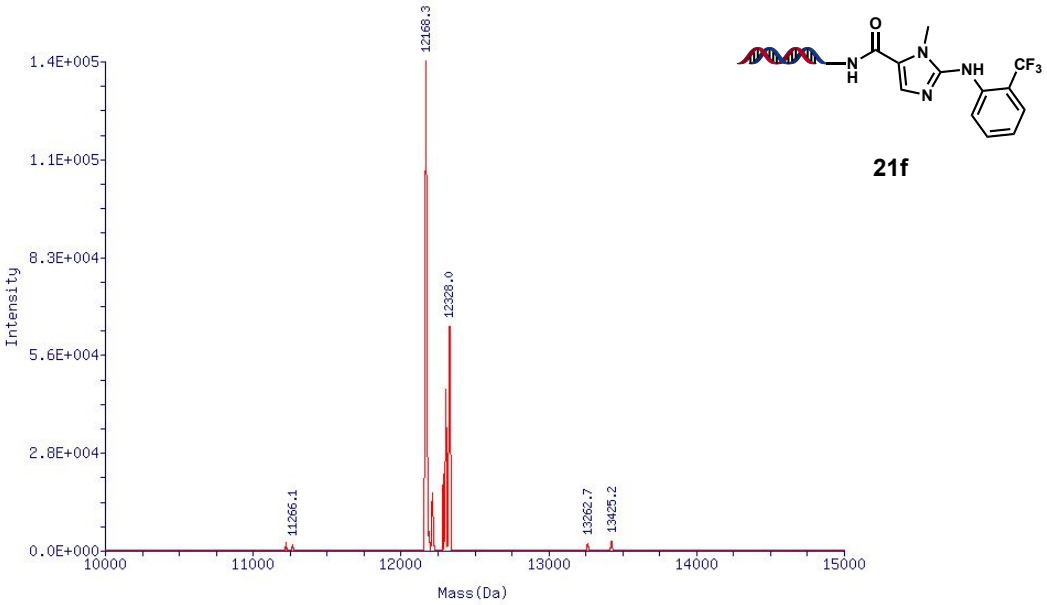


Figure S275. Deconvoluted mass spectrum of DNA **21f**, expected: 12327.2; observed 12328.

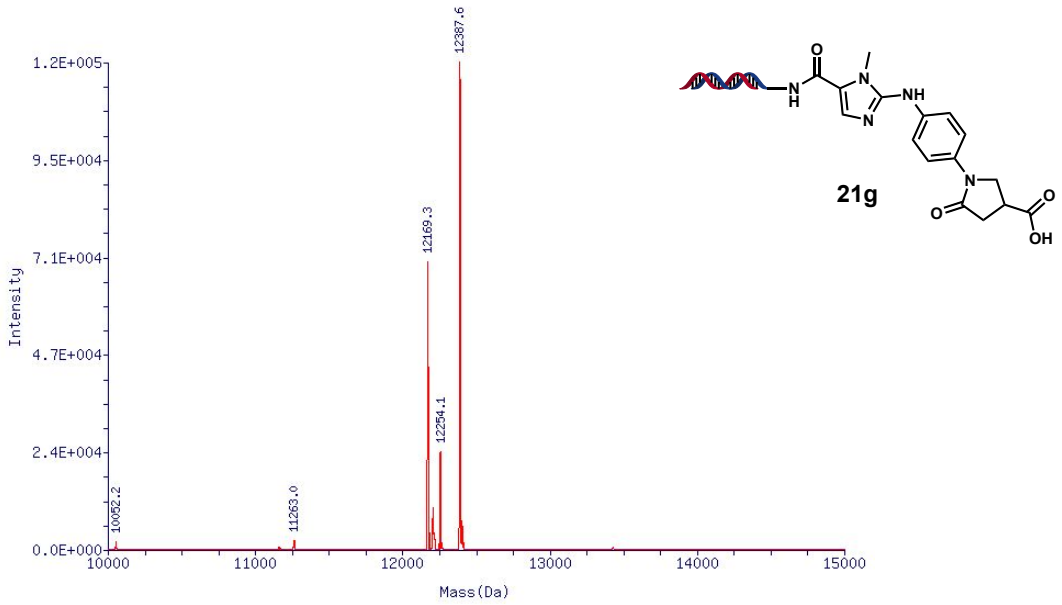


Figure S276. Deconvoluted mass spectrum of DNA **21g**, expected: 12386.2; observed 12387.6.

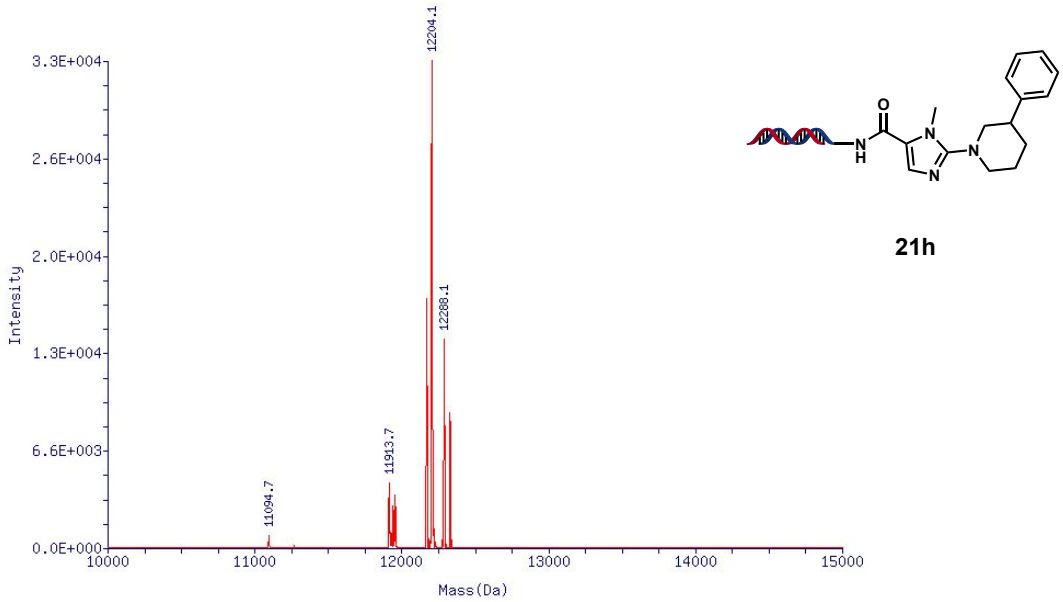


Figure S277. Deconvoluted mass spectrum of DNA **21h**, expected: 12327.3; observed 12327.7.

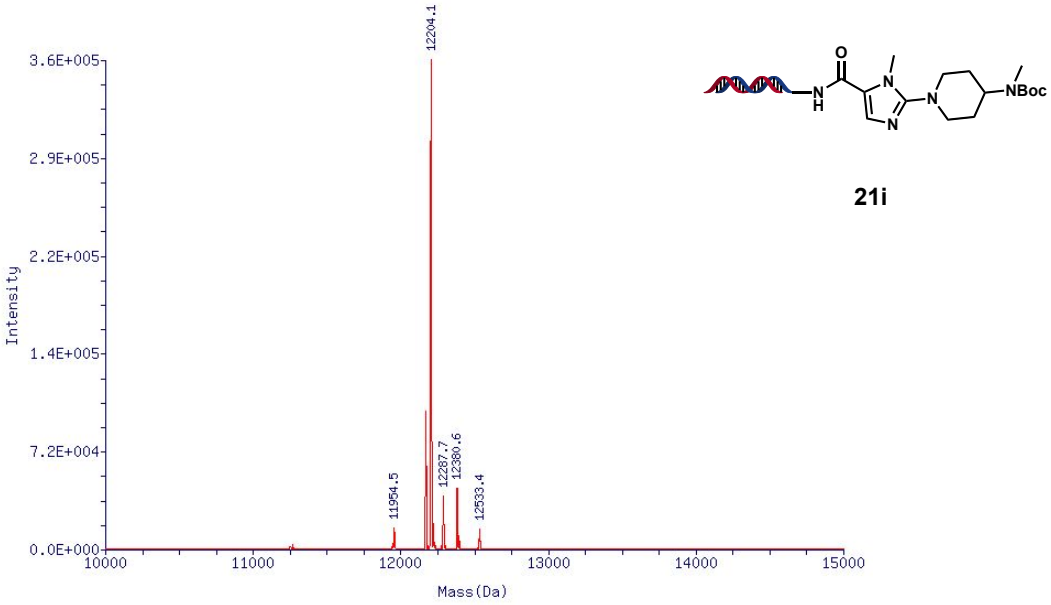


Figure S278. Deconvoluted mass spectrum of DNA **21i**, expected: 12380.4; observed 12380.6.

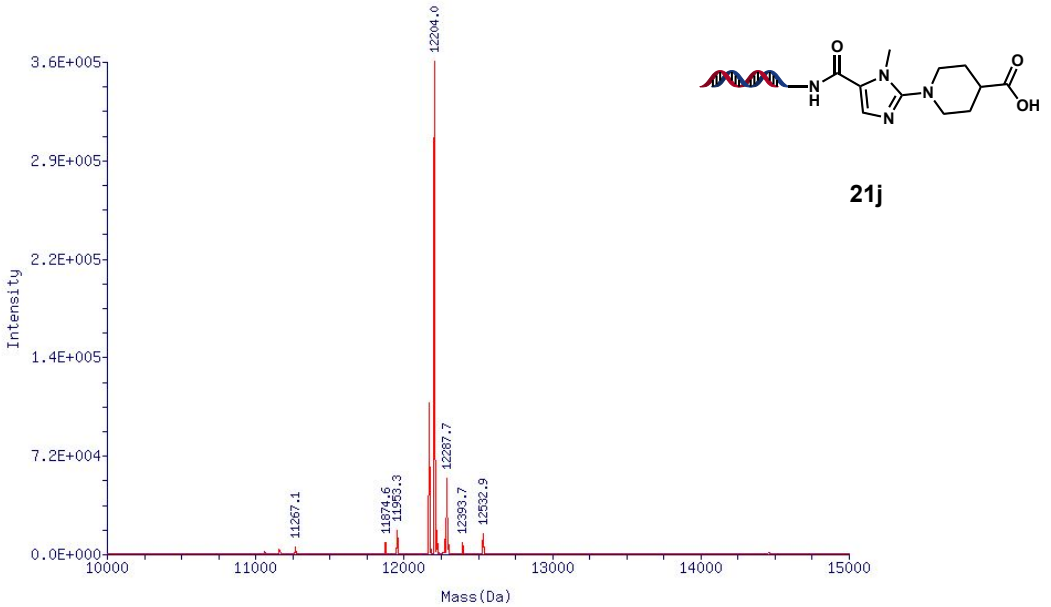


Figure S279. Deconvoluted mass spectrum of DNA **21j**, expected: 12295.2; no product observed.

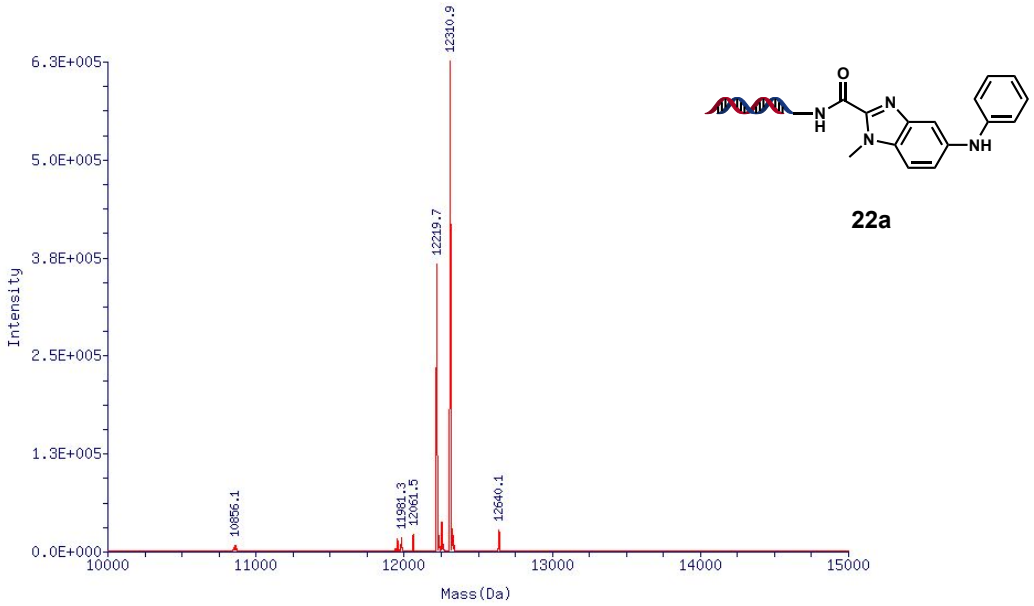


Figure S280. Deconvoluted mass spectrum of DNA **22a**, expected: 12309.3; observed 12310.9.

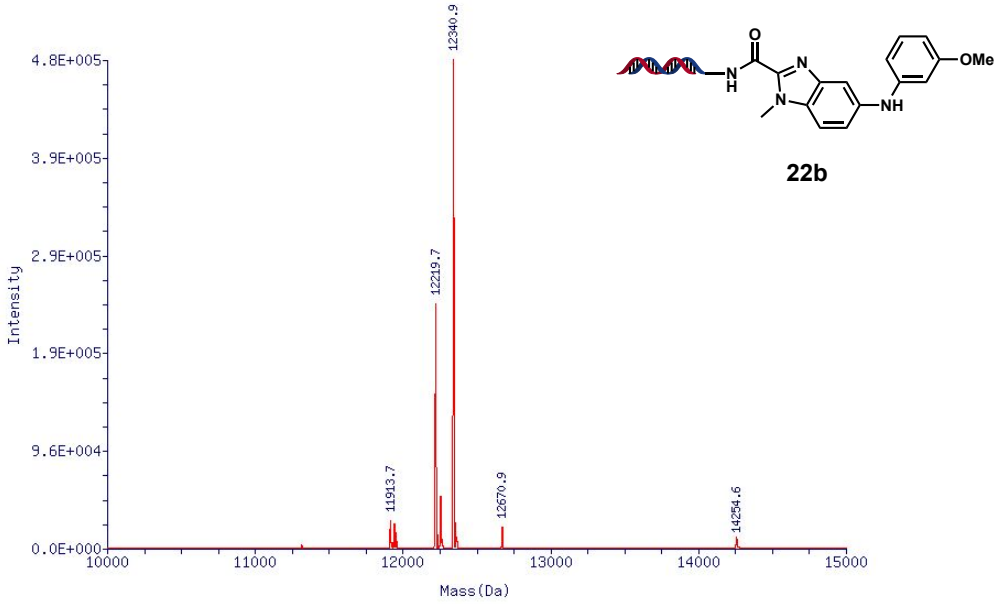


Figure S281. Deconvoluted mass spectrum of DNA **22b**, expected: 12339.3; observed 12340.9.

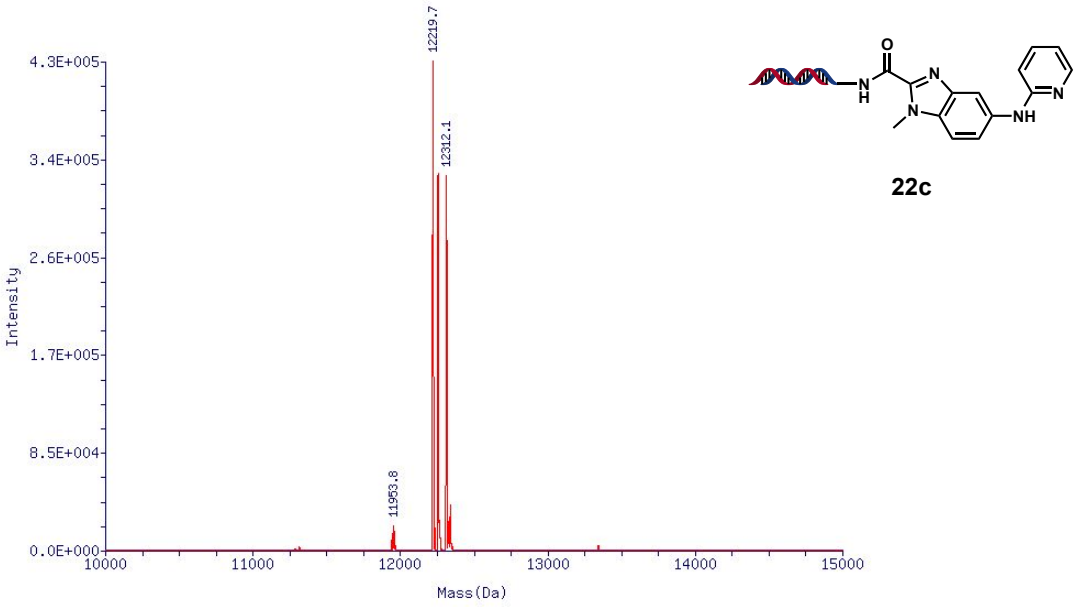


Figure S282. Deconvoluted mass spectrum of DNA **22c**, expected: 12310.3; observed 12312.1.

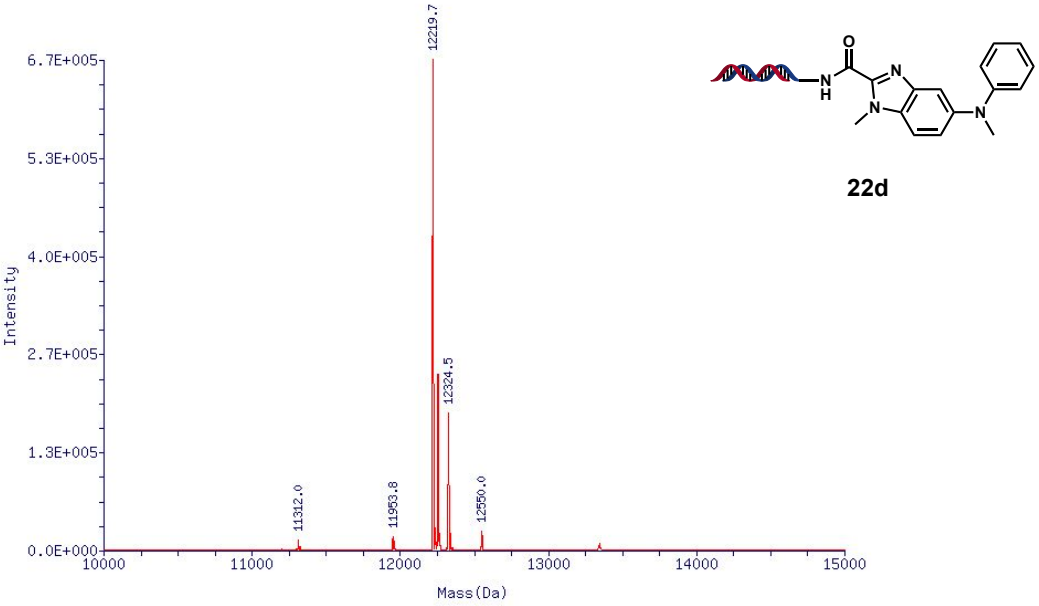


Figure S283. Deconvoluted mass spectrum of DNA **22d**, expected: 12323.3; observed 12324.5.

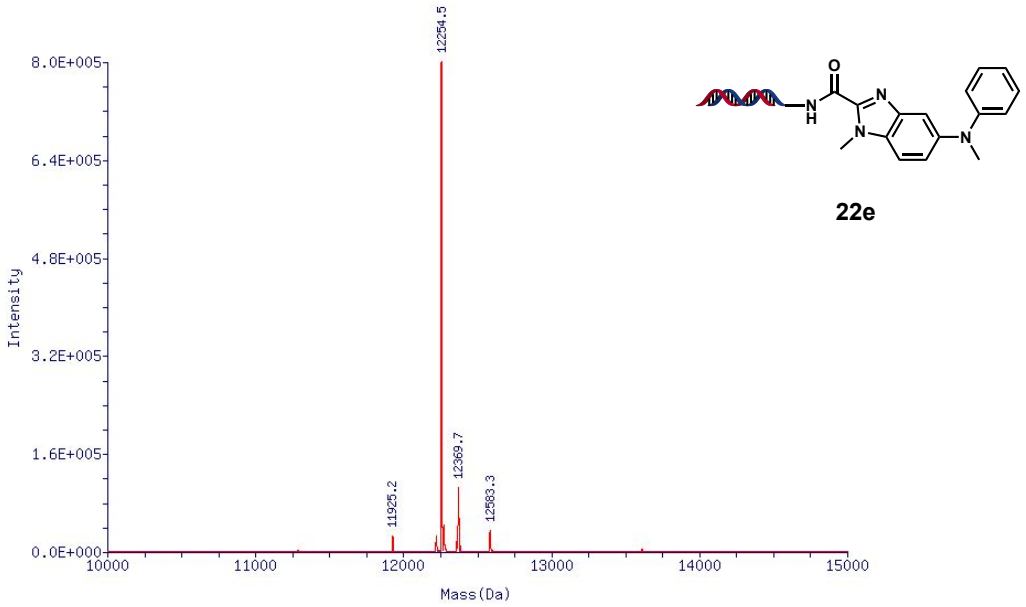


Figure S284. Deconvoluted mass spectrum of DNA **22e**, expected: 12368.3; observed 12369.7.

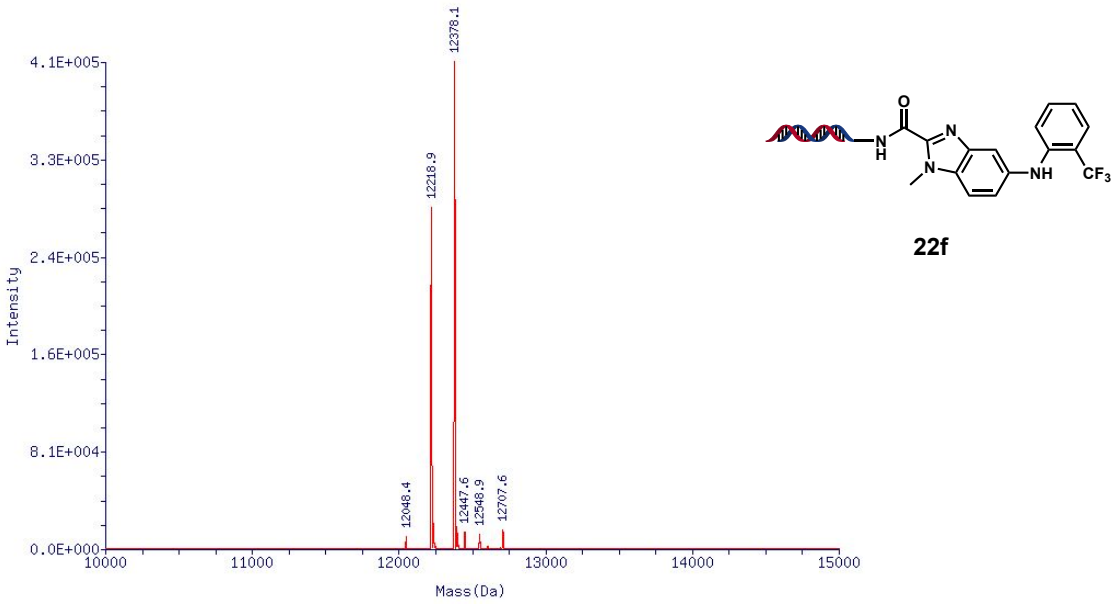


Figure S285. Deconvoluted mass spectrum of DNA **22f**, expected: 12377.3; observed 12378.1.

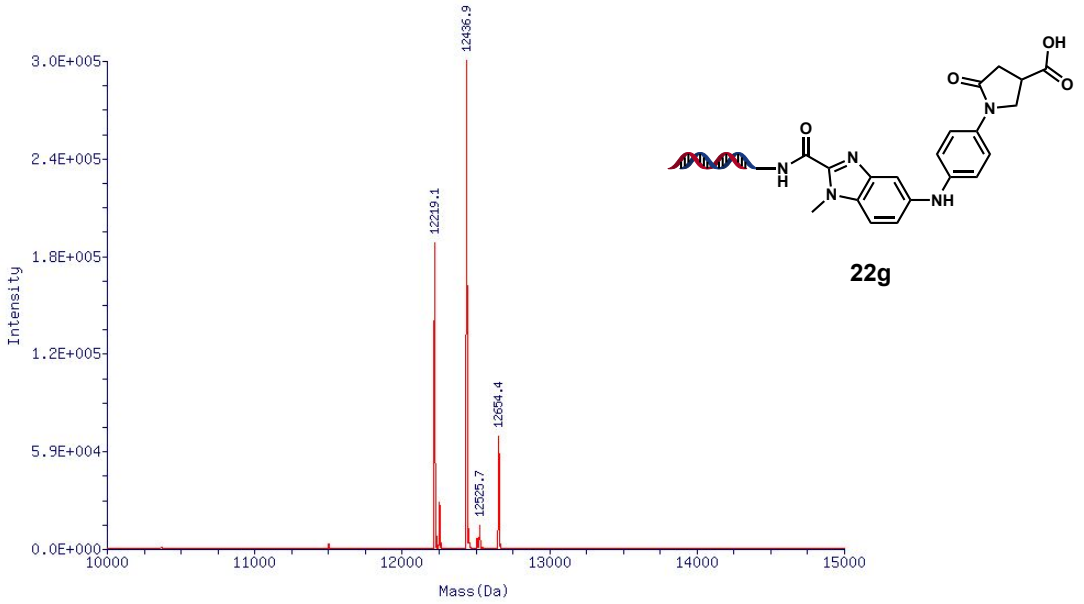


Figure S286. Deconvoluted mass spectrum of DNA **22g**, expected: 12436.3; observed 12436.9.

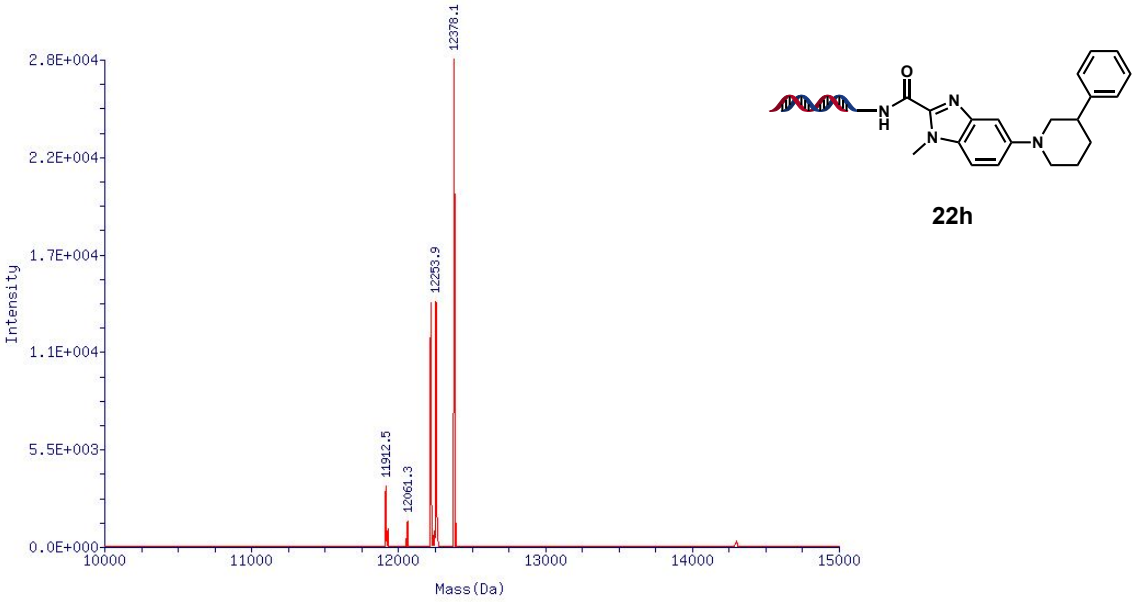


Figure S287. Deconvoluted mass spectrum of DNA **22h**, expected: 12377.4; observed 12378.1.

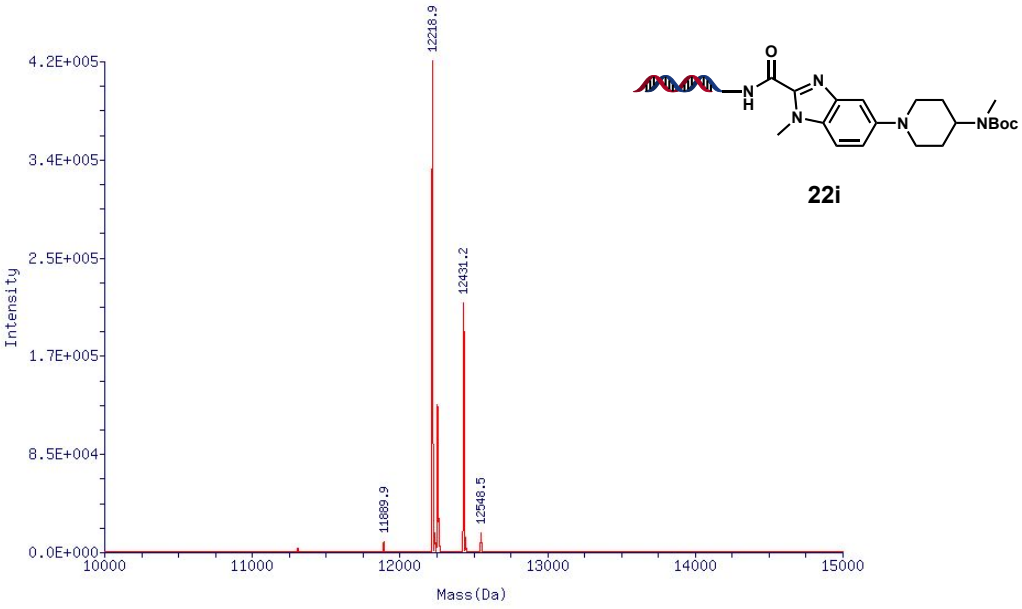


Figure S288. Deconvoluted mass spectrum of DNA **22i**, expected: 12430.5; observed 12431.2.

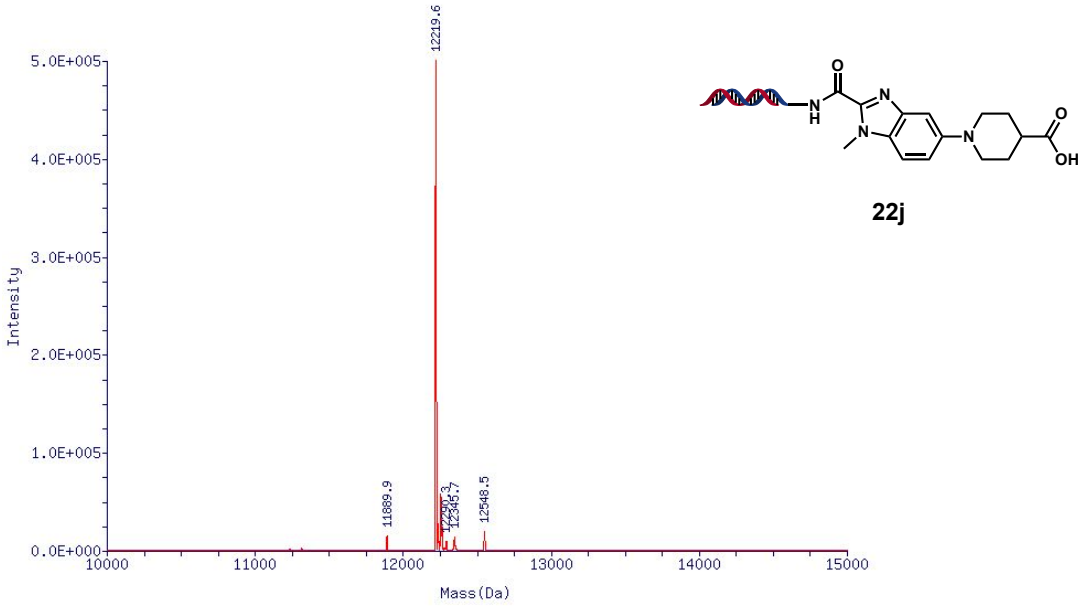


Figure S289. Deconvoluted mass spectrum of DNA **22j**, expected: 12345.3; no product observed.

