

Chemical and Linguistic Considerations for Encoding Chinese Characters: An Embodiment Using Chain-End Degradable Sequence-Defined Oligourethanes Created by Consecutive Solid Phase Click Chemistry

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I. General procedure and equipment

All materials used in the synthesis of each compound and related tests, were purchased from Sigma-Aldrich Chemical Co., Acros Organics, Tokyo Chemical Industry, Chem Impex International, etc. and used without further purification. Solvents (DCM, NMP, chloroform, DMSO, DMF, MeOH, MeCN, Isopropanol) were of reagent grade or HPLC grade quality and purchased from Fischer Scientific. NMR solvents (CDCl₃-*d*, MeOD-*d*₄) were purchased from Cambridge Isotope Laboratories.

Column chromatography was performed using silica gel 60 (230 ± 400 mesh, 0.040 ± 0.063 mm) from Dynamic Adsorbents.

TLC analyses were carried out using Silica TLC Plates Glass Backing 20 by 20 cm sheet UV active at 254 nm.

Reverse phase column chromatography and **HPLC** purifications were performed on Shimadzu Prominence HPLC system equipped with Zorbax SB-C18 preparatory column (21.2 x 250 mm) with 7.0 μm packing material. Analytical HPLC traces were also carried out using a Zorbax SB-C18 analytical column (4.6 x 250 mm) with 5.0 μm packing material. 5-95% gradient elution (MeCN/H₂O with 0.1% formic acid). Hydrophobic urethanes utilized 30-95% gradient elution (MeCN/H₂O with 0.1% formic acid).

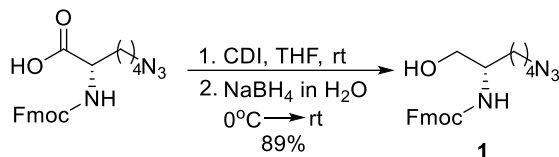
¹H and **¹³C** spectra were recorded on Bruker AVIII with a BBFO Prodigy liquid nitrogen CryoProbe 600 MHz NMR spectrometers. The NMR spectra were referenced to solvent and the spectroscopic solvents were purchased from Cambridge Isotope Laboratories.

Liquid Chromatography/Mass spectra were recorded on an Agilent Technologies 6120 Single Quadrupole or 6125B Single Quadrupole mass spectrometer interfaced with an Agilent 1200 series liquid chromatography system equipped with a diode-array detector. Column: Agilent ZORBAX Eclipse Plus S2 C18 narrow bore column; 2.1 mm internal diameter; 50 mm length; 5 micron particle size; P.N. 959746-902. Resulting spectra were analysed using Agilent LC/MSD ChemStation. Separations were achieved

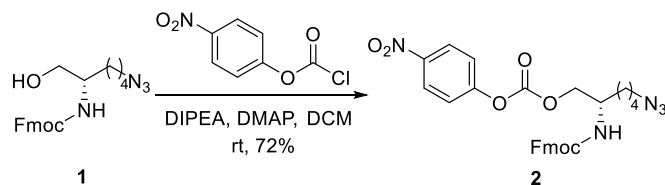
with a gradient elution from 5 to 95% organic, using MeCN and Water w/ 50 mM ammonium acetate as the eluents. **High resolution mass spectrometry** was performed by the UT-Austin Mass Spectrometry Facility using an Agilent Technologies 6530 Accurate-Mass Q-TOF (G6530A) with an Agilent Technologies Jet Stream ESI source, interfaced with an Agilent Technologies 1260 Infinity liquid chromatography system (G1312B). An Agilent Technologies 6546 Accurate-Mass Q-TOF (G6546A) with an Agilent Technologies Dual Jet Stream ESI source, interfaced with an Agilent Technologies 1260 Infinity II liquid chromatography system (G7112B), was used.

II. Synthesis and characterization

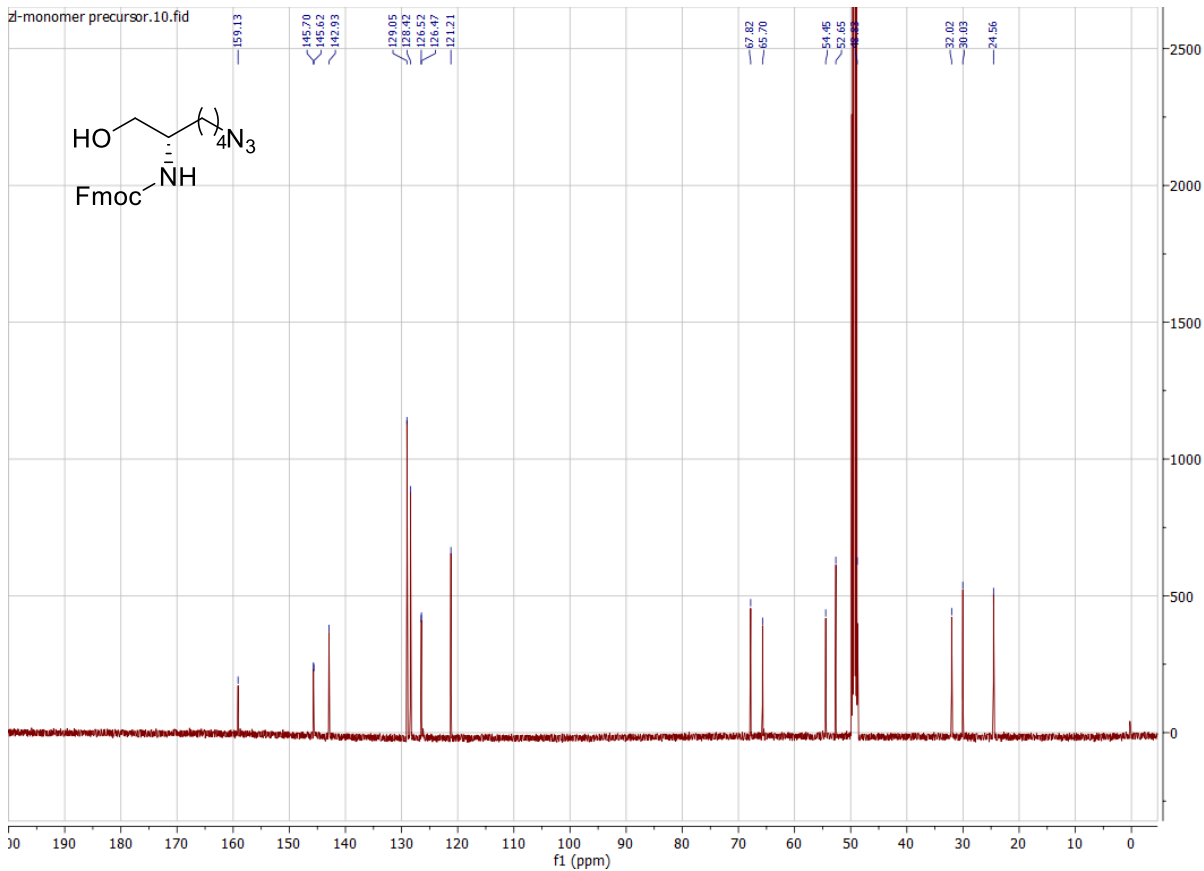
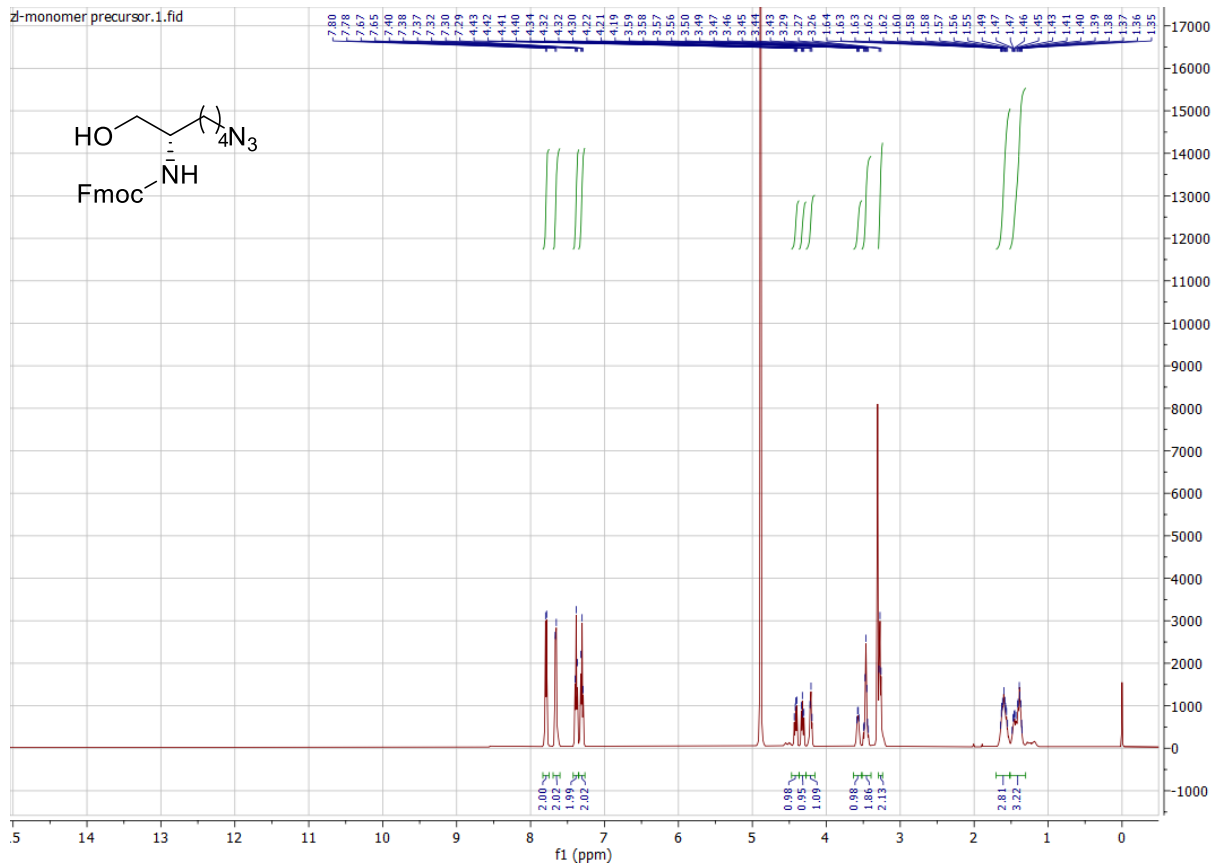
II(a). Synthesis and characterization of the monomer

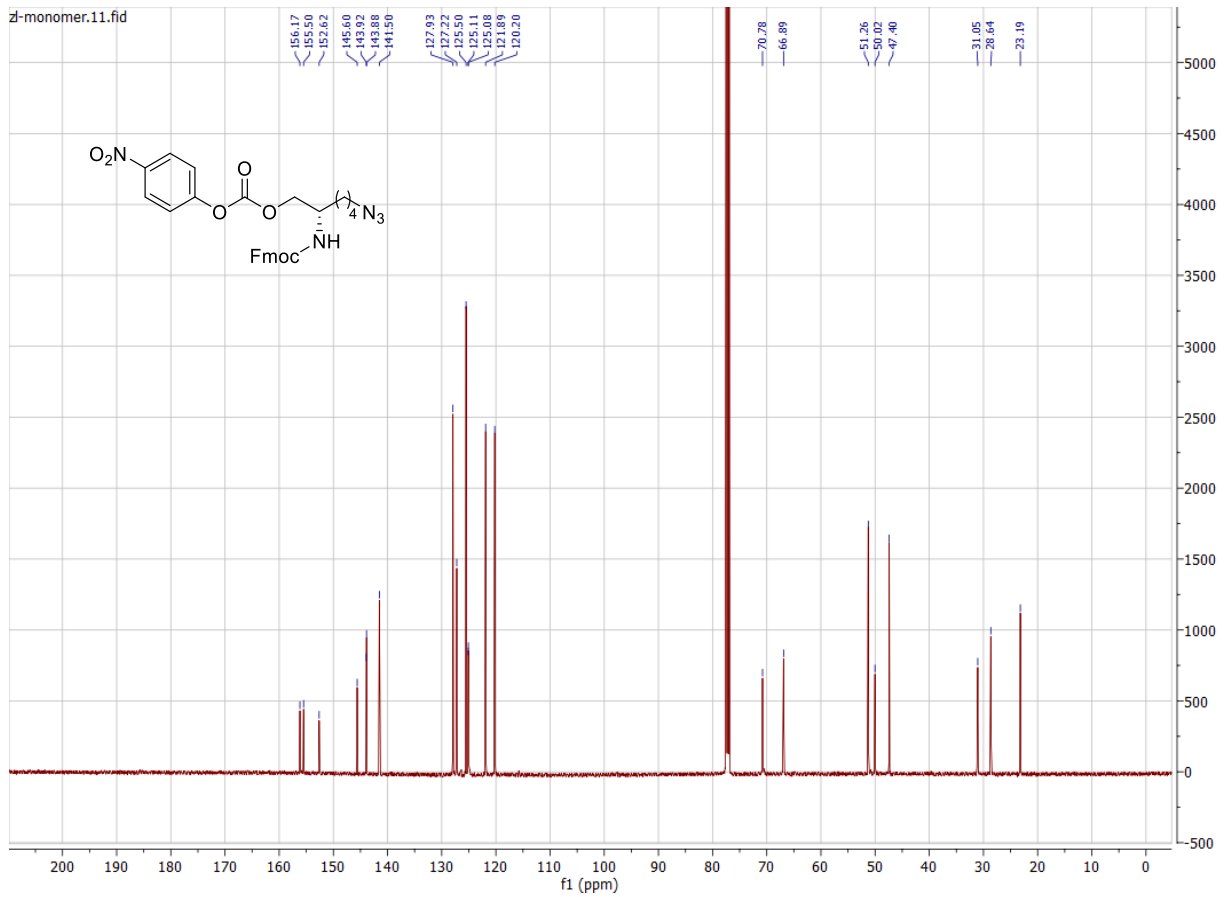
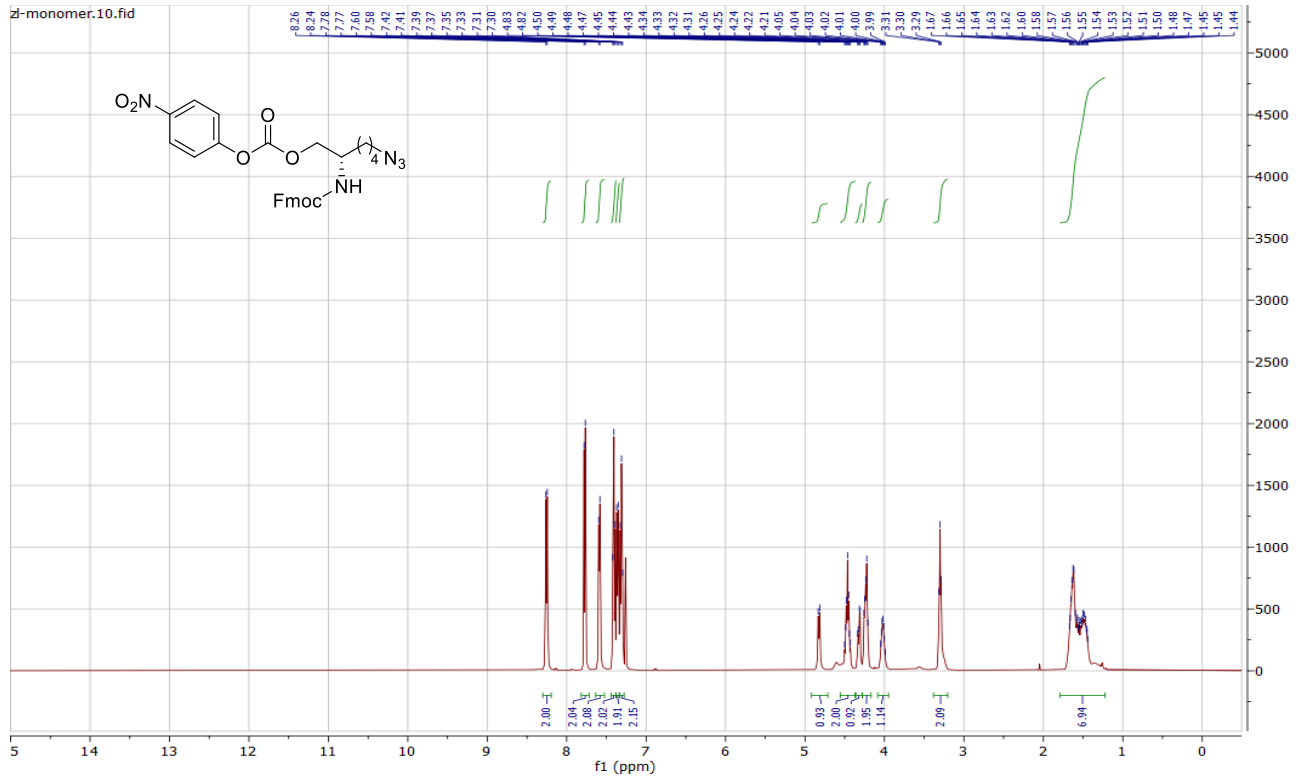


To a stirred solution of Fmoc-L-azidolysine (1.972 g, 5 mmol) in anhydrous THF (19 mL) was added N,N-carbonyldiimidazole (1.08 g, 6.7 mmol) at room temperature. The reaction stirred for at least 10 minutes and was then cooled to 0 °C. Next, a solution of NaBH₄ (311.7 mg, 8.24 mmol) in H₂O (8.32 mL) was added. The solution was stirred for at least 30 minutes, up to 1.5 hours. The reaction was quenched by addition of 1M HCl and extracted with EtOAc (3 x 65 mL). The combined organics were washed 1x with brine, dried over Na₂SO₄, and concentrated under vacuum. The crude product was purified by silica gel chromatography (1:1 Hexanes:EtOAc) to furnish a white solid (1.69 g, 89%). ¹H NMR (600 MHz, MeOD-*d*₄) δ 7.79 (d, *J* = 12 Hz, 2H), 7.66 (d, *J* = 12 Hz, 2H), 7.38 (t, *J* = 12 Hz, 2H), 7.30 (t, *J* = 12 Hz, 2H), 4.40-4.43 (m, 1H), 4.30-4.34 (m, 1H), 4.21 (t, *J* = 6 Hz, 1H), 3.56-3.59 (m, 1H), 3.43-3.50 (m, 2H), 3.27 (t, *J* = 6 Hz, 2H), 1.55-1.64 (m, 3H), 1.35-1.49 (m, 3H). ¹³C NMR (125 MHz, MeOD-*d*₄) δ 159.13, 145.70, 145.62, 142.93, 129.05, 128.42, 126.52, 126.47, 121.21, 67.82, 65.70, 54.45, 52.65, 49.83, 32.02, 30.03, 24.56. HRMS +ESI: calculated (C₂₁H₂₄N₄O₃Na⁺) 403.1746, found 403.1741. [M⁺Na].



To a stirring solution of **1** (1.69 g, 4.45 mmol) in anhydrous DCM (22 mL) was added pyridine (378 μL, 4.67 mmol) dropwise. Next, 4-nitrophenyl chloroformate (1.08 g, 6.67 mmol) was added, and the reaction left to stir overnight. Reaction was monitored by TLC (2:1 Hexanes:EtOAc) and upon consumption of the starting material, was diluted excessively in DCM and transferred to a separatory funnel. The organic layer was washed with 1M NaHSO₄ (2x), then 1M Na₂CO₃ (3x), and finally brine. The organic layer was dried over Na₂SO₄, filtered, and concentrated in vacuo. The product was purified by silica gel chromatography (2:1 Hexanes:EtOAc) and isolated as a white solid (1.75 g, 3.20 mmol). ¹H NMR (600 MHz, CDCl₃-*d*) δ 8.25 (d, *J* = 12 Hz, 2H), 7.78 (d, *J* = 6 Hz, 2H), 7.59 (d, *J* = 12 Hz, 2H), 7.41 (t, *J* = 12 Hz, 2H), 7.36 (d, *J* = 12 Hz, 2H), 7.31 (t, *J* = 12 Hz, 2H), 4.82 (d, *J* = 6 Hz, 1H), 4.43-4.50 (m, 2H), 4.31-4.34 (m, 1H), 4.21-4.26 (m, 2H), 3.99-4.05 (m, 1H), 3.30 (t, *J* = 6 Hz, 2H), 1.44-1.67 (m, 6H). ¹³C NMR (125 MHz, CDCl₃-*d*) δ 156.17, 155.50, 152.62, 145.60, 143.92, 143.88, 141.50, 127.93, 127.22, 125.50, 125.11, 125.08, 121.89, 120.20, 70.78, 66.89, 51.26, 50.02, 47.40, 31.05, 28.64, 23.19. HRMS +ESI: calculated (C₂₈H₂₇N₅O₇Na⁺) 568.1808, found 568.1799. [M⁺Na].





II(b). General procedure for the solid-supported synthesis of oligourethanes

Coupling: Phenylalaninol loaded (0.44 mmol/gram, 200-400 mesh) 2-chlorotrityl polystyrene resin (40 mg, 0.0176 mmol) was added to a small fritted solid phase synthesis apparatus (5mL). The apparatus was then evacuated and backfilled with argon. The resin was suspended in 0.5 mL of anhydrous N-methyl-2-pyrrolidinone (NMP) and left to swell for 10 minutes. Next, Hunig's base (4.4 μ L, 0.025 mmol) was added, followed by hydroxybenzotriazole (13.4 mg, 0.10 mmol). The suspension was swirled for 30 seconds until everything was dissolved. Finally, the activated amino alcohol **2** (33.2 mg, 0.05 mmol) was added. Reaction was shaken for 8 hours on a shaker at room temperature. Resin was washed with NMP (5x3 mL), then DCM (5x3 mL), and finally Et₂O (3x2 mL). Resin was dried overnight under vacuum. Test cleavages were effected with 1% TFA in DCM (5x0.2 mL) for 20 seconds each. Coupling efficiency was checked by LC/MS. NOTE: depending on the cleavage times and amounts of TFA used, the trifluoroacetic ester (presumably on the terminal alcohol) was observed by LC/MS. This ester was readily hydrolyzed by dissolving the sample in DCM and shaking with saturated NaHCO₃.

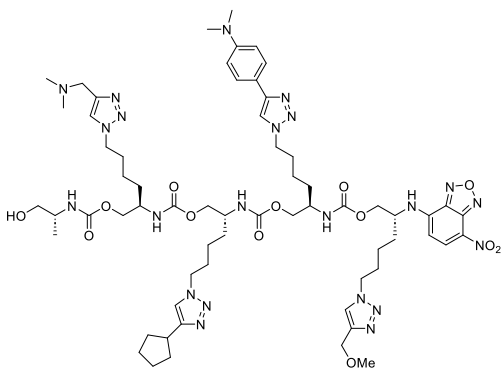
Solid phase CuAAC click chemistry: To the oligourethanes on the resin (about 40 mg resin, 0.0176 mmol) in the 5 mL fritted solid phase synthesis apparatus, a terminal alkyne (5.0 eq.), sodium ascorbate (1.0 eq.), TBTA (1.0 eq.) and copper iodide (0.5 eq.) were added along with 0.7 mL DMF. The solid phase synthesis apparatus was sealed with a septum and purged with N₂ gas for 15 minutes. After degassing, parafilm was used to seal the septum on the solid phase synthesis apparatus to prevent oxygen from going into the apparatus. The reaction was placed on the shaker and agitated for 18 hours at room temperature. The resin was then collected by vacuum filtration and washed with NMP (5x3 mL), then DCM (5x3 mL), and finally Et₂O (3x2 mL).

Deprotection: Resin loaded with terminal Fmoc-protected oligocarbamates (0.0176 mmol) suspended in 20% piperidine in DMF (3 mL) and shaken for 2 hours at room temperature. Cleavage of the dibenzofulvene-piperidine adduct was calculated by absorbance at 301 nm using Beer's Law. The resin was washed with DMF (5x3 mL), DCM (5x3 mL), Et₂O (3x2 mL), and dried overnight under vacuum.

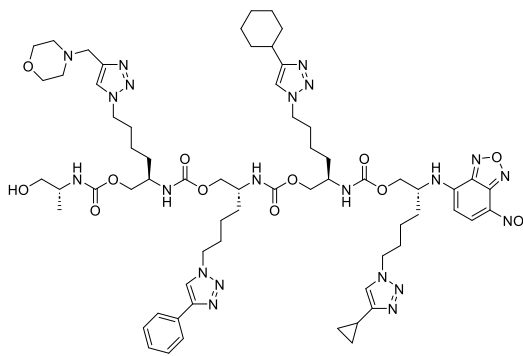
General procedure for labelling of the terminal amine with a NBD-Fluoride (on resin): To a fritted reaction vessel was added the oligomer (dimer, trimer or tetramer) on resin (0.0176 mmol). Vessel was evacuated and backfilled with argon. The resin was suspended and swelled in anhydrous DMF (2.4 mL) for 5 minutes. Next, DIPEA (41.76 μ L, 0.24 mmol) was added, followed by 4-fluoro-7-nitrobenzofurazan (33 mg, 0.179 mmol). Reaction was left to shake overnight. Resin was washed with DMF (5x16 mL), DCM (5x16 mL), and Et₂O (3x8 mL).

Cleavage procedure: Cleavages were effected with 1% TFA in DCM (5x1 mL) for 20 seconds each at room temperature. Resin was filtered off, and cleaved product was concentrated. Oligomer was purified by reverse-phase preparatory HPLC (5-95% MeCN/H₂O, 0.1% formic acid gradient elution).

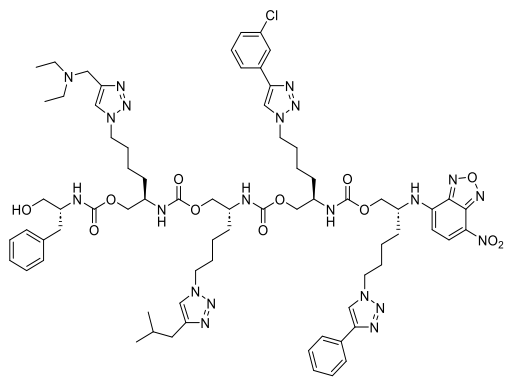
II(c). Determination of Conversions of Synthesized Oligourethanes



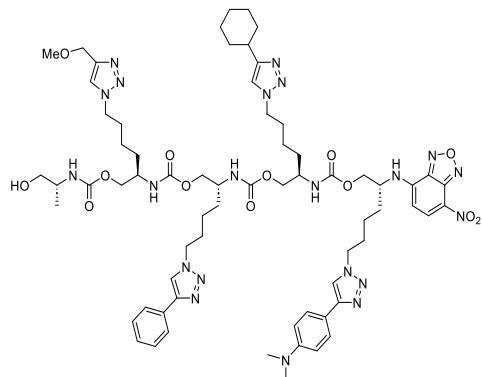
Oligomer 1: #6027



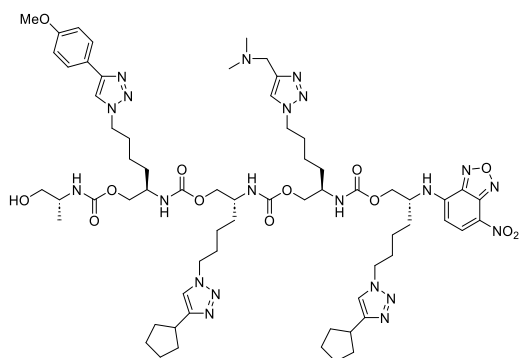
Oligomer 2: #8fd1



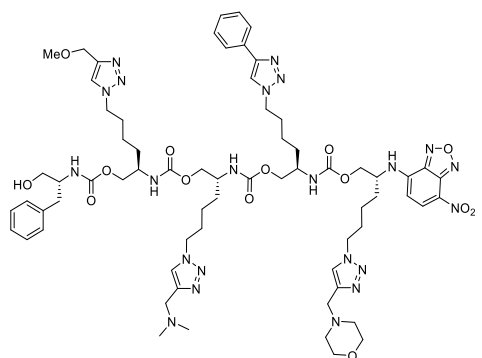
Oligomer 3: *BDRW



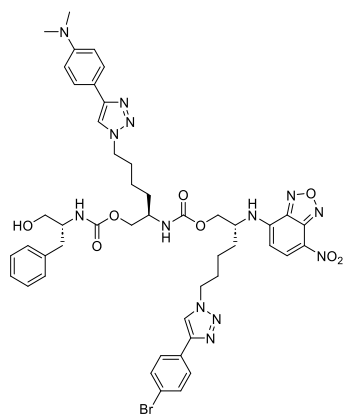
Oligomer 4: #7fd2



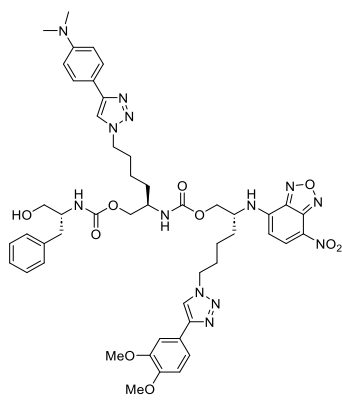
Oligomer 5: #9060



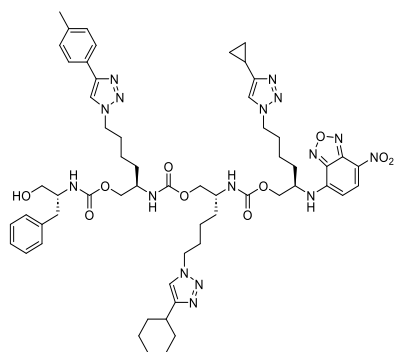
Oligomer 6: *76f8



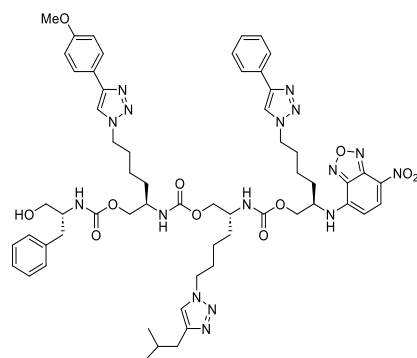
Oligomer Z1: *YI



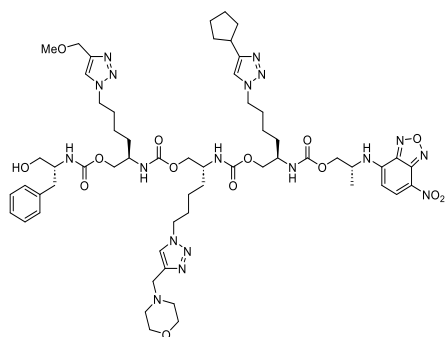
Oligomer Z2: *YT



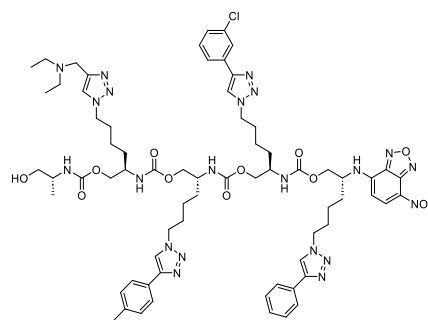
Oligomer Z3: *UMC



Oligomer Z4: *PDW



Oligomer Z5: *FLVV



Oligomer Z6_1: #4e5f

Table 1. The conversions of 12 synthesized oligourethanes

Oligourethane	Conversion ^a	Oligourethane	Conversion ^a
1	38%	Z1	80%
2	81%	Z2	90%
3	63%	Z3	83%
4	77%	Z4	65%
5	55%	Z5	65%
6	48%	Z6	68%

^aConversions were determined by the ratio of the peak area of product to the total peak area in LC trace.

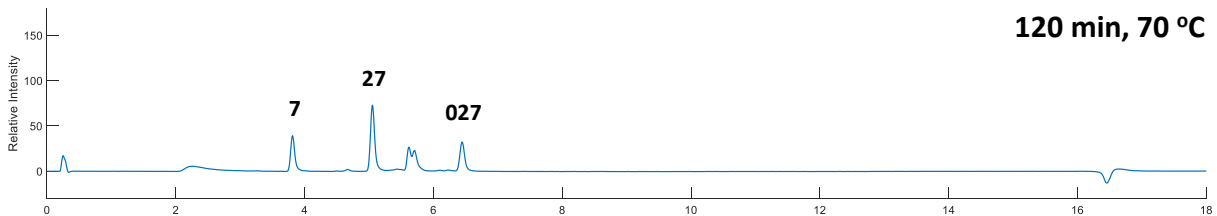
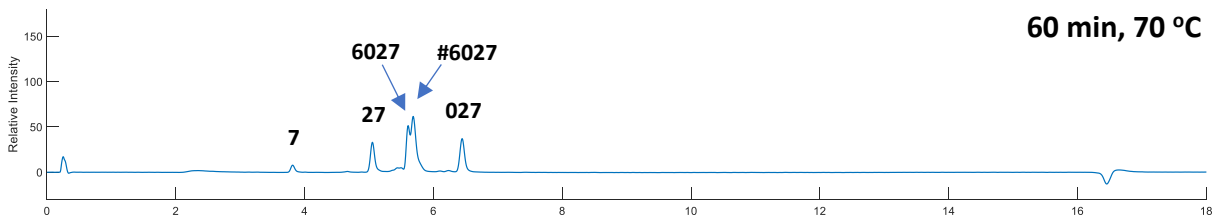
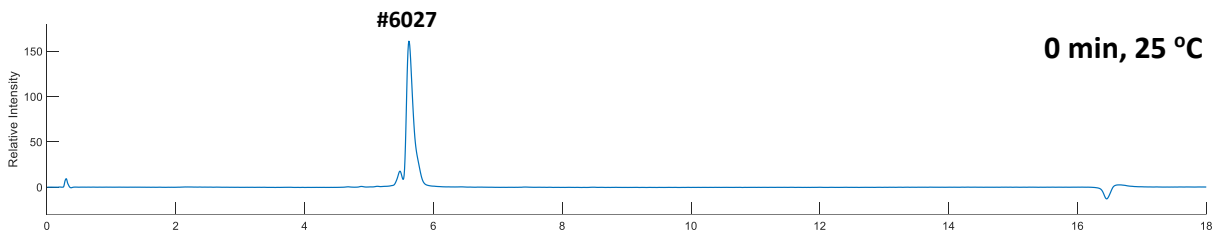
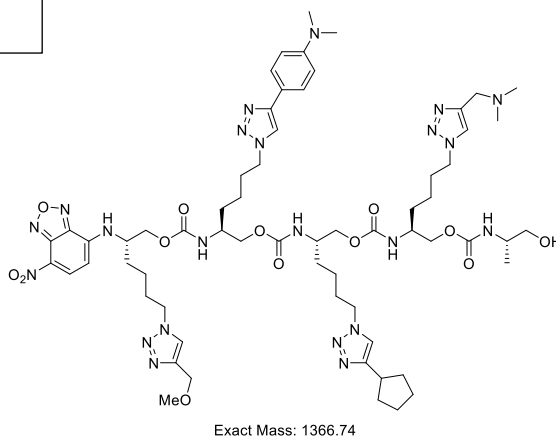
III. Sequencing experiments

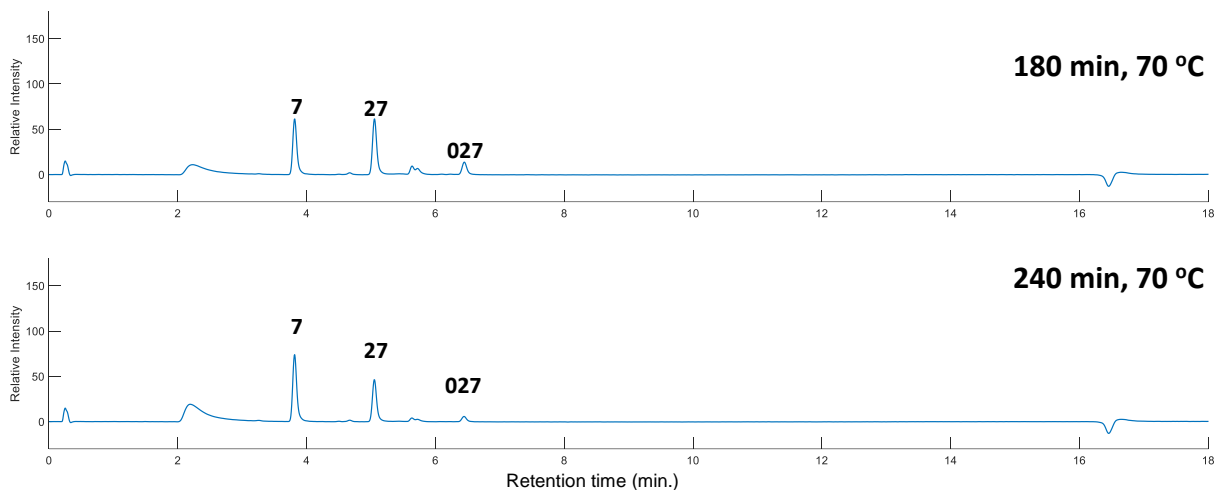
III(a). General procedure for self-degradation (sequencing)

The sequencing procedure is adapted from previous work.¹ The oligomer (measured to be at a final concentration between 0.5-1 mM) was dissolved in methanol and added to a vial. Next, potassium phosphate tribasic monohydrate was dissolved in water and then added to the reaction solution. The final concentration of base was approximately 30 mM. The final ratio of methanol and water was 1:2.5, respectively. Before placing the vial on the heated shaker, the reaction was sampled for LC/MS by taking 50 μ L of the reaction mixture and diluted into 50 μ L of a 1:1 methanol: water mixture. The reaction was ramped quickly to 70 °C in the heated shaker and held at the temperature. The reaction was sampled every 60 minutes for 240 minutes.

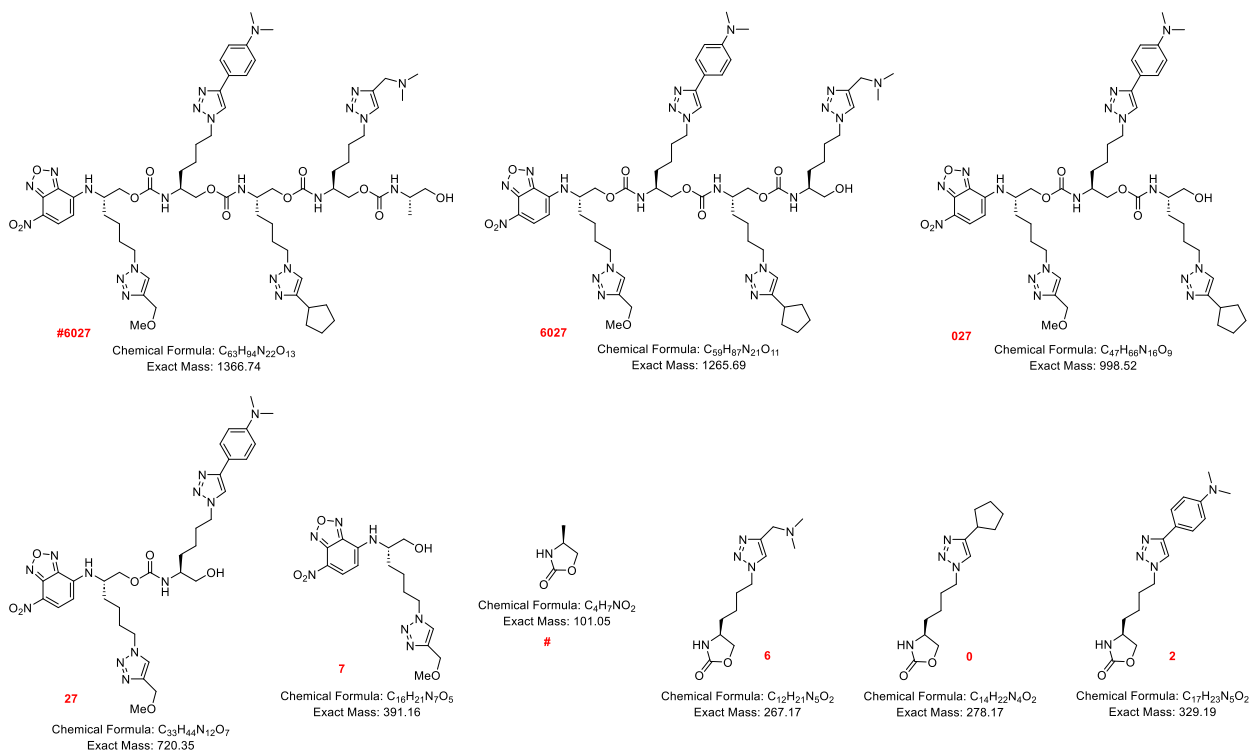
III(b). Oligomer Sequencing Data:

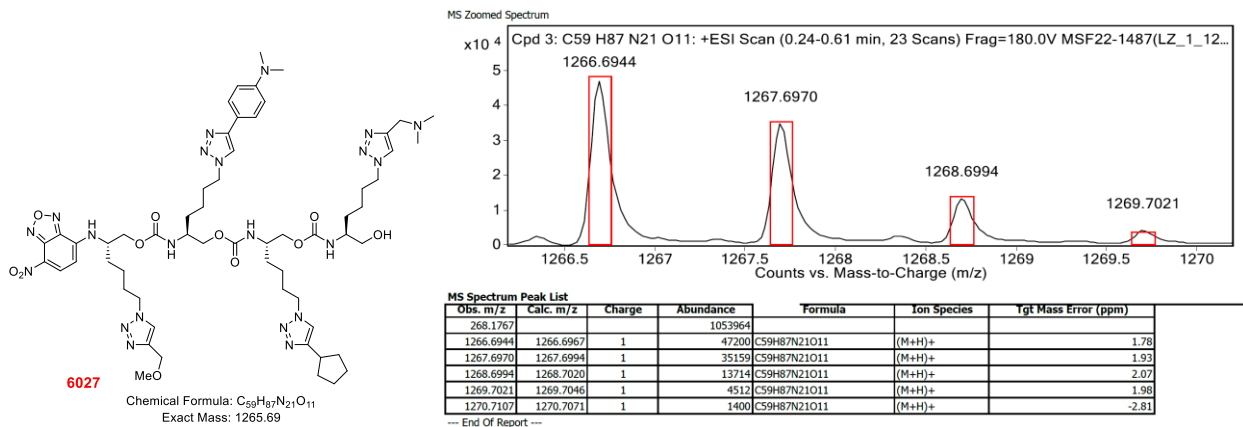
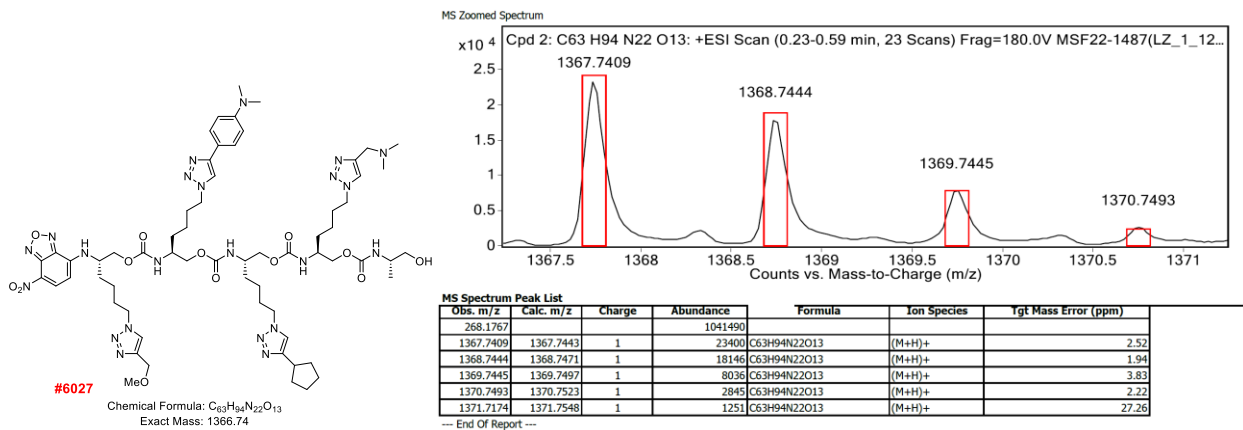
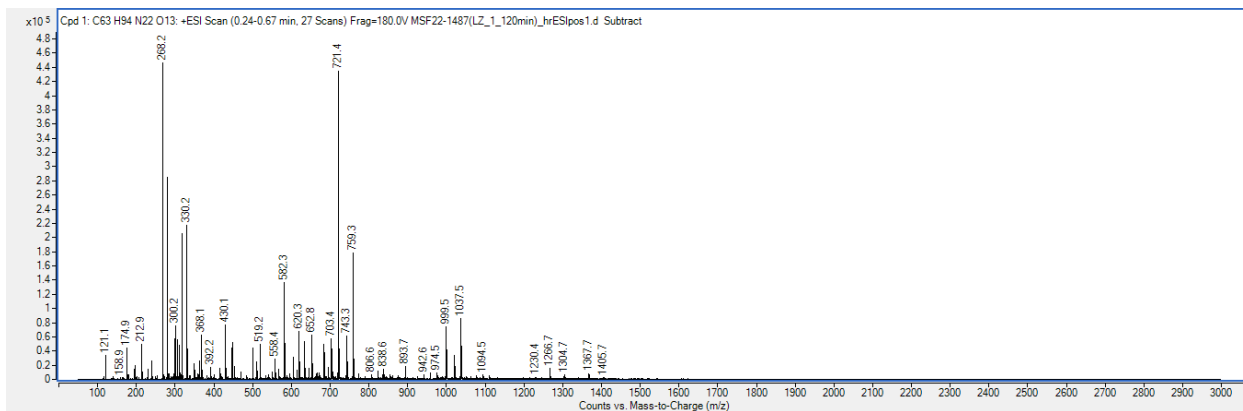
Oligomer 1: #6027

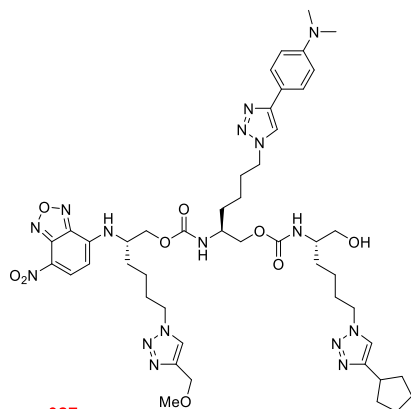




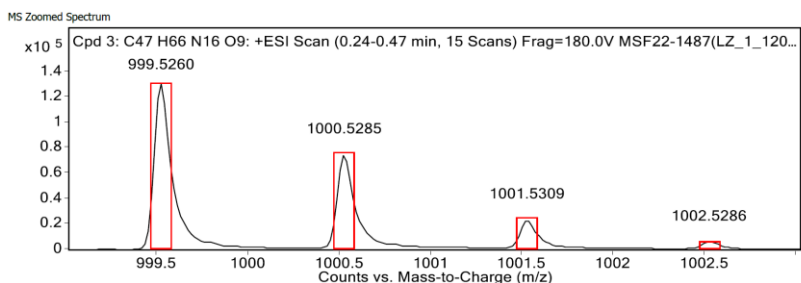
After 120 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.





