Section 1: General information

Materials sources:

All reagents for chemistry steps were obtained from Sigma or Acros. SuperFi DNA polymerase (Invitrogen), 2′-deoxyribonucleoside triphosphates (dNTP, set of dATP, dTTP, dGTP, dCTP, New England Biolabs), and T4 DNA ligase (New England Biolabs), were used as provided. Oligonucleotides (Integrated DNA Technologies) were obtained as desalted lyophilate and used without additional purification. FMOC-Cys(STmp)-OH, Sulfo-Cy5-azide were obtained from Sigma. Sulfo-Cy5-DBCO and monoBromobimane (mBBr) were obtained from Lumiprobe and Thermofisher, respectively. Filter plates (MultiScreen Solvinert 0.45 µm Hydrophobic PTFE) and BIS-Tris propane were purchased from EMD Millipore. 40% Acrylamide/Bis (19:1) was purchased from Bio-Rad.

Note: mBBr should be stored at -80°C in DMF. DMF or DMSO solutions of this dye lose efficiency over time. It is recommended to do titrations to find the optimal dye concentration for staining, if it was stored for an extended period.

Buffers

• BIS-Tris propane ligation buffer (BTPLB): 50 mM NaCl, 10 mM $MgCl_2$, 1 mM ATP, 0.02% Tween 20, 10 mM bis-tris, pH 7.6

• BIS-Tris propane wash buffer (BTPWB): 50 mM NaCl, 0.04% Tween 20, 10 mM bis-tris, pH 7.6

• BIS-Tris propane breaking buffer (BTPBB): 100 mM NaCl, 10 mM ethylenediaminetetraacetic acid, 1% SDS, 1% Tween 20, 10 mM bis-tris, pH 7.6

• Click reaction buffer (CRB): 50% DMSO, DI water, 1M triethylammonium acetate, 0.04% Tween 20, pH 7.4. Note: Mix DMSO and DI water (smells fishy) and then adjust pH (7.4) by addition of 1M TEAA buffer.

• 2X-PBS: 0.4 g/L KCl, 0.48 g/L KH_2PO_4, 16 g/L NaCl, 2.88 g/L Na_2HPO_4 (anhydrous), pH 7.4.

• 2X-PBST: 2X-PBS, 0.2% Tween-20.

• Annealing buffer: 1 mM BTP, pH 7.6, 50 mM NaCl

Note: CRB was made fresh prior to each N3-hDNA click reaction

Oligonucleotide sequences

Name	**Sequence (5' - 3')**
ABM062	/5AmMC6/GTGGCACAACAACTGGCGGGCAAAC
ABM063	GCCGCCCAGTCCTGCTCGCTTCGCTAC
ABM96	CGCCAGGGTTTTCCCAGTCACGACCAACCACCCAAACCACAAACCCAAACCC CAAACCCAACACACAACAACAGCCGCCCAGTCCTGCTCGCTTCGCTAC
ABM99	GTGGCACAACAACTG
ABM100	CCTCTCTATGGGCAGTCGGTGATGTGGCACAACAACTGGCGGGCAAAC
CES1	GTTTTCCCAGTCACGAC
U6-Rev	GACTATCATATGCTTACCGT

Frag_Fwd-1107[+]	/5Phos/GCCGCCCAGTCCTGCTCGCTTCGCTACATGGCAGAAGGA
Frag_Fwd-1107[-]	/5Phos/TGATCCTTCTGCCATGTAGCGAAGCGAGCAGGACTGGGCGGCGG
Frag_2209/1306/2406/1506[+]	/5Phos/TCATTCTTCATGTTATAGAGCCCTACATTTCAATTCATAGAGCC
Frag_2209/1306/2406/1506[-]	/5Phos/GCGGGCTCTATGAATTGAAATGTAGGGCTCTATAACATGAAGAA
Frag_2604/1707/2802[+]	/5Phos/CGCAACCCTACGTACAGAAGGATGGAACCTCAATCTAAGAGGCA
Frag_2604/1707/2802[-]	/5Phos/CTTTGCCTCTTAGATTGAGGTTCCATCCTTCTGTACGTAGGGTT
Frag_1901/2A01/Rev[+]	/5Phos/AAGCCTCCTAAGCCTGTTTGCCCGCCAGTTGTTGTGCCAC
Frag_1901/2A01/Rev[-]	/5Phos/GTGGCACAACAACTGGCGGGCAAACAGGCTTAGGAGG
ABM99_2A07-Rev	GTGGCACAACAACTGGCGGGCAAACAGGCCCGGAGGGCTT
P5_Univ_Fwd-2	AATGATACGGCGACCACCGAGATCTACACTCTTTCCCTACACGACGCTCTTCCGATCTNNNNNNNNNGCCGCCCAGTCCTGCTCGCTTCGCTAC
Illumina Index 1	CAAGCAGAAGACGGCATACGAGATCGTGATGTGACTGGAGTTCAGACGTGTGCTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC
Illumina Index 2	CAAGCAGAAGACGGCATACGAGATACATCGGTGACTGGAGTTCAGACGTGTGCTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC
Illumina Index 3	CAAGCAGAAGACGGCATACGAGATGCCTAAGTGACTGGAGTTCAGACGTGTGCTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC
Illumina Index 4	CAAGCAGAAGACGGCATACGAGATTGGTCAGTGACTGGAGTTCAGACGTGTGCTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC

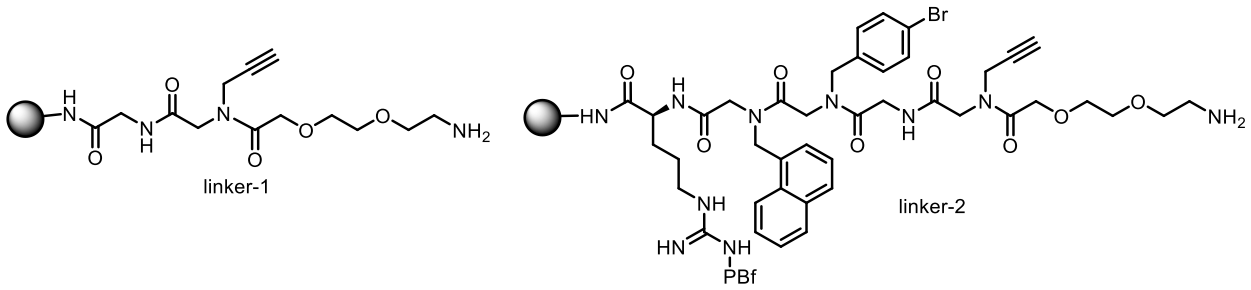
Section 2: Methods

2A: General solid phase synthesis protocol

Compounds were synthesized on TentaGel resin using general SPS protocol described below.

Linker-1, used for FACS studies and DEL synthesis, was synthesized on 10 µm TentaGel M NH_2 resin (Rapp-Polymere ,0.23 mmol/g). Linker-2, for mass analysis, was synthesized on 160 µm TentaGel MB RAM resin (0.41 mmol/g). TentaGel rink amide resin (160 µm, 0.41 mmol/g, 0.2 mmol, 50 mg, Rapp-Polymere) was transferred to a fritted spin-column (Mobicol Classic, large filter, 10 µm pore size) and swelled in DMF (1 h, RT). FMOC was removed with 20% piperidine in DMF (3x resin volume after swelling, 500 µL) at RT for 10 minutes, twice. It was then washed thoroughly with DMF, DCM and DMF, and successively coupled with either amino acids or peptoid units. In general, acids (5 times of resin capacity, 1.0 mmol) were pre-activated at RT for 5 minutes with DIC/Oxyma/Collidine (1.4/1.0/1.0 mmol) in DMF, added to the resin, incubated at 37°C for one hour, and washed with DMF, DCM (5 times each, 5x resin volume). FMOC was removed where applicable.

Figure S1: Linkers used in FACS and LCMS study



For peptoid units, bromoacetic acid (BAA) (1.0 M, DMF) and DIC (0.9 M) were added to the resin separately, vortexed, and incubated at 37°C for 1hr. Resin was washed thoroughly with DMF, DCM, and DMF and then sonicated in DMF for 2 minutes before further reactions. Amine (1.0 M, 1.5x resin volume, 500 µL DMF) was added successively and incubated at 37°C for 3 hrs., with agitation. ***Note***: Too concentrated BAA+DIC solution had incomplete addition. Longer reaction time (~1hr) with lower conc resulted better yield.

Linker-2 was synthesized upon addition of Fmoc-Arg(Pbf)-OH, BAA, 1-Naphthylmethyl amine, BAA, 4-bromobenzyl amine, Fmoc-Gly-OH, BAA, Propargyl amine, and Fmoc-EEAC, respectively, after swelling and FMOC removal.

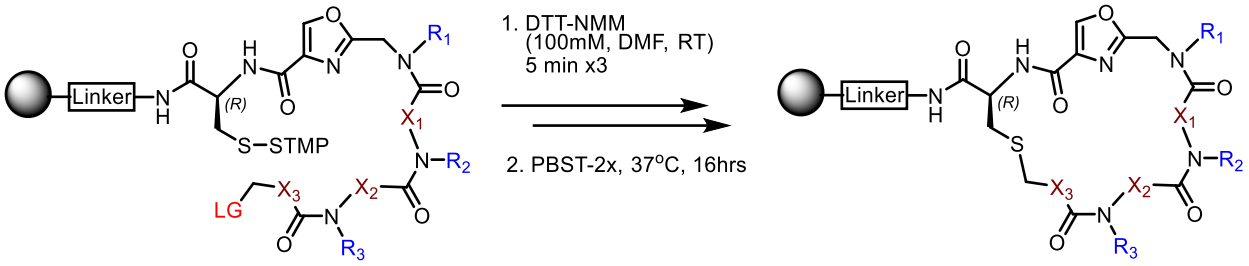
Linker-1 was synthesized upon addition of Fmoc-Gly-OH, BAA, Propargyl amine, and Fmoc-EEAC respectively.

2B: STMP group removal, cyclization and staining with mBBr.

After synthesis of linear precursor was complete, resin was washed 3 times each with MeOH, DCM and DMF. Mixture of DTT and N-methylmorpholine base (100 mM each in DMF) was added (500 µL for 50 mg, 10 µm beads, 150 µL for 0.5 mg of 10 µm beads in plate), incubated for 5 min at RT, washed with DMF & DCM and repeated for two more times. Beads were washed 3 times each with DMF, 50% DMF-PBS and PBS buffer. It was suspended in PBST (pH = 7.6) and incubated at 37°C for 8-16 hrs. for cyclization. For large scale preparation *N*-Methylmorpholine (100 mM in DMF) was used for cyclization.

After desired time of cyclization, mBBr (150.0 µL, 3.0 mM in DMF, 0.5 mg, 10 µm bead) was added in filter plate (MultiScreen Solvinert 0.45 µm Hydrophobic PTFE) and incubated at 37°C for one hour (9.0 mM, 2 hrs. when DNA tags are present). It was then washed with DMF, DCM, MeOH, suspended in PBST, and filtered into BD FACS tube for flow cytometry.

Figure S2: Standard protocol for OBOC thioether macrocyclization



2C: Copper based click (CuAAC) reaction to attach Cy5-azide dye and headpiece-DNA.

Cy5-azide dye was clicked to the alkyne in the linker region via CuAAC reaction before thiol deprotection, according to the Table **T2**. A similar procedure was followed for the azido-headpiece DNA (N3-hDNA).

In general, resin was suspended in freshly prepared CRB buffer (pH = 7.4) for one hour before the click reaction. $CuSO_4$-$5H_2O$ (500 mM in water) and Tris[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]amine (TBTA, 50 mM in DMSO) were mixed in a 1:1 molar ratio, in CRB buffer, to obtain a blue colored solution. To this was added 50% of the required Na-ascorbate. The solution was then incubated for 5 min at 37°C to prepare the click-mix. A second solution containing the azide-click partner and the remaining Na-ascrobate was then added to the click-mix, vortexed, added to the resin, and incubated at 37°C for 2-4 hrs. After the reaction was complete, the resin was washed with organic solvent (DMF, DCM, MeOH), then extensively with aqueous buffer (BTP-WB & BTP-BB) and was suspended in BTP-BB (breaking buffer) overnight to remove copper salt before further reactions. BTP-BB solution turns blueish after overnight suspension.

For dye addition, DMSO solution of Cy5-N_3 was added (final conc 0.11mM) to the click-mix and incubated for 2 hrs. at 37°C.

Headpiece DNA was added to batches of 30.0 mg Linker-1 beads in 2.0 ml Bio-Rad spin column fitted with a 10 µm filter. The click-mix was prepared according to Table **T1**, then incubated at 37°C for 5 min before being added to the resin. A solution of N_3-HDNA (3.0 mM, H_2O, 0.008 equiv. of resin capacity) was then added to the click-mix, vortexed, and incubated for 4 hrs. at 37°C.

Figure S3: General protocol to attach Cy5-azide dye and Azido headpiece DNA to the linker-alkyne

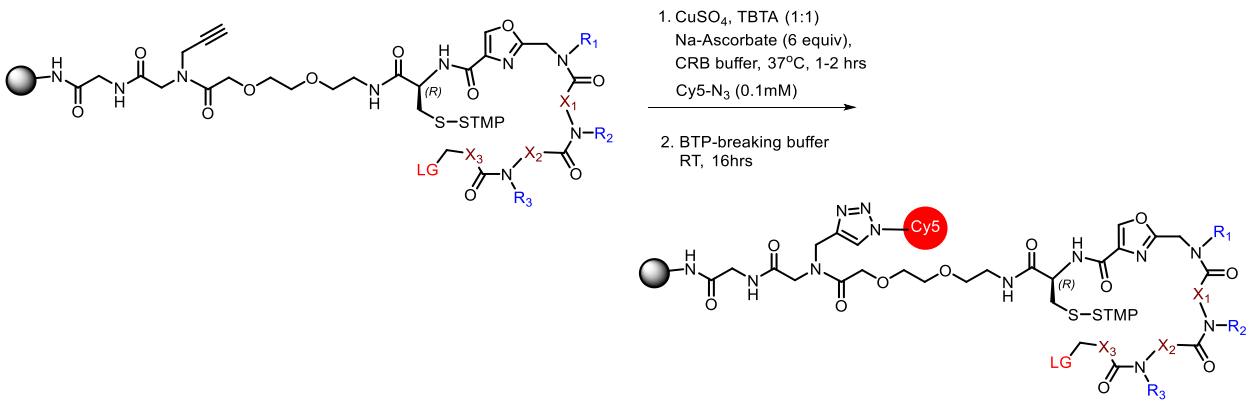


Table T1: General protocol for coupling Azido-HDNA with linker-1 beads via CuAAC reaction.

Azido-HDNA addition						
Reagents	Stock (mM)	equiv	mmols		amount	unit
Beads (10 uM) ~ loading 0.23			0.0069		30.00	mg
CuSO4 (H2O)	500	1.000	0.0069		13.80	ul
TBTA (DMSO)	50	1.000	0.0069		138.00	ul
Azido-peg-HDNA in TEAA buffer	3.1	0.008	0.0000552		17.81	ul
Na-Ascorbate (H2O)	500	6.000	0.0414		82.80	ul
CRB buffer					1747.59	ul
Total rxn vol					2000.00	ul

Table T2: General protocol for coupling Cy5-azide dye with linker beads via CuAAC reaction.

Cy5-N3 dye addition						
Reagents	Stock (mM)	equiv	mmols	Cy5(mM)	amount	unit
Beads (10 uM) ~ loading 0.23			0.000115		0.50	mg
CuSO4 (H2O)	500	1.000	0.000115		0.23	ul
TBTA (DMSO)	50	1.000	0.000115		2.30	ul
Cy5-N3 (DMSO)	12			0.11	1.38	ul
Na-Ascorbate (H2O)	500	6.000	0.00069		1.38	ul
CRB buffer					144.72	ul
Total rxn vol					150.00	ul

2D: General two-color staining protocol without a DNA tag

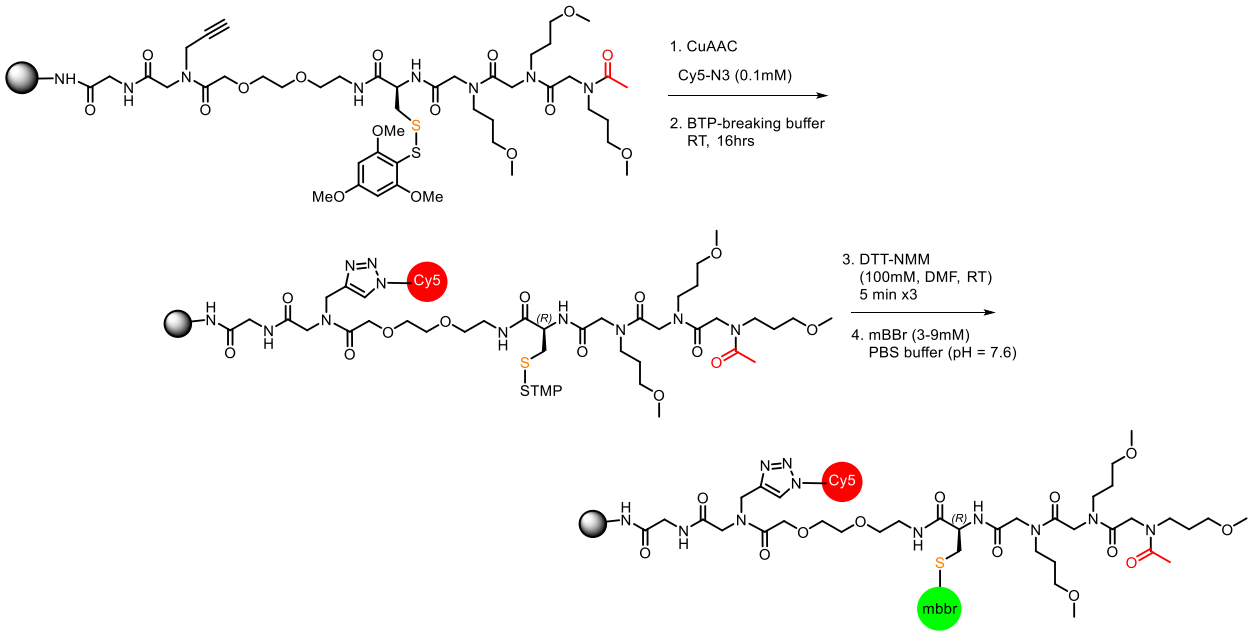
Cy5-azide dye was attached to the alkyne part of linear precursor via CuAAC reaction before thiol-protecting group was removed (Section **2C)**. Click-mix was prepared for total amount of resin according to Table **T2**, incubated at 37°C for 5 min, added to the resin (for filter plates, 150 µL, 0.5 mg/well) and incubated at 37°C for 2 hrs. Thiol-protecting STMP group was removed (Section **2B)** using 100 mM DTT-NMM, washed, and solvent exchanged to PBST buffer for cyclization. Resin was washed with 2X-PBS and re-suspended in

2X-PBS buffer and DMF solution of mBBr (final conc. 3.0 mM, 150.0 µL for 0.5mg, 10 µm beads) was added. It was incubated at 37°C for one hour before washing with DMF, DCM and DMF.

This general protocol was applied for staining control molecules and 64 scaffolds in the absence of DNA tags. For DNA-tagged control compound **2** & **3**, Cy5-azide dye (0.11 mM final conc. added 2 hrs. after N_3-HDNA addition) was clicked together with Azido-HDNA (0.002 equiv.), prior to thiol deprotection, at 37°C for 4 hrs. After thiol deprotection, the resin was transitioned to PBST, then a DMF solution of mBBr (final conc. 9.0 mM, PBST) was added and incubated for 2 hrs. at 37°C. It was then washed with MeOH, DCM and DMF.

For staining in the presence of DNA tags, please see Section **6**.

Figure S4: Two-color staining protocol without encoding DNA tags.



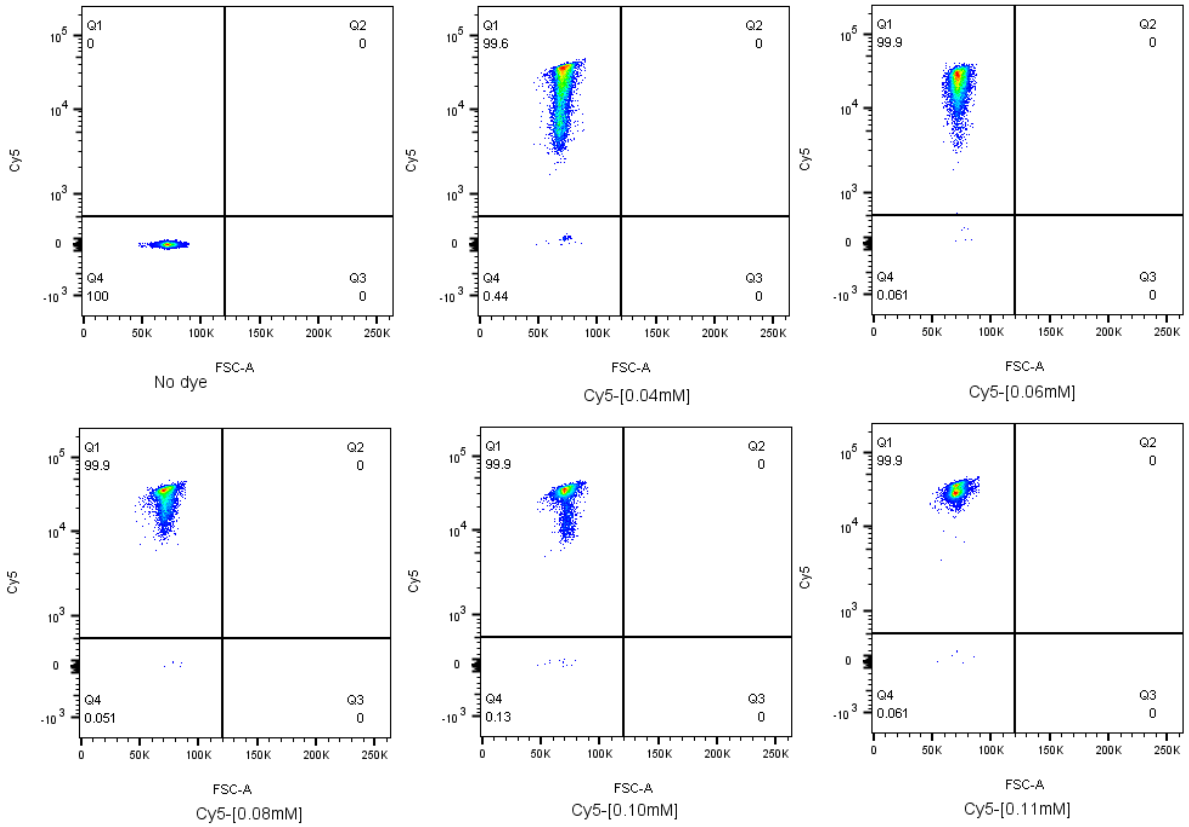
2E: DNA Ligations

DNA fragments are ordered as pairs of single-stranded DNA oligonucleotides, which are then annealed to form double-stranded fragments. The individual oligos are re-suspended at 1600 µM, mixed at equimolar ratios to 800 µM, then diluted to 80 µM in annealing buffer before being denatured and annealed (95°C, 2 min., -0.1°C/s to 25°C). The annealed oligos are mostly complementary but do have small 5' or 3' overhangs to permit directional ligation. The DNA fragments with complementary overhangs are then ligated to build the DNA barcode. Final ligation reactions included: 1X BTPLB, each dsDNA encoding fragment at an equimolar ratio to bead-bound HDNA, 2 µl T4 DNA ligase per mg of beads. Incubated at RT, with gentle agitation, 4 hours.

Section 3: Two-color staining and fluorescence measurements of control compounds

3A. Titration of Cy5-azide dye: Control compound **3** (0.5 mg, 0.11 µmols, 10 µm TentaGel M NH_2 resin) was transferred to separate wells in a filter plate (MultiScreen Solvinert 0.45 µm Hydrophobic PTFE) and suspended in CRB for one hour. Following general protocol described in section **2C,** click-mix solution was prepared in CRB according to Table **T2** and was added to each well (~150 µL). DMSO solution of Cy5-azide dye was added for final concentrations of (0.04 – 0.11 mM) and incubated for 2 hrs. at 37°C. Beads were washed, suspended in PBST, and filtered into BD FACS tube (~20,000 beads). Fluorescence intensity of these beads was measured (Red channel) to ensure it is under the linear range of flow cytometer. It appeared that the final Cy5 dye concentration of 0.11 mM is optimal and will be used in later studies.

Figure S5: Cy5-dye titration with compound 3.



3B. Optimization of mBBr concentration

Resin displaying control compound **2** (0.5 mg, 0.11 µmols, 10 µm TentaGel M NH_2 resin) was transferred to separate wells in a filter plate. The thiol-protecting STmp group was removed (Section **2B**) and the resin was washed and transitioned to PBST (pH = 7.6). A solution of mBBr (23.0 mM, in DMF) dye was added

to each well for final concentrations of 1.0 – 7.0 mM. The plate was then incubated at 37°C for one hour. It was washed with DMF, DCM, MeOH, and DMF-PBST (50%) buffer, re-suspended in PBST and filtered into BD FACS tubes (~20,000 beads) for FACS analysis (BV510).

Figure S6: Monobromobimane (mBBr) dye titration with compound 2.