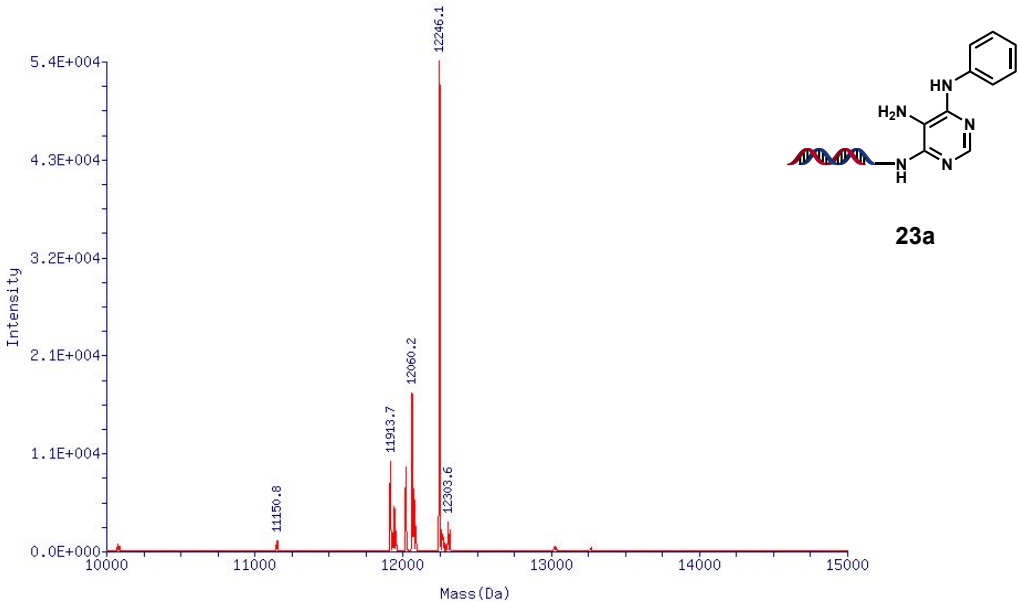


Figure S290. Deconvoluted mass spectrum of DNA **23a**, expected: 12244.2; observed 12246.1.

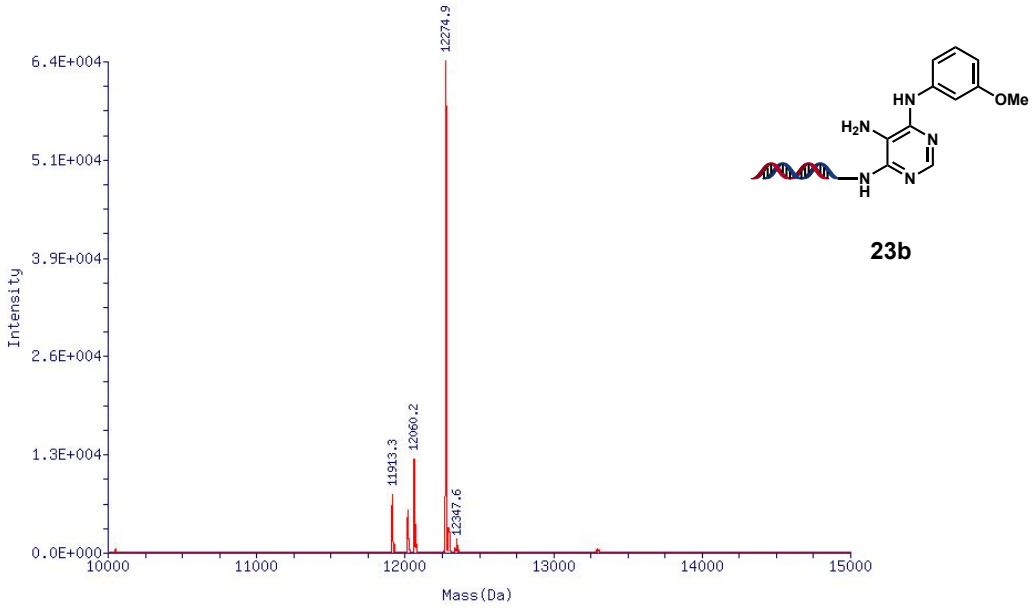


Figure S291. Deconvoluted mass spectrum of DNA **23b**, expected: 12274.2; observed 12274.9.

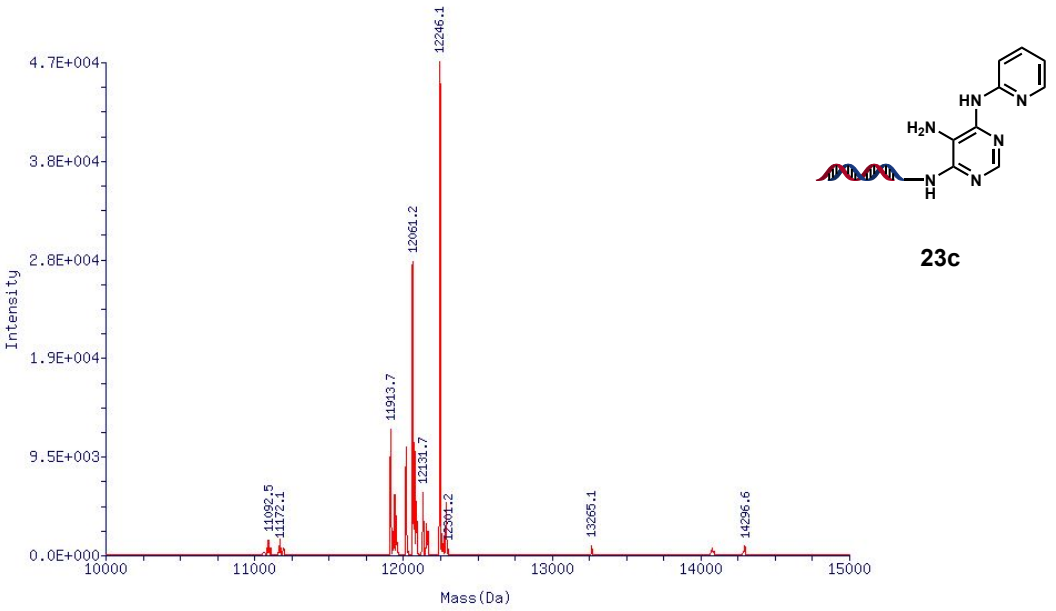


Figure S292. Deconvoluted mass spectrum of DNA **23c**, expected: 12245.2; observed 12246.1.

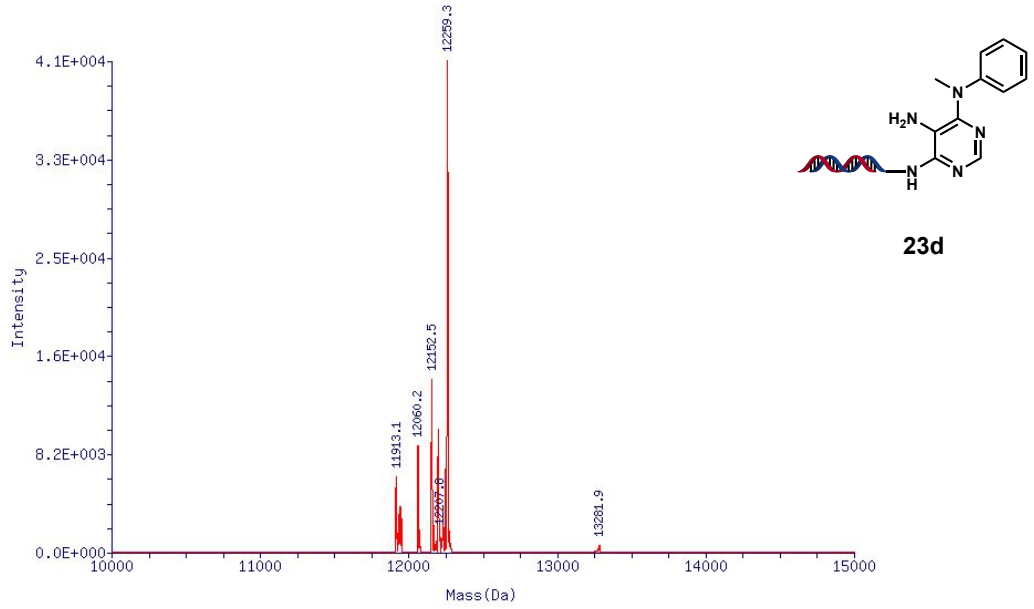
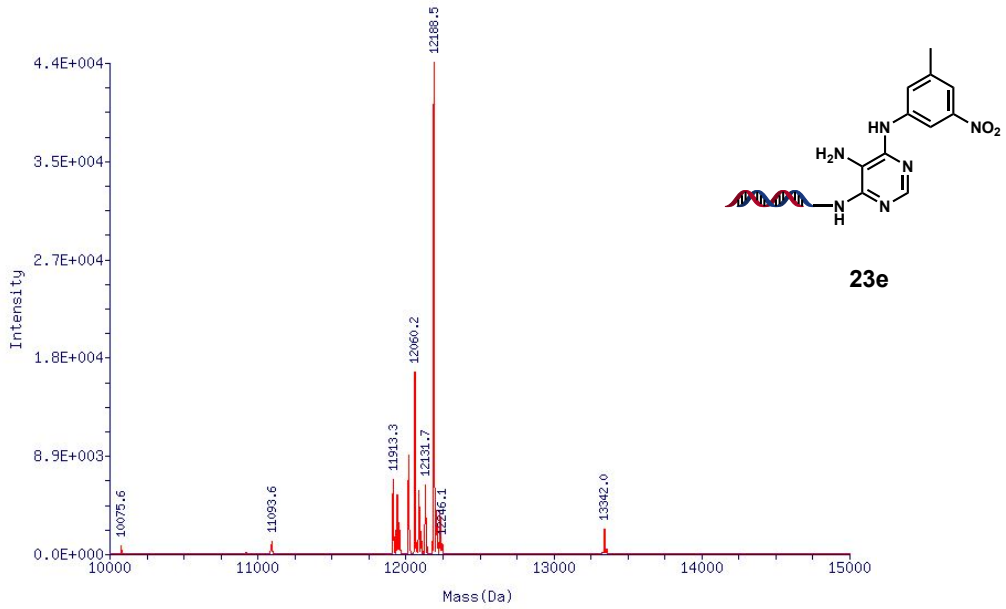
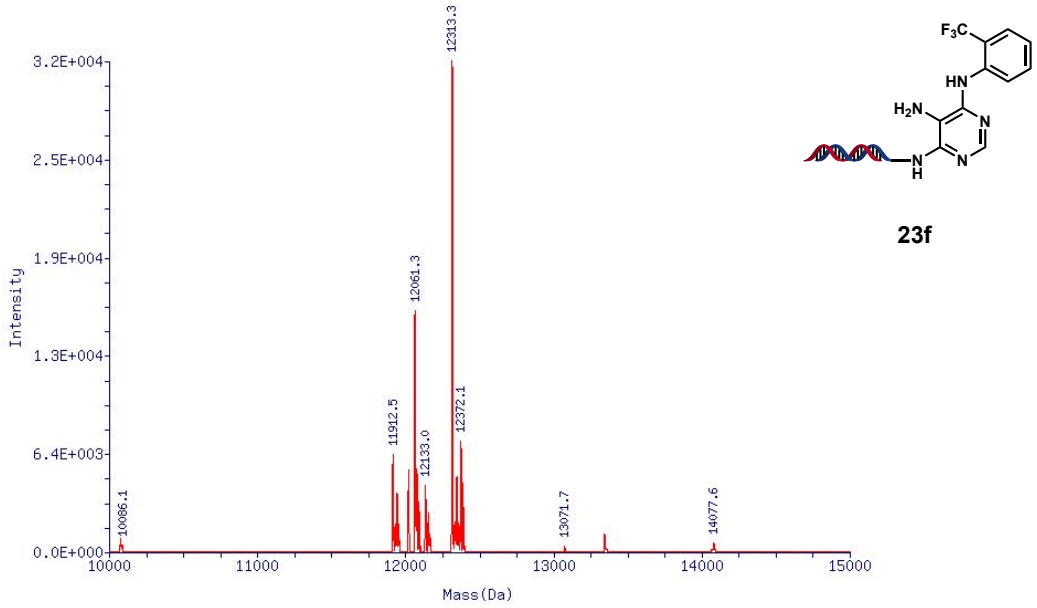


Figure S293. Deconvoluted mass spectrum of DNA **23d**, expected: 12258.2; observed 12259.3.



23e

Figure S294. Deconvoluted mass spectrum of DNA **23e**, expected: 12303.2; no product observed.



23f

Figure S295. Deconvoluted mass spectrum of DNA **23f**, expected: 12312.2; observed 12313.3.

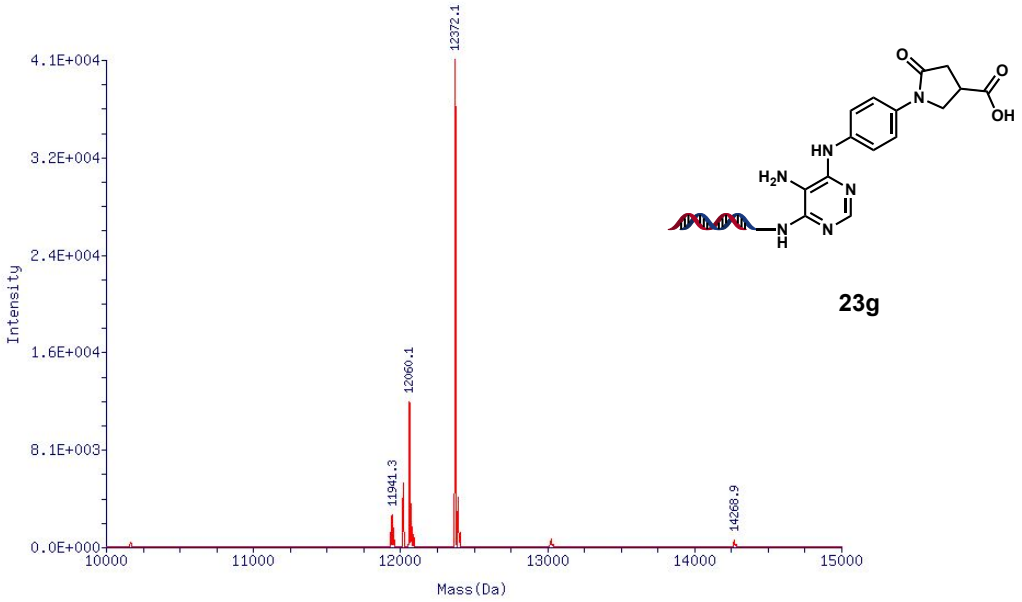


Figure S296. Deconvoluted mass spectrum of DNA **23g**, expected: 12371.2; observed 12372.1.

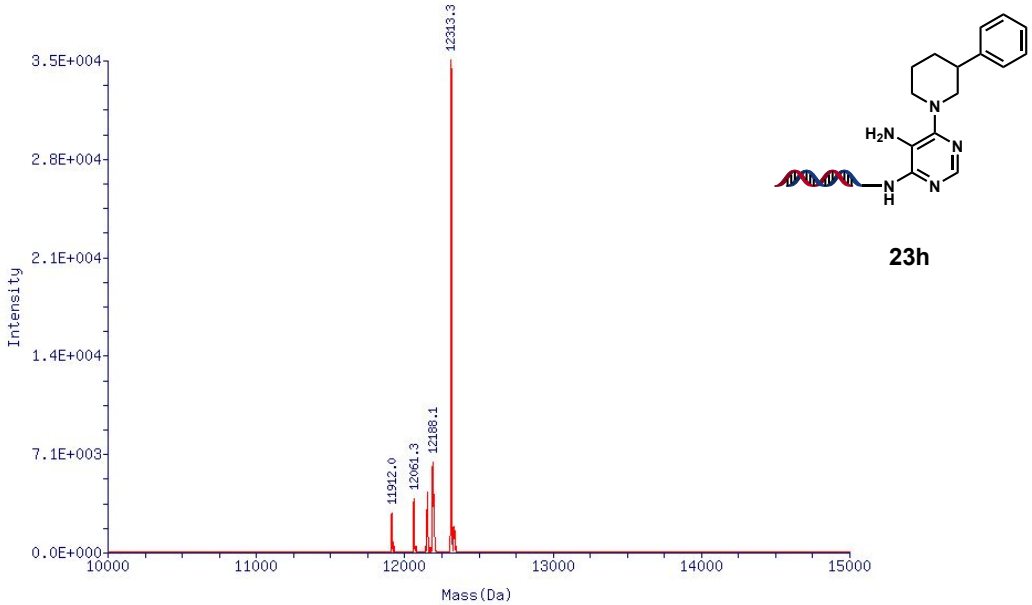


Figure S297. Deconvoluted mass spectrum of DNA **23h**, expected: 12312.3; observed 12313.3.

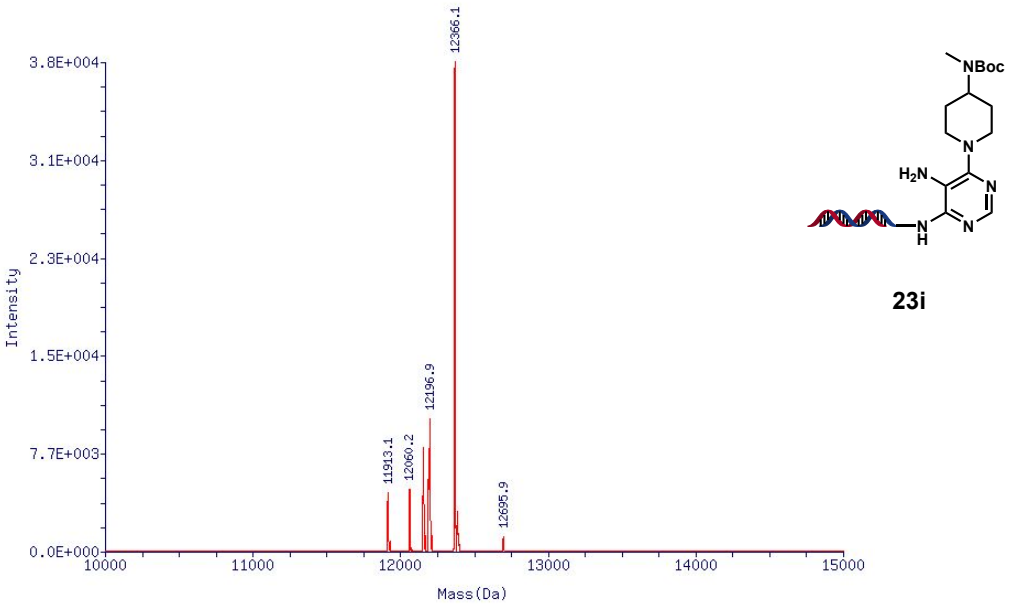


Figure S298. Deconvoluted mass spectrum of DNA **23i**, expected: 12365.4; observed 12366.1.

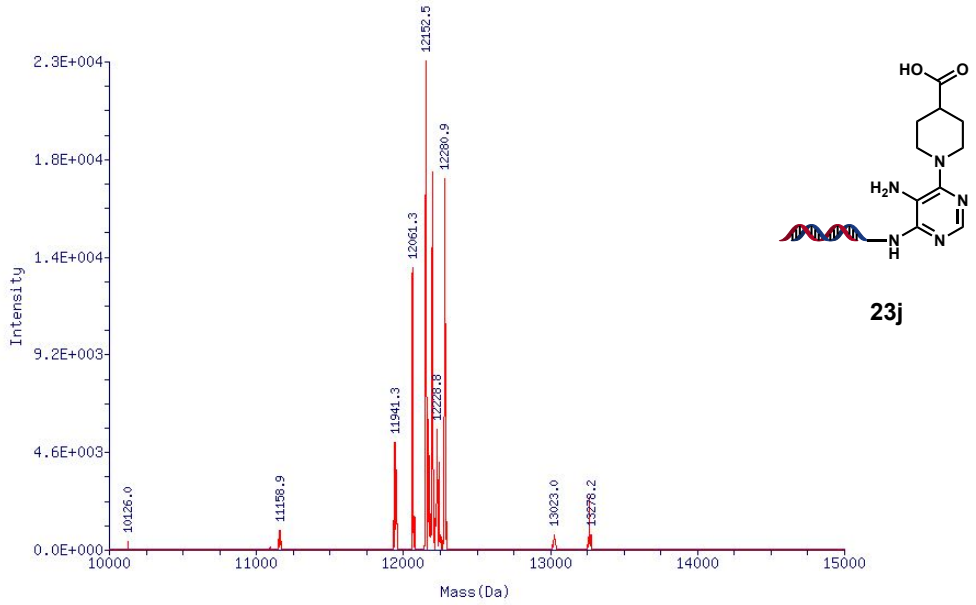


Figure S299. Deconvoluted mass spectrum of DNA **23j**, expected: 12280.2; observed 12280.9.

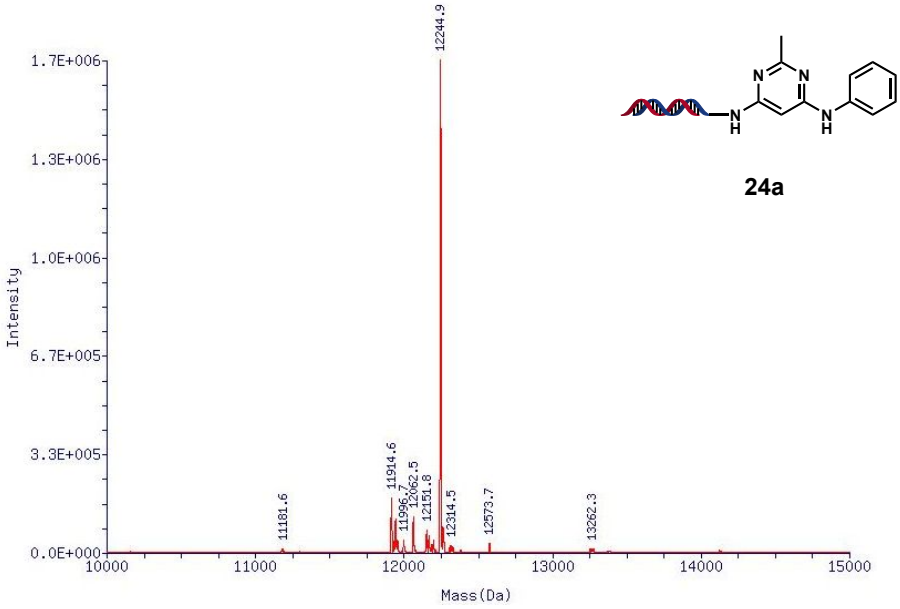


Figure S300. Deconvoluted mass spectrum of DNA **24a**, expected: 12243.2; observed 12244.9.

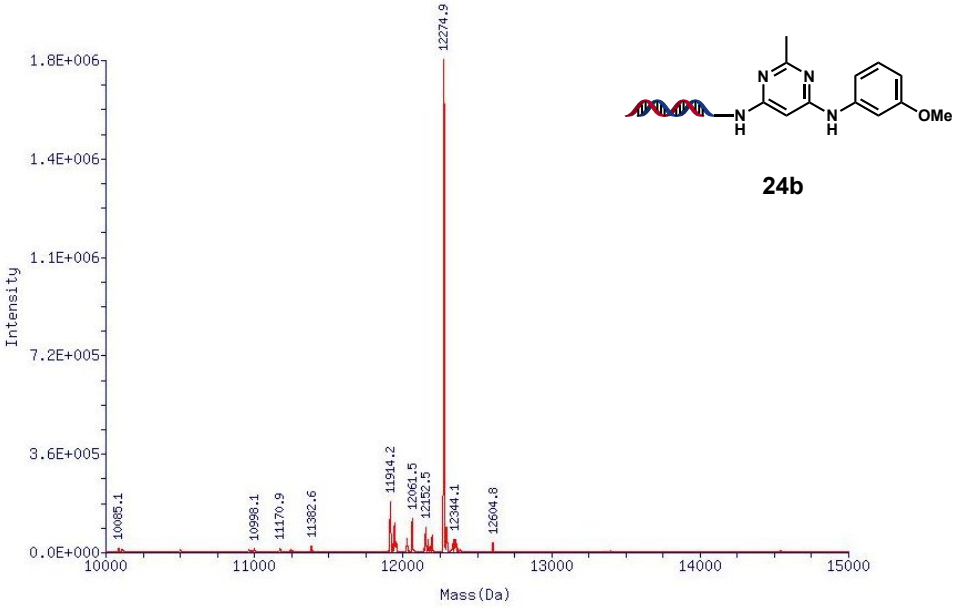


Figure S301. Deconvoluted mass spectrum of DNA **24b**, expected: 12273.2; observed 12274.9.

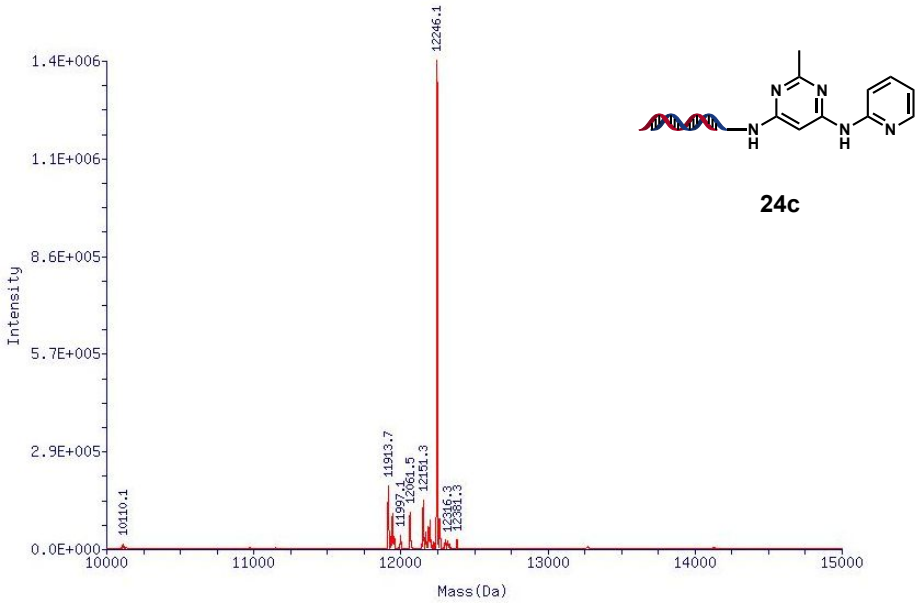


Figure S302. Deconvoluted mass spectrum of DNA **24c**, expected: 12244.2; observed 12246.1.

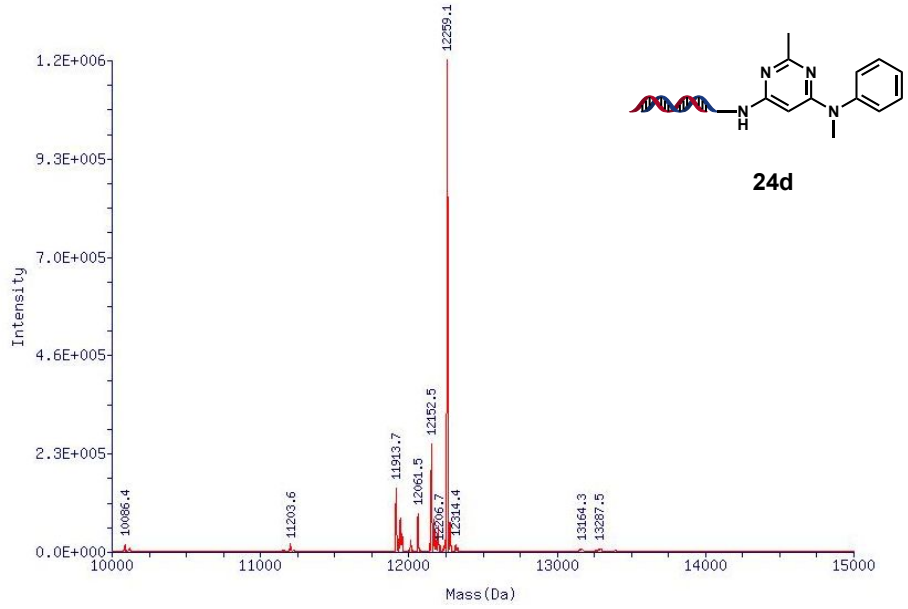


Figure S303. Deconvoluted mass spectrum of DNA **24d**, expected: 12257.2; observed 12259.1.

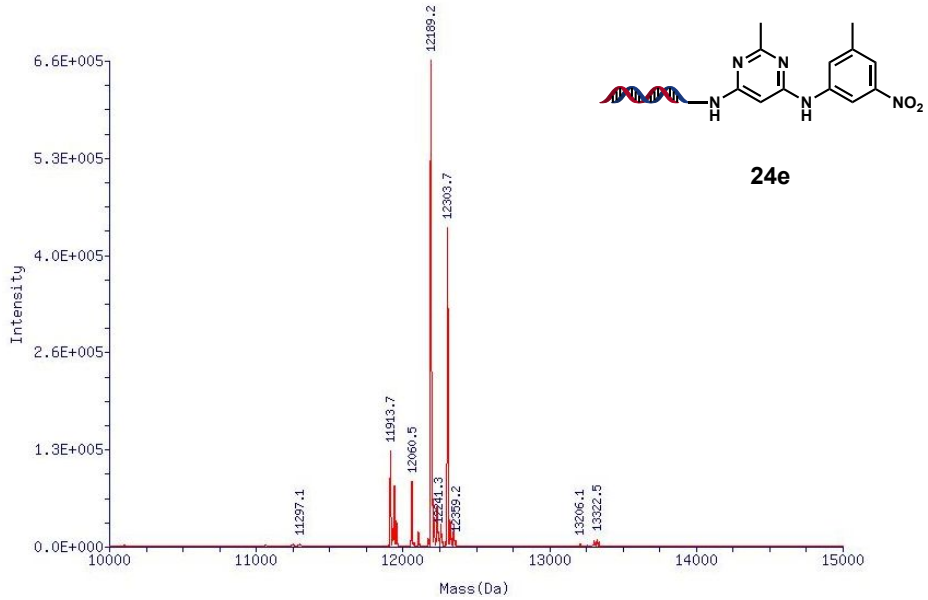


Figure S304. Deconvoluted mass spectrum of DNA **24e**, expected: 12302.2; observed 12303.7.