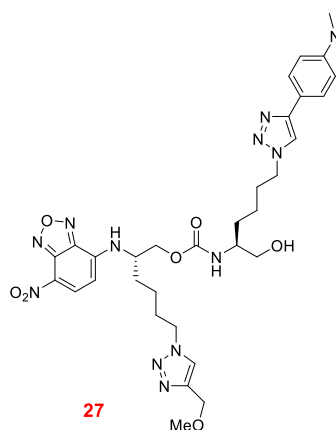


Chemical Formula: C₄₇H₆₆N₁₆O₉
Exact Mass: 998.52

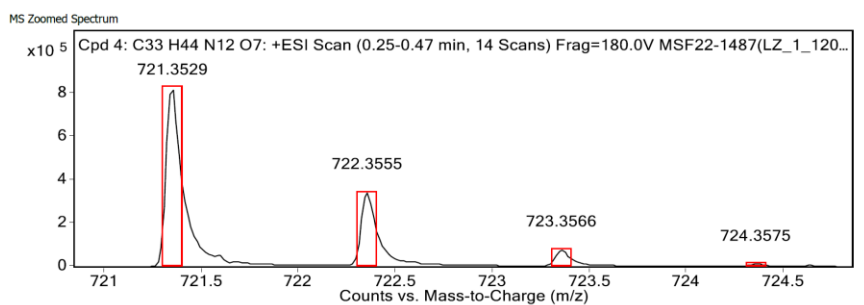


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
721.3529			771717			
999.5260	999.5271	1	130544	C ₄₇ H ₆₆ N ₁₆ O ₉	(M+H) ⁺	1.18
1000.5285	1000.5299	1	74346	C ₄₇ H ₆₆ N ₁₆ O ₉	(M+H) ⁺	1.37
1001.5309	1001.5325	1	23107	C ₄₇ H ₆₆ N ₁₆ O ₉	(M+H) ⁺	1.63
1002.5286	1002.5351	1	5701	C ₄₇ H ₆₆ N ₁₆ O ₉	(M+H) ⁺	6.43
1003.5350	1003.5376	1	1579	C ₄₇ H ₆₆ N ₁₆ O ₉	(M+H) ⁺	2.57

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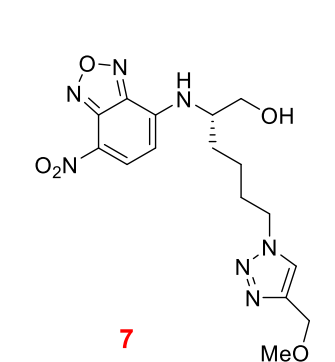


Chemical Formula: C₃₃H₄₄N₁₂O₇
Exact Mass: 720.35

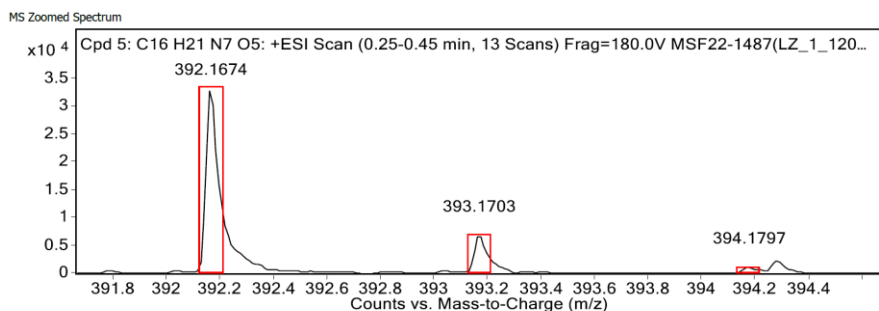


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
721.3529	721.3529	1	824867	C ₃₃ H ₄₄ N ₁₂ O ₇	(M+H) ⁺	-0.09
722.3555	722.3556	1	343106	C ₃₃ H ₄₄ N ₁₂ O ₇	(M+H) ⁺	0.11
723.3566	723.3581	1	78562	C ₃₃ H ₄₄ N ₁₂ O ₇	(M+H) ⁺	2.05
724.3575	724.3606	1	12158	C ₃₃ H ₄₄ N ₁₂ O ₇	(M+H) ⁺	4.25
725.3664	725.3630	1	1865	C ₃₃ H ₄₄ N ₁₂ O ₇	(M+H) ⁺	-4.7
726.3640	726.3654	1	489	C ₃₃ H ₄₄ N ₁₂ O ₇	(M+H) ⁺	1.81

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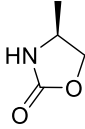


Chemical Formula: C₁₆H₂₁N₇O₅
Exact Mass: 391.16

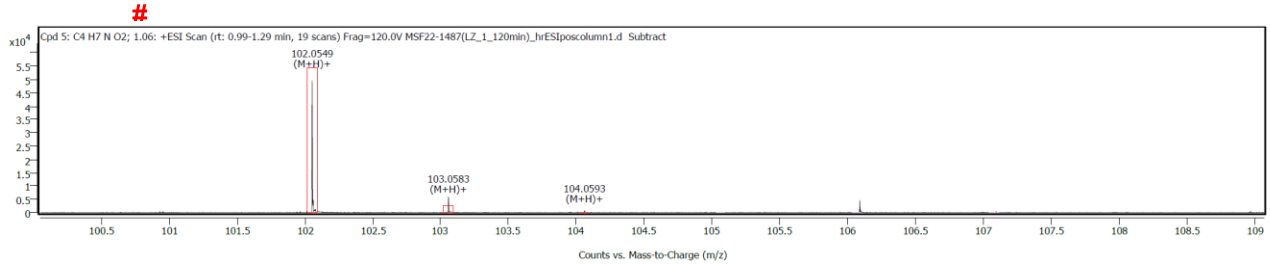


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
392.1674	392.1677	1	33332	C ₁₆ H ₂₁ N ₇ O ₅	(M+H) ⁺	0.65
393.1703	393.1703	1	6838	C ₁₆ H ₂₁ N ₇ O ₅	(M+H) ⁺	-0.01
394.1797	394.1725	1	1093	C ₁₆ H ₂₁ N ₇ O ₅	(M+H) ⁺	-18.26
721.3529			875111			

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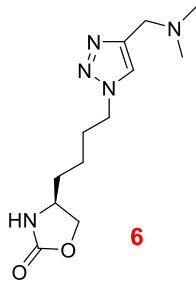
Chemical Formula: C₄H₇NO₂
Exact Mass: 101.05



Spectrum Peaks

Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
102.0549	102.0550	1	50756	C4H7NO2	(M+H)+	-0.76
103.0583	103.0579	1	5789	C4H7NO2	(M+H)+	3.83
104.0593	104.0595	1	629	C4H7NO2	(M+H)+	-2.17

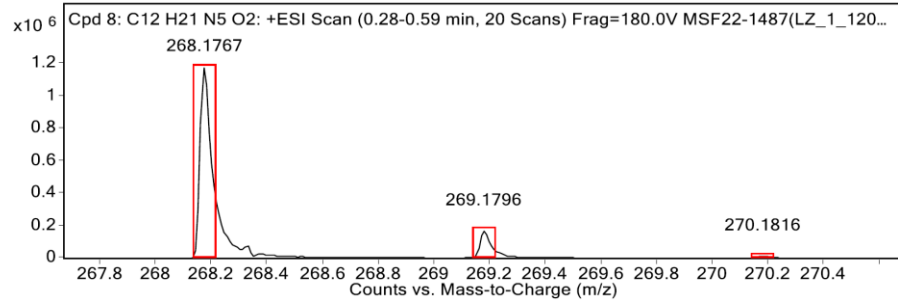
MassHunter Qual 10.0
(End of Report)



6

Chemical Formula: C₁₂H₂₁N₅O₂
Exact Mass: 267.17

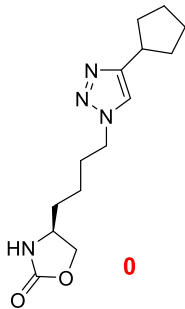
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1767	268.1768	1	1189627	C12H21N5O2	(M+H)+	0.35
269.1796	269.1794	1	172121	C12H21N5O2	(M+H)+	-0.64
270.1816	270.1818	1	16955	C12H21N5O2	(M+H)+	0.49
271.1826	271.1841	1	1973	C12H21N5O2	(M+H)+	5.51

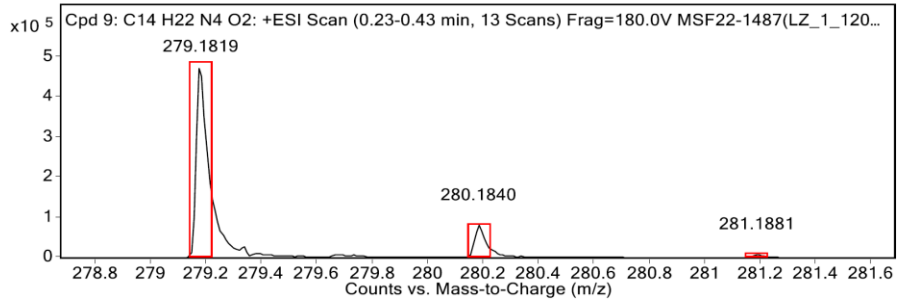
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0

Chemical Formula: C₁₄H₂₂N₄O₂
Exact Mass: 278.17

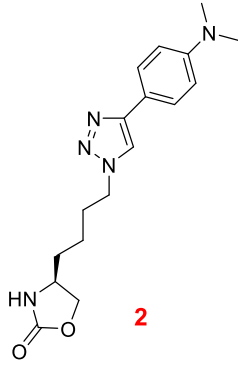
MS Zoomed Spectrum



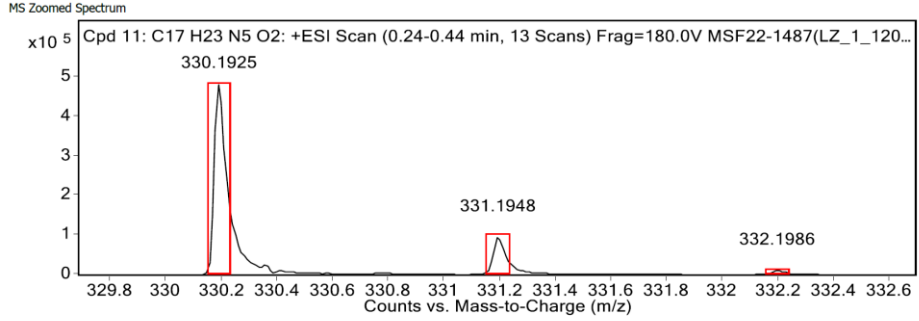
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1766			990696			
279.1819	279.1816	1	485039	C14H22N4O2	(M+H)+	-1.17
280.1840	280.1844	1	81153	C14H22N4O2	(M+H)+	1.49
281.1881	281.1869	1	8885	C14H22N4O2	(M+H)+	-4.25

--- End Of Report ---

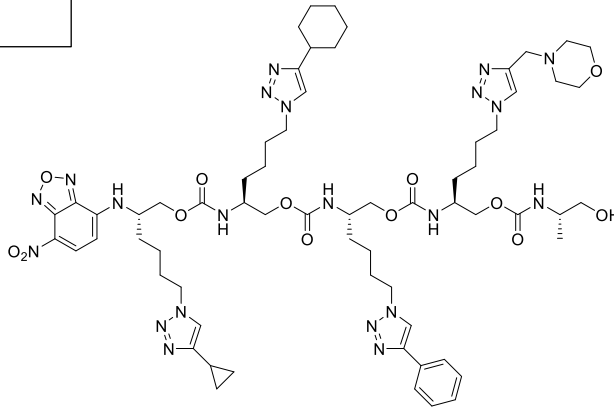


Chemical Formula: $C_{17}H_{23}N_5O_2$
 Exact Mass: 329.19

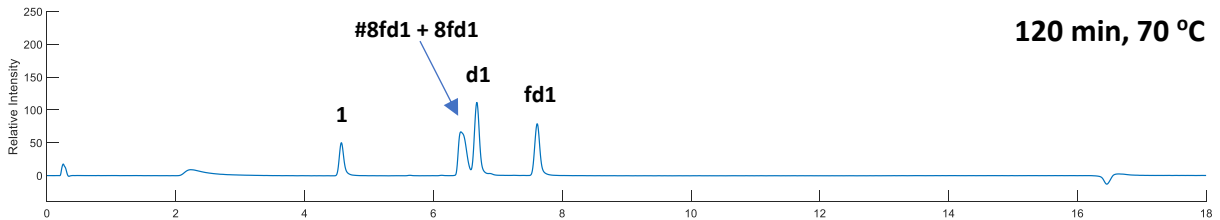
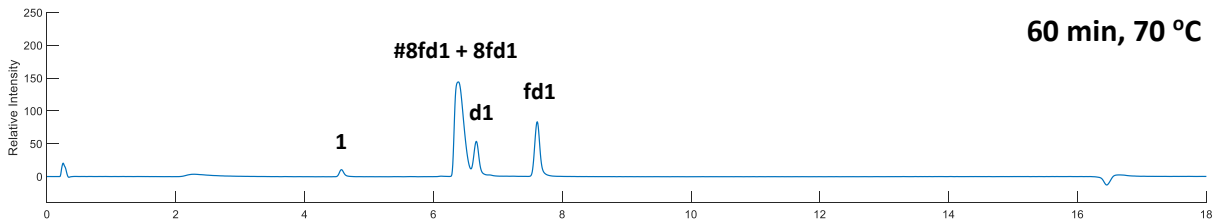
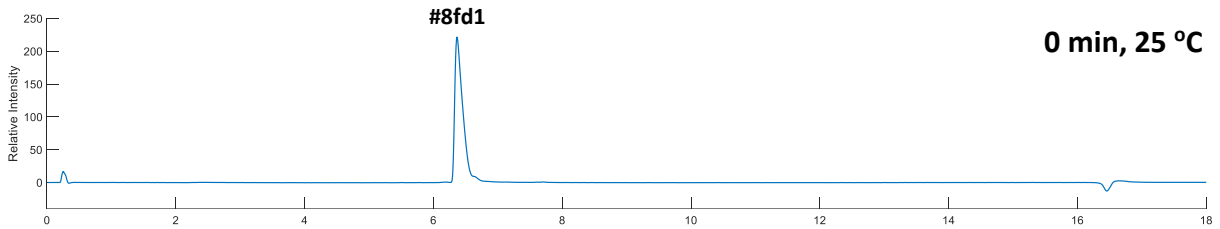


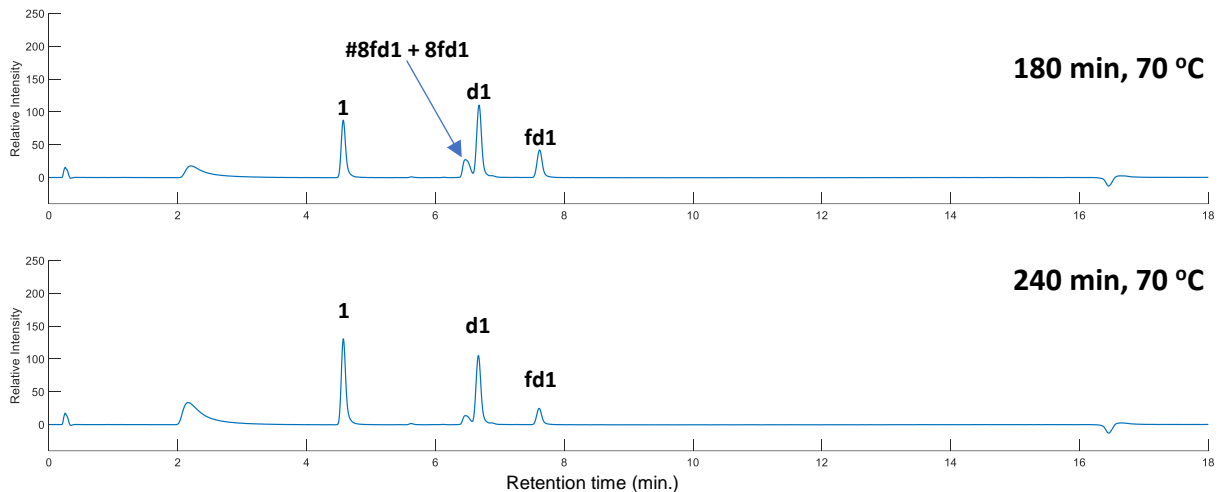
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1766			1147487			
330.1925	330.1925	1	483892	$C_{17}H_{23}N_5O_2$	(M+H) ⁺	-0.29
331.1948	331.1953	1	97276	$C_{17}H_{23}N_5O_2$	(M+H) ⁺	1.41
332.1986	332.1979	1	12985	$C_{17}H_{23}N_5O_2$	(M+H) ⁺	-2.29

Oligomer 2: #8fd1

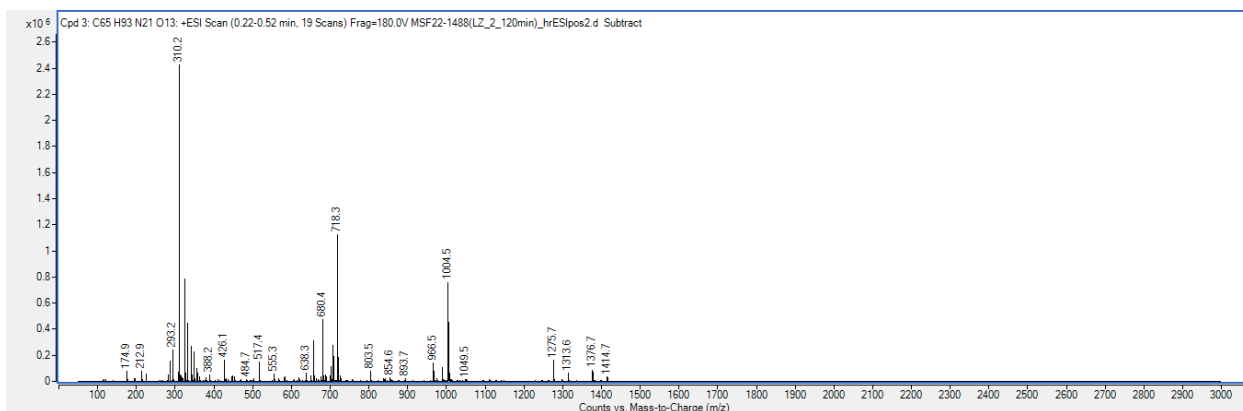
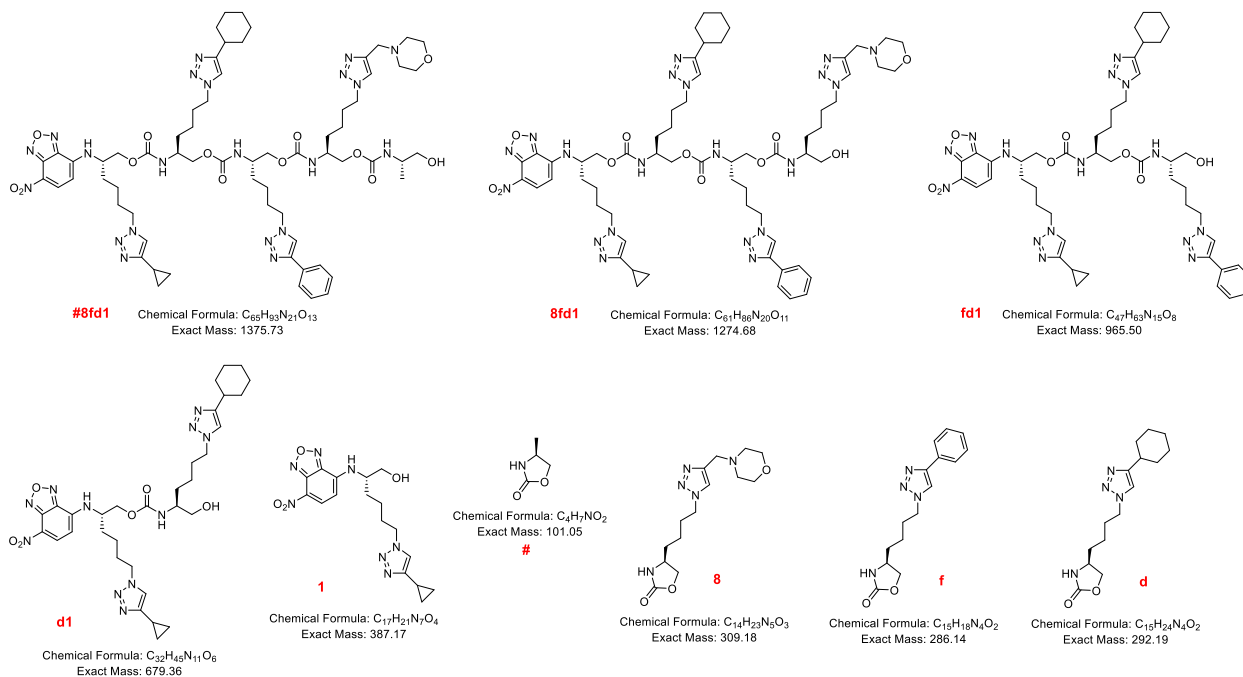


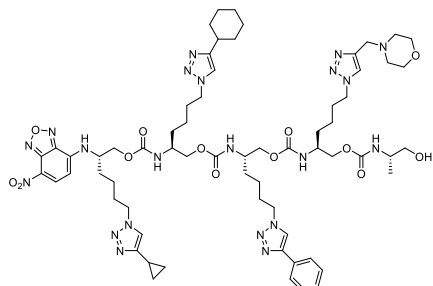
Exact Mass: 1375.73



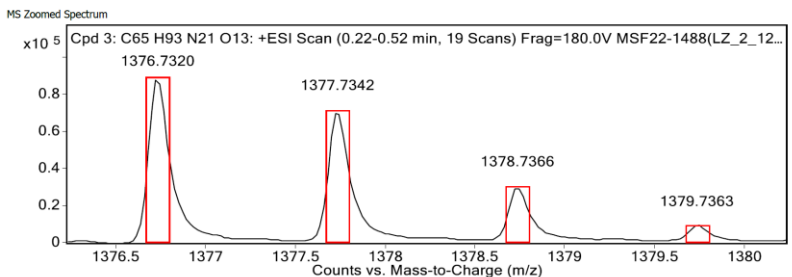


After 120 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.





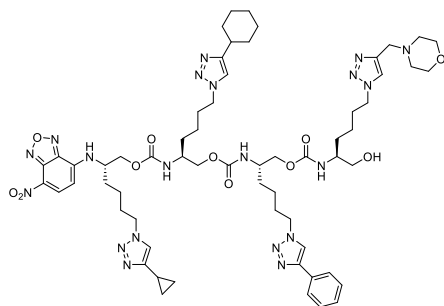
#8fd1 Chemical Formula: $C_{65}H_{93}N_{21}O_{13}$
Exact Mass: 1375.73



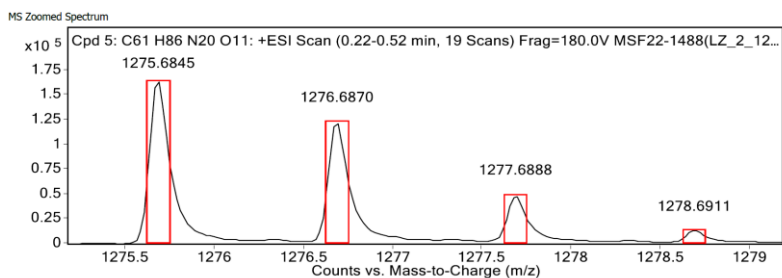
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1872			2446754			
1376.7320	1376.7334	1	89269	C65H93N21O13	(M+H)+	1.03
1377.7342	1377.7362	1	71284	C65H93N21O13	(M+H)+	1.52
1378.7366	1378.7389	1	30031	C65H93N21O13	(M+H)+	1.68
1379.7363	1379.7415	1	8537	C65H93N21O13	(M+H)+	3.78
1380.7370	1380.7441	1	2244	C65H93N21O13	(M+H)+	5.15
1381.7188	1381.7466	1	769	C65H93N21O13	(M+H)+	20.12

--- End Of Report ---



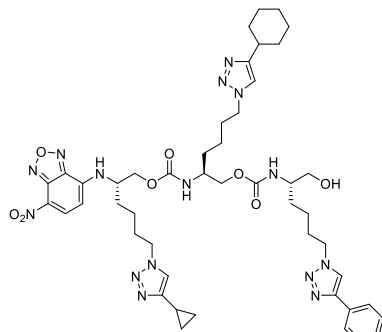
8fd1 Chemical Formula: $C_{61}H_{86}N_{20}O_{11}$
Exact Mass: 1274.68



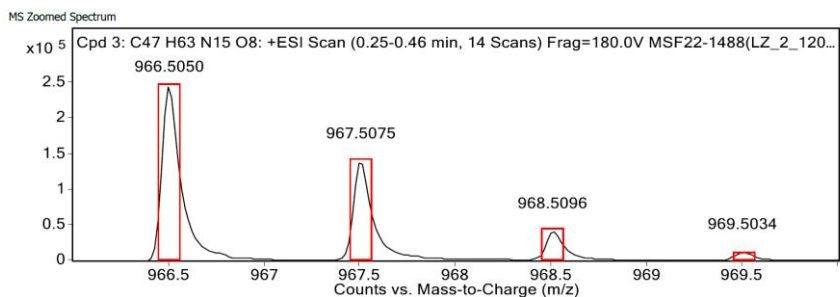
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1872			2446588			
1275.6845	1275.6858	1	164259	C61H86N20O11	(M+H)+	0.99
1276.6870	1276.6886	1	121823	C61H86N20O11	(M+H)+	1.24
1277.6888	1277.6912	1	48473	C61H86N20O11	(M+H)+	1.89
1278.6911	1278.6938	1	11885	C61H86N20O11	(M+H)+	2.15
1279.6918	1279.6964	1	3160	C61H86N20O11	(M+H)+	3.58
1280.6949	1280.6989	1	757	C61H86N20O11	(M+H)+	3.09

--- End Of Report ---



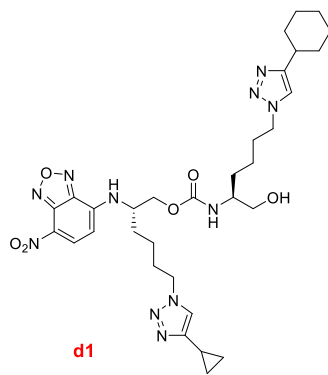
fd1 Chemical Formula: $C_{47}H_{63}N_{15}O_8$
Exact Mass: 965.50



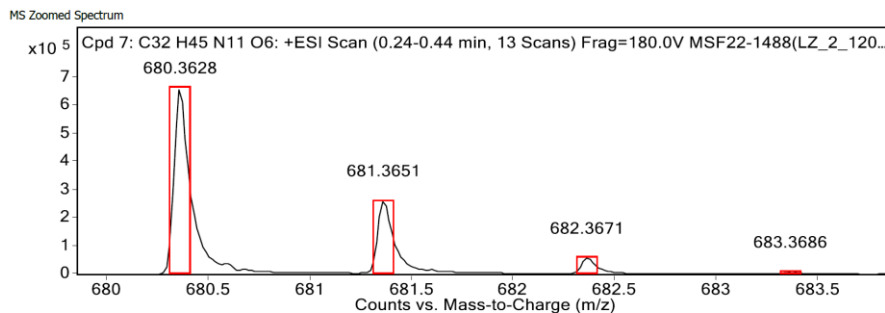
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1870			2305930			
966.5050	966.5057	1	246291	C47H63N15O8	(M+H)+	0.66
967.5075	967.5085	1	140196	C47H63N15O8	(M+H)+	1.02
968.5096	968.5111	1	41736	C47H63N15O8	(M+H)+	1.62
969.5034	969.5137	1	12513	C47H63N15O8	(M+H)+	10.61
970.4985	970.5162	1	4219	C47H63N15O8	(M+H)+	18.32

--- End Of Report ---



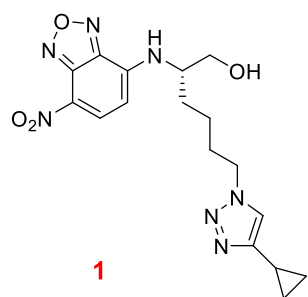
Chemical Formula: C₃₂H₄₅N₁₁O₆
Exact Mass: 679.36



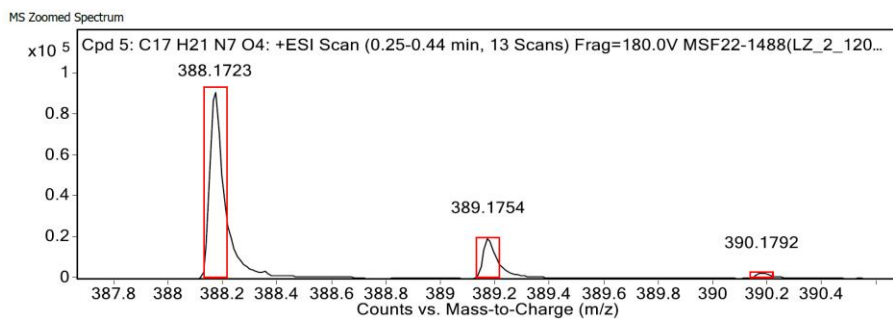
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1870			3191834			
680.3628	680.3627	1	661522	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	-0.07
681.3651	681.3655	1	262285	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	0.45
682.3671	682.3680	1	57962	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	1.35
683.3686	683.3705	1	8507	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	2.72

--- End Of Report ---



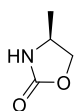
Chemical Formula: C₁₇H₂₁N₇O₄
Exact Mass: 387.17



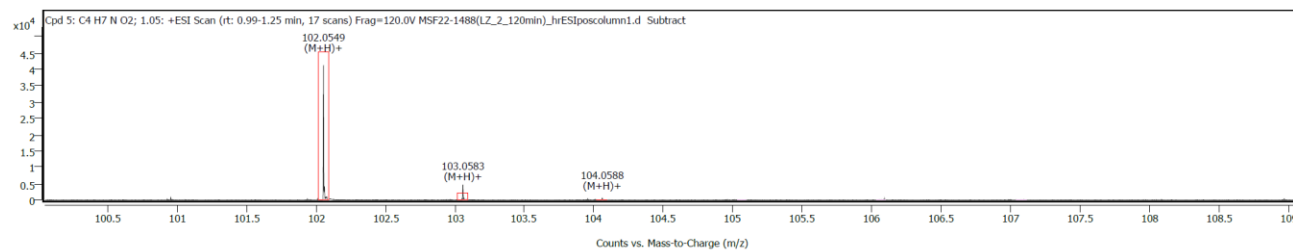
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1870			2367508			
388.1723	388.1728	1	92331	C ₁₇ H ₂₁ N ₇ O ₄	(M+H) ⁺	1.2
389.1754	389.1754	1	20048	C ₁₇ H ₂₁ N ₇ O ₄	(M+H) ⁺	-0.07
390.1792	390.1777	1	2938	C ₁₇ H ₂₁ N ₇ O ₄	(M+H) ⁺	-3.77

--- End Of Report ---



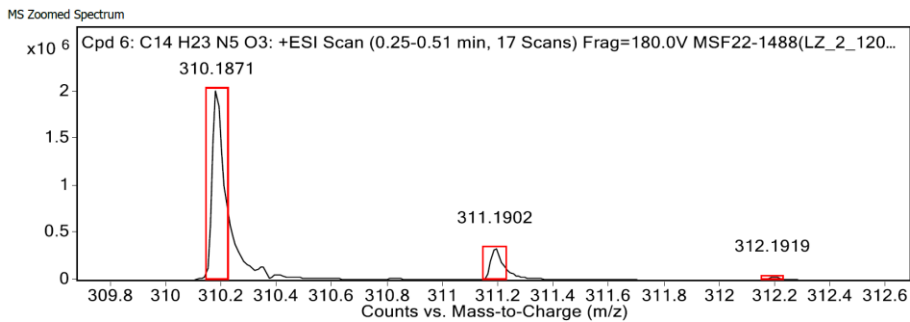
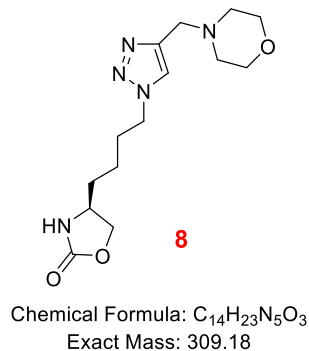
Chemical Formula: C₄H₇NO₂
Exact Mass: 101.05



Spectrum Peaks

Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
102.0549	102.0550	1	42443	C ₄ H ₇ NO ₂	(M+H) ⁺	-0.82
103.0583	103.0579	1	4632	C ₄ H ₇ NO ₂	(M+H) ⁺	3.39
104.0588	104.0595	1	531	C ₄ H ₇ NO ₂	(M+H) ⁺	-6.40

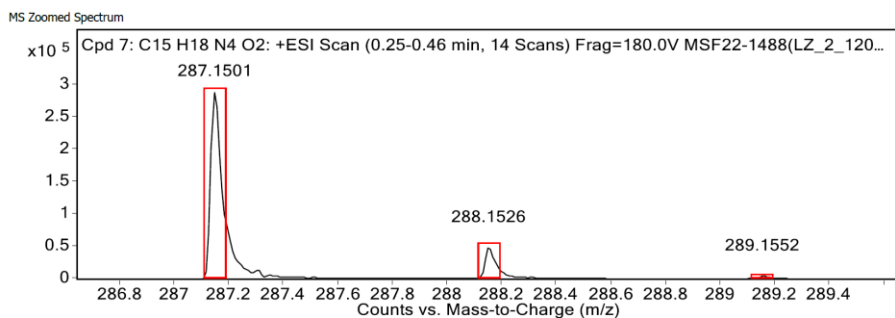
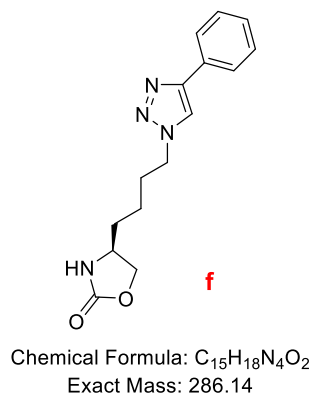
MassHunter Qual 10.0
(End of Report)



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1871	310.1874	1	2034225	$C_{14}H_{23}N_5O_3$	(M+H) ⁺	0.78
311.1902	311.1901	1	341235	$C_{14}H_{23}N_5O_3$	(M+H) ⁺	-0.45
312.1919	312.1924	1	39422	$C_{14}H_{23}N_5O_3$	(M+H) ⁺	1.67
313.1938	313.1948	1	3118	$C_{14}H_{23}N_5O_3$	(M+H) ⁺	3.32

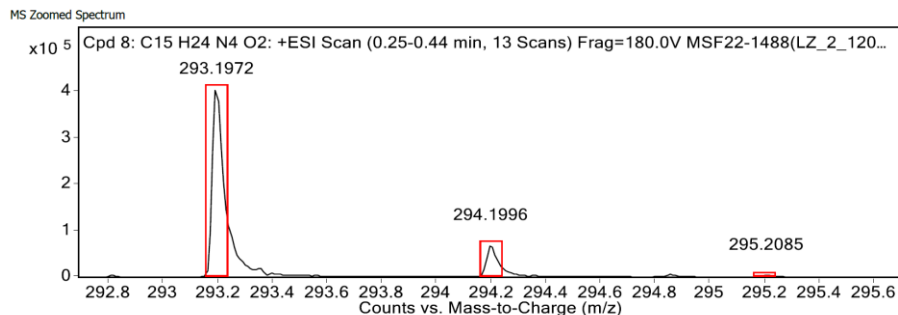
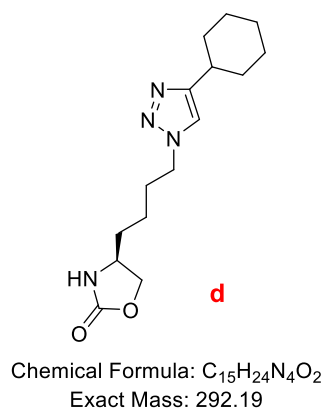
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
287.1501	287.1503	1	293256	$C_{15}H_{18}N_4O_2$	(M+H) ⁺	0.57
288.1526	288.1531	1	50002	$C_{15}H_{18}N_4O_2$	(M+H) ⁺	1.97
289.1552	289.1557	1	5938	$C_{15}H_{18}N_4O_2$	(M+H) ⁺	1.7
290.1221	290.1581	1	333	$C_{15}H_{18}N_4O_2$	(M+H) ⁺	124.14
310.1870			2299386			

--- End Of Report ---

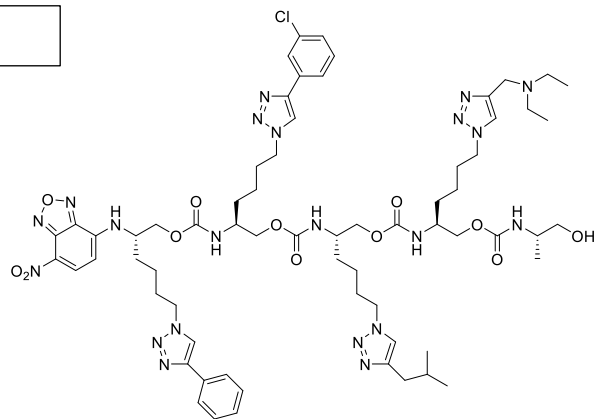


MS Spectrum Peak List

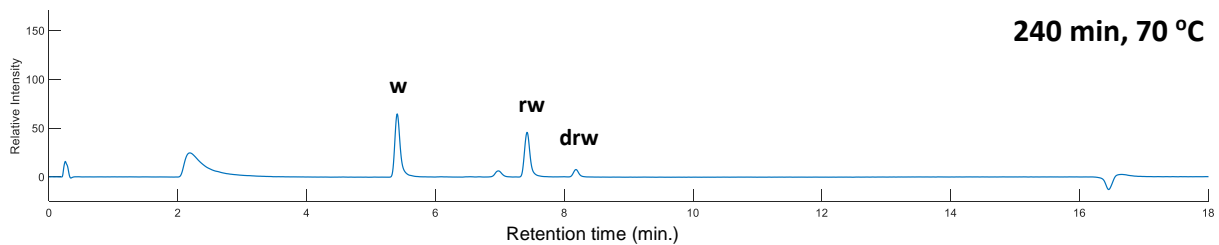
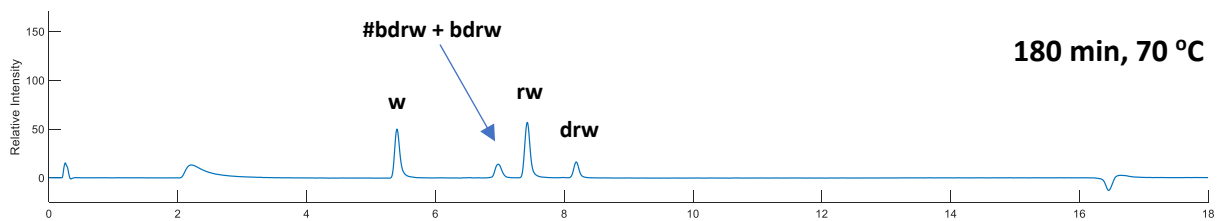
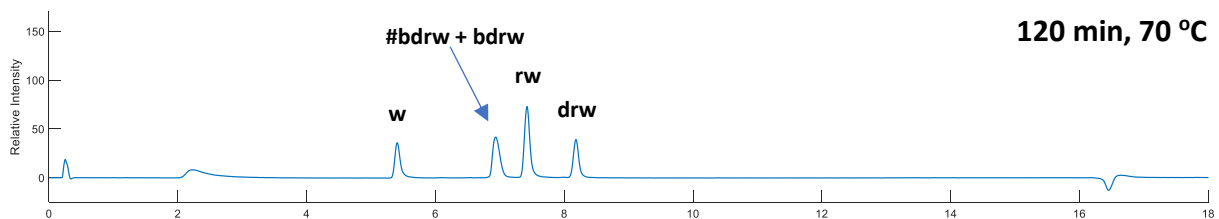
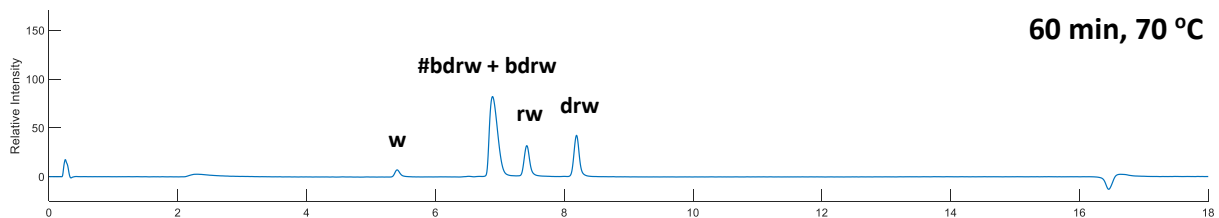
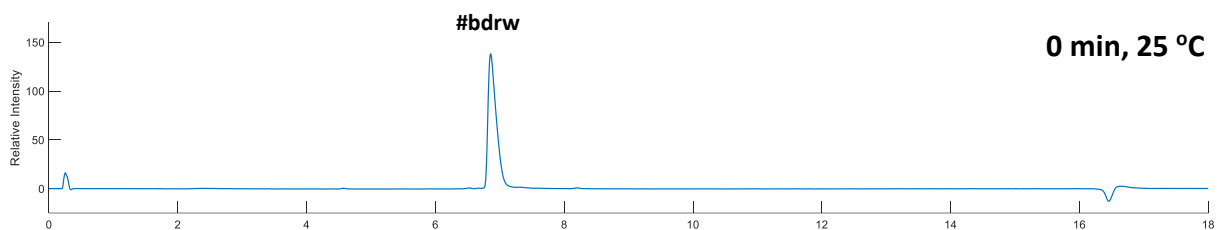
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
293.1972	293.1972	1	412036	$C_{15}H_{24}N_4O_2$	(M+H) ⁺	-0.03
294.1996	294.2001	1	69917	$C_{15}H_{24}N_4O_2$	(M+H) ⁺	1.67
295.2085	295.2026	1	5729	$C_{15}H_{24}N_4O_2$	(M+H) ⁺	-19.74
296.1461	296.2051	1	370	$C_{15}H_{24}N_4O_2$	(M+H) ⁺	199.05
310.1870			2368973			

--- End Of Report ---

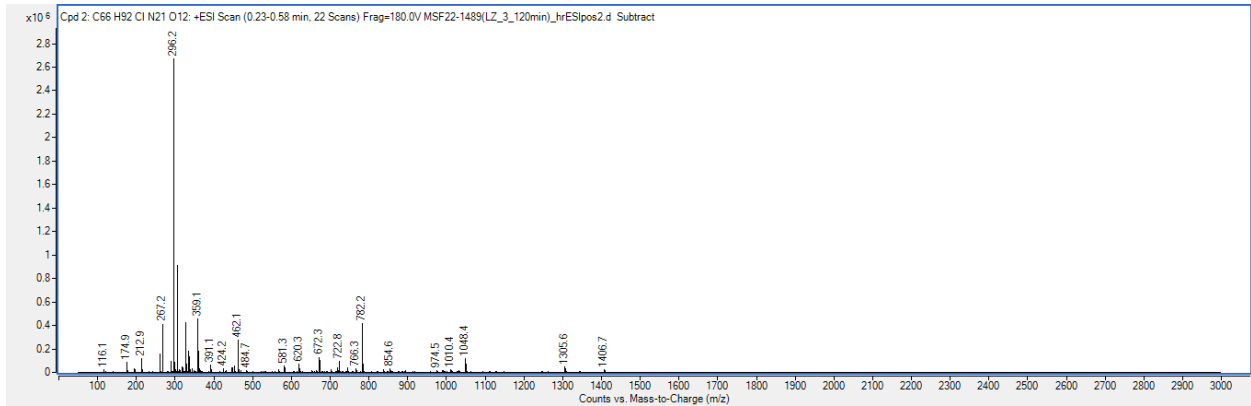
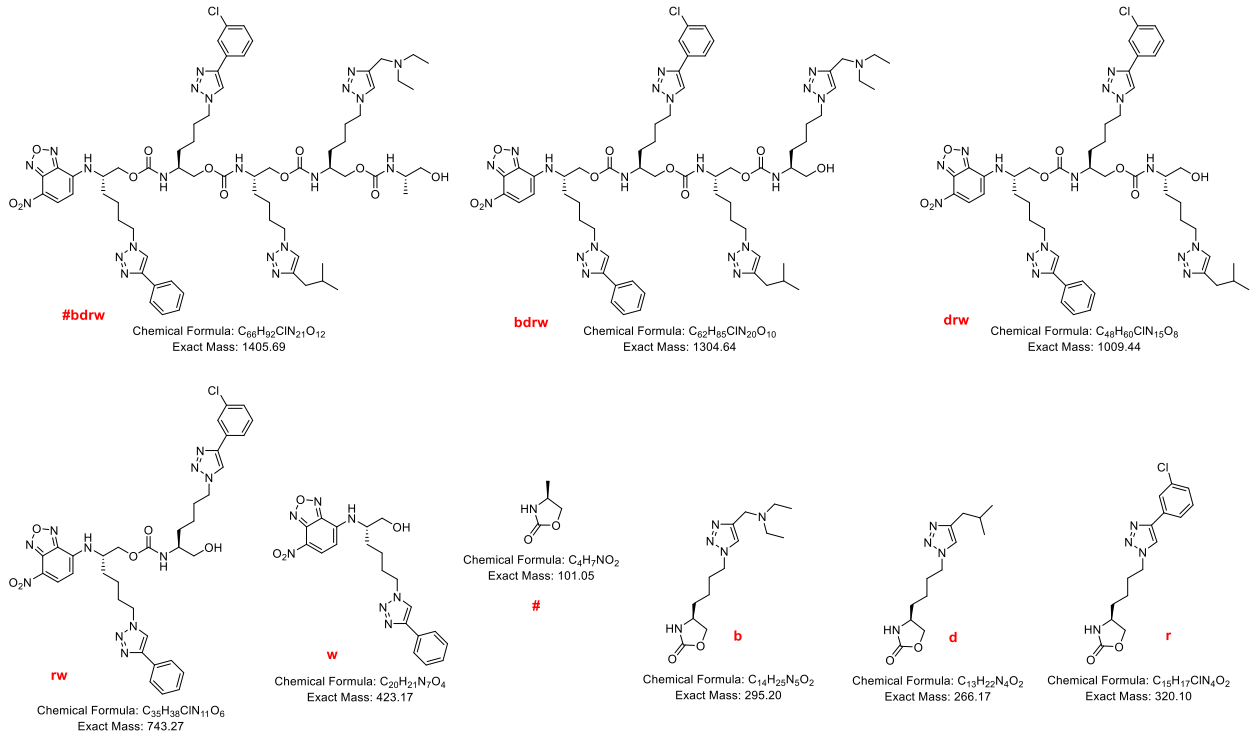
Oligomer 3: #bdrw

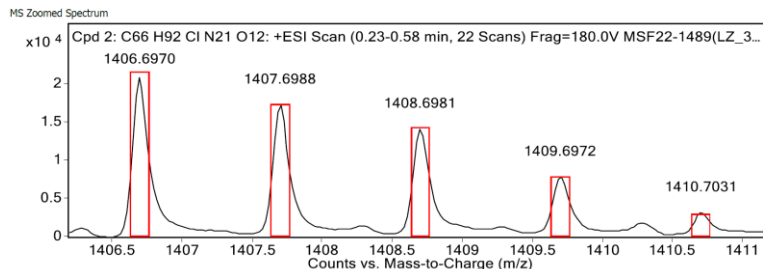
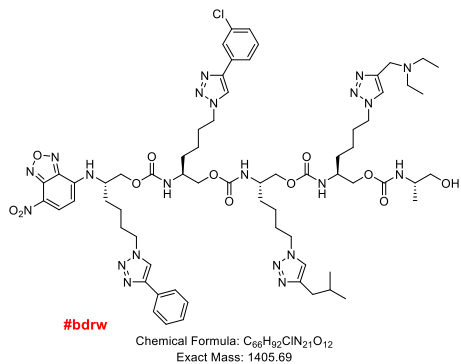


Exact Mass: 1405.69



After 120 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.