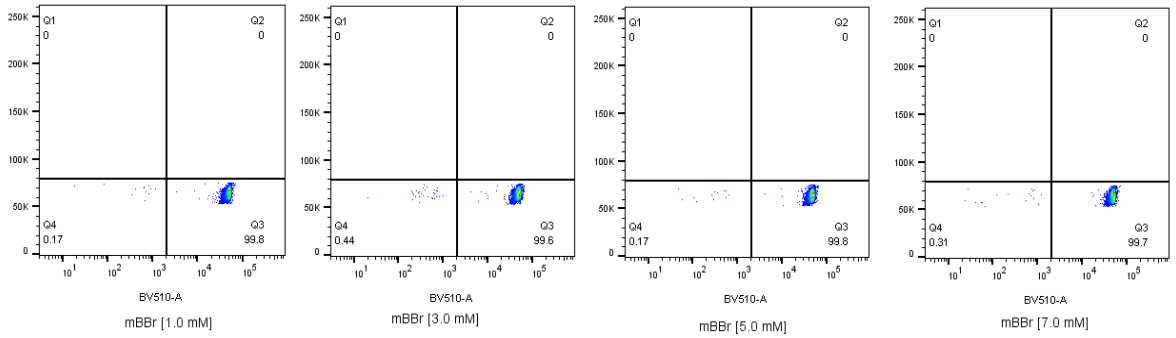
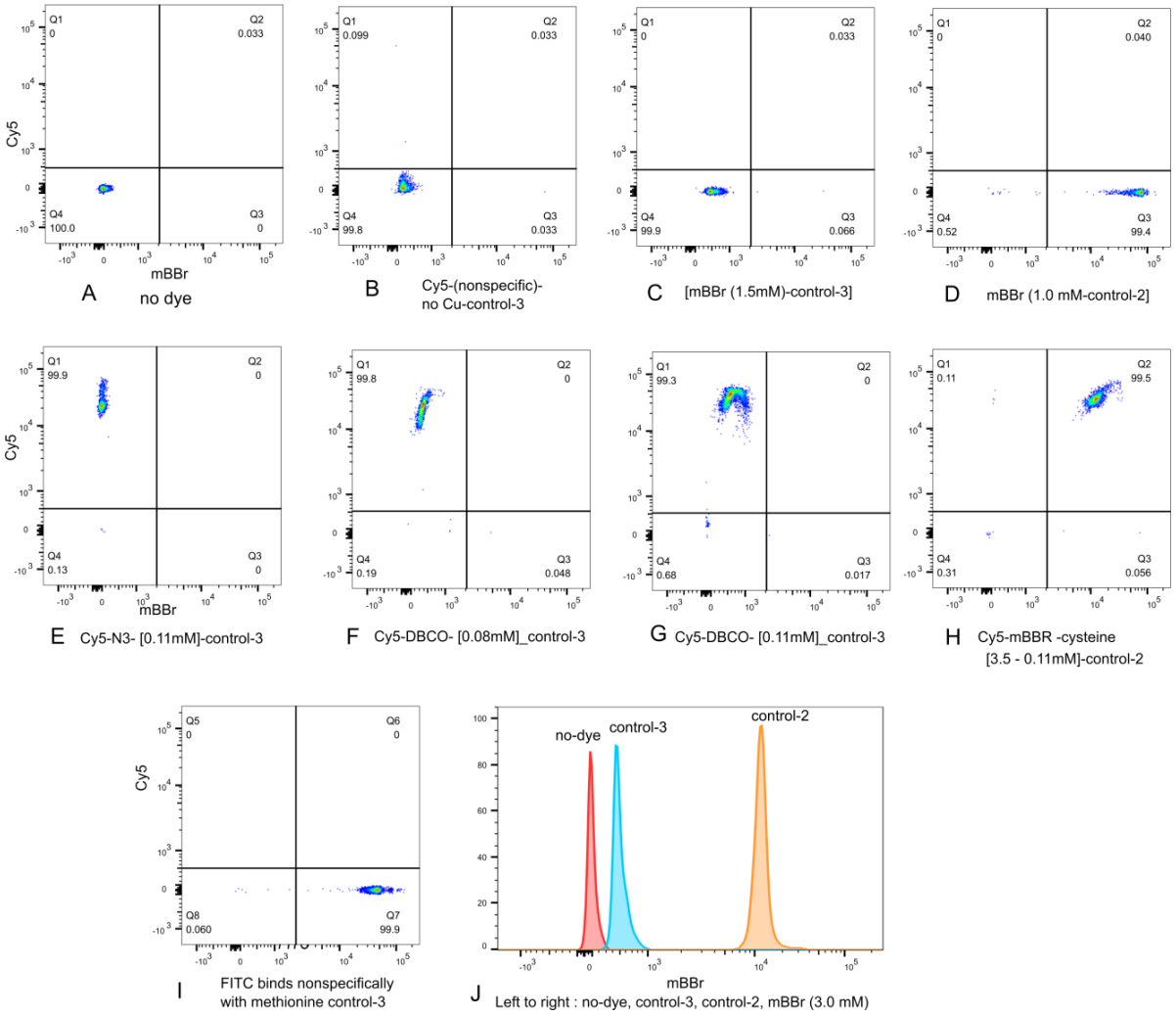


Figure S7: Summary for staining compound 2 & 3 with Cy5, mBBr and FITC dyes



After staining with mBBr, control compound **2,** which represents a linear model, fluoresces brightly in the green channel while compound **3** (cyclic model) shows almost no fluorescence (Figure **S7**, Panel C vs D) indicating high specificity of mBBr with free thiols but not with thioethers. In contrast, compound **2** & **3** both fluoresce brightly after staining with Fluorescein-5-Maleimide (FITC, panel I) which indicates FITC binds to the beads nonspecifically and therefore cannot be used in this assay. The sulfo-CY5 dyes tested did not show non-specific binding to the resin.

For two color staining, resin displaying compound **2** was first stained with Cy5 dye, followed by thiol deprotection and staining with mBBr. In the presence of Cy5, a higher amount of mBBr (3.5 mM, Panel H) was required to achieve similar fluorescence intensity without the Cy5 dye, although fluorescence compensation was not required. Under identical staining conditions as with mBBr, compound **2** fluoresces 100-fold more than compound **3** (Panel J).

Note: It was observed that, for fresh mBBr, a lower concentration (1.0- 3.0 mM) is optimal. However, over time mBBr loses efficiency and titration should be repeated to find the optimal dye concentration.

Section 4: Cyclization progress of DDA scaffold via LCMS/FACS

Scaffold **DDA** was synthesized on both 10 (linker-1) & 160 (linker-2) µm beads separately in spin columns (10 µm filter) after adding FMOC-Cys-(STmp)-OH, 2-(Chloromethyl)oxazole-4-carboxylic acid (3x) and 3-(Chloromethyl)-benzoic acid respectively following the general SPS protocol (Section **2A**). 3-methoxypropyl amine was used in all **X1-3** position (Figure S8A & B). After the linear precursor was synthesized, it was transferred to two separate filter plates (0.5 mg /well) and thiol protection was removed. Beads were washed with DMF, DCM, DMF-PBS (50%), and finally suspended in PBST.

Figure S8A: FACS analysis with 10 µm beads

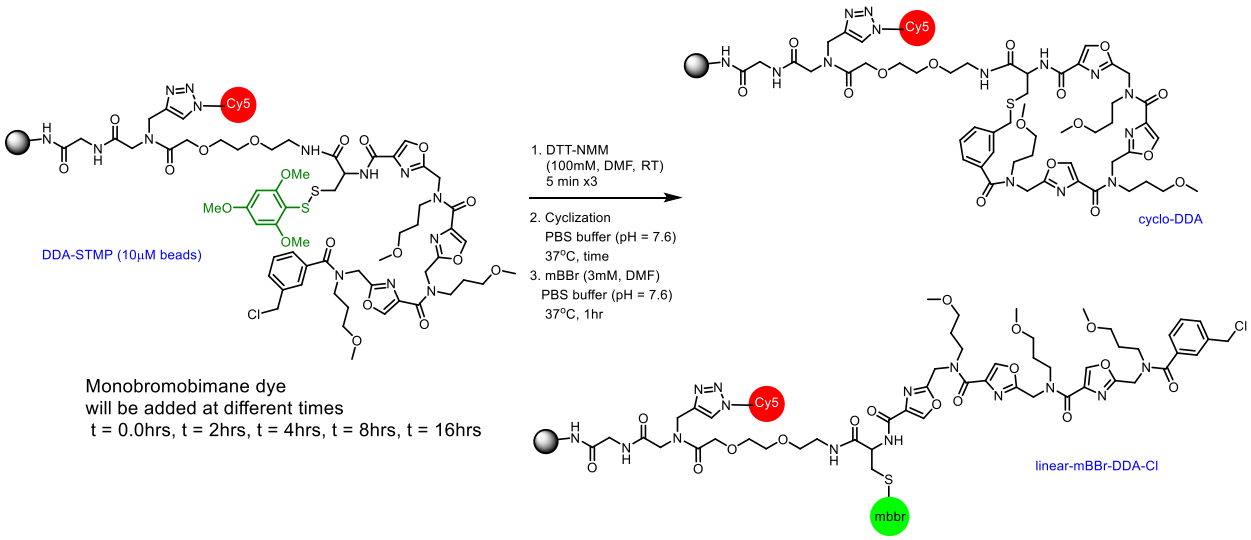
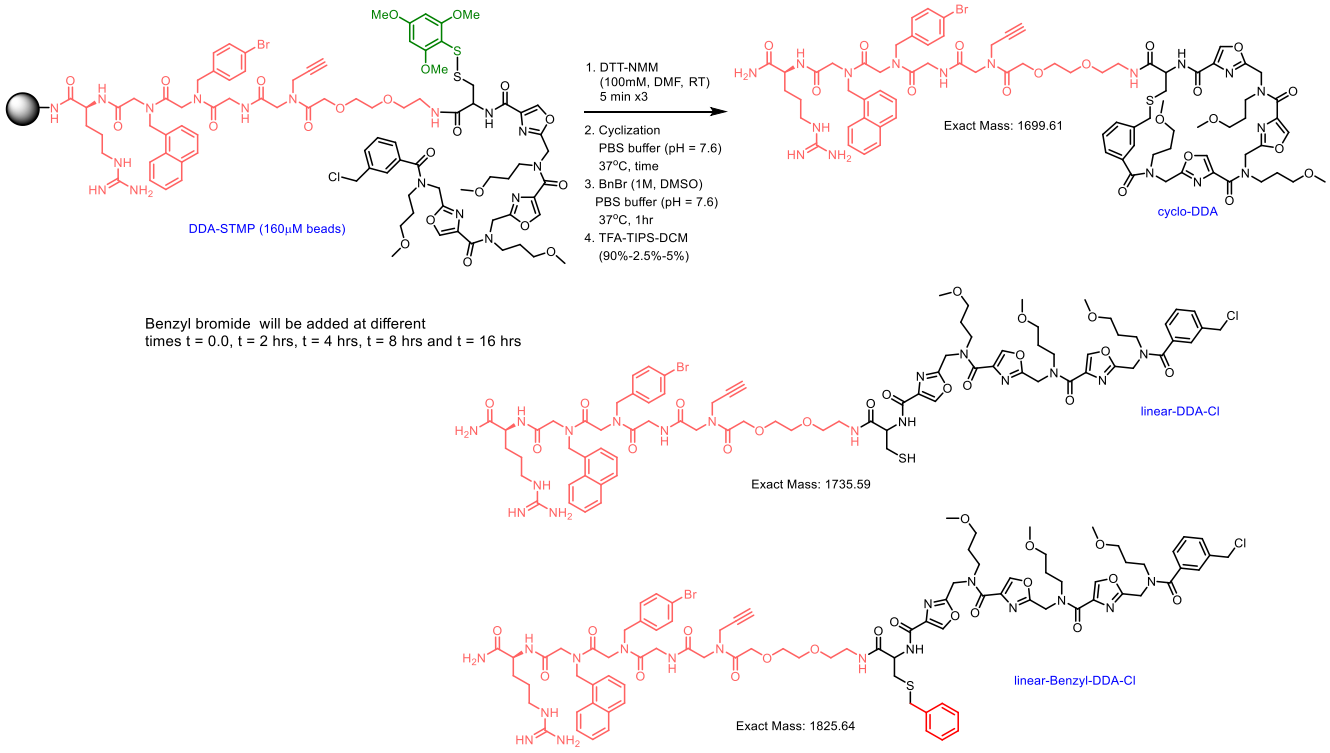
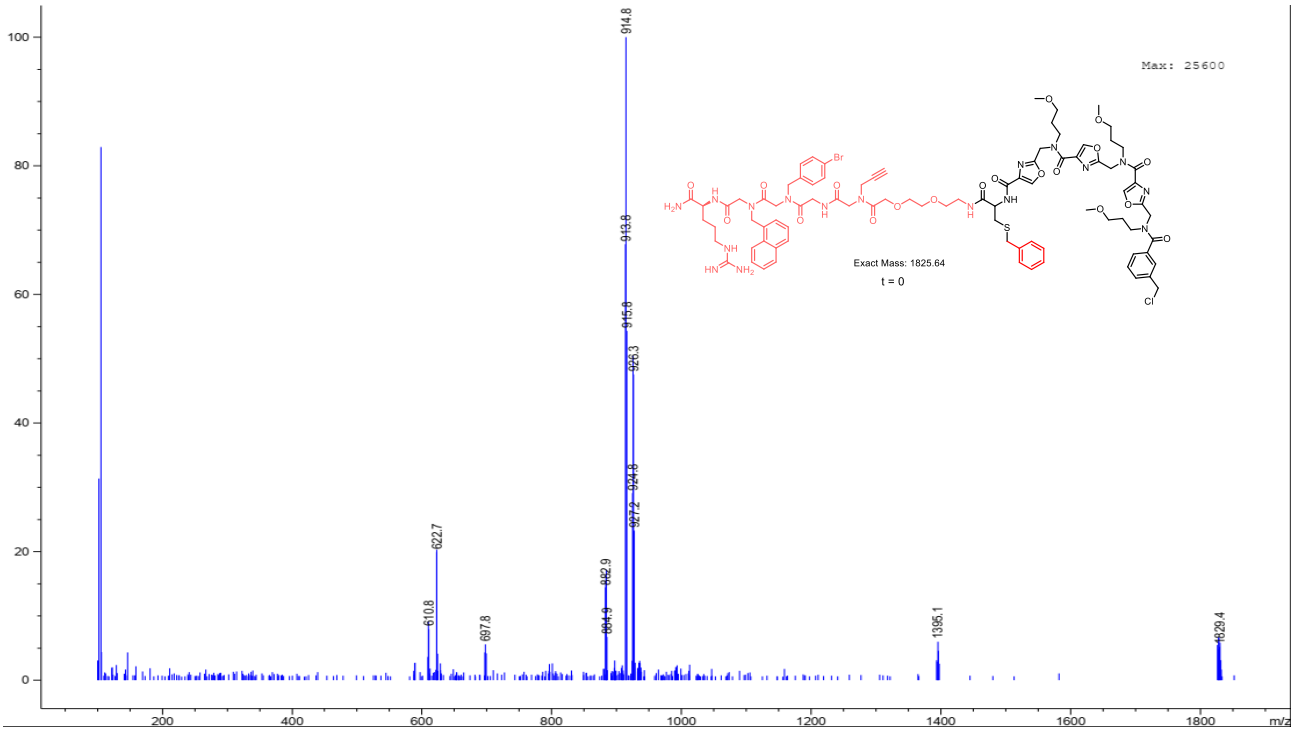


Figure S8B: LCMS analysis with 160 µm beads

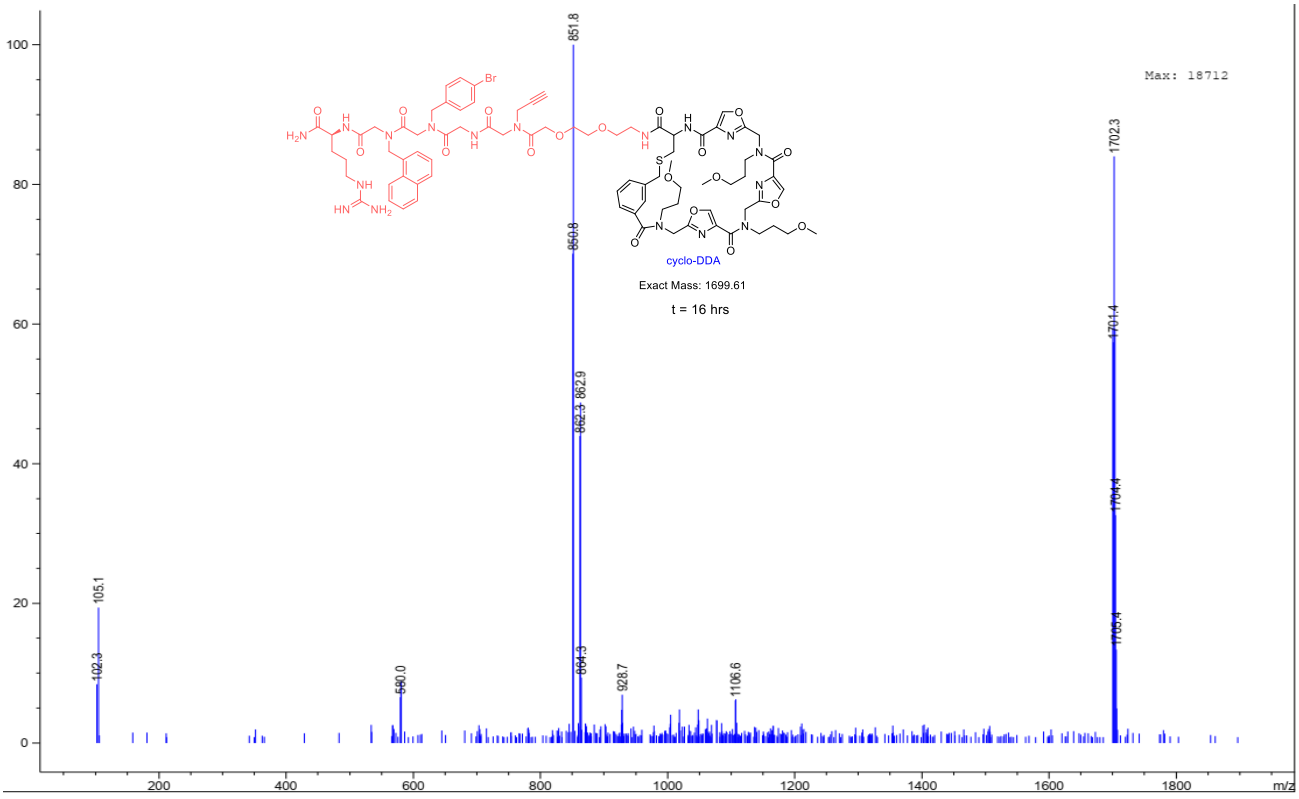


The ring closure process was monitored from point t= 0, onwards. After thiol exposure, mBBr (3.0 mM, 150 µL for 0.5mg /0.1 µmol of 10 µm TentaGel resin) and benzyl bromide (1.0 M, 150 µL for 0.5mg /0.2 µmol of 160 µm TentaGel resin) were added separately at t = 0, 2, 4, 6, 8 &16 hrs. and incubated at 37°C for one hour. After 16 hrs., the 160 µm beads were TFA-cleaved (90% TFA, 2.5% TIPS, 2.5% thioanisole and 5% DCM, 2hrs, RT) and analyzed by LCMS, while 10 µm beads were passed through a 35µm cells strainer and analyzed by FACS to measure fluorescence. As expected, at t = 0 hrs., mostly benzylated linear material (Figure **S8B**, Mw 1825) was obtained, while at t = 16 hrs., cyclo-**DDA** was obtained in major quantity. As cyclization progresses over time, absorbance for linear material (RT = 9.5 min) tend to diminish as expected.

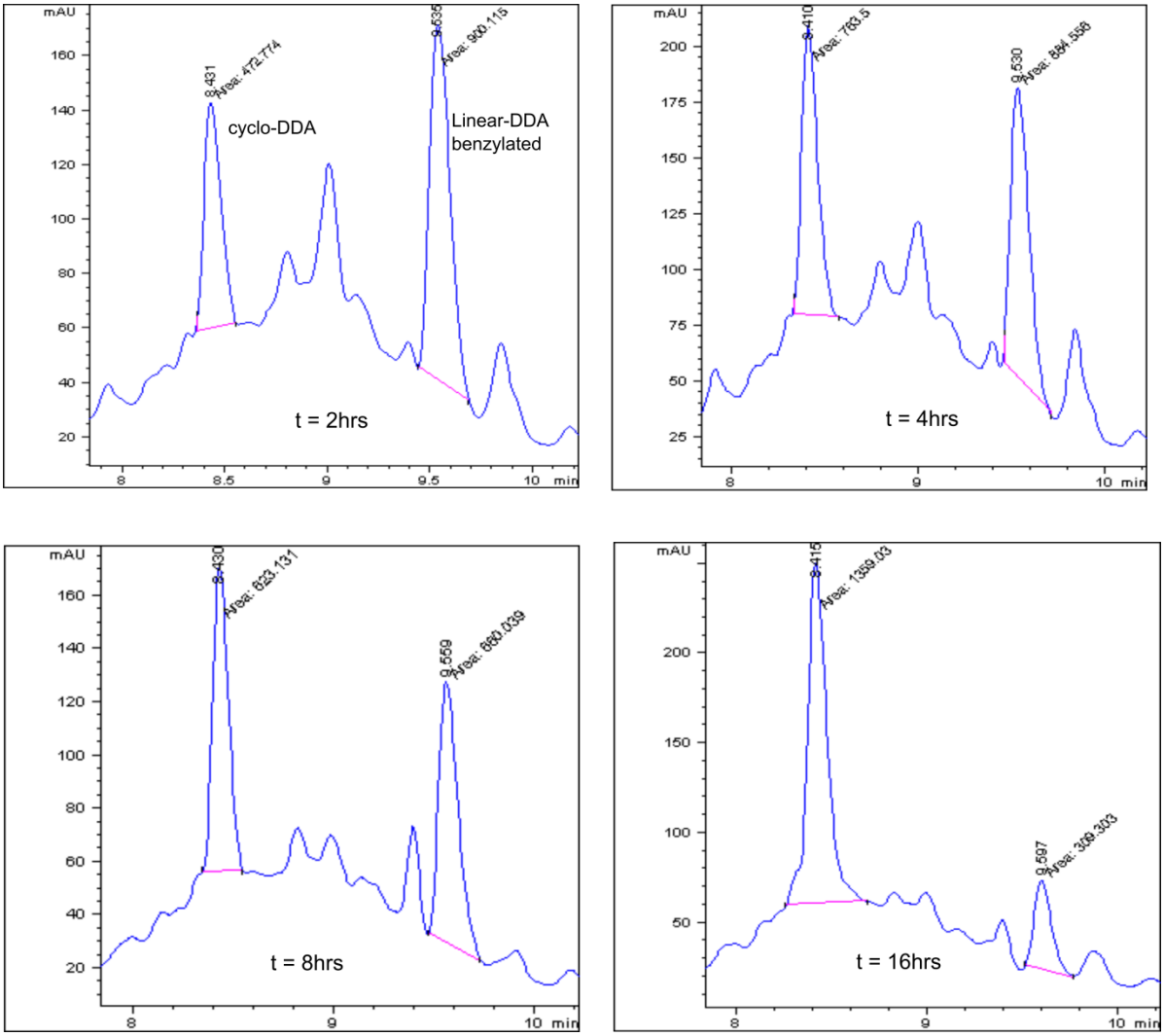
At t = 0, major ion corresponds to benzylated linear material.



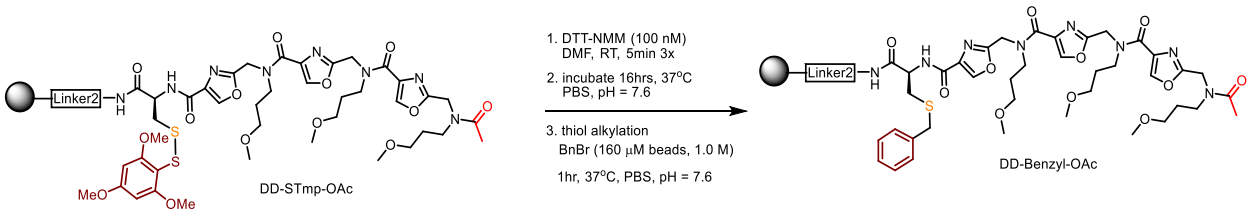
At t = 16 hrs., cyclo-DDA was obtained in major quantity.



Cyclization progress of DDA from t = 2 – 16 hrs.

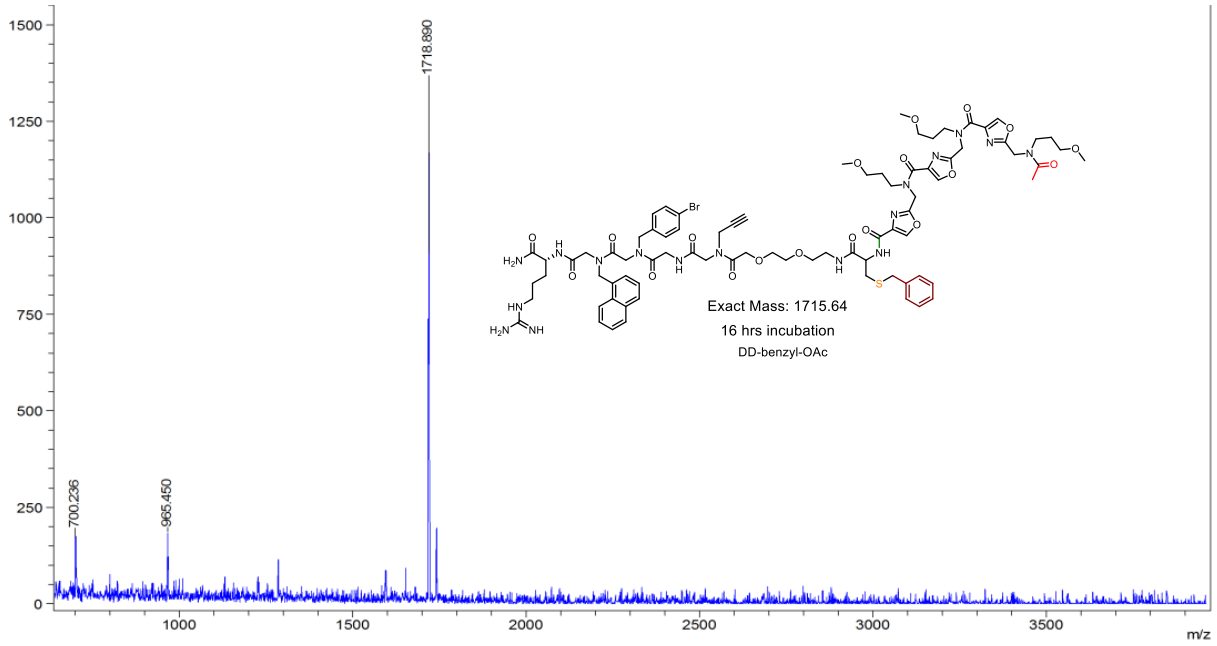


4C: Investigate stability of the sulfhydryl group after 16hrs. of incubation

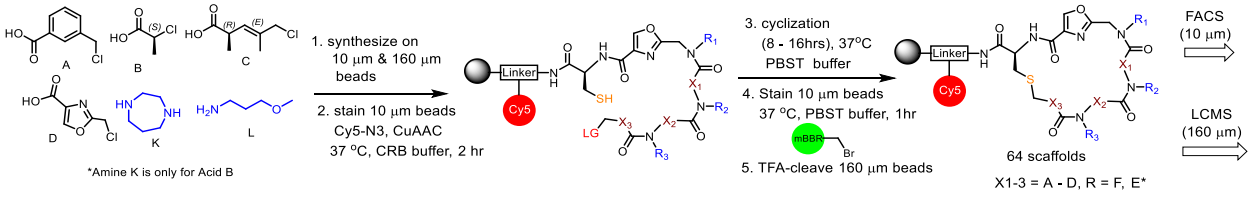


Due to concerns about general thiol oxidation occurring during 16 hours of cyclization, which would prevent mBBr addition and falsely indicate cyclization, an experiment was designed to test the stability of the sulfhydryl group. An acetylated version of the scaffold DD-STmp was synthesized on 160 µm beads (linker

2) after adding FMOC-Cys-(STmp)-OH. 2-(Chloromethyl)oxazole-4-carboxylic acid (3x) was the backbone unit, while 3-methoxypropyl amine was used in the amine positions. After the final amine addition, the compound was acetylated to prevent cyclization. The beads were then transferred to a filter plate (0.5mg/well), thiol protection was removed, and the resin was incubated at 37°C in PBST for 16 hrs. After 3 washes with PBST, the resin was treated with DMSO solution of benzyl bromide (final conc 1.0M, PBST) at 37°C for one hour, cleaved with TFA, and analyzed by MALDI. The data indicate that the sulfhydryl group remains intact and is able to react with the benzyl bromide, as observed below.