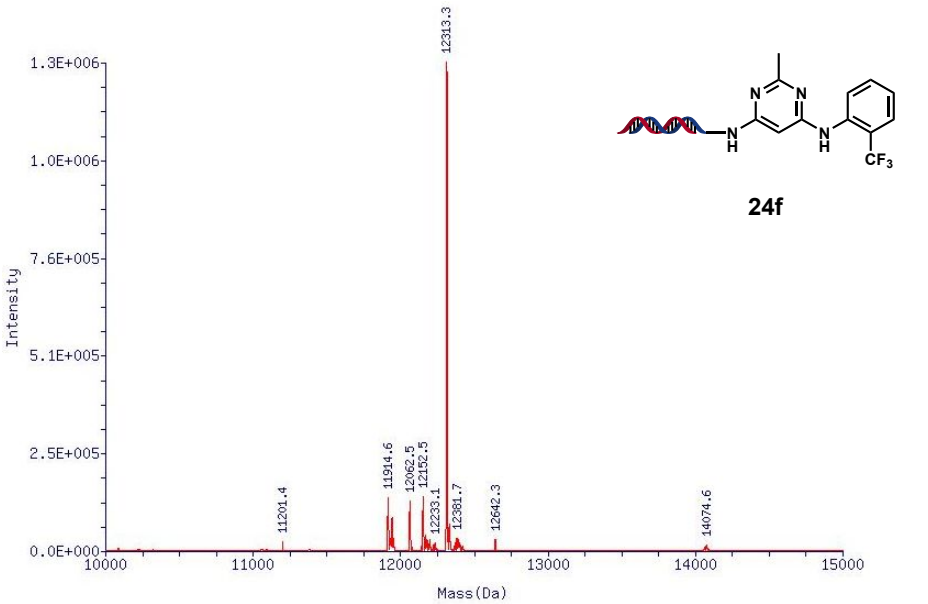


Figure S305. Deconvoluted mass spectrum of DNA **24f**, expected: 12311.2; observed 12313.3.

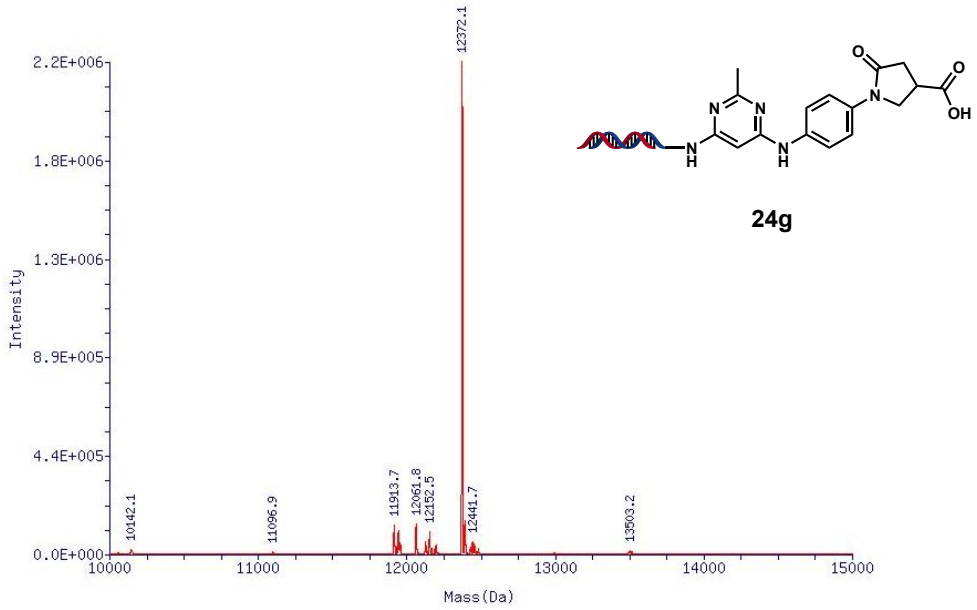


Figure S306. Deconvoluted mass spectrum of DNA **24g**, expected: 12370.2; observed 12372.1.

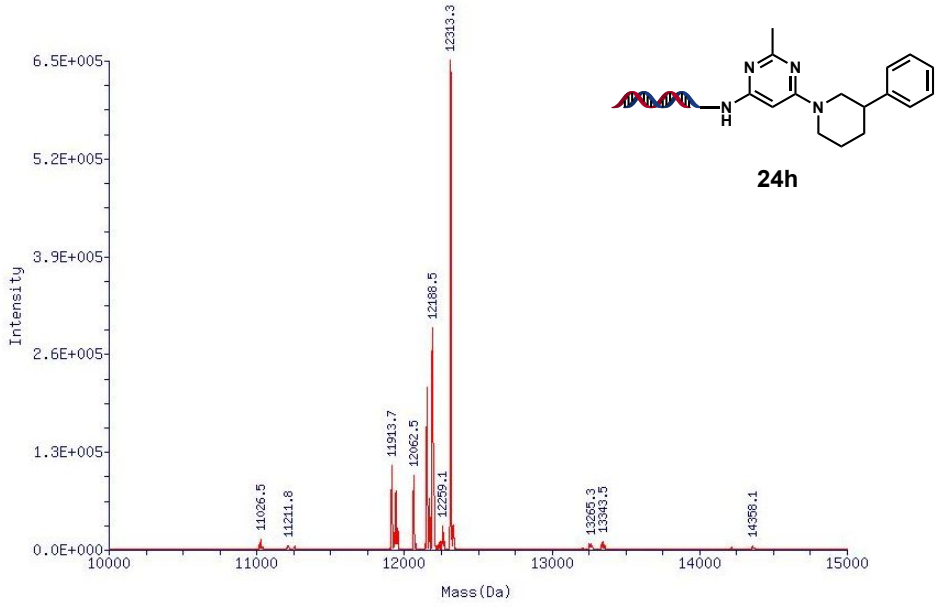


Figure S307. Deconvoluted mass spectrum of DNA **24h**, expected: 12311.3; observed 12313.3.

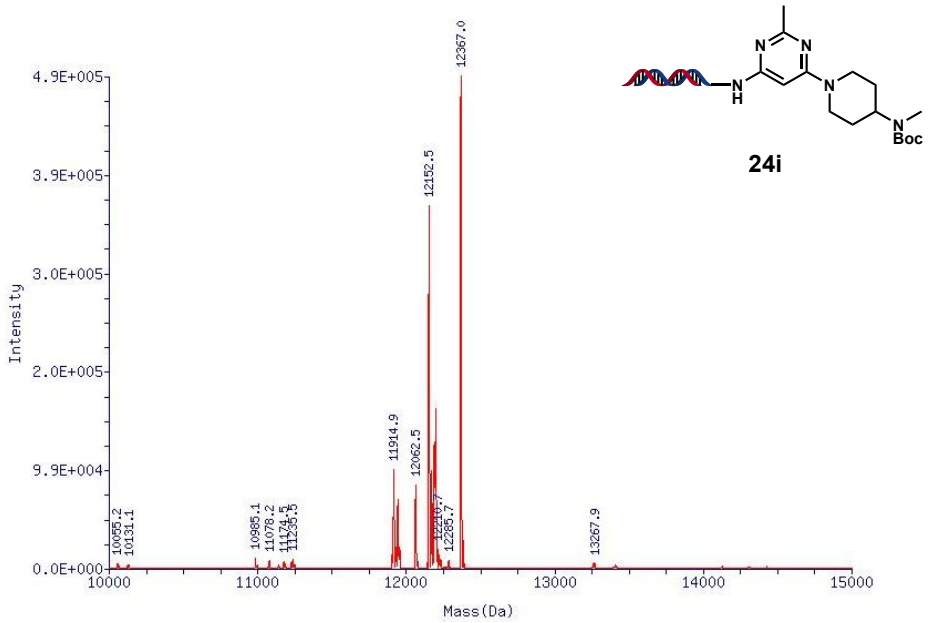


Figure S308. Deconvoluted mass spectrum of DNA **24i**, expected: 12364.4; observed 12367.

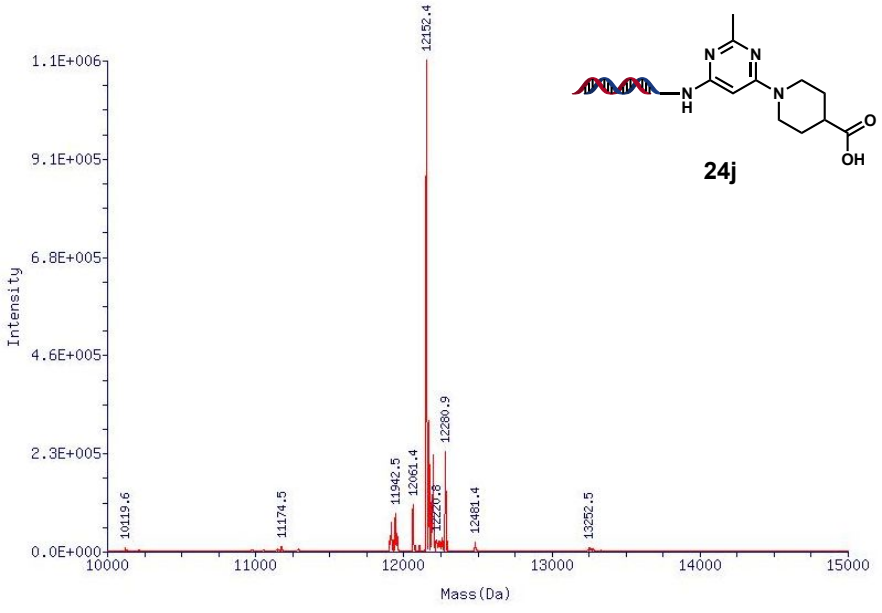


Figure S309. Deconvoluted mass spectrum of DNA **24j**, expected: 12279.2; observed 12280.9.

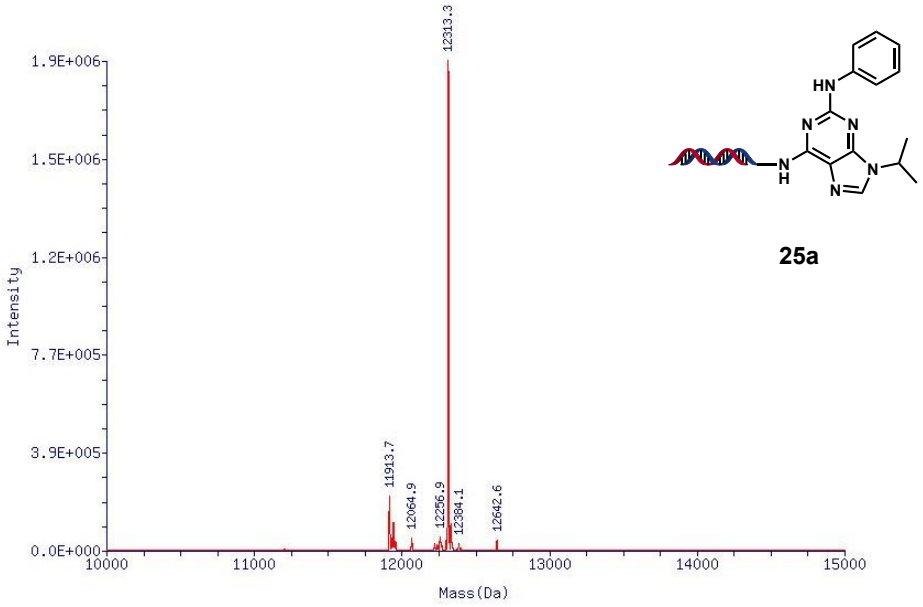


Figure S310. Deconvoluted mass spectrum of DNA **25a**, expected: 12311.3; observed 12313.3.

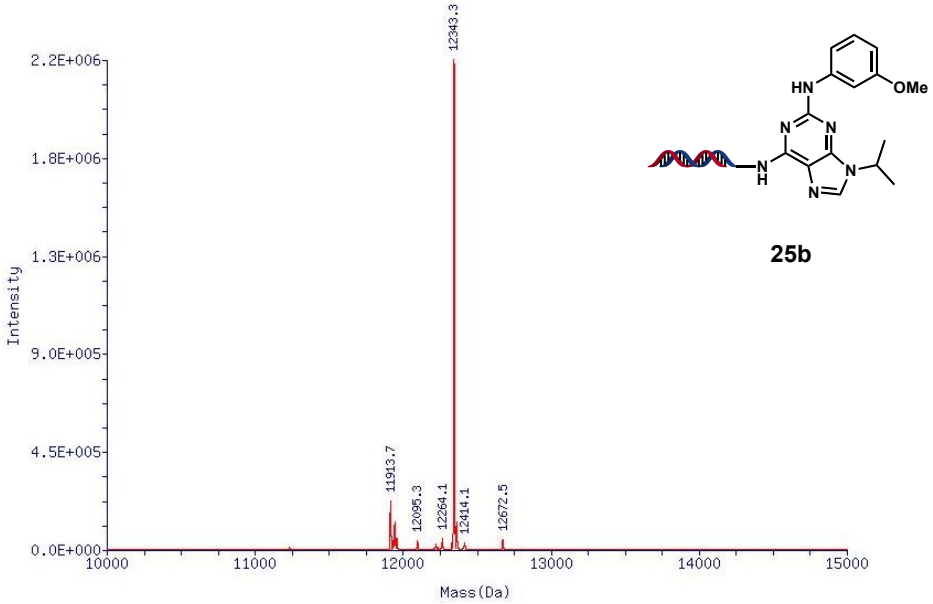


Figure S311. Deconvoluted mass spectrum of DNA **25b**, expected: 12341.3; observed 12343.3.

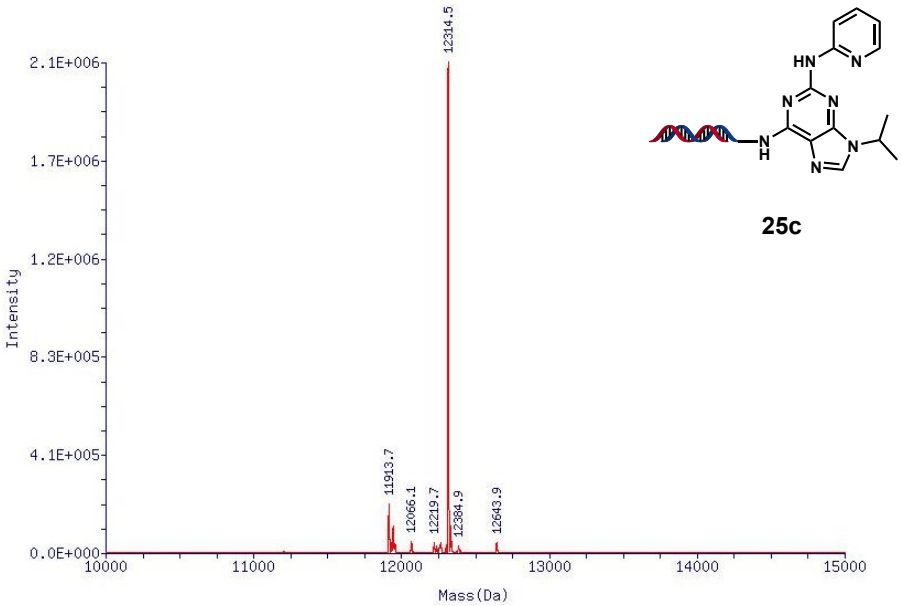


Figure S312. Deconvoluted mass spectrum of DNA **25c**, expected: 12312.3; observed 12314.5.

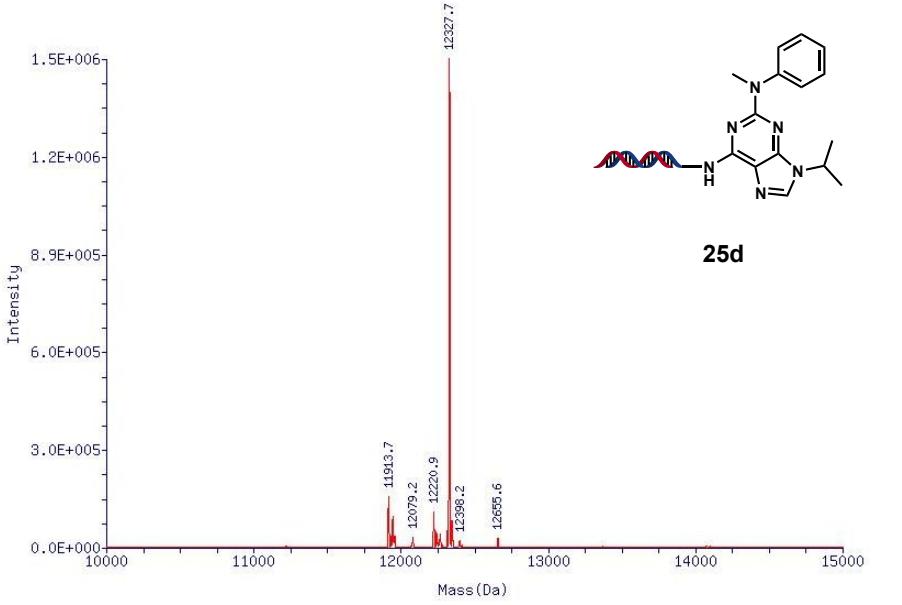


Figure S313. Deconvoluted mass spectrum of DNA **25d**, expected: 12325.3; observed 12327.7.

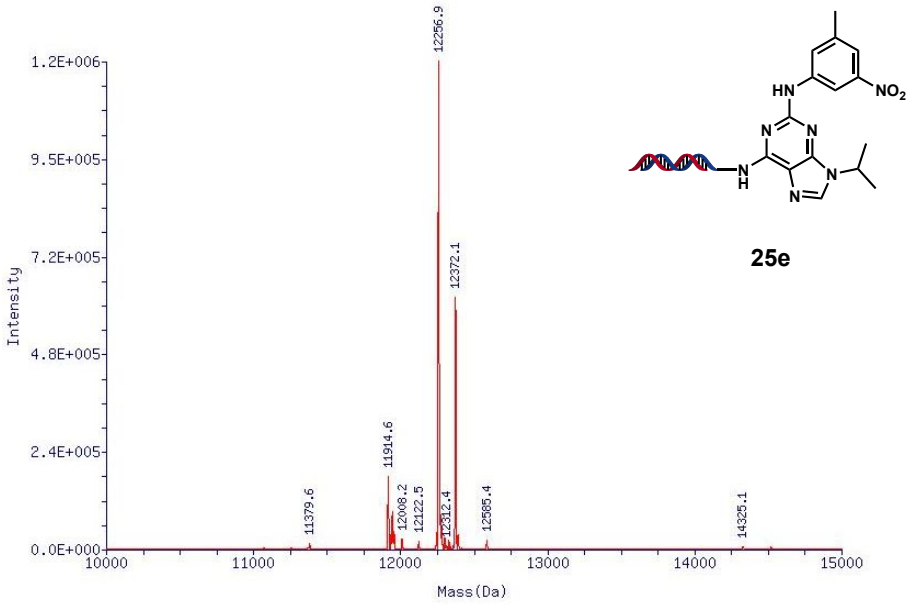


Figure S314. Deconvoluted mass spectrum of DNA **25e**, expected: 12370.3; observed 12372.1.

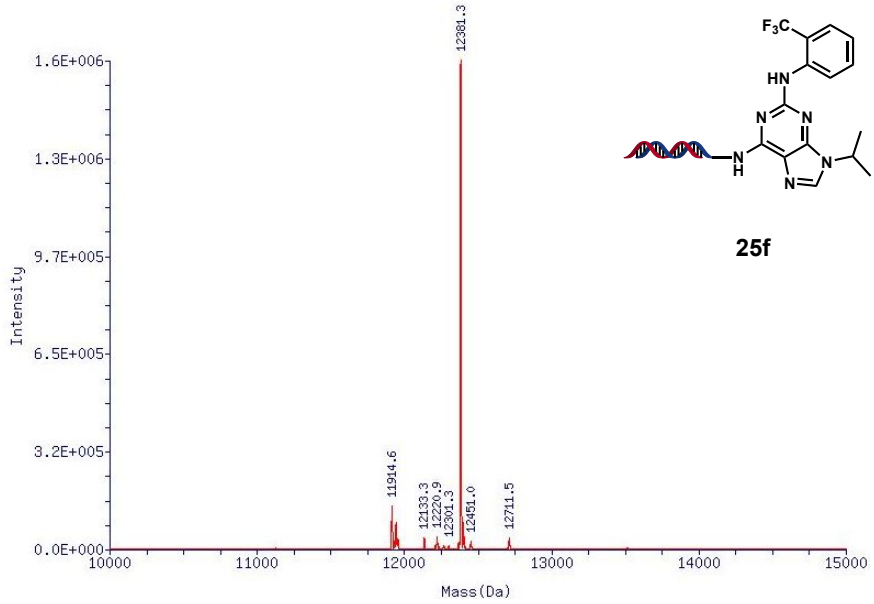


Figure S315. Deconvoluted mass spectrum of DNA **25f**, expected: 12379.3; observed 12381.3.

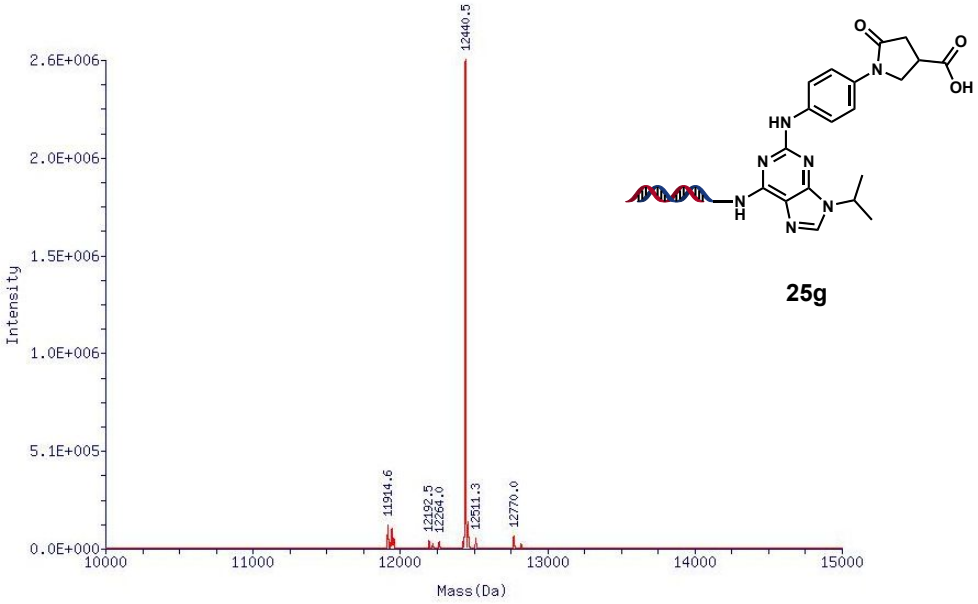


Figure S316. Deconvoluted mass spectrum of DNA **25g**, expected: 12438.3; observed 12400.5.

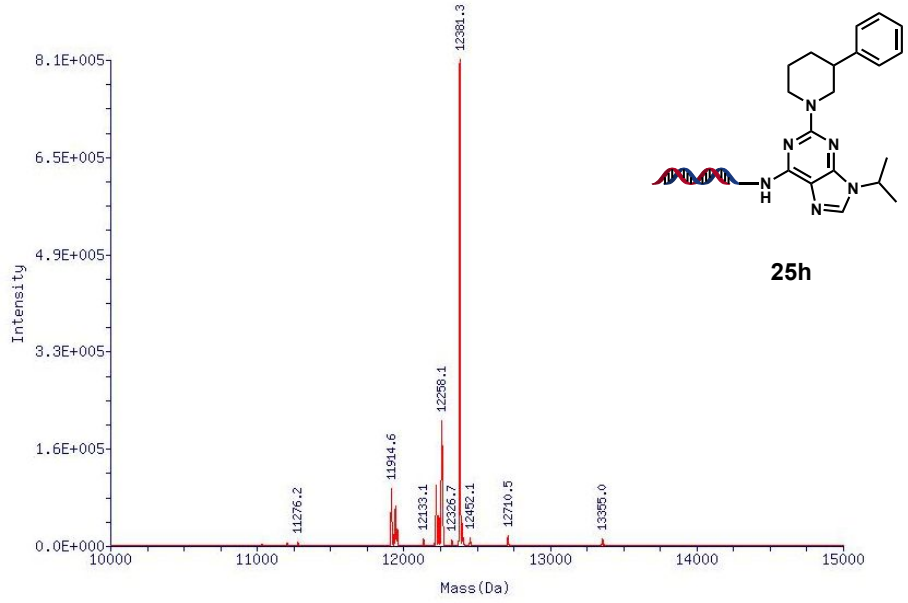


Figure S317. Deconvoluted mass spectrum of DNA **25h**, expected: 12379.4; observed 12381.3.

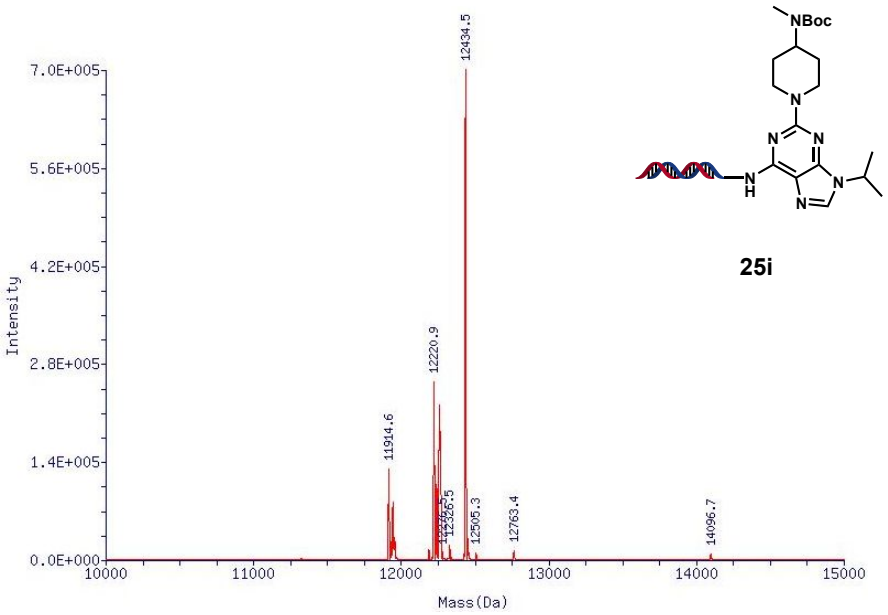


Figure S318. Deconvoluted mass spectrum of DNA **25i**, expected: 12432.5; observed 12434.5.

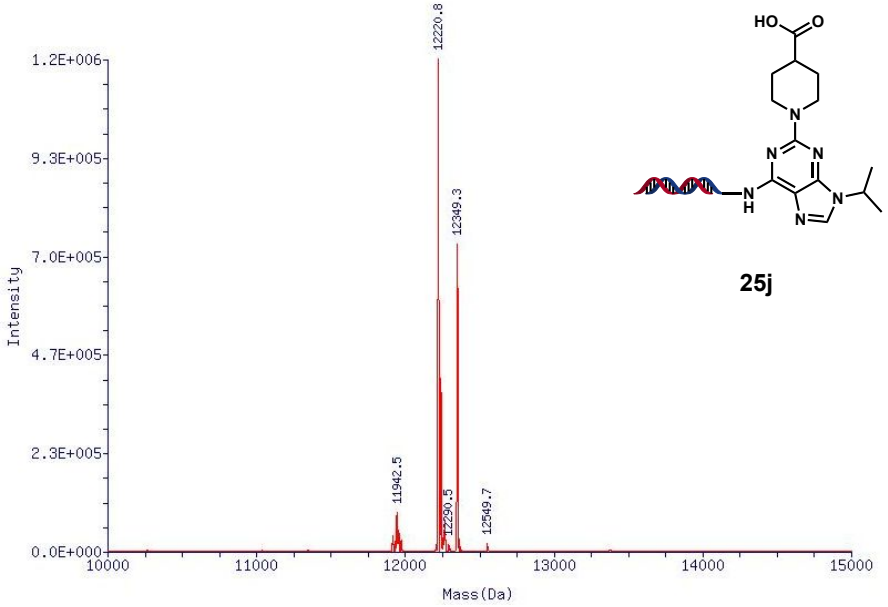


Figure S319. Deconvoluted mass spectrum of DNA **25j**, expected: 12347.3; observed 12349.3.

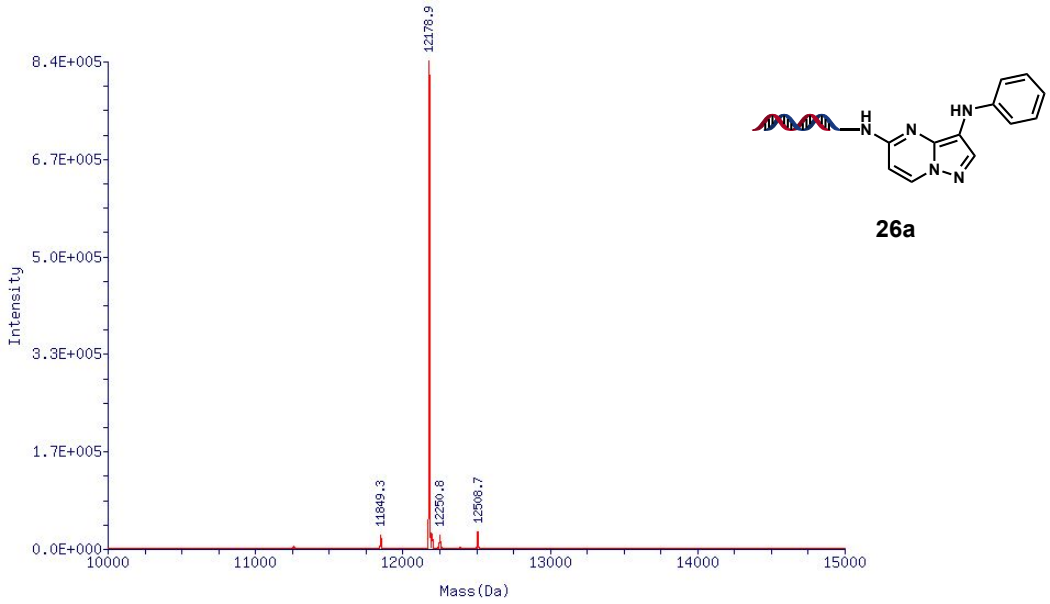


Figure S320. Deconvoluted mass spectrum of DNA **26a**, expected: 12268.2; no product observed.

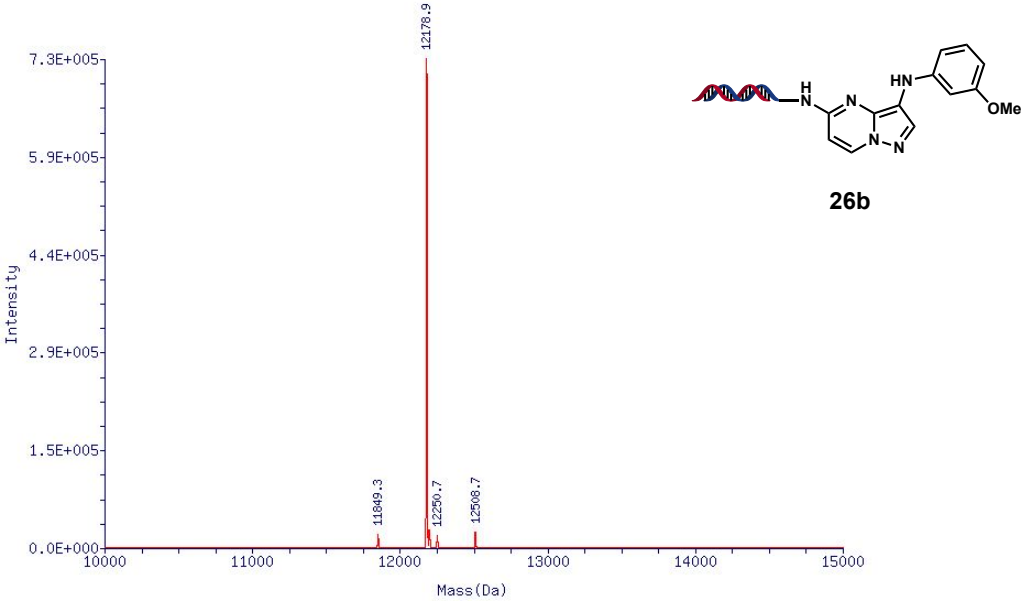


Figure S321. Deconvoluted mass spectrum of DNA **26b**, expected: 12298.3; no product observed.