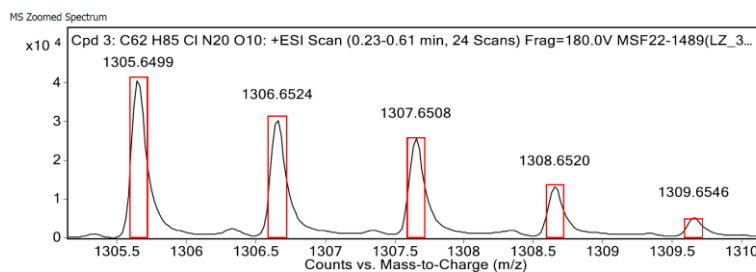
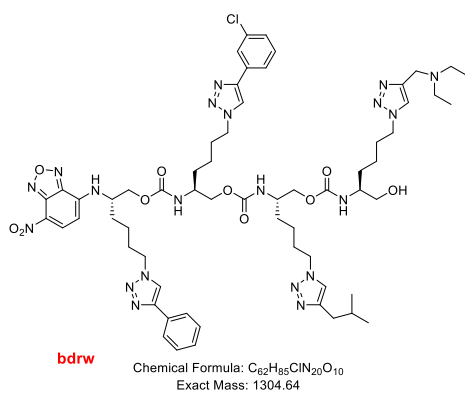




MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2078			2679292			
1406.6970	1406.6996	1	20946	C66H92ClN21O12	(M+H)+	1.85
1407.6988	1407.7024	1	17367	C66H92ClN21O12	(M+H)+	2.51
1408.6981	1408.7010	1	14207	C66H92ClN21O12	(M+H)+	2.03
1409.6972	1409.7018	1	7920	C66H92ClN21O12	(M+H)+	3.25
1410.7031	1410.7036	1	3249	C66H92ClN21O12	(M+H)+	0.34

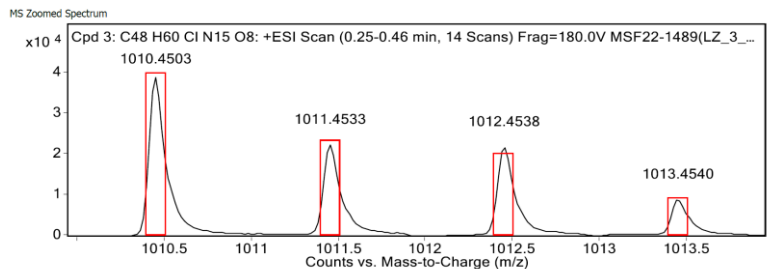
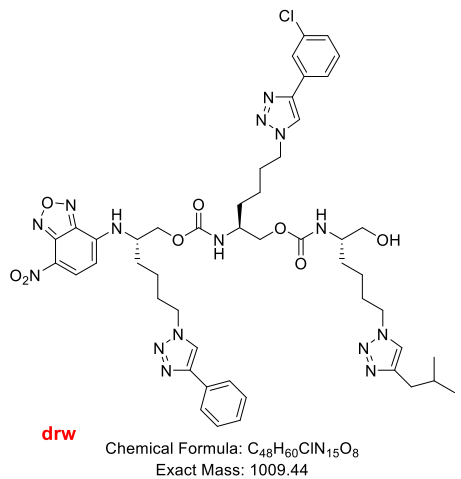
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2079			2522124			
1305.6499	1305.6519	1	41104	C62H85ClN20O10	(M+H)+	1.49
1306.6524	1306.6547	1	30654	C62H85ClN20O10	(M+H)+	1.74
1307.6508	1307.6530	1	25815	C62H85ClN20O10	(M+H)+	1.72
1308.6520	1308.6539	1	13524	C62H85ClN20O10	(M+H)+	1.46
1309.6546	1309.6557	1	5413	C62H85ClN20O10	(M+H)+	0.89
1310.6685	1310.6579	1	1761	C62H85ClN20O10	(M+H)+	-8.07

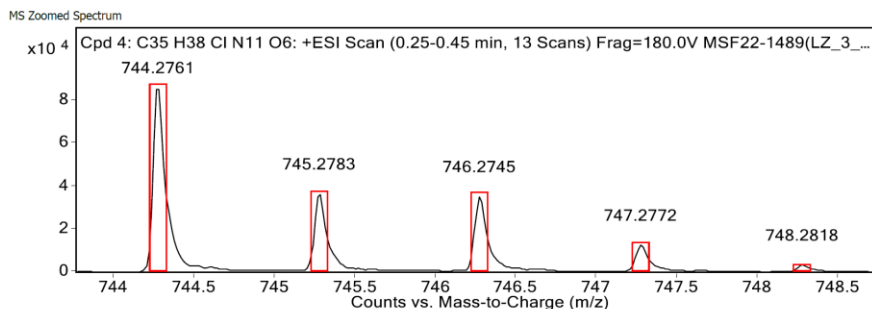
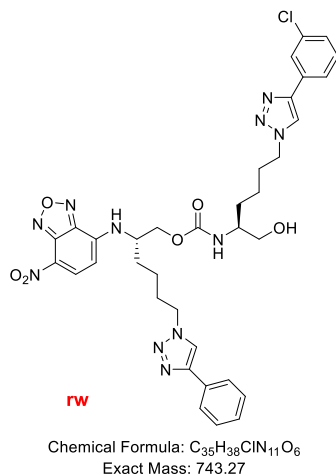
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2081			1284984			
1010.4503	1010.4511	1	38940	C48H60ClN15O8	(M+H)+	0.73
1011.4533	1011.4539	1	22411	C48H60ClN15O8	(M+H)+	0.51
1012.4538	1012.4512	1	21849	C48H60ClN15O8	(M+H)+	-2.62
1013.4540	1013.4524	1	8944	C48H60ClN15O8	(M+H)+	-1.57

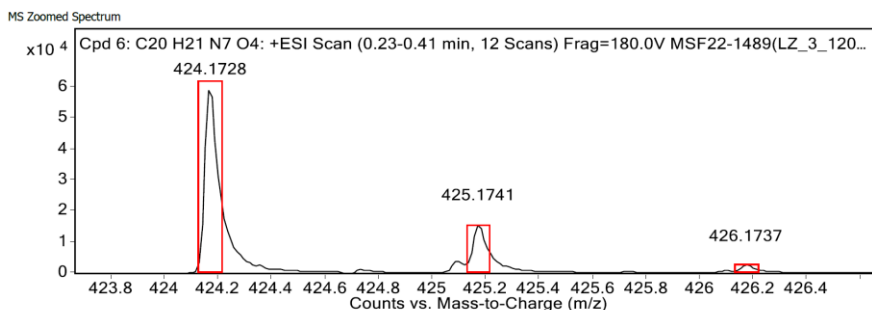
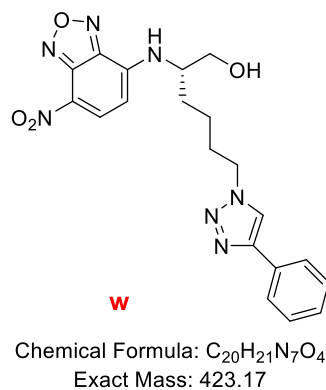
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2081			1166541			
744.2761	744.2768	1	87262	$C_{35}H_{38}ClN_{11}O_6$	(M+H) ⁺	0.91
745.2783	745.2796	1	36653	$C_{35}H_{38}ClN_{11}O_6$	(M+H) ⁺	1.68
746.2745	746.2758	1	35366	$C_{35}H_{38}ClN_{11}O_6$	(M+H) ⁺	1.79
747.2772	747.2775	1	12712	$C_{35}H_{38}ClN_{11}O_6$	(M+H) ⁺	0.43
748.2818	748.2798	1	3413	$C_{35}H_{38}ClN_{11}O_6$	(M+H) ⁺	-2.74
749.2948	749.2821	1	804	$C_{35}H_{38}ClN_{11}O_6$	(M+H) ⁺	-16.85

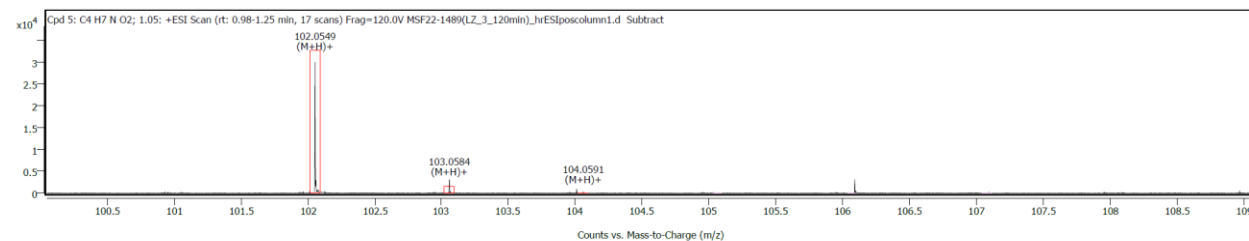
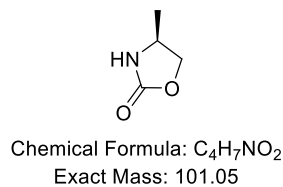
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2077			2624516			
424.1728	424.1728	1	60499	$C_{20}H_{21}N_7O_4$	(M+H) ⁺	-0.02
425.1741	425.1755	1	15791	$C_{20}H_{21}N_7O_4$	(M+H) ⁺	3.29
426.1737	426.1780	1	2589	$C_{20}H_{21}N_7O_4$	(M+H) ⁺	9.88
427.1766	427.1803	1	427	$C_{20}H_{21}N_7O_4$	(M+H) ⁺	8.66

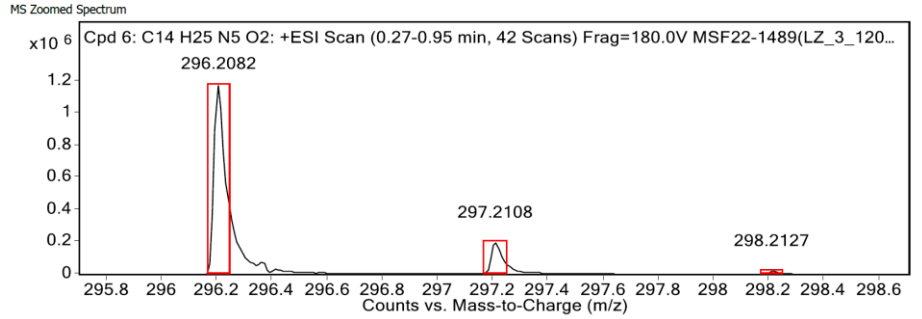
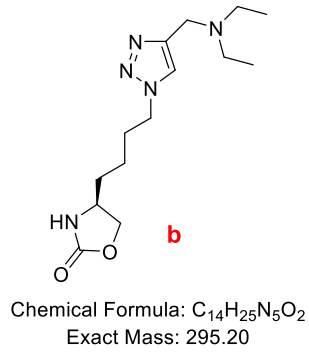
--- End Of Report ---



Spectrum Peaks

Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
102.0549	102.0550	1	30805	$C_4H_7NO_2$	(M+H) ⁺	-0.41
103.0584	103.0579	1	3115	$C_4H_7NO_2$	(M+H) ⁺	5.21
104.0591	104.0595	1	236	$C_4H_7NO_2$	(M+H) ⁺	-3.23

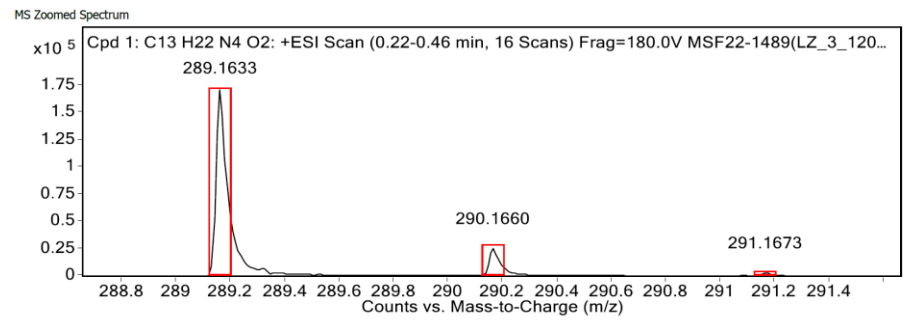
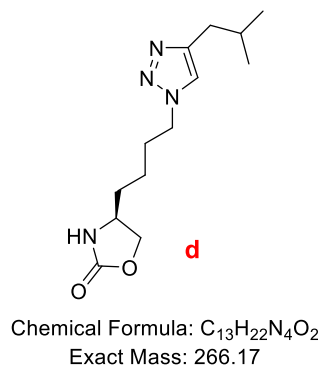
MassHunter Qual 10.0
(End of Report)



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2082	296.2081	1	1178381	C ₁₄ H ₂₅ N ₅ O ₂	(M+H) ⁺	-0.29
297.2108	297.2108	1	197531	C ₁₄ H ₂₅ N ₅ O ₂	(M+H) ⁺	0.1
298.2127	298.2133	1	20996	C ₁₄ H ₂₅ N ₅ O ₂	(M+H) ⁺	1.84

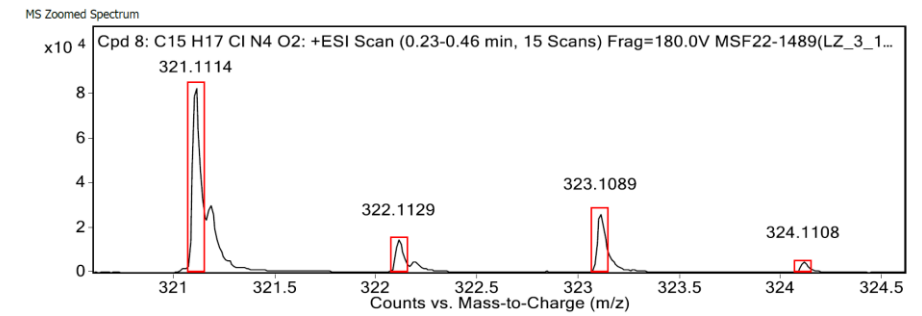
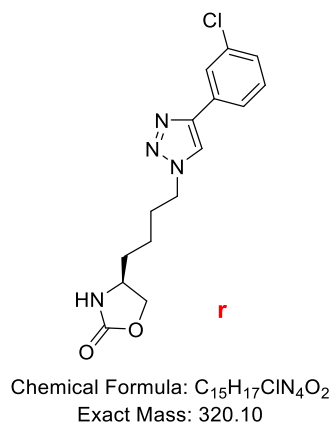
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
289.1633	289.1635	1	171372	C ₁₃ H ₂₂ N ₄ O ₂	(M+Na) ⁺	0.83
290.1660	290.1663	1	25126	C ₁₃ H ₂₂ N ₄ O ₂	(M+Na) ⁺	1
291.1673	291.1687	1	2814	C ₁₃ H ₂₂ N ₄ O ₂	(M+Na) ⁺	4.88
292.1706	292.1711	1	307	C ₁₃ H ₂₂ N ₄ O ₂	(M+Na) ⁺	1.98
296.2081			1067585			

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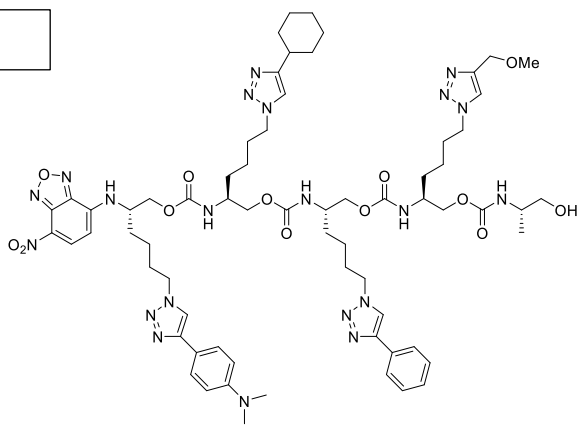


MS Spectrum Peak List

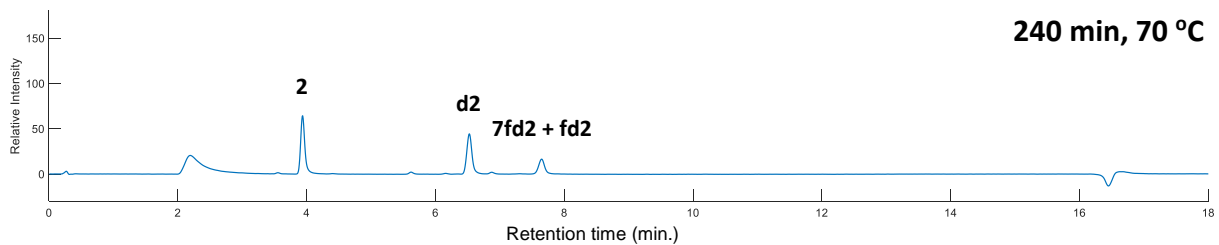
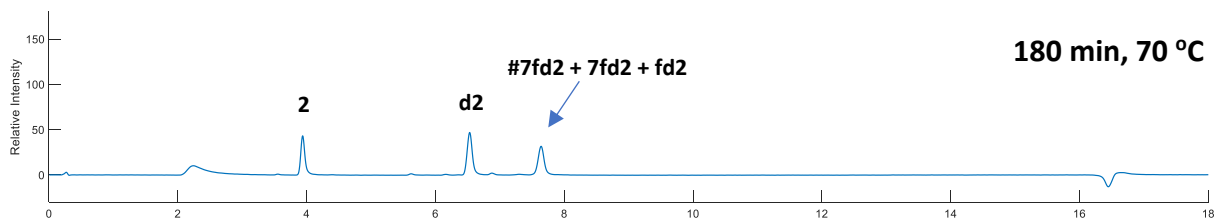
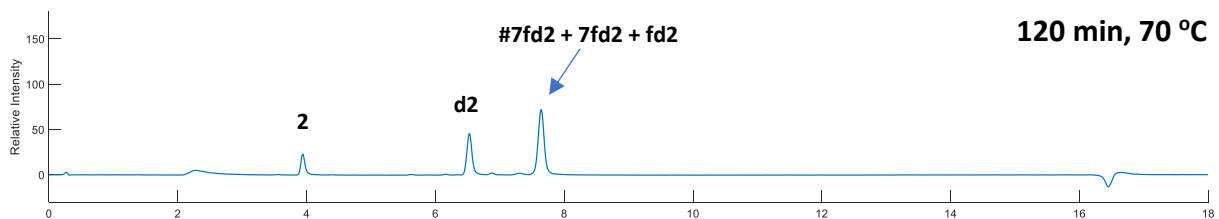
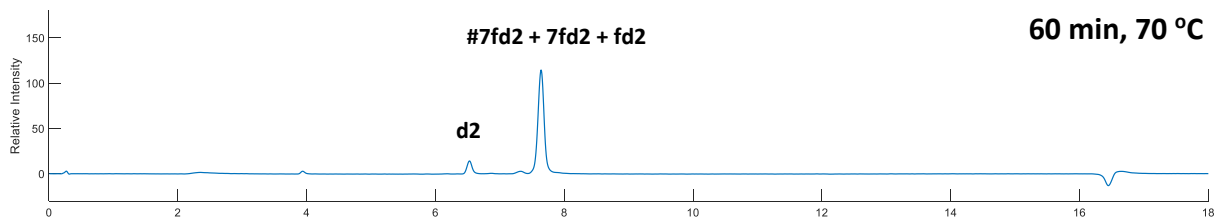
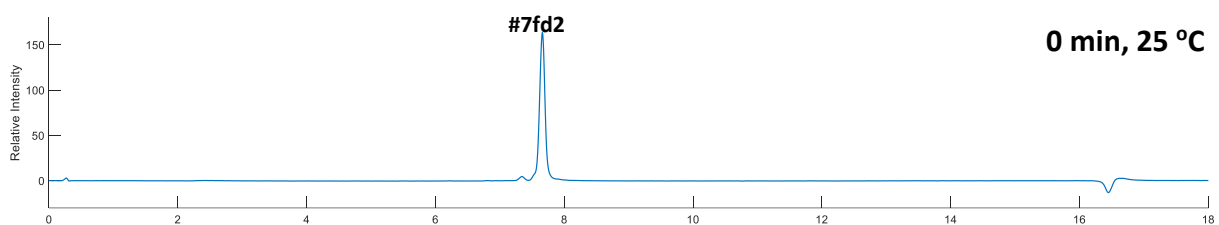
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2081			1101688			
321.1114	321.1113	1	83930	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+H) ⁺	-0.3
322.1129	322.1142	1	14904	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+H) ⁺	3.77
323.1089	323.1088	1	26472	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+H) ⁺	-0.44
324.1108	324.1114	1	4739	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+H) ⁺	1.92
325.1073	325.1139	1	3819	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+H) ⁺	20.22
326.1111	326.1163	1	815	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+H) ⁺	15.7

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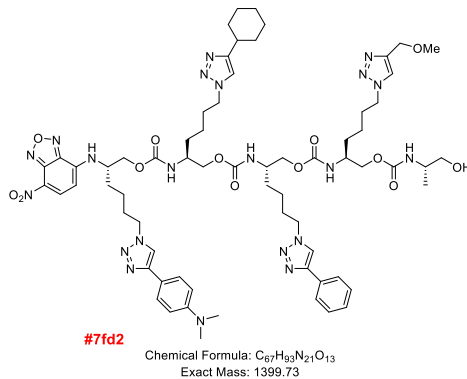
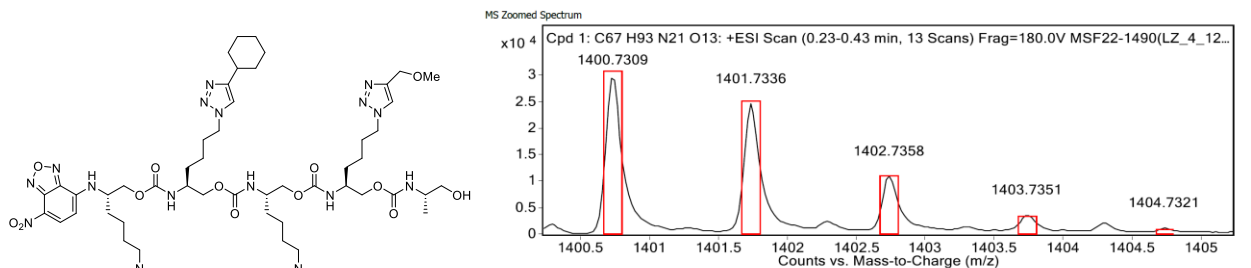
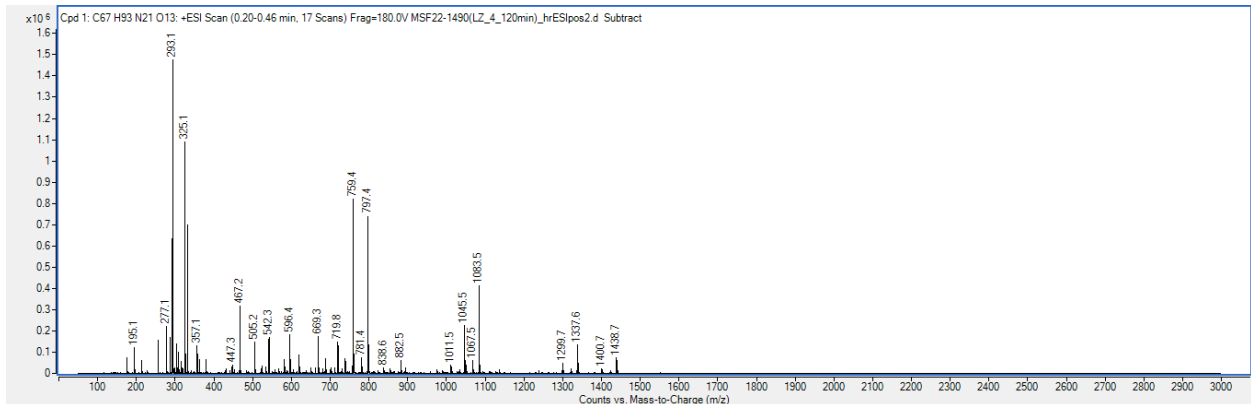
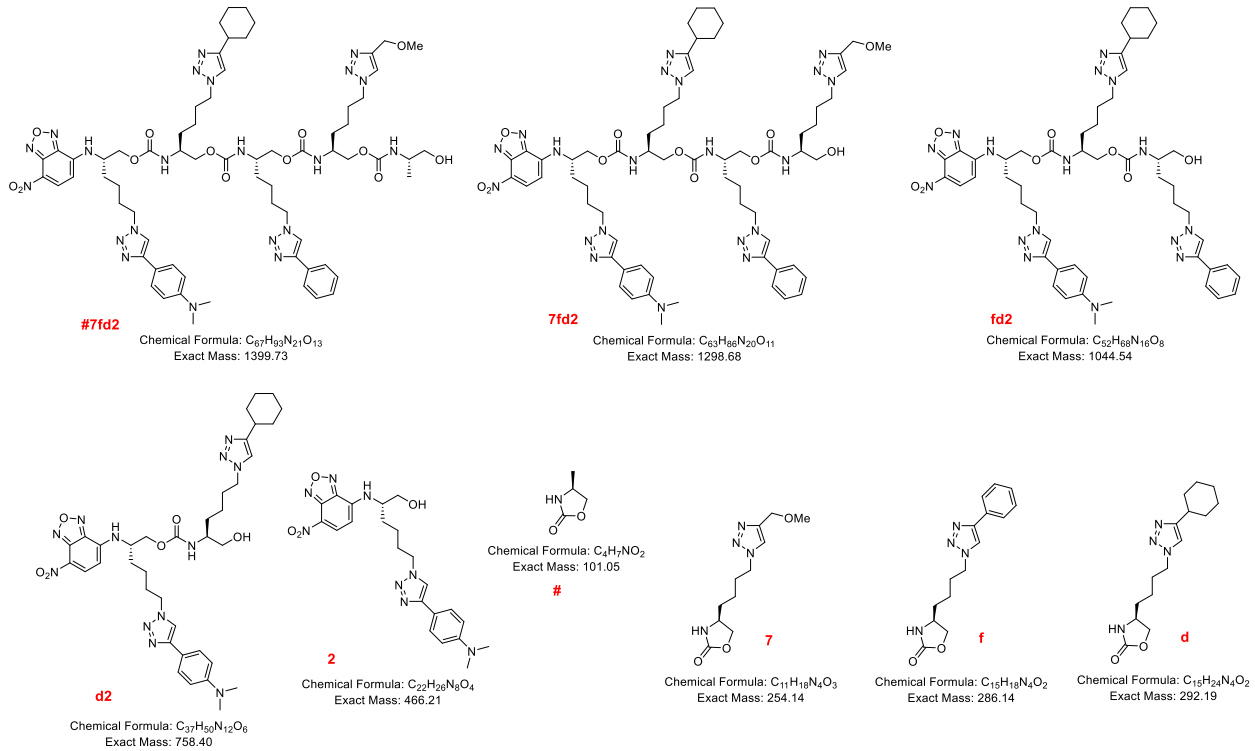
Oligomer 4: #7fd2



Exact Mass: 1399.73

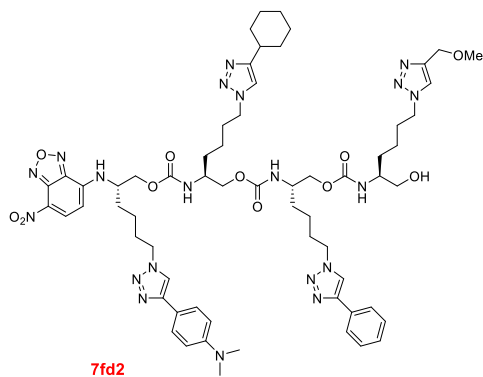


After 120 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.

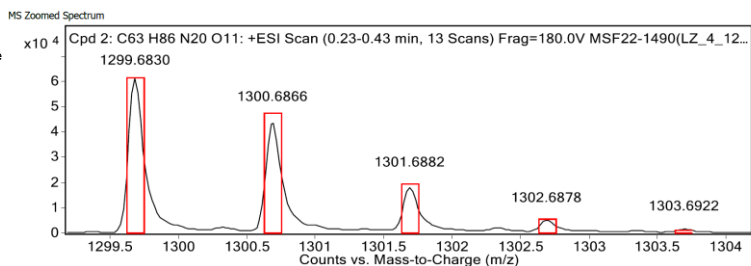


MS Spectrum Peak List						
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
293.1010			1779023			
1400.7309	1400.7334	1	30107	$C_{67}H_{93}N_{21}O_{13}$	(M+H) ⁺	1.8
1401.7336	1401.7363	1	24759	$C_{67}H_{93}N_{21}O_{13}$	(M+H) ⁺	1.87
1402.7358	1402.7389	1	11096	$C_{67}H_{93}N_{21}O_{13}$	(M+H) ⁺	2.24
1403.7351	1403.7416	1	3793	$C_{67}H_{93}N_{21}O_{13}$	(M+H) ⁺	4.61
1404.7321	1404.7441	1	1357	$C_{67}H_{93}N_{21}O_{13}$	(M+H) ⁺	8.58

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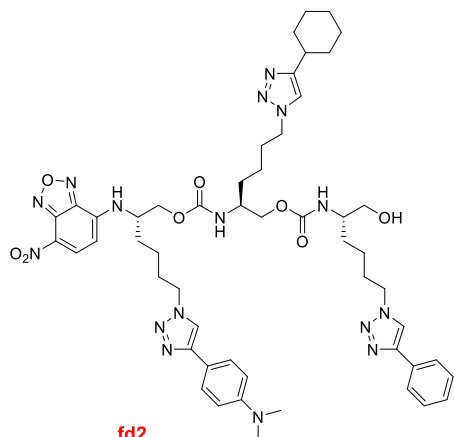


Chemical Formula: C₆₃H₈₆N₂₀O₁₁
Exact Mass: 1298.68

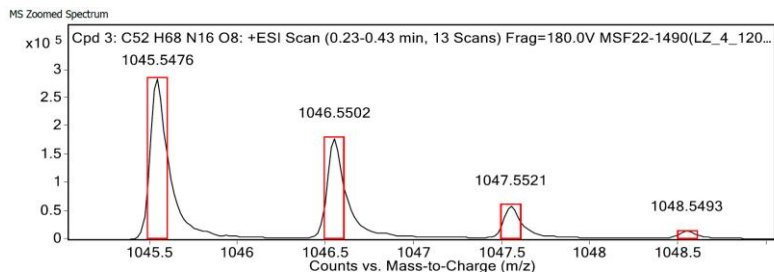


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
293.1010			1779991			
1299.6830	1299.6858	1	61539	C ₆₃ H ₈₆ N ₂₀ O ₁₁	(M+H) ⁺	2.1
1300.6866	1300.6886	1	44497	C ₆₃ H ₈₆ N ₂₀ O ₁₁	(M+H) ⁺	1.53
1301.6882	1301.6913	1	18568	C ₆₃ H ₈₆ N ₂₀ O ₁₁	(M+H) ⁺	2.34
1302.6878	1302.6939	1	4546	C ₆₃ H ₈₆ N ₂₀ O ₁₁	(M+H) ⁺	4.67
1303.6922	1303.6964	1	1229	C ₆₃ H ₈₆ N ₂₀ O ₁₁	(M+H) ⁺	3.26
1304.6768	1304.6990	1	248	C ₆₃ H ₈₆ N ₂₀ O ₁₁	(M+H) ⁺	17

--- End Of Report ---

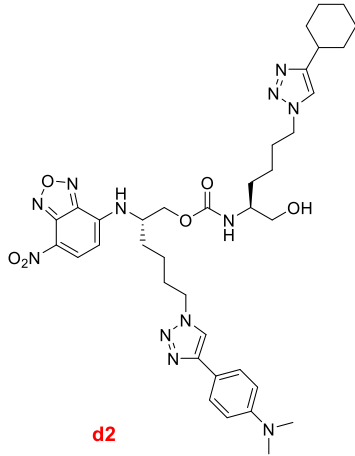


Chemical Formula: C₅₂H₆₈N₁₆O₈
Exact Mass: 1044.54

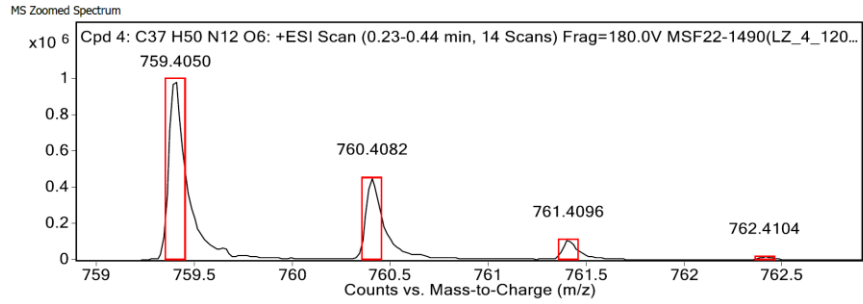


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
293.1010			1777930			
1045.5476	1045.5479	1	285185	C ₅₂ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	0.22
1046.5502	1046.5507	1	178740	C ₅₂ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	0.52
1047.5521	1047.5534	1	58956	C ₅₂ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	1.27
1048.5493	1048.5560	1	13187	C ₅₂ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	6.43

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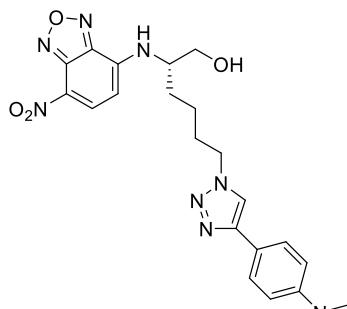


d2
 Chemical Formula: C₃₇H₅₀N₁₂O₆
 Exact Mass: 758.40

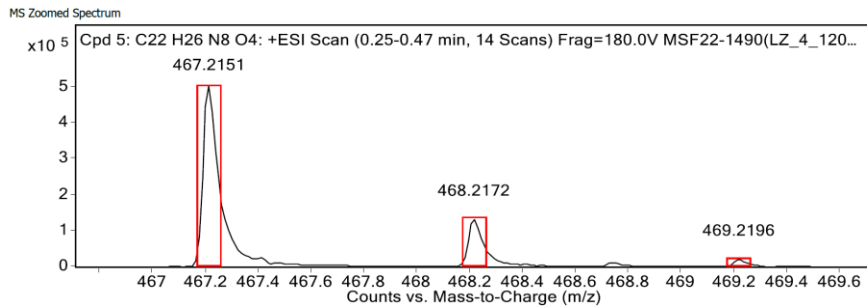


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
293.1010			1773373			
759.4050	759.4049	1	1002280	C ₃₇ H ₅₀ N ₁₂ O ₆	(M+H) ⁺	-0.13
760.4082	760.4077	1	455872	C ₃₇ H ₅₀ N ₁₂ O ₆	(M+H) ⁺	-0.73
761.4096	761.4103	1	111402	C ₃₇ H ₅₀ N ₁₂ O ₆	(M+H) ⁺	0.92
762.4104	762.4129	1	17271	C ₃₇ H ₅₀ N ₁₂ O ₆	(M+H) ⁺	3.16
763.4086	763.4153	1	2466	C ₃₇ H ₅₀ N ₁₂ O ₆	(M+H) ⁺	8.86

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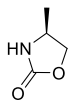


2
 Chemical Formula: C₂₂H₂₆N₈O₄
 Exact Mass: 466.21

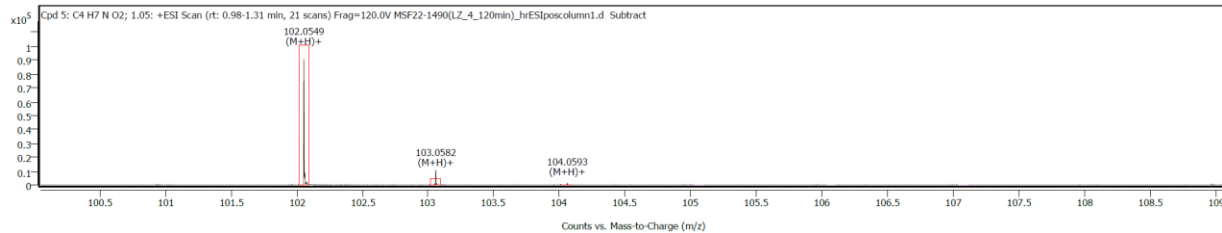


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
467.2151	467.2150	1	503378	C ₂₂ H ₂₆ N ₈ O ₄	(M+H) ⁺	-0.35
468.2172	468.2177	1	131744	C ₂₂ H ₂₆ N ₈ O ₄	(M+H) ⁺	1.04
469.2196	469.2202	1	20692	C ₂₂ H ₂₆ N ₈ O ₄	(M+H) ⁺	1.17
470.2523	470.2226	1	2501	C ₂₂ H ₂₆ N ₈ O ₄	(M+H) ⁺	-63.31
471.2134	471.2249	1	569	C ₂₂ H ₂₆ N ₈ O ₄	(M+H) ⁺	24.42
759.4044			1429557			

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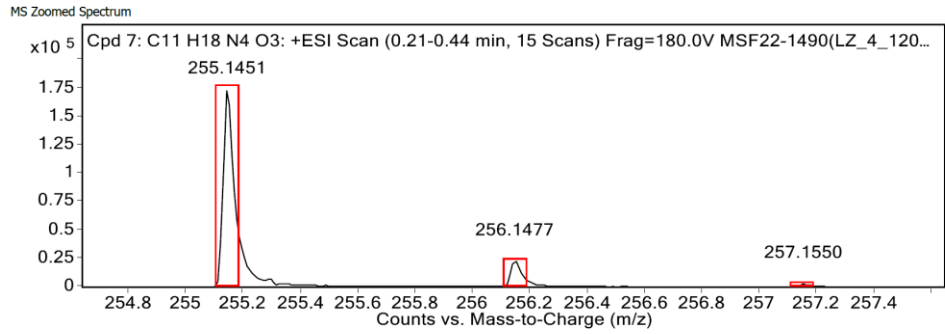
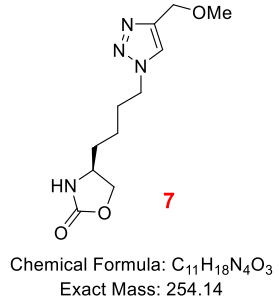


#
 Chemical Formula: C₄H₇NO₂
 Exact Mass: 101.05



Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
102.0549	102.0550	1	94820	C ₄ H ₇ NO ₂	(M+H) ⁺	-0.58
103.0582	103.0579	1	10733	C ₄ H ₇ NO ₂	(M+H) ⁺	2.96
104.0593	104.0595	1	1258	C ₄ H ₇ NO ₂	(M+H) ⁺	-1.74

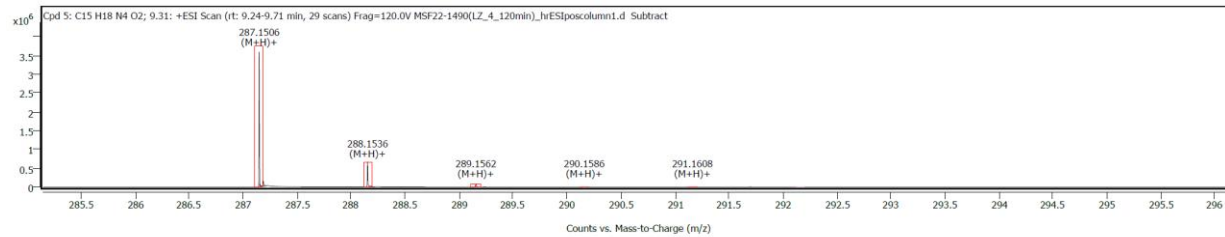
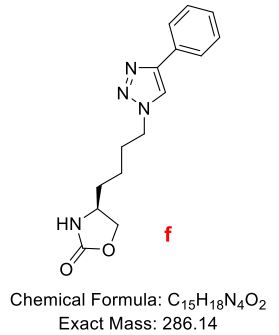
MassHunter Qual 10.0
 (End of Report)



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
255.1451	255.1452	1	176362	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	0.35
256.1477	256.1479	1	22645	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	0.96
257.1550	257.1501	1	2804	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	-19.13
258.1715	258.1524	1	421	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	-73.93
293.1010			1625527			

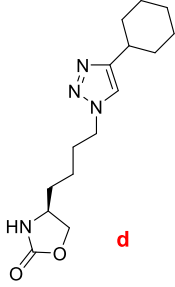
--- End Of Report ---



Spectrum Peaks

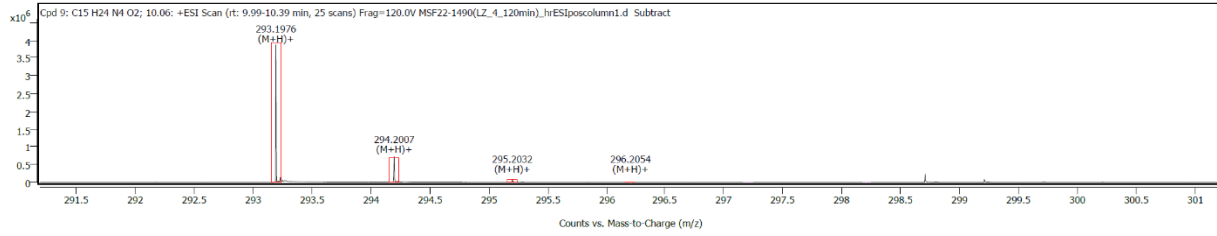
Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
287.1506	287.1503	1	3714401	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	1.17
288.1536	288.1531	1	685425	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	1.75
289.1562	289.1557	1	75108	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	1.72
290.1586	290.1581	1	5989	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	1.58
291.1608	291.1606	1	445	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	0.62

MassHunter Qual 10.0
(End of Report)



d

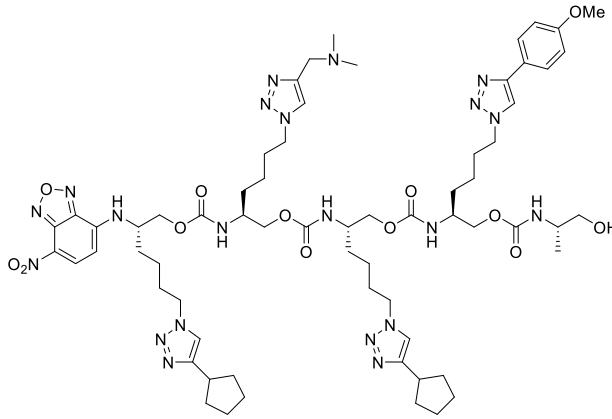
Chemical Formula: C₁₅H₂₄N₄O₂
Exact Mass: 292.19



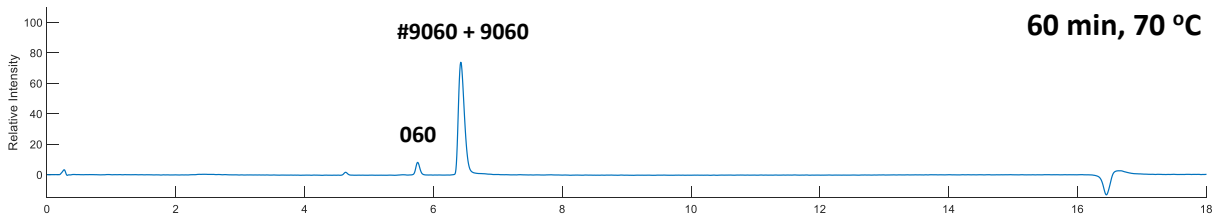
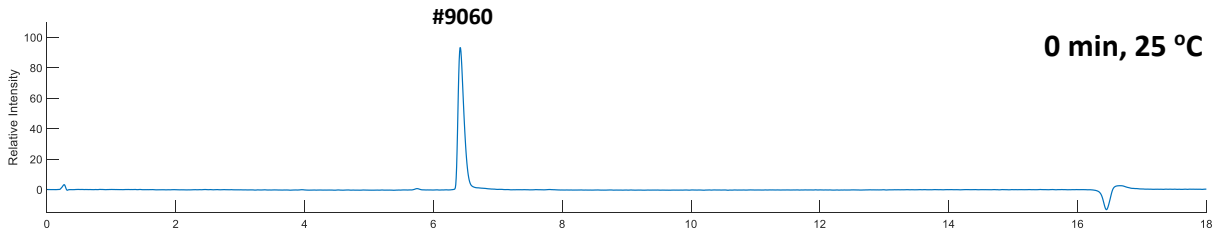
Spectrum Peaks

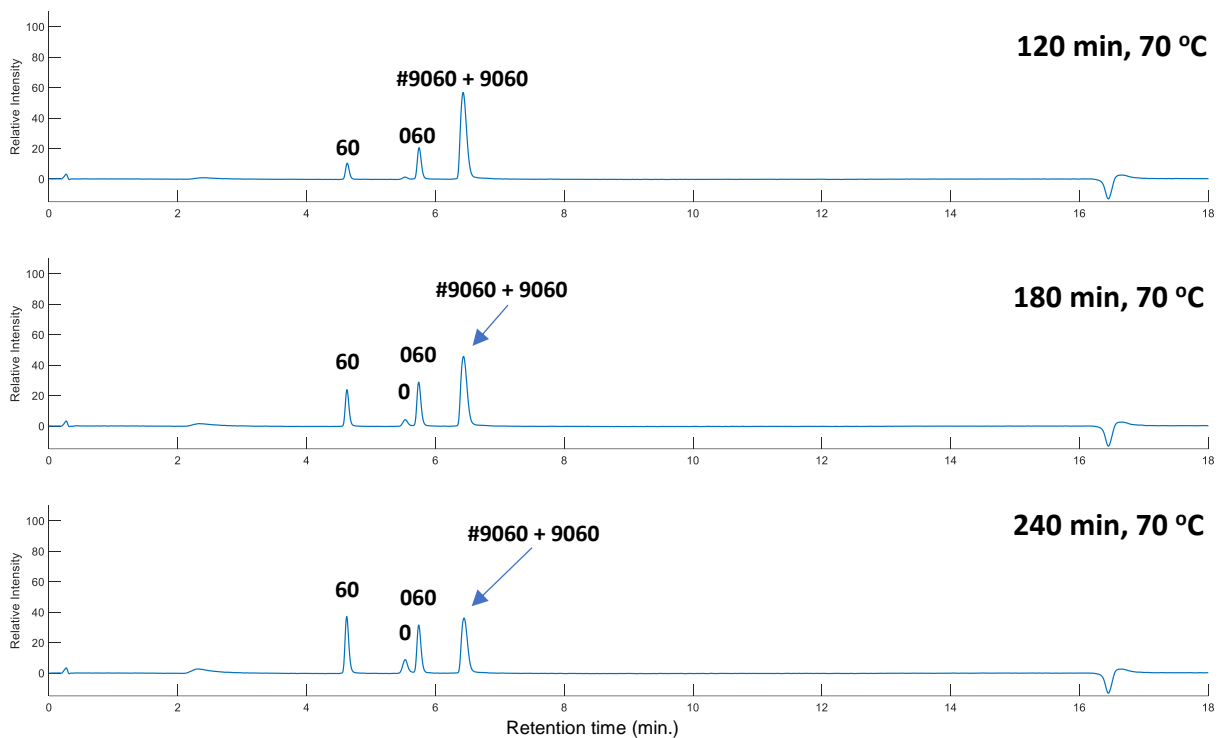
Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
293.1976	293.1972	1	3885574	C ₁₅ H ₂₄ N ₄ O ₂	(M+H) ⁺	1.37
294.2007	294.2001	1	729886	C ₁₅ H ₂₄ N ₄ O ₂	(M+H) ⁺	1.97
295.2032	295.2026	1	80608	C ₁₅ H ₂₄ N ₄ O ₂	(M+H) ⁺	1.93
296.2054	296.2051	1	6756	C ₁₅ H ₂₄ N ₄ O ₂	(M+H) ⁺	1.04

MassHunter Qual 10.0
(End of Report)

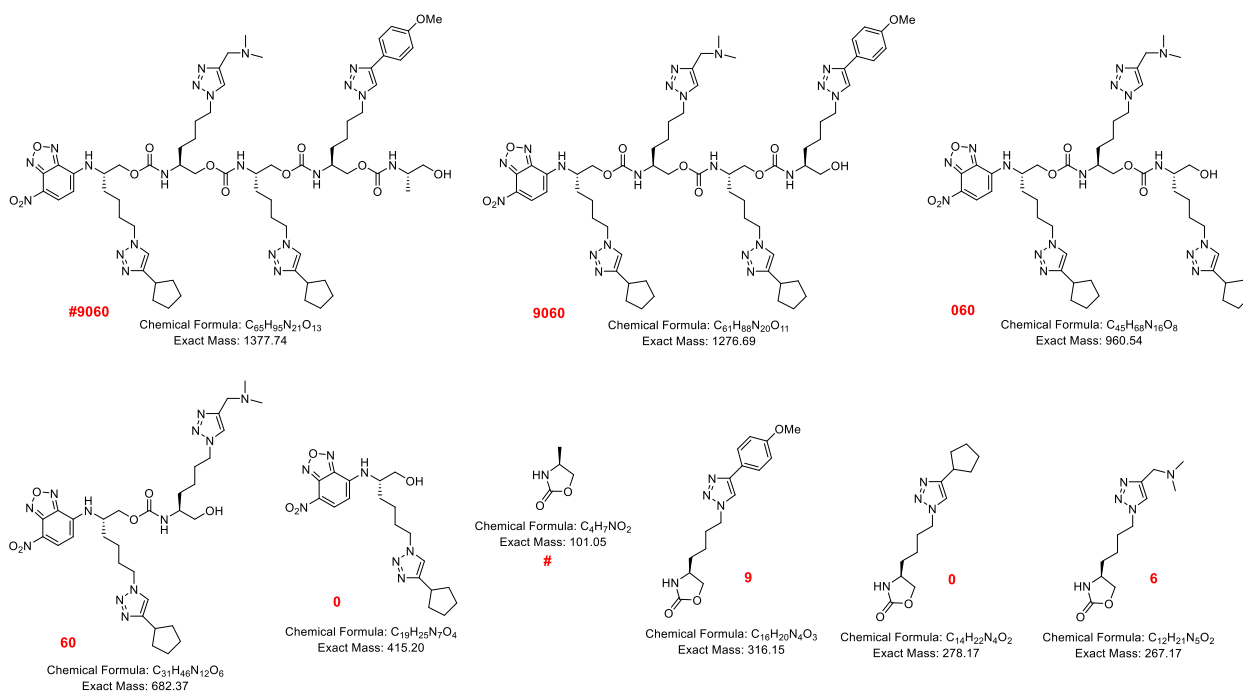


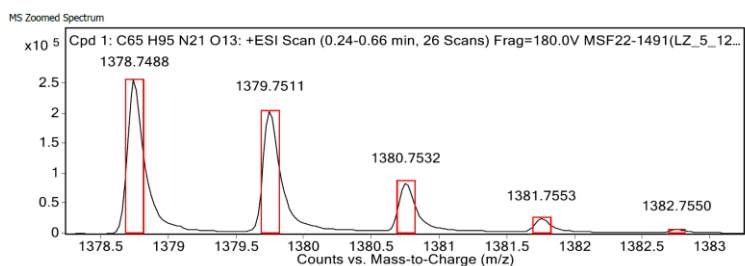
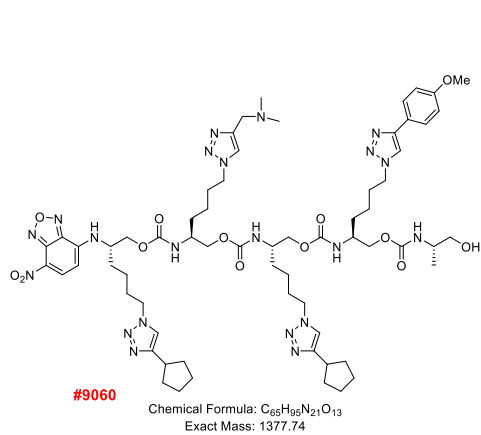
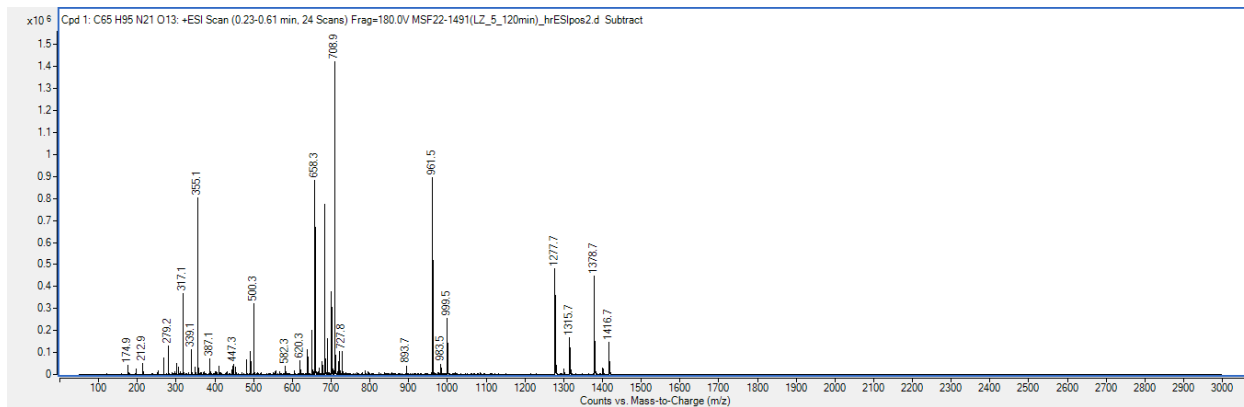
Exact Mass: 1377.74





After 120 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.