Section 5: Cyclization efficiency of 64 PICCO scaffolds



Synthesis & characterization of 64 scaffolds: 64 PICCO scaffolds (3.5-mer) were synthesized, in parallel, on 10 (linker-1) & 160 (linker-2) µm TentaGel resins in separate filter plates (MultiScreen Solvinert 0.45 µm Hydrophobic PTFE). Linkers 1 & 2 were functionalized with FMOC-Cys-(STmp)-OH, then acid D, and distributed into the filter plate (0.5 mg / well). Scaffold synthesis was completed by iterative couplings of the various acids (A-D, preactivated for 5 minutes with oxyma/DEC/collidine, 1 hr., 37°C) and 3-methoxypropyl amine (1.0 M, 3 hrs., 37°C). Cy5-azide was then clicked onto the 10 µm resin only, followed by copper salt removal with BTP-BB, overnight. Thiol protection was then removed on both 10 µm and 160

µm resins with 100 mM DTT and 100 mM NMM, in DMF solution (3 x 5 min) at RT. The beads were then washed with DMF, DCM, and DMF-PBS, then suspended in PBST (pH = 7.6) buffer and incubated for 8 hrs. at 37°C, for cyclization. With synthesis complete, the 10 µm beads were then washed with and transitioned to PBST, labeled with mBBr (3.0 mM, 37°C, 1 hr), washed with DMF, DCM, and DMF-PBS buffer, then resuspended in PBST and filtered (35 µm) into 64 FACS tubes for FACS analysis. The 160 µm beads, meanwhile, were washed, suspended in DMF for one hour, and cleaved (90% TFA, 2.5% TIPS, 2.5% thioanisole and 5% DCM) for mass analysis.

Table T4: Ring closure summary (FACS & LCMS) of 64 Scaffolds

	1	2	3	4	7	8	9	10
K	AAA	ABA	ACA	ADA	AAB	ABB	ACB	ADB
L	BAA	BBA	BCA	BDA	BAB	BBB	BCB	BDB
M	CAA	CBA	CCA	CDA	CAB	CBB	CCB	CDB
N	DAA	DBA	DCA	DDA	DAB	DBB	DCB	DDB
O	AAD	ABD	ACD	ADD	AAC	ABC	ACC	ADC
P	BAD	BBD	BCD	BDD	BAC	BBC	BCC	BDC
Q	CAD	CBD	CCD	CDD	CAC	CBC	CCC	CDC
R	DAD	DBD	DCD	DDD	DAC	DBC	DCC	DDC

Note1: “3.5-mer” means the scaffold has four acids and three amines, but the first acid is always acid D. “2.5-mer means” scaffold has three acids and two amines.

Note2: Although 160 µm beads had 8 hrs. incubation time, cyclization may continue during and after TFA cleavage reaction. However, cyclization was frozen for the selected two-color population on 10 µm bead after mBBr addition, but continued during TFA cleavage. This indicates that few scaffolds have more conformational constraint than others and need more time to cyclize.

Note3: Some scaffolds cyclized as it is (3.5-mer to 3.5-mer) and some has incomplete acid addition residues, which in most cases also cyclized (2.5-mer).

5A: Ring closure analysis - summary of 64 scaffolds:

Each scaffold is analyzed by how much linear starting material (3.5-mer) is left after cyclization for 8 hrs. If a scaffold had 90% cyclization, it was considered complete. If it had 40% or more linear material left, it was considered incomplete. Due to incomplete synthesis reactions, some “2.5-mer” scaffolds were generated (ABA, ABB, BBA). Regardless, these compounds mostly cyclized as well. Ring closure is primarily reviewed for 3.5-mer compounds and examined that any 2.5-mer linear fragments contributed as false positive. In the LCMS analysis, combined area of all the cyclic compounds are compared against combined area of all the linear compounds.

Table T5: LCMS analysis of ring closure of 64 scaffolds

			cyclization status		linear SM		nature	
En-try	Posi-tion	Scaffold	FACS	mass-spec	left(%)	cyclic: linear	of scaffold	comment
1	K1	AAA	incomplete	complete	7.5	93.0:7.0		
2	K2	ABA	complete	complete				
3	K3	ACA	incomplete	complete				
4	K4	ADA	complete	complete	3.8	96.2:3.7		
5	K7	AAB	complete	incomplete	70.7	58.5: 41.4	difficult to cyclize	
6	K8	ABB	complete	incomplete	17.2	85.4: 14.7		
7	K9	ACB	incomplete	incomplete	28.8	69.6:20.1		
8	K10	ADB	incomplete	incomplete	20.9	82.6: 17.3		
9	L1	BAA	incomplete	complete				
10	L2	BBA	complete	complete				
11	L3	BCA	complete	complete				
12	L4	BDA	complete	complete				
13	L7	BAB	complete	complete	9.7	91.0: 8.9		
14	L8	BBB	complete	complete				
15	L9	BCB	complete	complete	4.7	95.5:4.5		Linear-2.5 mer
16	L10	BDB	complete	incomplete	30.8	76.4: 23.6		
17	M1	CAA	complete	complete				
18	M2	CBA	complete	complete				
19	M3	CCA	complete	complete				
20	M4	CDA	complete	complete				
21	M7	CAB	complete	incomplete	45	69.0: 31.0	difficult to cyclize	
22	M8	CBB	complete	incomplete	33.4	74.7: 25.2		linear- 3.0 mer
23	M9	CCB	incomplete	incomplete	66.7	60.0: 40.2	difficult to cyclize	
24	M10	CDB	complete	incomplete	27.2	78.5: 21.4		
25	N1	DAA	complete	complete				
26	N2	DBA	complete	complete				
27	N3	DCA	complete	complete				
28	N4	DDA	complete	complete				
29	N7	DAB	complete	incomplete	27.7	78.4: 21.6		
30	N8	DBB	complete	incomplete	34	74.6: 25.4		
31	N9	DCB	incomplete	incomplete	13.4	88.1: 11.8		
32	N10	DDB	complete	complete				
33	O1	AAD	incomplete	complete				

34	O2	ABD	complete	complete				
35	O3	ACD	incomplete	complete				
36	O4	ADD	complete	complete				
37	O7	AAC	complete	complete	2	98.1: 2.0		
38	O8	ABC	complete	complete				
39	O9	ACC	complete	complete				
40	O10	ADC	incomplete	complete	5	95.2: 4.8		
41	P1	BAD	complete	complete				
42	P2	BBD	complete	complete				
43	P3	BCD	complete	complete				
44	P4	BDD	complete	complete				
45	P7	BAC	complete	complete				
46	P8	BBC	complete	complete				
47	P9	BCC	complete	complete				
48	P10	BDC	incomplete	complete				
49	Q1	CAD	complete	complete				
50	Q2	CBD	complete	complete				
51	Q3	CCD	complete	complete				
52	Q4	CDD	complete	complete				
53	Q7	CAC	incomplete	complete				
54	Q8	CBC	complete	complete				
55	Q9	CCC	incomplete	complete				
56	Q10	CDC	incomplete	complete				
57	R1	DAD	complete	complete				
58	R2	DBD	complete	complete				
59	R3	DCD	complete	complete				
60	R4	DDD	complete	complete				
61	R7	DAC	complete	complete				
62	R8	DBC	complete	complete				
63	R9	DCC	complete	complete				
64	R10	DDC	complete	complete				

For fluorescence and LCMS data, please see section 9.

Section 6: Monitor on-resin cyclization progress in presence of DNA

To test for inhibition of macrocyclization by the encoding DNAs, cyclization progress was measured on resins that displayed full-length barcodes. Compounds **DDD**, **DDA**, **DDE** and **EBB** were synthesized on 10 & 160 µm beads (~5.0 mg). Headpiece DNA (0.008 equiv.) & 1,3-azidopropane (1.5 equiv., added two hours after azido-HDNA addition) were clicked together via a CuAAC reaction, and a full length, test-DNA tag was ligated onto the 10 µm beads. After linear precursor synthesis was complete, Cy5-DBCO was attached (final conc. 0.11mM, 150 µL CRB buffer, for 0.5 mg, 10 µm beads, ON, 37°C) via SPAAC reaction in a filter plate. The thiol-protecting STMP group was then removed and the compounds were cyclized for 16 hrs. at 37°C. The 10 µm beads were then treated with mBBr (final conc. 9.0 mM, 150 µL PBST, 2 hrs., 37°C) while the 160 µm beads were treated with benzyl bromide (1.0 M, 150 µL PBST, 2 hrs., 37°C) to freeze cyclization during or after TFA cleavage. DNA tags from the 10 µm beads were then PCR-amplified and Sanger sequenced. Ring closure status was then analyzed by FACS and MALDI.

Figure S10: Cyclization and staining in the presence of a DNA tag

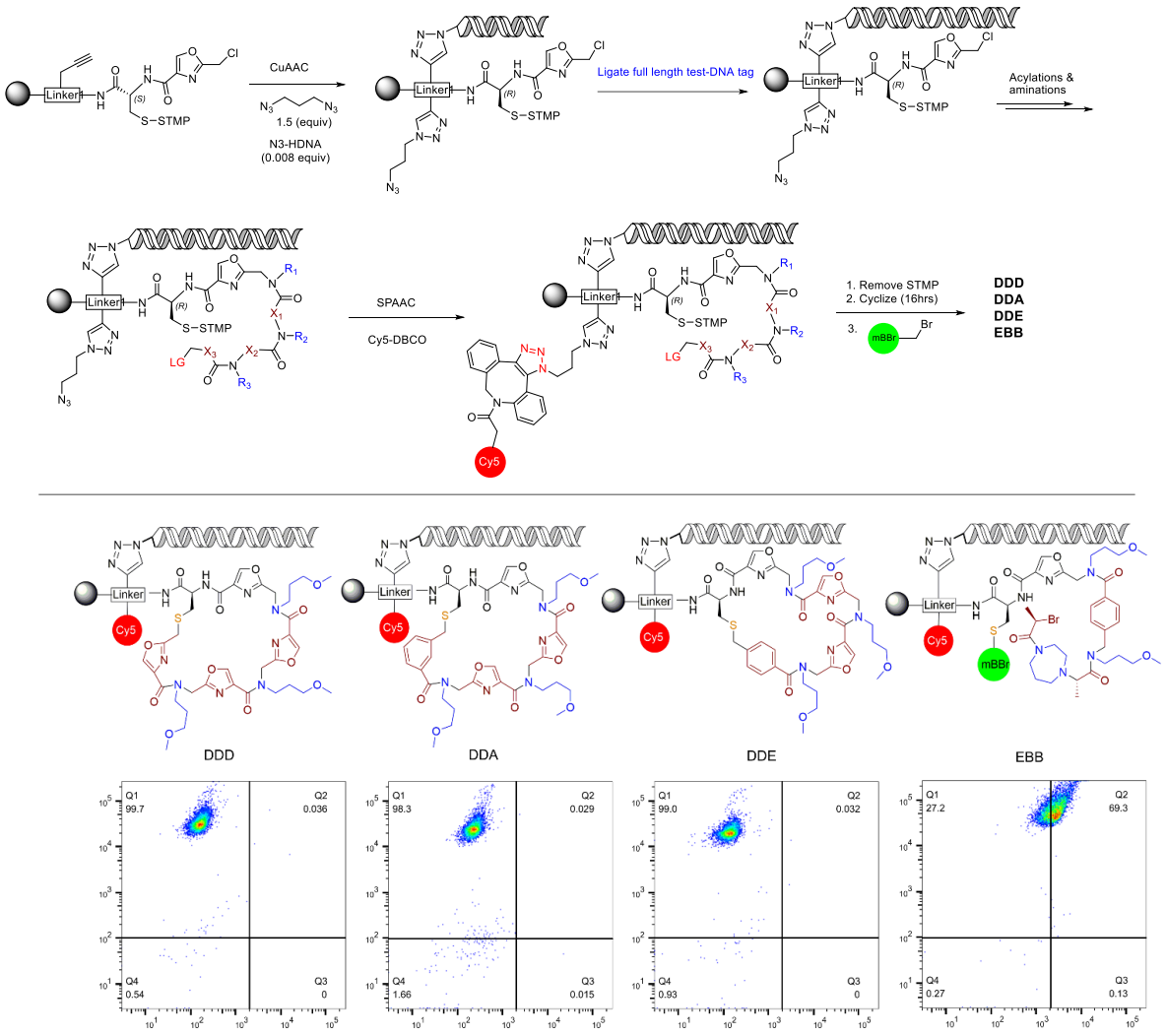
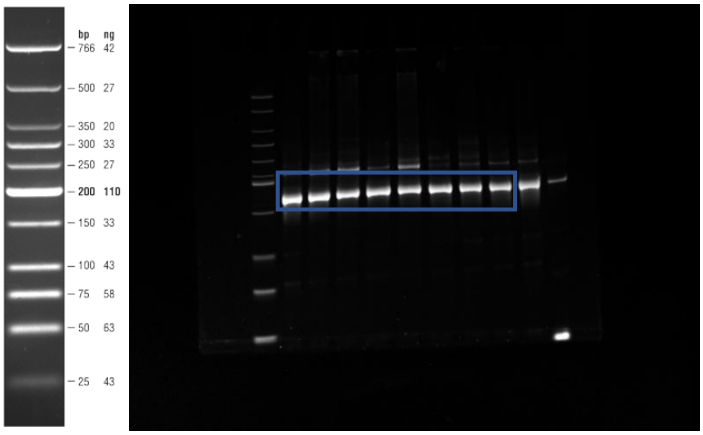


Figure S11: DNA tag amplification of compounds DDD, DDA, DDE and EBB from 10 µm beads (1500 beads) in two replicates followed by controls (+ve, -ve) and Sanger sequencing results.

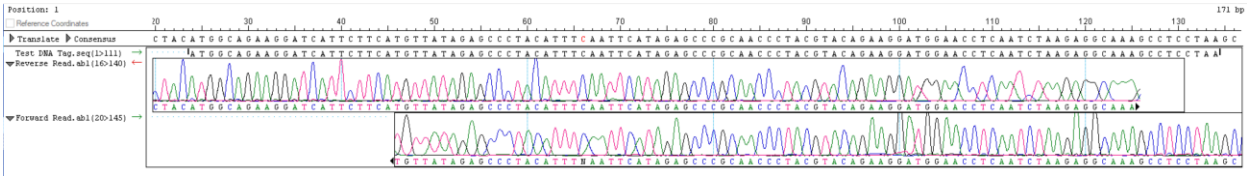


Test-DNA tags of these beads were amplified (Table **T7**, 1st PCR), purified (5.0 µL) by native PAGE gel extraction (6%, 1 x TBE, 4 W, 60 min), with 1X SYBR Gold staining. Gel slices containing 167bp DNA products were excised and suspended in DI water (50.0 µL) in a clean tube overnight. The samples were then centrifuged (5 min, 10,000 RCF), and the supernatants were transferred to clean tubes, diluted 1:10000 in BTPWB, and used as template for Sanger-primer-addition PCRs. The samples were again gel purified by native PAGE gel extraction (233bp DNA), suspended in DI water, centrifuged, and sent for Sanger sequencing (GENEWIZ).

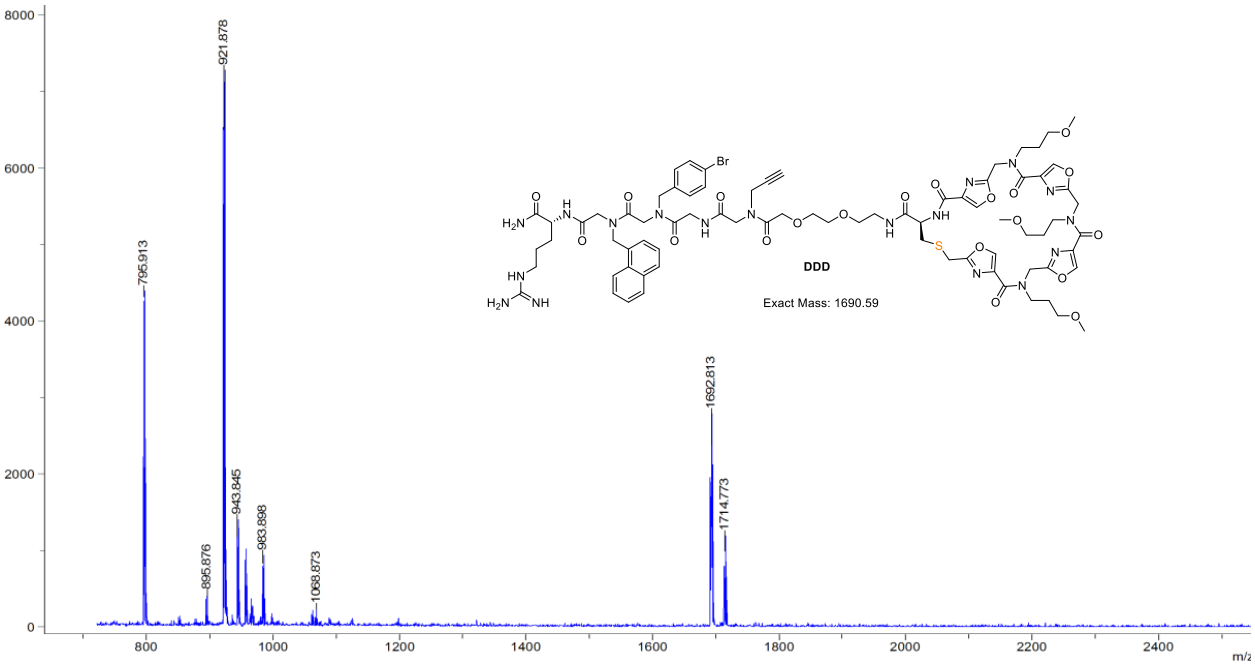
All four samples had same test-DNA tag. They are shown below.

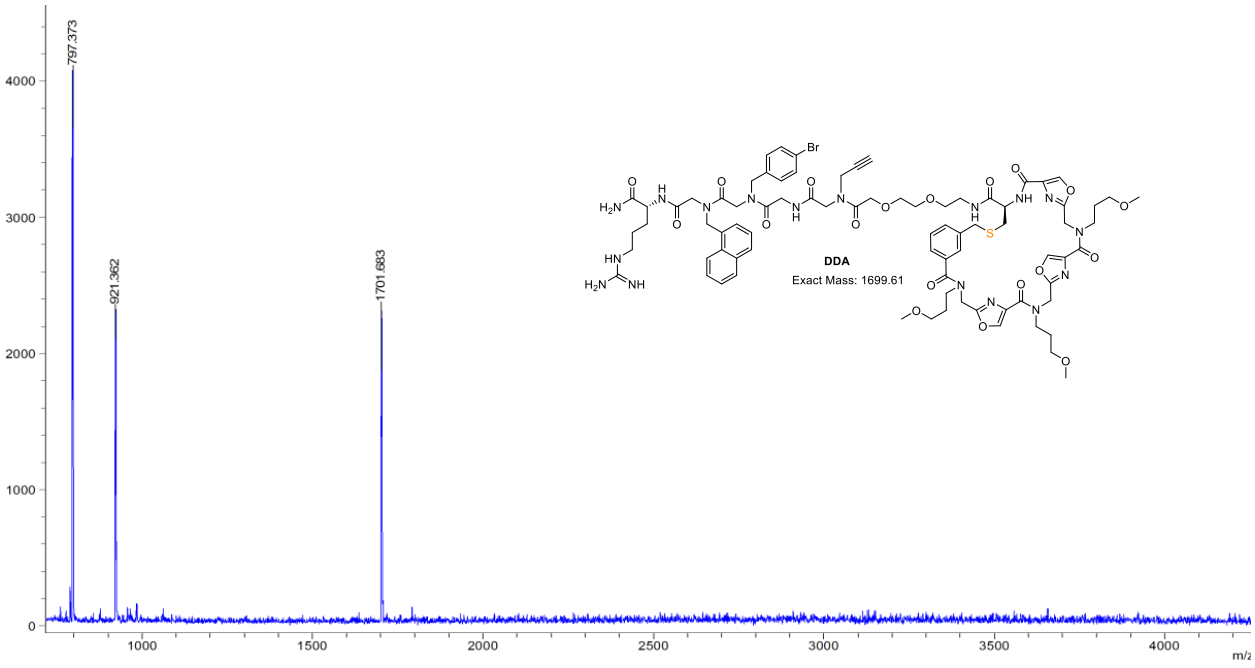
Expected DNA sequence :
1107[+],2209[+],1306[+],2406[+],1506[+],2604[+],1707[+],2802[+],1901[+],2A01[+]

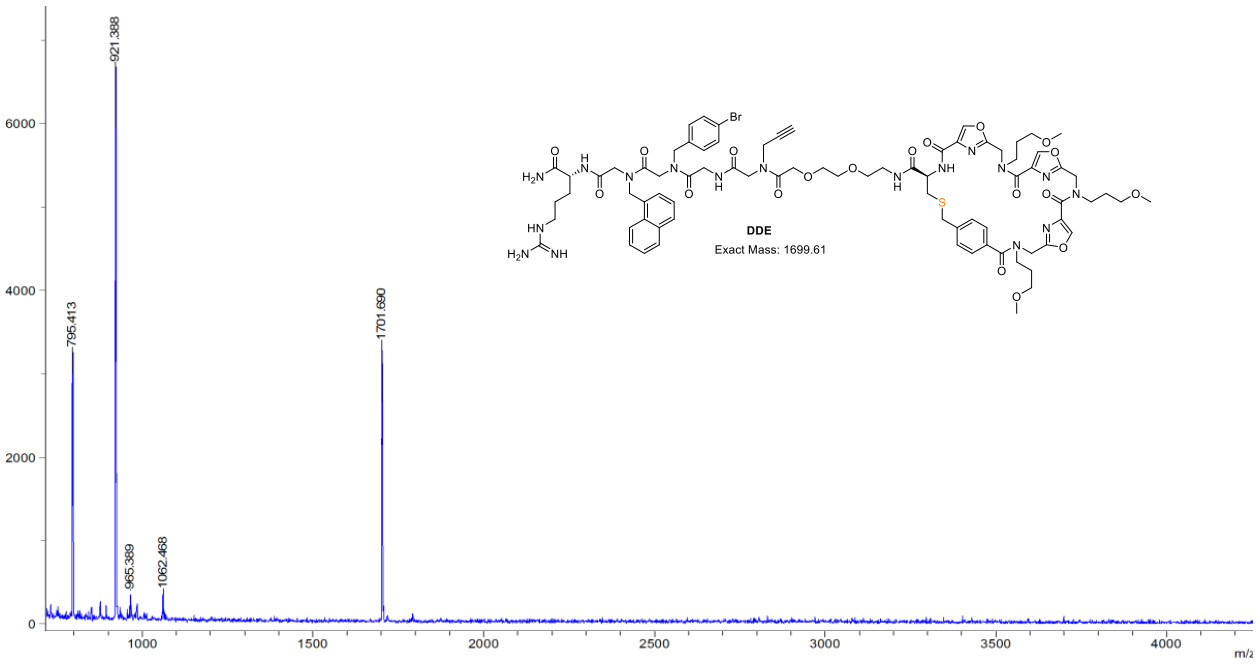
Found sequence as expected. All 4 samples had same test DNA tag below.

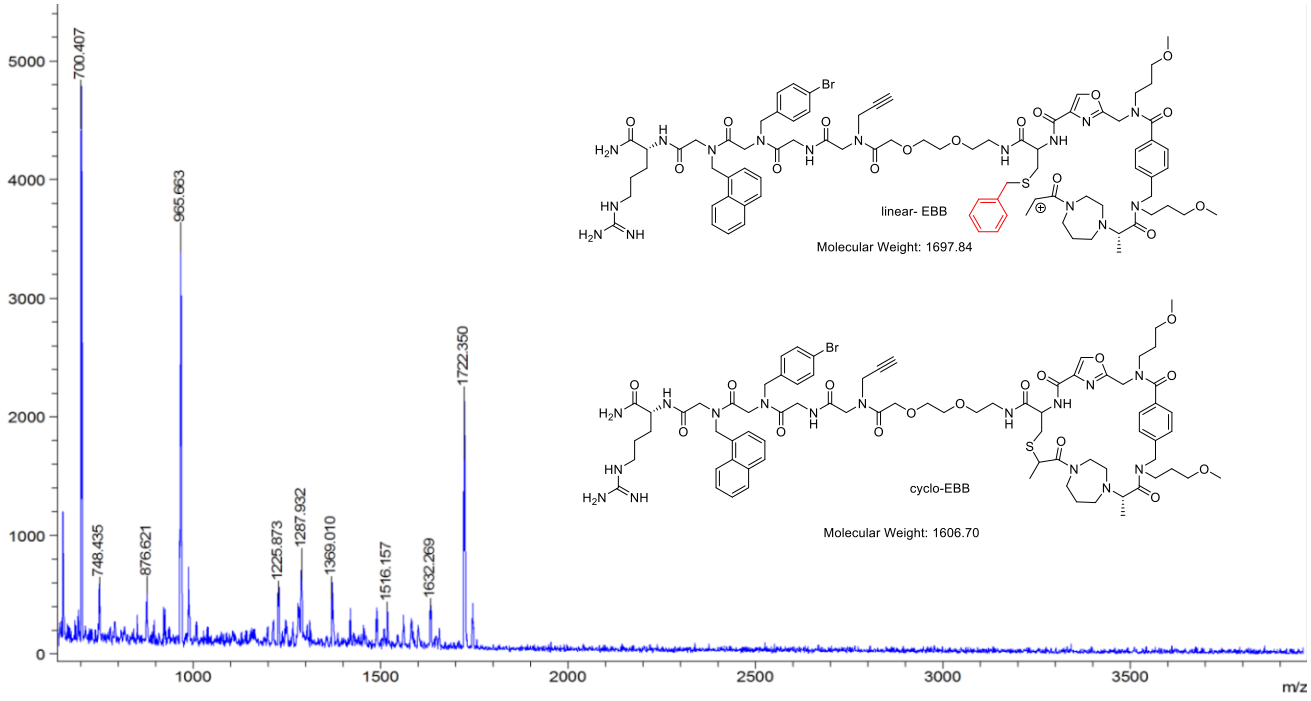


6A: Mass analysis of compounds **DDD**, **DDA**, **DDE** and **EBB**

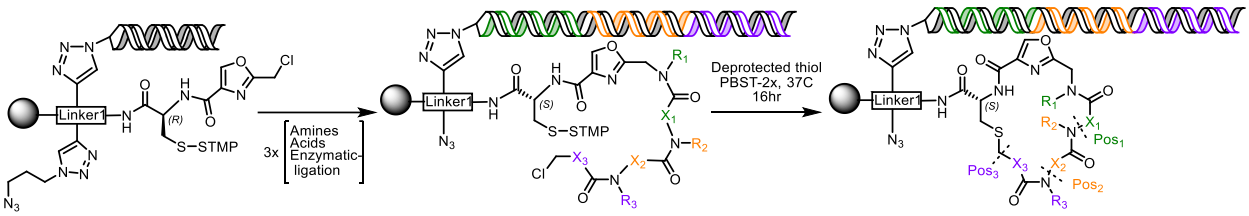




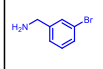
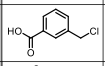
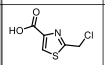
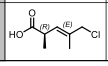

921.388
795.413
1701.890
965.389
1062.468
6000
4000
2000
0
1000
1500
2000
2500
3000
3500
4000
m/z
DDE
Exact Mass: 1699.61


700.407
965.663
1722.350
748.435
876.621
1225.873
1287.932
1369.010
1516.157
1632.269
5000
4000
3000
2000
1000
0
1000
1500
2000
2500
3000
3500
m/z
linear- EBB
Molecular Weight: 1697.84
cyclo-EBB
Molecular Weight: 1606.70

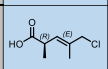
Section 7: Synthesis & quality control of OBOC thioether macrocyclic DEL for ring closure.