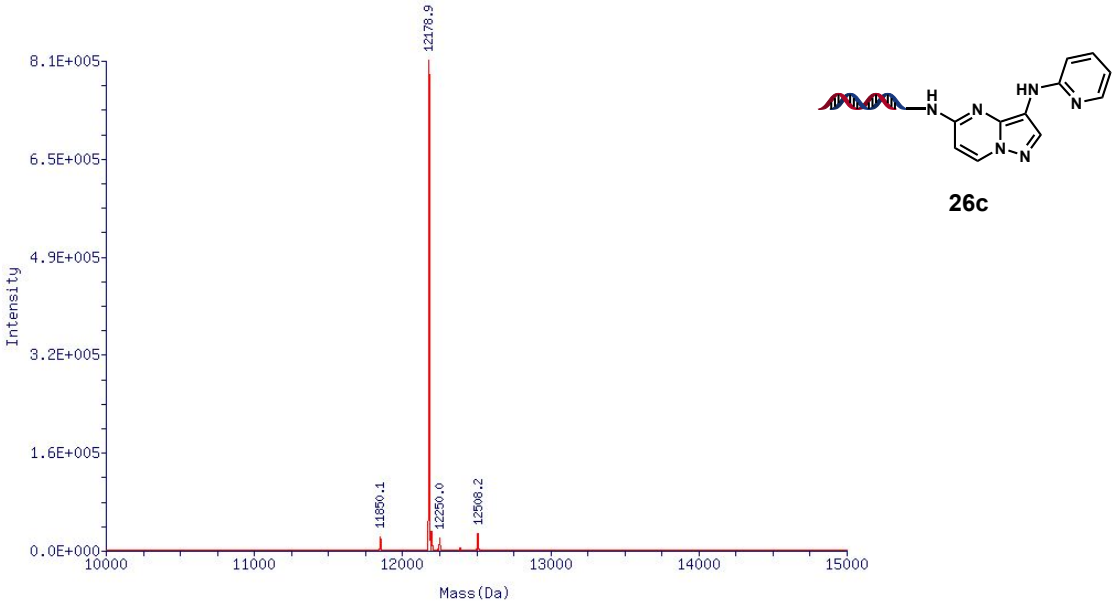


Figure S322. Deconvoluted mass spectrum of DNA **26c**, expected: 12269.2; no product observed.

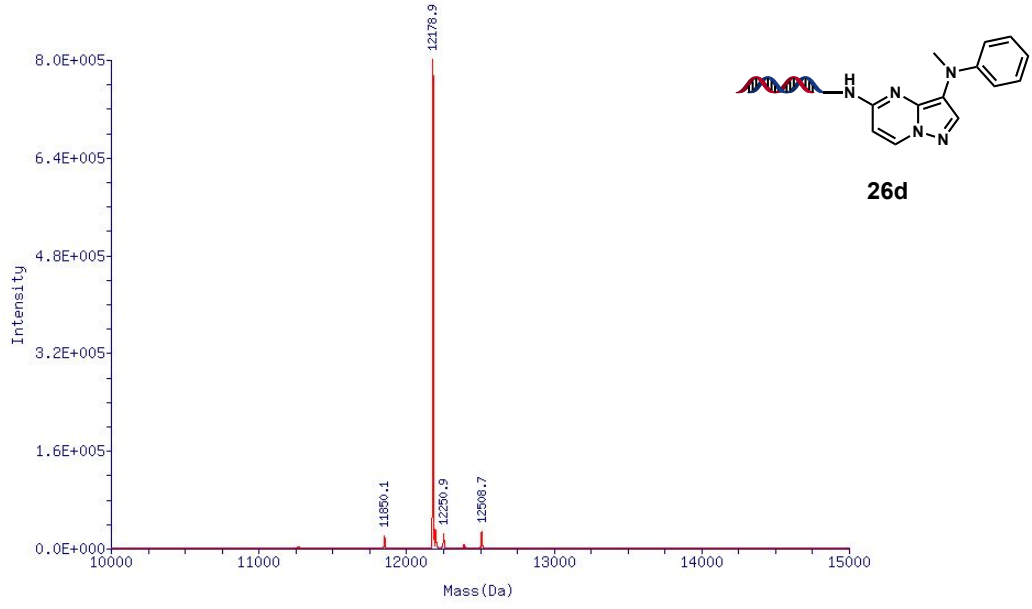


Figure S323. Deconvoluted mass spectrum of DNA **26d**, expected: 12282.3; no product observed.

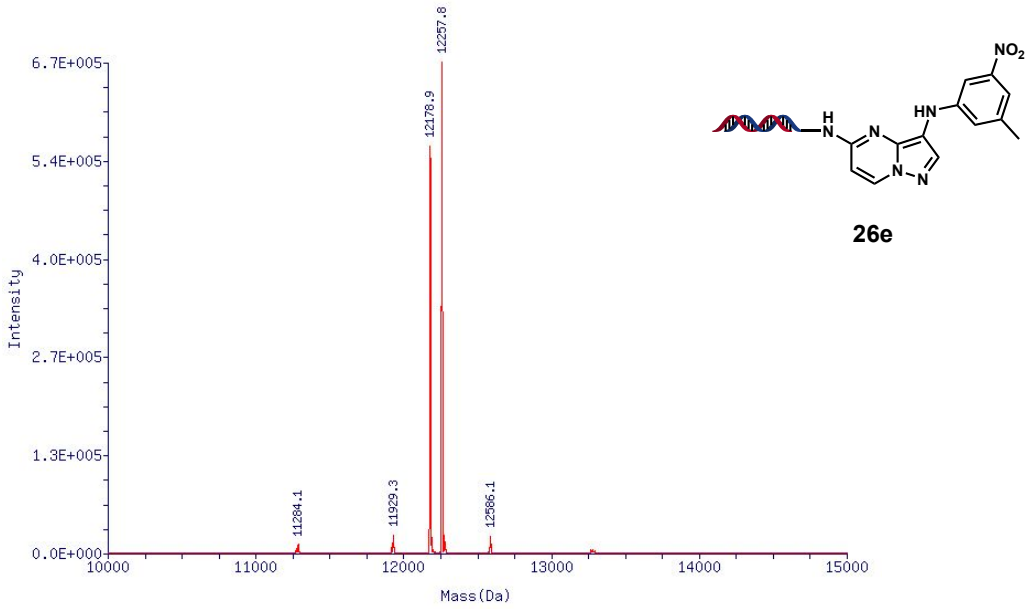


Figure S324. Deconvoluted mass spectrum of DNA **26e**, expected: 12327.3; no product observed.

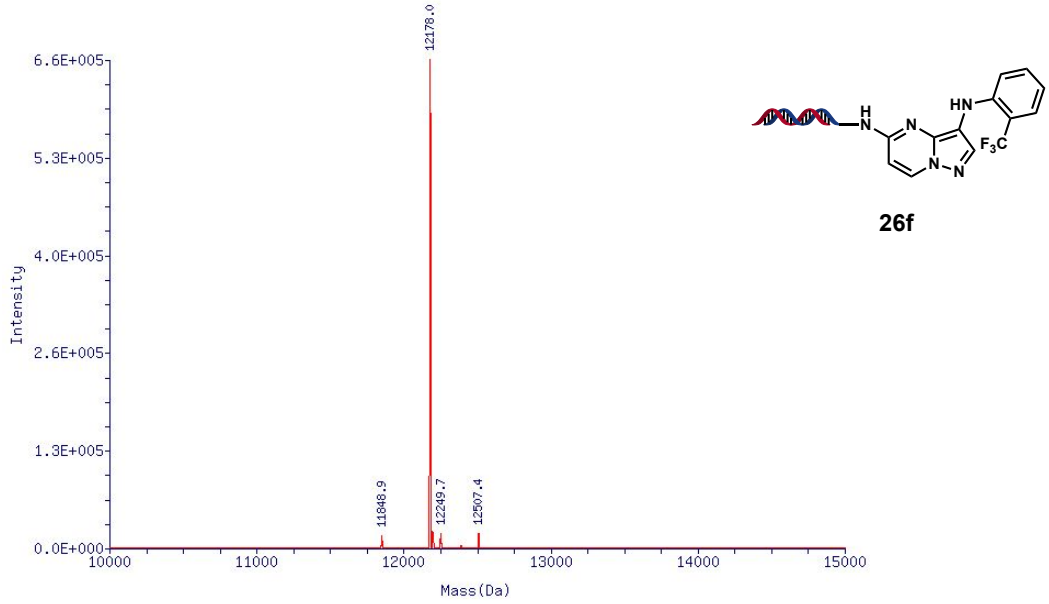


Figure S325. Deconvoluted mass spectrum of DNA **26f**, expected: 12336.2; no product observed.

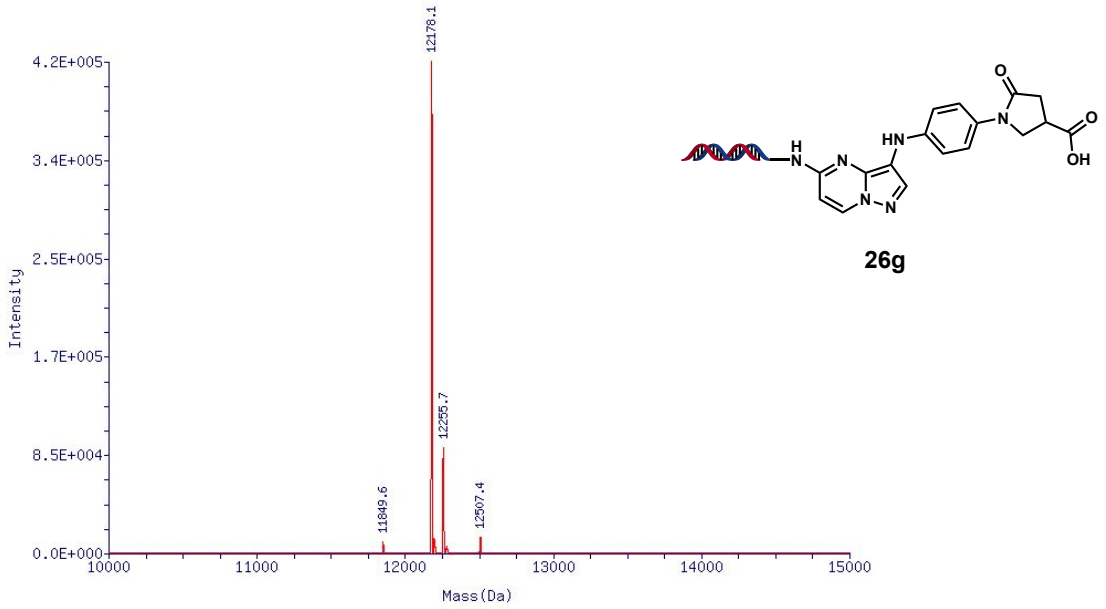


Figure S326. Deconvoluted mass spectrum of DNA **26g**, expected: 12395.2; no product observed.

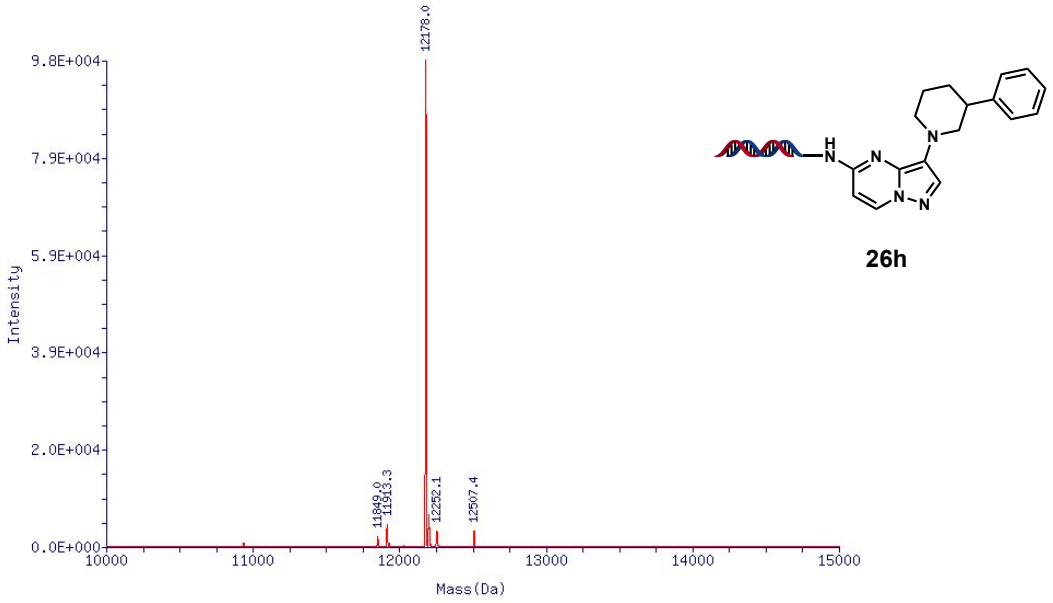


Figure S327. Deconvoluted mass spectrum of DNA **26h**, expected: 12336.4; no product observed.

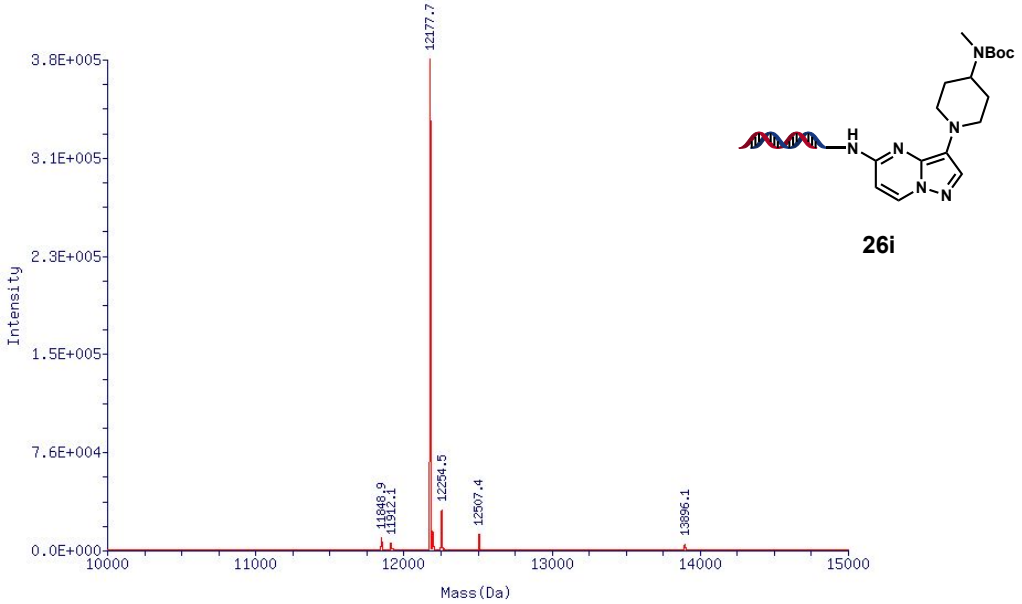


Figure S328. Deconvoluted mass spectrum of DNA **26i**, expected: 12389.4; no product observed.

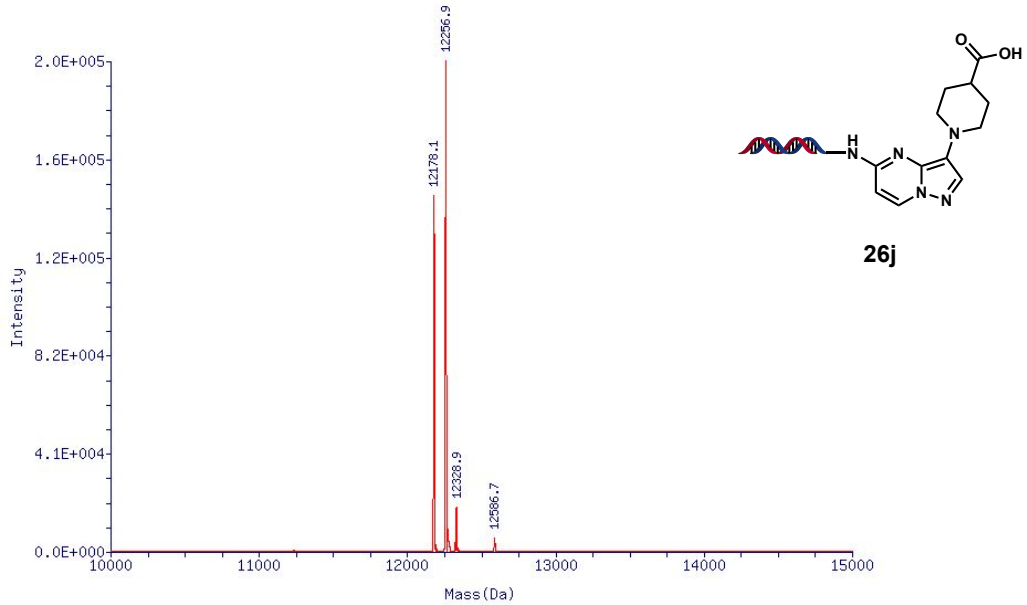


Figure S329. Deconvoluted mass spectrum of DNA **26j**, expected: 12304.3; no product observed.

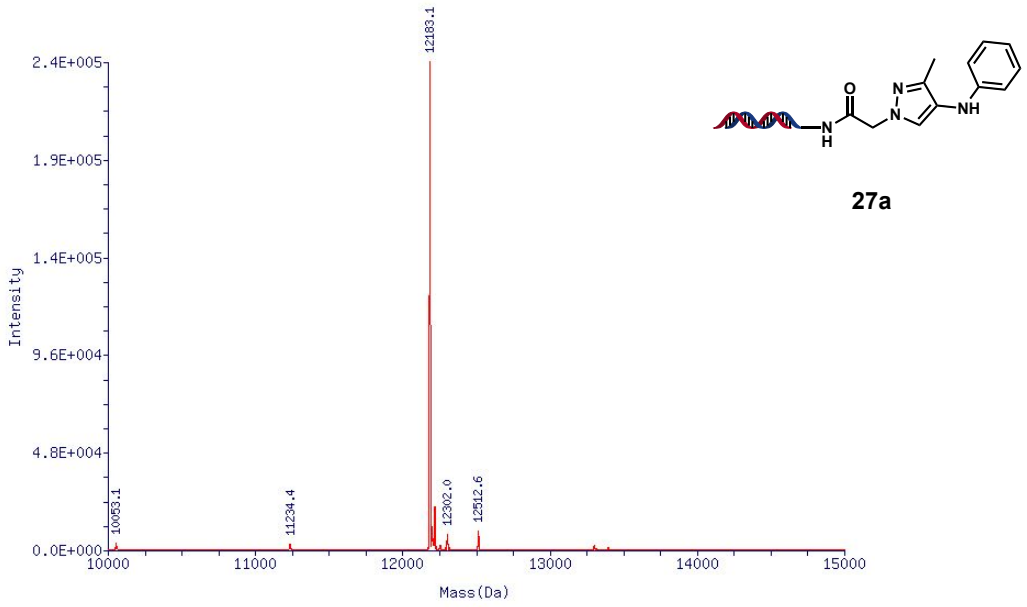


Figure S330. Deconvoluted mass spectrum of DNA **27a**, expected: 12273.2; no product observed.

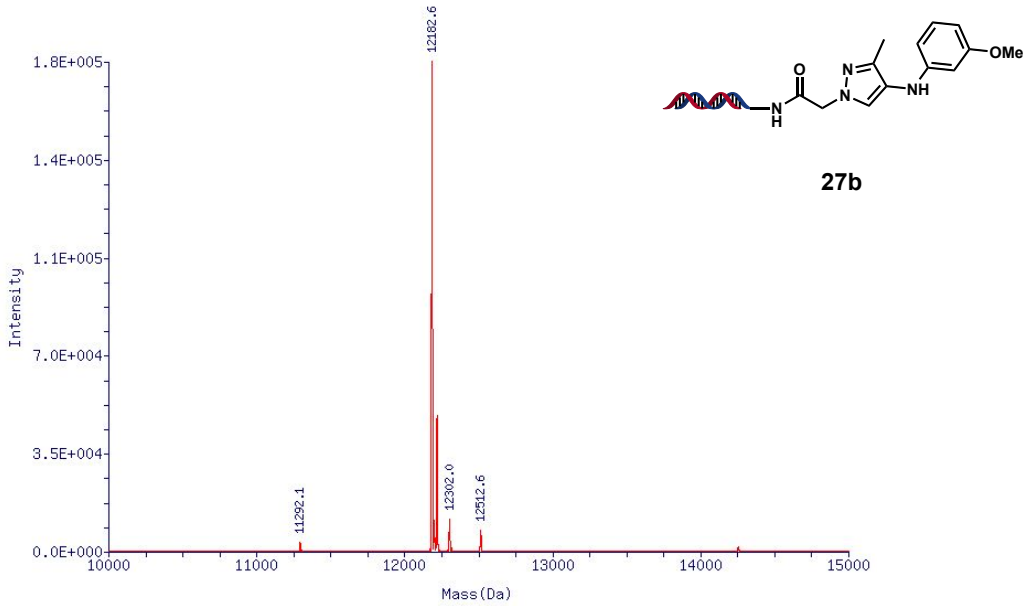
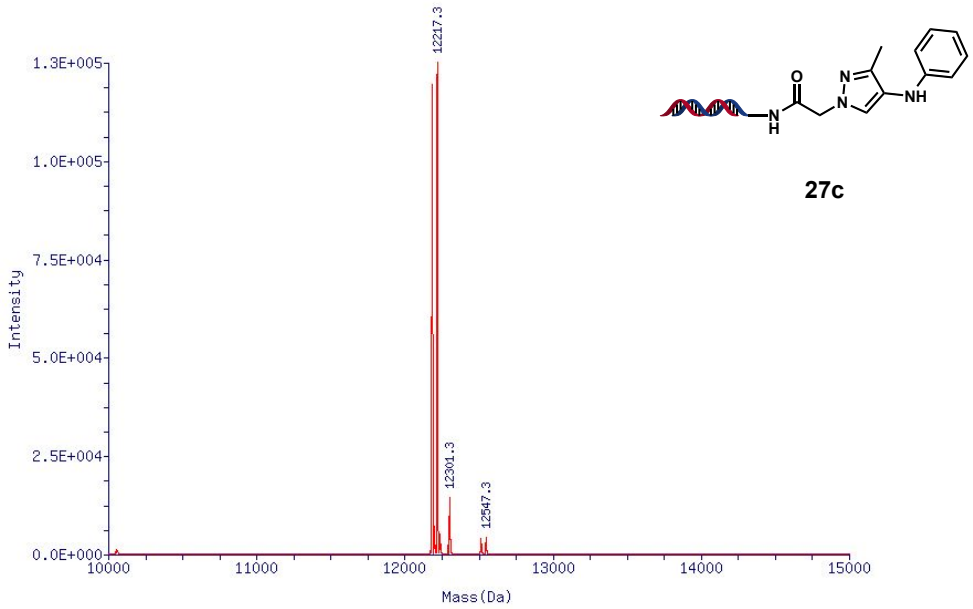
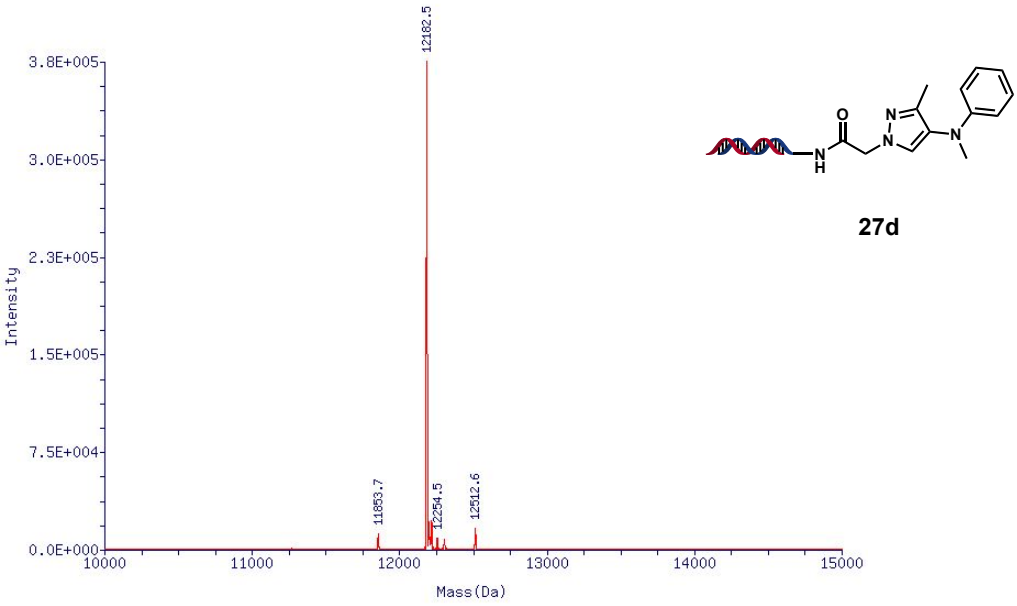


Figure S331. Deconvoluted mass spectrum of DNA **27b**, expected: 12303.3; no product observed.



27c

Figure S332. Deconvoluted mass spectrum of DNA **27c**, expected: 12274.2; no product observed.



27d

Figure S333. Deconvoluted mass spectrum of DNA **27d**, expected: 12287.3; no product observed.

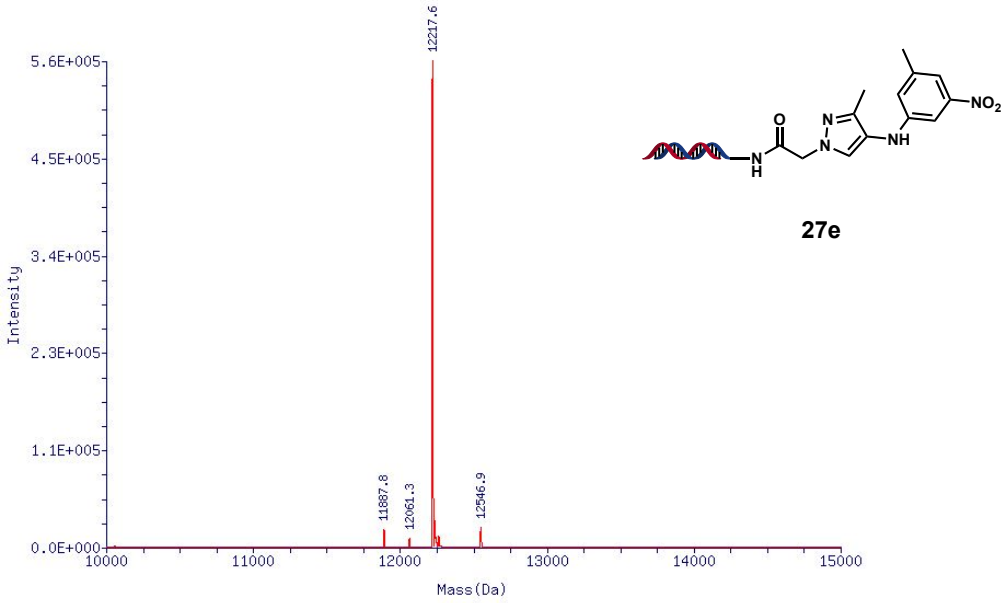


Figure S334. Deconvoluted mass spectrum of DNA **27e**, expected: 12332.3; no product observed.

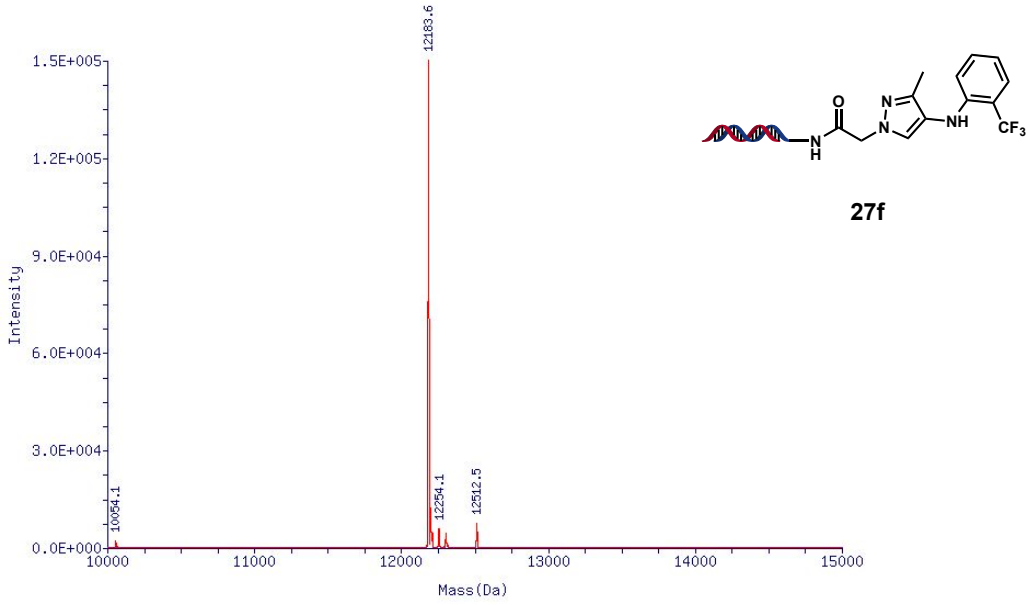


Figure S335. Deconvoluted mass spectrum of DNA **27f**, expected: 12341.2; no product observed.

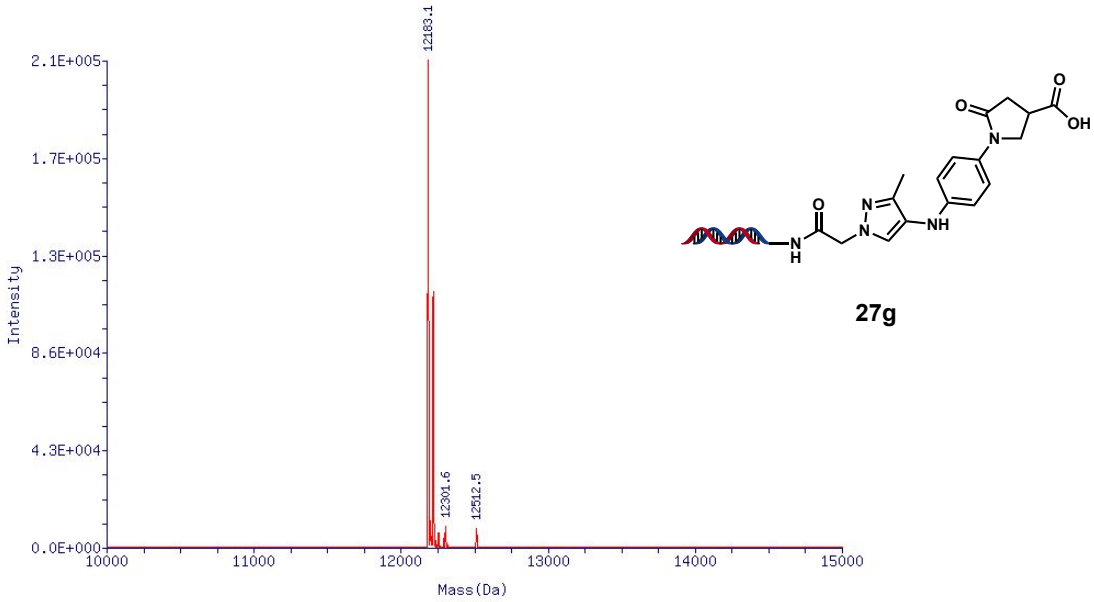


Figure S336. Deconvoluted mass spectrum of DNA **27g**, expected: 12400.3; no product observed.