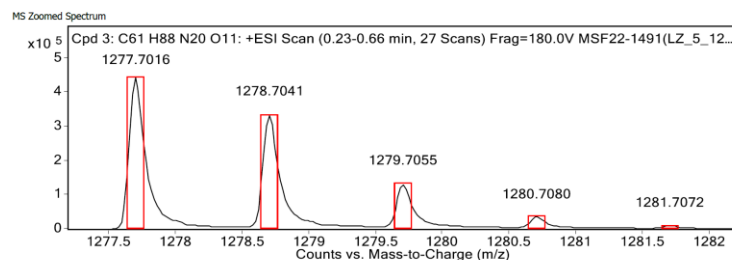
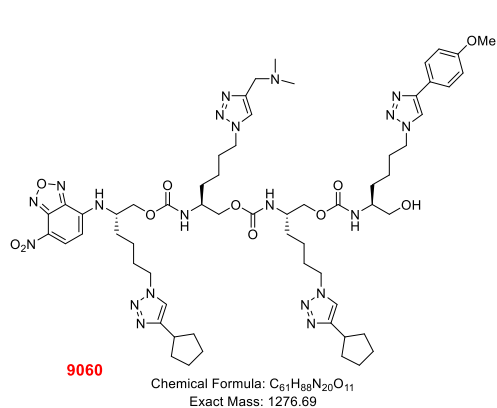




MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
708.8576			786927			
1378.7488	1378.7491	1	257452	C ₆₅ H ₉₅ N ₂₁ O ₁₃	(M+H) ⁺	0.24
1379.7511	1379.7519	1	205424	C ₆₅ H ₉₅ N ₂₁ O ₁₃	(M+H) ⁺	0.56
1380.7532	1380.7546	1	85241	C ₆₅ H ₉₅ N ₂₁ O ₁₃	(M+H) ⁺	0.99
1381.7553	1381.7572	1	22253	C ₆₅ H ₉₅ N ₂₁ O ₁₃	(M+H) ⁺	1.38
1382.7550	1382.7597	1	5388	C ₆₅ H ₉₅ N ₂₁ O ₁₃	(M+H) ⁺	3.43
1383.7472	1383.7622	1	1195	C ₆₅ H ₉₅ N ₂₁ O ₁₃	(M+H) ⁺	10.84
1384.7199	1384.7647	1	391	C ₆₅ H ₉₅ N ₂₁ O ₁₃	(M+H) ⁺	32.4

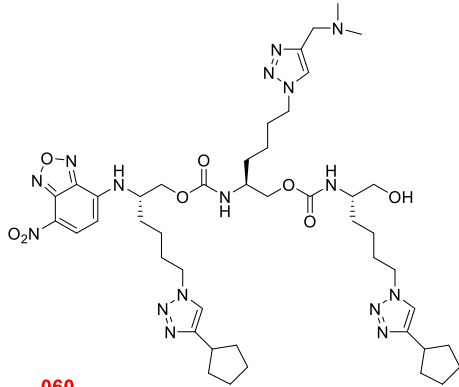
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
708.8569			1373255			
1277.7016	1277.7014	1	444067	C ₆₁ H ₈₈ N ₂₀ O ₁₁	(M+H) ⁺	-0.1
1278.7041	1278.7042	1	332958	C ₆₁ H ₈₈ N ₂₀ O ₁₁	(M+H) ⁺	0.11
1279.7055	1279.7069	1	130646	C ₆₁ H ₈₈ N ₂₀ O ₁₁	(M+H) ⁺	1.04
1280.7080	1280.7095	1	31737	C ₆₁ H ₈₈ N ₂₀ O ₁₁	(M+H) ⁺	1.17
1281.7072	1281.7120	1	7262	C ₆₁ H ₈₈ N ₂₀ O ₁₁	(M+H) ⁺	3.76
1282.7086	1282.7145	1	1469	C ₆₁ H ₈₈ N ₂₀ O ₁₁	(M+H) ⁺	4.67

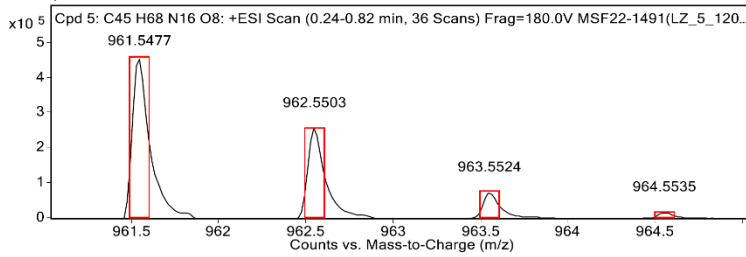
--- End Of Report ---



060

Chemical Formula: C₄₅H₆₈N₁₆O₈
Exact Mass: 960.54

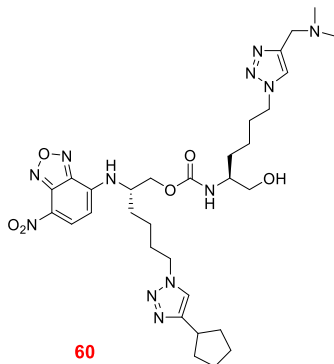
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
708.8576	721214					
961.5477	961.5479	1	455760	C ₄₅ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	0.18
962.5503	962.5506	1	257267	C ₄₅ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	0.29
963.5524	963.5532	1	74346	C ₄₅ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	0.84
964.5535	964.5558	1	17695	C ₄₅ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	2.33
965.5507	965.5582	1	3226	C ₄₅ H ₆₈ N ₁₆ O ₈	(M+H) ⁺	7.82

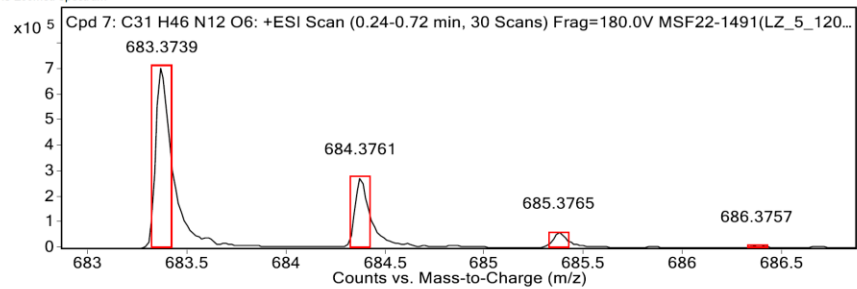
--- End Of Report ---



60

Chemical Formula: C₃₁H₄₆N₁₂O₆
Exact Mass: 682.37

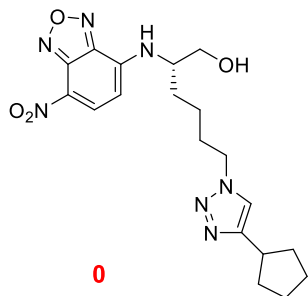
MS Zoomed Spectrum



MS Spectrum Peak List

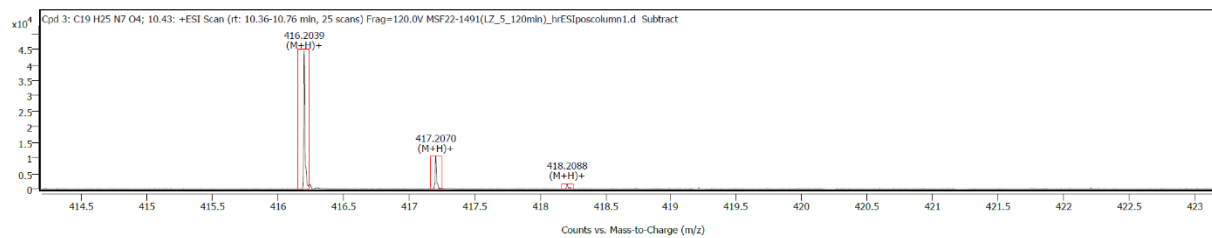
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
683.3739	683.3736	1	711672	C ₃₁ H ₄₆ N ₁₂ O ₆	(M+H) ⁺	-0.47
684.3761	684.3763	1	274587	C ₃₁ H ₄₆ N ₁₂ O ₆	(M+H) ⁺	0.3
685.3765	685.3788	1	62449	C ₃₁ H ₄₆ N ₁₂ O ₆	(M+H) ⁺	3.41
686.3757	686.3812	1	9978	C ₃₁ H ₄₆ N ₁₂ O ₆	(M+H) ⁺	8.04
687.3494	687.3836	1	2431	C ₃₁ H ₄₆ N ₁₂ O ₆	(M+H) ⁺	49.82
708.8570			1317642			

--- End Of Report ---



0

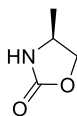
Chemical Formula: C₁₉H₂₅N₇O₄
Exact Mass: 415.20



Spectrum Peaks

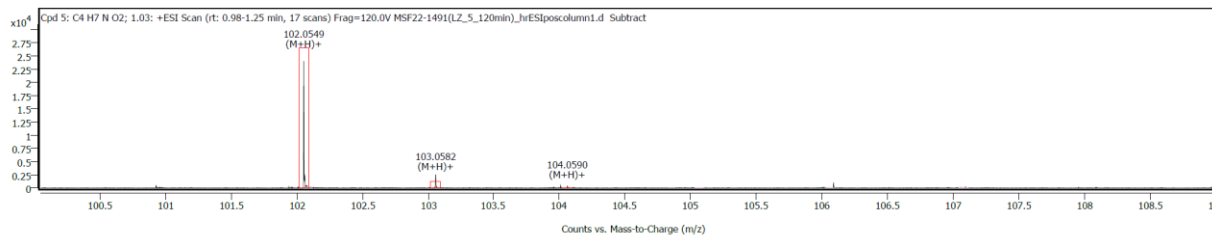
Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
416.2039	416.2041	1	44601	C ₁₉ H ₂₅ N ₇ O ₄	(M+H) ⁺	-0.54
417.2070	417.2068	1	10731	C ₁₉ H ₂₅ N ₇ O ₄	(M+H) ⁺	0.46
418.2088	418.2092	1	1547	C ₁₉ H ₂₅ N ₇ O ₄	(M+H) ⁺	-0.85
481.2778			61066			

MassHunter Qual 10.0
(End of Report)



Chemical Formula: C₄H₇NO₂
Exact Mass: 101.05

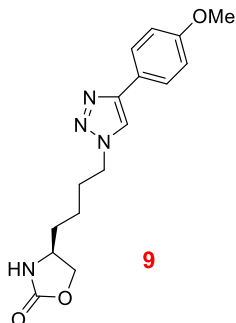
#



Spectrum Peaks

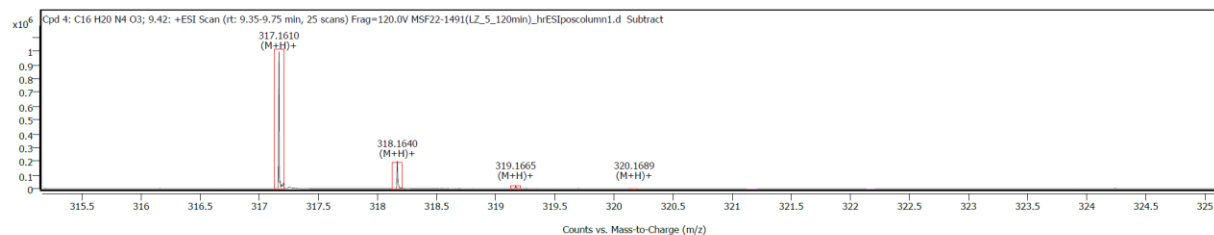
Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
102.0549	102.0550	1	24958	C ₄ H ₇ NO ₂	(M+H) ⁺	-0.36
103.0582	103.0579	1	2557	C ₄ H ₇ NO ₂	(M+H) ⁺	2.59
104.0590	104.0595	1	363	C ₄ H ₇ NO ₂	(M+H) ⁺	-5.09
922.0036			37361			

MassHunter Qual 10.0
(End of Report)



9

Chemical Formula: C₁₆H₂₀N₄O₃
Exact Mass: 316.15

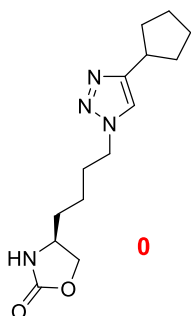
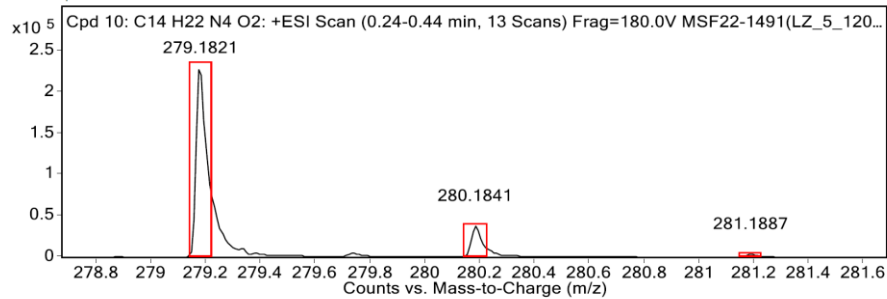


Spectrum Peaks

Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
317.1610	317.1608	1	1001021	C ₁₆ H ₂₀ N ₄ O ₃	(M+H) ⁺	0.63
318.1640	318.1637	1	202360	C ₁₆ H ₂₀ N ₄ O ₃	(M+H) ⁺	0.82
319.1665	319.1662	1	24087	C ₁₆ H ₂₀ N ₄ O ₃	(M+H) ⁺	0.79
320.1689	320.1687	1	2224	C ₁₆ H ₂₀ N ₄ O ₃	(M+H) ⁺	0.71

MassHunter Qual 10.0
(End of Report)

MS Zoomed Spectrum



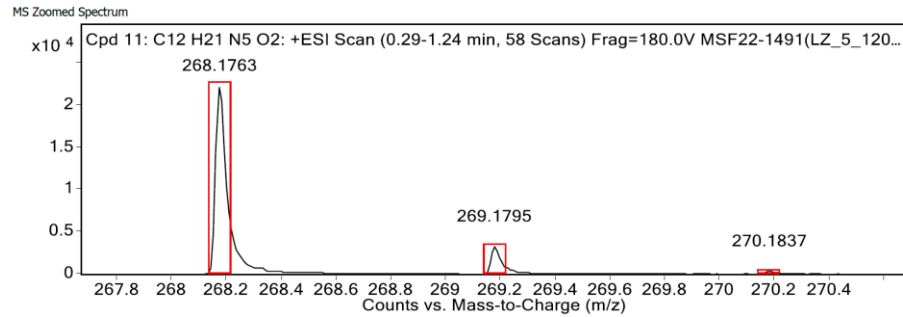
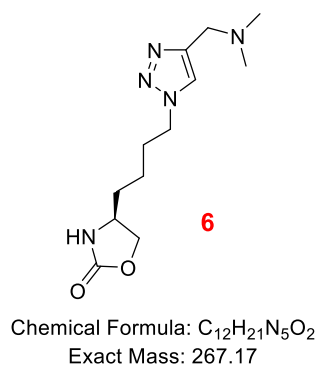
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Chemical Formula: C₁₄H₂₂N₄O₂
Exact Mass: 278.17

MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
279.1821	279.1816	1	234825	C ₁₄ H ₂₂ N ₄ O ₂	(M+H) ⁺	-2.05
280.1841	280.1844	1	38205	C ₁₄ H ₂₂ N ₄ O ₂	(M+H) ⁺	1.15
281.1887	281.1869	1	4162	C ₁₄ H ₂₂ N ₄ O ₂	(M+H) ⁺	-6.49
708.8570			1426713			

--- End Of Report ---

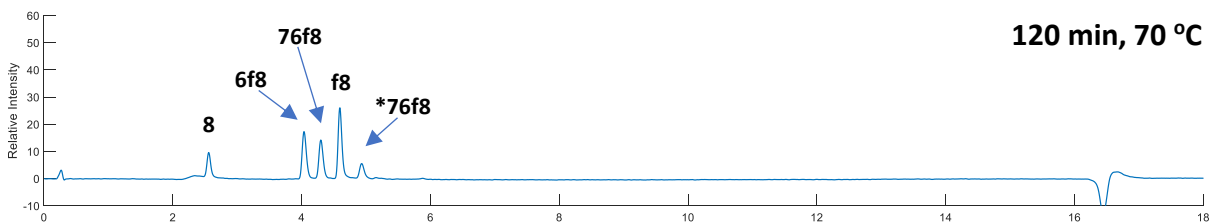
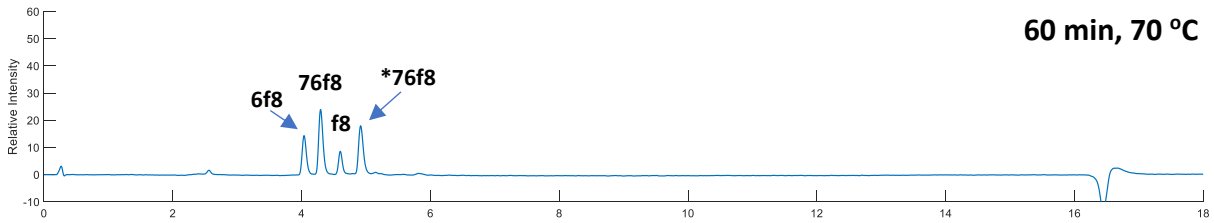
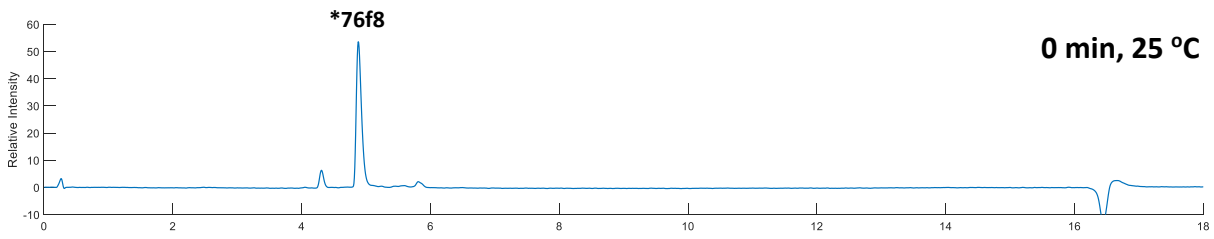
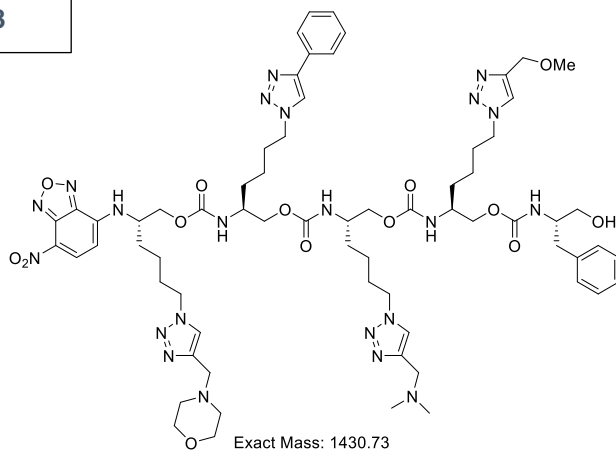


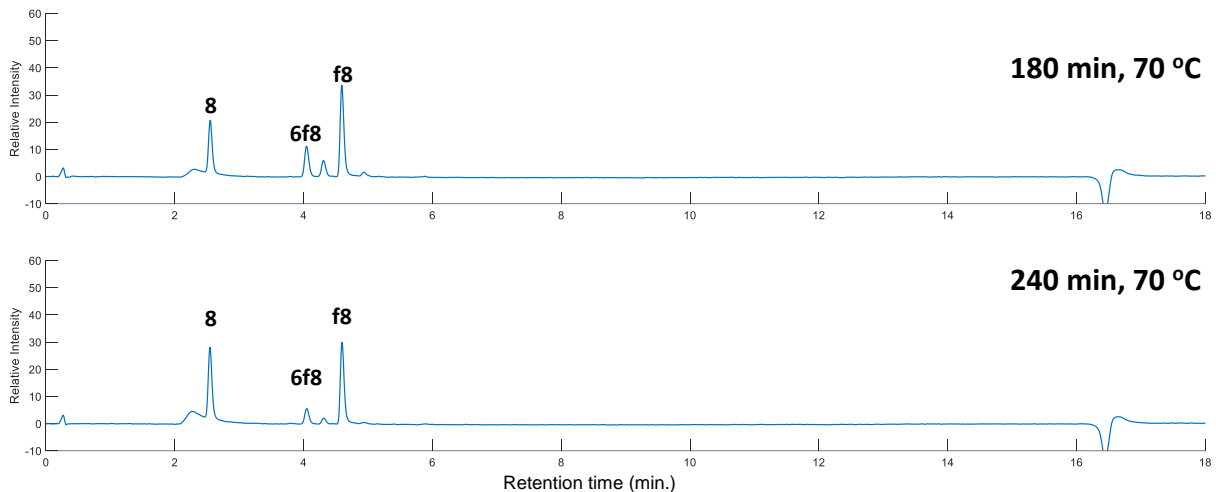
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1763	268.1768	1	22578	$C_{12}H_{21}N_5O_2$	(M+H) ⁺	1.89
269.1795	269.1794	1	3329	$C_{12}H_{21}N_5O_2$	(M+H) ⁺	-0.05
270.1837	270.1818	1	398	$C_{12}H_{21}N_5O_2$	(M+H) ⁺	-7.03
708.8576			525030			

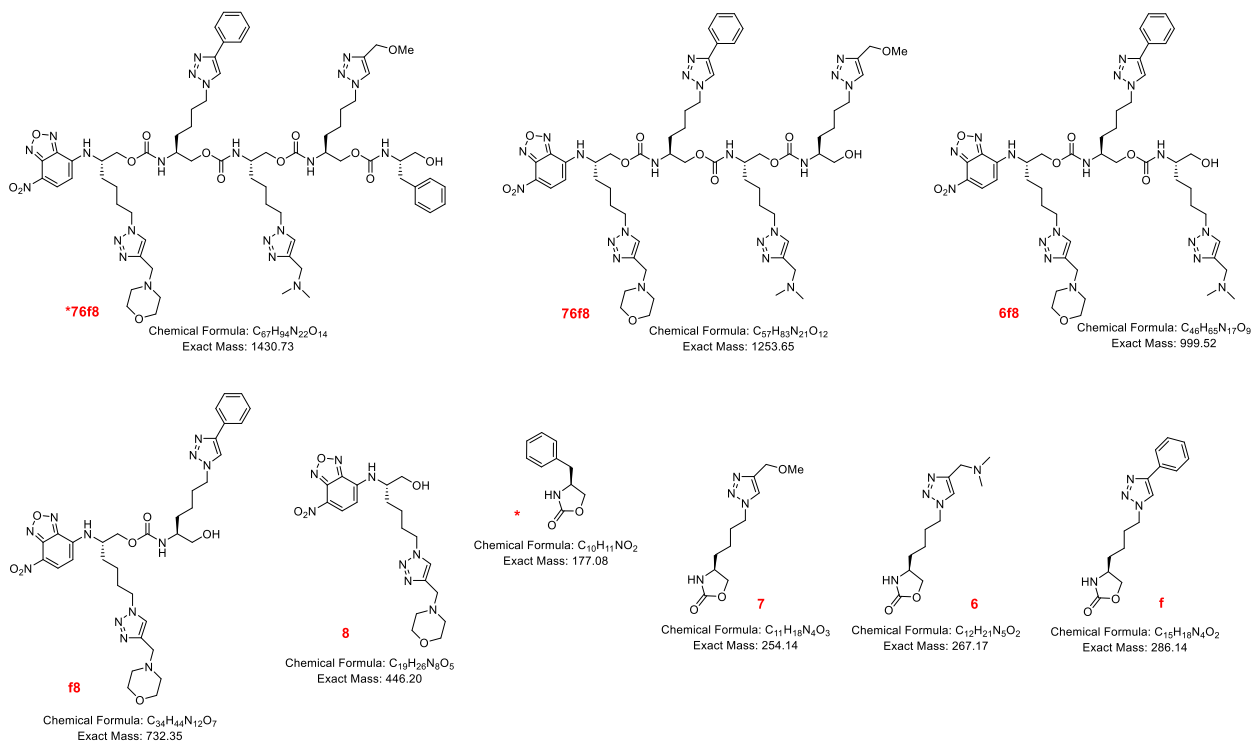
--- End Of Report ---

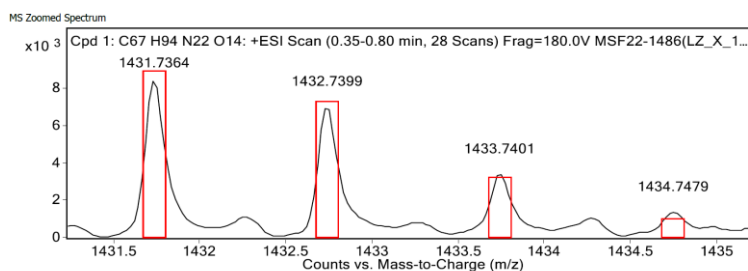
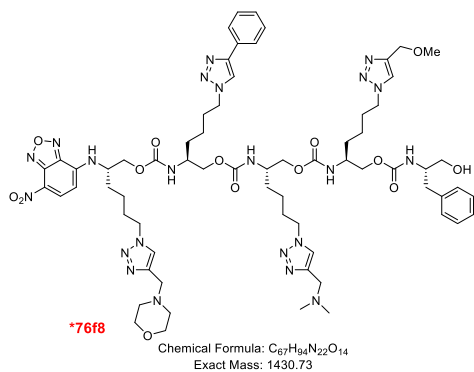
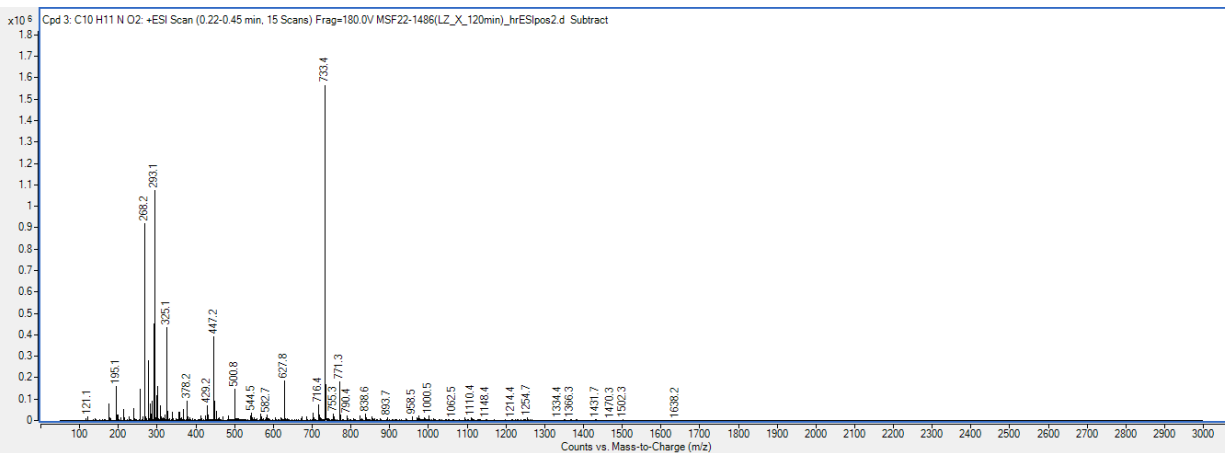
Oligomer 6_1: *76f8





After 120 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.

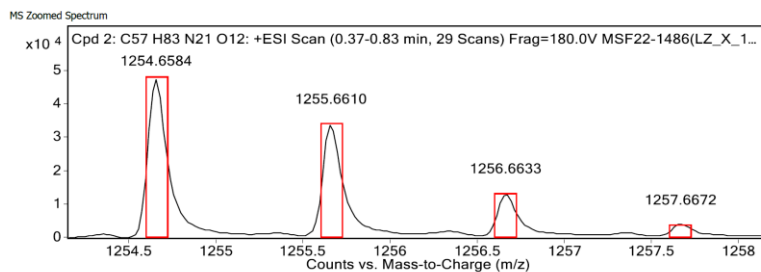
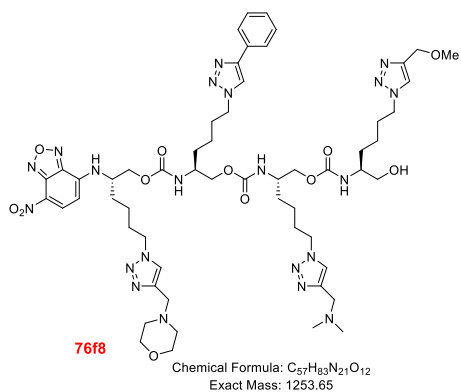




MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1768			877491			
1431.7364	1431.7393	1	8465	C ₆₇ H ₉₄ N ₂₂ O ₁₄	(M+H) ⁺	2.03
1432.7399	1432.7420	1	7071	C ₆₇ H ₉₄ N ₂₂ O ₁₄	(M+H) ⁺	1.5
1433.7401	1433.7447	1	3455	C ₆₇ H ₉₄ N ₂₂ O ₁₄	(M+H) ⁺	3.19
1434.7479	1434.7473	1	1425	C ₆₇ H ₉₄ N ₂₂ O ₁₄	(M+H) ⁺	-0.4

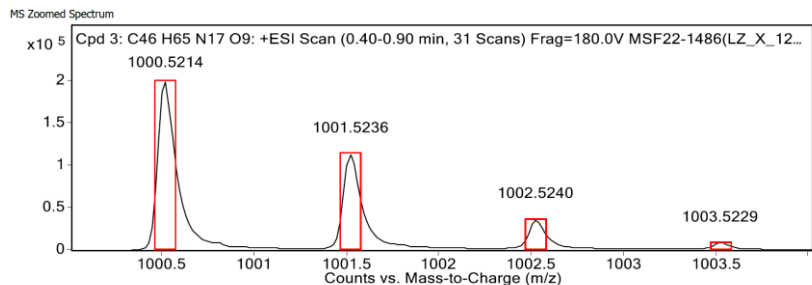
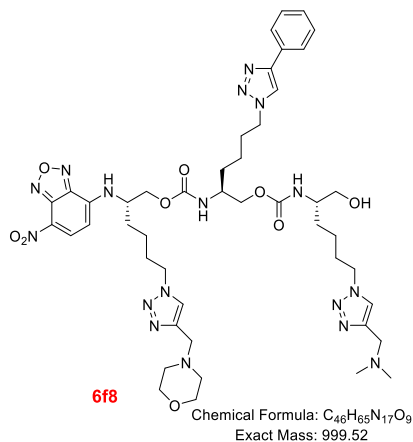
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1768			810816			
1254.6584	1254.6603	1	47537	C ₅₇ H ₈₃ N ₂₁ O ₁₂	(M+H) ⁺	1.51
1255.6610	1255.6630	1	34020	C ₅₇ H ₈₃ N ₂₁ O ₁₂	(M+H) ⁺	1.59
1256.6633	1256.6656	1	13186	C ₅₇ H ₈₃ N ₂₁ O ₁₂	(M+H) ⁺	1.8
1257.6672	1257.6681	1	3804	C ₅₇ H ₈₃ N ₂₁ O ₁₂	(M+H) ⁺	0.74
1258.6924	1258.6706	1	931	C ₅₇ H ₈₃ N ₂₁ O ₁₂	(M+H) ⁺	-17.35

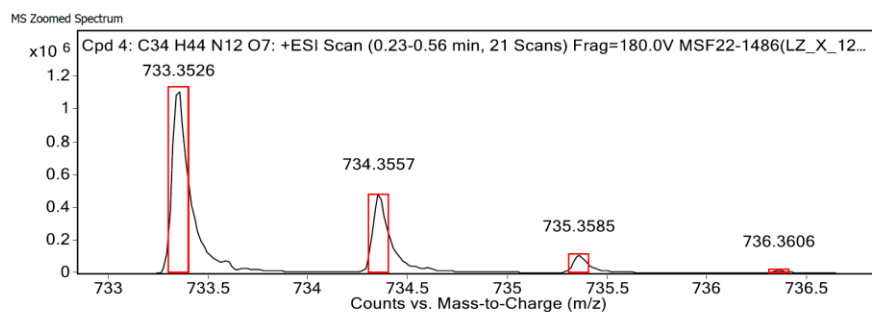
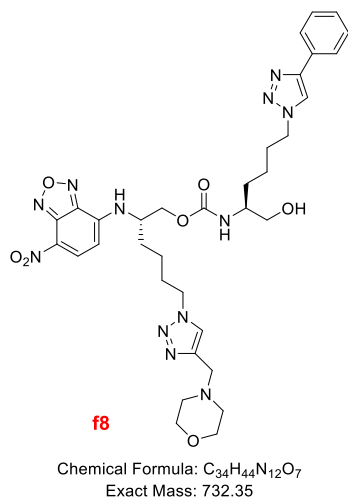
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1768			671398			
1000.5214	1000.5224	1	200279	$C_{46}H_{65}N_{17}O_9$	(M+H) ⁺	0.95
1001.5236	1001.5251	1	113494	$C_{46}H_{65}N_{17}O_9$	(M+H) ⁺	1.47
1002.5240	1002.5277	1	35910	$C_{46}H_{65}N_{17}O_9$	(M+H) ⁺	3.71
1003.5229	1003.5302	1	7840	$C_{46}H_{65}N_{17}O_9$	(M+H) ⁺	7.26
1004.4888	1004.5326	1	2248	$C_{46}H_{65}N_{17}O_9$	(M+H) ⁺	43.6

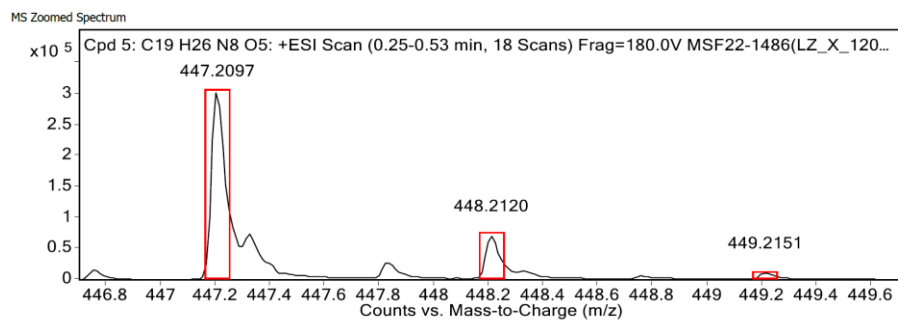
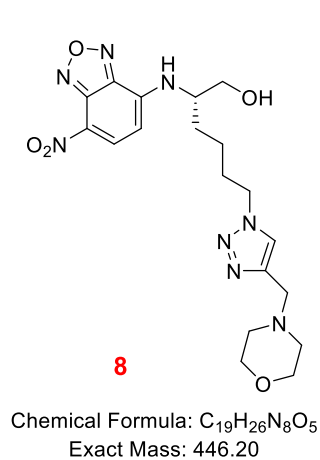
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
733.3526	733.3529	1	1126879	$C_{34}H_{44}N_{12}O_7$	(M+H) ⁺	0.43
734.3557	734.3556	1	489317	$C_{34}H_{44}N_{12}O_7$	(M+H) ⁺	-0.1
735.3585	735.3581	1	110820	$C_{34}H_{44}N_{12}O_7$	(M+H) ⁺	-0.46
736.3606	736.3606	1	17291	$C_{34}H_{44}N_{12}O_7$	(M+H) ⁺	0.08
737.3570	737.3630	1	2994	$C_{34}H_{44}N_{12}O_7$	(M+H) ⁺	8.2
738.3585	738.3654	1	858	$C_{34}H_{44}N_{12}O_7$	(M+H) ⁺	9.38

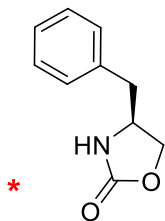
--- End Of Report ---



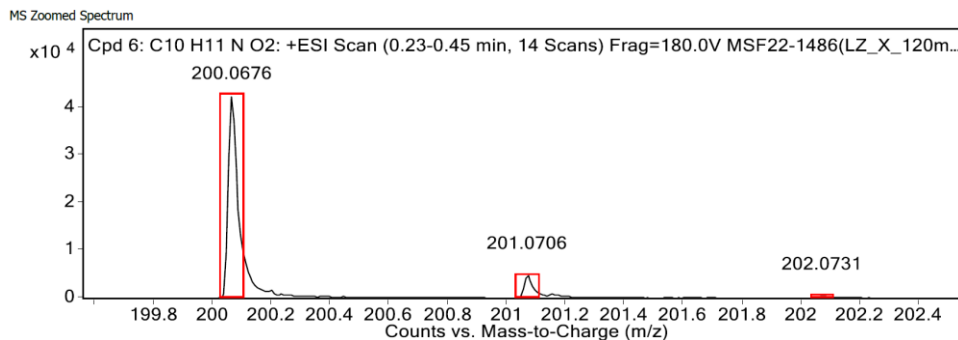
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
447.2097	447.2099	1	305704	$C_{19}H_{26}N_8O_5$	(M+H) ⁺	0.46
448.2120	448.2125	1	70604	$C_{19}H_{26}N_8O_5$	(M+H) ⁺	1.21
449.2151	449.2148	1	10564	$C_{19}H_{26}N_8O_5$	(M+H) ⁺	-0.6
450.2183	450.2172	1	1816	$C_{19}H_{26}N_8O_5$	(M+H) ⁺	-2.56
733.3526			1270069			

--- End Of Report ---

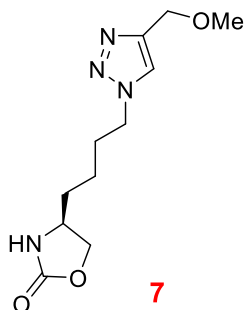


Chemical Formula: $C_{10}H_{11}NO_2$
Exact Mass: 177.08

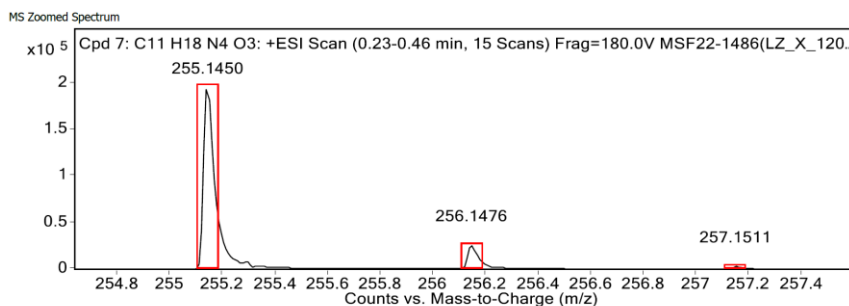


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
200.0676	200.0682	1	42671	$C_{10}H_{11}NO_2$	(M+Na)+	3
201.0706	201.0714	1	4777	$C_{10}H_{11}NO_2$	(M+Na)+	3.72
202.0731	202.0737	1	442	$C_{10}H_{11}NO_2$	(M+Na)+	3.13
733.3523			1368605			

--- End Of Report ---

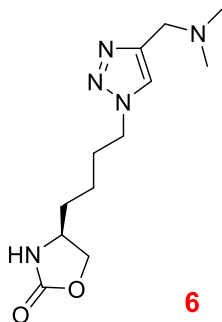


Chemical Formula: $C_{11}H_{18}N_4O_3$
Exact Mass: 254.14

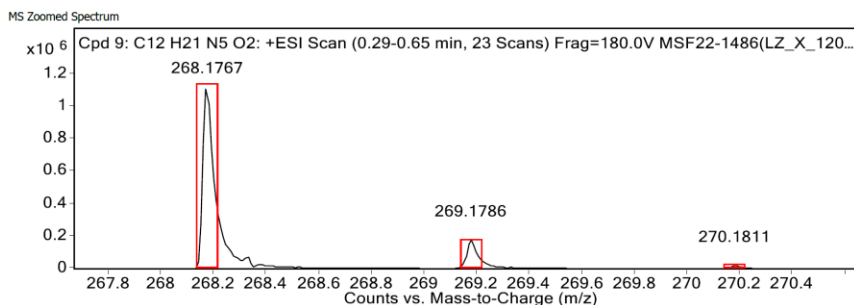


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
255.1450	255.1452	1	197367	$C_{11}H_{18}N_4O_3$	(M+H)+	0.72
256.1476	256.1479	1	25928	$C_{11}H_{18}N_4O_3$	(M+H)+	1.16
257.1511	257.1501	1	3100	$C_{11}H_{18}N_4O_3$	(M+H)+	-3.98
258.1586	258.1524	1	426	$C_{11}H_{18}N_4O_3$	(M+H)+	-23.88
733.3524			1352653			

--- End Of Report ---

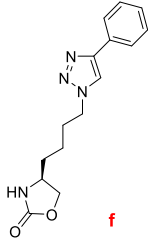


Chemical Formula: $C_{12}H_{21}N_5O_2$
Exact Mass: 267.17

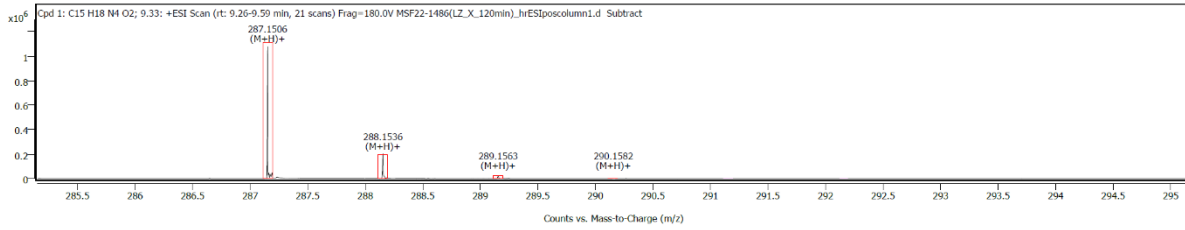


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
268.1767	268.1768	1	1121969	$C_{12}H_{21}N_5O_2$	(M+H)+	0.31
269.1786	269.1794	1	176131	$C_{12}H_{21}N_5O_2$	(M+H)+	3.1
270.1811	270.1818	1	18622	$C_{12}H_{21}N_5O_2$	(M+H)+	2.3
271.1675	271.1841	1	3471	$C_{12}H_{21}N_5O_2$	(M+H)+	61.2

--- End Of Report ---



Chemical Formula: C₁₅H₁₈N₄O₂
Exact Mass: 286.14

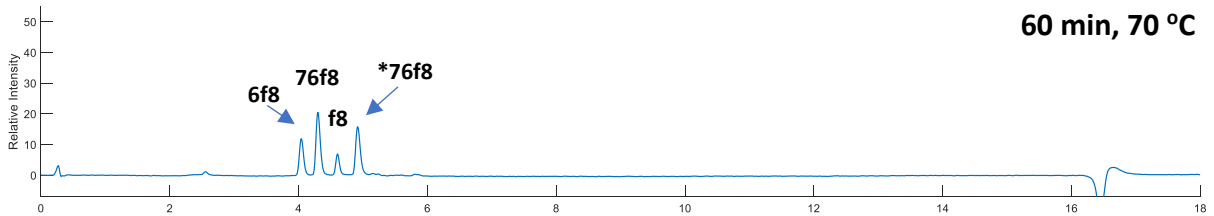
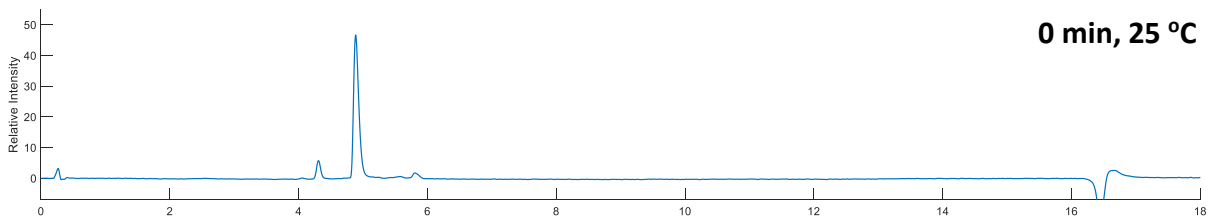
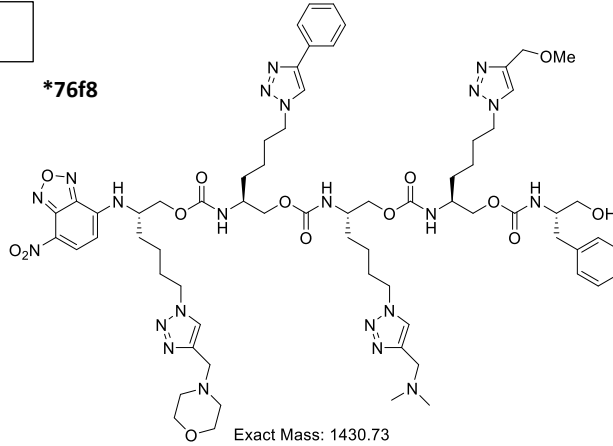