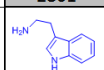
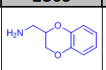
Position 1

1st amine-acid	2401	2402	2403	2404	2405	2406	2407	2408	2409	2410		1309	1310
													
1301											2401		
1302											2402		
1303											2403		
1304											2404		

Position 2

2nd amine-acid	2601	2602	2603	2604	2605	2606	2607	2608	2609	2610		1509	1510
													
1501											2601		
1502											2602		
1503											2603		
1504											2604		

Position 3

3rd amine-acid	2801	2802	2803	2804	2805	2806	2807	2808	2809	2810		1709	1710
													
1701											2801		
1702											2802		
1703											2803		
1704											2804		

Synthesis & analysis: Linker-**1** was synthesized on 25.0 mg of 10 µm TentaGel amine beads, FMOC-Cys(STmp)-OH and acid **D** were then added, in succession. Azido headpiece-DNA and 1, 3-diazidopropane

were attached via CuAAC reaction following general method **2C**. The beads were then distributed into a filter plate (0.5 mg/ well, 48 wells, Millipore MultiScreen Solvinert 0.45 µm Hydrophobic PTFE). Subsequently, FWD primer along with 11xx-22xx primers were ligated, beads were pooled and redistributed. Amines (1.0 M, 150.0 µL, 3 hrs., 37°C) were reacted first, followed by acid additions for each position **X1-3** (Acid/DIC/Oxyma/Collidine: 80/126/80/80mM, pre-activated, 150.0 µL, 3hrs., 37˚C) following the general scheme **7A**. Beads were then washed (150.0 µL, DMF, DCM, DMF, BTP-WB) and suspended in BTP-WB overnight before encoding.

X1-3 positions were encoded with primers 13xx-24xx, 15xx-26xx and 17xx-28xx, respectively. In general, an encoding oligonucleotide ligation mixture containing T4 DNA ligase (15000 U) in BTP-LB (1.35X) was prepared and aliquoted into all plate wells (110 µL). Stocks of ≈13XX[±] (Table **T5**) and ≈24XX[±]were annealed and then added to the appropriate wells (final conc for each codes ~10mM, total vol 150uL) the plate was sealed with adhesive foil, and incubated with agitation (4h, RT, 800 rpm).

After each ligation, beads were transitioned to and equilibrated in DMF overnight before the chemistry steps. The library- id (1901-2A07) and reverse primer were then ligated to complete the DNA barcodes. The beads were then washed with and equilibrated with BTP-WB buffer, overnight. An aliquot of the library (~5.0 mg) was transferred to a fritted spin-column (Bio-Rad, large filter, 10-µm pore size) and re-suspended in CRB, DMSO solution of Cy5-DBCO (final conc 0.11 mM, 150uL) was added and incubated at 37°C for overnight (2hr also works). The beads were then washed with BTPWB, DMF, and DCM before re-suspending in DMF for overnight. The thiol-protecting STmp group was then removed (100.0 mM DTT-NMM in DMF, 500 µL, 3x, RT). The beads were then suspended in PBST (1.00 ml) and incubated at 37°C to monitor cyclization. After 8, 12 & 16 hrs., aliquots of beads were transferred to a filter pate, stained with mBBr (9.0 mM, DMF, 37°C, 2hrs) , and analyzed by flow cytometry. Beads that have higher fluorescence intensities than control-**3** (due to incomplete cyclization) were separated and collected.

Sorted beads were transferred from the FACS collection tubes to clean centrifuge tubes (0.2 mL) and concentrated (to ~5.0 µL). Encoding DNA tags were amplified (Table **T7**, 1st PCR) and purified (5.0 µL) by native PAGE gel extraction (6%, 1 x TBE, 4 W, 60 min). Gel slices containing 167bp DNA products were excised and suspended in DI water (50.0 µL) in a clean tube overnight. The samples were then centrifuged (5 min, 10,000 RCF), transferred to a clean tube, diluted to (1:10000 in BTPWB), and used as template for Illumina primer addition PCRs. Illumina index primers, along with the P5-univ-FWD primer, SuperFi buffer, SuperFI DNAP, and dNTP mix were premixed, 1.0 µL of the template from the 1st PCR was added, and the mixture was thermally cycled (Table **T7**). The samples were again gel purified (289bp DNA), eluted with DI water, and deep sequenced.

Table T6. Oligonucleotide sequence lookup table.

Overhangs

Overhang #	Sequence
≈X1XX[+]	/5Phos/ATGG
≈X1XX[-]	/5Phos/TGA
≈X2XX[+]	/5Phos/TCA
≈X2XX[-]	/5Phos/AAC
≈X3XX[+]	/5Phos/GTT
≈X3XX[-]	/5Phos/TAG
≈X4XX[+]	/5Phos/CTA
≈X4XX[-]	/5Phos/GAA
≈X5XX[+]	/5Phos/TTC
≈X5XX[-]	/5Phos/GCG
≈X6XX[+]	/5Phos/CGC
≈X6XX[-]	/5Phos/AAC
≈X7XX[+]	/5Phos/GTT
≈X7XX[-]	/5Phos/TAG
≈X8XX[+]	/5Phos/CTA
≈X8XX[-]	/5Phos/AGGC

Coding Sequences

Identifier #	Sequence
≈1X01[+]	AAGAGAGG
≈1X01[-]	CCTCTCTT
≈1X02[+]	ACGGAGCA
≈1X02[-]	TGCTCCGT
≈1X03[+]	ACAAAGAG
≈1X03[-]	CTCTTTGT
≈1X04[+]	AAGGAGGT
≈1X04[-]	ACCTCCTT
≈1X05[+]	AGAAAGCA
≈1X05[-]	TGCTTTCT
≈1X06[+]	ATAAAGGT
≈1X06[-]	ACCTTTAT
≈1X07[+]	ATAGAAGG
≈1X07[-]	CCTTCTAT
≈1X08[+]	ATGGGAGT
≈1X08[-]	ACTCCCAT
≈1X09[+]	GCAAAGGA
≈1X09[-]	TCCTTTGC
≈1X10[+]	TTGAGGAT
≈1X10[-]	ATCCTCAA

Identifier #	Sequence
≈2X01[+]	AGTTTCAG
≈2X01[-]	CTGAAACT
≈2X02[+]	AACCTCAA
≈2X02[-]	TTGAGGTT
≈2X03[+]	AATCCCAT
≈2X03[-]	ATGGGATT
≈2X04[+]	AACCCTAC
≈2X04[-]	GTAGGGTT
≈2X05[+]	ATCCTCTC
≈2X05[-]	GAGAGGAT
≈2X06[+]	ATTCTCCG
≈2X06[-]	CGGAGAAT
≈2X07[+]	CGCCTTCA
≈2X07[-]	TGAAGGCG
≈2X08[+]	CGTTCCTG
≈2X08[-]	CAGGAACG
≈2X09[+]	CTCTCCAC
≈2X09[-]	GTGGAGAG
≈2X10[+]	TCCTCTTA
≈2X10[-]	TAAGAGGA

Primers

PCR Primer #	Sequence
≈0001[+]	/5Phos/GCCGCCCAGTCCTGCTCGCTTCGCTAC
≈0001[-]	/5Phos/CCATGTAGCGAAGCGAGCAGGACTGGGCGGCGG
≈0901[+]	/5Phos/GCCTGTTTGCCCGCCAGTTGTTGTGCCAC
≈0901[-]	/5AmMC6/GTGGCACAACAACTGGCGGGCAAAC

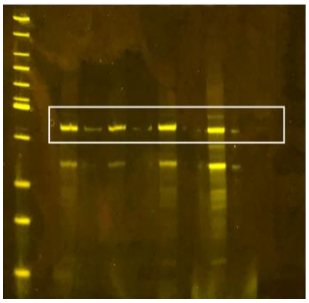
Table T7: PCR amplification of encoding DNA tags from beads.

1st PCR: Amplification of encoding DNA tags from beads						
rxn volume:	50	**total rxns:**	6			
reagent	**vol**	**stock**	**MM volume**		**Cycle:**	
initial vol	**10**		**60**			
5X SuperFi Buffer	10.0	**5X**	60.0		1	98°C, 30 sec
0.2 mM dNTP Mix	1.0	**10 mM**	6.0		2	98°C, 10 sec.
0.3 µM ABM99-2A-07*	1.5	**10 uM**	9.0		3	46°C, 10 sec.
0.3 µM ABM063	1.5	**10 uM**	9.0		4	72°C, 15 s
SuperFi DNAP	0.5	**2U/ul**	3.0		5	Goto 2, 25 times
ddH20	25.5	**ddH20**	153.0		6	4° hold
total	50.0	**total**	300.0			
*library specific rev primer						

Table T8: NGS sample preparation- addition of Illumina index primer

2nd PCR- add illumina rev-index and fwd primers						
rxn volume:	50	**total rxns:**	9			
reagent	**vol**	**stock**	**MM volume**		**Cycle 2:**	
5X SuperFi Buffer	10.0	**5X**	90.0		1	98°C, 2 min
0.2 mM dNTP Mix	1.0	**10 mM**	9.0		2	98°C, 10 sec.
0.3 µM P5 Univ Fwd2	1.5	**10 uM**	13.5		3	36°C, 10 sec.
0.3 µM Index Rev (1-4)*	1.5	**10 uM**			4	72°C, 15 s
SuperFi DNAP	0.5	**2U/ul**	4.5		5	Goto 2, 25 times
DNA Template (1k & 10k)fold diluted	1.0				6	4° hold
ddH20	34.5	**ddH20**	310.5			
total	50.0	**total**	427.5			
*Illumina index						

1st PCR: 25 Cycles



2nd PCR: Illumina primer addition, 10Kx dilution

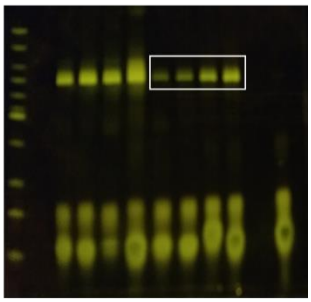
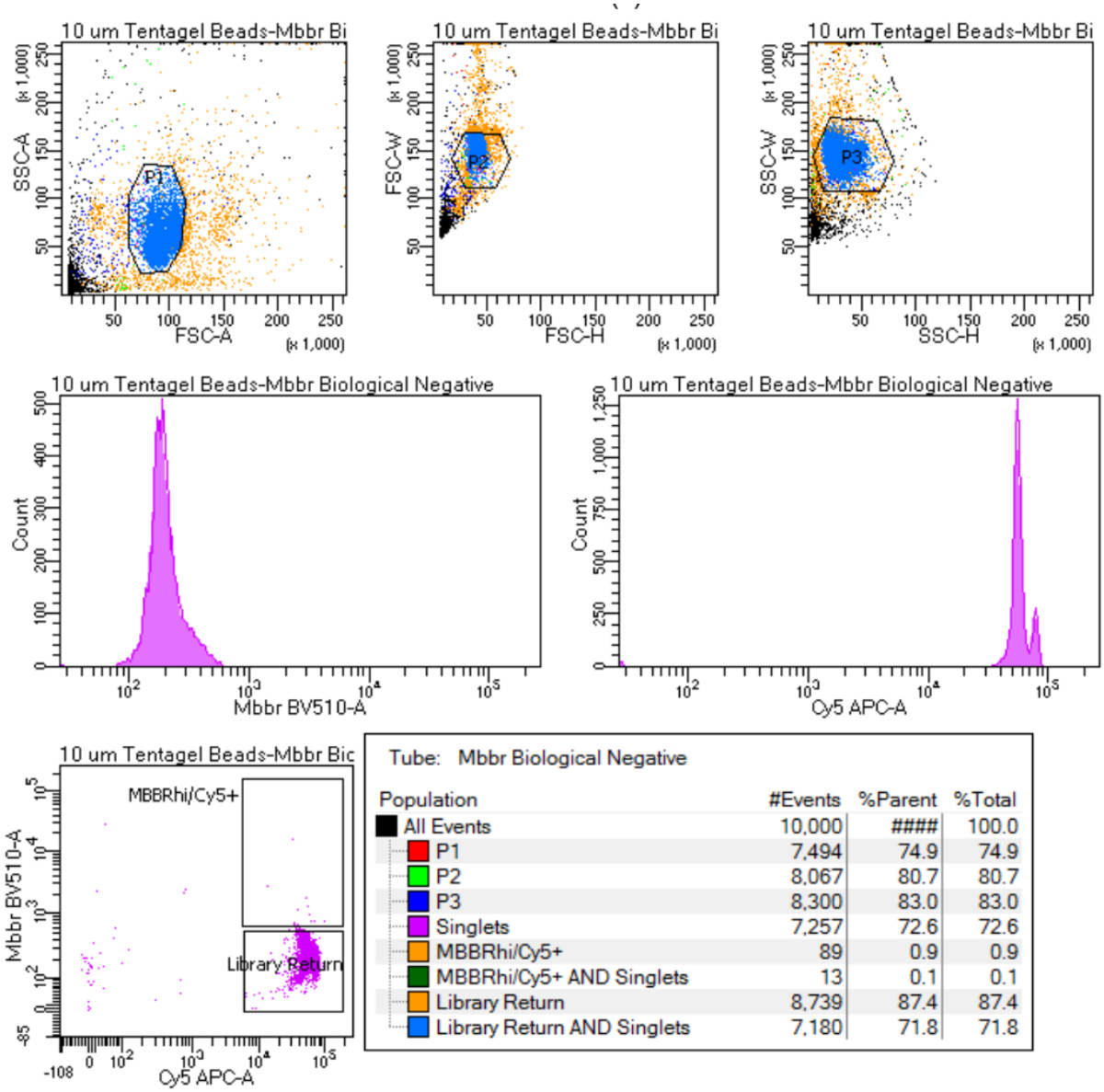
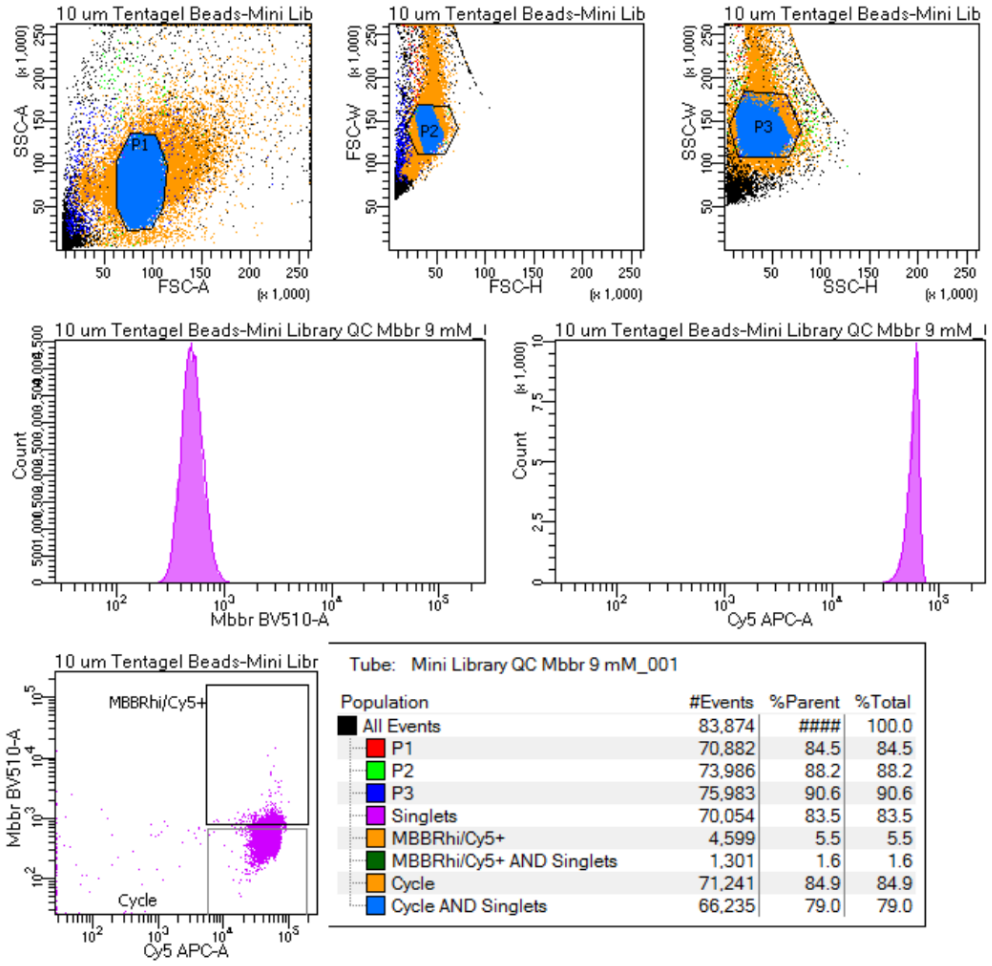


Figure S12: Fluorescence readout of DNA-linked control-**3**. Methionine-DNA-CY5 beads were treated with mBBr and analyzed by FACS. This is a negative control for analyzing OBOC macrocyclic DEL through a flow cytometer.

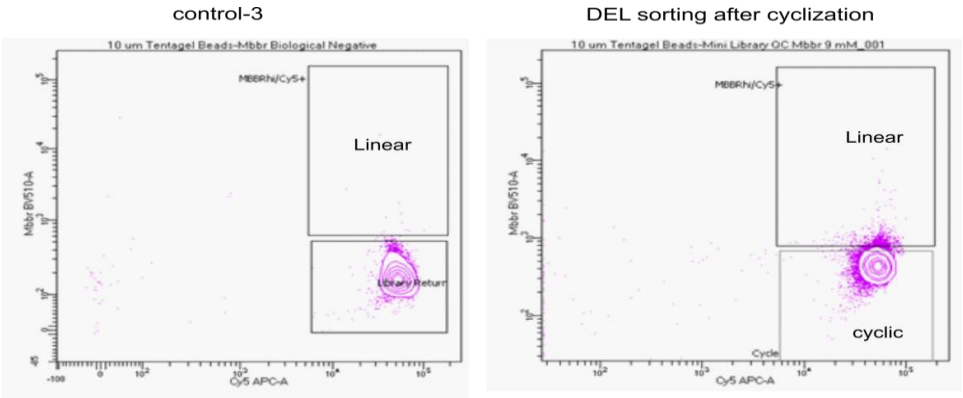


Population	#Events	%Parent	%Total
All Events	10,000	####	100.0
P1	7,494	74.9	74.9
P2	8,067	80.7	80.7
P3	8,300	83.0	83.0
Singlets	7,257	72.6	72.6
MBBRhi/Cy5+	89	0.9	0.9
MBBRhi/Cy5+ AND Singlets	13	0.1	0.1
Library Return	8,739	87.4	87.4
Library Return AND Singlets	7,180	71.8	71.8

Figure S13: Fluorescence readout of beads from the macrocyclic DEL. After cyclization, beads were stained with Cy5-DBCO and MBBR (9.0 mM) and analyzed by FACS.

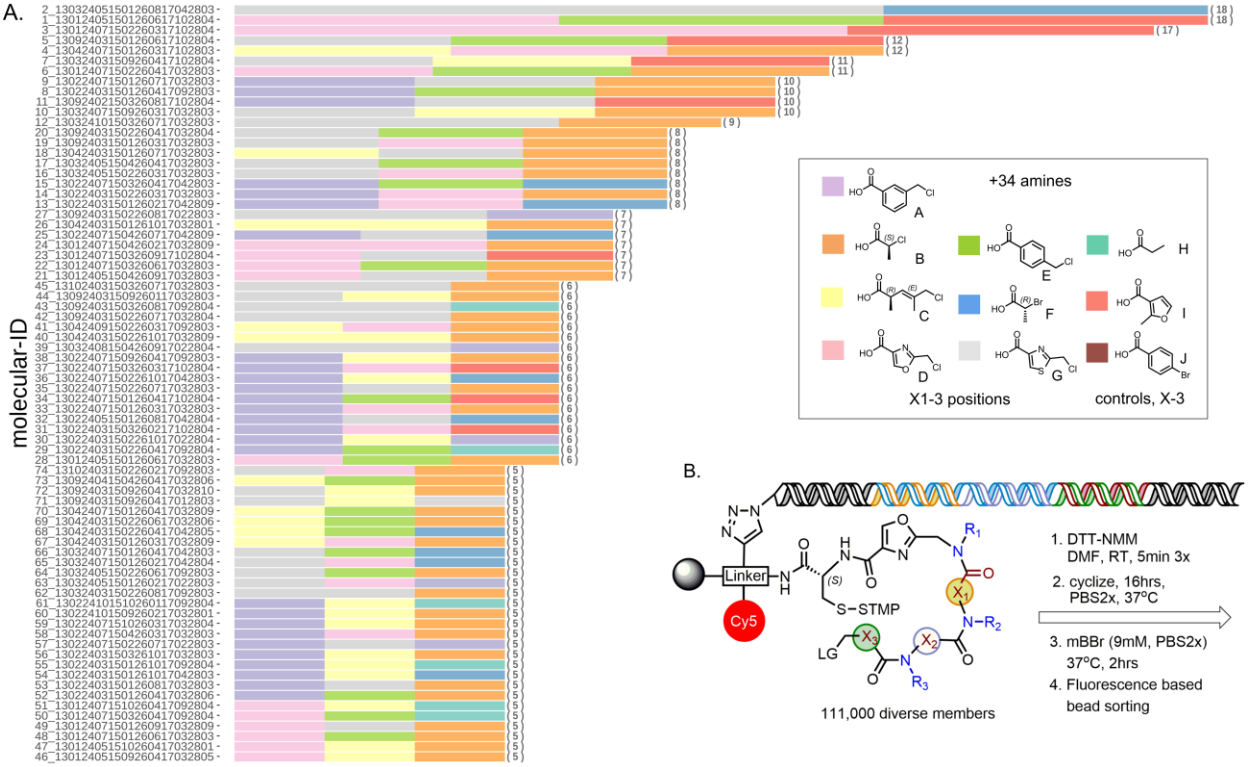


Sorting result: Beads that appeared in the cyclic region (MBBR/Cy5+) were collected and their encoding tags were deep sequenced.



For sequencing analysis of naïve and FACS-sorted beads, please see **Sections 10** & **11,** respectively.

Figure S14: (A) After deep sequencing, difficult to cyclize scaffolds were arranged by count (up to 5 copies, 74 scaffolds). Each line indicates a combination of three acids at position X1-3 for a scaffold along with its molecular ID (left) and the number of times it was present in the collected pool (right). (**B)** Acids A – G and amines were used in position X1-X3 to construct DEL scaffolds. 4% of DEL members were capped with acid H & I to keep them as linear controls for FACS analysis.