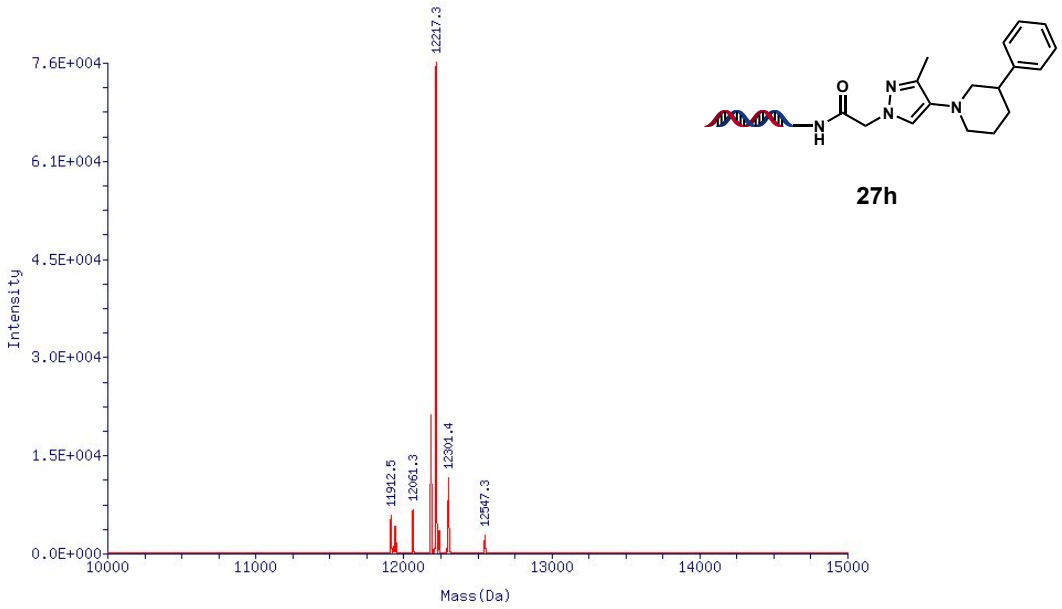


Figure S337. Deconvoluted mass spectrum of DNA **27h**, expected: 12341.4; no product observed.

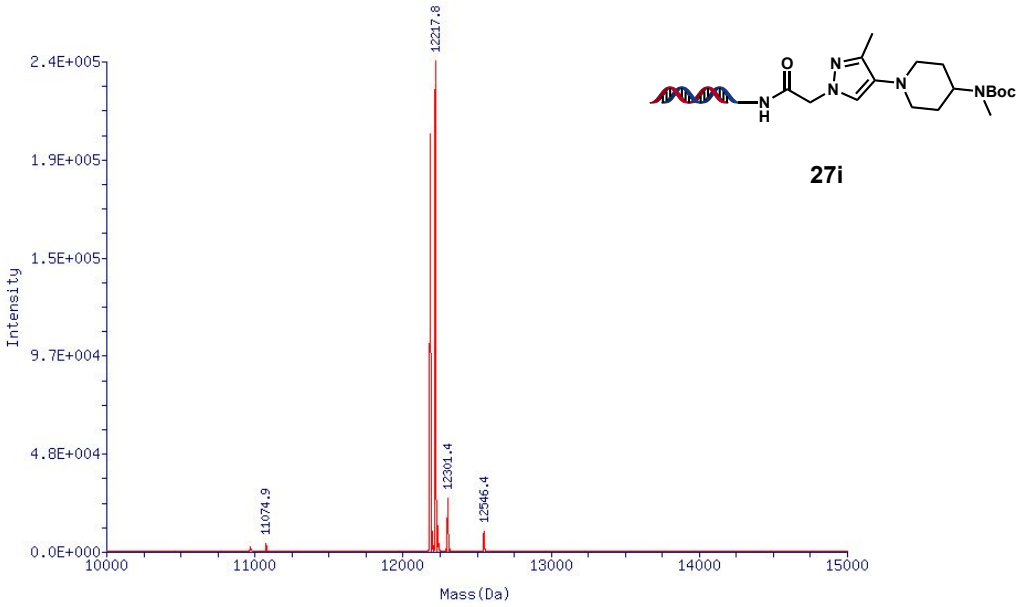


Figure S338. Deconvoluted mass spectrum of DNA **27i**, expected: 12394.4; no product observed.

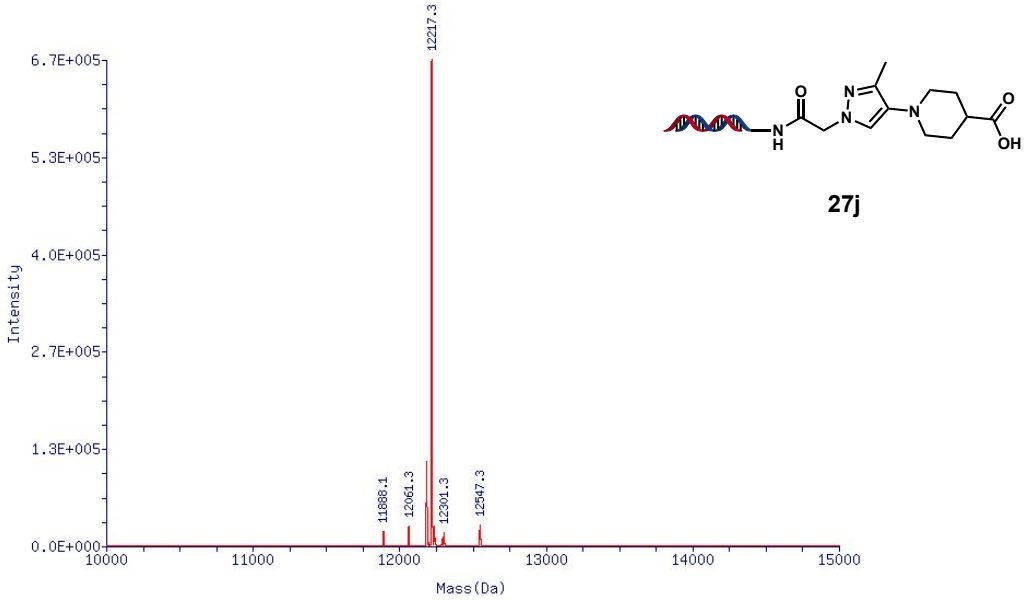


Figure S339. Deconvoluted mass spectrum of DNA **27j**, expected: 12309.3; no product observed.

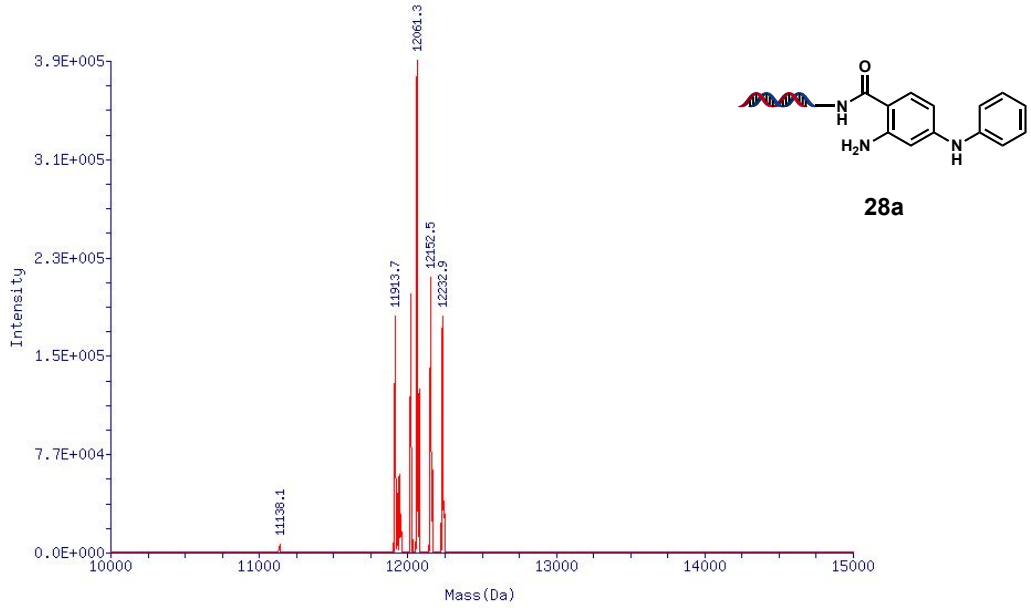


Figure S340. Deconvoluted mass spectrum of DNA **28a**, expected: 12242.2; no product observed.

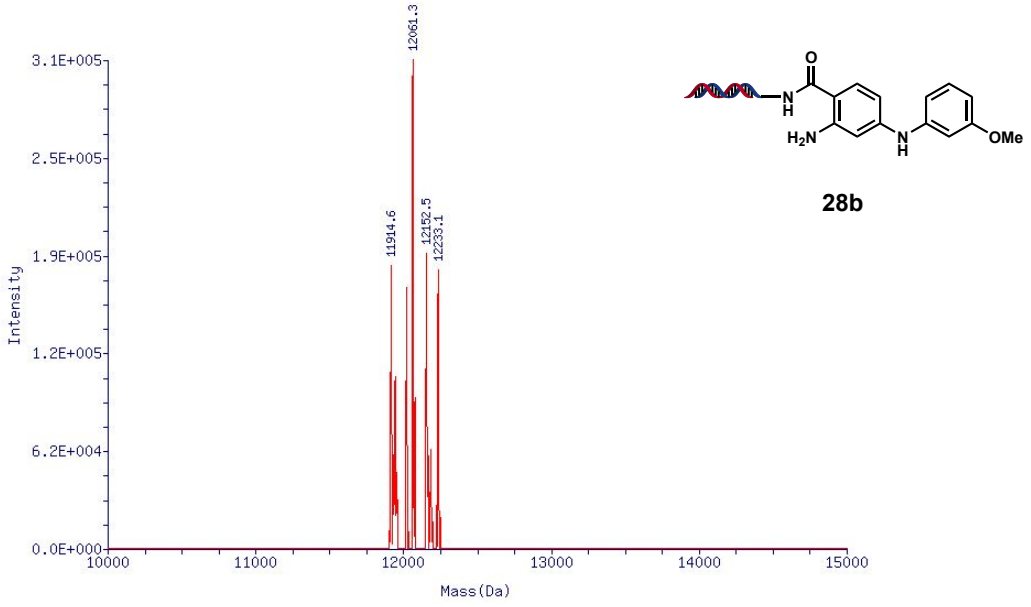


Figure S341. Deconvoluted mass spectrum of DNA **28b**, expected: 12272.2; no product observed.

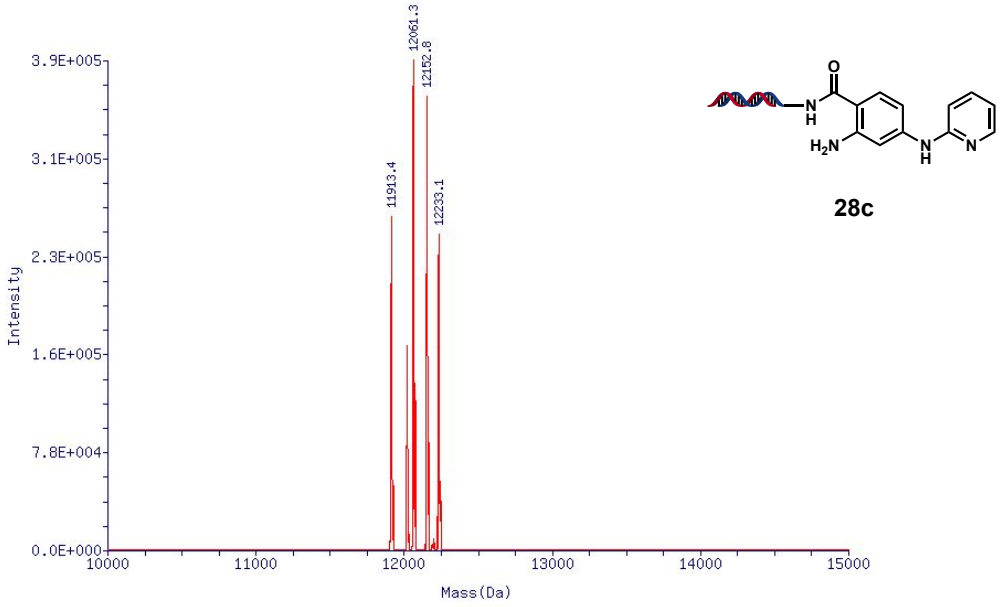


Figure S342. Deconvoluted mass spectrum of DNA **28c**, expected: 12243.2; no product observed.

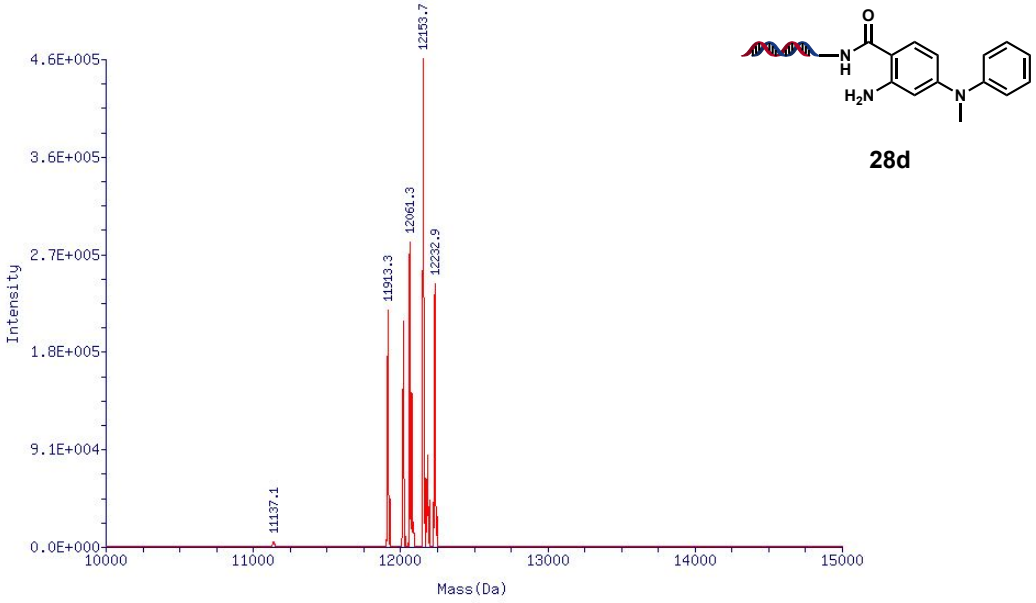


Figure S343. Deconvoluted mass spectrum of DNA **28d**, expected: 12256.3; no product observed.

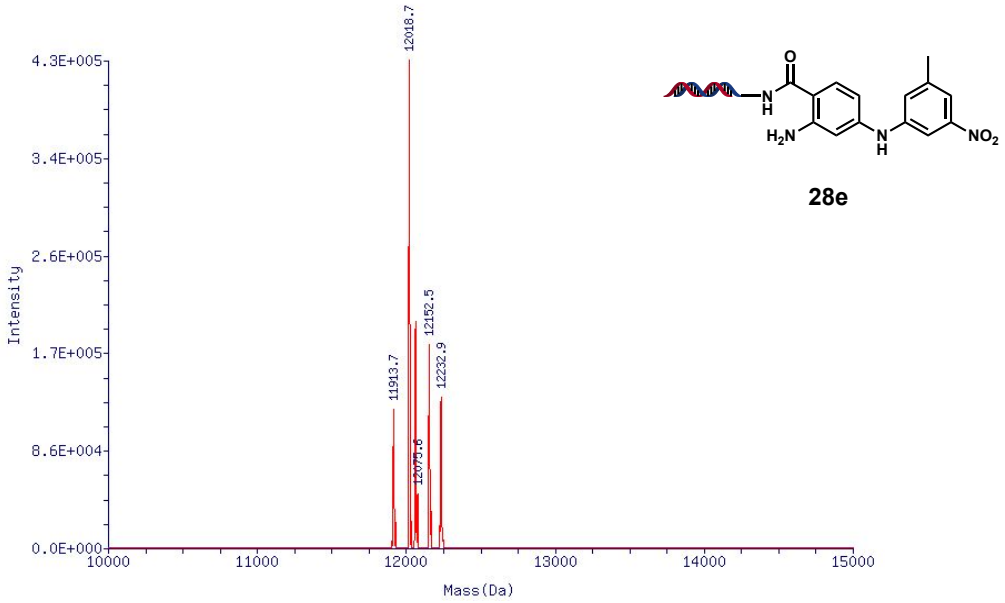


Figure S344. Deconvoluted mass spectrum of DNA **28e**, expected: 12301.2; no product observed.

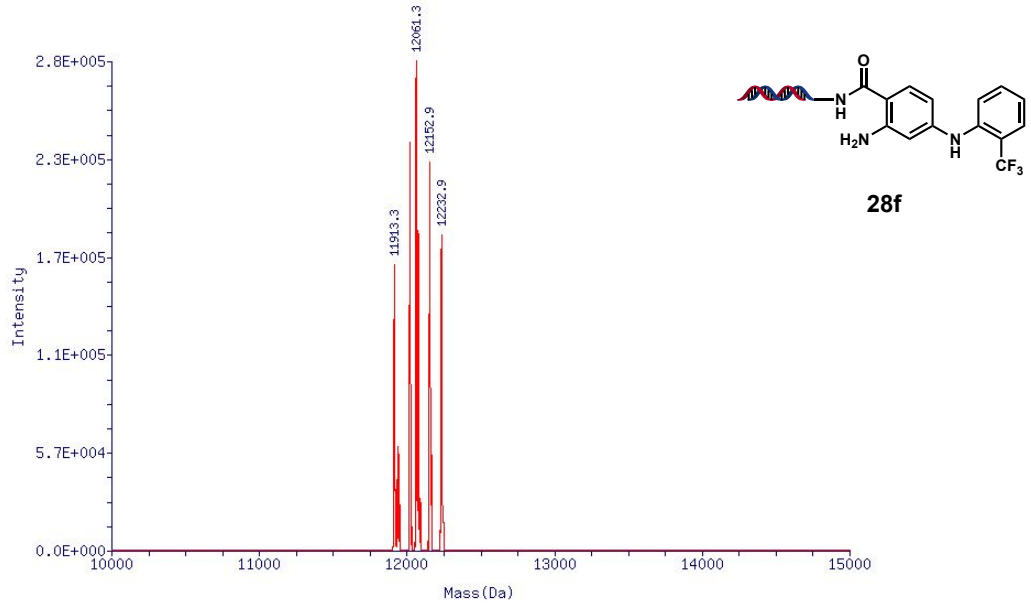


Figure S345. Deconvoluted mass spectrum of DNA **28f**, expected: 12310.2; no product observed.

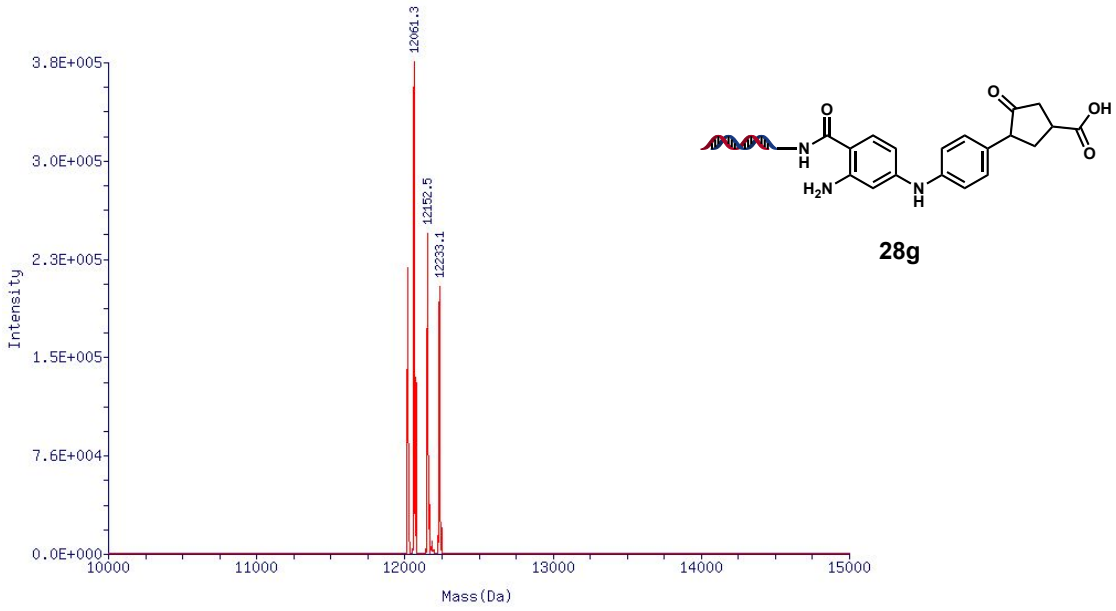


Figure S346. Deconvoluted mass spectrum of DNA **28g**, expected: 12369.2; no product observed.

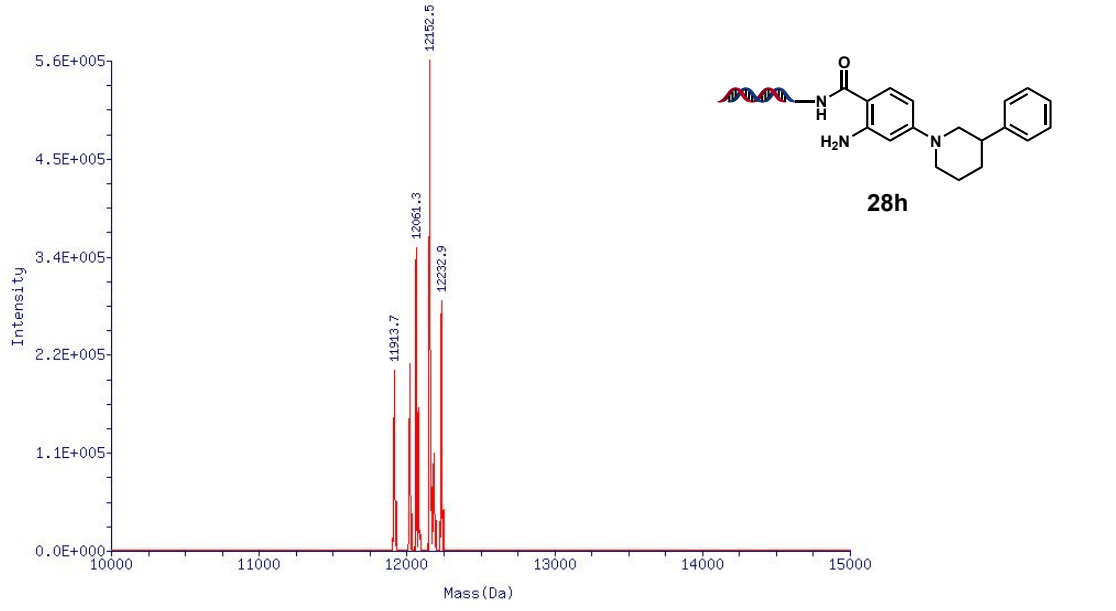


Figure S347. Deconvoluted mass spectrum of DNA **28h**, expected: 12310.3; no product observed.

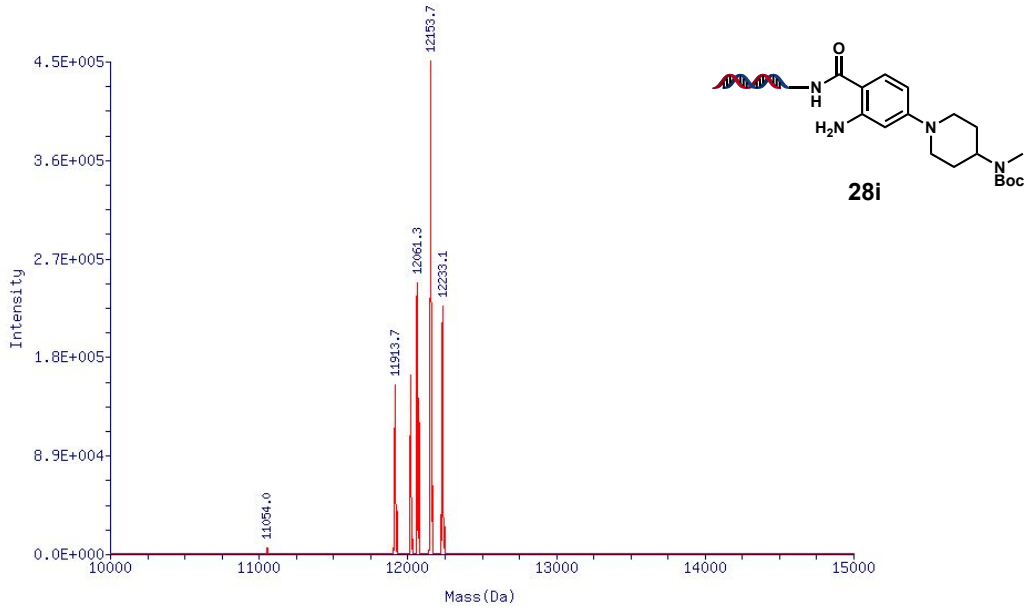


Figure S348. Deconvoluted mass spectrum of DNA **28i**, expected: 12363.4; no product observed.

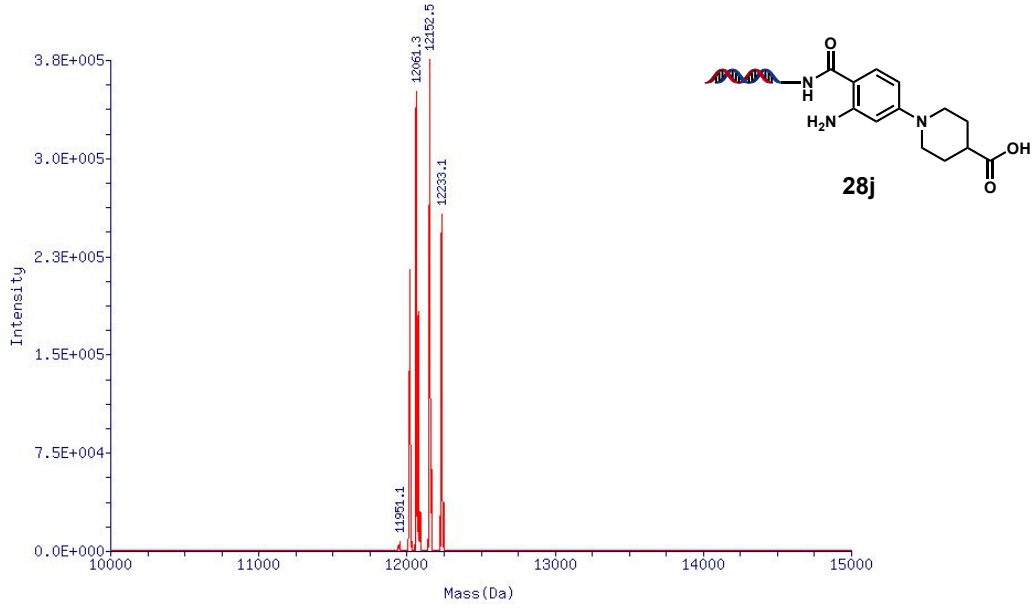


Figure S349. Deconvoluted mass spectrum of DNA **28j**, expected: 12278.3; no product observed.

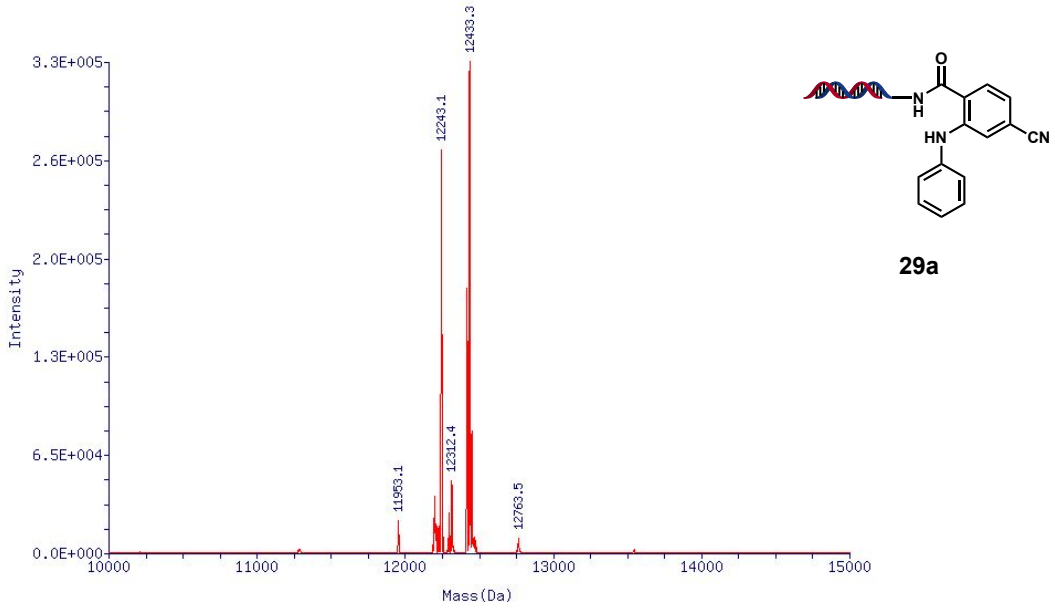


Figure S350. Deconvoluted mass spectrum of DNA **29a**, expected: 12280.2; no product observed.

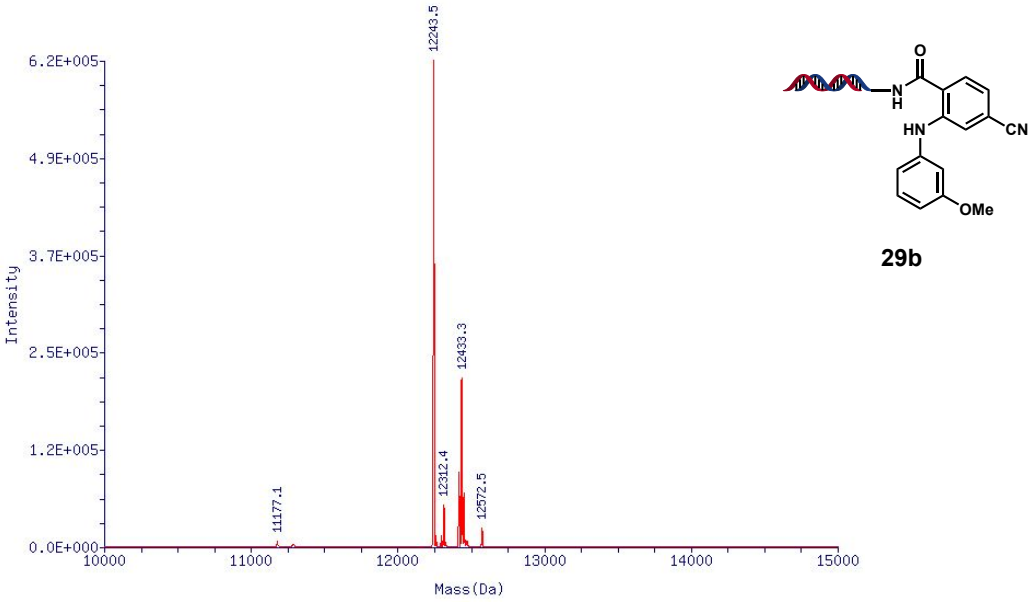


Figure S351. Deconvoluted mass spectrum of DNA **29b**, expected: 12310.3; no product observed.