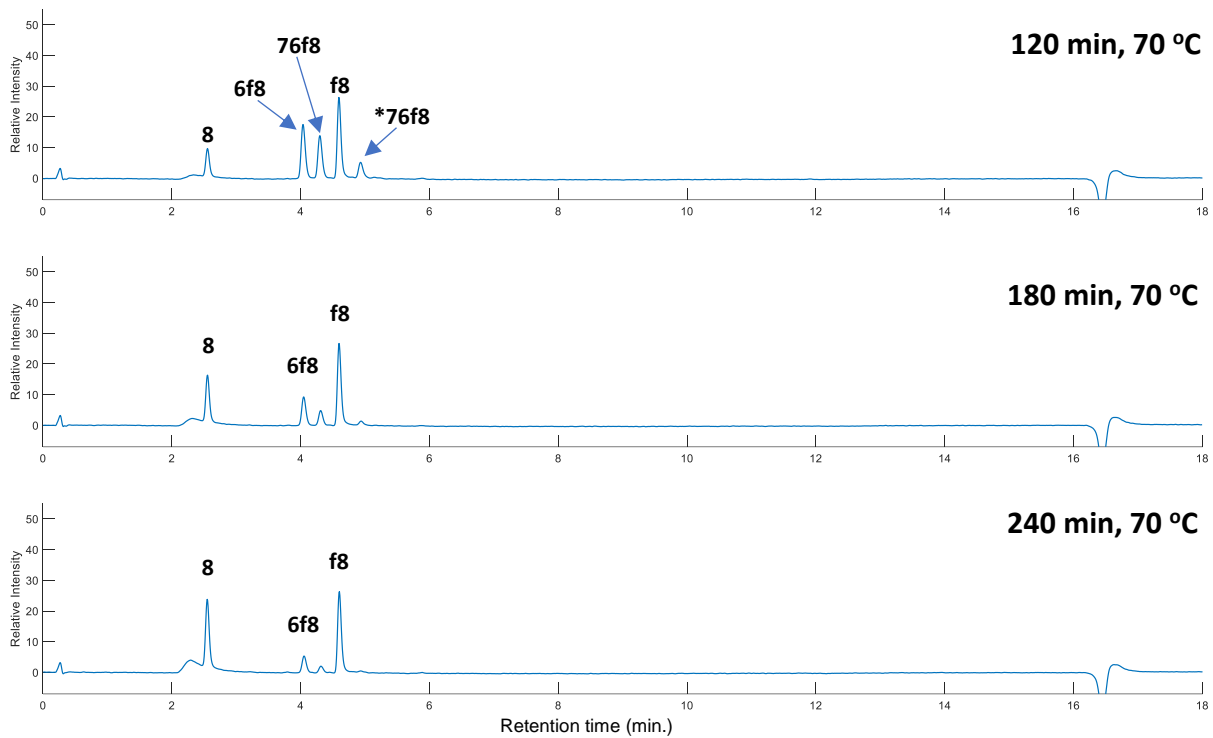
Spectrum Peaks

Obs. m/z	Calc. m/z	Charge	Abund	Formula	Ion Species	Tgt Mass Error (PPM)
287.1506	287.1503	1	1100940	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	1.14
288.1536	288.1531	1	205374	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	1.73
289.1563	289.1557	1	22564	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	2.31
290.1582	290.1581	1	1424	C ₁₅ H ₁₈ N ₄ O ₂	(M+H) ⁺	0.22
733.3531			1177512			

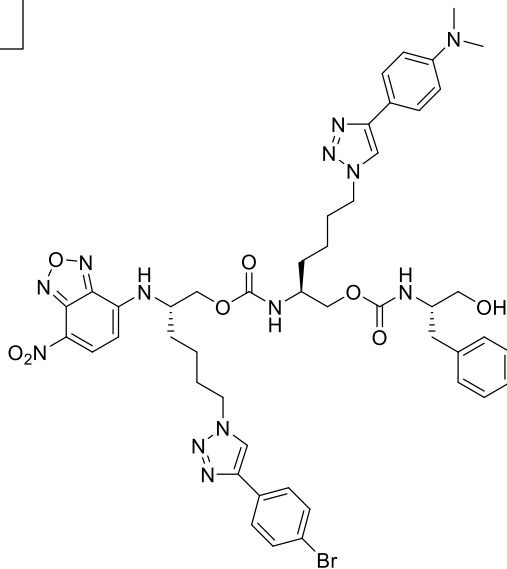
MassHunter Qual 10.0
(End of Report)

Oligomer 6_2: *76f8

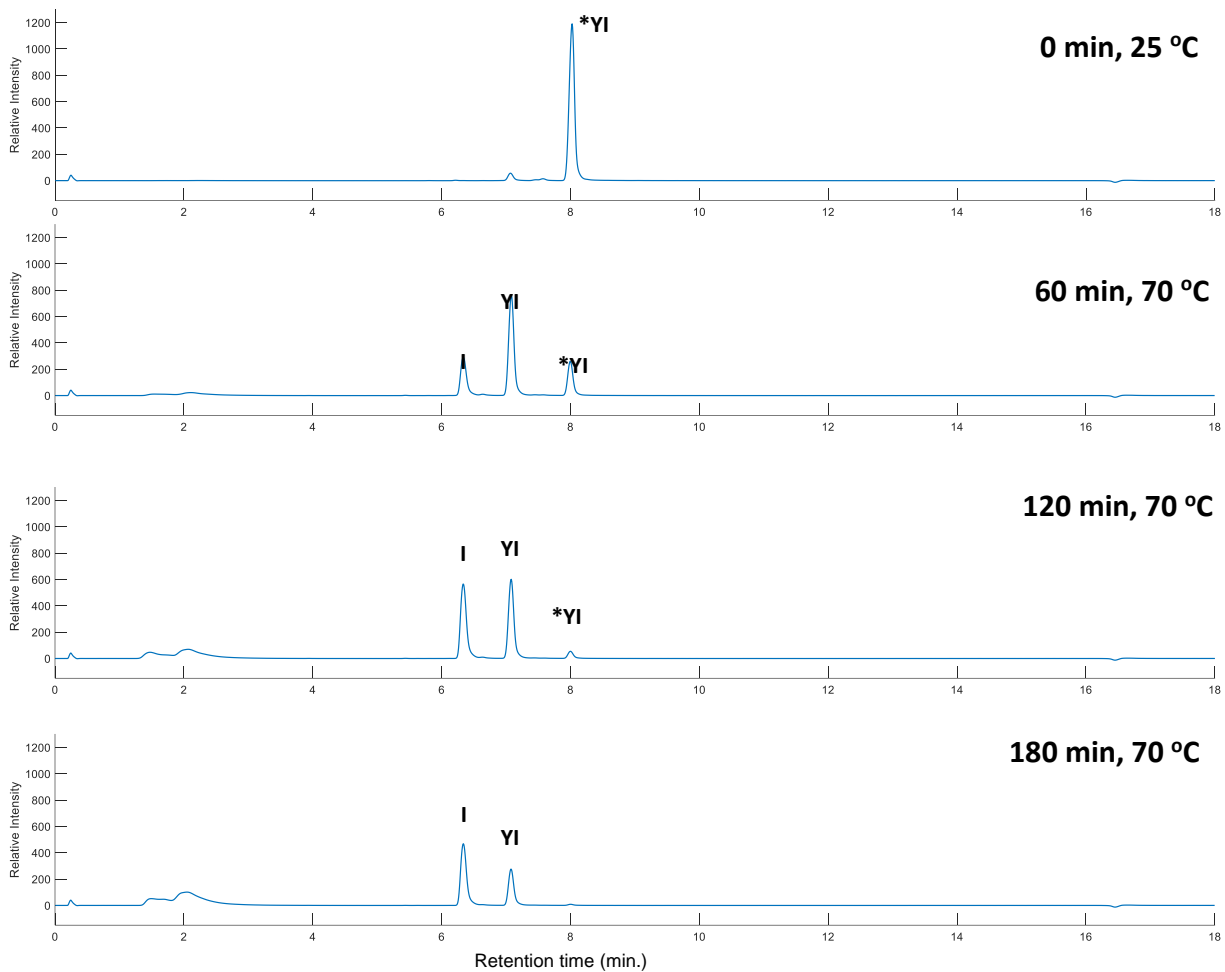




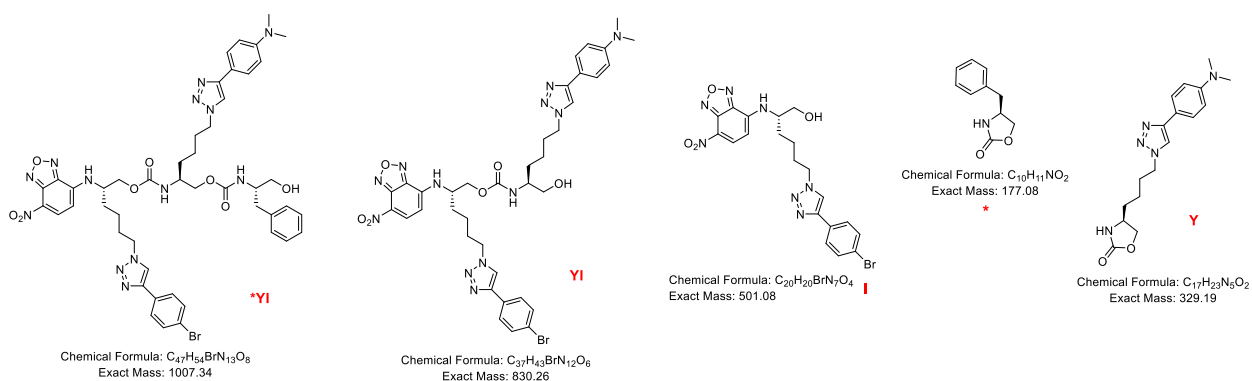
Oligomer Z1_1: *YI

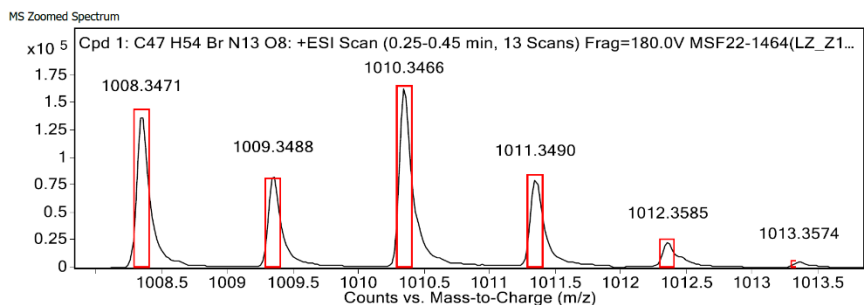
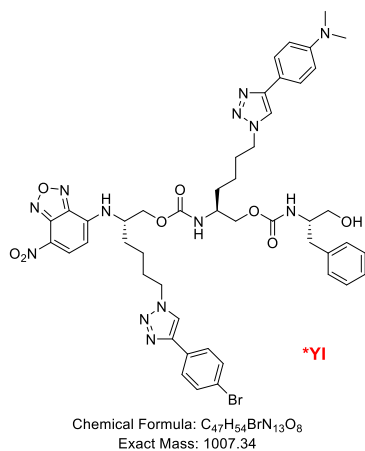
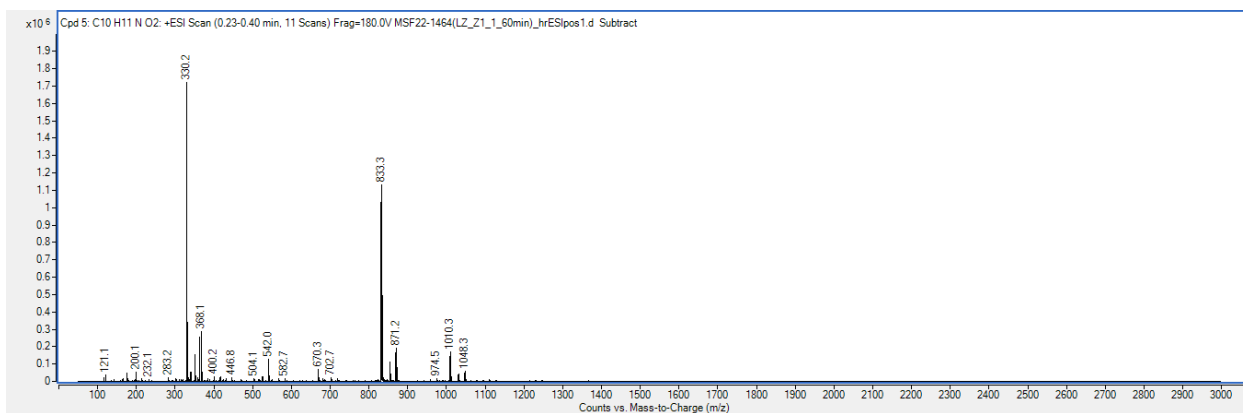


Exact Mass: 1007.34



After 60 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.

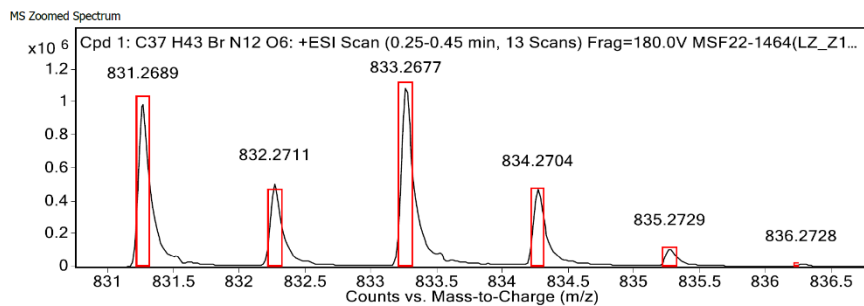
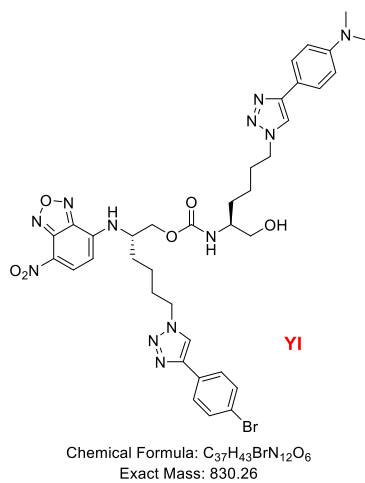




MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
330.1927			1631671			
1008.3471	1008.3474	1	139751	C47H54BrN13O8	(M+H)+	0.32
1009.3488	1009.3503	1	84139	C47H54BrN13O8	(M+H)+	1.51
1010.3466	1010.3466	1	164479	C47H54BrN13O8	(M+H)+	-0.02
1011.3490	1011.3487	1	80795	C47H54BrN13O8	(M+H)+	-0.25
1012.3585	1012.3512	1	23911	C47H54BrN13O8	(M+H)+	-7.14
1013.3574	1013.3538	1	5160	C47H54BrN13O8	(M+H)+	-3.59

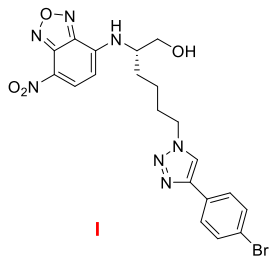
--- End Of Report ---



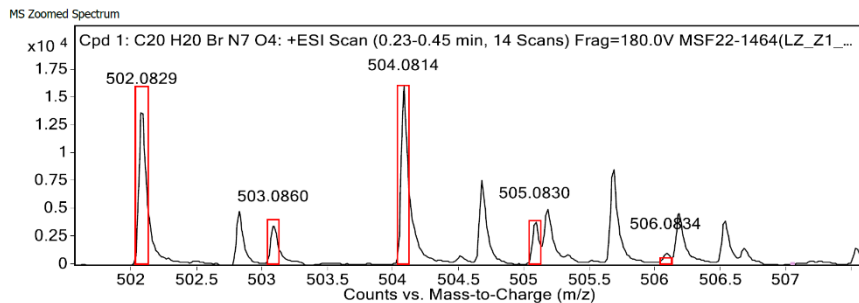
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
330.1927			1631767			
831.2689	831.2685	1	1006838	C37H43BrN12O6	(M+H)+	-0.48
832.2711	832.2712	1	509775	C37H43BrN12O6	(M+H)+	0.18
833.2677	833.2672	1	1108627	C37H43BrN12O6	(M+H)+	-0.59
834.2704	834.2695	1	473370	C37H43BrN12O6	(M+H)+	-1.07
835.2729	835.2720	1	114724	C37H43BrN12O6	(M+H)+	-1.11
836.2728	836.2745	1	16771	C37H43BrN12O6	(M+H)+	1.97
837.2740	837.2769	1	2459	C37H43BrN12O6	(M+H)+	3.53

--- End Of Report ---

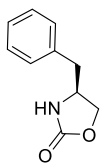


Chemical Formula: C₂₀H₂₀BrN₇O₄
Exact Mass: 501.08

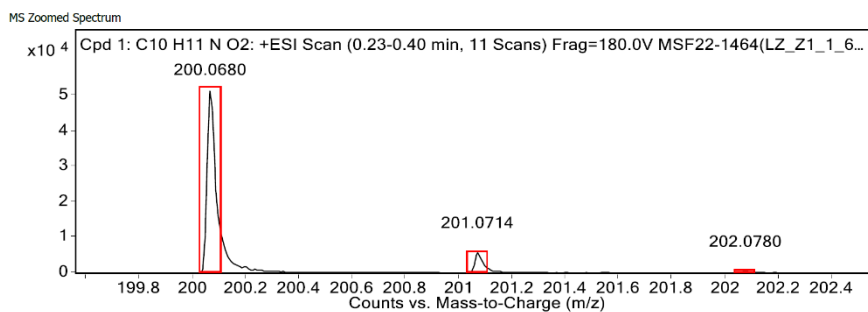


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
330.1927			1516400			
502.0829	502.0833	1	14174	C ₂₀ H ₂₀ BrN ₇ O ₄	(M+H) ⁺	0.78
503.0860	503.0860	1	3568	C ₂₀ H ₂₀ BrN ₇ O ₄	(M+H) ⁺	-0.03
504.0814	504.0815	1	16105	C ₂₀ H ₂₀ BrN ₇ O ₄	(M+H) ⁺	0.14
505.0830	505.0841	1	3865	C ₂₀ H ₂₀ BrN ₇ O ₄	(M+H) ⁺	2.07
506.0834	506.0865	1	1086	C ₂₀ H ₂₀ BrN ₇ O ₄	(M+H) ⁺	6.12

--- End Of Report ---

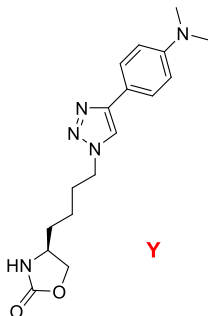


Chemical Formula: C₁₀H₁₁NO₂
Exact Mass: 177.08

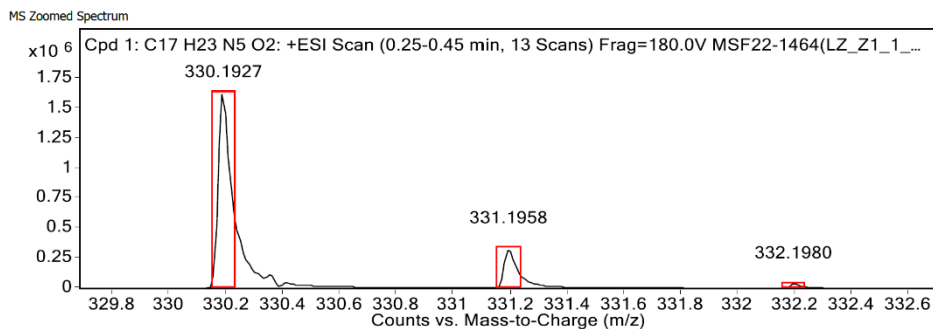


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
200.0680	200.0682	1	52132	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	0.88
201.0714	201.0714	1	5911	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	0.04
202.0780	202.0737	1	628	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-21.08
330.1926			1735902			

--- End Of Report ---



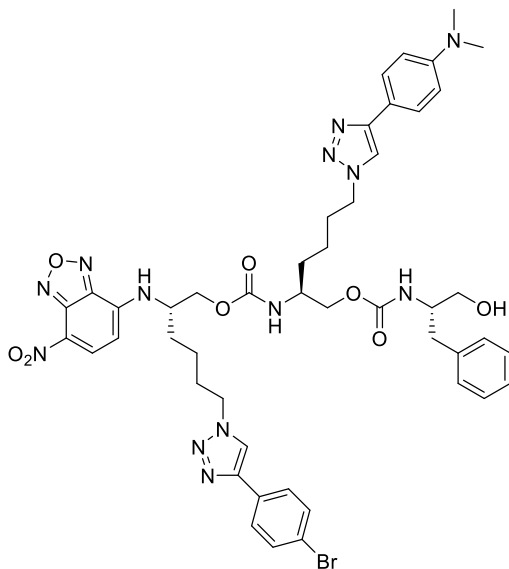
Chemical Formula: C₁₇H₂₃N₅O₂
Exact Mass: 329.19



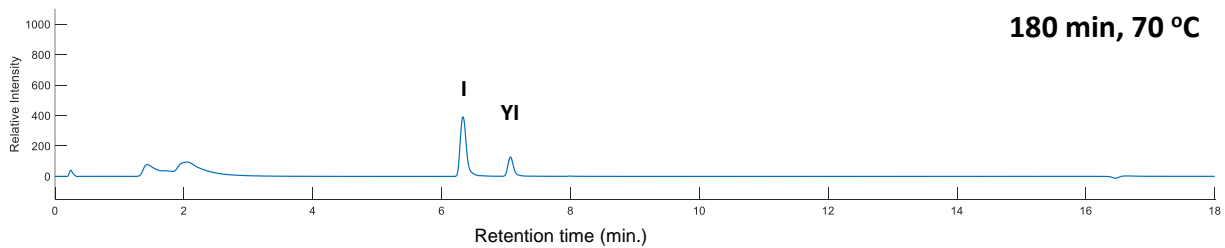
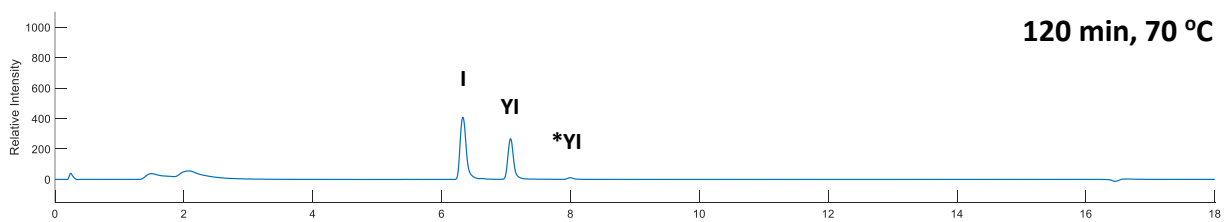
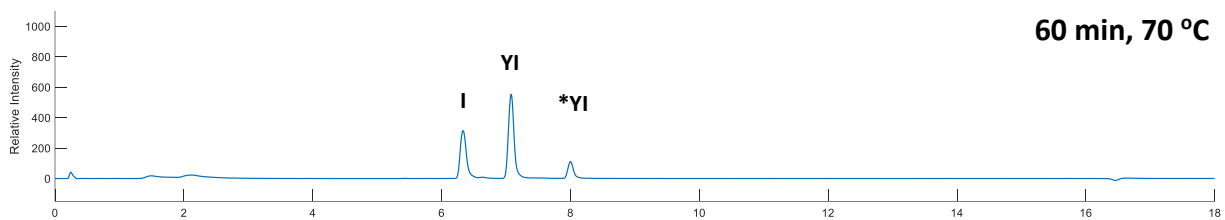
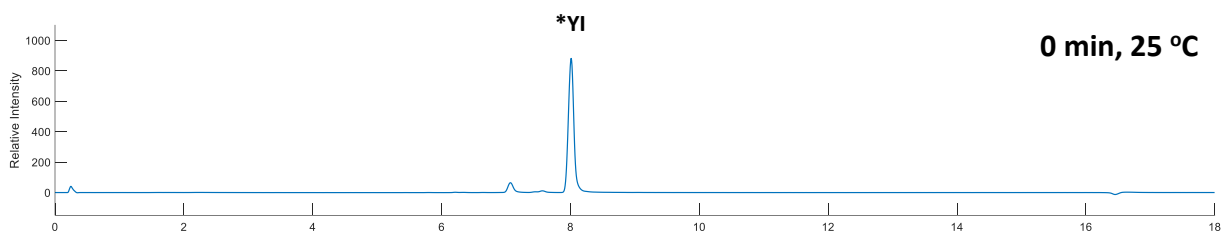
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
330.1927	330.1925	1	1631610	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	-0.83
331.1958	331.1953	1	329494	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	-1.67
332.1980	332.1979	1	36961	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	-0.44
333.2098	333.2003	1	5255	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	-28.5
334.2105	334.2028	1	1033	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	-23.2

--- End Of Report ---

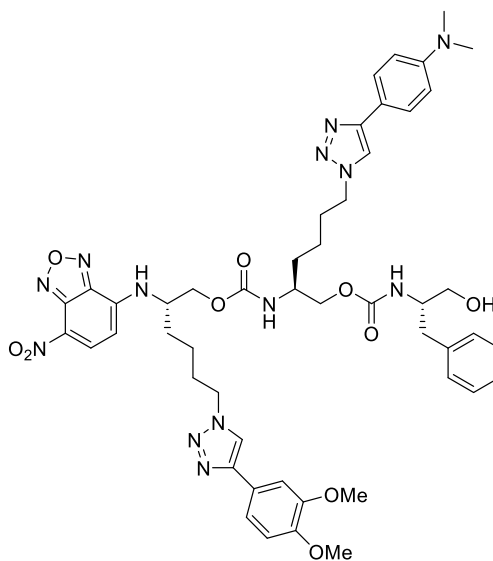
Oligomer Z1_2: *YI



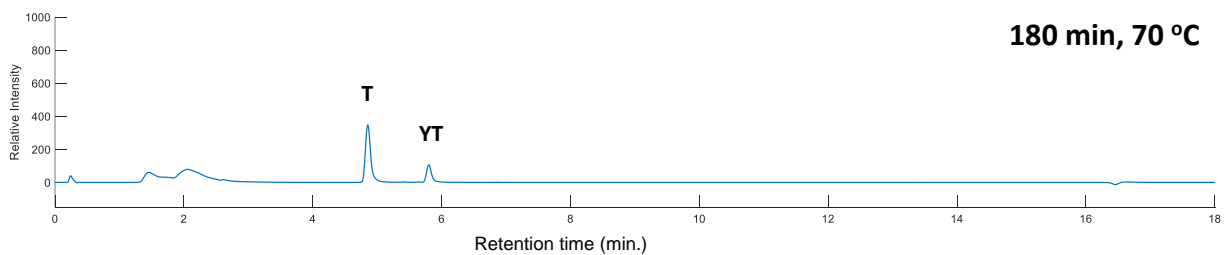
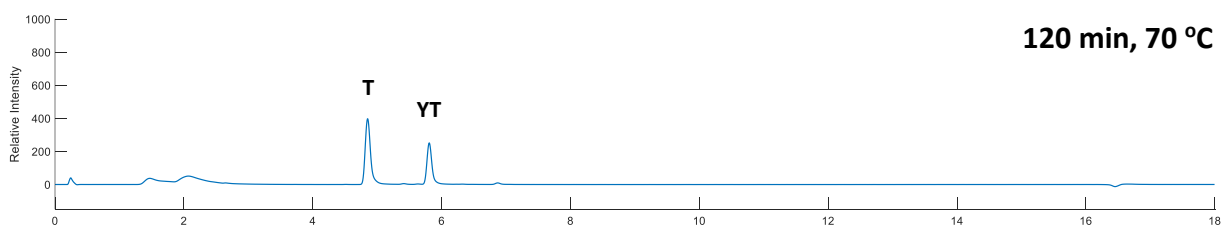
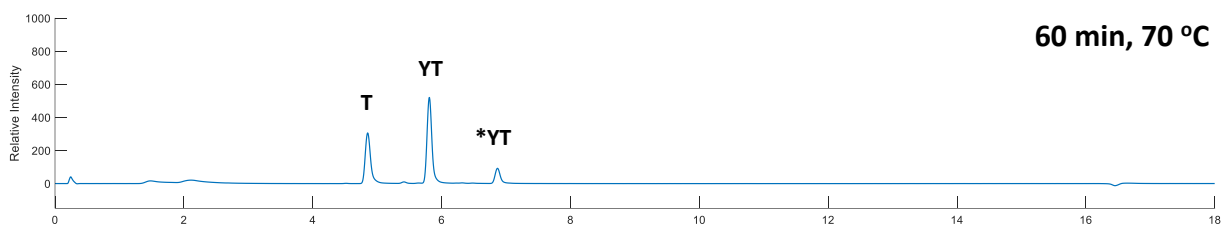
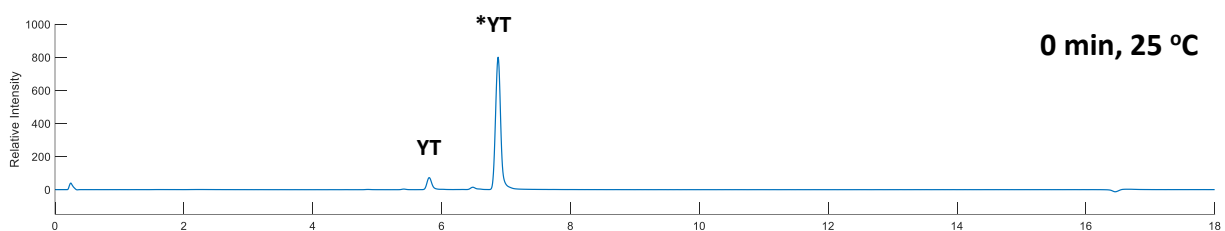
Exact Mass: 1007.34



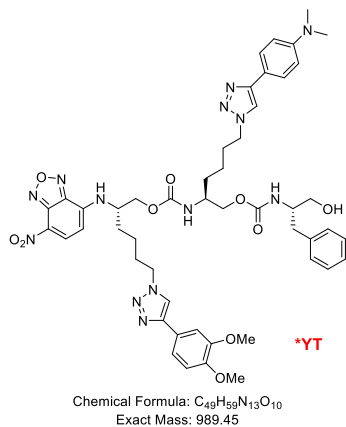
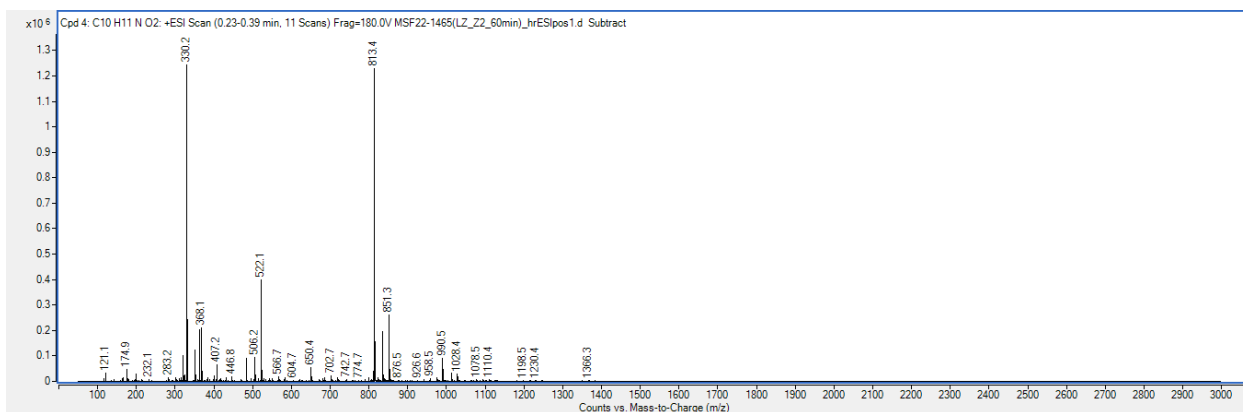
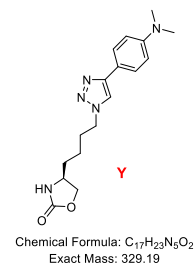
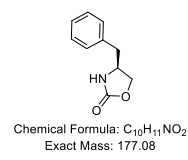
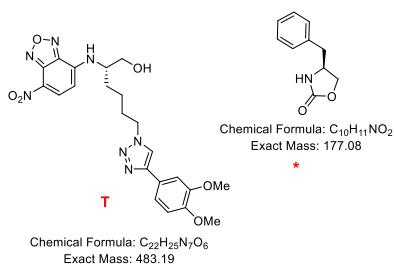
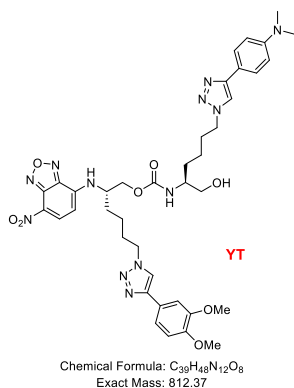
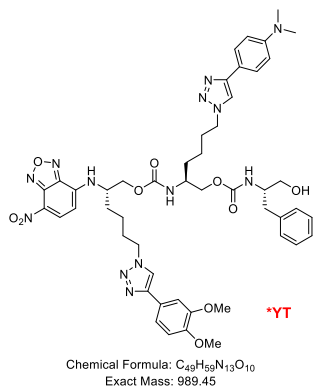
Oligomer Z2: *YT



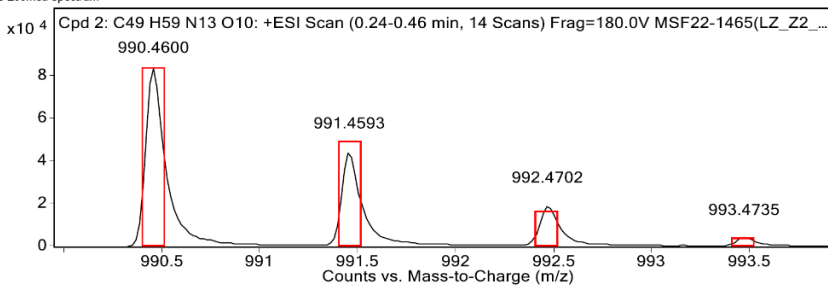
Exact Mass: 989.45



After 60 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.



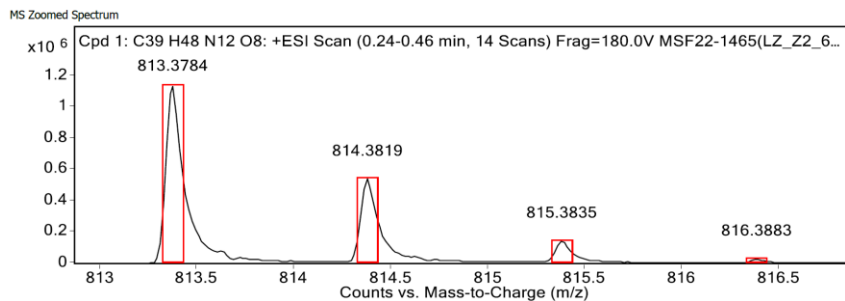
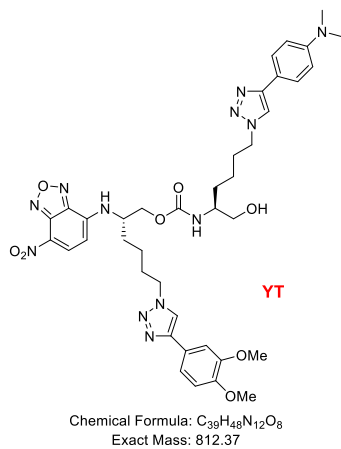
MS Zoomed Spectrum



MS Spectrum Peak List

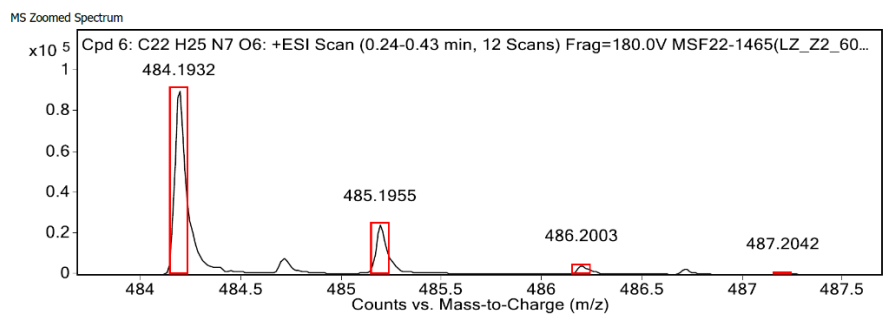
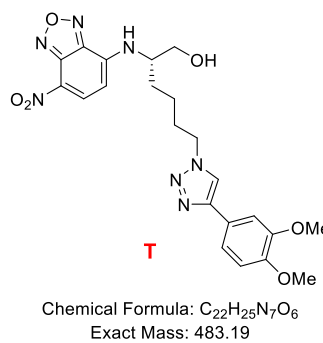
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
813.3784			1139089			
990.4600	990.4581	1	83810	C ₄₉ H ₅₉ N ₁₃ O ₁₀	(M+H) ⁺	-1.93
991.4593	991.4609	1	44582	C ₄₉ H ₅₉ N ₁₃ O ₁₀	(M+H) ⁺	1.68
992.4702	992.4637	1	19087	C ₄₉ H ₅₉ N ₁₃ O ₁₀	(M+H) ⁺	-6.6
993.4735	993.4663	1	3922	C ₄₉ H ₅₉ N ₁₃ O ₁₀	(M+H) ⁺	-7.26

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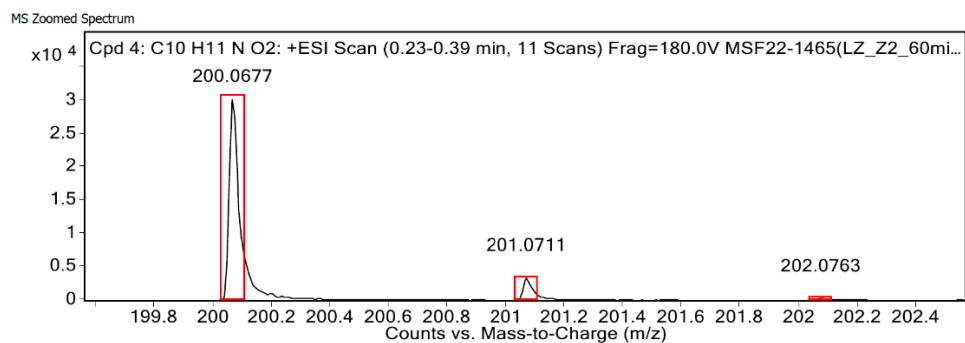
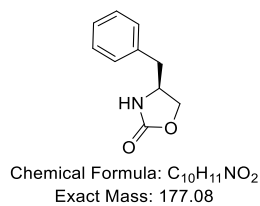
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
813.3784	813.3791	1	1139112	C ₃₉ H ₄₈ N ₁₂ O ₈	(M+H) ⁺	0.8
814.3819	814.3819	1	538590	C ₃₉ H ₄₈ N ₁₂ O ₈	(M+H) ⁺	0.02
815.3835	815.3845	1	142767	C ₃₉ H ₄₈ N ₁₂ O ₈	(M+H) ⁺	1.23
816.3883	816.3870	1	28719	C ₃₉ H ₄₈ N ₁₂ O ₈	(M+H) ⁺	-1.52
817.3810	817.3895	1	4115	C ₃₉ H ₄₈ N ₁₂ O ₈	(M+H) ⁺	10.47
818.3698	818.3920	1	824	C ₃₉ H ₄₈ N ₁₂ O ₈	(M+H) ⁺	27.06

--- End Of Report ---



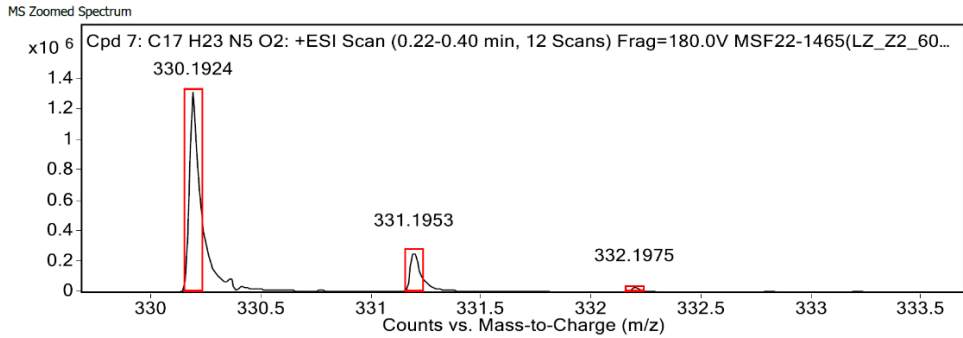
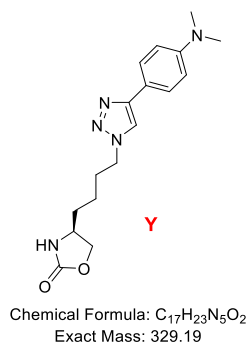
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
484.1932	484.1939	1	91353	C ₂₂ H ₂₅ N ₇ O ₆	(M+H) ⁺	1.52
485.1955	485.1967	1	24078	C ₂₂ H ₂₅ N ₇ O ₆	(M+H) ⁺	2.39
486.2003	486.1991	1	4524	C ₂₂ H ₂₅ N ₇ O ₆	(M+H) ⁺	-2.47
487.2042	487.2015	1	632	C ₂₂ H ₂₅ N ₇ O ₆	(M+H) ⁺	-5.38
813.3784			1274478			

--- End Of Report ---



Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
200.0677	200.0682	1	30751	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	2.41
201.0711	201.0714	1	3465	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	1.55
202.0763	202.0737	1	382	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-12.94
330.1922			1253860			

--- End Of Report ---

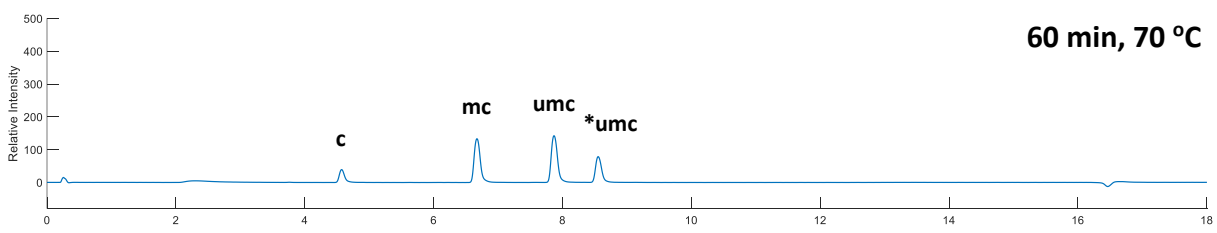
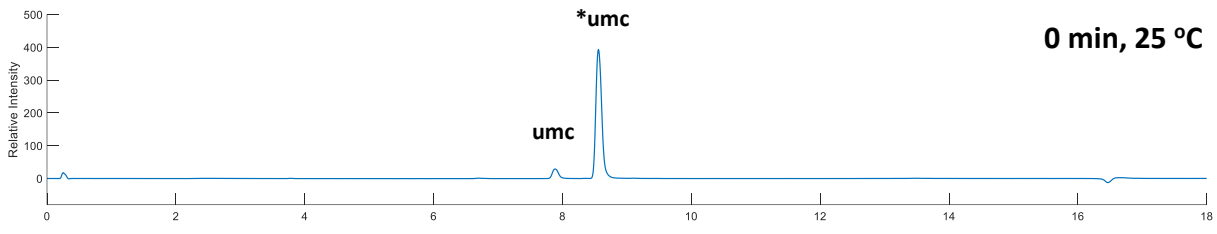
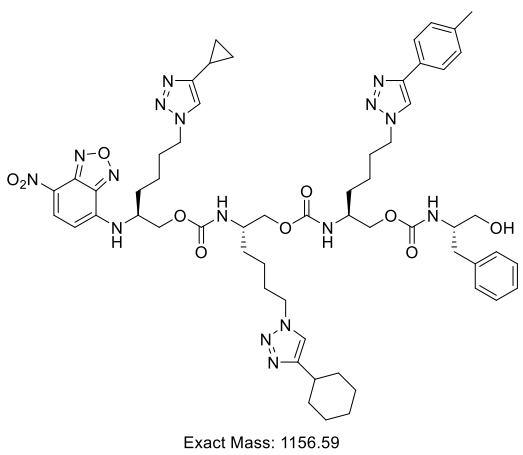


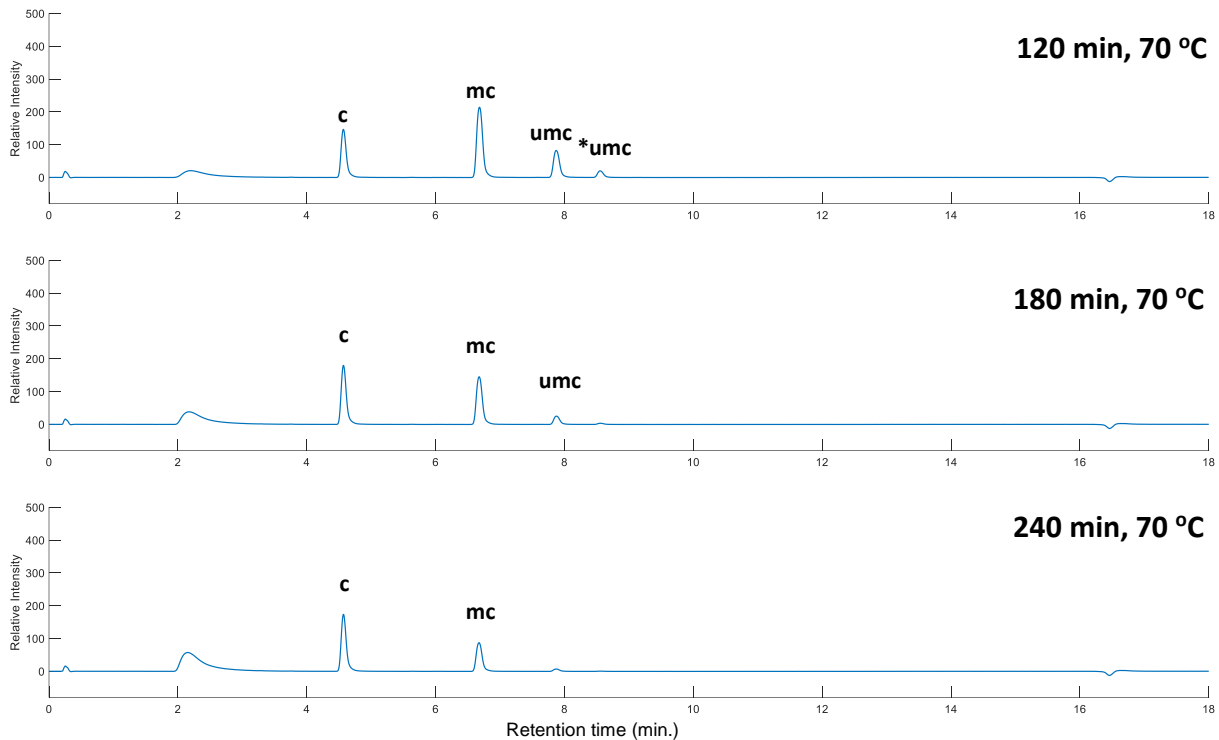
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Ygt Mass Error (ppm)
330.1924	330.1925	1	1327937	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	0.13
331.1953	331.1953	1	263087	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	-0.15
332.1975	332.1979	1	29321	C ₁₇ H ₂₃ N ₅ O ₂	(M+H) ⁺	0.98
813.3784			1360110			

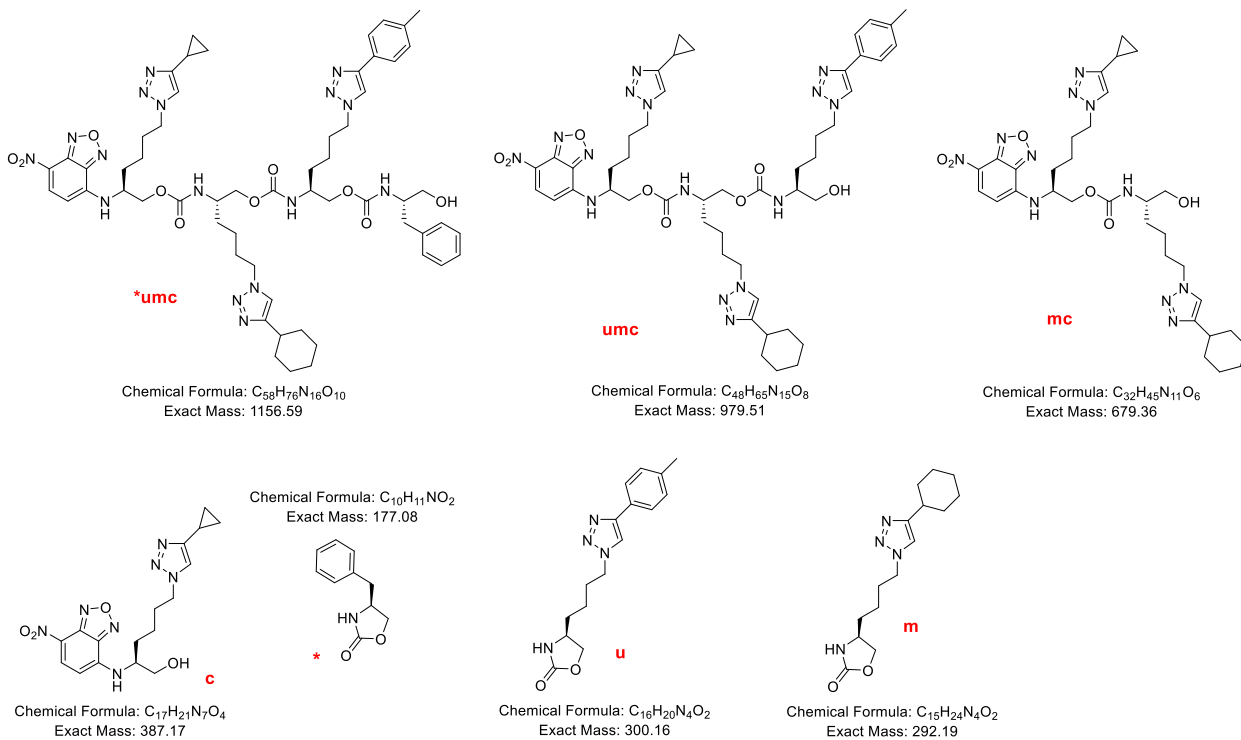
--- End Of Report ---

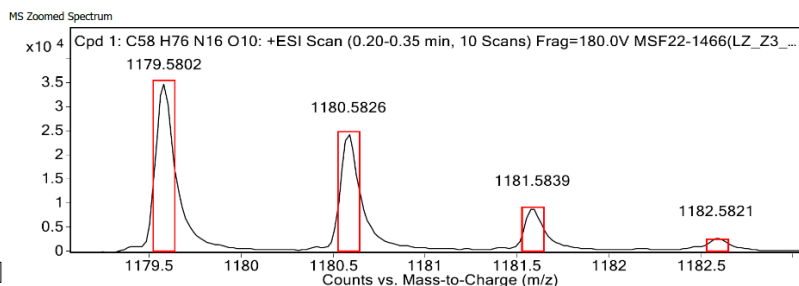
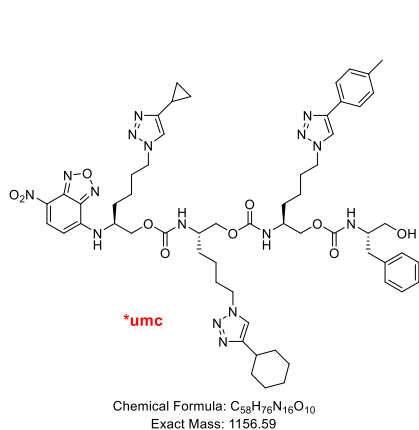
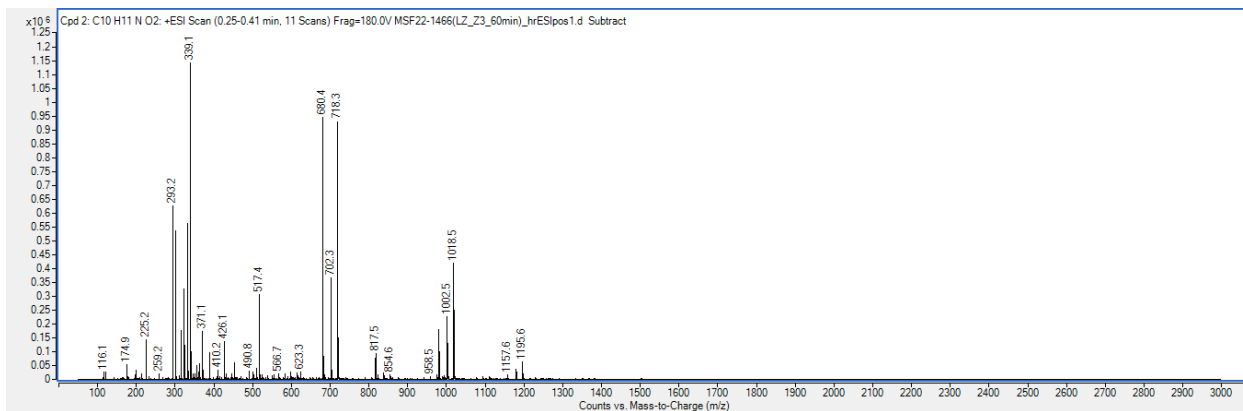
Oligomer Z3: *umc





After 60 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.