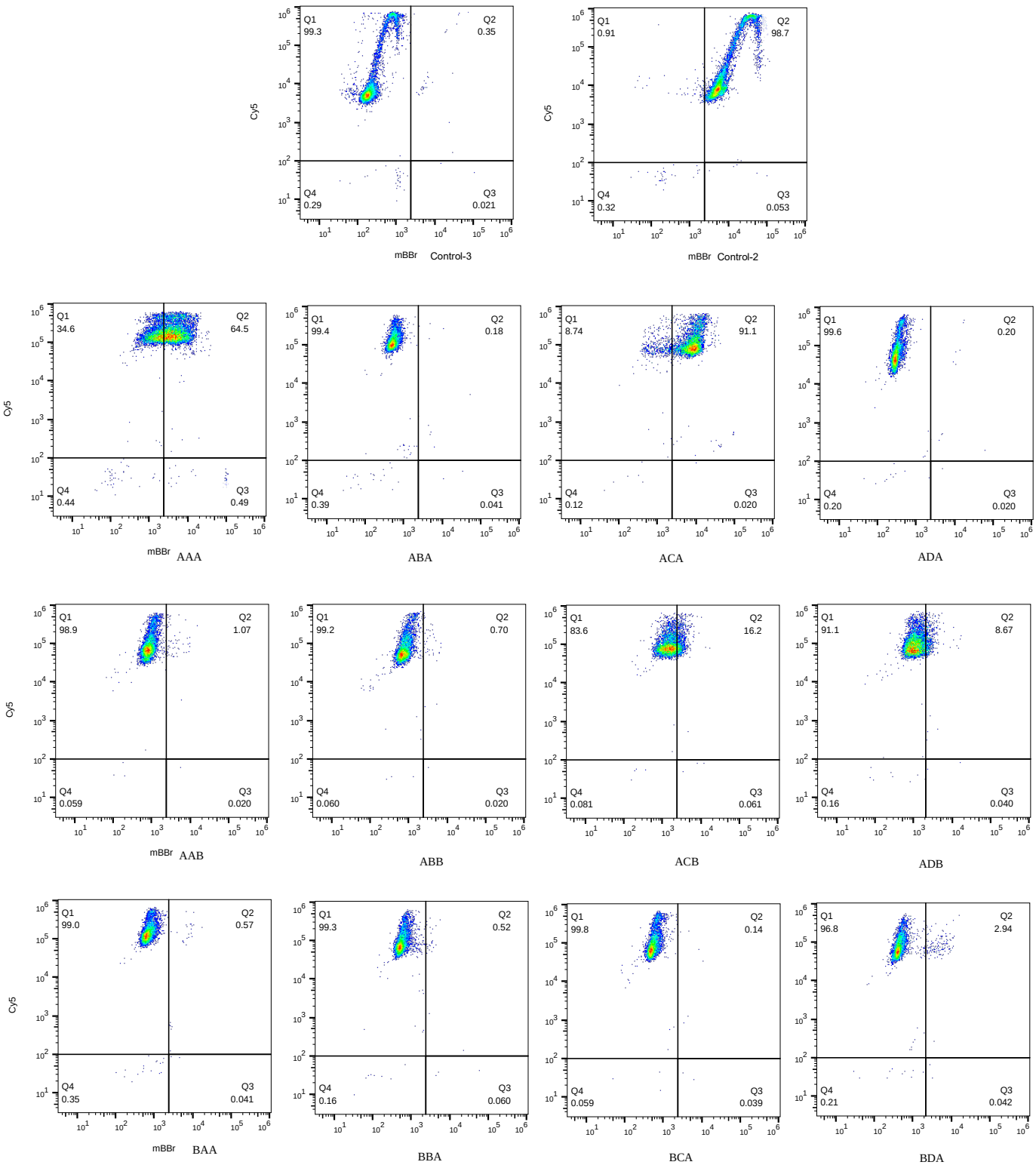
Section 8: FACS & LCMS analysis of 64-scaffolds

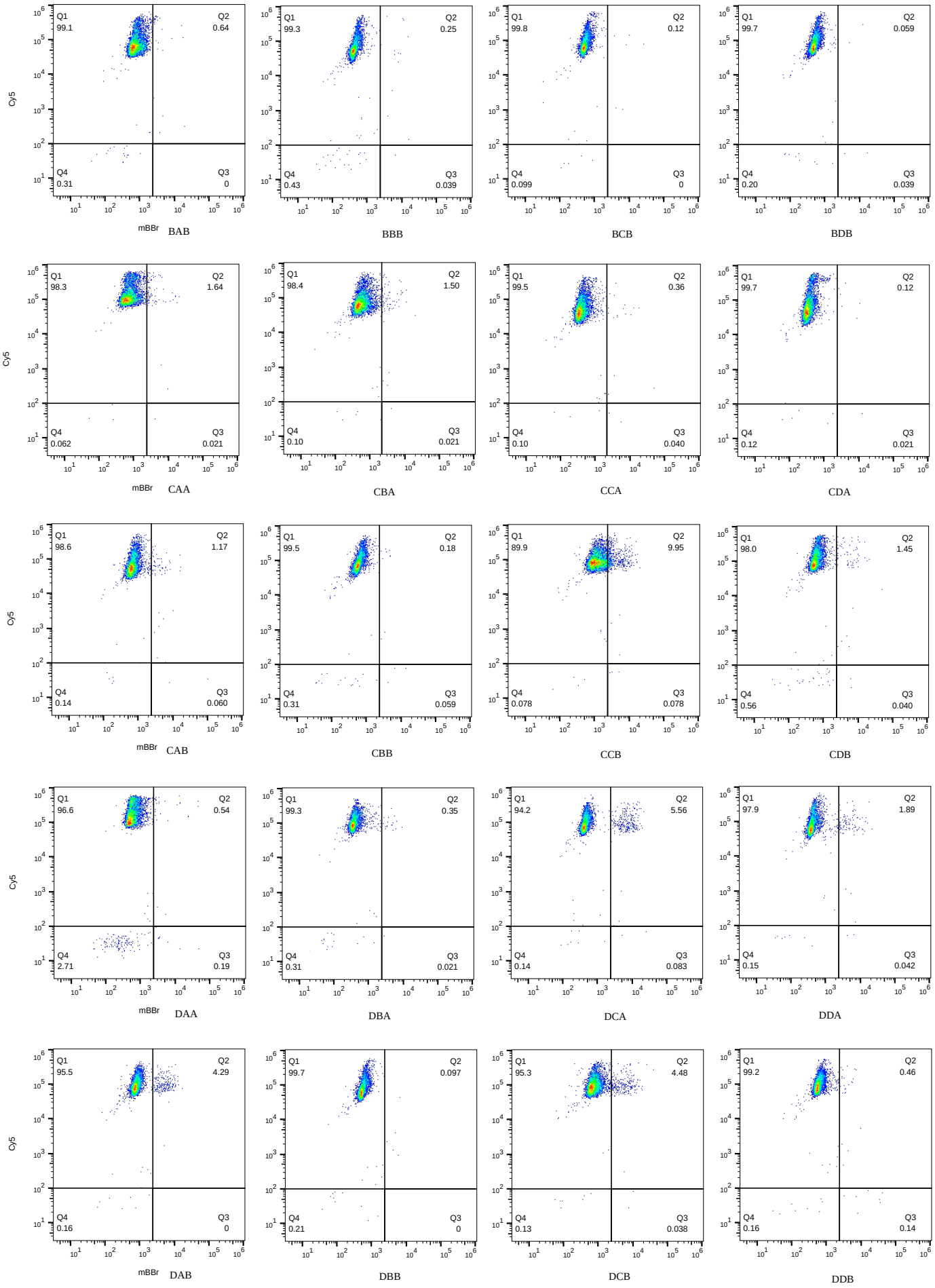
Fluorescence data analysis of 64 PICCO scaffolds after cyclization

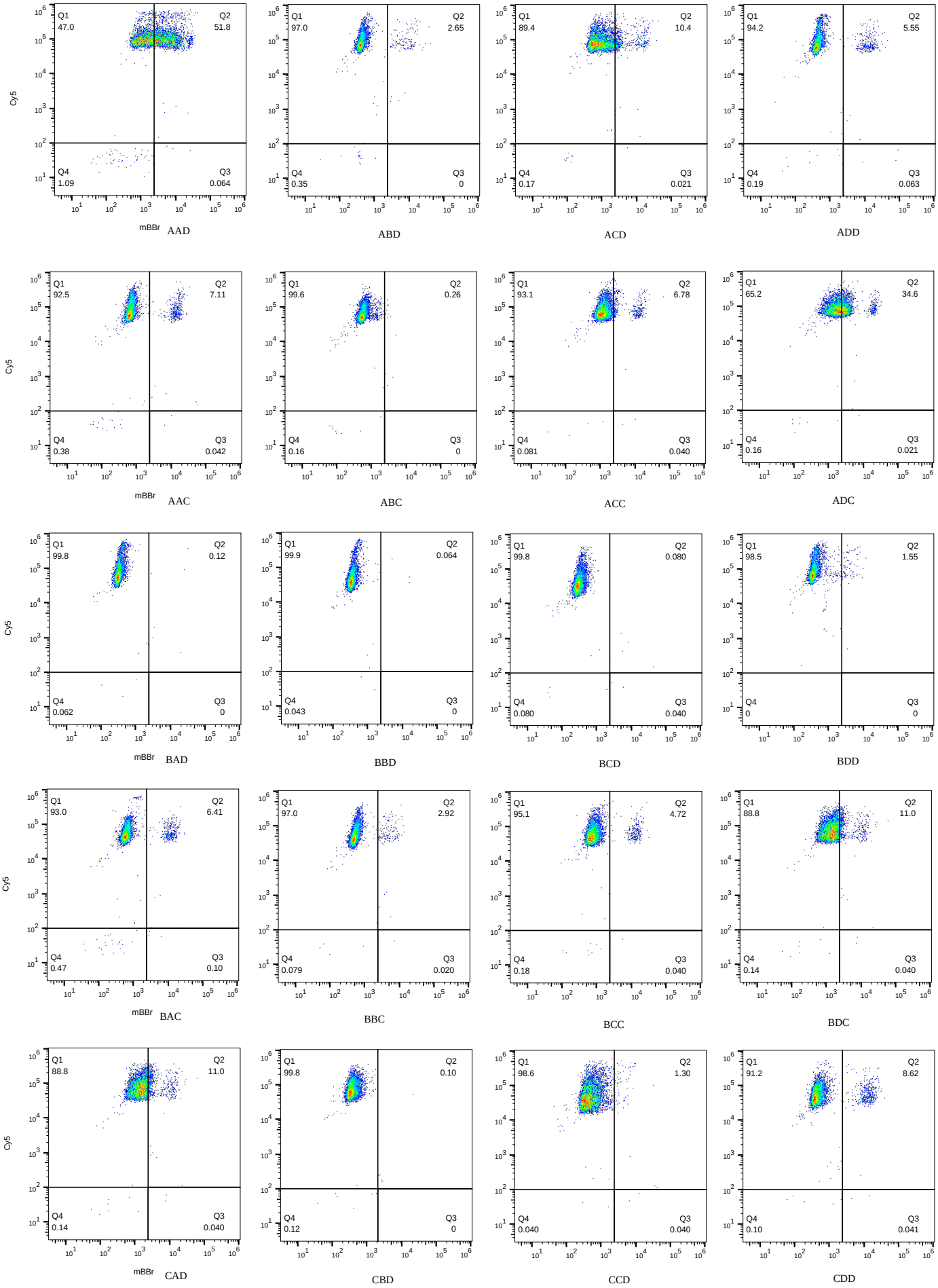
Fluorescence readouts were recorded for each of the 64 scaffolds. Status of ring closures were determined by FACS and cross-referenced with mass spectra to see if there is any linear starting material remaining. The goal was to ultimately gauge the state of cyclization from FACS data by locating the majority of the bead population, without cleaving compounds from beads.

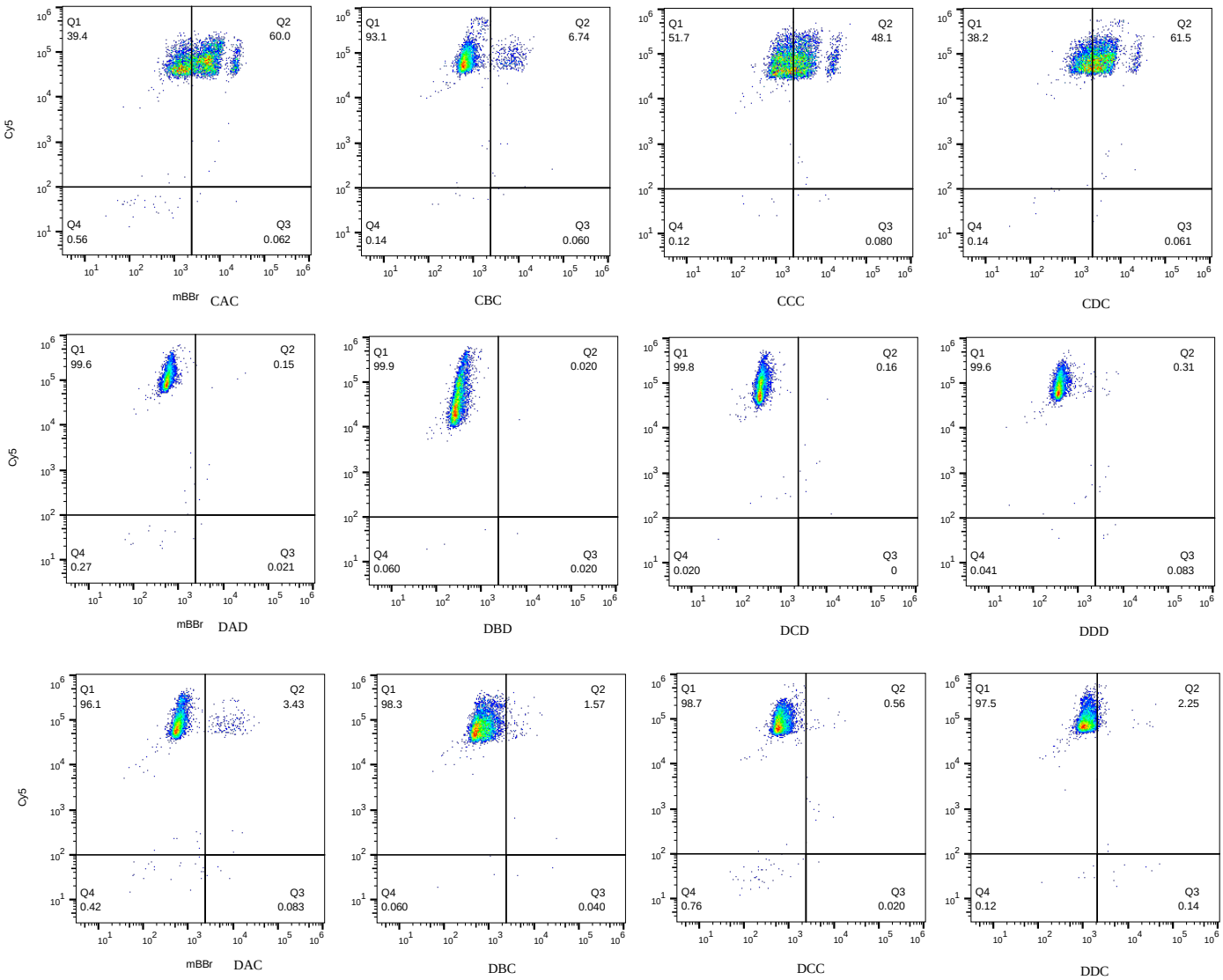
Each FACS plot is divided into 4 quadrants; Q1-Q4. After cyclization and two dye additions, if the majority of the bead population for a particular scaffold stays in Q1 (Cy5 +, MBBR -), cyclization will be considered as complete. If the scaffold does not cyclize efficiently, it will have unreacted thiol groups and will be present in Q2 (Cy5 +, MBBR +), as it will pick up both dyes. Negative control beads that were not treated with any dye will stay in Q4 (Cy5 -, MBBR -). These populations are gated based on the fluorescence intensity of control compound **3**.

Section-9A: Fluorescence readout of 64 scaffolds after cyclization.



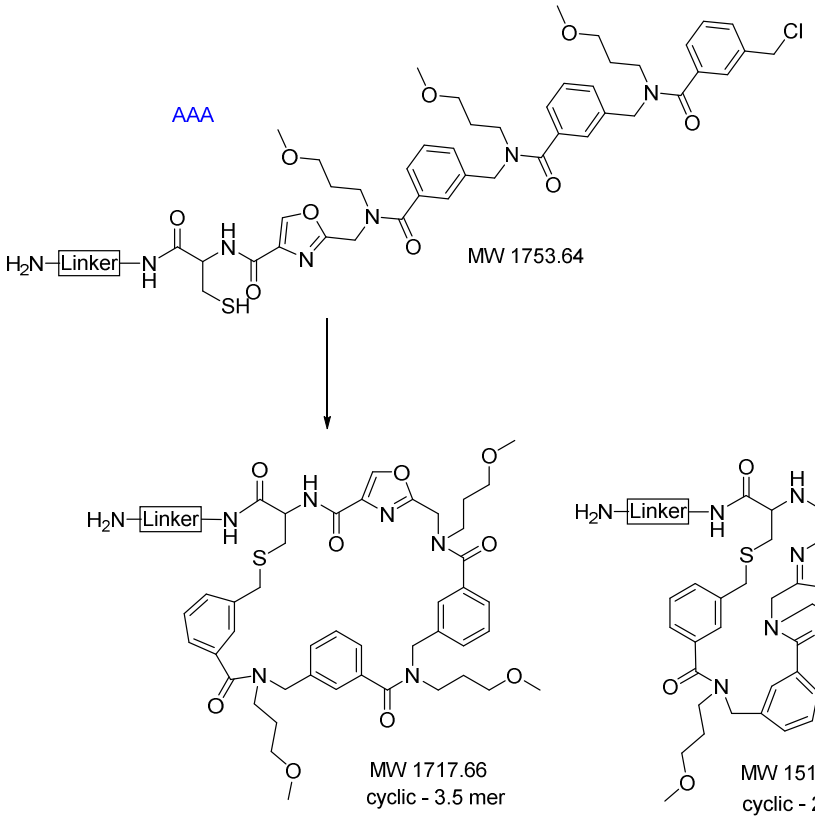

Cy5
mBBr
BAB
Q1 99.1
Q2 0.64
Q4 0.31
Q3 0
BBB
Q1 99.3
Q2 0.25
Q4 0.43
Q3 0.039
BCB
Q1 99.8
Q2 0.12
Q4 0.099
Q3 0
BDB
Q1 99.7
Q2 0.059
Q4 0.20
Q3 0.039
CAA
Q1 98.3
Q2 1.64
Q4 0.062
Q3 0.021
CBA
Q1 98.4
Q2 1.50
Q4 0.10
Q3 0.021
CCA
Q1 99.5
Q2 0.36
Q4 0.10
Q3 0.040
CDA
Q1 99.7
Q2 0.12
Q4 0.12
Q3 0.021
CAB
Q1 98.6
Q2 1.17
Q4 0.14
Q3 0.060
CBB
Q1 99.5
Q2 0.18
Q4 0.31
Q3 0.059
CCB
Q1 89.9
Q2 9.95
Q4 0.078
Q3 0.078
CDB
Q1 98.0
Q2 1.45
Q4 0.56
Q3 0.040
DAA
Q1 96.6
Q2 0.54
Q4 2.71
Q3 0.19
DBA
Q1 99.3
Q2 0.35
Q4 0.31
Q3 0.021
DCA
Q1 94.2
Q2 5.56
Q4 0.14
Q3 0.083
DDA
Q1 97.9
Q2 1.89
Q4 0.15
Q3 0.042
DAB
Q1 95.5
Q2 4.29
Q4 0.16
Q3 0
DBB
Q1 99.7
Q2 0.097
Q4 0.21
Q3 0
DCB
Q1 95.3
Q2 4.48
Q4 0.13
Q3 0.038
DDB
Q1 99.2
Q2 0.46
Q4 0.16
Q3 0.14

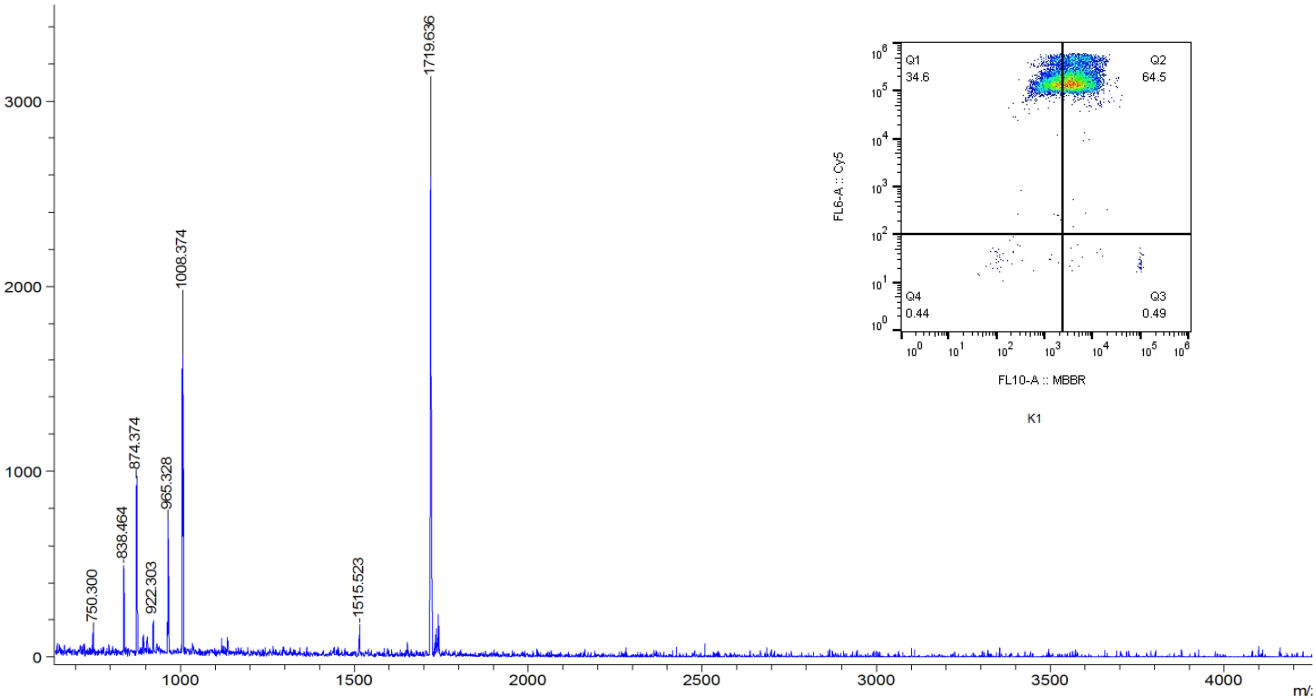

Cy5
mBBr
AAD
Q1 47.0
Q2 51.8
Q4 1.09
Q3 0.064
ABD
Q1 97.0
Q2 2.65
Q4 0.35
Q3 0
ACD
Q1 89.4
Q2 10.4
Q4 0.17
Q3 0.021
ADD
Q1 94.2
Q2 5.55
Q4 0.19
Q3 0.063
AAC
Q1 92.5
Q2 7.11
Q4 0.38
Q3 0.042
ABC
Q1 99.6
Q2 0.26
Q4 0.16
Q3 0
ACC
Q1 93.1
Q2 6.78
Q4 0.081
Q3 0.040
ADC
Q1 65.2
Q2 34.6
Q4 0.16
Q3 0.021
BAD
Q1 99.8
Q2 0.12
Q4 0.062
Q3 0
BBD
Q1 99.9
Q2 0.064
Q4 0.043
Q3 0
BCD
Q1 99.8
Q2 0.080
Q4 0.080
Q3 0.040
BDD
Q1 98.5
Q2 1.55
Q4 0
Q3 0
BAC
Q1 93.0
Q2 6.41
Q4 0.47
Q3 0.10
BBC
Q1 97.0
Q2 2.92
Q4 0.079
Q3 0.020
BCC
Q1 95.1
Q2 4.72
Q4 0.18
Q3 0.040
BDC
Q1 88.8
Q2 11.0
Q4 0.14
Q3 0.040
CAD
Q1 88.8
Q2 11.0
Q4 0.14
Q3 0.040
CBD
Q1 99.8
Q2 0.10
Q4 0.12
Q3 0
CCD
Q1 98.6
Q2 1.30
Q4 0.040
Q3 0.040
CDD
Q1 91.2
Q2 8.62
Q4 0.10
Q3 0.041

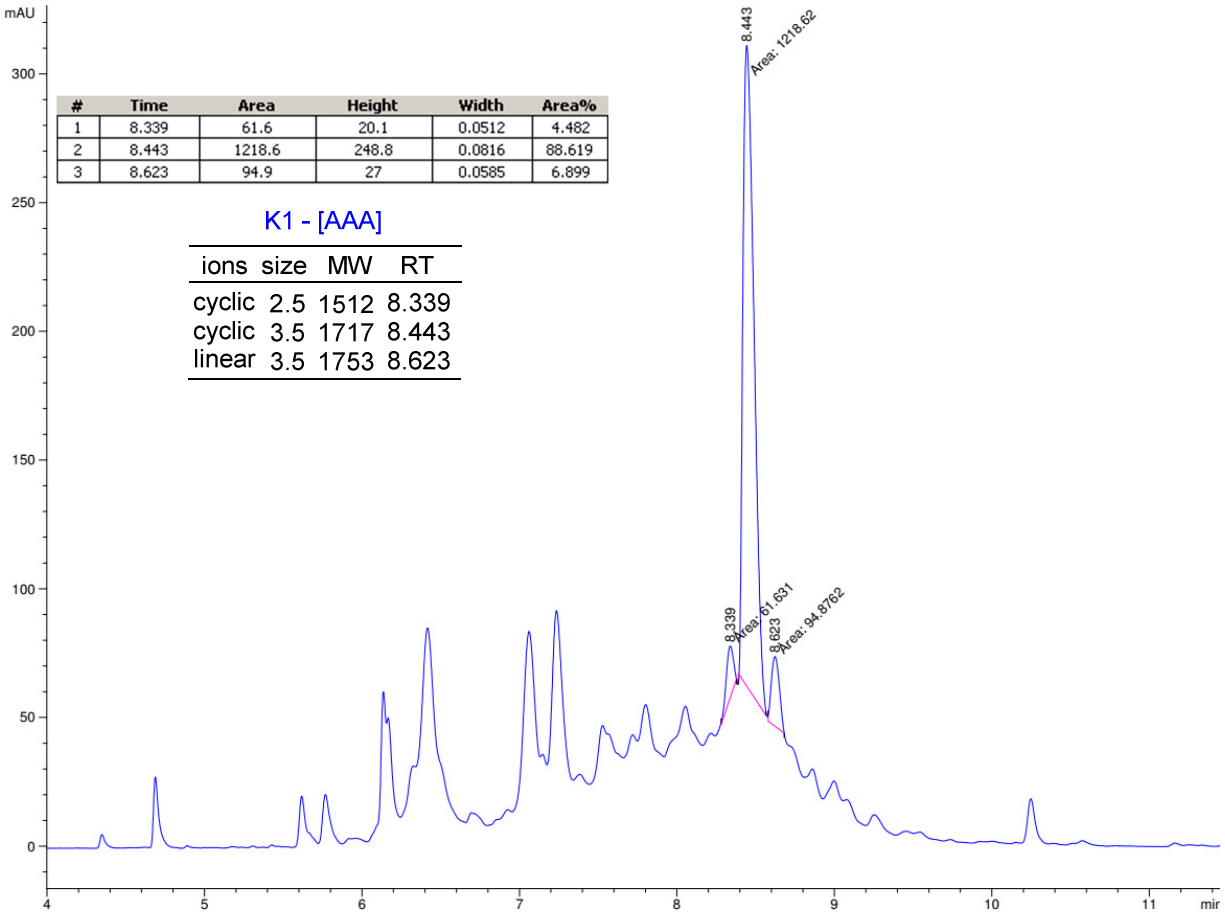

Cy5
mBBr
Q1 39.4
Q2 60.0
Q4 0.56
Q3 0.062
CAC
Q1 93.1
Q2 6.74
Q4 0.14
Q3 0.060
CBC
Q1 51.7
Q2 48.1
Q4 0.12
Q3 0.080
CCC
Q1 38.2
Q2 61.5
Q4 0.14
Q3 0.061
CDC
Q1 99.6
Q2 0.15
Q4 0.27
Q3 0.021
DAD
Q1 99.9
Q2 0.020
Q4 0.060
Q3 0.020
DBD
Q1 99.8
Q2 0.16
Q4 0.020
Q3 0
DCD
Q1 99.6
Q2 0.31
Q4 0.041
Q3 0.083
DDD
Q1 96.1
Q2 3.43
Q4 0.42
Q3 0.083
DAC
Q1 98.3
Q2 1.57
Q4 0.060
Q3 0.040
DBC
Q1 98.7
Q2 0.56
Q4 0.76
Q3 0.020
DCC
Q1 97.5
Q2 2.25
Q4 0.12
Q3 0.14
DDC

Section-9B: Mass analysis of 64-scaffolds

K1-[AAA]: Incomplete cyclization was detected on 10 µm but was >90% complete on 160 µm beads.