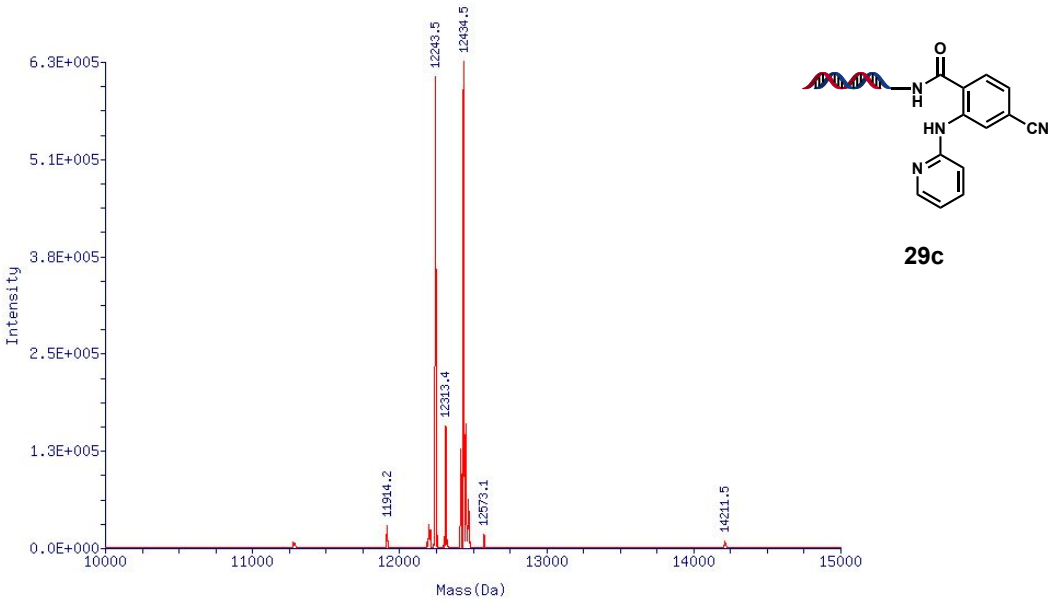


Figure S352. Deconvoluted mass spectrum of DNA **29c**, expected: 12281.2; no product observed.

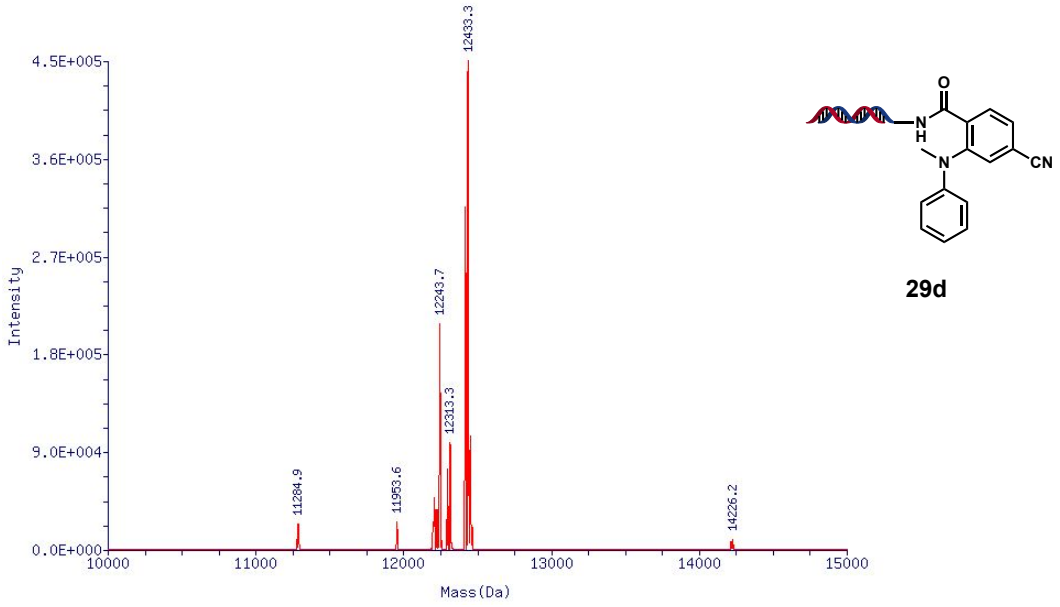


Figure S353. Deconvoluted mass spectrum of DNA **29d**, expected: 12294.3; no product observed.

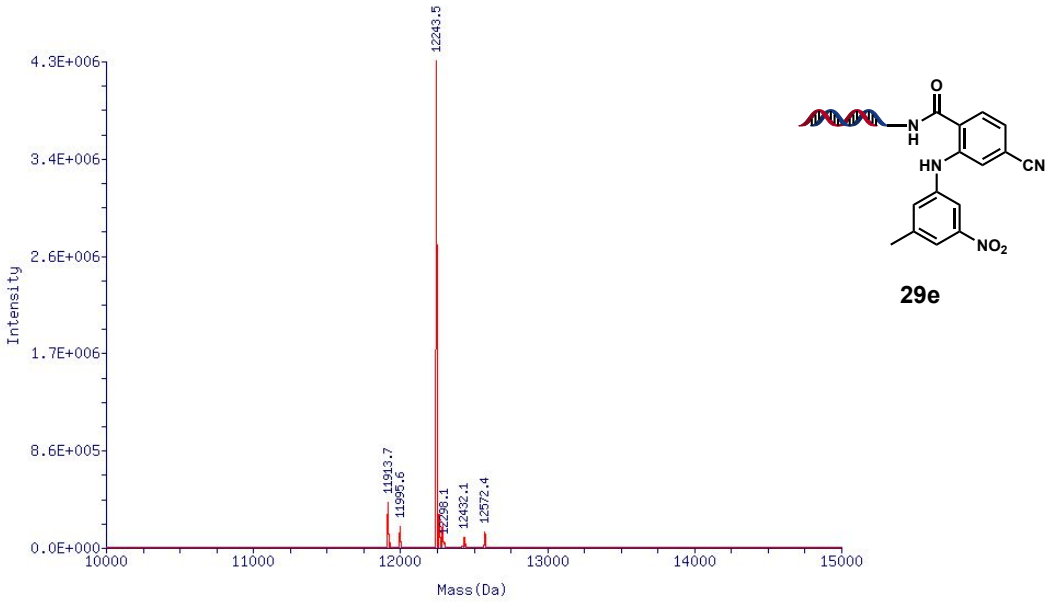


Figure S354. Deconvoluted mass spectrum of DNA **29e**, expected: 12339.3; no product observed.

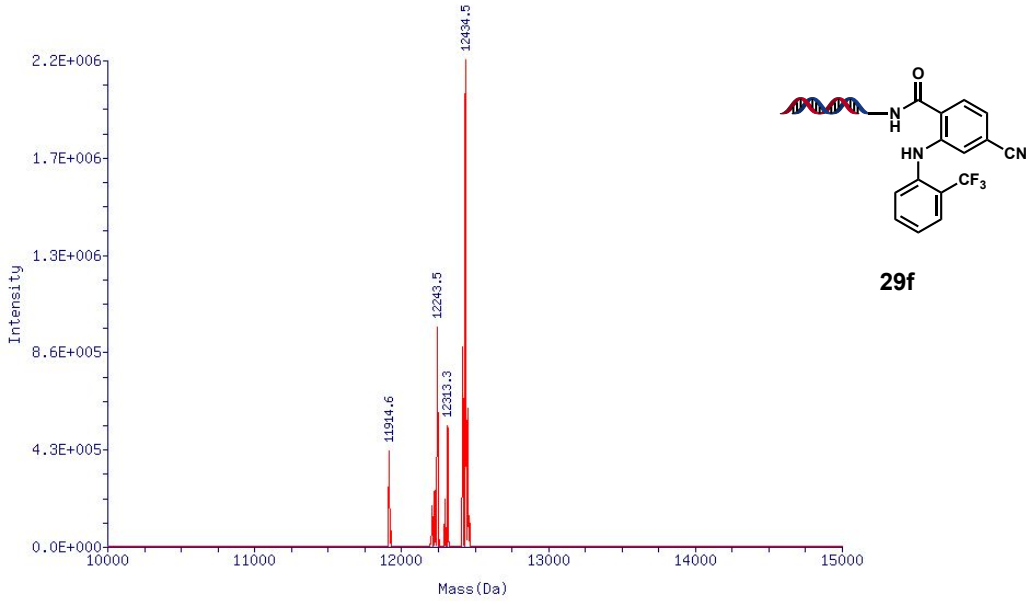


Figure S355. Deconvoluted mass spectrum of DNA **29f**, expected: 12348.2; no product observed.

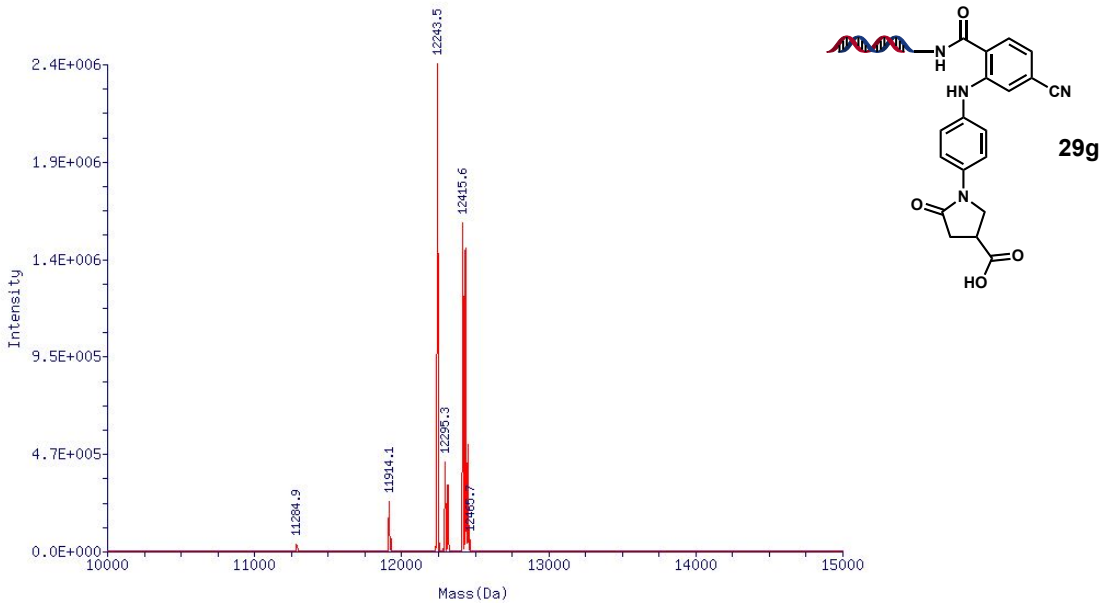


Figure S356. Deconvoluted mass spectrum of DNA **29g** , expected: 12407.2; no product observed

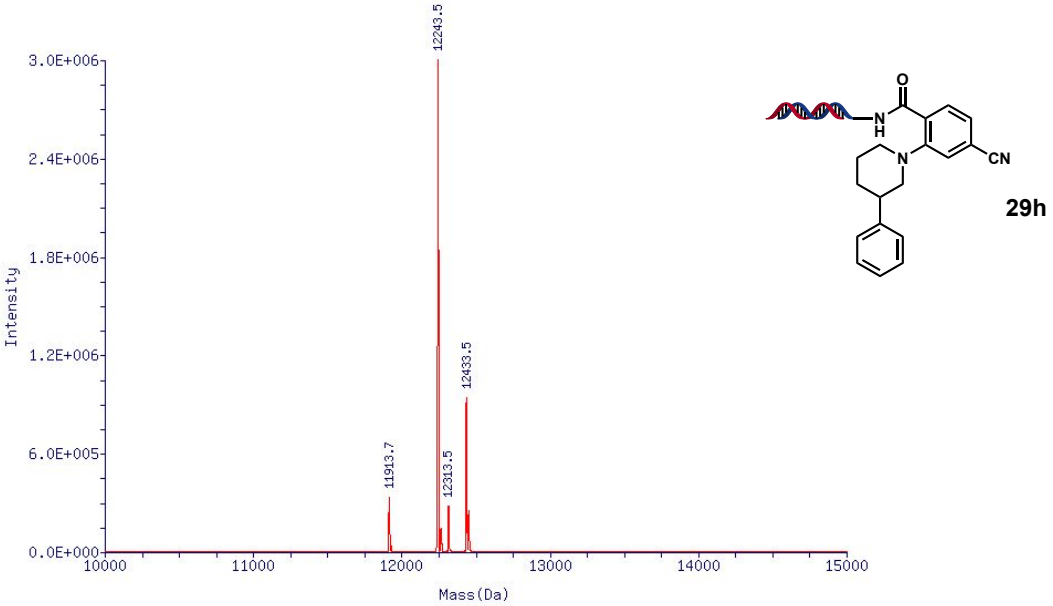
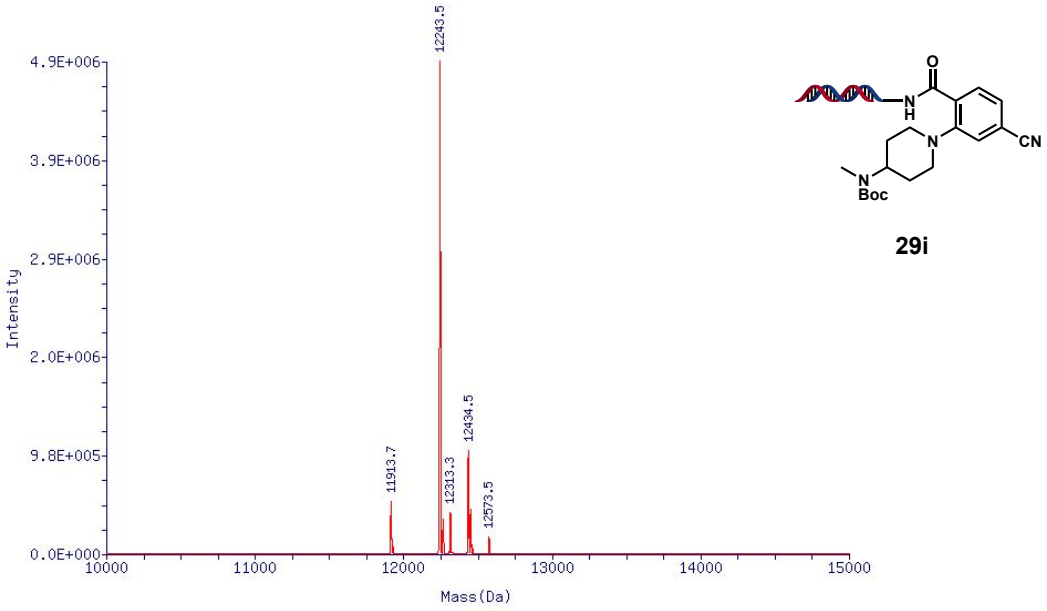
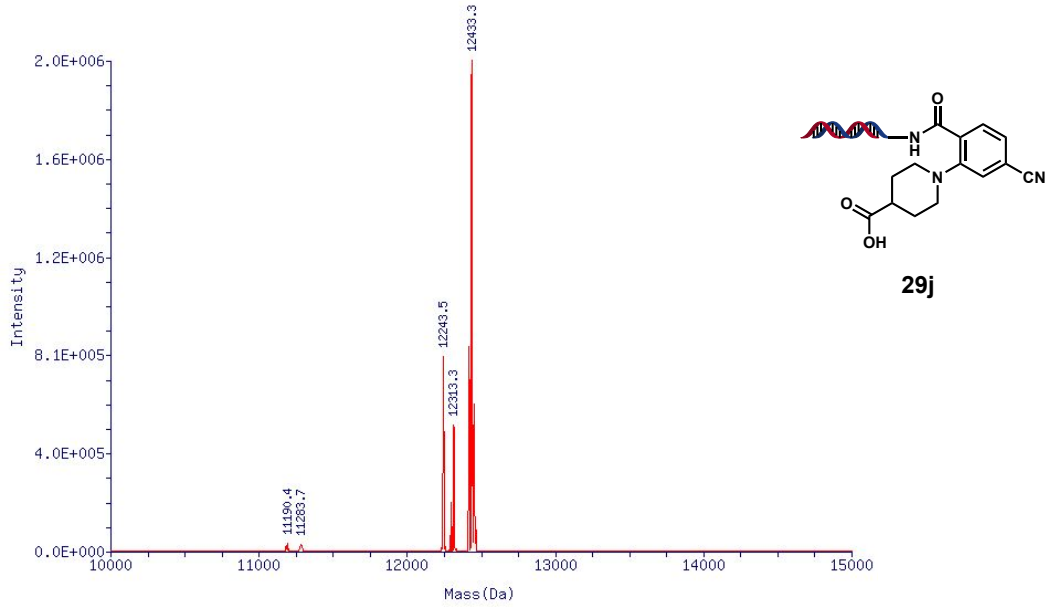


Figure S357. Deconvoluted mass spectrum of DNA **29h**, expected: 12348.4; no product observed.



29i

Figure S358. Deconvoluted mass spectrum of DNA **29i**, expected: 12401.4; no product observed.



29j

Figure S359. Deconvoluted mass spectrum of DNA **29j**, expected: 12316.3; no product observed.

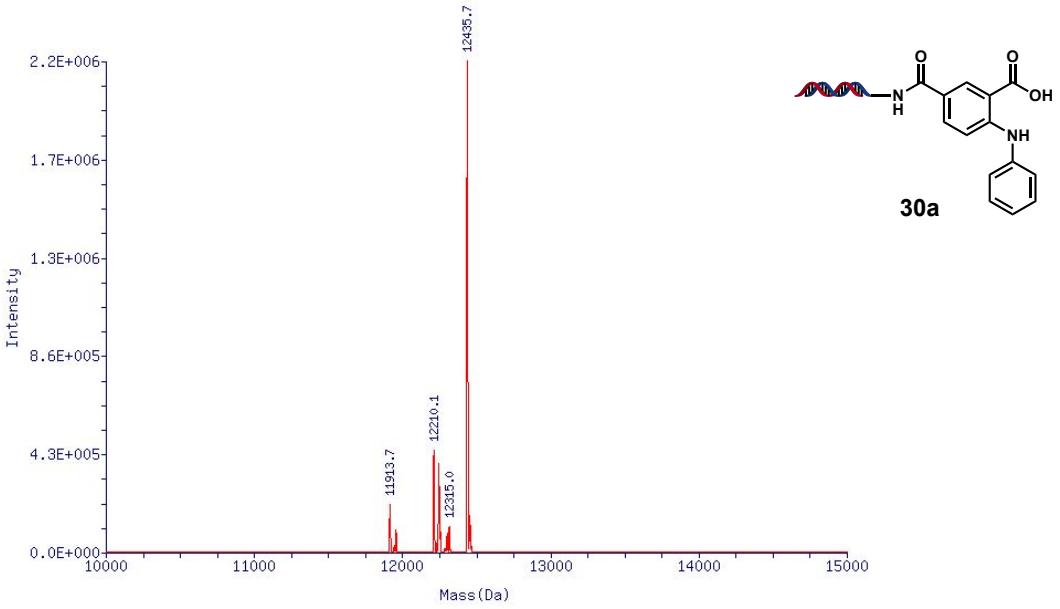


Figure S360. Deconvoluted mass spectrum of DNA **30a**, expected: 12299.2; no product observed.

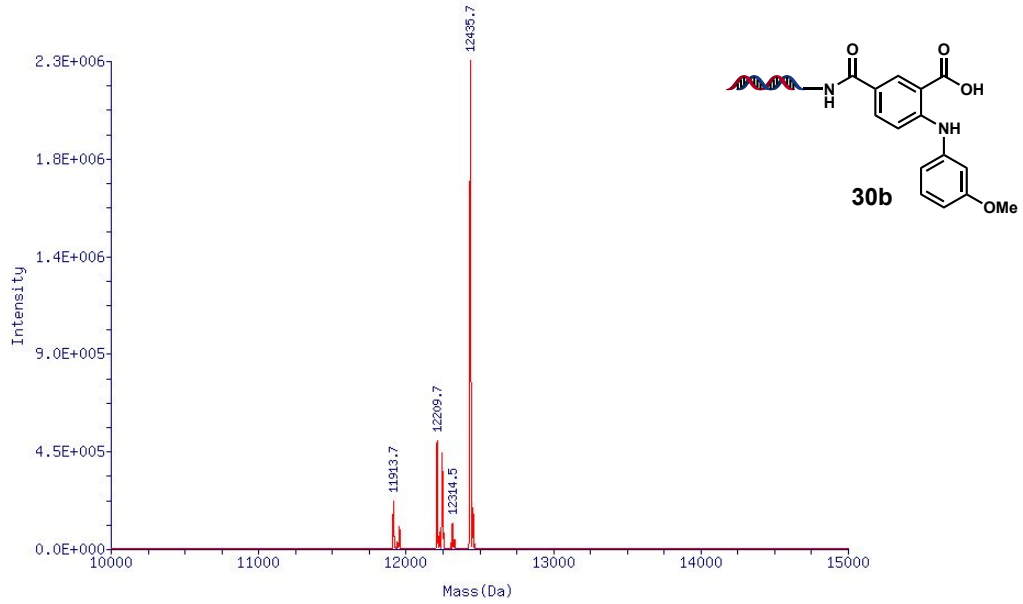


Figure S361. Deconvoluted mass spectrum of DNA **30b**, expected: 12329.3; no product observed.

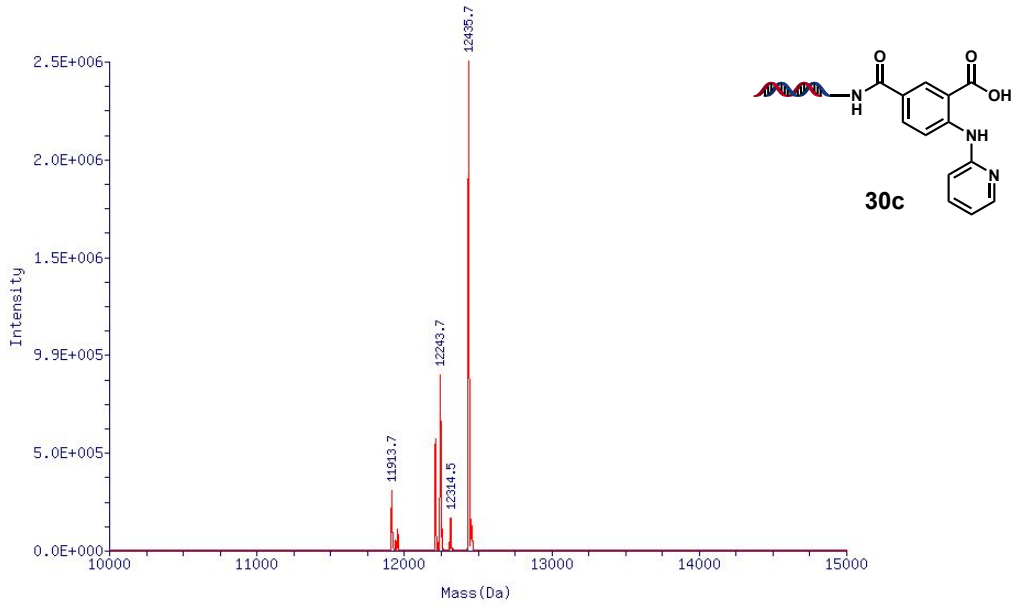


Figure S362. Deconvoluted mass spectrum of DNA **30c**, expected: 12300.2; no product observed.

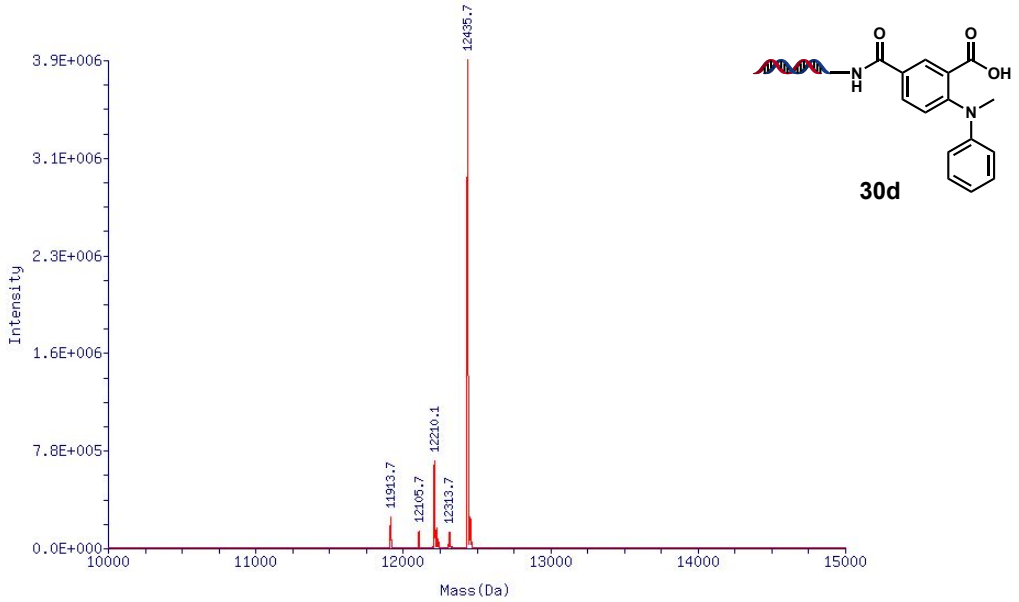


Figure S363. Deconvoluted mass spectrum of DNA **30d**, expected: 12313.3; no product observed.

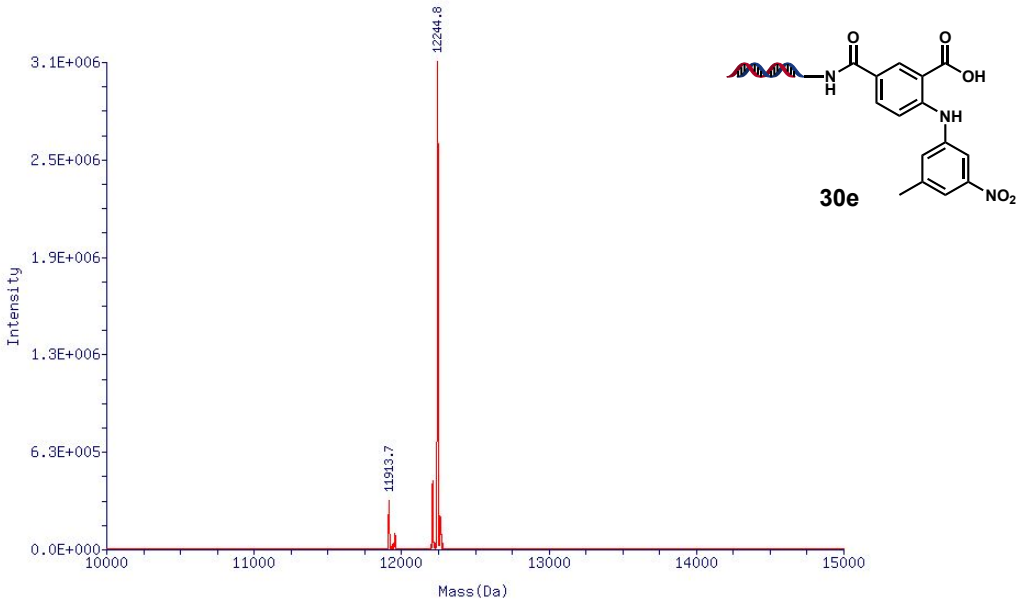


Figure S364. Deconvoluted mass spectrum of DNA **30e**, expected: 12358.3; no product observed.

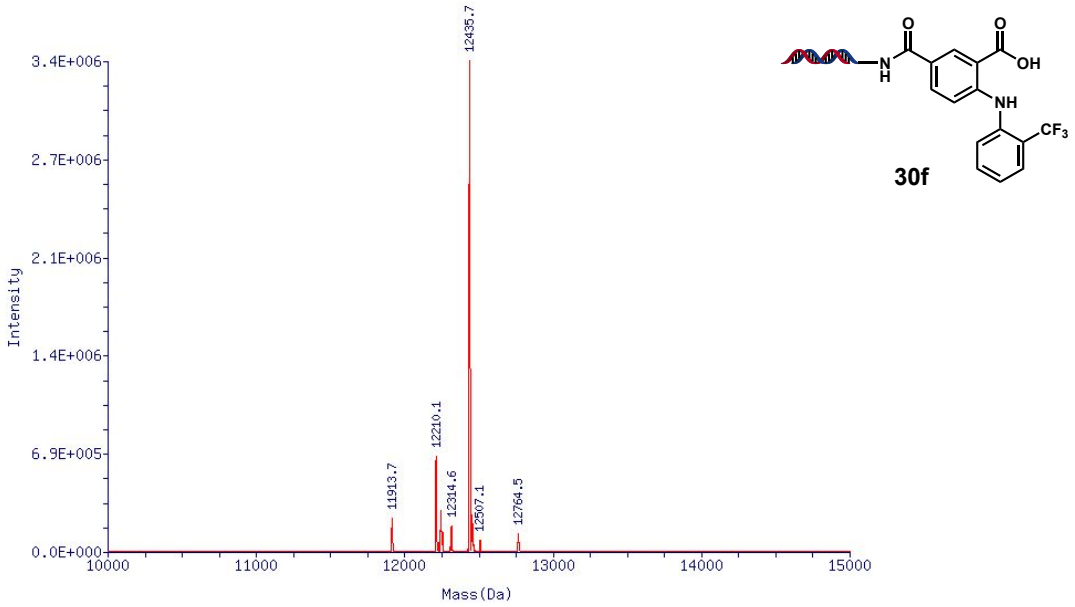


Figure S365. Deconvoluted mass spectrum of DNA **30f**, expected: 12367.2; no product observed.

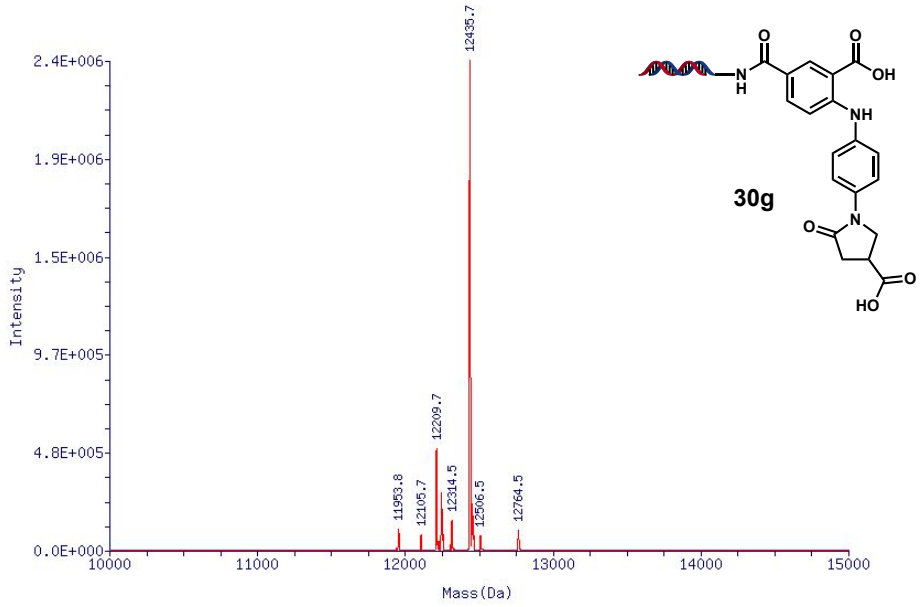


Figure S366. Deconvoluted mass spectrum of DNA **30g**, expected: 12426.2; no product observed.