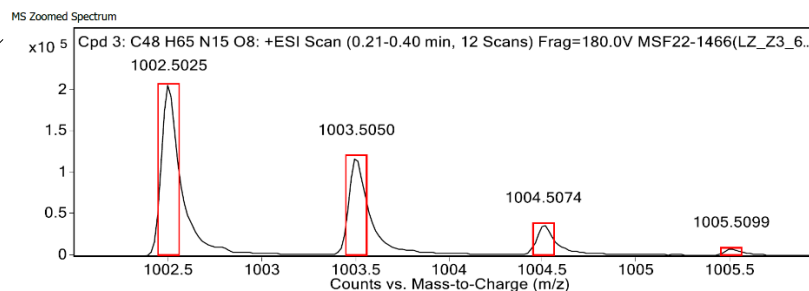
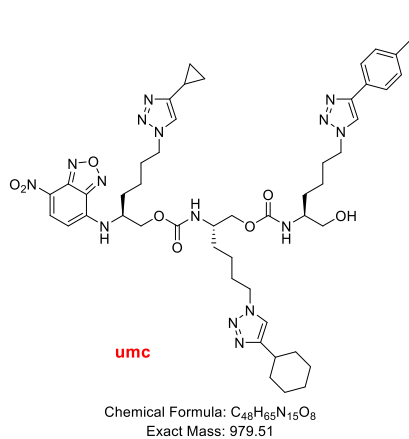




MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
339.1217			1248861			
1179.5802	1179.5823	1	34878	C58H76N16O10	(M+Na)+	1.74
1180.5826	1180.5851	1	24409	C58H76N16O10	(M+Na)+	2.14
1181.5839	1181.5879	1	9213	C58H76N16O10	(M+Na)+	3.39
1182.5821	1182.5905	1	2914	C58H76N16O10	(M+Na)+	7.1
1183.5960	1183.5931	1	772	C58H76N16O10	(M+Na)+	-2.43

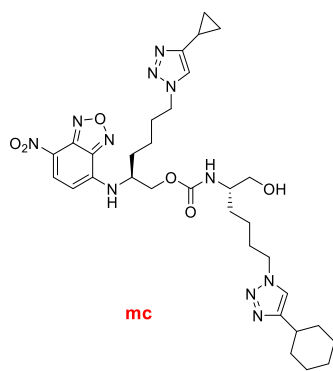
--- End of Report ---



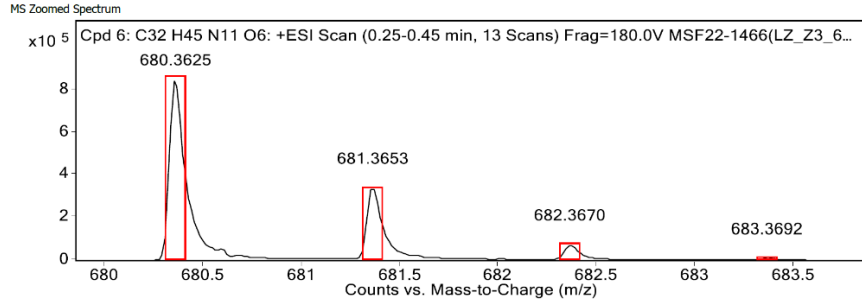
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
339.1217			955617			
1002.5025	1002.5033	1	207380	C48H65N15O8	(M+Na)+	0.75
1003.5050	1003.5061	1	119381	C48H65N15O8	(M+Na)+	1.11
1004.5074	1004.5088	1	37382	C48H65N15O8	(M+Na)+	1.37
1005.5099	1005.5113	1	7696	C48H65N15O8	(M+Na)+	1.47
1006.5170	1006.5139	1	1636	C48H65N15O8	(M+Na)+	-3.09

--- End of Report ---



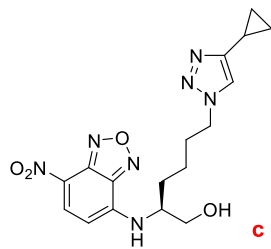
mc
 Chemical Formula: C₃₂H₄₅N₁₁O₆
 Exact Mass: 679.36



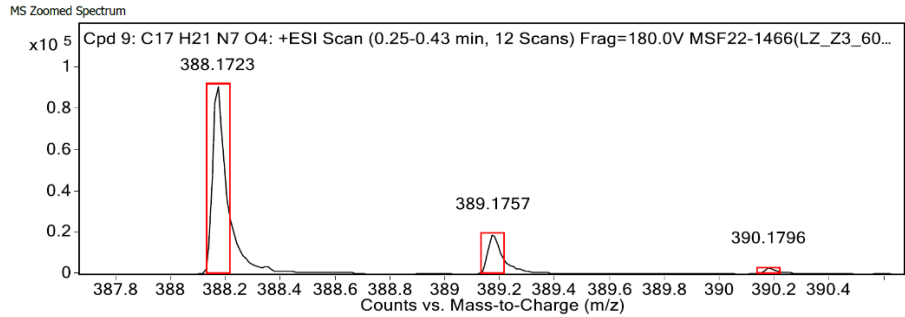
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
339.1218			1143050			
680.3625	680.3627	1	858821	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	0.34
681.3653	681.3655	1	341434	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	0.23
682.3670	682.3680	1	74733	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	1.5
683.3692	683.3705	1	11149	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	1.88
684.3711	684.3729	1	1753	C ₃₂ H ₄₅ N ₁₁ O ₆	(M+H) ⁺	2.72

--- End Of Report ---



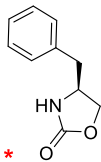
C
 Chemical Formula: C₁₇H₂₁N₇O₄
 Exact Mass: 387.17



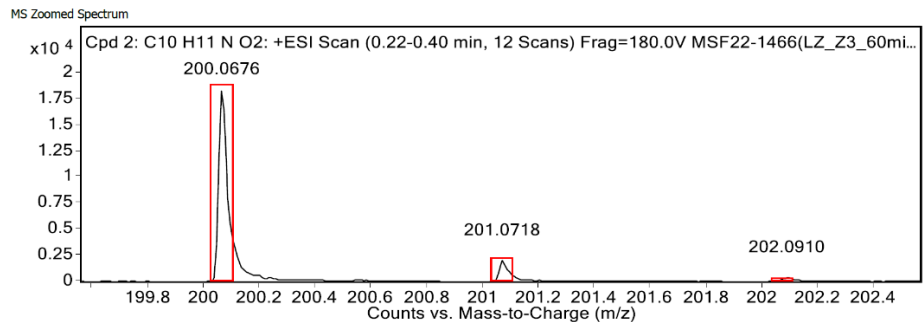
MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
339.1218			1172686			
388.1723	388.1728	1	91609	C ₁₇ H ₂₁ N ₇ O ₄	(M+H) ⁺	1.27
389.1757	389.1754	1	19532	C ₁₇ H ₂₁ N ₇ O ₄	(M+H) ⁺	-0.81
390.1796	390.1777	1	3009	C ₁₇ H ₂₁ N ₇ O ₄	(M+H) ⁺	-4.64

--- End Of Report ---



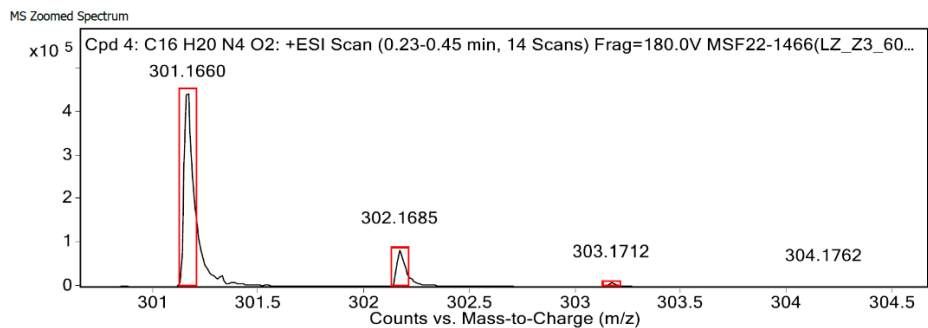
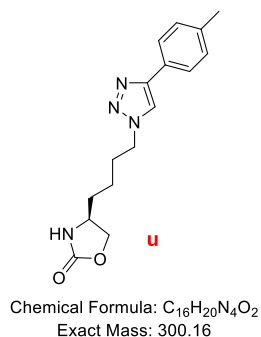
 Chemical Formula: C₁₀H₁₁NO₂
 Exact Mass: 177.08



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
200.0676	200.0682	1	18592	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	2.95
201.0718	201.0714	1	2041	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-1.88
202.0910	202.0737	1	414	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-85.41
339.1217			1652829			

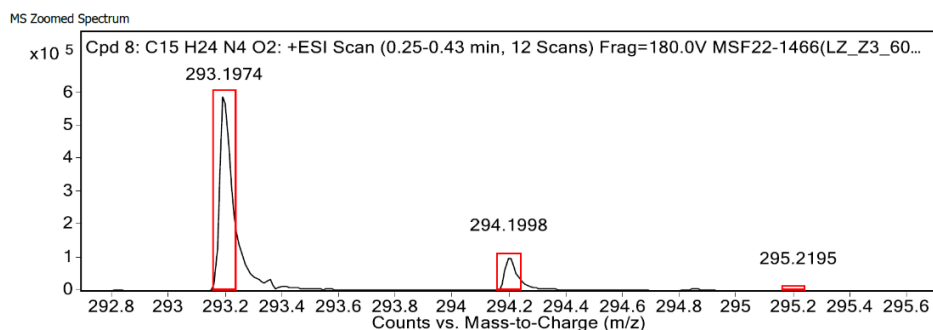
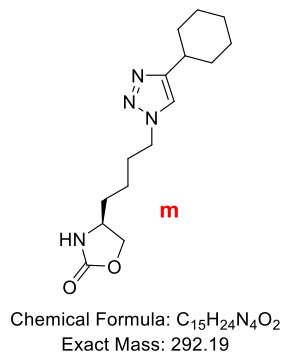
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
301.1660	301.1659	1	452094	$C_{16}H_{20}N_4O_2$	(M+H) ⁺	-0.47
302.1685	302.1688	1	85743	$C_{16}H_{20}N_4O_2$	(M+H) ⁺	0.99
303.1712	303.1714	1	9452	$C_{16}H_{20}N_4O_2$	(M+H) ⁺	0.69
304.1762	304.1739	1	828	$C_{16}H_{20}N_4O_2$	(M+H) ⁺	-7.61
339.1218			1080400			

--- End Of Report ---

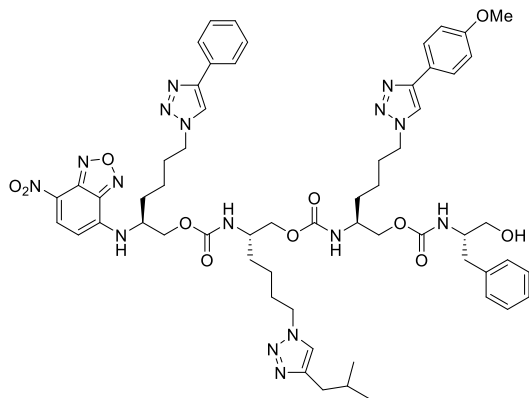


MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
293.1974	293.1972	1	607055	$C_{15}H_{24}N_4O_2$	(M+H) ⁺	-0.74
294.1998	294.2001	1	104470	$C_{15}H_{24}N_4O_2$	(M+H) ⁺	1.04
295.2195	295.2026	1	3072	$C_{15}H_{24}N_4O_2$	(M+H) ⁺	-56.96
339.1218			1178658			

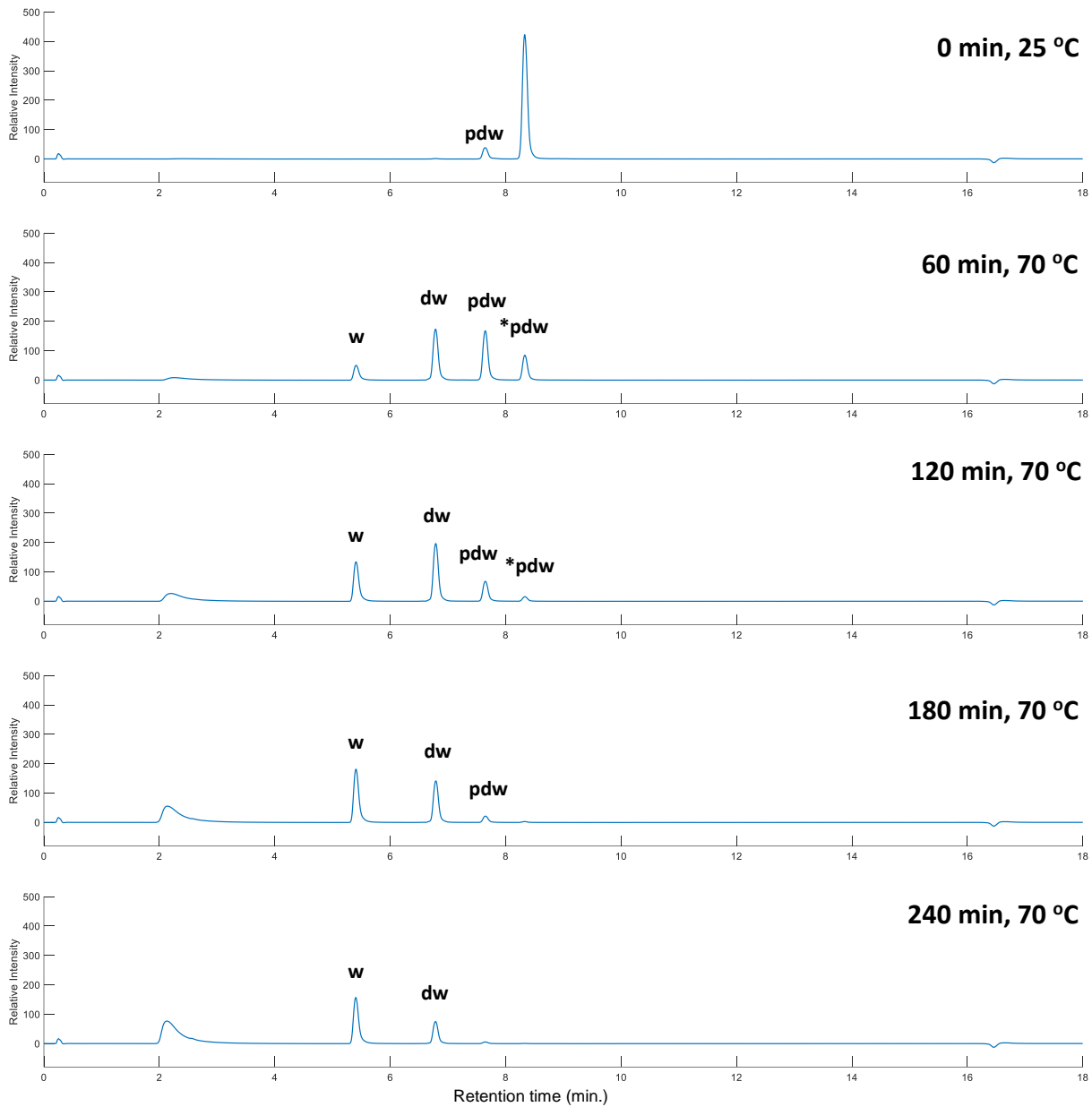
--- End Of Report ---

Oligomer Z4: *pdw

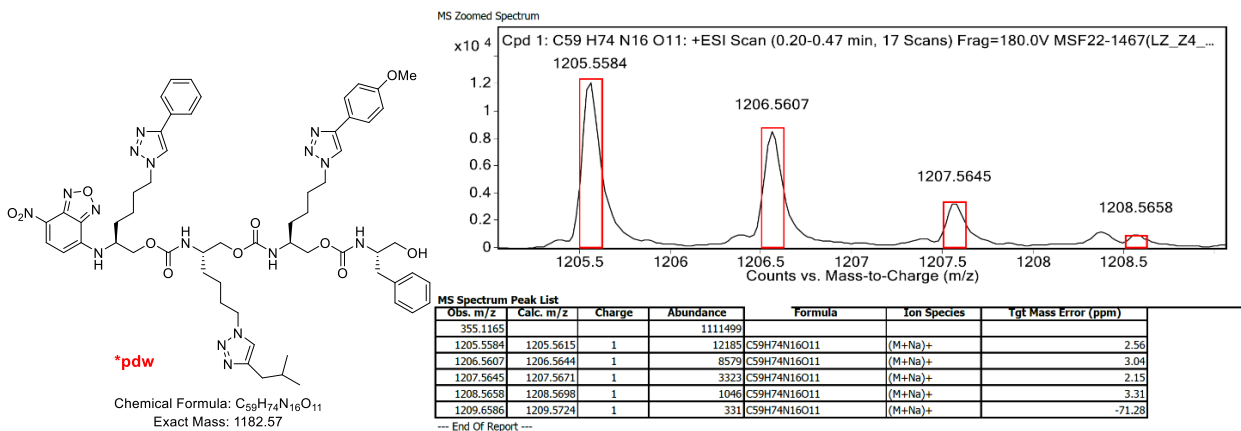
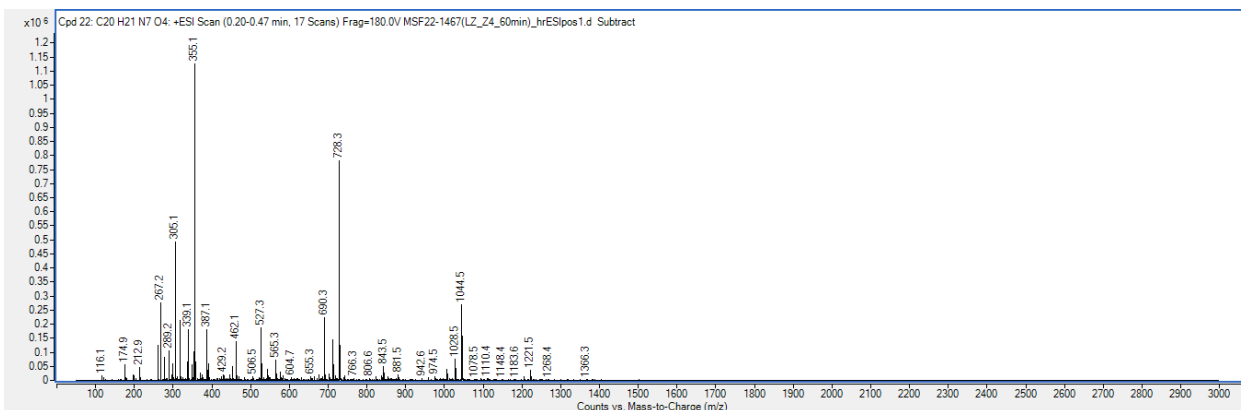
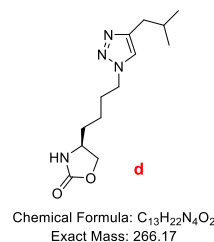
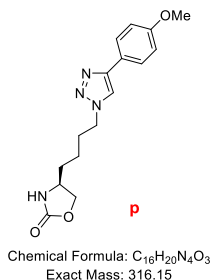
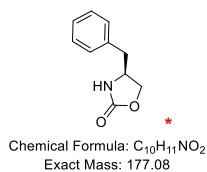
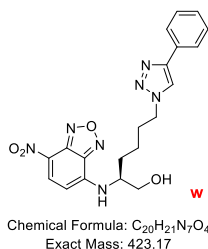
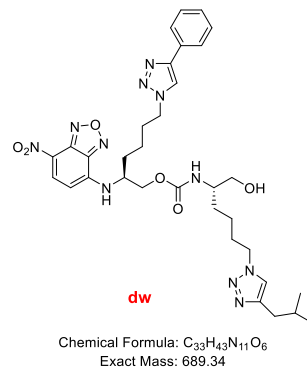
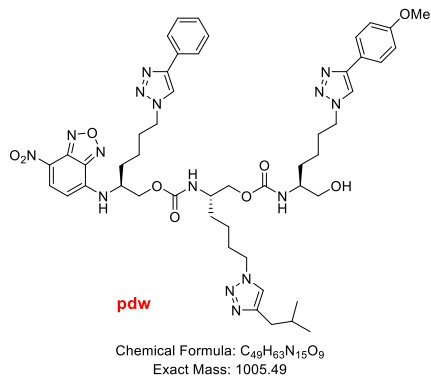
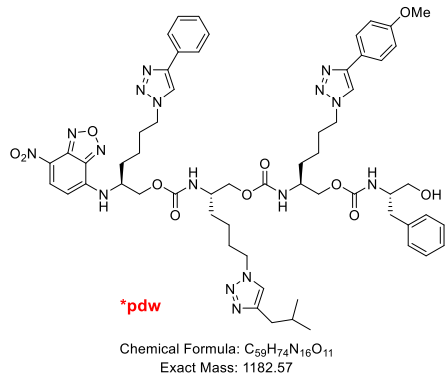


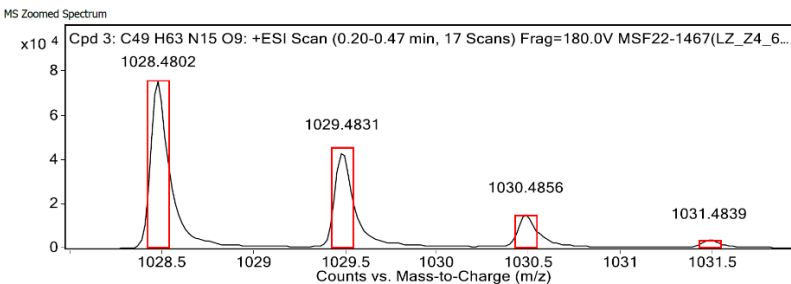
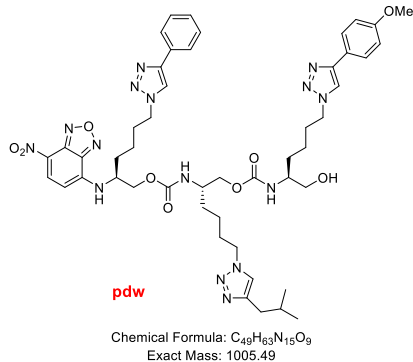
Exact Mass: 1182.57

*pdw



After 60 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.

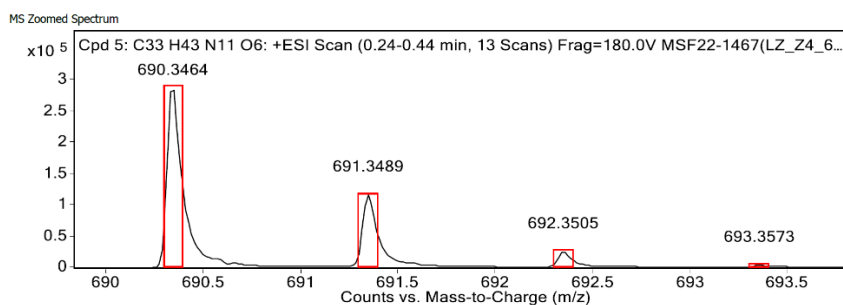
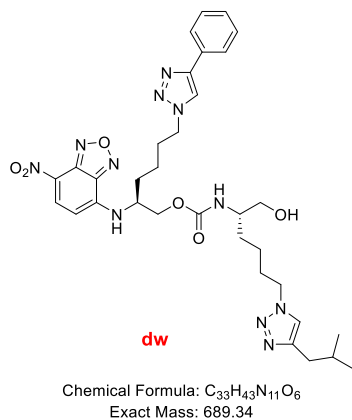




MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
355.1165			1124680			
1028.4802	1028.4825	1	75801	C ₄₉ H ₆₃ N ₁₅ O ₉	(M+Na) ⁺	2.23
1029.4831	1029.4854	1	43996	C ₄₉ H ₆₃ N ₁₅ O ₉	(M+Na) ⁺	2.17
1030.4856	1030.4880	1	15425	C ₄₉ H ₆₃ N ₁₅ O ₉	(M+Na) ⁺	2.35
1031.4839	1031.4906	1	3558	C ₄₉ H ₆₃ N ₁₅ O ₉	(M+Na) ⁺	6.54

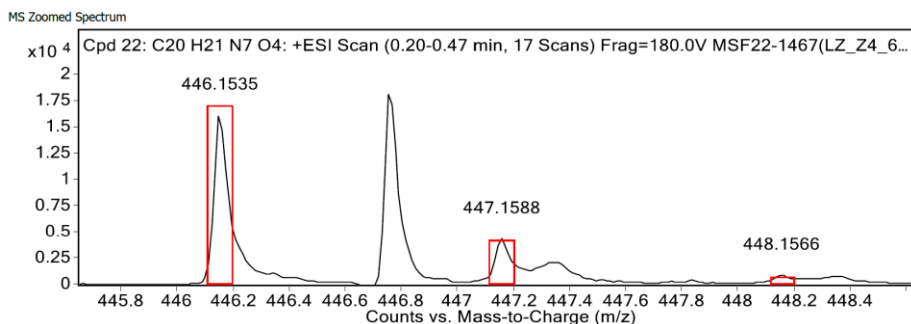
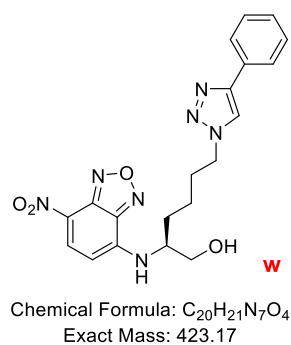
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
355.1164			1347538			
690.3464	690.3471	1	289473	C ₃₃ H ₄₃ N ₁₁ O ₆	(M+H) ⁺	0.92
691.3489	691.3498	1	116937	C ₃₃ H ₄₃ N ₁₁ O ₆	(M+H) ⁺	1.4
692.3505	692.3524	1	25994	C ₃₃ H ₄₃ N ₁₁ O ₆	(M+H) ⁺	2.7
693.3573	693.3549	1	4339	C ₃₃ H ₄₃ N ₁₁ O ₆	(M+H) ⁺	-3.5
694.4222	694.3574	1	1039	C ₃₃ H ₄₃ N ₁₁ O ₆	(M+H) ⁺	-93.42

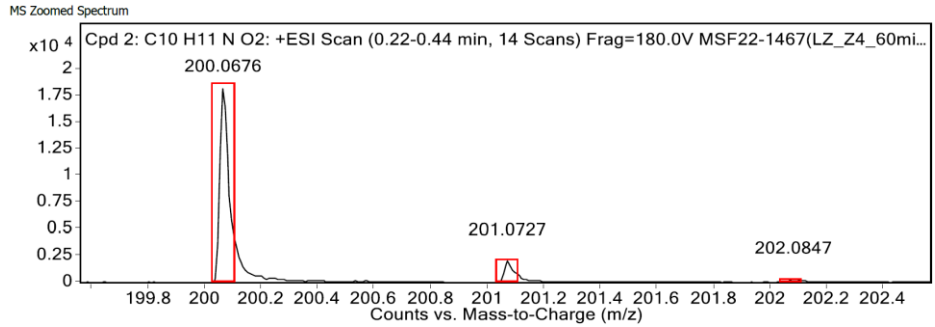
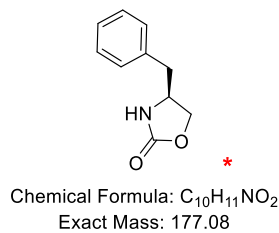
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
355.1165			1136338			
446.1535	446.1547	1	16223	C ₂₀ H ₂₁ N ₇ O ₄	(M+Na) ⁺	2.78
447.1588	447.1575	1	4480	C ₂₀ H ₂₁ N ₇ O ₄	(M+Na) ⁺	-2.93
448.1566	448.1599	1	978	C ₂₀ H ₂₁ N ₇ O ₄	(M+Na) ⁺	7.33

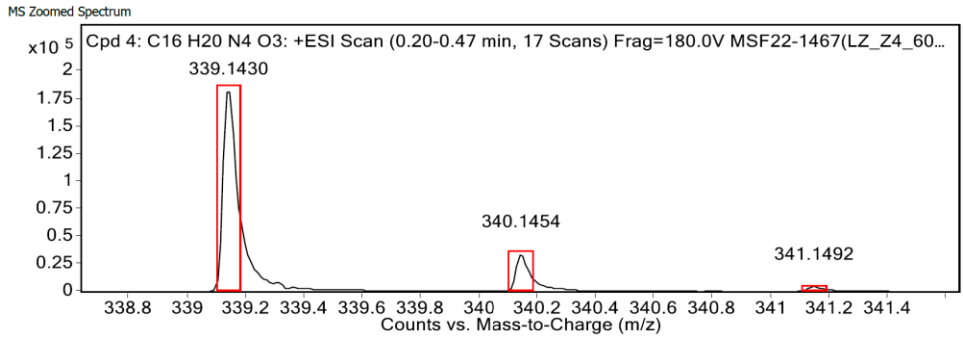
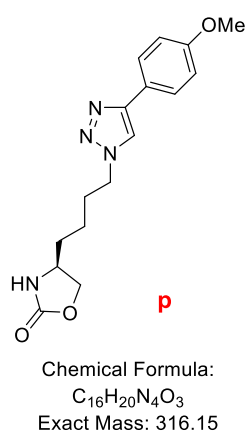
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
200.0676	200.0682	1	18515	$C_{10}H_{11}NO_2$	(M+Na)+	2.84
201.0727	201.0714	1	2042	$C_{10}H_{11}NO_2$	(M+Na)+	-6.72
202.0847	202.0737	1	328	$C_{10}H_{11}NO_2$	(M+Na)+	-54.36
355.1164			1249394			

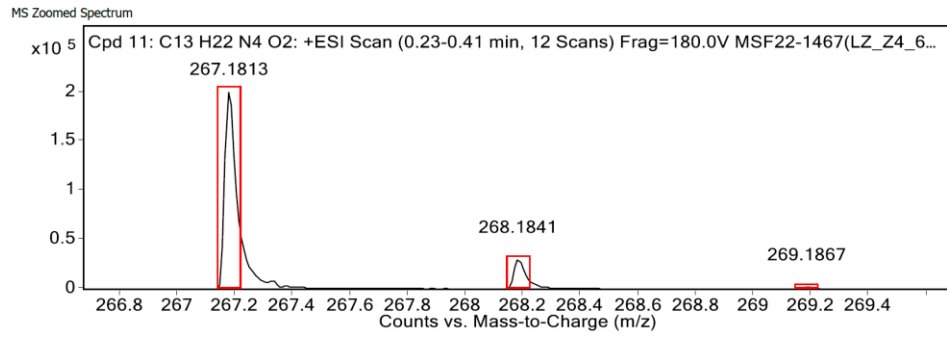
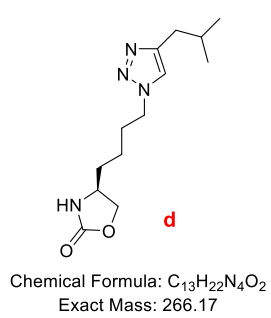
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
339.1430	339.1428	1	185836	$C_{16}H_{20}N_4O_3$	(M+Na)+	-0.63
340.1454	340.1457	1	34678	$C_{16}H_{20}N_4O_3$	(M+Na)+	0.74
341.1492	341.1481	1	5105	$C_{16}H_{20}N_4O_3$	(M+Na)+	-3.15
342.1561	342.1506	1	694	$C_{16}H_{20}N_4O_3$	(M+Na)+	-16.18
355.1165			1126090			

--- End Of Report ---

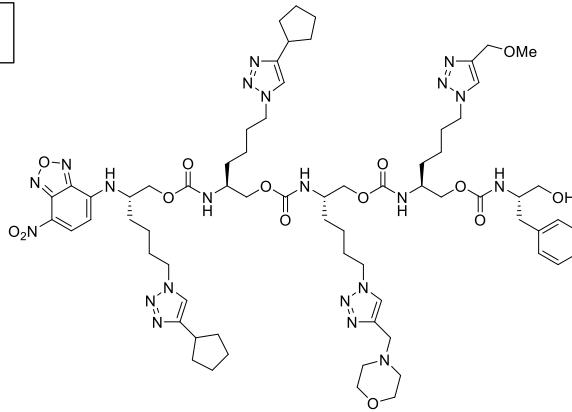


MS Spectrum Peak List

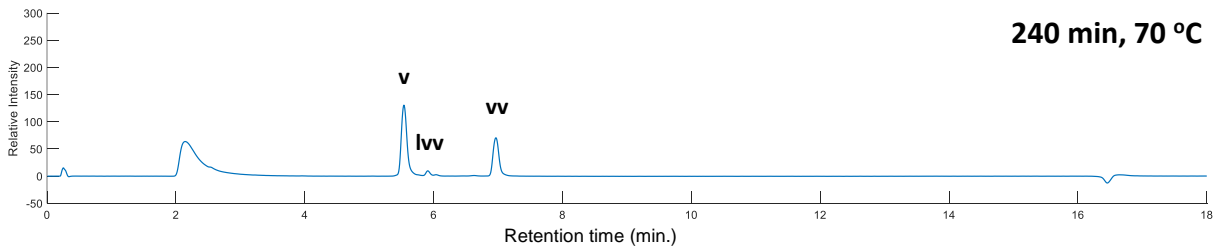
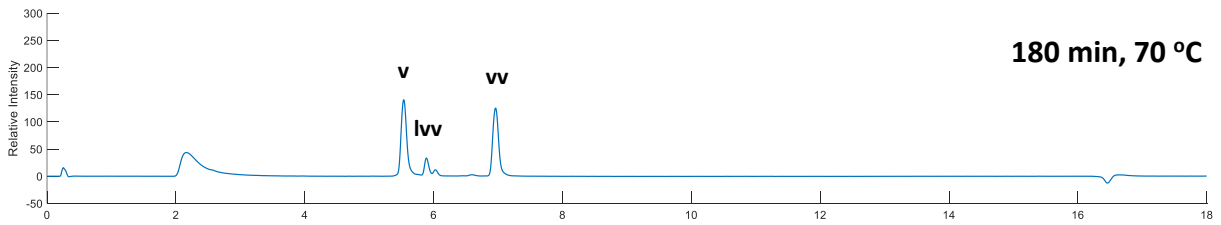
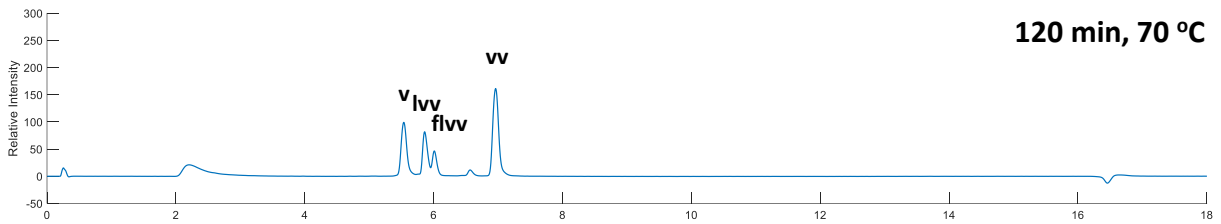
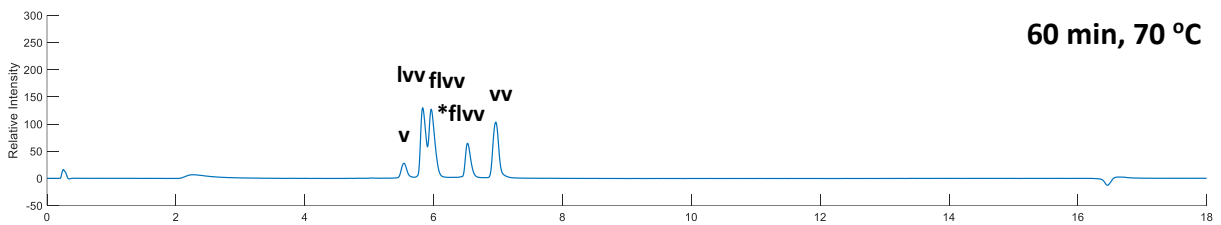
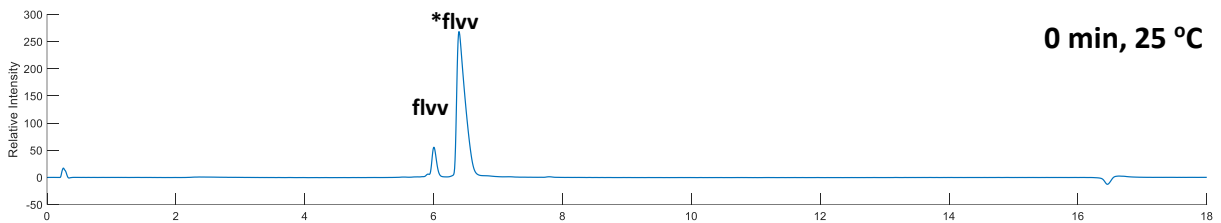
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
267.1813	267.1816	1	204025	$C_{13}H_{22}N_4O_2$	(M+H)+	0.81
268.1841	268.1844	1	30711	$C_{13}H_{22}N_4O_2$	(M+H)+	0.9
269.1867	269.1868	1	2803	$C_{13}H_{22}N_4O_2$	(M+H)+	0.55
270.1926	270.1892	1	295	$C_{13}H_{22}N_4O_2$	(M+H)+	-12.45
355.1164			2138946			

--- End Of Report ---

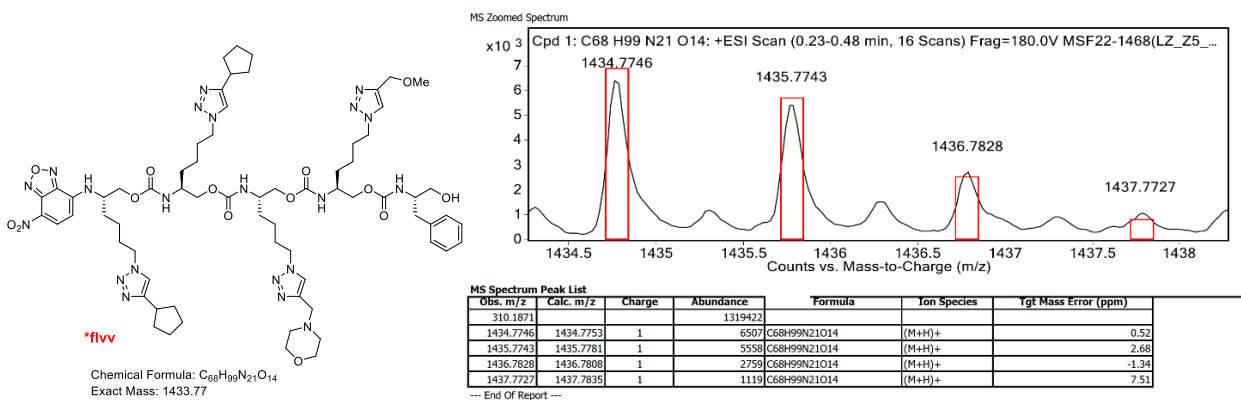
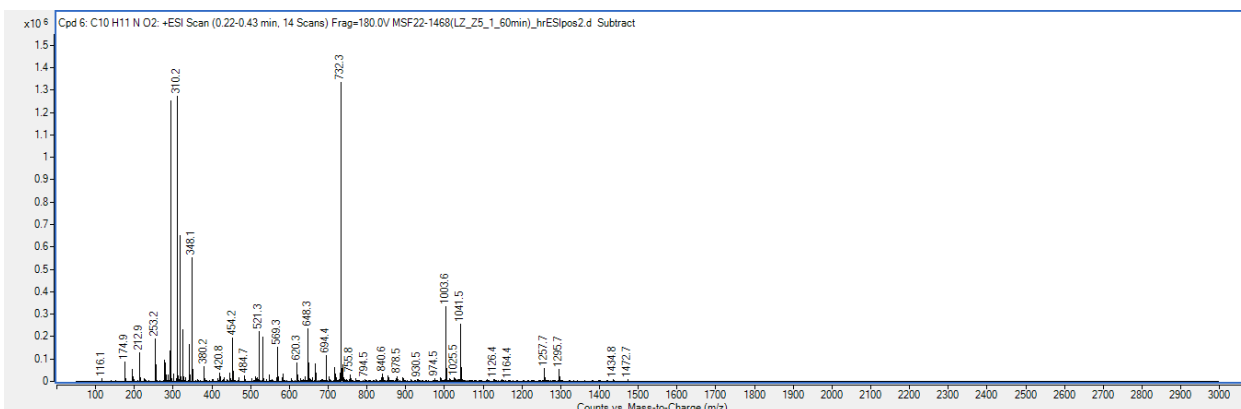
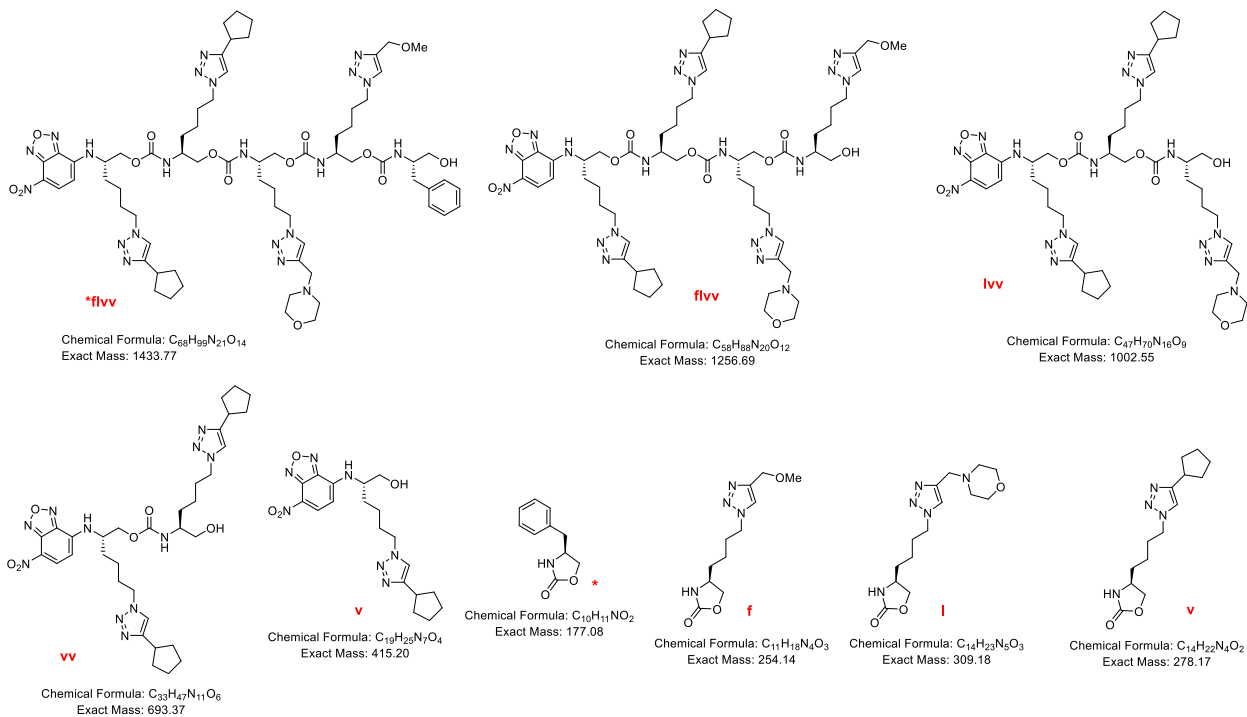
Oligomer Z5_1: *flvv

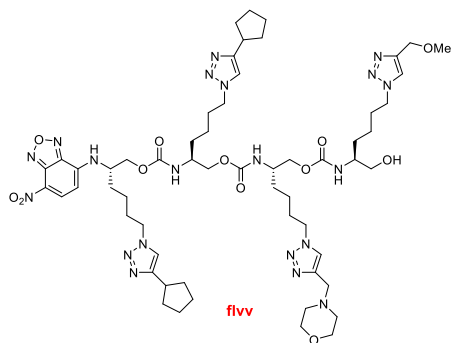


Exact Mass: 1433.77



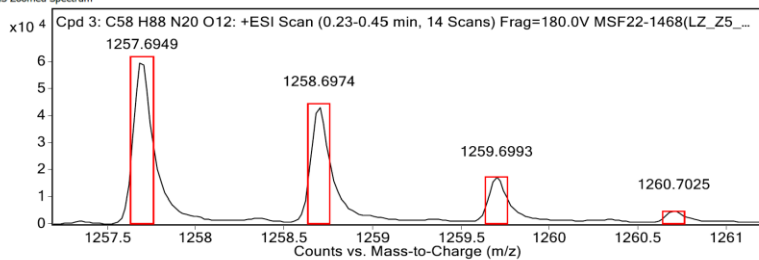
After 60 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.