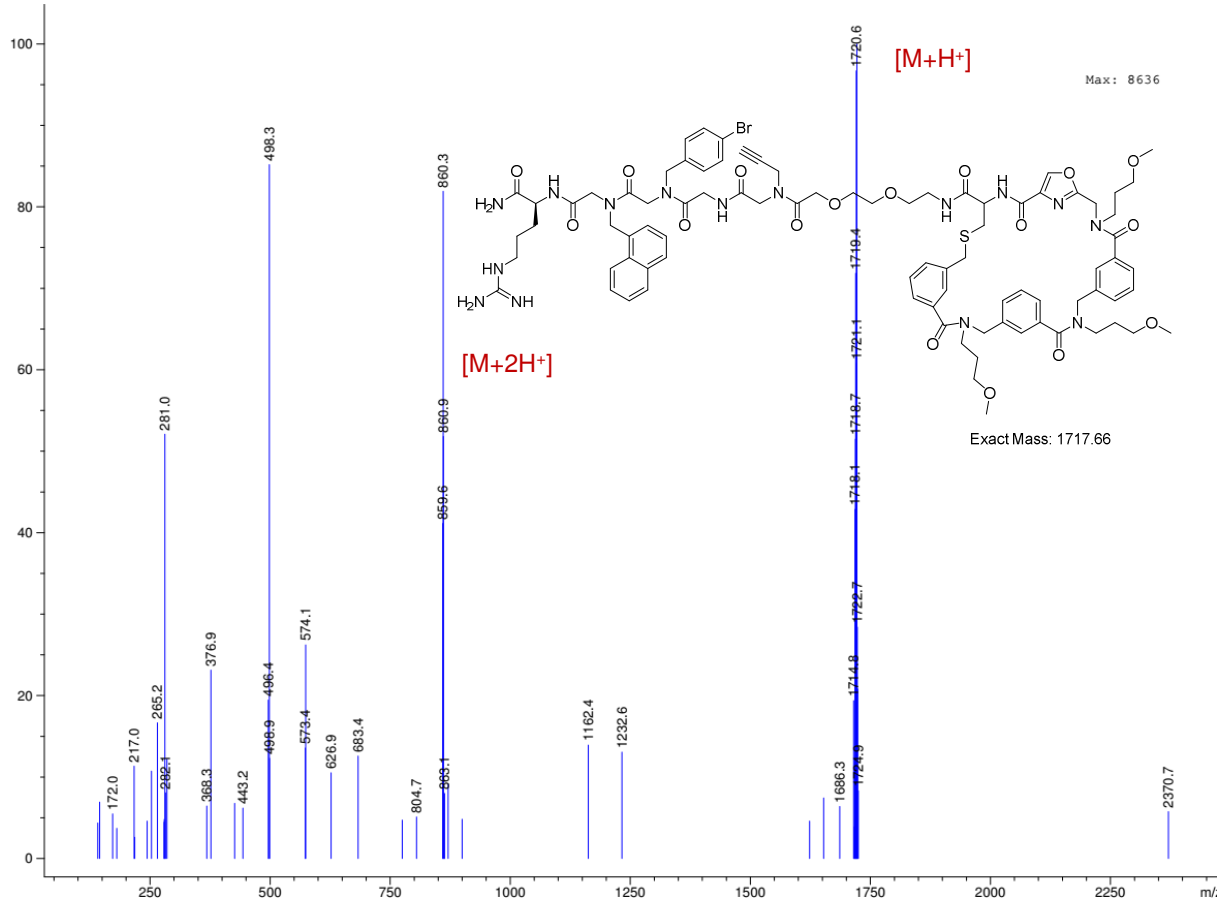


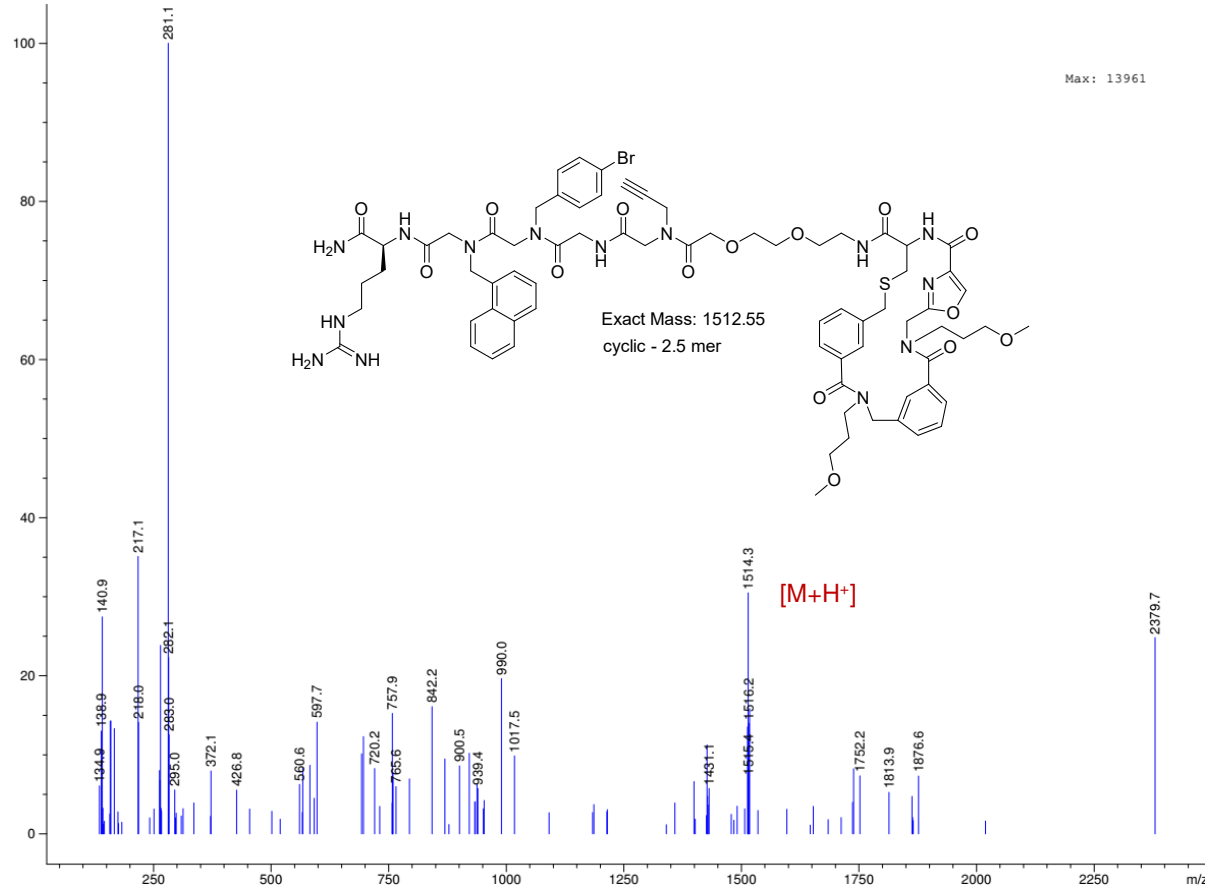


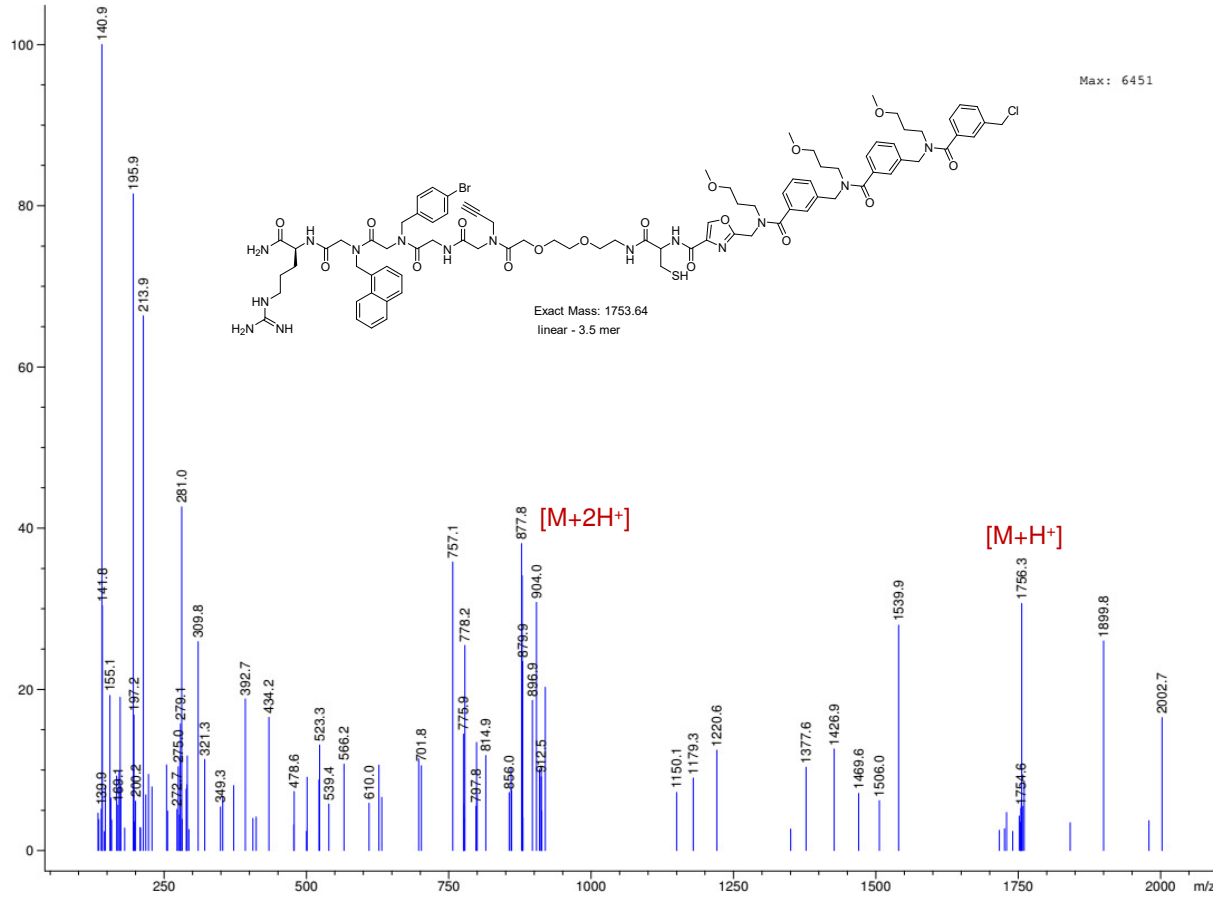
#	Time	Area	Height	Width	Area%
1	8.339	61.6	20.1	0.0512	4.482
2	8.443	1218.6	248.8	0.0816	88.619
3	8.623	94.9	27	0.0585	6.899

K1 - [AAA]

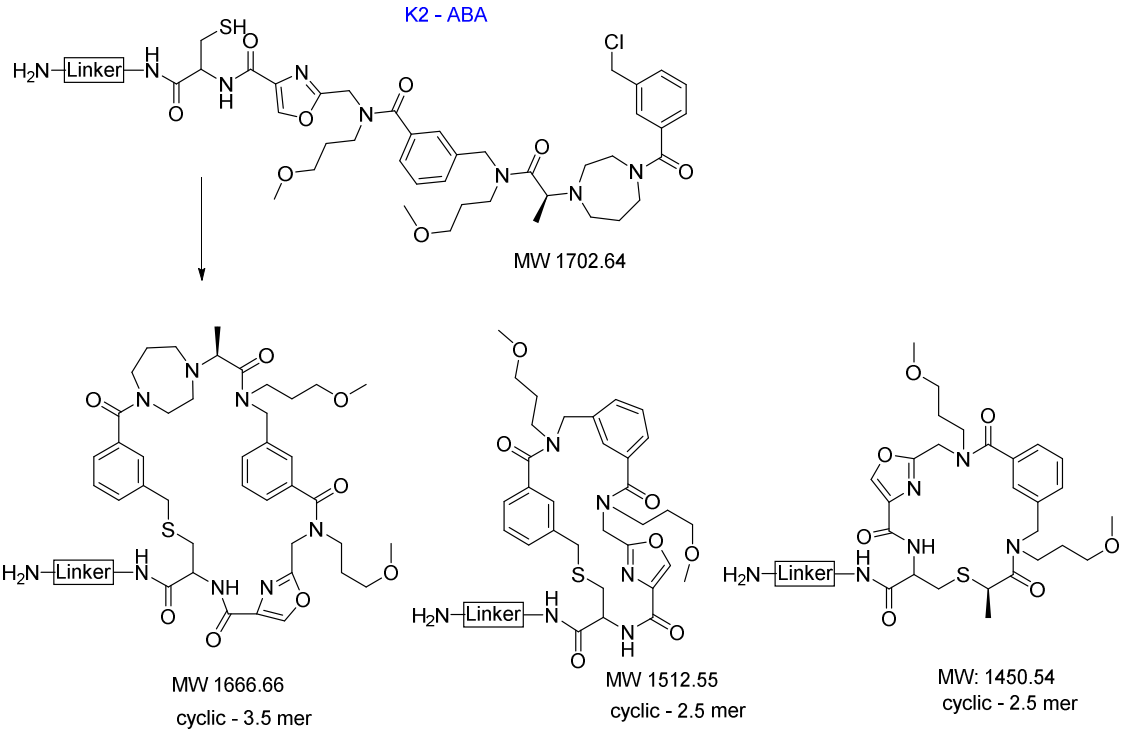
ions	size	MW	RT
cyclic	2.5	1512	8.339
cyclic	3.5	1717	8.443
linear	3.5	1753	8.623

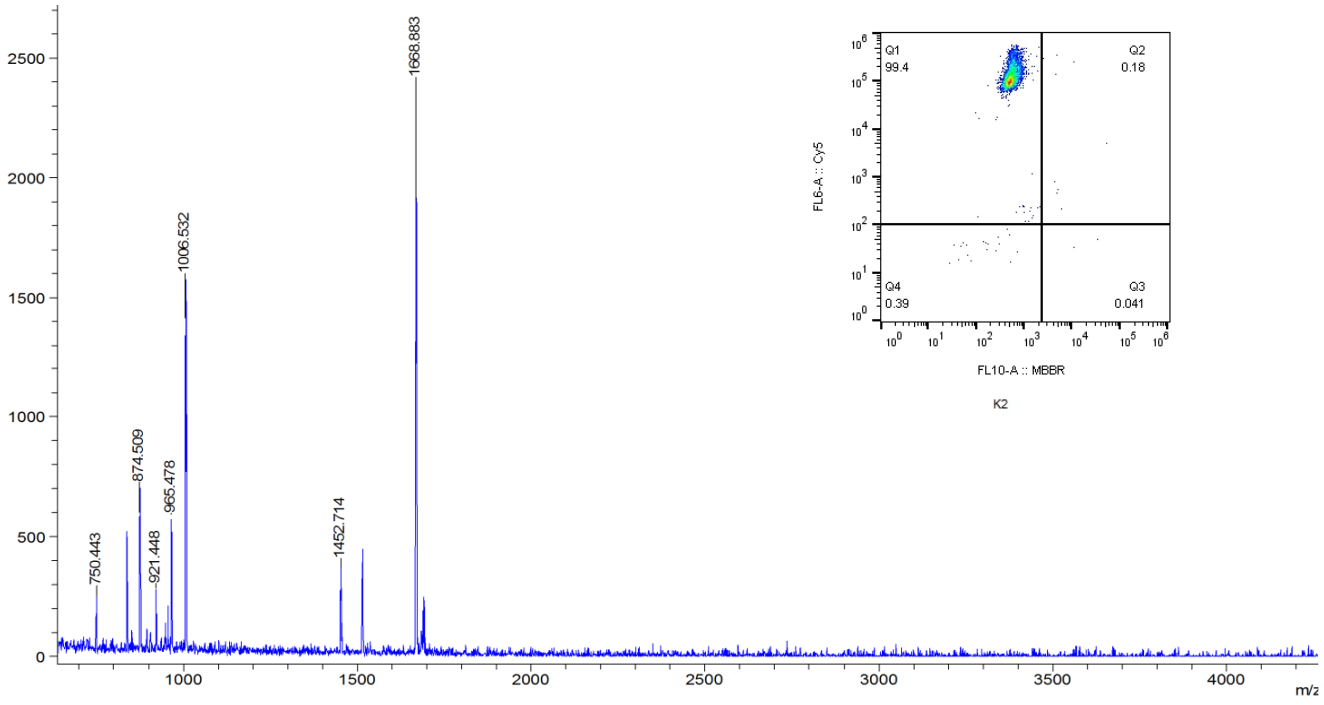


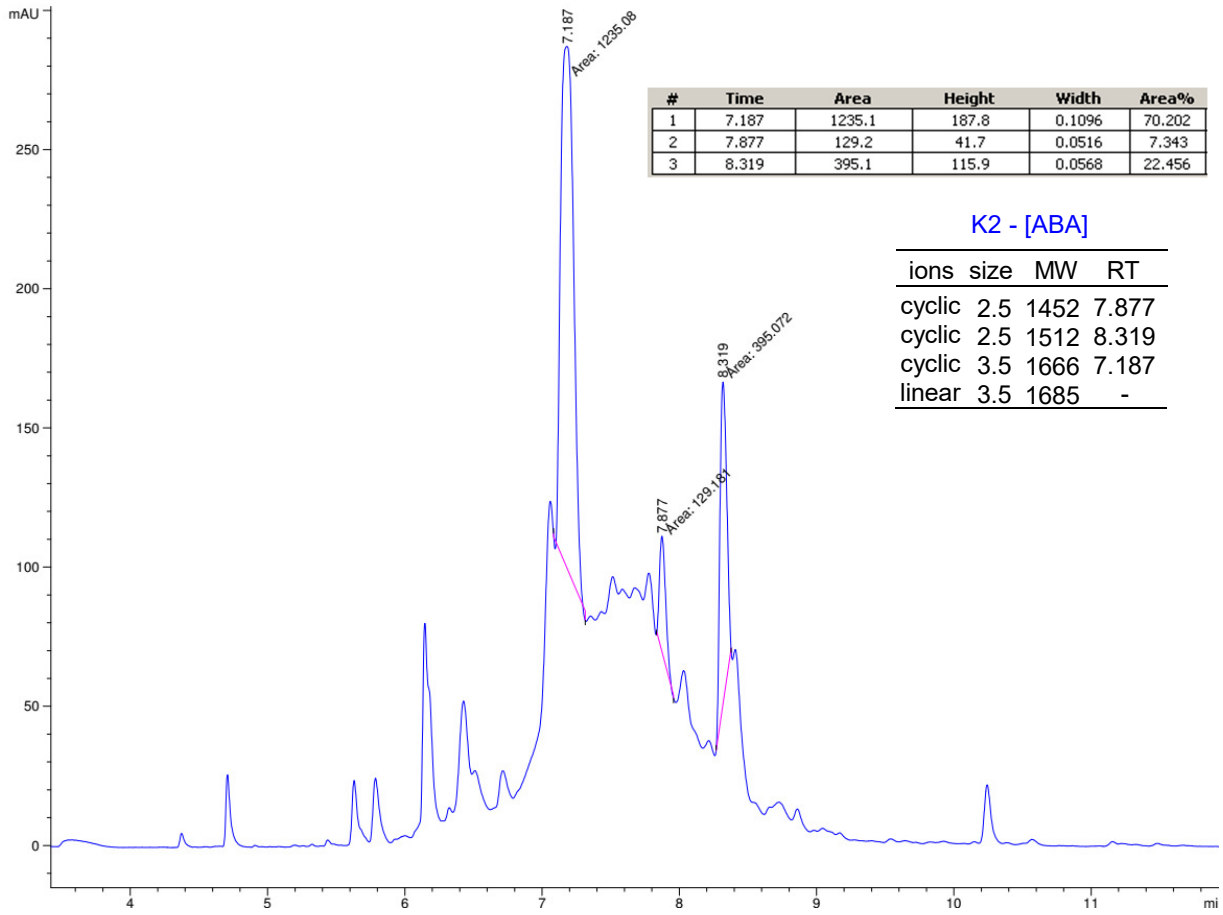

Max: 13961
Exact Mass: 1512.55
cyclic - 2.5 mer
[M+H+]
281.1
217.1
140.9
514.3
2379.7
990.0
842.2
757.9
597.7
1752.2
1876.6
1813.9
m/z


Max: 6451
Exact Mass: 1753.64
linear - 3.5 mer
[M+2H+]
[M+H+]
140.9
195.9
213.9
281.0
757.1
877.8
904.0
778.2
309.8
1539.9
1756.3
1899.8
2002.7
m/z

K2-[ABA]: Complete cyclization was observed on 10 µm & 160 µm beads.