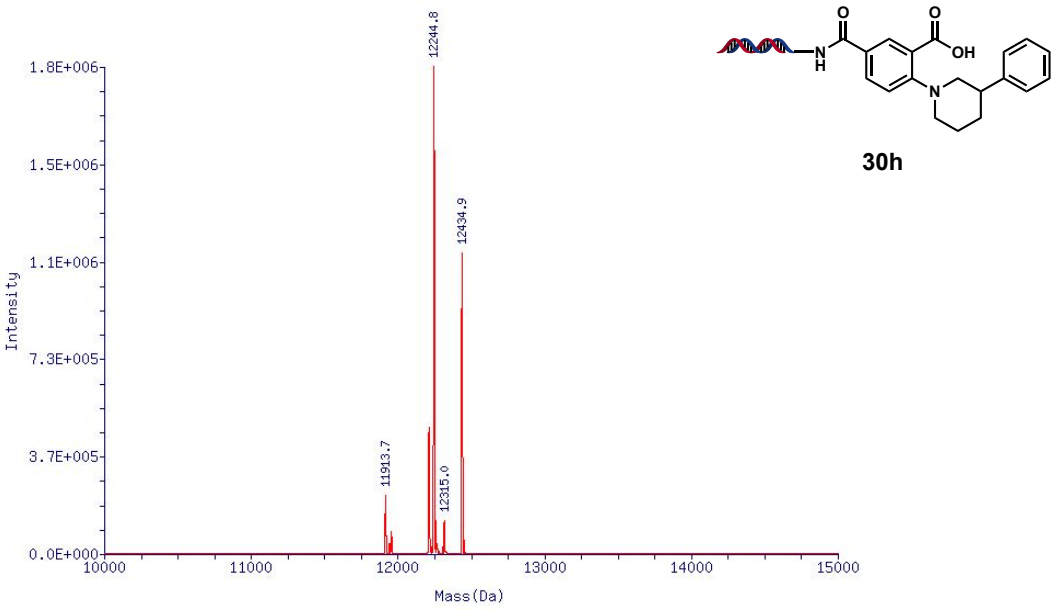


Figure S367. Deconvoluted mass spectrum of DNA **30h**, expected: 12367.4; no product observed.

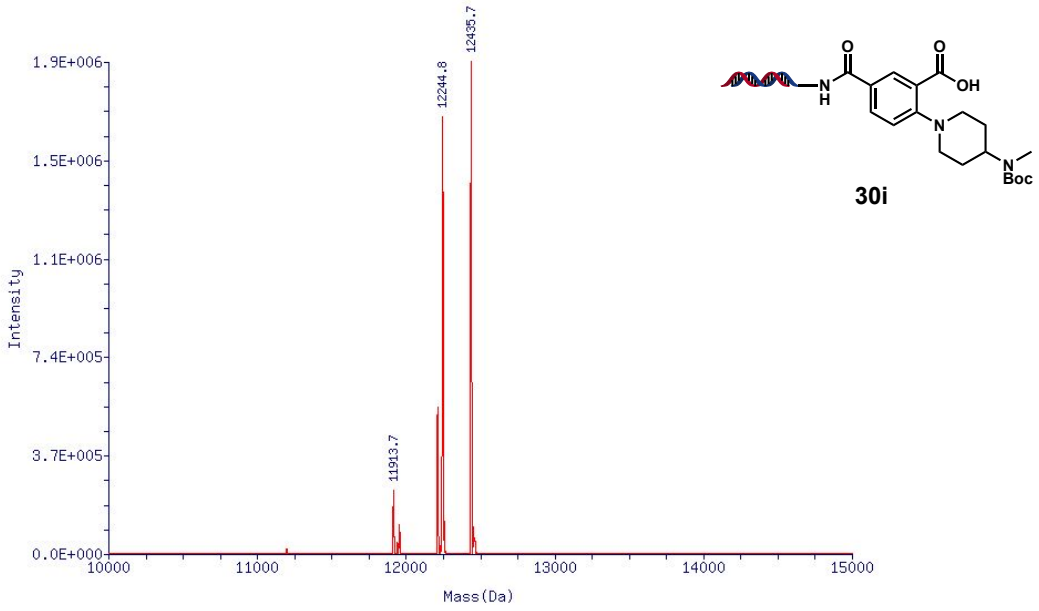


Figure S368. Deconvoluted mass spectrum of DNA **30i**, expected: 12420.4; no product observed.

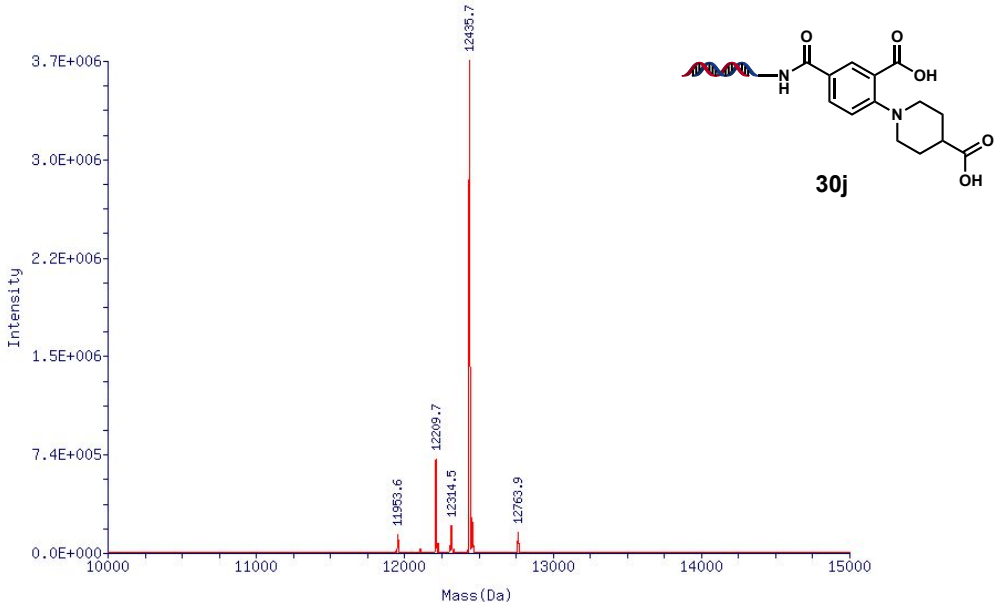
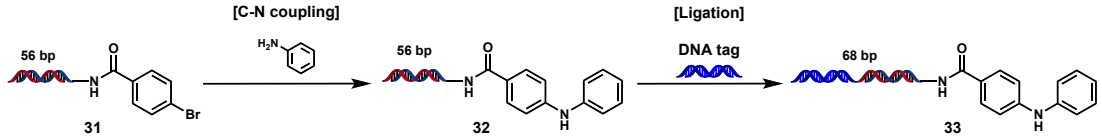


Figure S369. Deconvoluted mass spectrum of DNA **30j**, expected: 12335.3; no product observe

6. DNA stability and ligation test



Scheme S1. Validation of C–N coupling on substrate **31** to form product **32** and the subsequent DNA tag ligation to afford **33**.

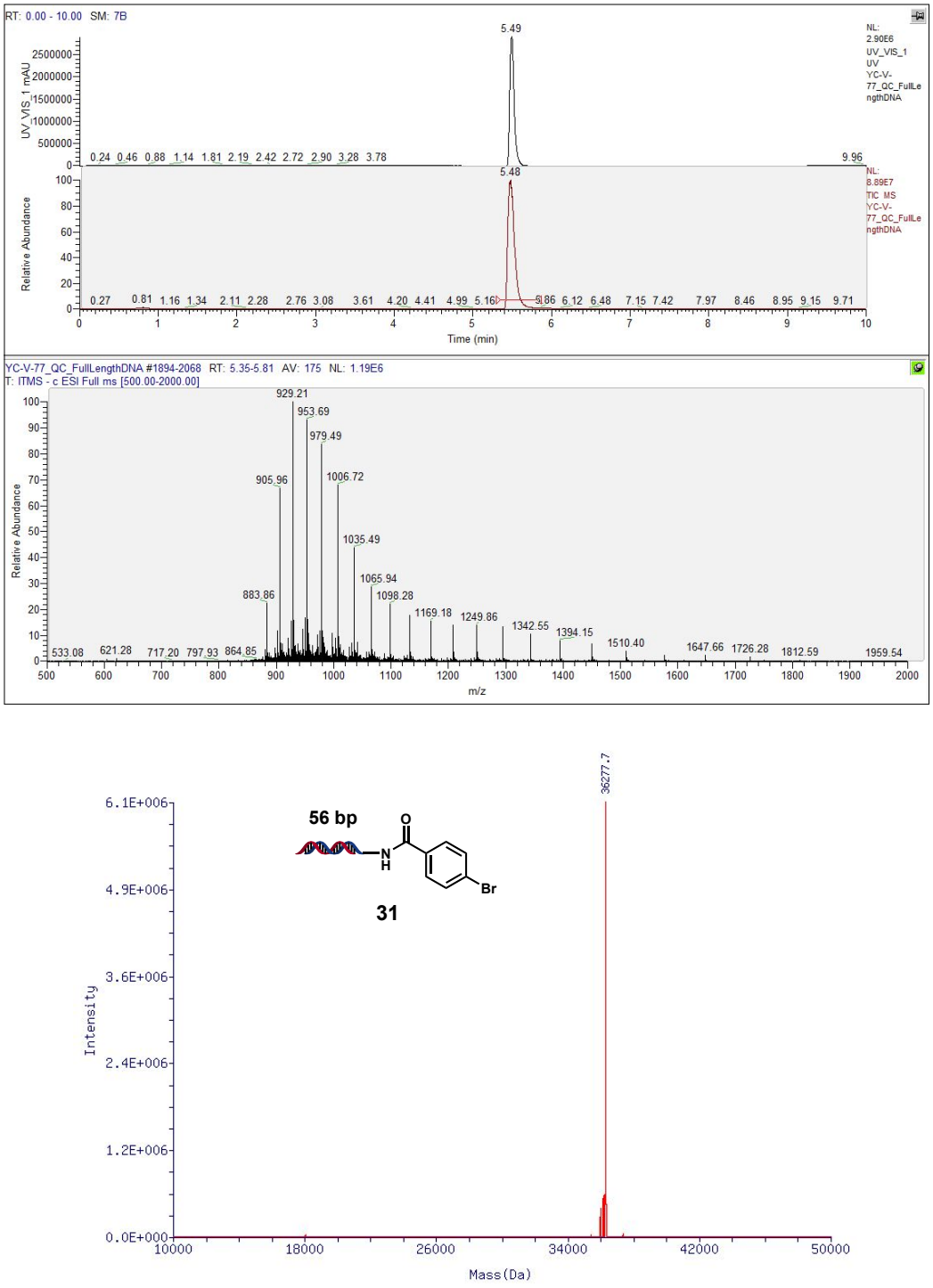
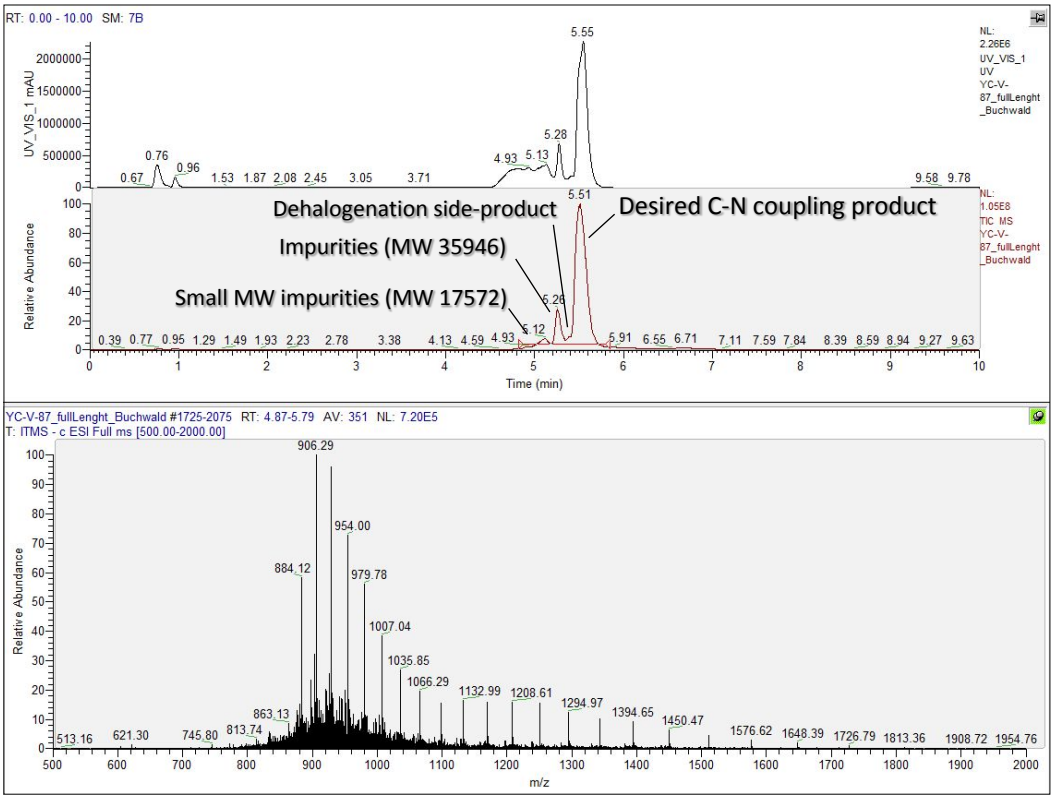


Figure S370. Deconvoluted mass spectrum of full length DNA-conjugated 4-bromo benzoate **31** purified by HPLC, expected: 36275; Observed: 36277.7.



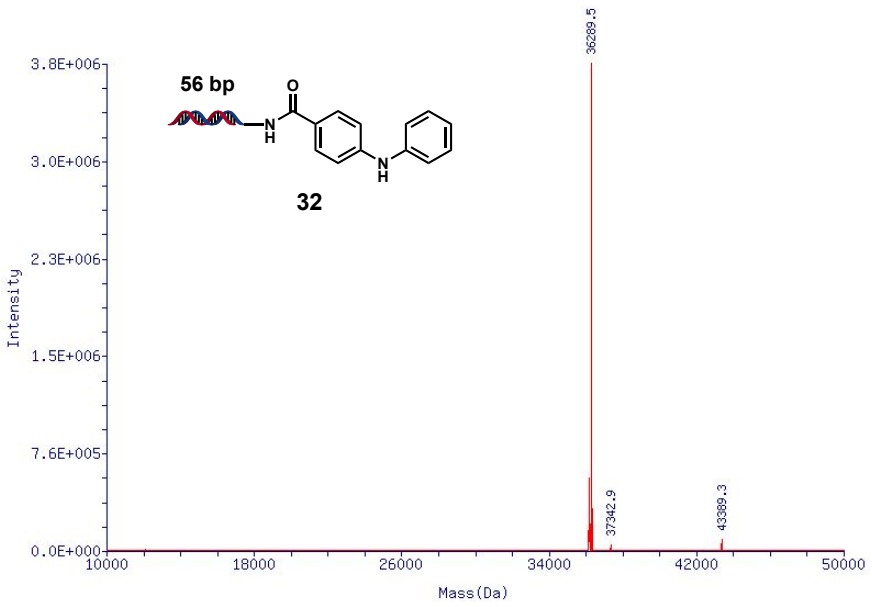
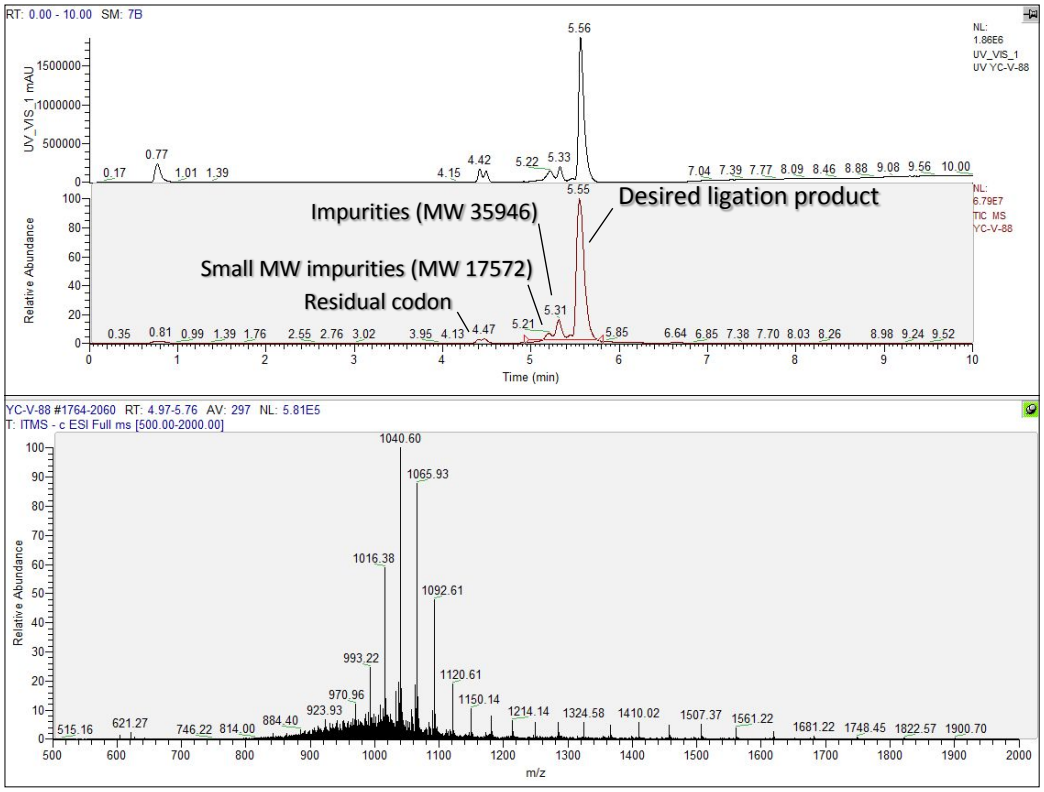


Figure S371. Deconvoluted mass spectrum of DNA-conjugated product **32** after C–N coupling, expected: 36287.22; Observed: 36289.5.



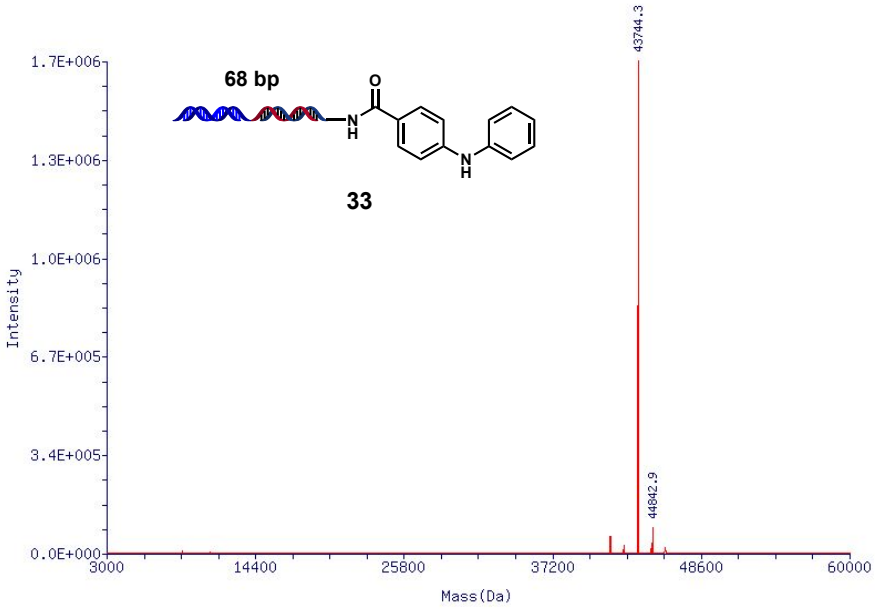


Figure S372. Deconvoluted mass spectrum of ligation product **33** after Buchwald coupling, expected: 43742.05; Observed: 43744.3.

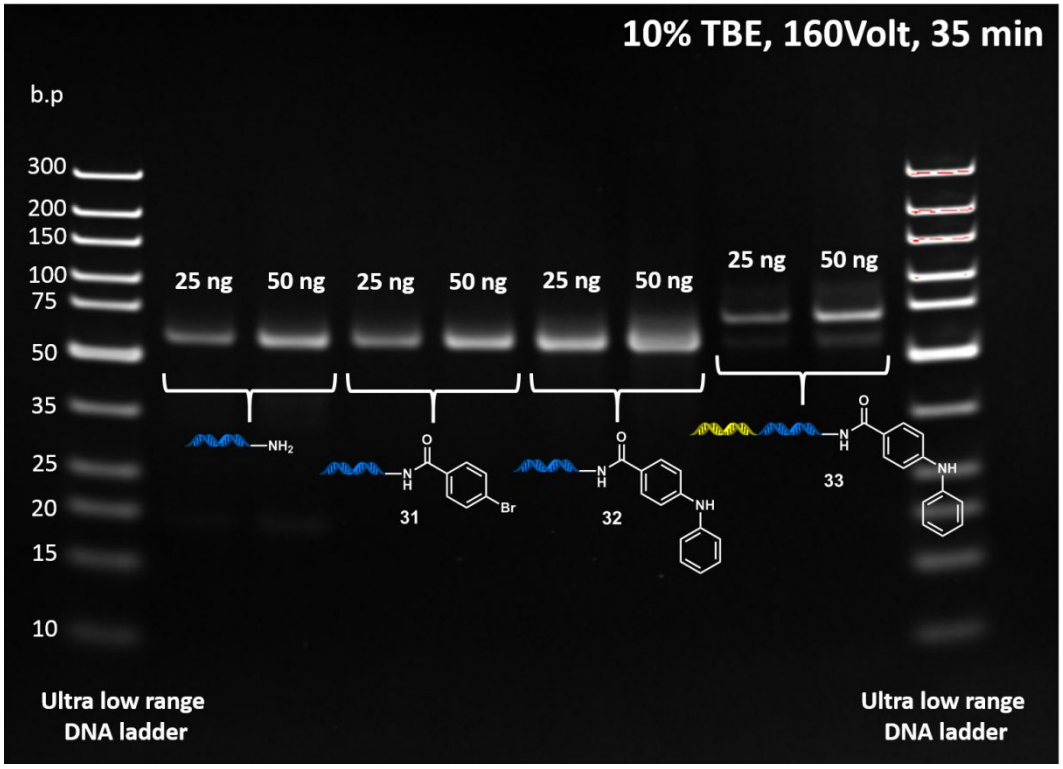


Figure S373. Gel electrophoresis image comparing the starting DNA unit, starting material **31**, C–N coupling product **32** and the subsequent ligation product **33**.

7. Synthesis of a DNA-Encoded Chemical Library (DECL) using C–N coupling condition

7a. Architecture of the Main Library build. The DECL was produced as a three-cycle library. It was built through three iterative cycles, each containing a chemical transformation, corresponding DNA oligonucleotide (codon) encoding ligation phase and material pooling and splitting for the subsequent cycle. The library is constructed on HP **S2** (shown here as combination of DTSU, first overhang, forward primer unit, and second overhang, Figure S374), which had been further diversified on the small molecule end with various amino- or carboxy-terminating linkers. Overhangs between codons are two base pairs and encoding regions within codons feature eleven base pairs. Specific details and principles related to the overall oligonucleotide sequence design utilized in our DECL production pipeline have been discussed previously.[3]

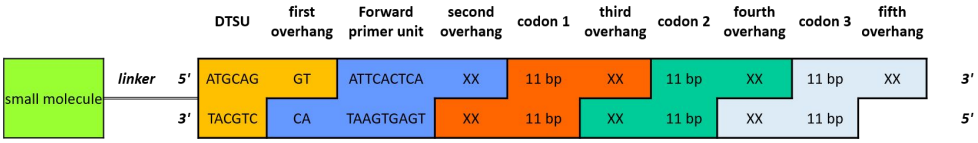


Figure S374. Architecture of the main library build. Separately assembled/ligated oligonucleotides (codons) are shown in different colors.

7b. Building block diversity analysis. To identify a good building block set to employ in a library build, we first scanned a database of commercially available compounds for the requested chemical functionality with an in-house substructure match script utilizing SMARTS patterns. During this scan, we also limited the molecular weight of building blocks to 350 Da and filtered out building blocks containing functional groups that might interfere with the planned reactions. We eliminated the functionalities that would lead to multiple, ambiguous products at any stage along the library synthesis. The database we used for this purpose was the most up-to-date version of the Aldrich Market Select Full Release. This first pass of filtering reduced the size of the building block pool significantly, which was further reduced upon application of cost, minimum available amount, and delivery time filters. The resulting pool of building blocks was further examined for functional groups that might pose liabilities for on-DNA chemistry and medicinal chemistry optimizations, and these groups were eliminated from the pool. Additional physical property filters such as number of ring components, aromatic rings, the fraction of sp3-hybridized carbons to the rest of the carbons, and chiral center counts were imposed. The library chemists perused the set in development to give feedback about the compatibility with the design and possible built-in structure-activity relationship potential. If there were certain building blocks that they specifically would like to include, we ensured the retention of these building blocks. The set was analyzed for diversity by generating histograms of the examined physical and other computed properties including calculated logP and Murcko scaffolds. This filtered set of building blocks was then reviewed by the library chemists for compatibility with the library design.

Bifunctional building blocks, in which both functionalities would take part in separate reactions within the library build, were also subject to evaluation of the variety in their shapes via exit vector analysis.[12-15] The exit vectors were assumed to lie along the two functional groups pivoting from where they were attached to the main chemical scaffold (e. g. a ring). The distance between these pivot points, the angle spanned by the first functional group vector and the vector connecting the two pivot points, the angle spanned by the second functional group vector and the vector connecting the two pivot points, and the dihedral angle spanned by the relative alignment of the two functional group vectors were calculated for each building block. These properties were binned to assess their

distributions through histograms. With this exercise, the goal was to ensure the functional groups were presented to the reactions in diverse ways.

7c. General procedures utilized in the DECL build. General information listed previously of procedures for material preparation, oligonucleotide analysis, ethanol precipitation, and ligation were applied in the library build (see sections 1a–1e). Cholesterol-tagged DNA oligomer ("spike in") was employed in cycle 2 and cycle 3 to monitor reactions in pooled library manner, which provided different retention time in LC-MS. Other general procedures related to chemical transformations were performed as followed:

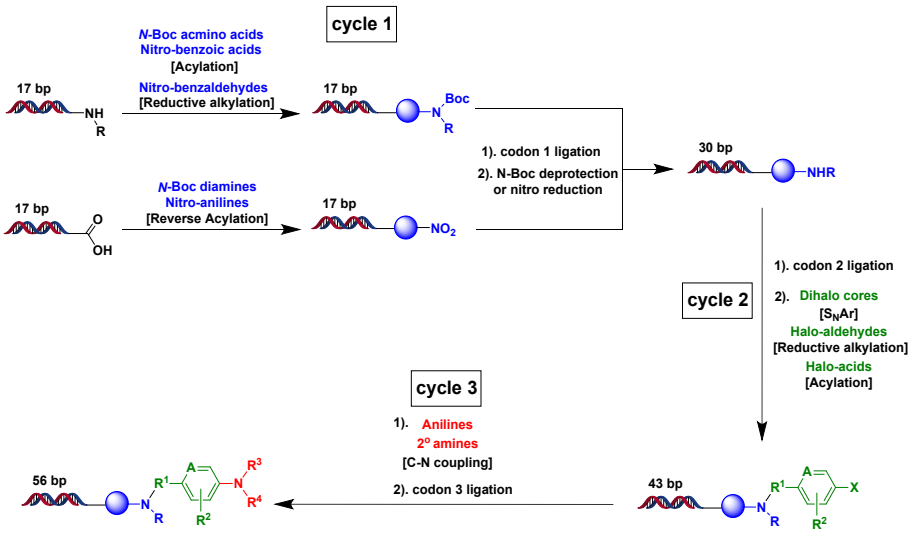
Reverse Acylation: To an on-DNA carboxylic acid (35 nmol, 32 μL, 1.1 mM in H_2O) in pH 5.8 MES buffer (17500 nmol, 35 μL, 500 equiv), additional water (29.3 μL) and acetonitrile (43.8 μL) were added 100 equivalents of amino-building block (17.5 μL, 200 mM in MeCN) and 100 equivalents of DMTMM (17.5 μL, 200 mM in water). The solution was allowed to incubate for 18 h at room temperature. The reactions were assessed for completion and precipitated by EtOH precipitation.

Nitro Reduction (hypodiboric acid)[4]: To a solution of nitro-containing DNA conjugate (3 μL, 1.0 mM in water) was added 500 equivalents of NaOH solution (1 μL, 1500 mM in water), water (2 μL) and EtOH (4.5 μL), followed by the addition of 150 equivalents of $B_2(OH)_4$ (4.5 μL, 100 mM in water). The reaction mixture was incubated at room temperature for 2 h prior to EtOH precipitation. Second EtOH precipitation was performed after reconstitution the DNA pellet with water in order to remove residual building blocks and salts before further ligation. The solution of $B_2(OH)_4$ in neutral water was prepared freshly from vortexing or brief sonication before use.

Nucleophilic aromatic substitution (DABCO): To amino-terminated DNA (47.7 nmol, 50 μL, 1 equiv, soln in H_2O), NaOH (47620 nmol, 9.52 μL, 1000 equiv, 5M in H_2O), and additional water (100 μL) were added. Then an electrophilic dihaloarene (14286 nmol, 71 μL, 300 equiv, 200 mM in CH_3CN) and DABCO (476 nmol, 4.76 μL, 10 equiv, 100 mM in CH_3CN) were added and the solution was incubated at room temperature overnight. The reactions were then assessed for completion and/or precipitated by the general procedures.

Buchwald–Hartwig cross coupling: see section 2b.

7d. Synthetic sequence of the library build.



Scheme S2. Synthetic sequence of the Main Build. Cycle 1 is shown in blue, cycle 2 is shown in green and cycle 3 is shown in red.

Procedure for Cycle 1. Various linker-functionalized **S2** (35 nmol/well) were plated individually into wells in 96-well plates. *N*-Boc amino acids (57) and nitro benzoic acids (23) were acylated onto four different amine-terminating DNA substrates. Nitro benzaldehydes (14) were attached through reductive amination onto four different amino-terminating DNA substrates in separate wells. *N*-Boc diamines (183) and nitro anilines (23) were attached by reverse acylation to two different carboxylic acid terminated DNA substrates in separate wells. In addition, blanks were included as controls of building block-free and/or reagent-free conditions. After precipitation, each chemical transformation was encoded through the ligation with a unique pair of 13-mer duplexed DNA oligonucleotides (codon 1) in separate wells. Finally, the *N*-Boc carbamates and nitroarenes were deprotected in well using the general procedures for *N*-Boc deprotection or nitro reduction, respectively. Each well was carefully analyzed by LC-MS before being quenched. After pooling and additional ethanol precipitation, approximately 24 μmol of the cycle 1 library pool was recovered.

Procedure for Cycle 2. After splitting a portion of the cycle 1 pool into 336 wells (47.6 nmol/well), each well underwent codon 2 ligation by the general procedure. A Series of dihaloarenes (33) were attached through nucleophilic substitution using both the pH 9.5 heating and DABCO promoted methods. A Series of carboxyl aryl halides (99) were acylated employing both the DEPBT and DMTMM methods, and a series of aldehyde aryl halides (33) were attached by reductive amination using both the $NaCNBH_3$ and $NaBH_4$ methods. The conditions of these methods are described in sections previously mentioned and all methods were separately encoded with unique codons. In addition, blanks to encode the no reaction or reagent related side products were included. After pooling and additional precipitation, approximately 14.6 μmol of the Cycle 2 pool was recovered.

Procedure for Cycle 3. After splitting a portion of the cycle 2 pool into 482 wells (11 nmol/well), a series of anilines (386) and secondary amines (96) were attached by Buchwald–Hartwig cross coupling. In addition, several blanks were included without building block and/or reagents in order to incorporate possible side-products. After EtOH precipitation, chemical transformation in each well was encoded with the ligation of codon 3 DNA tags. After pooling

and additional precipitation, approximately 3.9 μmol of the Cycle 3 pool was recovered (72% recovery yield after cycle3 chemistry and codon3 ligation).