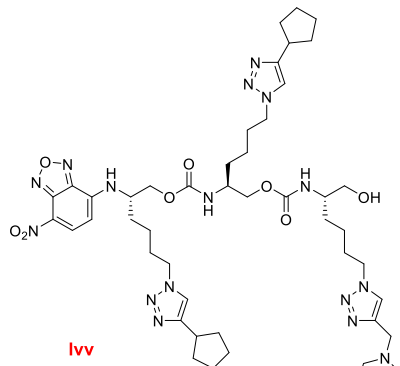
Chemical Formula: C₅₈H₈₈N₂₀O₁₂

MS Zoomed Spectrum



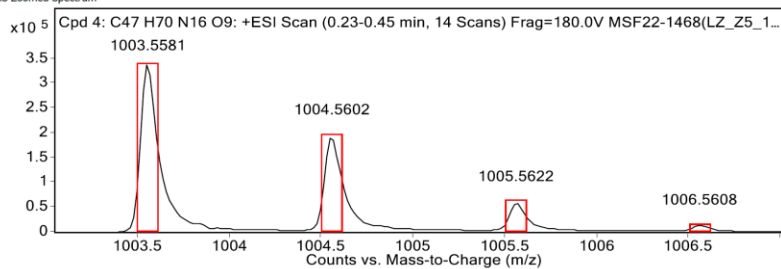
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
732.3339			1417106			
1257.6949	1257.6963	1	60978	C ₅₈ H ₈₈ N ₂₀ O ₁₂	(M+H) ⁺	1.15
1258.6974	1258.6991	1	43406	C ₅₈ H ₈₈ N ₂₀ O ₁₂	(M+H) ⁺	1.37
1259.6993	1259.7017	1	17361	C ₅₈ H ₈₈ N ₂₀ O ₁₂	(M+H) ⁺	1.89
1260.7025	1260.7043	1	5165	C ₅₈ H ₈₈ N ₂₀ O ₁₂	(M+H) ⁺	1.45
1261.6976	1261.7068	1	1822	C ₅₈ H ₈₈ N ₂₀ O ₁₂	(M+H) ⁺	7.32

--- End Of Report ---



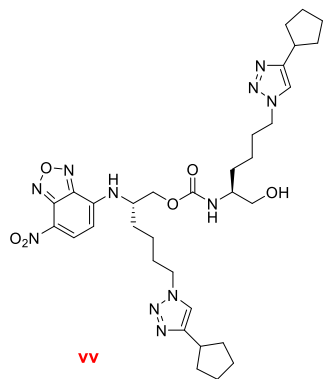
Chemical Formula: C₄₇H₇₀N₁₆O₉
Exact Mass: 1002.55

MS Zoomed Spectrum



Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
732.3339			1417495			
1003.5581	1003.5584	1	339733	C ₄₇ H ₇₀ N ₁₆ O ₉	(M+H) ⁺	0.34
1004.5602	1004.5612	1	193654	C ₄₇ H ₇₀ N ₁₆ O ₉	(M+H) ⁺	0.96
1005.5622	1005.5638	1	58838	C ₄₇ H ₇₀ N ₁₆ O ₉	(M+H) ⁺	1.61
1006.5608	1006.5664	1	11576	C ₄₇ H ₇₀ N ₁₆ O ₉	(M+H) ⁺	5.53
1007.5708	1007.5689	1	2325	C ₄₇ H ₇₀ N ₁₆ O ₉	(M+H) ⁺	-1.89
1008.6315	1008.5713	1	351	C ₄₇ H ₇₀ N ₁₆ O ₉	(M+H) ⁺	-59.63

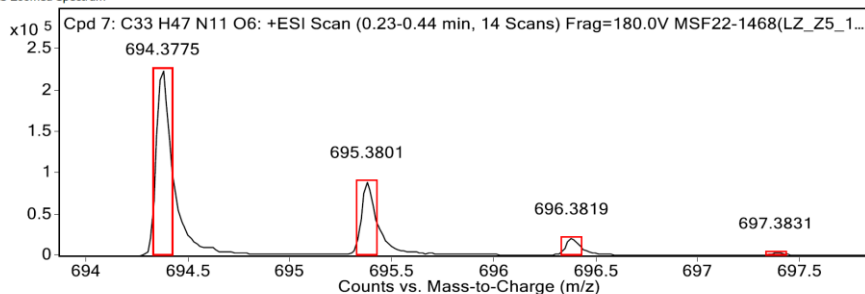
--- End Of Report ---



Chemical Formula: C₃₃H₄₇N₁₁O₆
Exact Mass: 693.37

VV

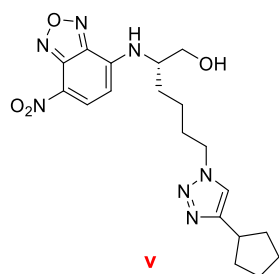
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1870			1466951			
694.3775	694.3784	1	225503	C ₃₃ H ₄₇ N ₁₁ O ₆	(M+H) ⁺	1.23
695.3801	695.3811	1	89447	C ₃₃ H ₄₇ N ₁₁ O ₆	(M+H) ⁺	1.55
696.3819	696.3837	1	21247	C ₃₃ H ₄₇ N ₁₁ O ₆	(M+H) ⁺	2.63
697.3831	697.3862	1	3503	C ₃₃ H ₄₇ N ₁₁ O ₆	(M+H) ⁺	4.52
698.3601	698.3887	1	826	C ₃₃ H ₄₇ N ₁₁ O ₆	(M+H) ⁺	40.92

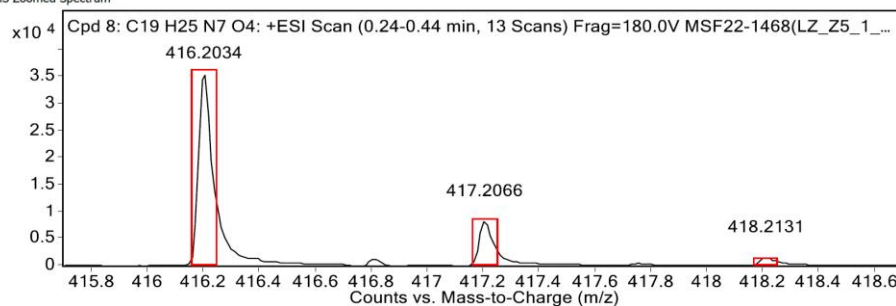
--- End Of Report ---



Chemical Formula: C₁₉H₂₅N₇O₄
Exact Mass: 415.20

V

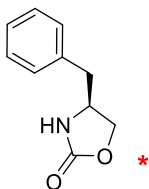
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1870			1579303			
416.2034	416.2041	1	35990	C ₁₉ H ₂₅ N ₇ O ₄	(M+H) ⁺	1.74
417.2066	417.2068	1	8355	C ₁₉ H ₂₅ N ₇ O ₄	(M+H) ⁺	0.35
418.2131	418.2092	1	1581	C ₁₉ H ₂₅ N ₇ O ₄	(M+H) ⁺	-9.4

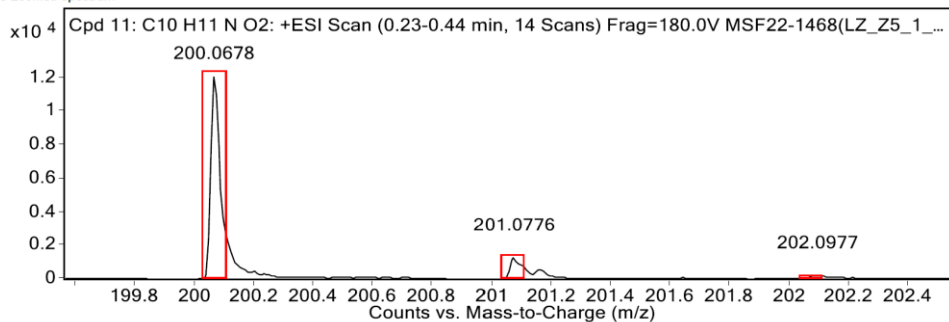
--- End Of Report ---



Chemical Formula: C₁₀H₁₁NO₂
Exact Mass: 177.08

*

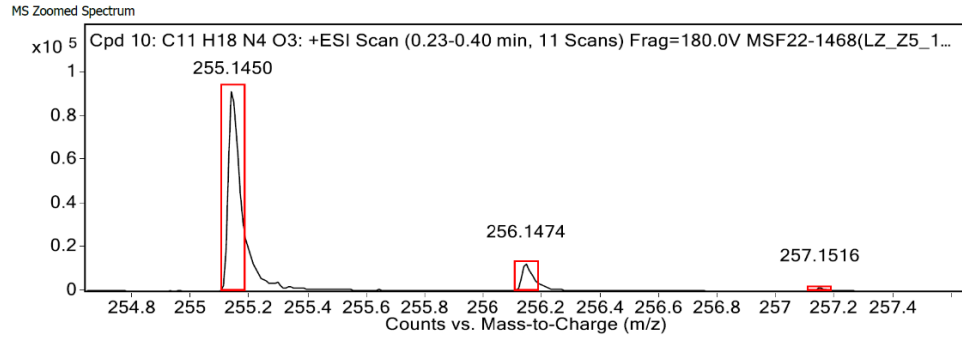
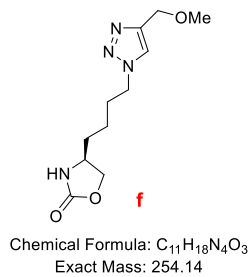
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
200.0678	200.0682	1	12276	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	1.99
201.0776	201.0714	1	1312	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-30.94
202.0977	202.0737	1	245	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-118.93
310.1870			1466891			

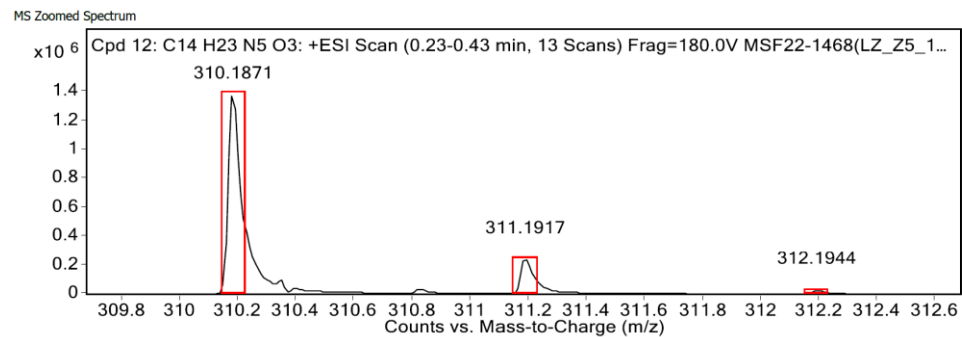
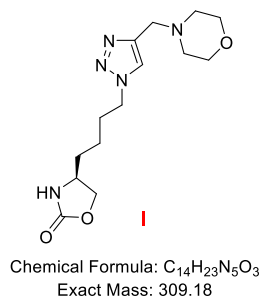
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
255.1450	255.1452	1	93982	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	0.59
256.1474	256.1479	1	12553	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	1.83
257.1516	257.1501	1	1635	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	-5.79
258.1549	258.1524	1	296	C ₁₁ H ₁₈ N ₄ O ₃	(M+H) ⁺	-9.36
310.1871			1547083			

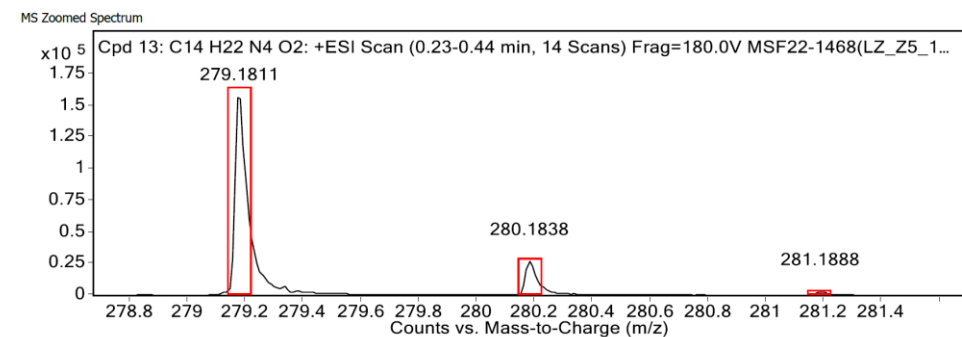
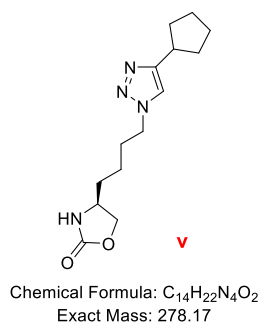
--- End Of Report ---



MS Spectrum Peak List

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
310.1871	310.1874	1	1395079	C ₁₄ H ₂₃ N ₅ O ₃	(M+H) ⁺	0.79
311.1917	311.1901	1	242452	C ₁₄ H ₂₃ N ₅ O ₃	(M+H) ⁺	-5
312.1944	312.1924	1	28381	C ₁₄ H ₂₃ N ₅ O ₃	(M+H) ⁺	-6.15
313.2042	313.1948	1	2587	C ₁₄ H ₂₃ N ₅ O ₃	(M+H) ⁺	-29.88
732.3339			1437123			

--- End Of Report ---

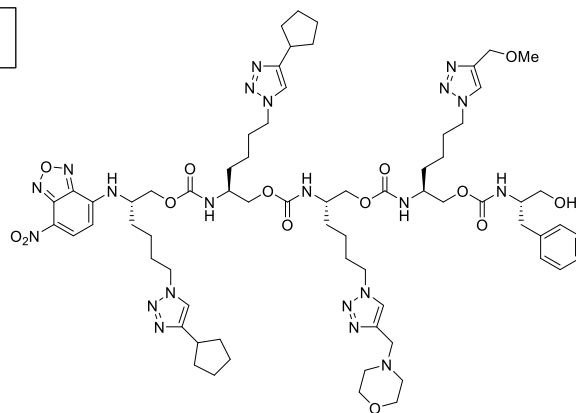


MS Spectrum Peak List

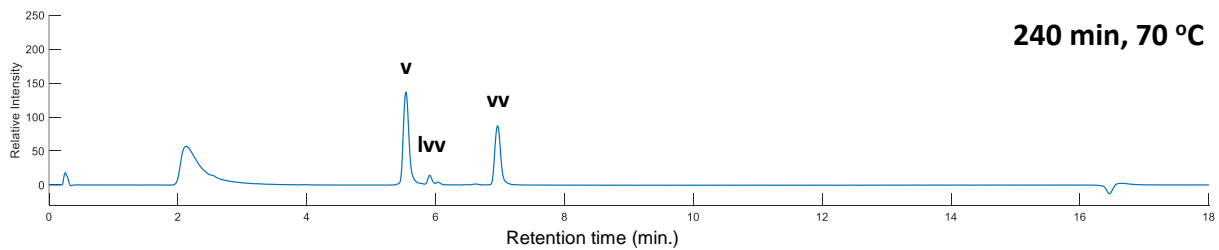
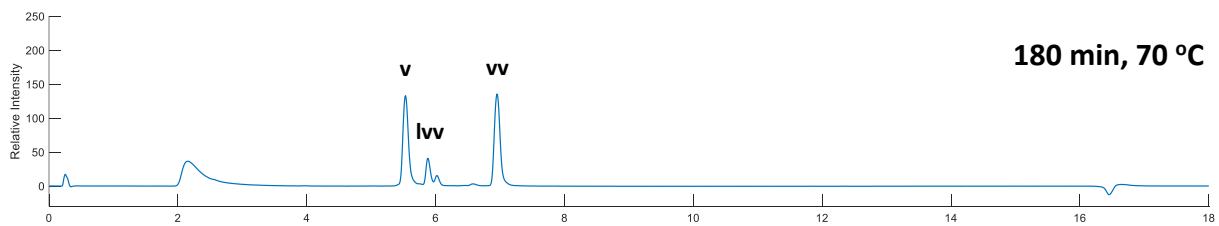
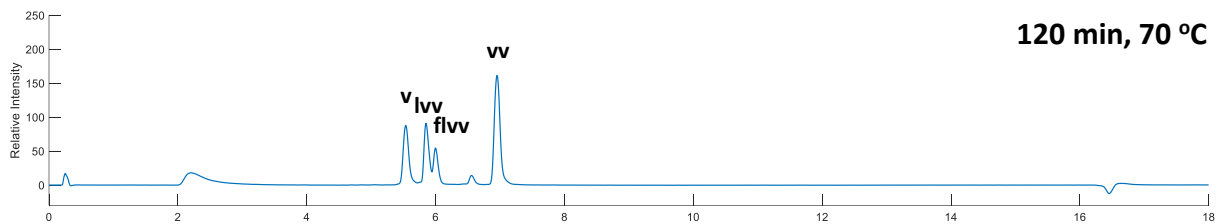
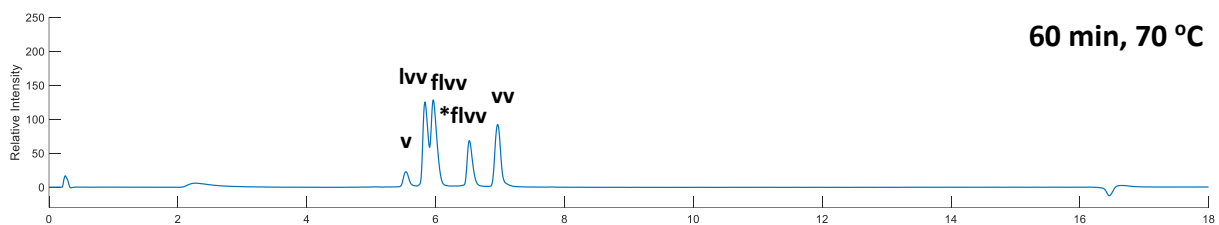
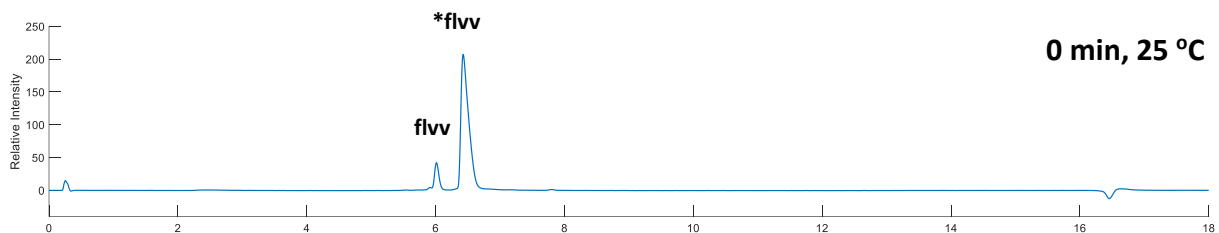
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
279.1811	279.1816	1	163805	C ₁₄ H ₂₂ N ₄ O ₂	(M+H) ⁺	1.59
280.1838	280.1844	1	27120	C ₁₄ H ₂₂ N ₄ O ₂	(M+H) ⁺	2.32
281.1888	281.1869	1	3208	C ₁₄ H ₂₂ N ₄ O ₂	(M+H) ⁺	-6.59
310.1870			1466986			

--- End Of Report ---

Oligomer Z5_2: *flvv

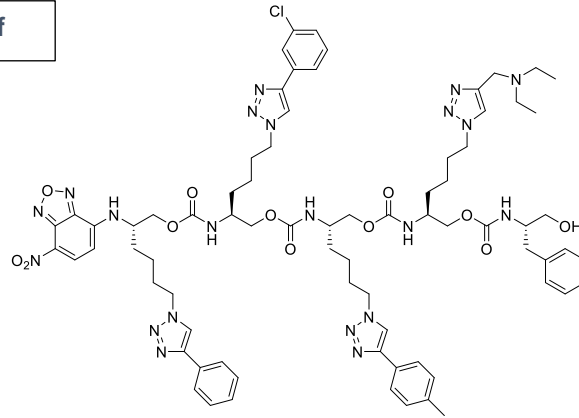


Exact Mass: 1433.77

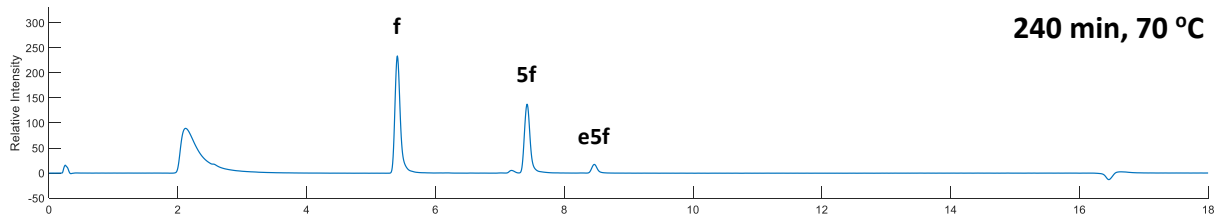
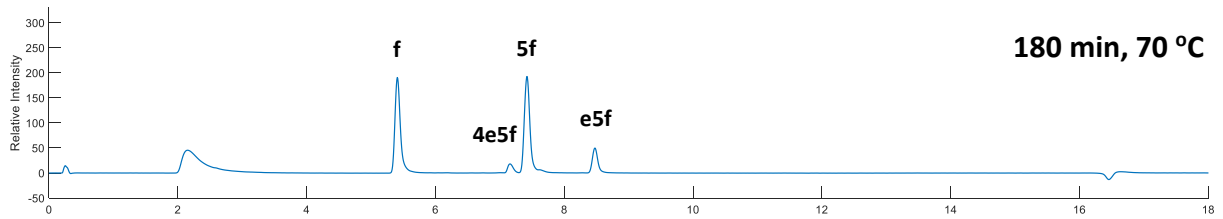
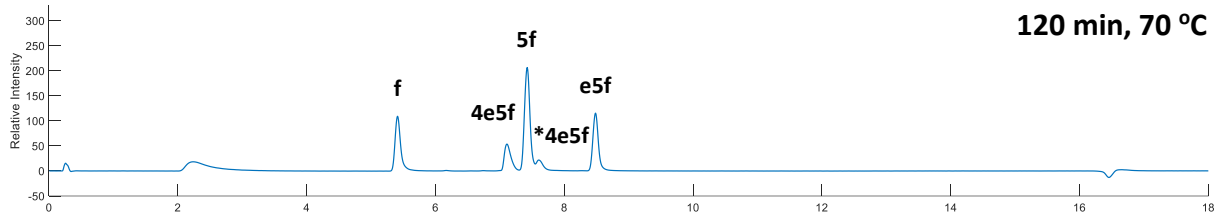
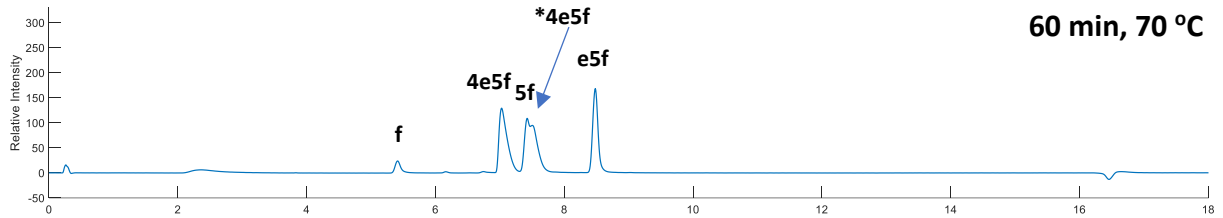
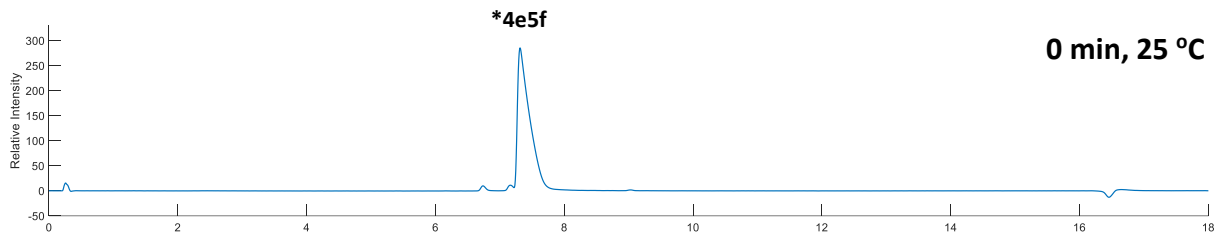


Retention time (min.)

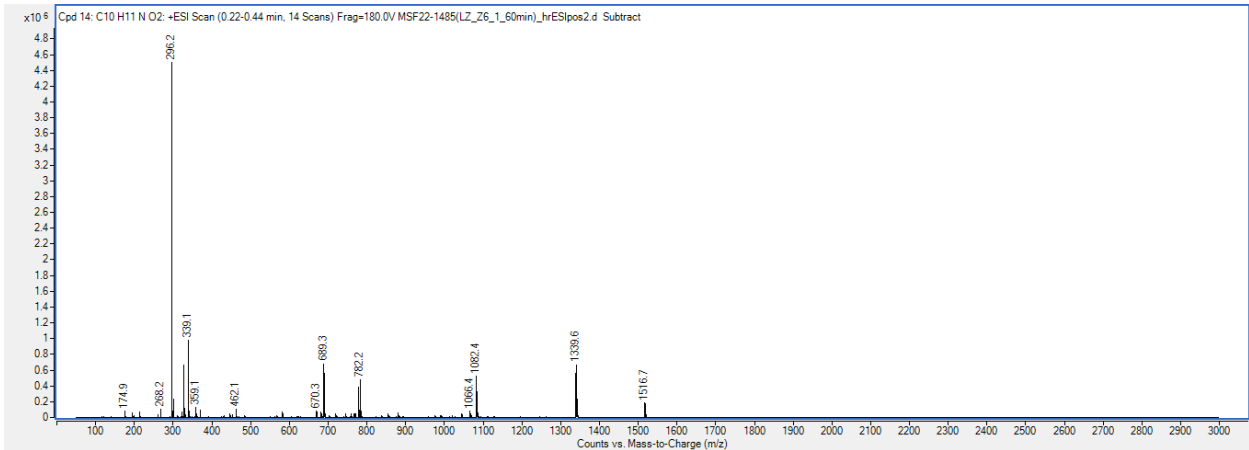
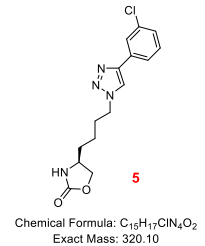
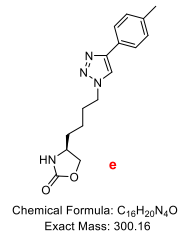
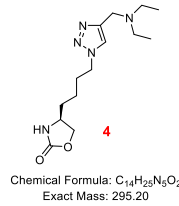
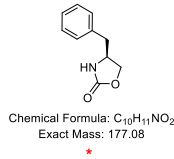
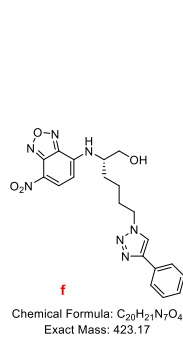
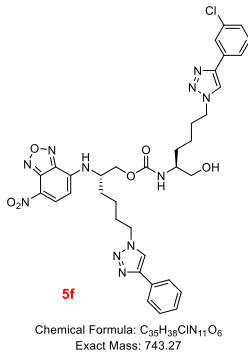
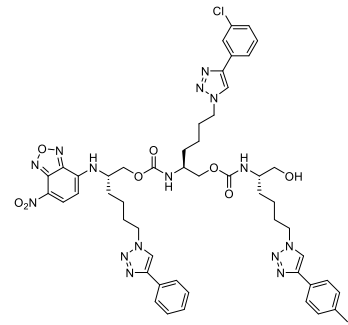
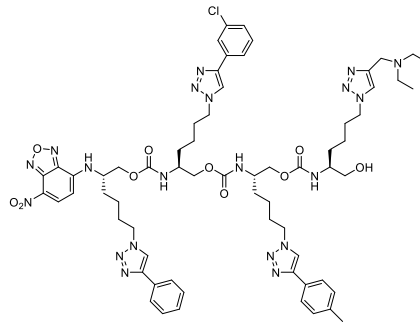
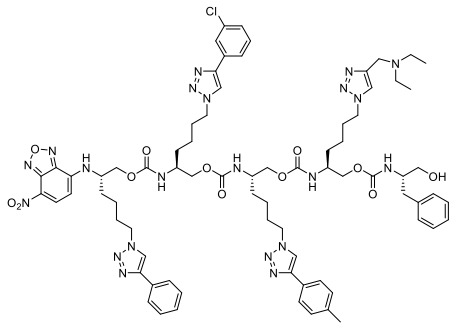
Oligomer Z6_1: *4e5f

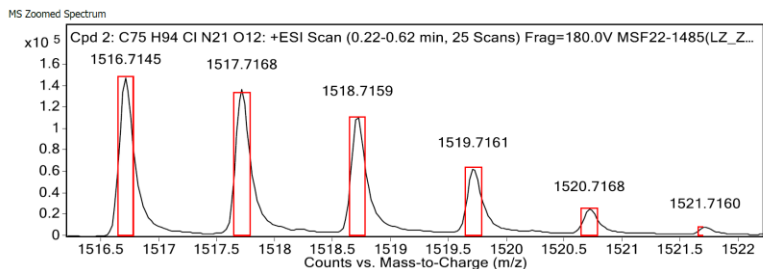
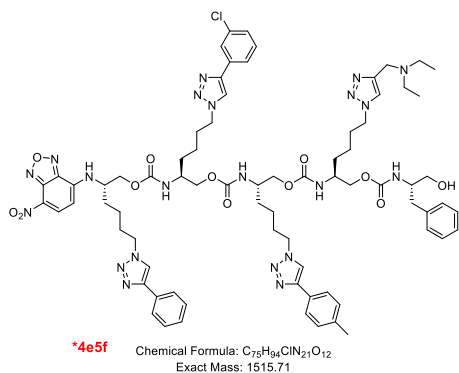


Exact Mass: 1515.71



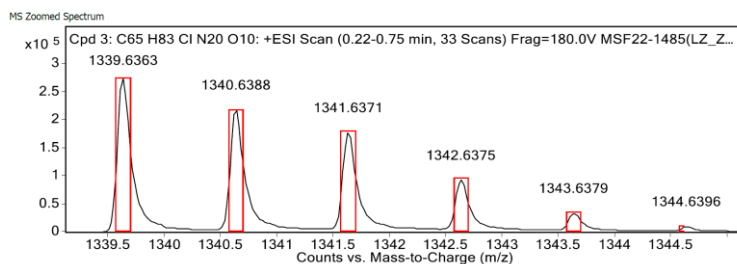
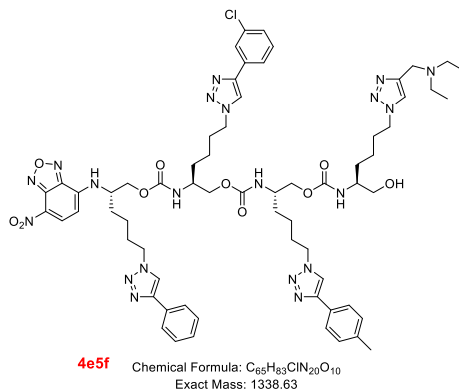
After 60 minutes of sequencing, all the following molecules are observed in the solution and analyzed via High-Res MS.





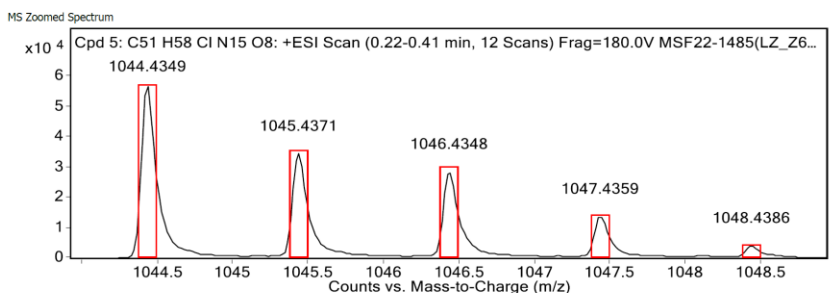
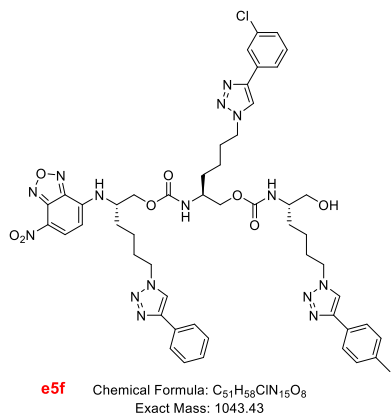
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2077			4027732			
1516.7145	1516.7152	1	147801	C75H94ClN21O12	(M+H)+	0.47
1517.7168	1517.7181	1	136649	C75H94ClN21O12	(M+H)+	0.84
1518.7159	1518.7172	1	111863	C75H94ClN21O12	(M+H)+	0.83
1519.7161	1519.7179	1	63748	C75H94ClN21O12	(M+H)+	1.2
1520.7168	1520.7196	1	22808	C75H94ClN21O12	(M+H)+	1.86
1521.7160	1521.7218	1	6843	C75H94ClN21O12	(M+H)+	3.76
1522.7186	1522.7241	1	1843	C75H94ClN21O12	(M+H)+	3.62
1523.6572	1523.7265	1	550	C75H94ClN21O12	(M+H)+	45.5

--- End Of Report ---



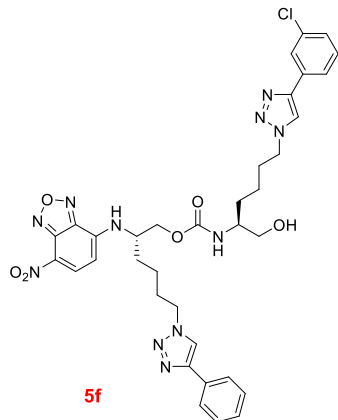
Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2077			2549357			
1339.6363	1339.6362	1	274774	C65H83ClN20O10	(M+H)+	-0.06
1340.6388	1340.6390	1	218795	C65H83ClN20O10	(M+H)+	0.16
1341.6371	1341.6376	1	178187	C65H83ClN20O10	(M+H)+	0.36
1342.6375	1342.6384	1	93068	C65H83ClN20O10	(M+H)+	0.66
1343.6379	1343.6402	1	34085	C65H83ClN20O10	(M+H)+	1.69
1344.6396	1344.6424	1	10338	C65H83ClN20O10	(M+H)+	2.12
1345.6400	1345.6447	1	3456	C65H83ClN20O10	(M+H)+	3.52

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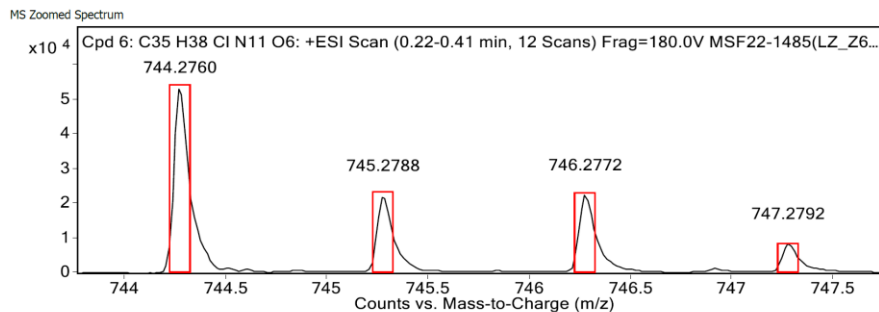


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2077			4116022			
1044.4349	1044.4354	1	57102	C51H58ClN15O8	(M+H)+	0.47
1045.4371	1045.4382	1	34677	C51H58ClN15O8	(M+H)+	1.08
1046.4348	1046.4358	1	28709	C51H58ClN15O8	(M+H)+	0.93
1047.4359	1047.4369	1	13870	C51H58ClN15O8	(M+H)+	0.92
1048.4386	1048.4389	1	4234	C51H58ClN15O8	(M+H)+	0.37
1049.4423	1049.4413	1	1288	C51H58ClN15O8	(M+H)+	-1.03

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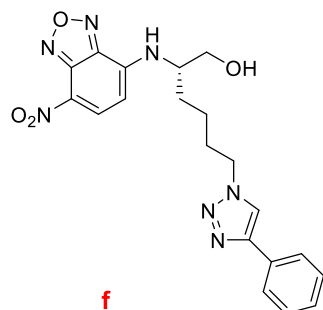


Chemical Formula: C₃₅H₃₈ClN₁₁O₆
Exact Mass: 743.27

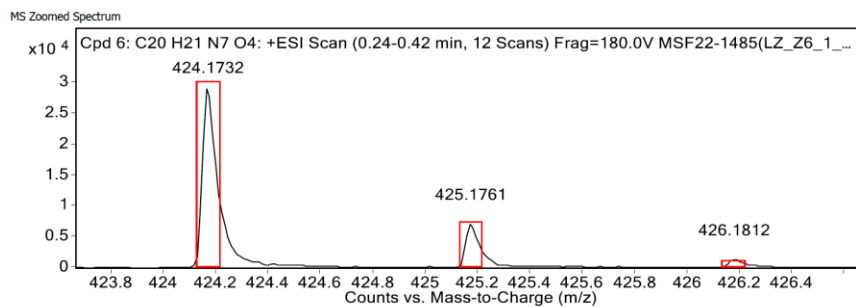


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2077			4130249			
744.2760	744.2768	1	54173	C ₃₅ H ₃₈ ClN ₁₁ O ₆	(M+H) ⁺	1.12
745.2788	745.2796	1	22515	C ₃₅ H ₃₈ ClN ₁₁ O ₆	(M+H) ⁺	1.02
746.2772	746.2758	1	22706	C ₃₅ H ₃₈ ClN ₁₁ O ₆	(M+H) ⁺	-1.78
747.2792	747.2775	1	8634	C ₃₅ H ₃₈ ClN ₁₁ O ₆	(M+H) ⁺	-2.19
748.2913	748.2798	1	2091	C ₃₅ H ₃₈ ClN ₁₁ O ₆	(M+H) ⁺	-15.44

--- End Of Report ---

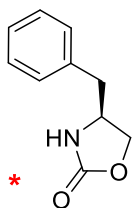


Chemical Formula: C₂₀H₂₁N₇O₄
Exact Mass: 423.17

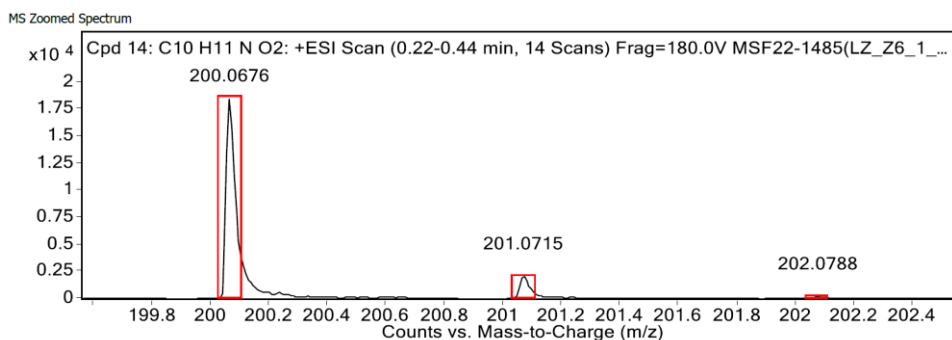


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2074			2614340			
424.1732	424.1728	1	29717	C ₂₀ H ₂₁ N ₇ O ₄	(M+H) ⁺	-1.04
425.1761	425.1755	1	7217	C ₂₀ H ₂₁ N ₇ O ₄	(M+H) ⁺	-1.28
426.1812	426.1780	1	1448	C ₂₀ H ₂₁ N ₇ O ₄	(M+H) ⁺	-7.56
427.2155	427.1803	1	210	C ₂₀ H ₂₁ N ₇ O ₄	(M+H) ⁺	-82.23

--- End Of Report ---

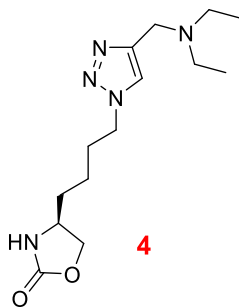


Chemical Formula:
C₁₀H₁₁NO₂
Exact Mass: 177.08

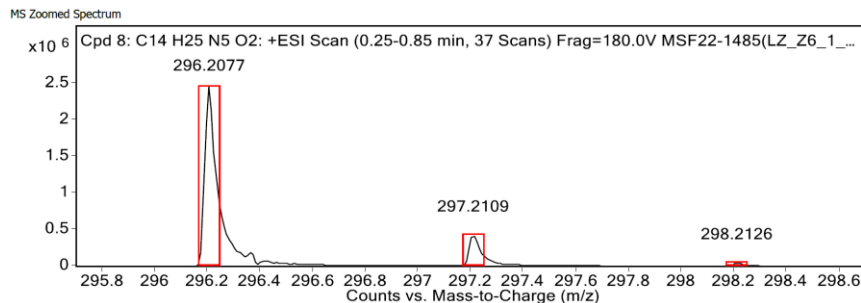


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
200.0676	200.0682	1	18541	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	3
201.0715	201.0714	1	2145	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-0.5
202.0788	202.0737	1	287	C ₁₀ H ₁₁ NO ₂	(M+Na) ⁺	-25.33
296.2077			4499905			

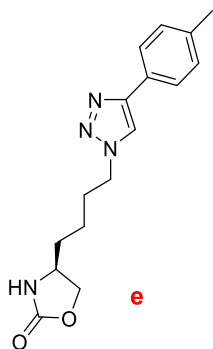
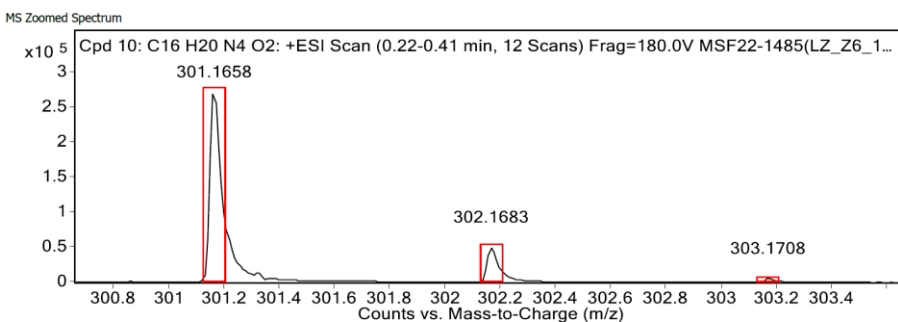
--- End Of Report ---



Chemical Formula: C₁₄H₂₅N₅O₂
Exact Mass: 295.20

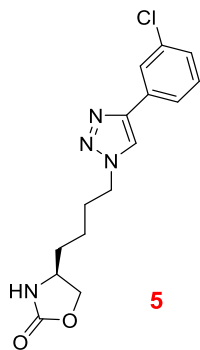


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2077	296.2081	1	2459419	C ₁₄ H ₂₅ N ₅ O ₂	(M+H) ⁺	1.26
297.2109	297.2108	1	422901	C ₁₄ H ₂₅ N ₅ O ₂	(M+H) ⁺	-0.18
298.2126	298.2133	1	44286	C ₁₄ H ₂₅ N ₅ O ₂	(M+H) ⁺	2.37
299.2148	299.2156	1	3356	C ₁₄ H ₂₅ N ₅ O ₂	(M+H) ⁺	2.67

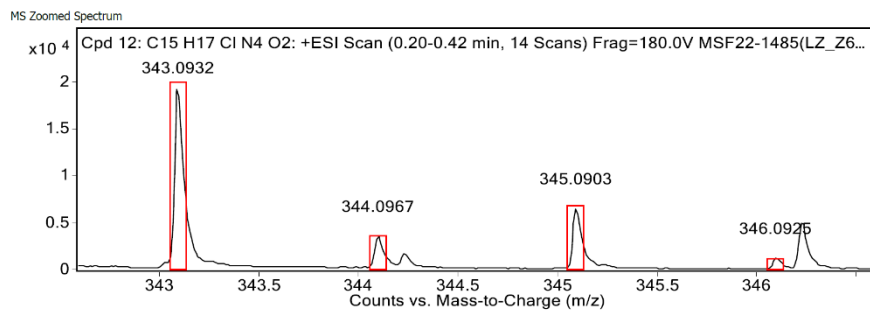


Chemical Formula: C₁₆H₂₀N₄O₂
Exact Mass: 300.16

Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2077			4192038			
301.1658	301.1659	1	276416	C ₁₆ H ₂₀ N ₄ O ₂	(M+H) ⁺	0.23
302.1683	302.1688	1	50363	C ₁₆ H ₂₀ N ₄ O ₂	(M+H) ⁺	1.67
303.1708	303.1714	1	5711	C ₁₆ H ₂₀ N ₄ O ₂	(M+H) ⁺	1.83
304.1100	304.1739	1	381	C ₁₆ H ₂₀ N ₄ O ₂	(M+H) ⁺	210.05

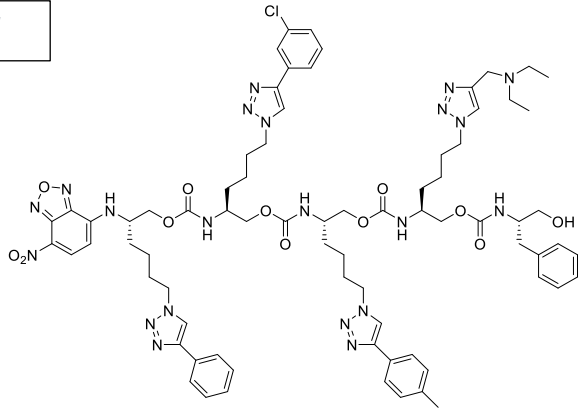


Chemical Formula: C₁₅H₁₇ClN₄O₂
Exact Mass: 320.10

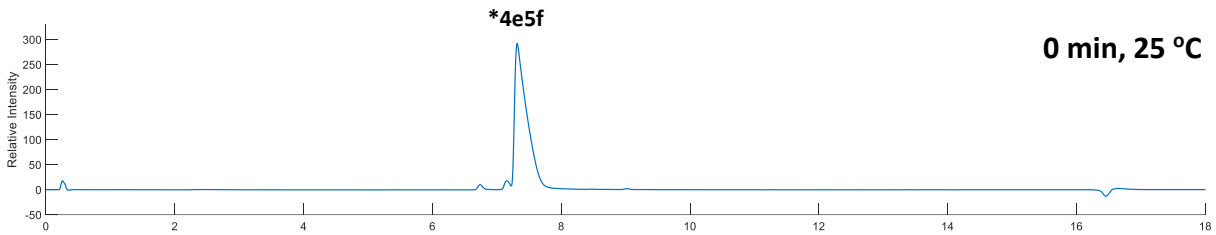


Obs. m/z	Calc. m/z	Charge	Abundance	Formula	Ion Species	Tgt Mass Error (ppm)
296.2074			2117257			
343.0932	343.0932	1	19791	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+Na) ⁺	0.01
344.0967	344.0961	1	3716	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+Na) ⁺	-1.85
345.0903	345.0908	1	6641	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+Na) ⁺	1.29
346.0925	346.0934	1	1370	C ₁₅ H ₁₇ ClN ₄ O ₂	(M+Na) ⁺	2.61

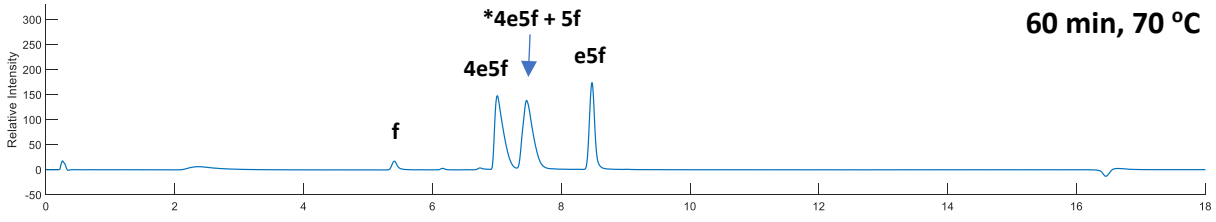
Oligomer Z6_2: *4e5f



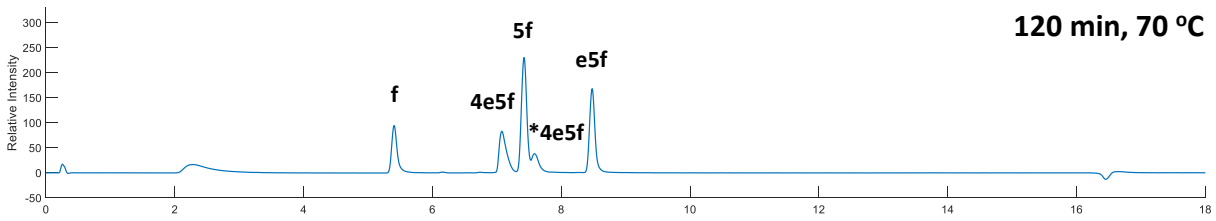
Exact Mass: 1515.71



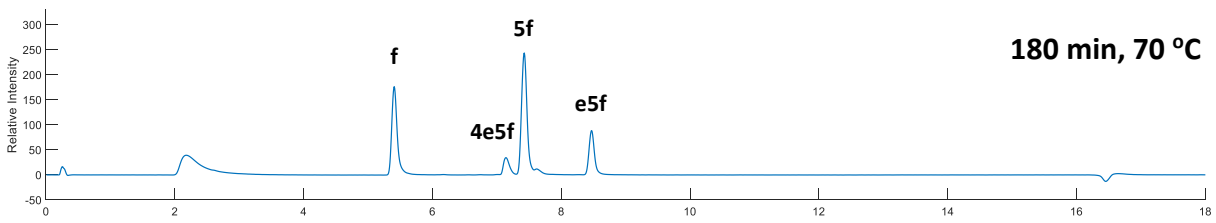
0 min, 25 °C



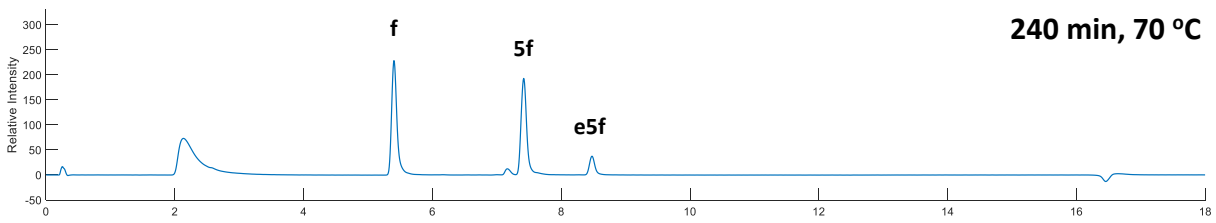
60 min, 70 °C



120 min, 70 °C



180 min, 70 °C



240 min, 70 °C

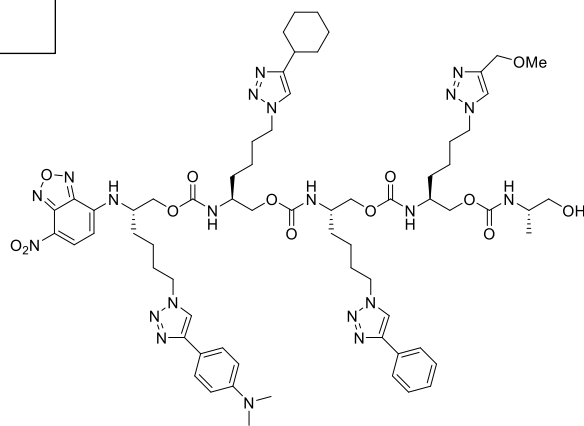
Retention time (min.)