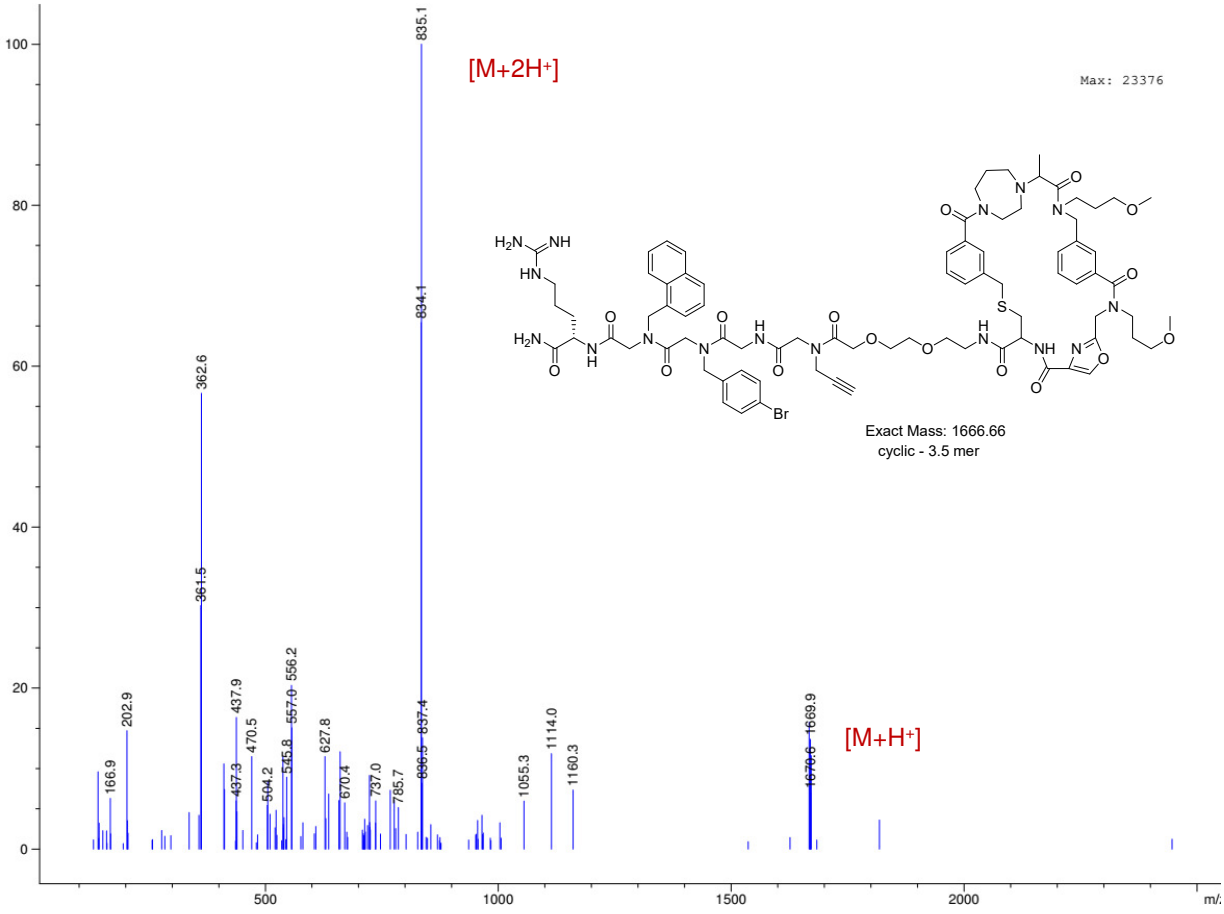


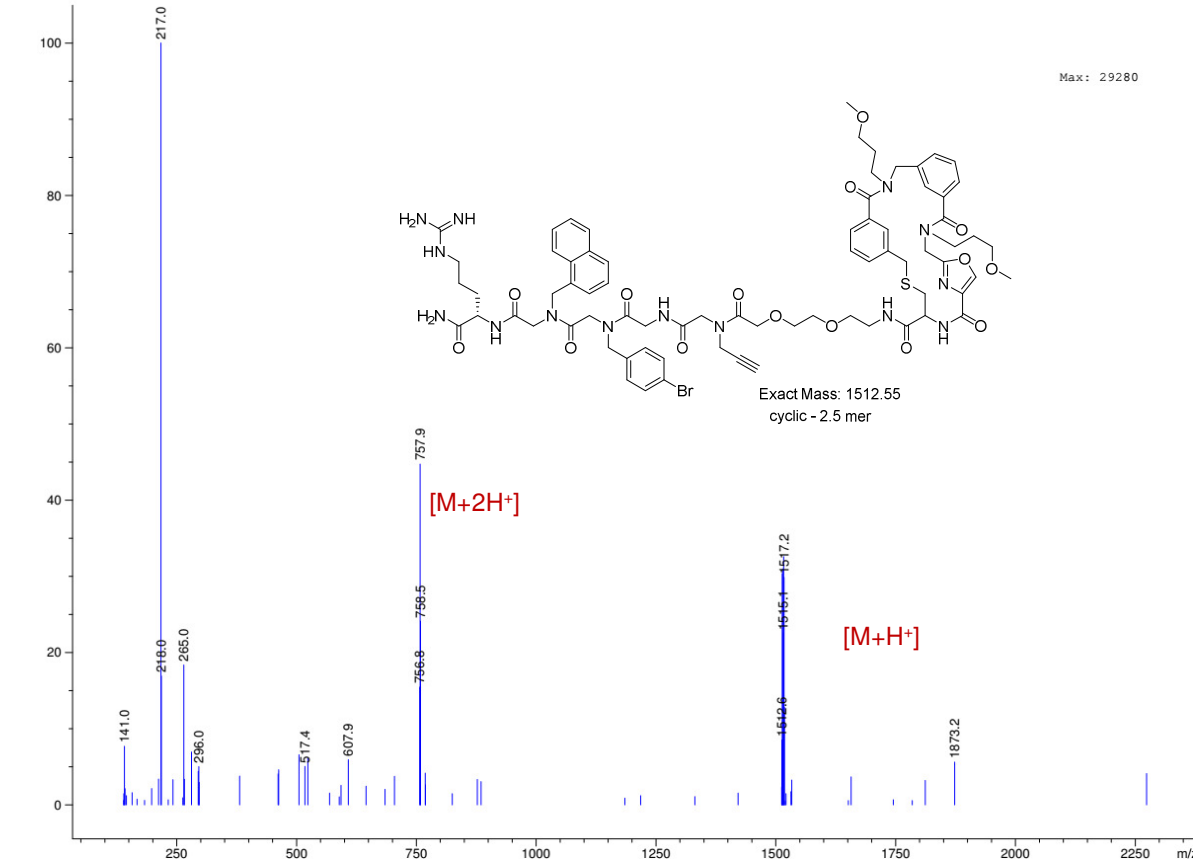


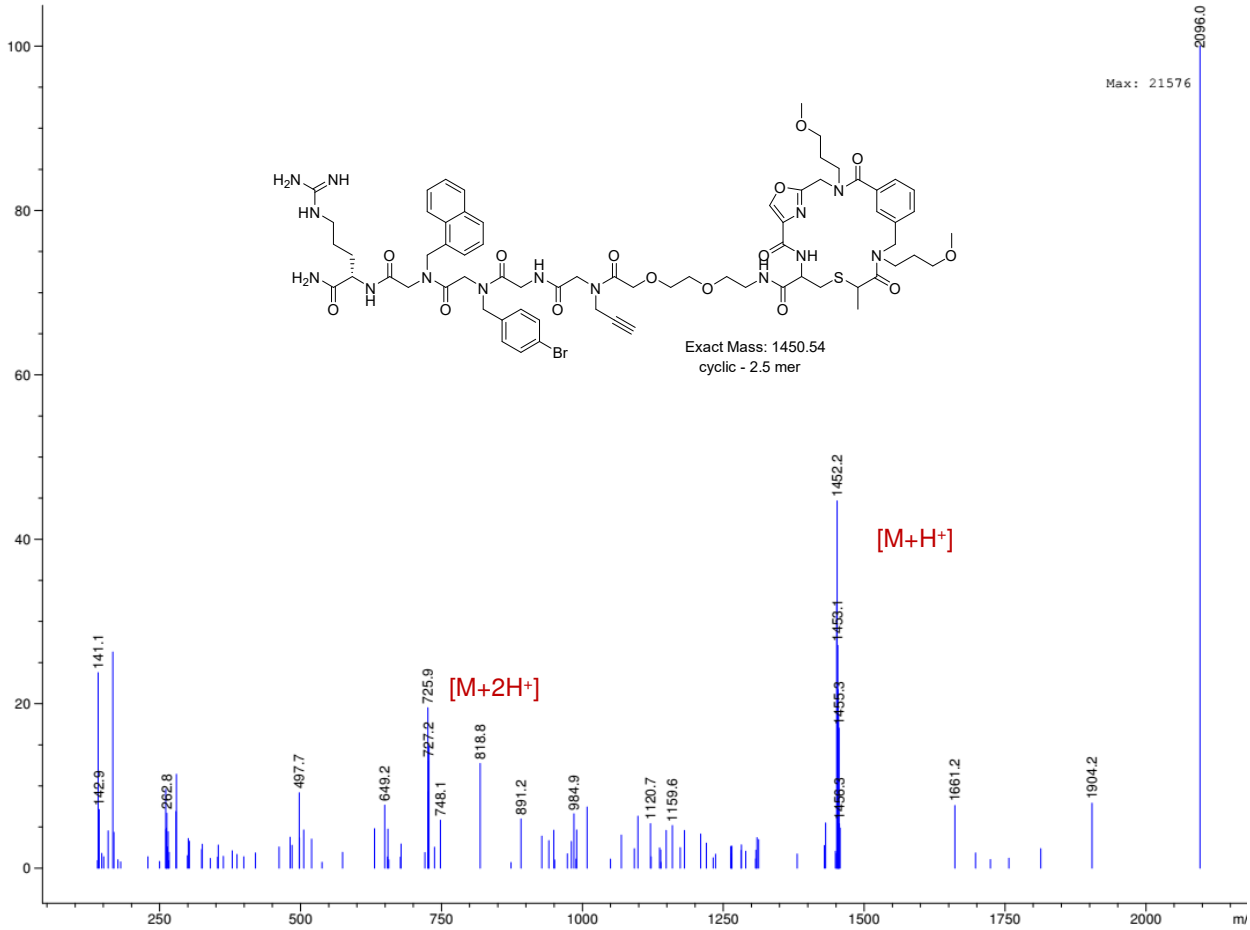
#	Time	Area	Height	Width	Area%
1	7.187	1235.1	187.8	0.1096	70.202
2	7.877	129.2	41.7	0.0516	7.343
3	8.319	395.1	115.9	0.0568	22.456

K2 - [ABA]

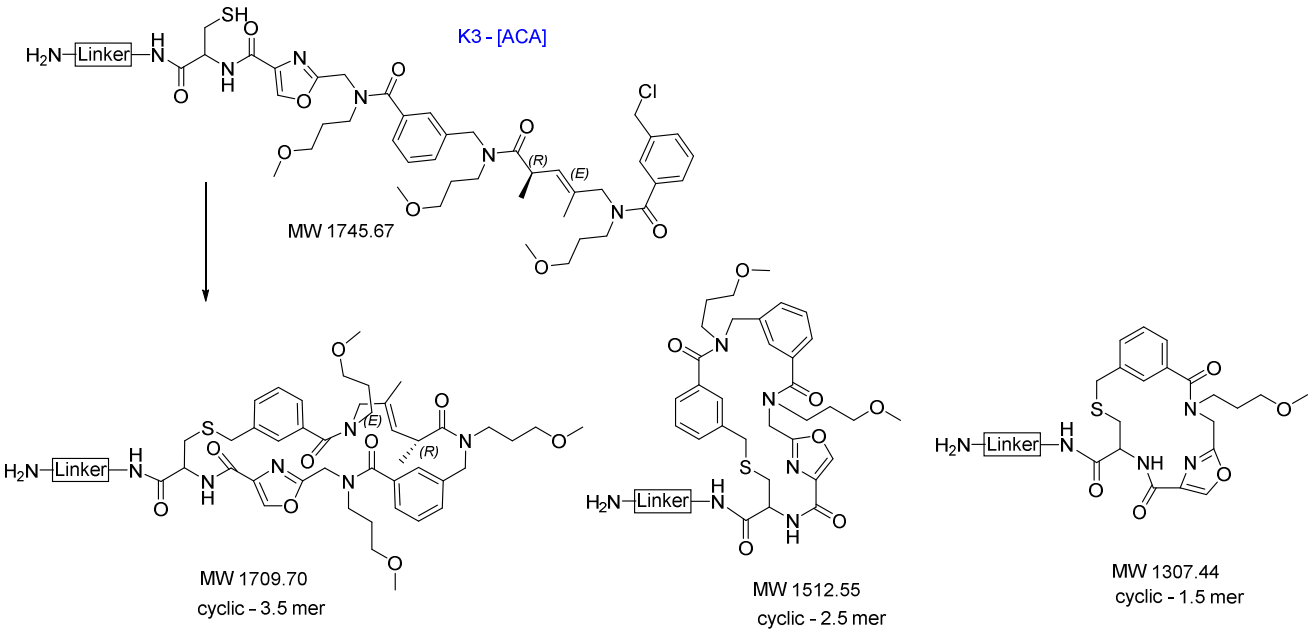
ions	size	MW	RT
cyclic	2.5	1452	7.877
cyclic	2.5	1512	8.319
cyclic	3.5	1666	7.187
linear	3.5	1685	-

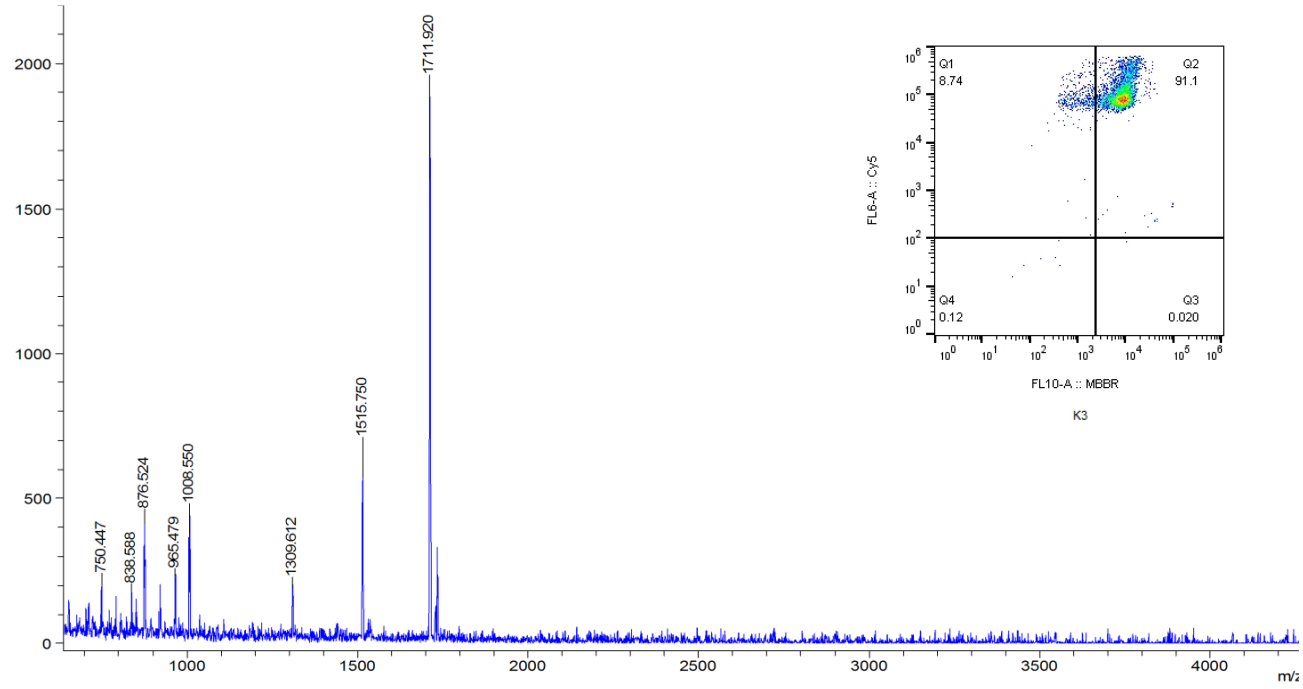


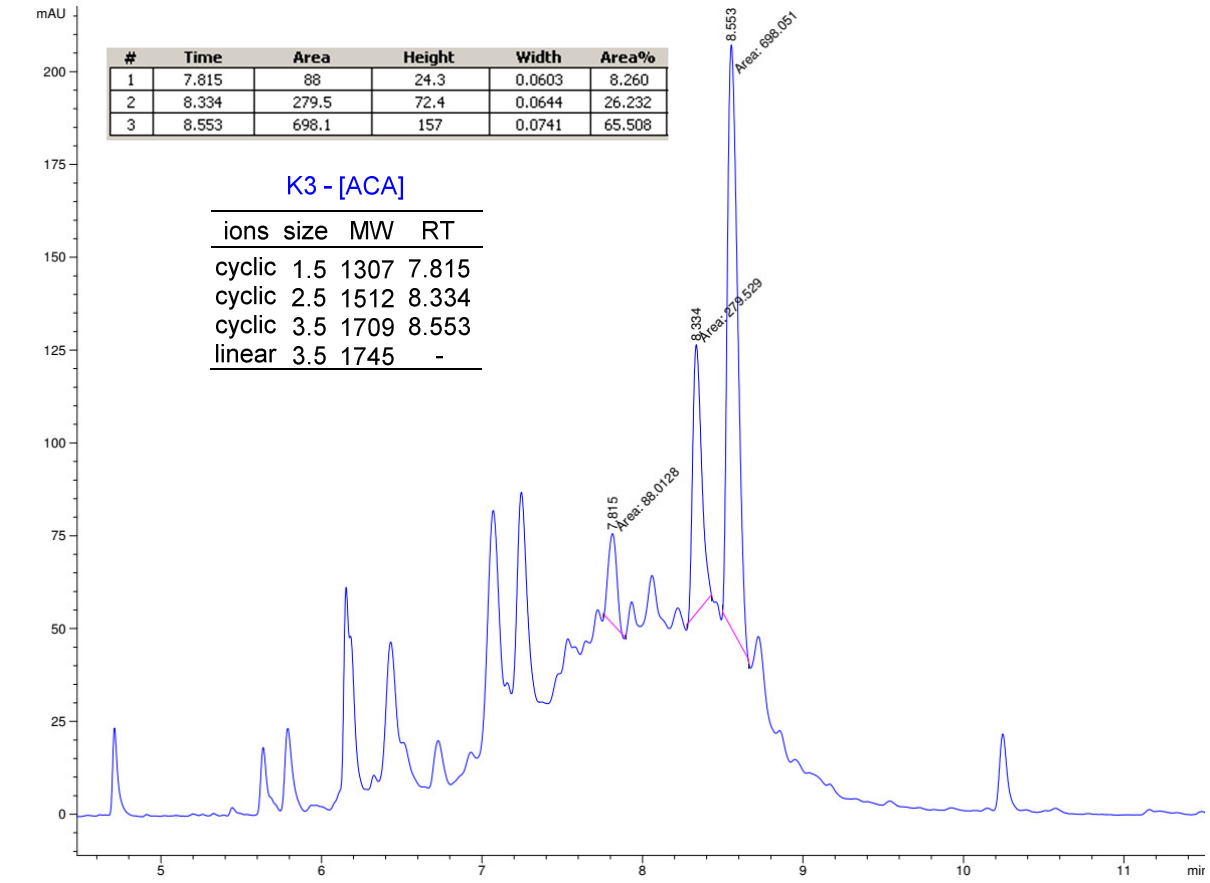

Max: 29280
Exact Mass: 1512.55
cyclic - 2.5 mer
[M+2H+]
[M+H+]
217.0
757.9
1517.2
1516.1
758.5
756.8
265.0
218.0
141.0
296.0
517.4
607.9
1512.6
1873.2


Max: 21576
Exact Mass: 1450.54
cyclic - 2.5 mer
[M+H+]
[M+2H+]
2096.0
1452.2
1453.1
1455.3
725.9
727.2
818.8
141.1
142.9
262.8
497.7
649.2
748.1
891.2
984.9
1120.7
1159.6
1661.2
1904.2

K3-[ACA]: Incomplete cyclization was observed on both 10 µm and 160 µm beads.



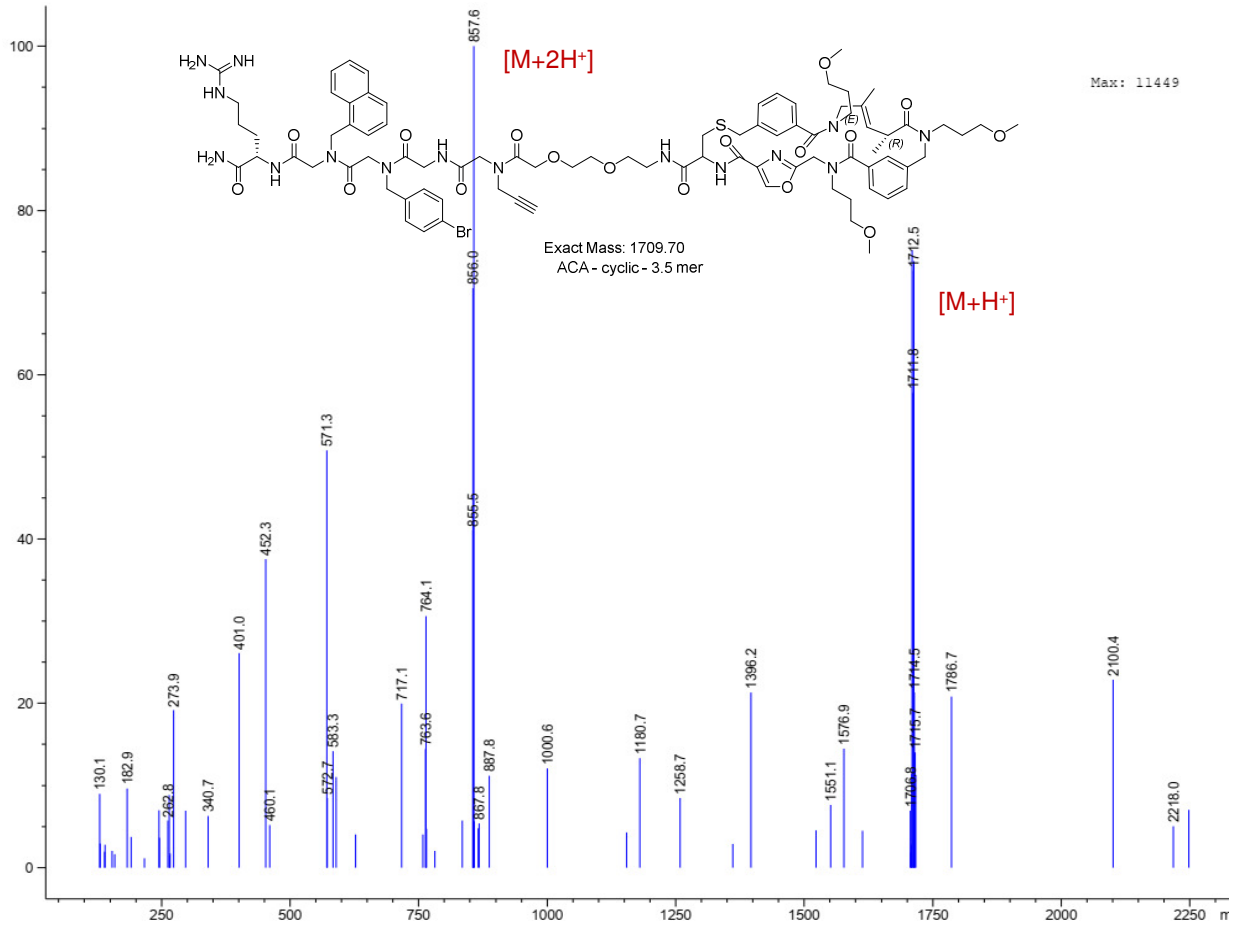


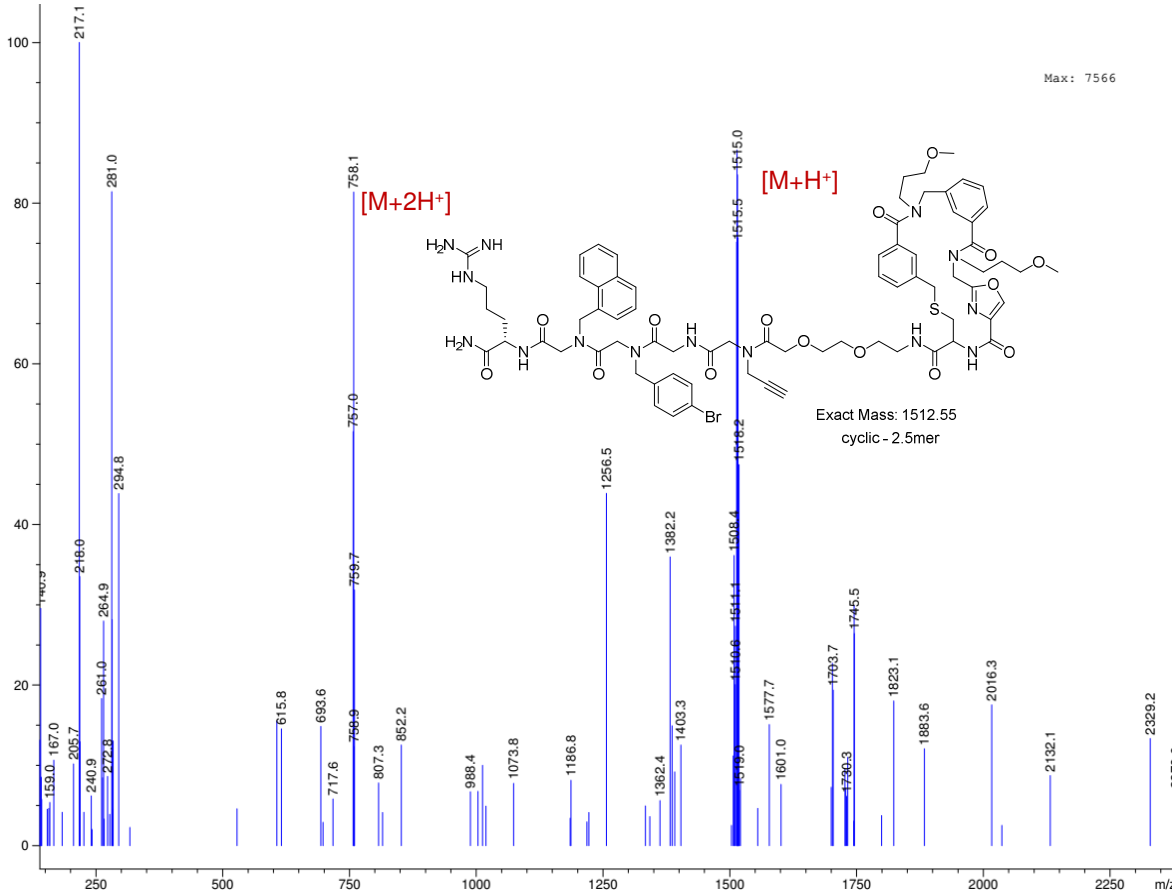


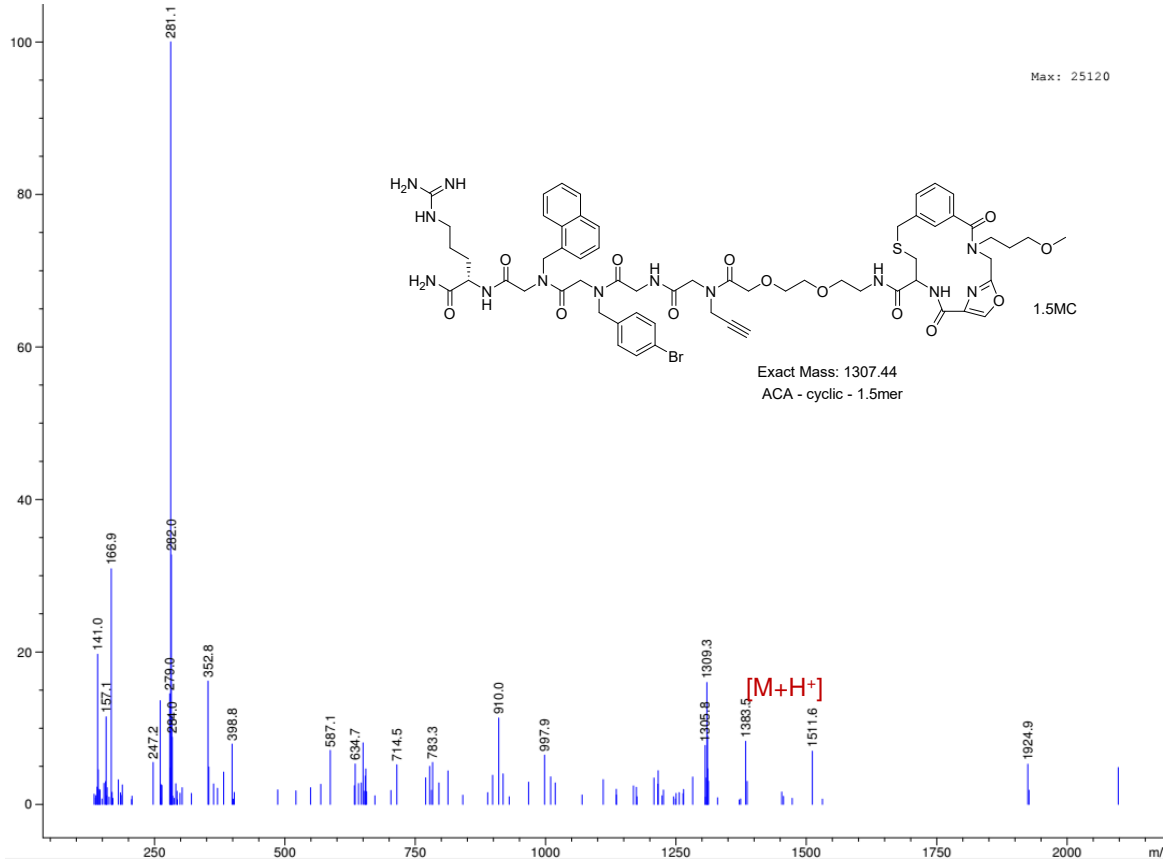
#	Time	Area	Height	Width	Area%
1	7.815	88	24.3	0.0603	8.260
2	8.334	279.5	72.4	0.0644	26.232
3	8.553	698.1	157	0.0741	65.508

K3 - [ACA]

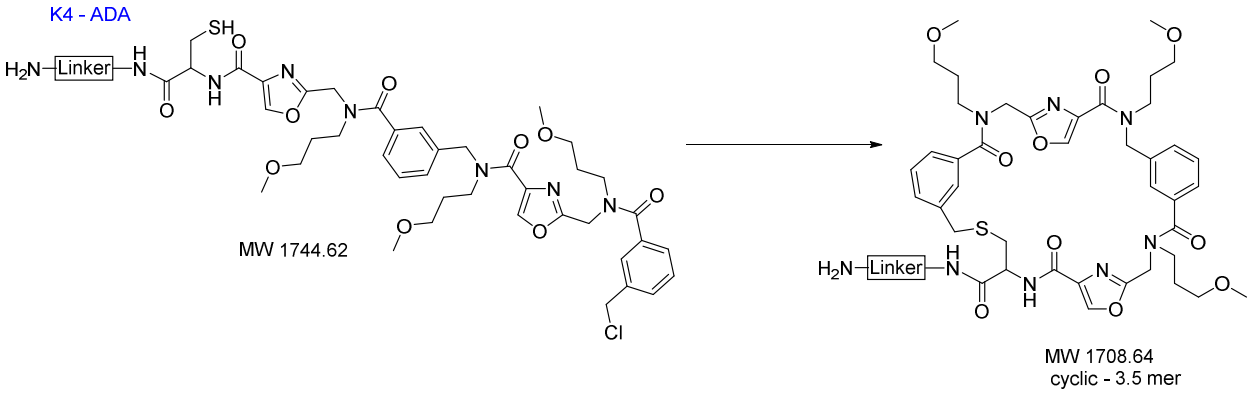
ions	size	MW	RT
cyclic	1.5	1307	7.815
cyclic	2.5	1512	8.334
cyclic	3.5	1709	8.553
linear	3.5	1745	-