Preparation of amplifiable DECL samples ("shots") for experiments. After completion of the main library builds, the entire library material was ligated with a duplexed pair of 12-mer DNA oligonucleotides to encode the overall library structure/design. After EtOH precipitation, partial material underwent sequential ligation with two DNA oligonucleotides, containing a region to encode selection experiment, a degenerate region as an amplification control, a segment to increase sequencing base diversity, and a reverse primer region for post-selection PCR amplification (the purposes/design of these components are discussed in our previous publication[3]).

8. DECL sequencing and selection experiments

Naïve Amplification:

An amplifiable DECL shot was quantified by quantitative Real-Time PCR (qPCR) and then a total of $1.54X10^7$ DNA copies were amplified by PCR with primers adaptors to add the sequences compatible with Illumina sequencing flowcells. Platinum Taq DNA Polymerase High Fidelity (Thermo Fisher Scientific) PCR reagent was used for PCR amplification. A total of 16 PCR cycles were used for amplification and the following PCR conditions were used (Initial denaturation at 95 °C for 2.5 min, denaturation at 95 °C for 30 s, annealing at 58 °C for 30 s, extension at 72 °C for 1 min and final extension at 72 °C for 10 min). PCR library temple was purified using Agencount AMPure XP SPRI beads according to the manufacturer's instructions. The purified library was analyzed in Bioanalyzer 2100 (Agilent Technologies, Santa Clara, CA) by using Agilent high sensitivity DNA kit to verify library size and concentration before clustering. Illumina NextSeq 500 was used for sequencing.

To ensure the integrity of DNA barcodes in our libraries, we routinely perform a sequencing of the "naive" or unscreened library material. We compare the "perfect read" rate with previous library data, and we examine the distributions of codon populations for each synthetic cycle. No anomalies were observed in our analysis of the library material, and the % perfect rate observed (69%) was close to our historical average (76%). It should be noted this analysis was performed on *non-HPLC purified* library material and thus reflects the total integrity of the library material within the build.

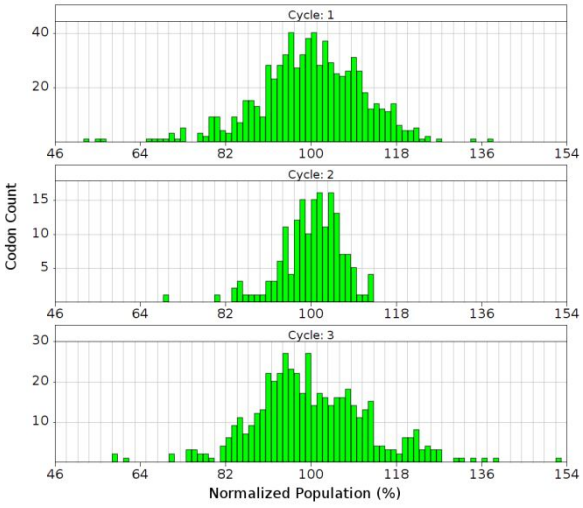


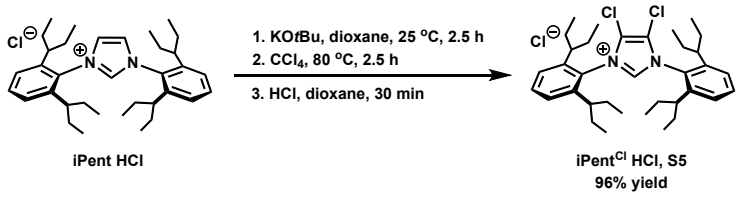
Figure S375. Distributions of observed codon populations from sequencing an unscreened library sample. For each synthetic cycle, the total count for each codon sequence was evaluated and normalized by the mean count for that

cycle, and reported as a percentage. Each histogram therefore shows the variation in codon populations about the mean count per cycle.

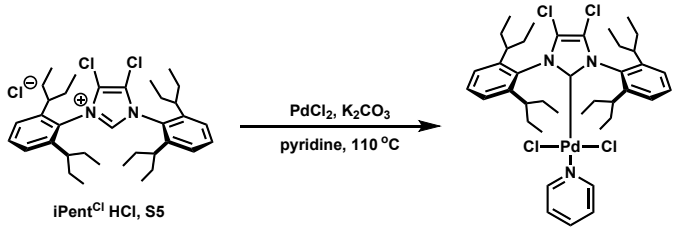
Sequencing analysis:

Raw DNA sequence reads (in the form of FASTQ files), quality metrics, and sequencing index-to-sample attribute value pairs were obtained from Illumina BaseSpace at the conclusion of sequencing. Samples were linked to their respective FASTQ files based on their sequencing index (DTSU) and were expanded into individual experiments if they were part of a larger pool. Individual samples were then decoded by perfectly matching individual oligonucleotide sub-structures without gaps and in the order defined by the known DNA encoding structure (Main Library Build). Valid DNA barcodes were annotated with the corresponding oligonucleotide sequence-to-building block lookup for each of the three codon cycles, which collectively represent a distinct small molecule within a specific DECL. The degenerate UMI (unique molecular identifier) portions of the DNA barcodes were accumulated into a list of UMIs for each unique codon tuple as a method to distinguish experimental vs. amplification events. Unique molecule counts were then evaluated using a directed-graph counting model as described previously.[3] The set of unique codon tuples with unique molecule counts was then aggregated across all possible combinations of codons (all *n-synthons*), and enrichment for each *n-synthon* was evaluated independently. Enrichment was evaluated with a normalized *z-score* metric which normalizes for sampling and library diversity.[3]

9. Representative procedures for the preparation of Pd-PEPPSI-iPent^{Cl}-pyr



iPent^{Cl} HCl S5. The procedure used for the preparation of **S5** was adapted from the work of Pompeo et al and Arduengo et al.[16,17] A flask charged with potassium *tert*-butoxide (0.251 g, 2.24 mmol, 1.2 equiv) and iPent HCl (1.000 g, 1.86 mmol, 1 equiv) was dried overnight under high vacuum. An atmosphere of N_2 was introduced and then dry 1,4-dioxane (7.44 mL, 0.25 M) was added and the solution was stirred for 2.5 h at 21 °C. Dry CCl_4 (7 mL) was then added, and the solution was heated to 80 °C for 2.5 h. After cooling, HCl (~1 mL, 4 M in 1,4-dioxane, ~3.72 mmol, ~2 equiv) was added slowly and the resulting slurry was stirred for 30 min at 21 °C. The reaction mixture was diluted with CH_2Cl_2 (30 mL), and then filtered through a Celite pad with additional CH_2Cl_2 washes. After concentration of the filtrate under reduced pressure, the resulting solids were triturated with small amounts of hexanes and diethyl ether to give nearly pure **S5** (1.082 g, 1.79 mmol, 96% yield) that spectroscopically consistent with previously reported characterization data.[17] **S5**: ^{1}H NMR (600 MHz, $CDCl_3$) δ = 12.99 (bs, 1H), 7.59 (t, *J* = 7.79 Hz, 2H), 7.31 (d, *J* = 7.79 Hz, 4H), 1.99 (bs, 4H), 1.81 (bs, 8H), 1.67 (m, 8H), 0.92 (bs, 12H), 0.87 (t, *J* = 7.32 Hz, 12H) ppm.



Pd-PEPPSI-iPent^{Cl}-pyr S6. The procedure used for the preparation of **S6** was adapted from the work of Pompeo et al.[9] An oven-dried flask charged with iPent^{Cl} HCl (0.200 g, 0.330 mmol, 1 equiv), $PdCl_2$ (0.058 g, 0.330 mmol, 1 equiv), and K_2CO_3 (0.228 g, 1.65 mmol, 5 equiv, **mortar-and-pestle crushed**), was placed under high-vacuum for several hours to dry all components. After the addition of an N_2 atmosphere, dry pyridine (2.2 mL, 0.15 mM) was added and the reaction was heated to 110 °C for 3 h. After cooling, the reaction slurry was filtered through a silica plug with additional CH_2Cl_2 washes and the filtrate was concentrated. After trituration with hexanes to remove residual pyridine, purification by flash column chromatography (silica, 10:0 → 4:6 hexanes:CH_2Cl_2) provided **S6** (0.220 g, 0.266 mmol, 81% yield) as a solid that spectroscopically consistent with the previously reported characterization data.[9] **S6**: R_f = 0.2 (silica, 1:1 hexanes:CH_2Cl_2); ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.52–8.50 (m, 2H), 7.53 (t, *J* = 7.40 Hz, 1H), 7.49 (t, *J* = 7.90 Hz, 2H), 7.29 (d, *J* = 7.90 Hz, 4H), 7.09 (t, *J* = 7.17 Hz, 2H), 2.97–2.91 (m, 4H), 2.06–1.97 (m, 4H), 1.94–1.84 (m, 4H), 1.71–1.62 (m, 4H), 1.55–1.45 (m, 4H), 1.13 (t, *J* = 7.43 Hz , 12 H), 0.84 (t, *J* = 7.43 Hz, 12H) ppm.

10. NMR spectra

General description:

NMR spectra were recorded at room temperature using an Avance III HD 600 MHz spectrometer (^{1}H NMR at 600 MHz and ^{13}C NMR at 150 MHz). Chemical shifts (δ) are given in parts per million (ppm) with reference to solvent signals [^{1}H-NMR: DMSO-d_6 (2.50 ppm); ^{13}C-NMR: DMSO-d_6 (39.50 ppm)]. Signal patterns are reported as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad). Coupling constants (*J*) are given in Hz.

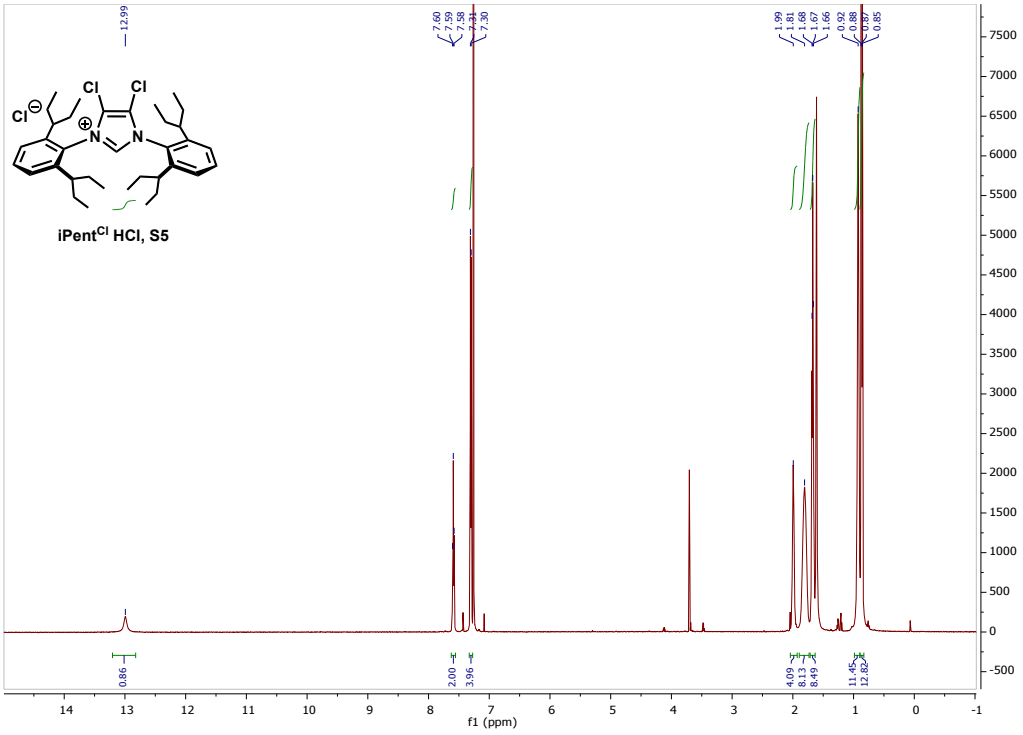


Figure S376. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of iPent^{Cl} HCl **S5.**

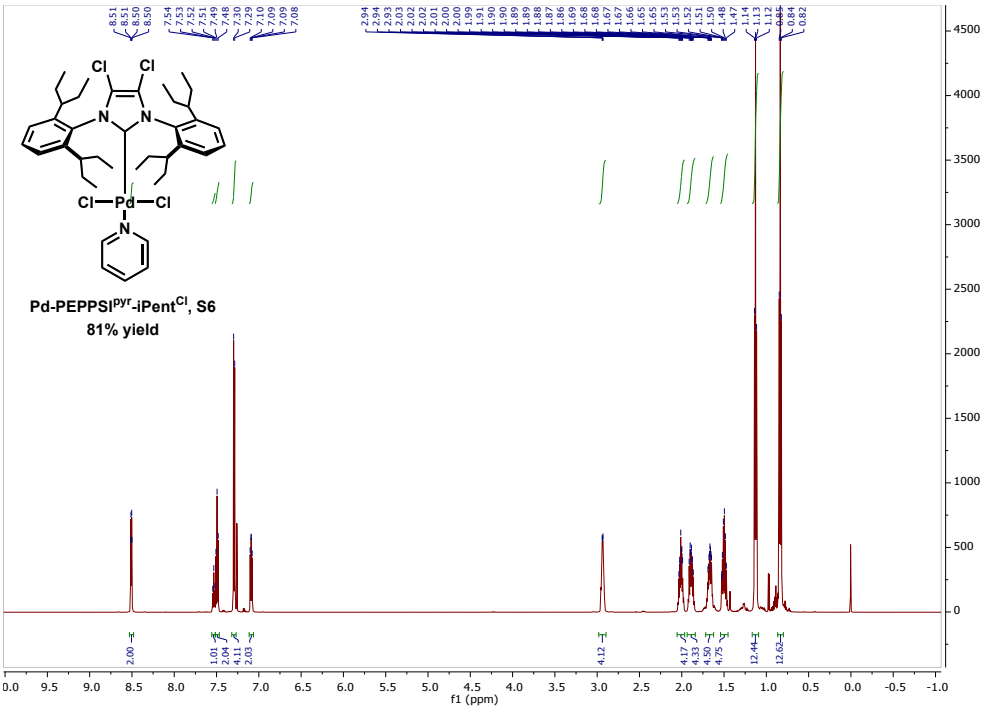
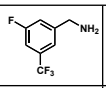
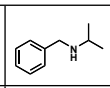
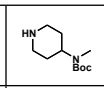
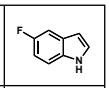
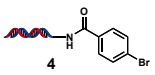
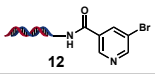


Figure S377. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of Pd-PEPPSI-iPent^{Cl}-pyr **S6**.

11. Representative results of C–N coupling on aliphatic amines and indoles

Table S4. Screening results of C–N cross coupling against 1° and 2° amines

									
 4	21%	24%	9%	35%	0%	63%	68%	66%	58%
 12	13%	11%	0%	18%	0%	52%	26%	17%	18%

12. Tables of screening results of C–N coupling

General description:

The screening of C–N coupling to substrate **4** and **12** were carried out on 5 nmol scale in 96-well plate. The conversions reported in table S1 were determined by LC/MS. The reported conversions for the ester-containing building blocks were generally observed as hydrolyzed carboxylic acid.

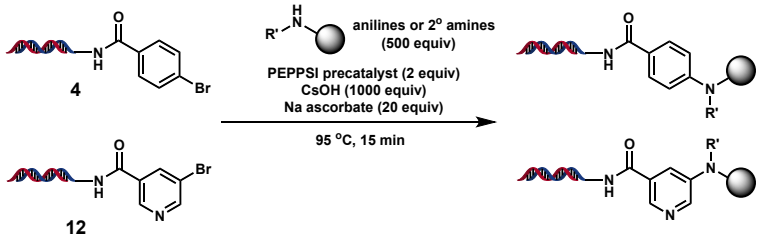
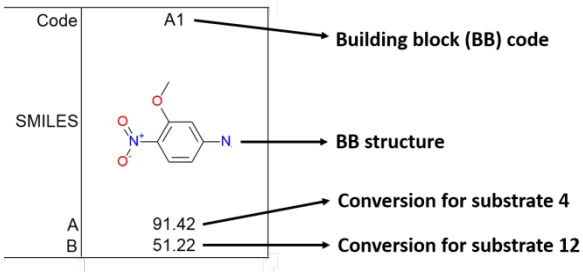
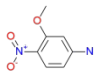
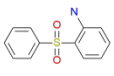
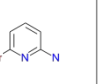
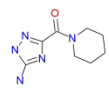
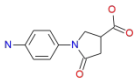
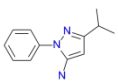
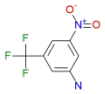
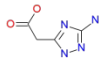
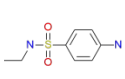
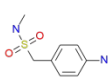
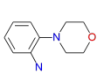
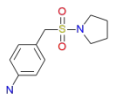
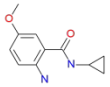
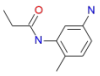
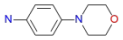
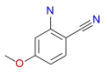
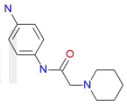
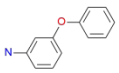
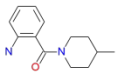
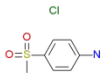
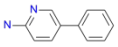
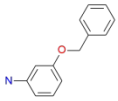
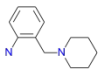
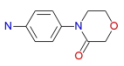
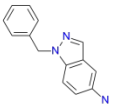
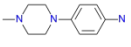
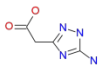
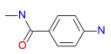
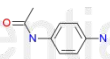
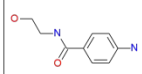
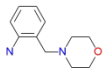
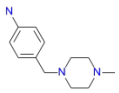
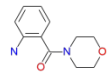
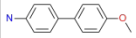
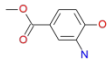
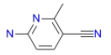
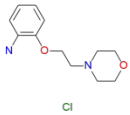
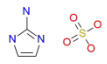
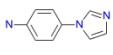
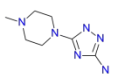
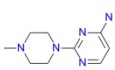
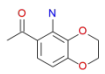
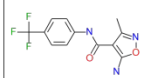
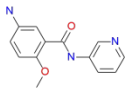
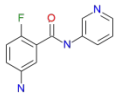
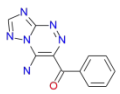
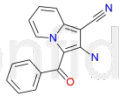
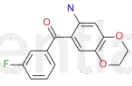
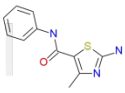
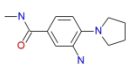


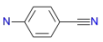
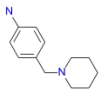
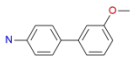
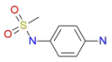
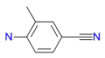
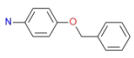
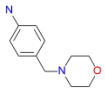
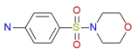
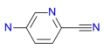
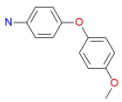
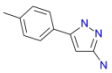
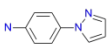
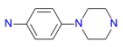
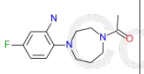
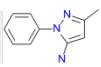
Table S5. Screening results of C–N cross coupling against aniline and 2° amines

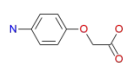
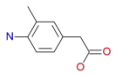
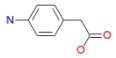
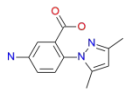
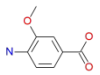
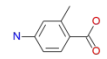
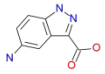
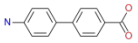
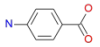
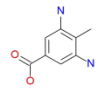
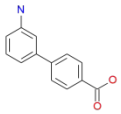
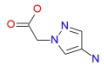
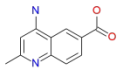
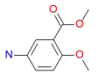
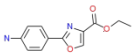
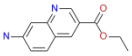
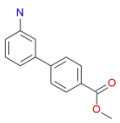
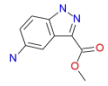
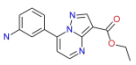
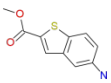
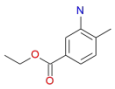
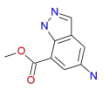
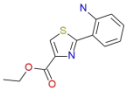
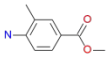
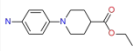
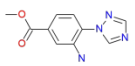
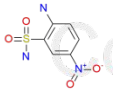
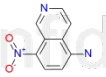
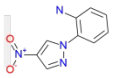
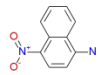
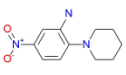


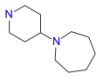
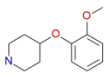
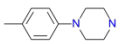
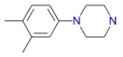
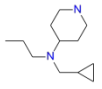
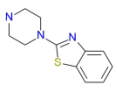
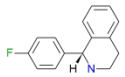
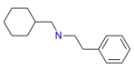
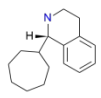
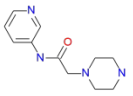
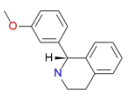
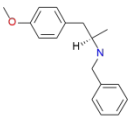
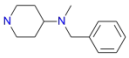
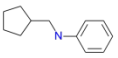
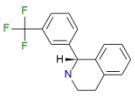
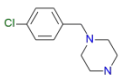
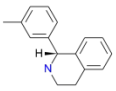
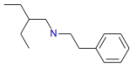
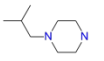
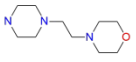
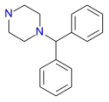
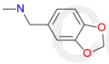
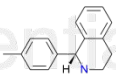
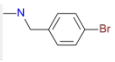
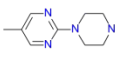
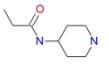
Code	A1	A2	A3	A4	A5	A6	A7	A8
SMILES								
A	91.42	67.05	0	58.98	0	88.9	0	43.58
B	51.22	100	13.81	45.79	0	33.23	0	40.49
Code	A9	A10	A11	A12	A13	A14	A15	A16
SMILES								
A	85.67	78.05	100	88.58	65.23	0	0	86.3
B	74.3	58.98	91.9	75.97	80.9	0	0	38.64
Code	A17	A18	A19	A20	A21	A22	A23	A24
SMILES								
A	100	78.67	100	100	39.1	100	100	86.95
B	76.42	25.5	40.5	31	0	90.45	89.87	78.45
Code	A25	A26	A27	A28	A29	A30	A31	A32
SMILES								
A	0	43.45	100	100	100	100	0	100
B	0	0	23.95	76.55	22.88	86.97	0	83.95
Code	A33	A34	A35	A36	A37	A38	A39	A40
SMILES								
A	40.48	86.94	100	100	100	100	15.9	100
B	26.13	52.4	88.98	85.37	100	100	0	92.37
Code	A41	A42	A43	A44	A45	A46	A47	A48
SMILES								
A	100	0	83.35	100	26.67	93.05	95.1	100
B	86	0	44.29	89.85	58.26	72.74	100	92.92
Code	A49	A50	A51	A52	A53	A54	A55	A56
SMILES								
A	100	100	100	0	92.48	0	86.37	100
B	100	100	73.32	0	84.26	0	68.7	100
Code	A57	A58	A59	A60	A61	A62	A63	A64
SMILES								
A	0	100	100	0	51.57	100	100	92.35
B	0	73.2	100	0	14.93	87.52	84.23	68.38
Code	A65	A66	A67	A68	A69	A70	A71	A72
SMILES								
A	45.44	82.53	100	100	0	6.02	100	35.97
B	23.99	38.75	100	87.49	0	60.7	42.12	100

Code	A73	A74	A75	A76	A77	A78	A79	A80
SMILES								
A	61.23	93.87	100	100	0	100	0	7.32
B	51.68	62.77	100	92.26	6.82	45	0	0
Code	A81	A82	A83	A84	A85	A86	A87	A88
SMILES								
A	0	95.18	100	100	86.55	100	0	6.46
B	0	91.44	55.85	94.37	93.74	74.82	0	8.31
Code	A89	A90	A91	A92	A93	A94	A95	A96
SMILES								
A	100	100	100	100	0	89.78	100	13.83
B	79.13	71.92	64.9	74.61	0	85.55	72.48	0
Code	A97	A98	A99	A100	A101	A102	A103	A104
SMILES								
A	100	100	100	78.81	100	100	100	0
B	91.69	91.65	81.94	54.2	84.68	81.56	84.63	0
Code	A105	A106	A107	A108	A109	A110	A111	A112
SMILES								
A	100	66.91	0	100	100	100	83.73	100
B	54.26	15.11	0	62.5	63.21	100	15.04	76.69
Code	A113	A114	A115	A116	A117	A118	A119	A120
SMILES								
A	100	100	91.23	100	82.47	61.93	52.94	53.41
B	81.6	36.48	26.07	50.52	62.45	0	37.94	50.14
Code	A121	A122	A123	A124	A125	A126	A127	A128
SMILES								
A	42.34	95.05	89.94	31.86	0	100	63.03	69.67
B	0	78.5	74.34	22.11	0	45.26	88.45	51.14
Code	A129	A130	A131	A132	A133	A134	A135	A136
SMILES								
A	100	100	0	92.44	67.57	100	22.9	100
B	77.73	58.8	0	68.09	30.39	87.38	17.2	76.09
Code	A137	A138	A139	A140	A141	A142	A143	A144
SMILES								
A	100	73.55	0	41.28	100	66.7	100	100
B	91.96	73.2	0	10.8	48.51	43.6	21.57	89.95

Code	A145	A146	A147	A148	A149	A150	A151	A152
SMILES								
A	0	81.63	64.6	100	100	100	92.42	100
B	0	59.63	32.35	39.03	90.49	100	49.37	92.05
Code	A153	A154	A155	A156	A157	A158	A159	A160
SMILES								
A	70.18	100	89.31	100	6.99	70.77	70	100
B	20.8	100	60.07	67.84	0	26.42	100	90.2
Code	A161	A162	A163	A164	A165	A166	A167	A168
SMILES								
A	0	30.87	0	100	100	9.14	93.43	32.69
B	0	0	20.18	88.15	81.1	0	76.91	16.72
Code	A169	A170	A171	A172	A173	A174	A175	A176
SMILES								
A	10.98	64.4	0	0	100	58.8	84.75	0
B	0	30.52	0	0	87.86	64.95	82.99	0
Code	A177	A178	A179	A180	A181	A182	A183	A184
SMILES								
A	9.58	0	59.16	33.43	77.11	0	0	89.64
B	10.28	0	76.96	0	100	0	0	68.57
Code	A185	A186	A187	A188	A189	A190	A191	A192
SMILES								
A	91.6	100	0	0	0	100	100	100
B	62.18	89.5	0	0	0	100	95.19	87.94
Code	A193	A194	A195	A196	A197	A198	A199	A200
SMILES								
A	0	100	100	100	84.84	0	100	78.7
B	0	86.56	85.3	71.71	72.13	0	94.48	50.22
Code	A201	A202	A203	A204	A205	A206	A207	A208
SMILES								
A	0	13.75	100	88.87	0	92.67	89.66	35.35
B	0	14.67	93.66	35.9	0	80.87	39.5	0
Code	A209	A210	A211	A212	A213	A214	A215	A216
SMILES								
A	28.39	52.64	100	100	80.27	74.33	88.59	41.37
B	54.31	33.8	77.5	100	86.88	64.88	59.38	31.27

Code	A217	A218	A219	A220	A221	A222	A223	A224
SMILES								
A	100	100	100	14.37	0	47.8	58.14	100
B	83.5	53.66	26.77	0	0	8.42	43.18	94.82
Code	A225	A226	A227	A228	A229	A230	A231	A232
SMILES								
A	100	39.3	100	74.96	94.1	82.12	100	72.18
B	57.65	30.23	64.12	76.41	70.46	84.58	87.94	82.65
Code	A233	A234	A235	A236	A237	A238	A239	A240
SMILES								
A	93.84	0	13.09	100	94.35	39.59	100	100
B	88.29	0	24.13	60.74	91.52	78.19	80.9	75
Code	A241	A242	A243	A244	A245	A246	A247	A248
SMILES								
A	93.22	3.6	0	0	100	100	83.38	18.03
B	58.85	0	0	0	85.98	69.28	43	46.61
Code	A249	A250	A251	A252	A253	A254	A255	A256
SMILES								
A	100	46.34	59.63	100	0	100	0	52.62
B	65.9	0	75.62	na	na	na	na	na
Code	A257	A258	A259	A260	A261	A262	A263	A264
SMILES								
A	0	0	100	100	40.62	18.73	61	72.75
B	na	na	na	na	na	na	na	na
Code	A265	A266	A267	A268	A269	A270	A271	A272
SMILES								
A	14.6	93.9	84.88	72.56	10.38	81.42	47.56	100
B	na	na	na	na	na	na	na	na
Code	A273	A274	A275	A276	A277	A278	A279	A280
SMILES								
A	0	100	7.32	56.16	17.41	75.62	61.88	82.96
B	na	na	na	na	na	na	na	na
Code	A281	A282	A283	A284	A285	A286	A287	A288
SMILES								
A	83.4	100	100	100	51.23	82.93	100	0
B	na	na	na	na	na	na	na	0

Code	A289	A290	A291	A292	A293	A294	A295	A296
SMILES								
A	71.43	100	100	100	100	15.33	100	100
B	16.45	84.57	89.64	95	75.37	0	88.47	92.53
Code	A297	A298	A299	A300	A301	A302	A303	A304
SMILES								
A	0	100	100	100	65.24	100	0	90.62
B	0	100	84.59	91.05	34.03	100	52.37	7.29
Code	A305	A306	A307	A308	A309	A310	A311	A312
SMILES								
A	0	0	0	100	100	95	100	0
B	42.91	0	0	82	77	66	87	0
Code	A313	A314	A315	A316	A317	A318	A319	A320
SMILES								
A	100	0	94	81	94	28	90	100
B	80	0	85	28	64	10	88	80
Code	A321	A322	A323	A324	A325	A326	A327	A328
SMILES								
A	90	77	0	10.11	0	63.05	66.74	0
B	77	27	0	10	17.86	94.06	0	0
Code	A329	A330	A331	A332	A333	A334	A335	A336
SMILES								
A	42	0	12	68	82	64	53	0
B	20	0	5	66	62	48	40	0
Code	A337	A338	A339	A340	A341	A342	A343	A344
SMILES								
A	63	100	60	51	0	0	60	0
B	50	100	52	30	0	0	56	0
Code	A345	A346	A347	A348	A349	A350	A351	A352
SMILES								
A	48	0	100	78	0	48	100	34
B	93	0	100	86	0	85	0	36
Code	A353	A354	A355	A356	A357	A358	A359	A360
SMILES								
A	100	96	0	48	16	0	100	0
B	100	0	0	92	0	0	100	0

Code	A361	A362	A363	A364	A365	A366	A367	A368
SMILES								
A	7	0	100	61	0	100	72	78
B	0	0	100	36	0	100	53	61
Code	A369	A370	A371	A372	A373	A374	A375	A376
SMILES								
A	9	100	0	45	0	0	58	100
B	0	100	0	76	0	0	42	0
Code	A377	A378	A379	A380	A381	A382	A383	A384
SMILES								
A	0	0	6	0	0	0	100	0
B	0	0	5	0	0	0	0	0
Code	A385	A386	A387	A388	A389	A390	A391	A392
SMILES								
A	0	0	0	0	0	100	0	0
B	0	0	0	0	0	0	0	0
Code	A393	A394	A395	A396	A397	A398	A399	A400
SMILES								
A	58	100	0	0	0	0	82	26
B	41	0	0	0	0	0	0	12
Code	A401	A402	A403	A404	A405	A406	A407	A408
SMILES								
A	35	20	0	5	0	0	0	45
B	25	8	11	21	0	0	0	35
Code	A409	A410	A411	A412	A413	A414	A415	A416
SMILES								
A	0	66	21	39	0	0	62	100
B	0	39	18	11	0	0	41	100
Code	A417	A418	A419	A420	A421	A422	A423	A424
SMILES								
A	100	0	100	0	0	100	93	0
B	100	0	100	0	0	0	0	0

13. References

1. Du, H.-C., and Huang, H. (2017) DNA-compatible nitro reduction and synthesis of benzimidazoles. *Bioconjugate Chem. 28*, 2575–2580.

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