References

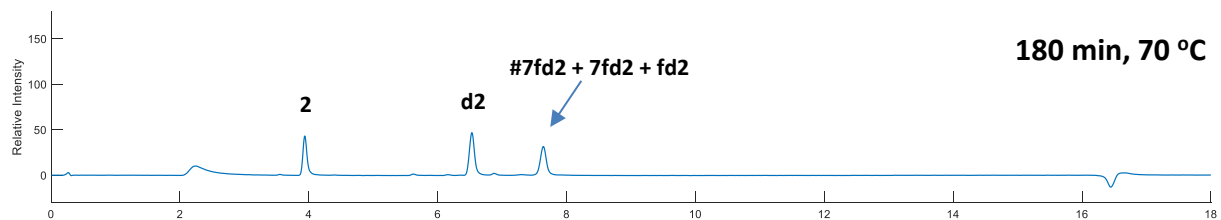
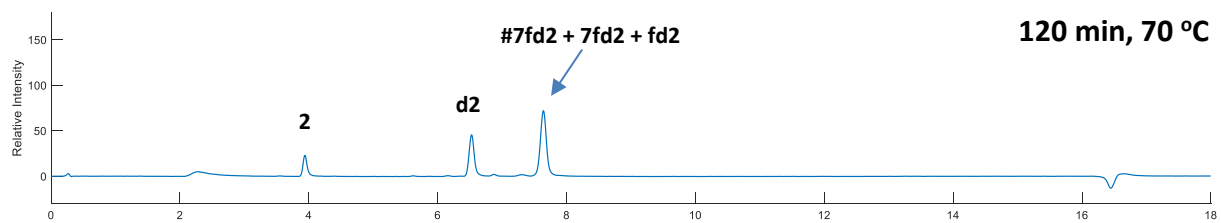
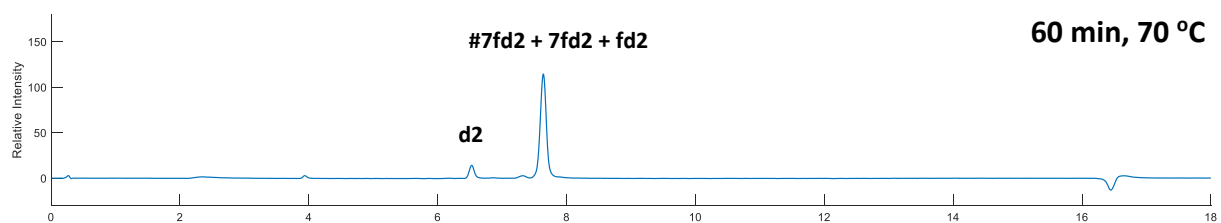
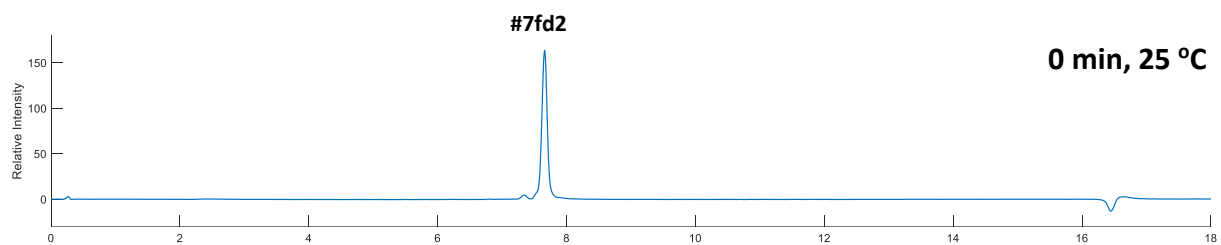
1. Dahlhauser, S. D.; Escamilla, P. R.; Vandewalle, A. N.; York, J. T.; Rapagnani, R. M.; Shei, J. S.; Glass, S. A.; Coronado, J. N.; Moor, S. R.; Saunders, D. P.; Anslyn, E. V. *J. Am. Chem. Soc.* **2020**, *142* (6), 2744–2749.

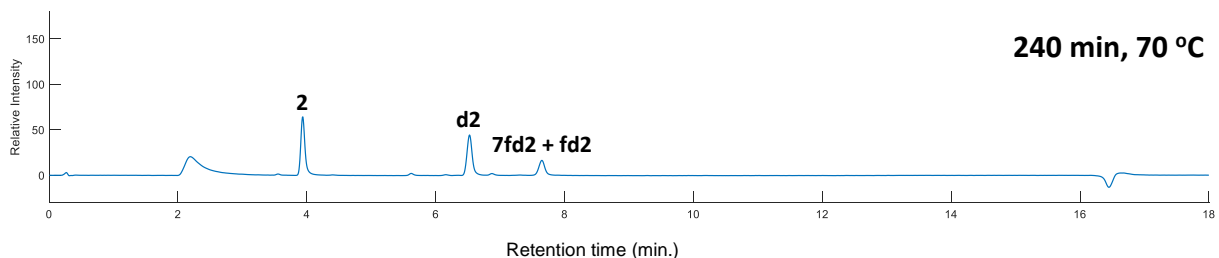
III(c). Sequencing the oligomers with overlapping truncated oligomers of similar polarities in LC

Oligomer 4: **#7fd2**



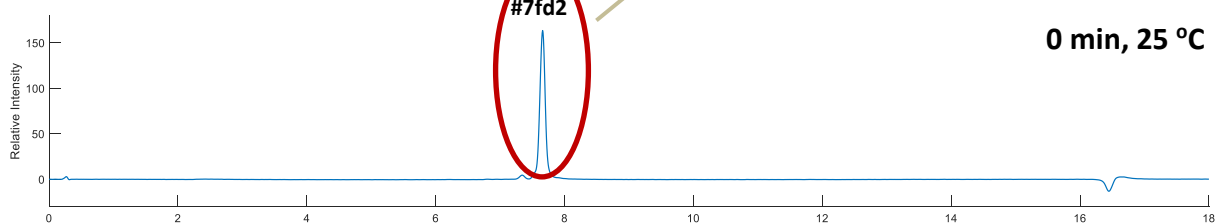
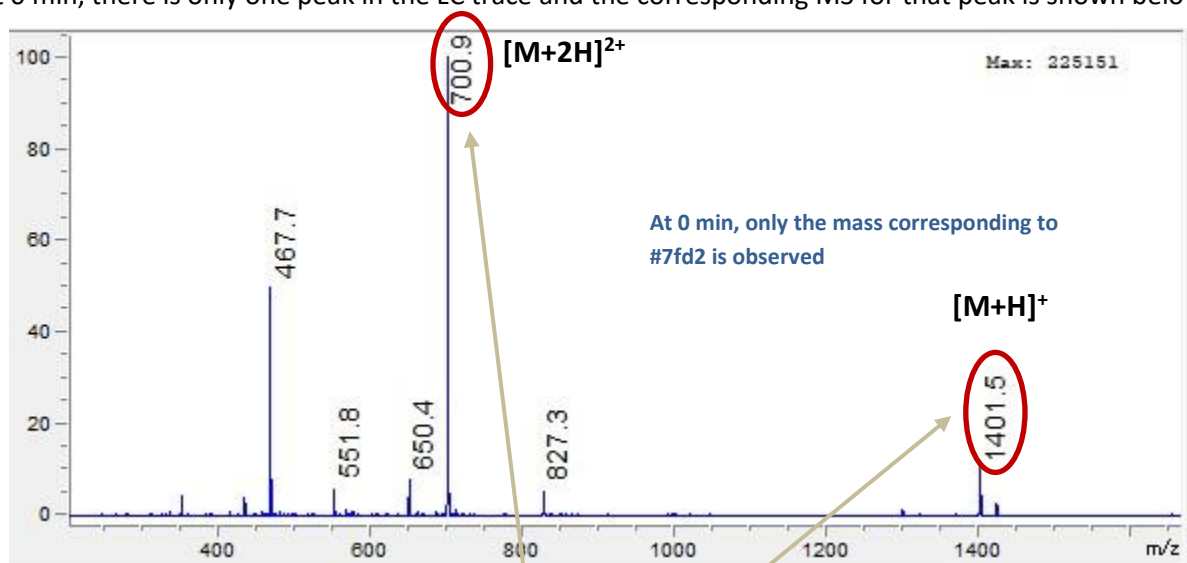
Exact Mass: 1399.73



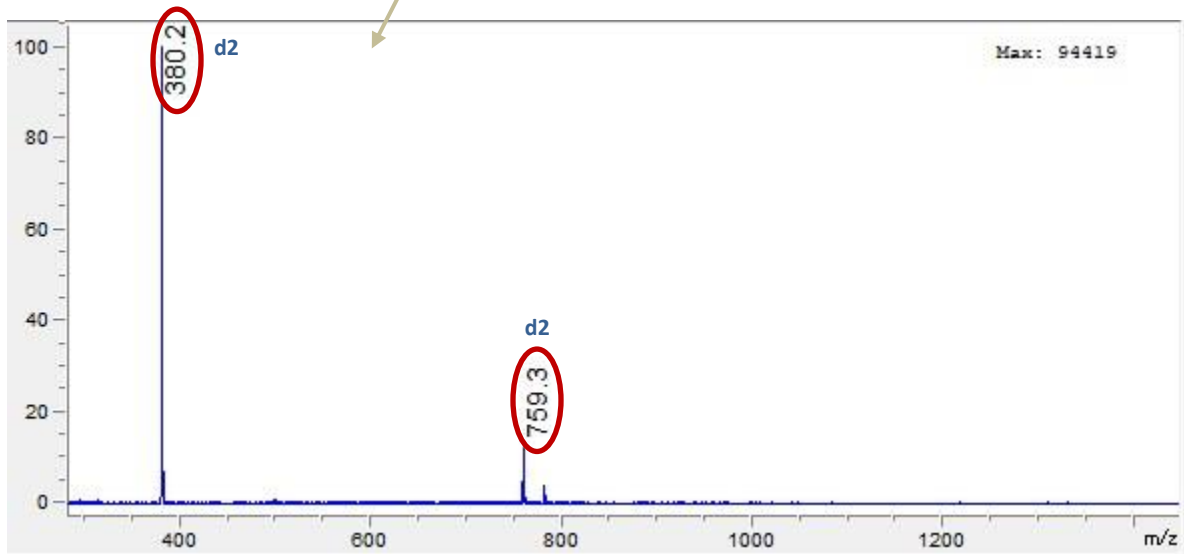
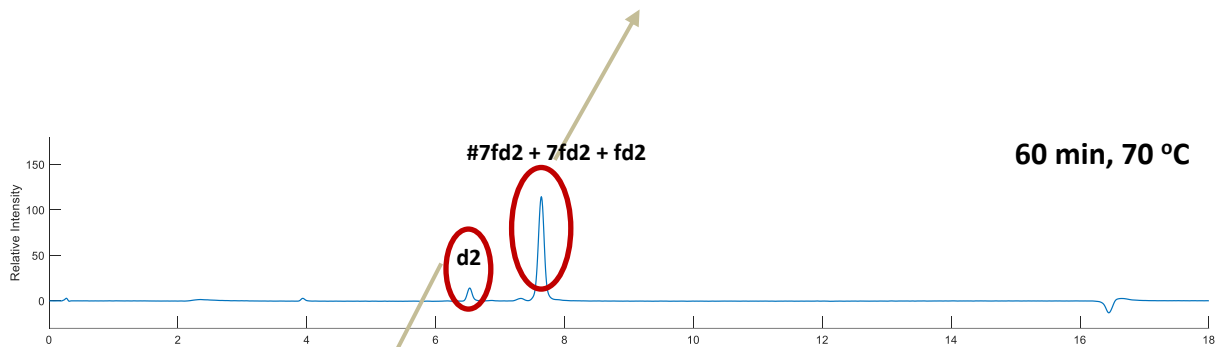
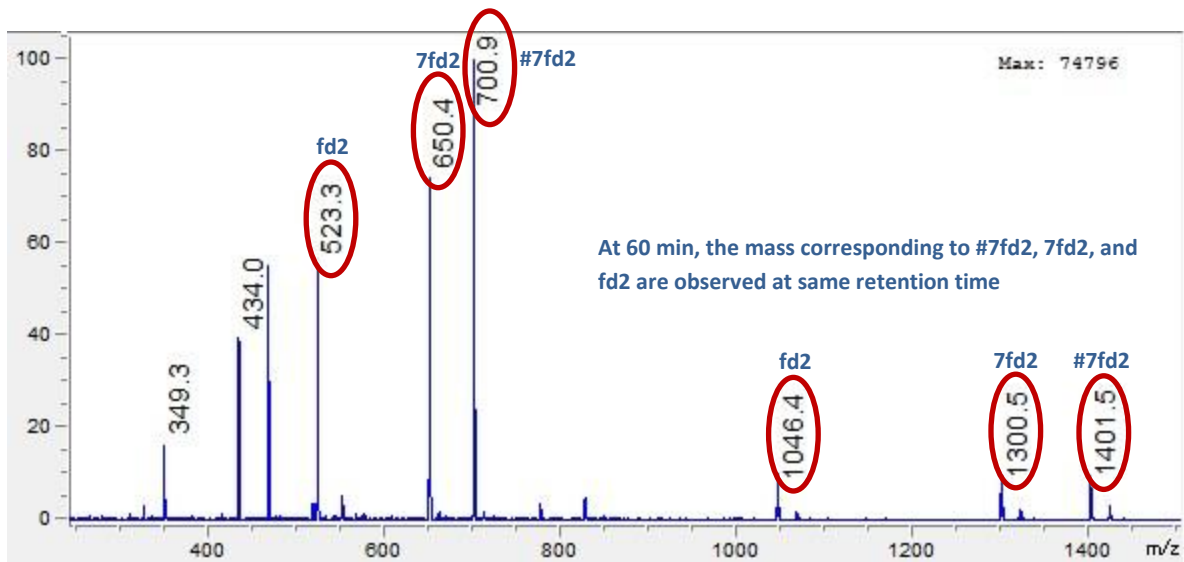


The sequencing of Oligomer 4 (#7fd2) is a scenario where multiple peaks overlap. In this case, it can be difficult to identify what peaks are overlapping, and what is the order in which these peaks show up in LC-MS. The MS data can help in deconvolute that. The process is shown below:

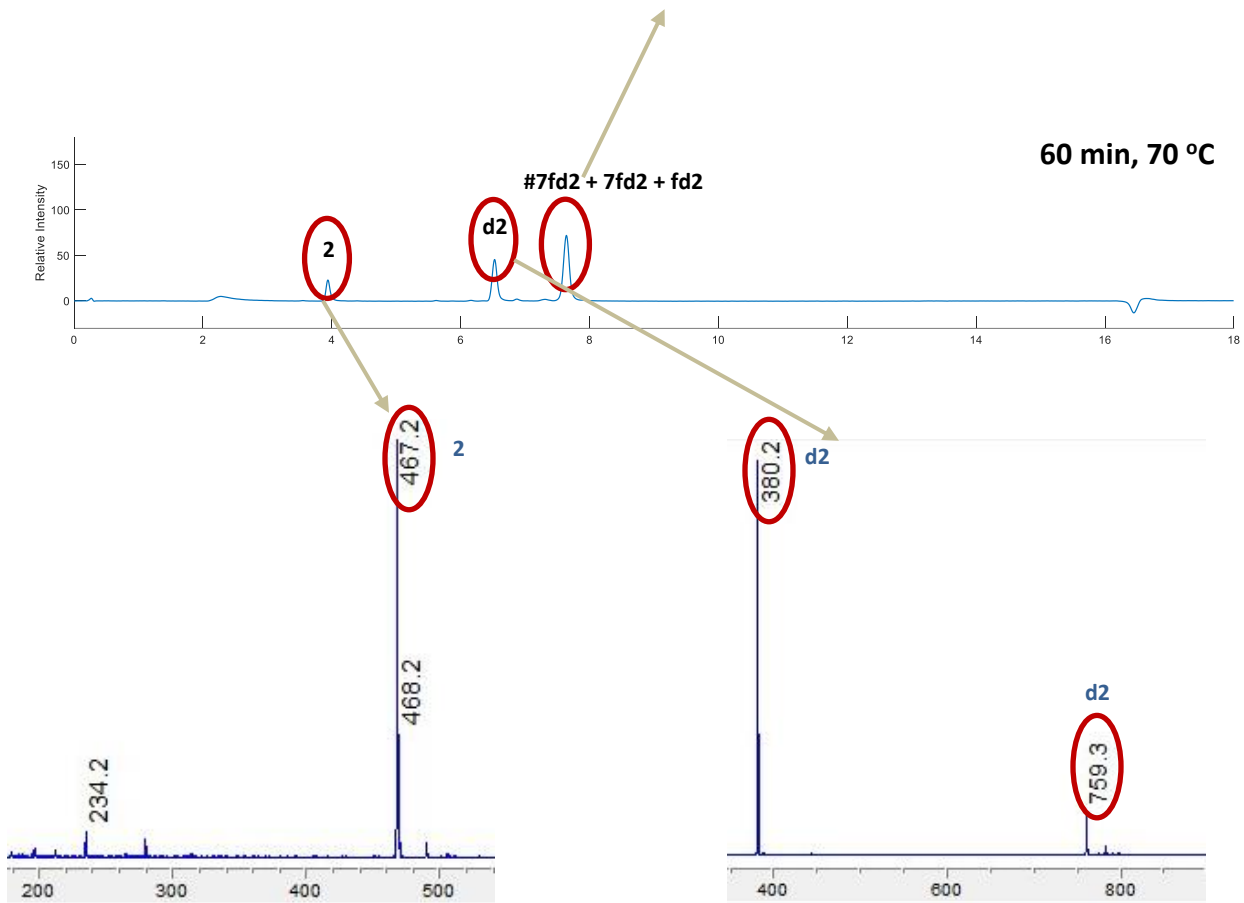
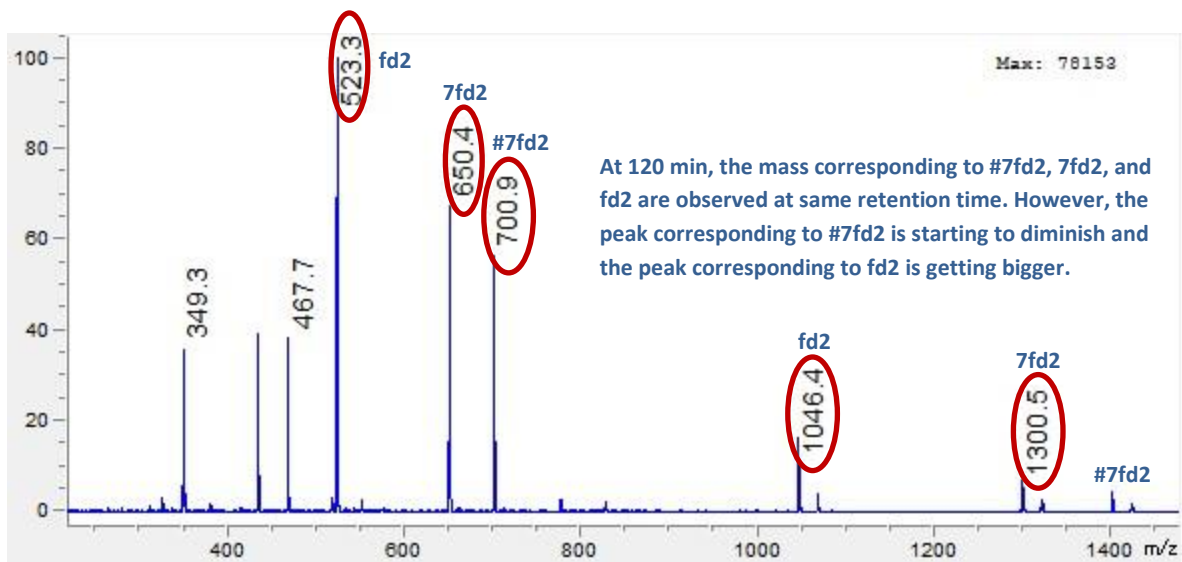
At 0 min, there is only one peak in the LC trace and the corresponding MS for that peak is shown below:



At 60 min, there are two peaks in the LC trace, and the corresponding MS for these peaks are shown below:

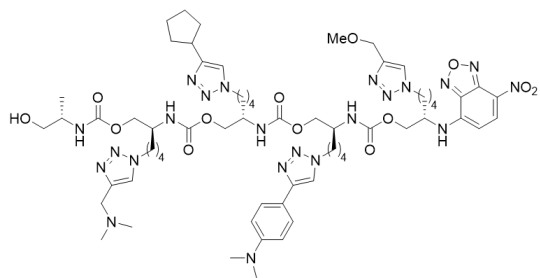


At 120 min, there are three peaks in the LC trace, and the corresponding MS for these peaks are shown below:

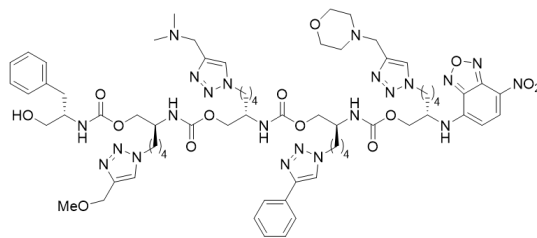


As we keep observing the LC trace and the corresponding MS peaks for the 180 and 240 minutes, we can confidently say what peaks are overlapping and what is the order of their appearance and disappearance. From this observation, the accurate sequence of the given oligomer can be determined.

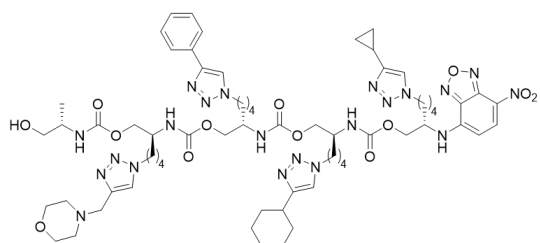
III(d). The oligomers and corresponding Chinese characters.



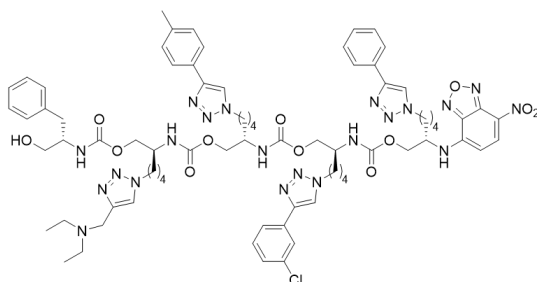
6027
性



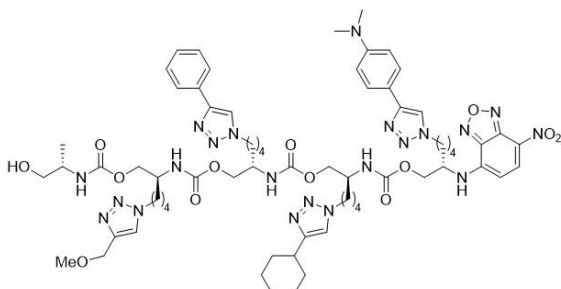
76f8
相



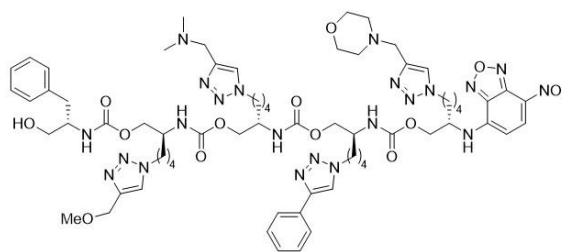
8fd1
近



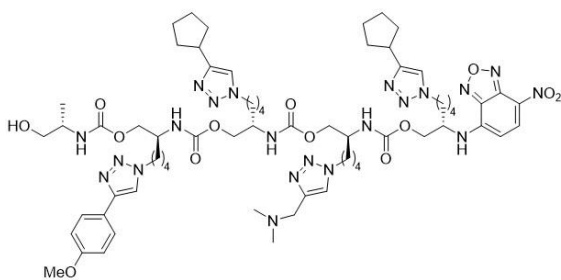
4e5f
也



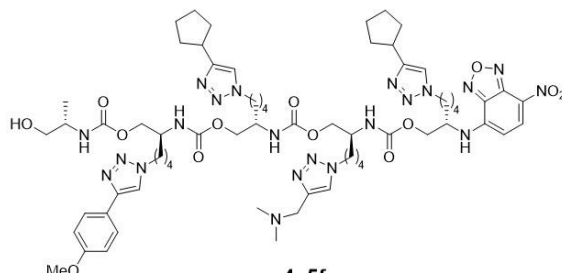
7fd2
習



76f8
相

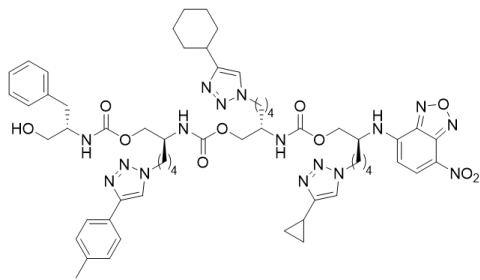


9060
遠

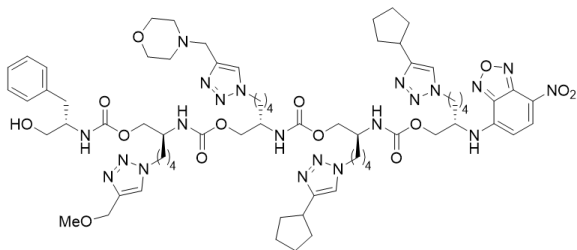


4e5f
也

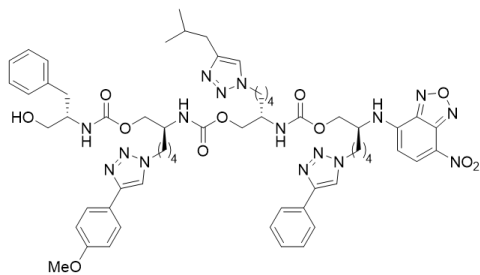
(1) Unicode encoding



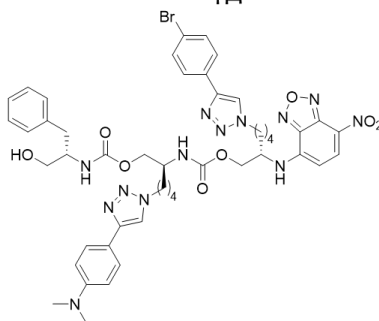
UMC
性



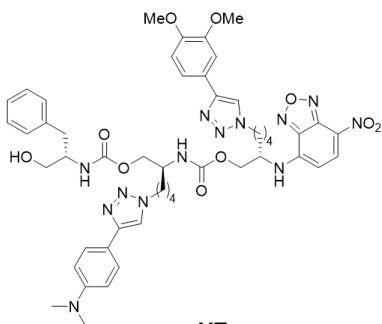
FLVW
相



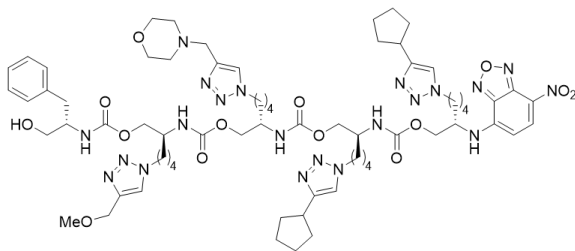
PDW
近



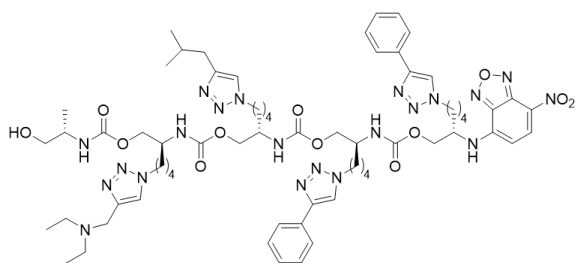
YI
也



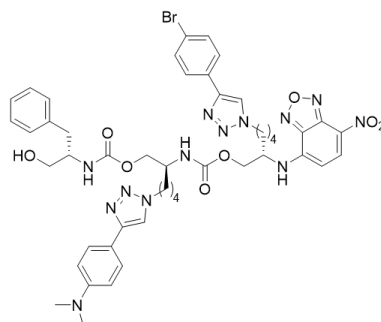
YT
习



FLVW
相



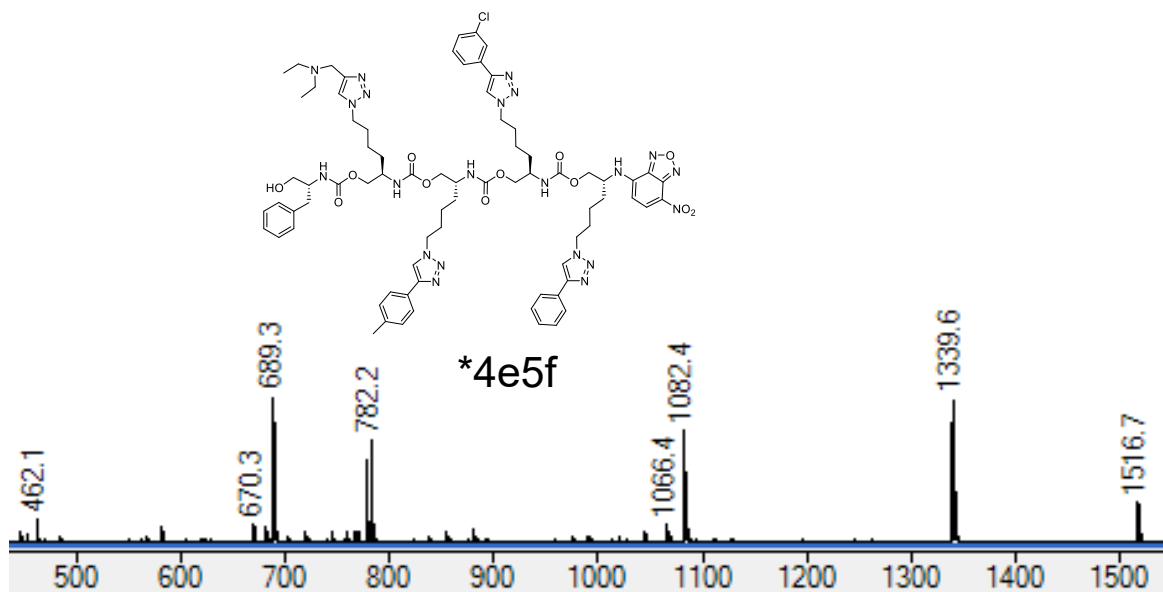
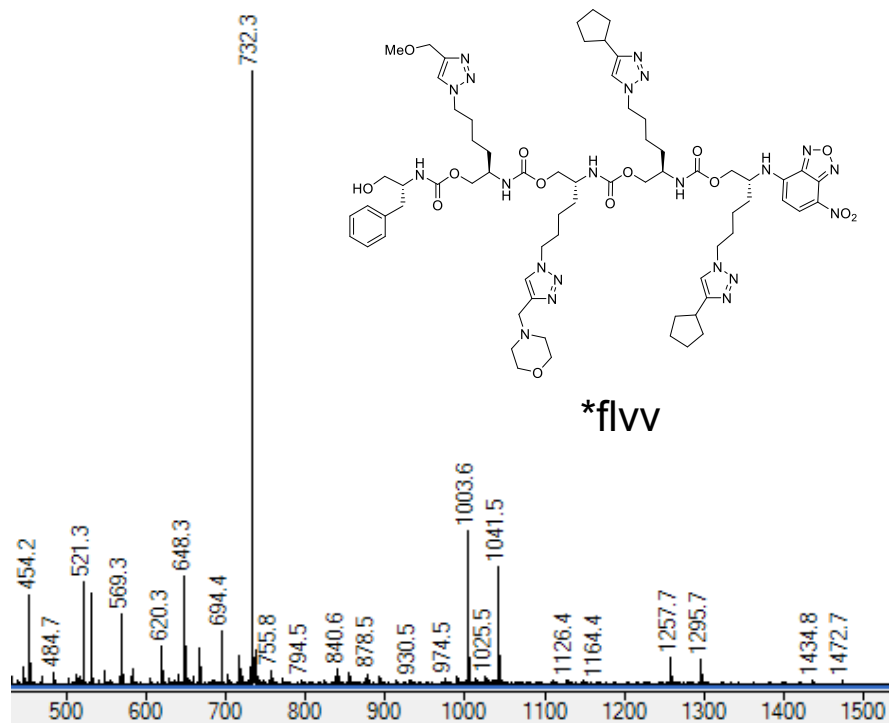
BDRW
远



YI
也

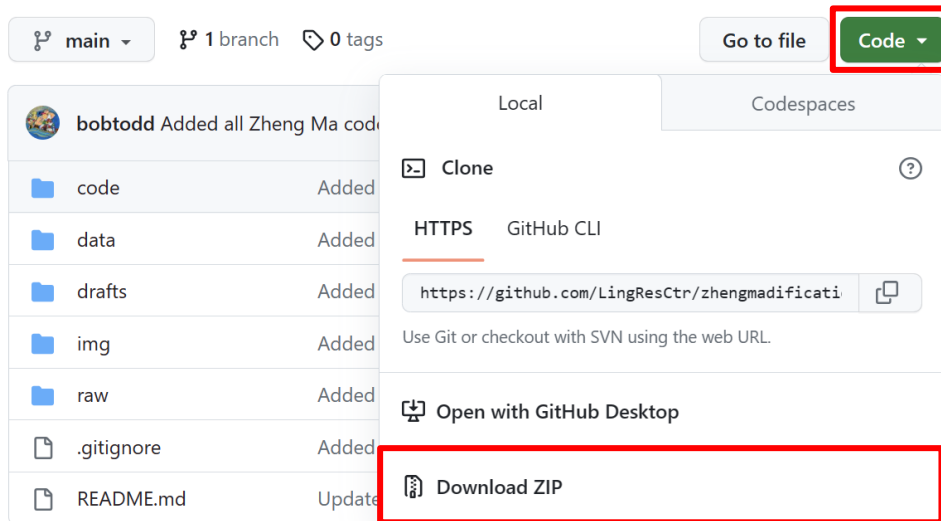
(2) Zhengma encoding

III(e). The zoomed in mass spectra of Oligomer Z5 (*flvv) and Z6 (*4e5f).



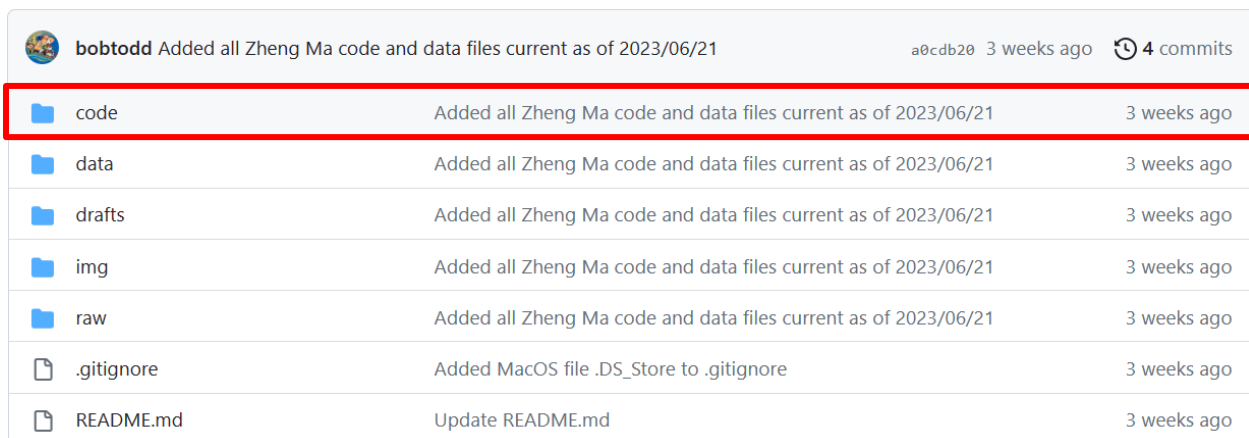
IV. User manual for Python scripts

To use this program, download the zip file, which can be located by clicking on “Code” on the GitHub website.



- To convert from Chinese characters to Zhengma codes

1. Go to the “code” folder.



2. Open the “4_converter.ipynb” file.

Name	Last commit message	Last commit date
..		
1_background.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
2_data.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
3_tests.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
4_converter.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
zm_helpers.py	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago

3. Load and run the codes 1-4 shown below.

```
In [1]: # If running in Google Colab
#from google.colab import drive
#drive.mount('/content/gdrive')
#
#path_prefix = "/content/gdrive/My Drive/CoLab Notebooks/zhengma/raw/"
#data_prefix = '/content/gdrive/My Drive/CoLab Notebooks/zhengma/data/'
```

```
In [2]: # If running on local system
path_prefix = "../raw/"
data_prefix = '../data/'
```

```
In [3]: import pickle

# Load pickle
with open(data_prefix + 'df_zm_merged.pkl', 'rb') as pickle_file:
    df_zm_merged = pickle.load(pickle_file)
```

```
In [4]: def characters_to_codes_simplistic(cjk_string, zm_dataframe, db_column='RIME Characters', zm_column='ZM Codes'):
# Input:
# string of CJK characters
# database of Zheng Ma codes as a pandas DataFrame
# name of column to check for characters
# name of column containing Zheng Ma codes
# Output:
# list (dictionary?) of Zheng Ma codes
# - In case of multiple code correspondences, choose the longest

characters = cjk_string.strip().replace(' ', '')

codes = []

for character in characters:
# Find any rows in the desired column that have the desired character
# Take the ZM codes in those rows as a list
possible_codes = zm_dataframe[z_m_dataframe[db_column] == character][zm_column].tolist()

# Choose the **longest code** in that list of ZM codes
max_code = max(possible_codes, key=len) if possible_codes else None
# There could be several, so order alphabetically and pick the first
desired_codes = [c for c in possible_codes if len(c) == len(max_code)] if max_code else None
desired_code = sorted(desired_codes)[0] if desired_codes else 'N/A: no match'
codes.append([character, desired_code])

return codes
```

4. In code line 5, enter the Chinese characters to be encoded, encased in quotation marks as shown in the red box. The example below reads “Zhengma Method” in Chinese.

```
In [5]: new_test_string1 = '郑码输入法'
```









5. Run code 6 to obtain the Zhengma codes that correlate to the Chinese characters.

```
In [6]: new_test_codes_output1 = characters_to_codes_simplistic(new_test_string1, df_zm_merged)
print(new_test_codes_output1)






[['郑', 'uagy'], ['码', 'gxvv'], ['输', 'heqk'], ['入', 'oda'], ['法', 'vbzs']]
```

- To convert from Zhengma codes to Chinese characters

1. Go to the “code” folder.

 bobtodd	Added all Zheng Ma code and data files current as of 2023/06/21	a0cdb20 3 weeks ago	🕒 4 commits
 code	Added all Zheng Ma code and data files current as of 2023/06/21		3 weeks ago
 data	Added all Zheng Ma code and data files current as of 2023/06/21		3 weeks ago
 drafts	Added all Zheng Ma code and data files current as of 2023/06/21		3 weeks ago
 img	Added all Zheng Ma code and data files current as of 2023/06/21		3 weeks ago
 raw	Added all Zheng Ma code and data files current as of 2023/06/21		3 weeks ago
 .gitignore	Added MacOS file .DS_Store to .gitignore		3 weeks ago
 README.md	Update README.md		3 weeks ago

2. Open the “4_converter.ipynb” file.

Name	Last commit message	Last commit date
..		
 1_background.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
 2_data.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
 3_tests.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
 4_converter.ipynb	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago
 zm_helpers.py	Added all Zheng Ma code and data files current as of 2023/06/21	3 weeks ago

3. Load and run the codes 1-3 and 8 shown below.

```
In [1]: # If running in Google Colab
#from google.colab import drive
#drive.mount('/content/gdrive')
#
#path_prefix = "/content/gdrive/My Drive/Colab Notebooks/zhengma/raw/"
#data_prefix = '/content/gdrive/My Drive/Colab Notebooks/zhengma/data/'
```

```
In [2]: # If running on local system
path_prefix = "../raw/"
data_prefix = '../data/'
```

```
In [3]: import pickle

# Load pickle
with open(data_prefix + 'df_zm_merged.pkl', 'rb') as pickle_file:
    df_zm_merged = pickle.load(pickle_file)
```

```
In [8]: def codes_to_characters_simplistic(code_list, zm_dataframe, db_column='RIME Characters', zm_column='ZM Codes'):
# Input:
# List of ZM codes
# database of Zheng Ma codes as a pandas DataFrame
# name of column to check for characters
# name of column containing Zheng Ma codes
# Output:
# string of CJK characters
# - In case of multiple character correspondences for a code, choose...

cjk_string = ''

for code in code_list:
# Make sure the code is a valid ZM code:
# - fewer than 5 letters
# - no spaces
if ' ' not in code:
if len(code) < 5:
# Get the characters for that code
possible_characters = zm_dataframe[z_m_dataframe[z_m_column] == code][db_column].tolist()
# Remove any empty strings
viable_characters = [x for x in possible_characters if (len(x) > 0)]
# Add the smallest string (hopefully 1 character)
# ... watch out: there might be more than one minimum...
# ... what does min() do? return the first it finds in the list?
cjk_string += min(viable_characters, key=len)
else:
print('Code too long: {}'.format(code))
else:
print('Code should not contain spaces: {}'.format(code))

return cjk_string
```

4. In code line 10, enter the Zhengma codes to be decoded back to Chinese characters as shown in the red box below. Each Zhengma code should be encased in quotation marks as well as separated from the other Zhengma codes by commas. Then, all Zhengma codes should be encased in a pair of brackets. Running this code will return the Chinese characters correlating to the Zhengma codes.

```
In [10]: new_test_string_output1 = codes_to_characters_simplistic(['uagy', 'gxvv', 'heqk', 'oda', 'vbzs'], df_zm_merged)
print(new_test_string_output1)
```

郑码输入法