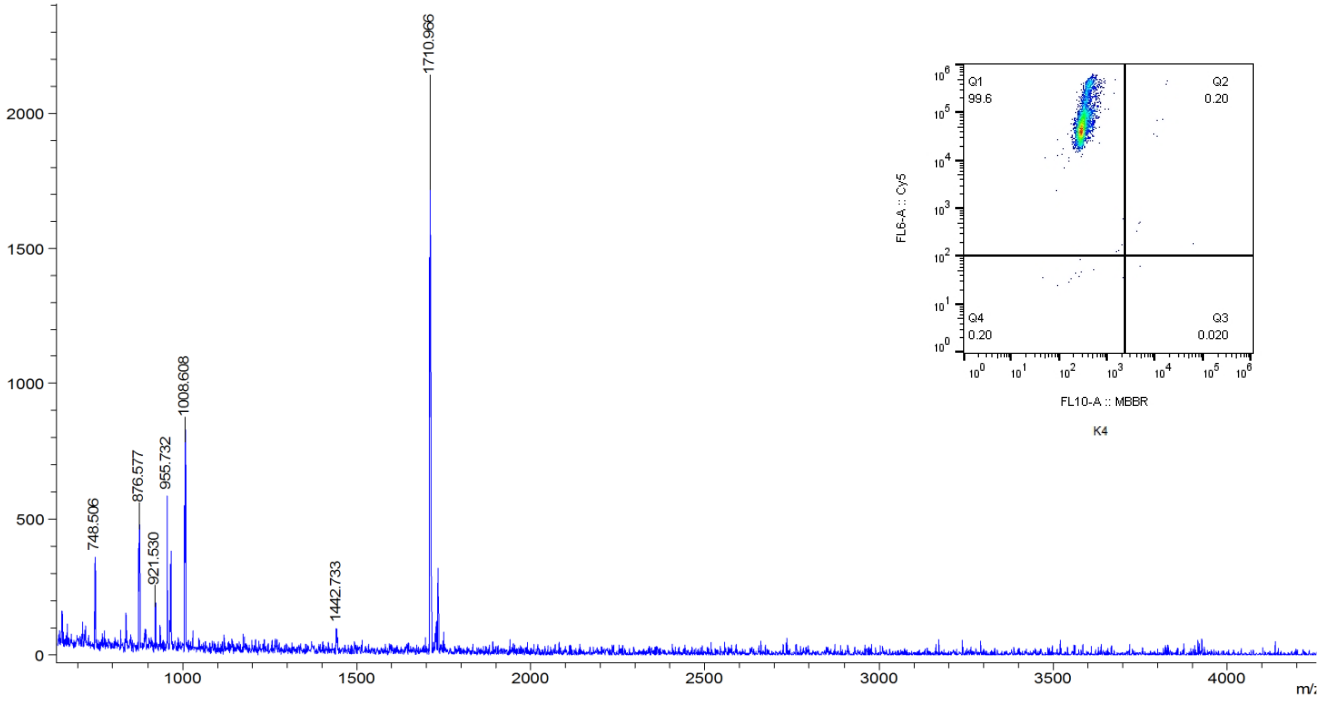


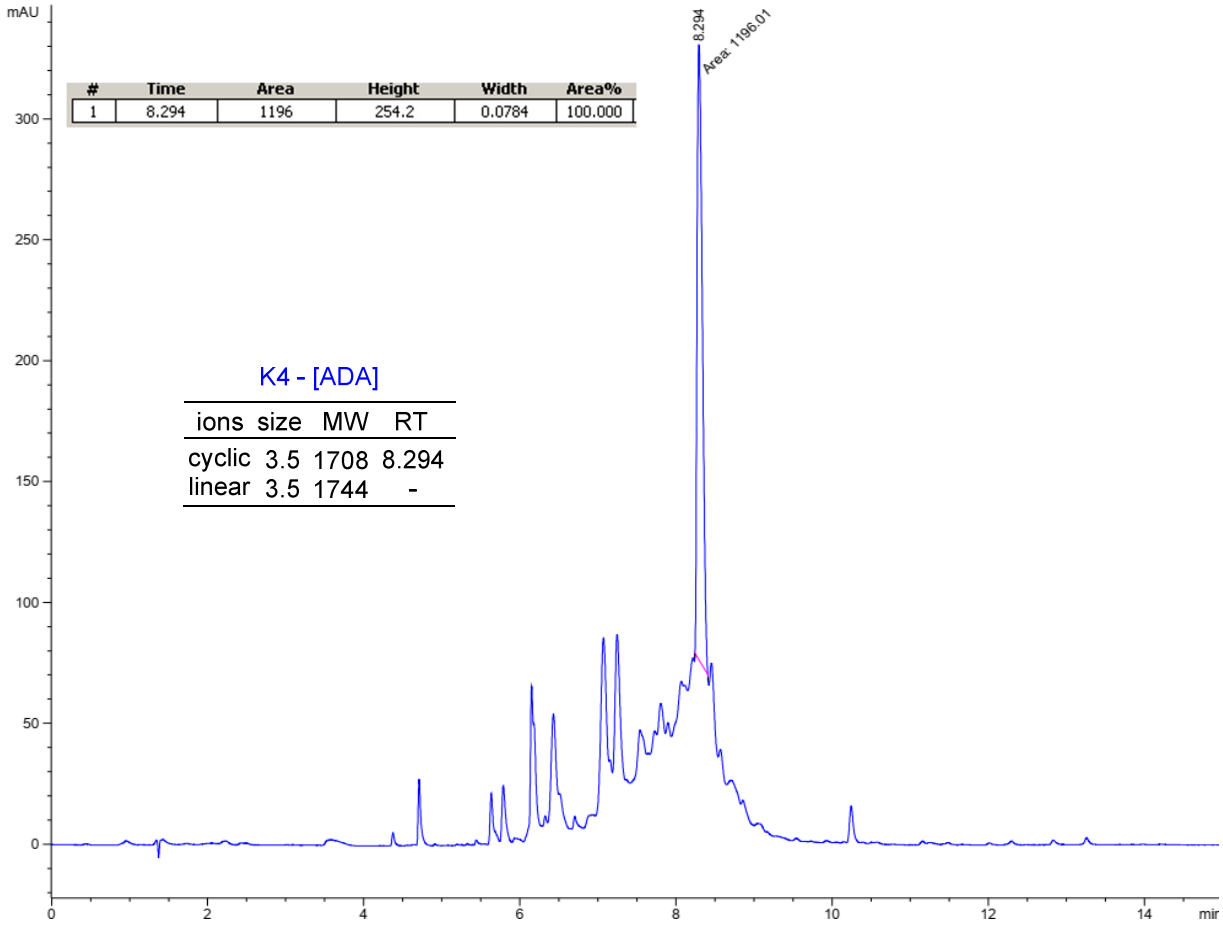

Max: 7566
[M+2H+]
[M+H+]
Exact Mass: 1512.55
cyclic - 2.5mer

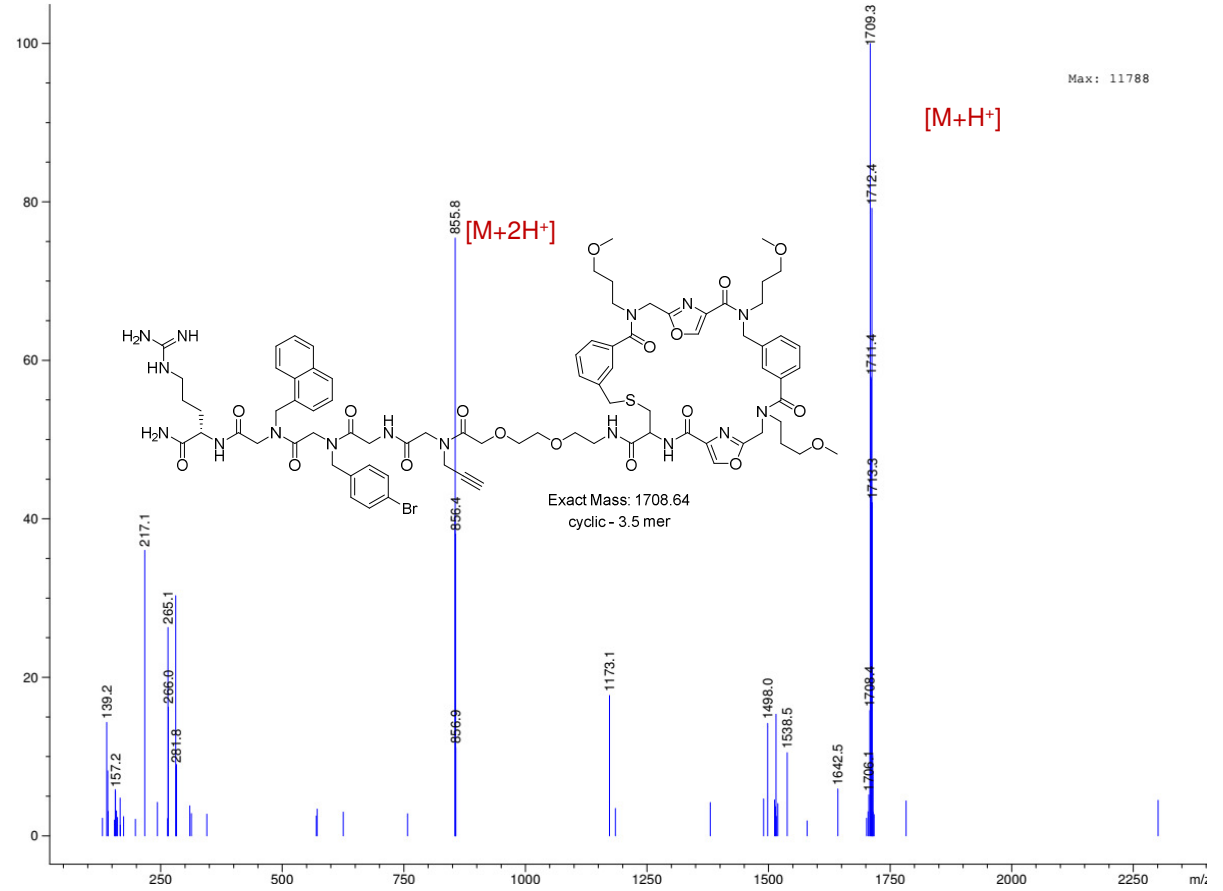

Max: 25120
1.5MC
Exact Mass: 1307.44
ACA - cyclic - 1.5mer
[M+H+]

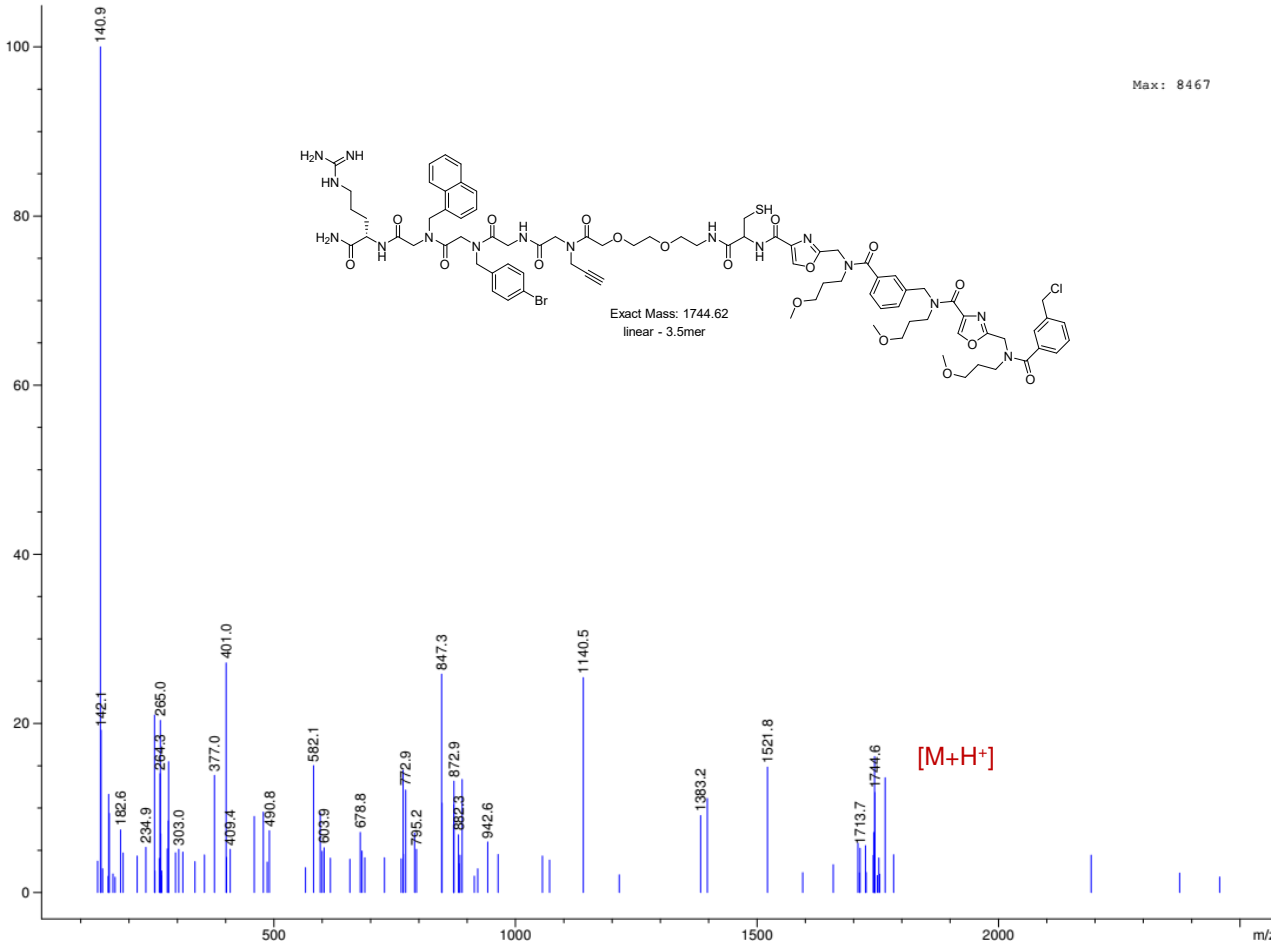
K4-[ADA]: Complete cyclization was observed 10 µm & 160 µm beads.



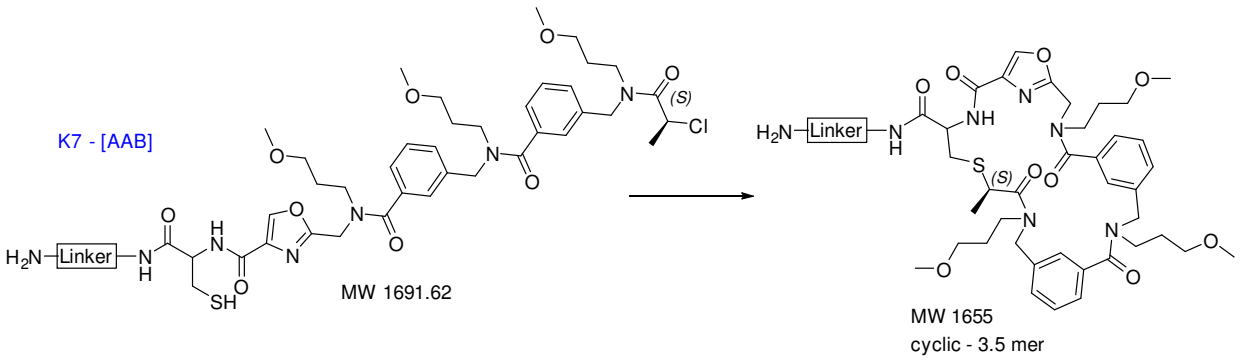


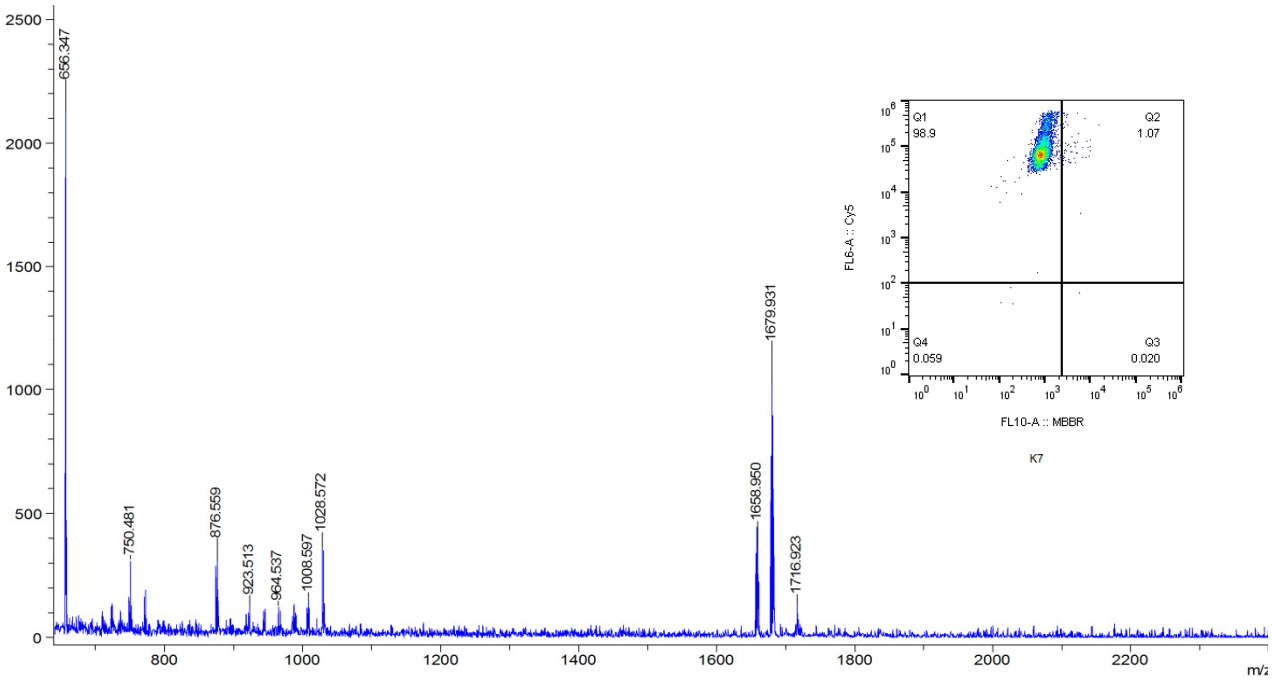

mAU
8.294
Area: 1196.01
Time Area Height Width Area%
1 8.294 1196 254.2 0.0784 100.000
K4 - [ADA]
ions size MW RT
cyclic 3.5 1708 8.294
linear 3.5 1744 -
min

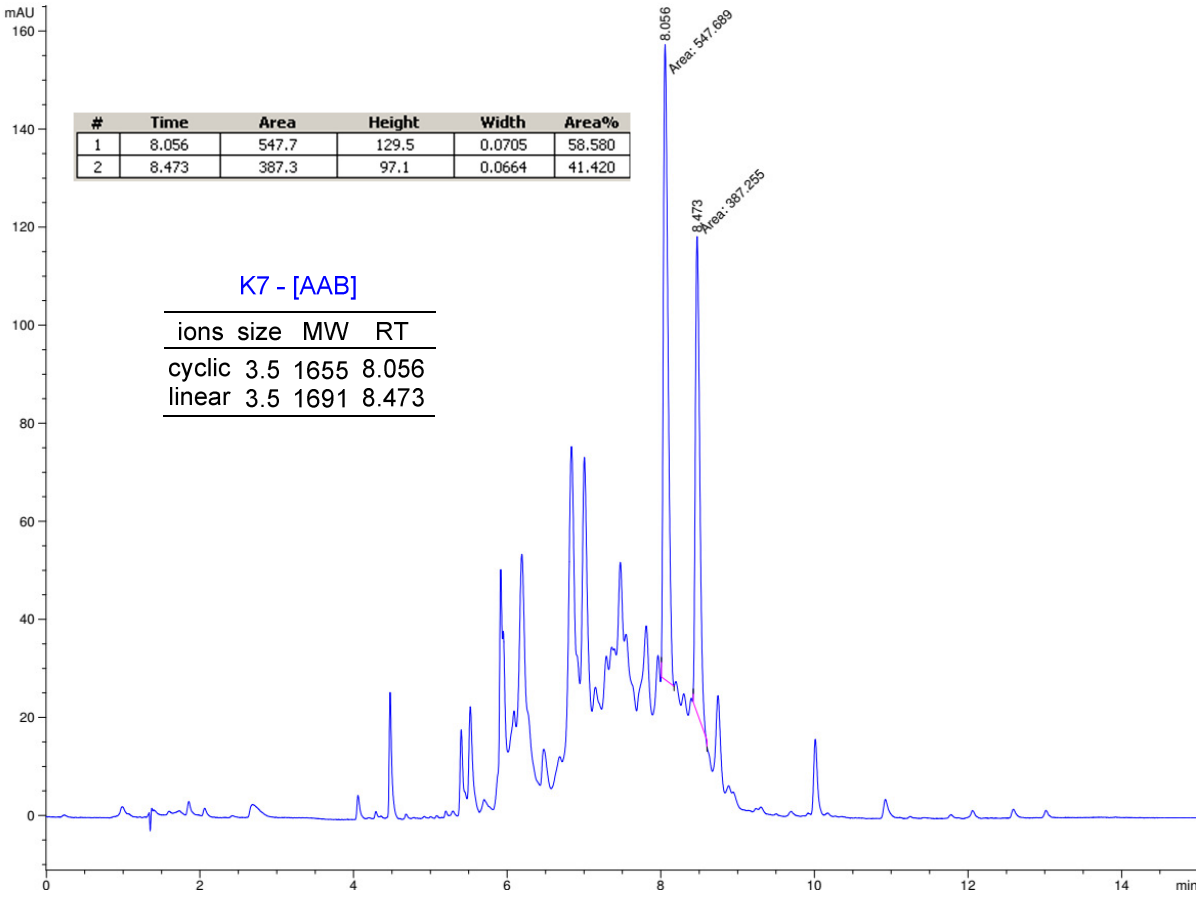

[M+H+]
[M+2H+]
Max: 11788
1709.3
855.8
856.4
856.9
217.1
265.1
266.0
281.8
139.2
157.2
1173.1
1498.0
1538.5
1642.5
Exact Mass: 1708.64
cyclic - 3.5 mer
m/z



K7-[AAB]: Incomplete cyclization was observed on 10 µm but was complete on 160 µm beads.



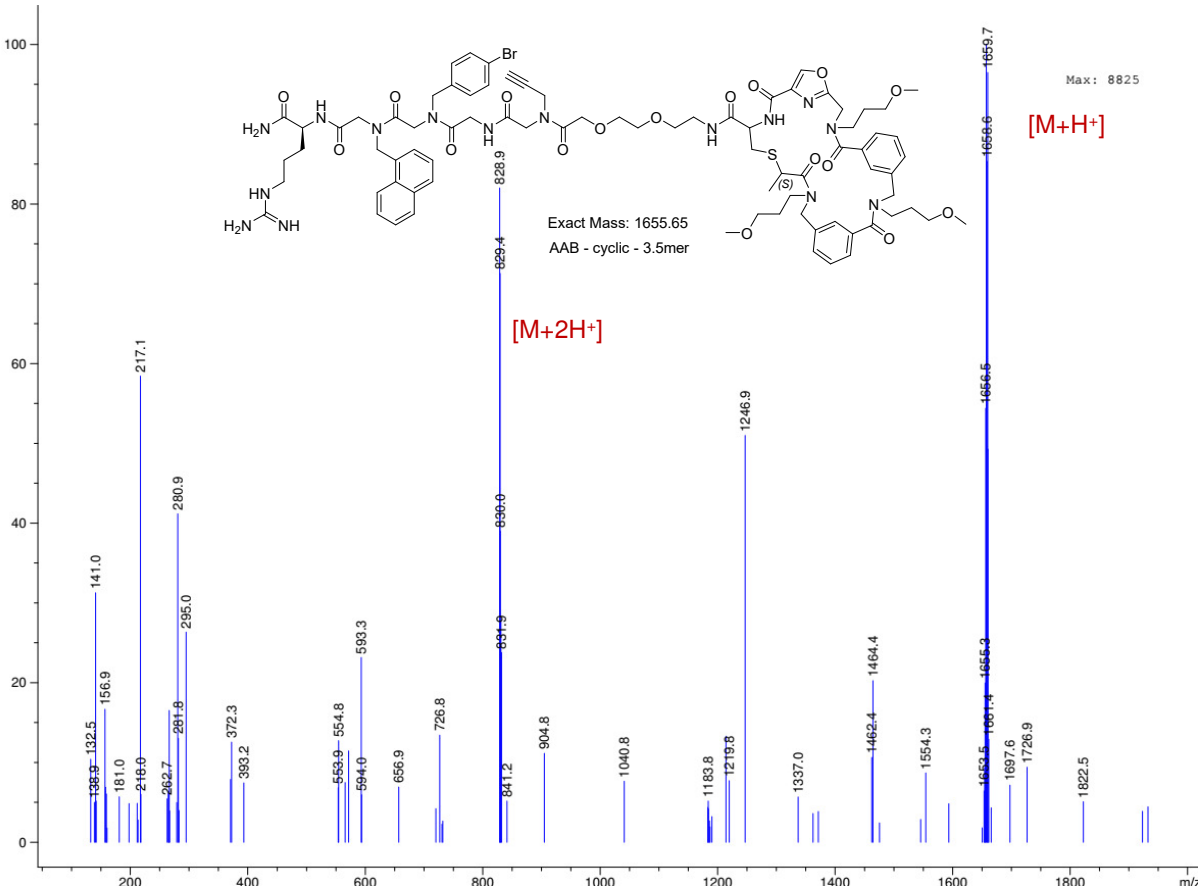


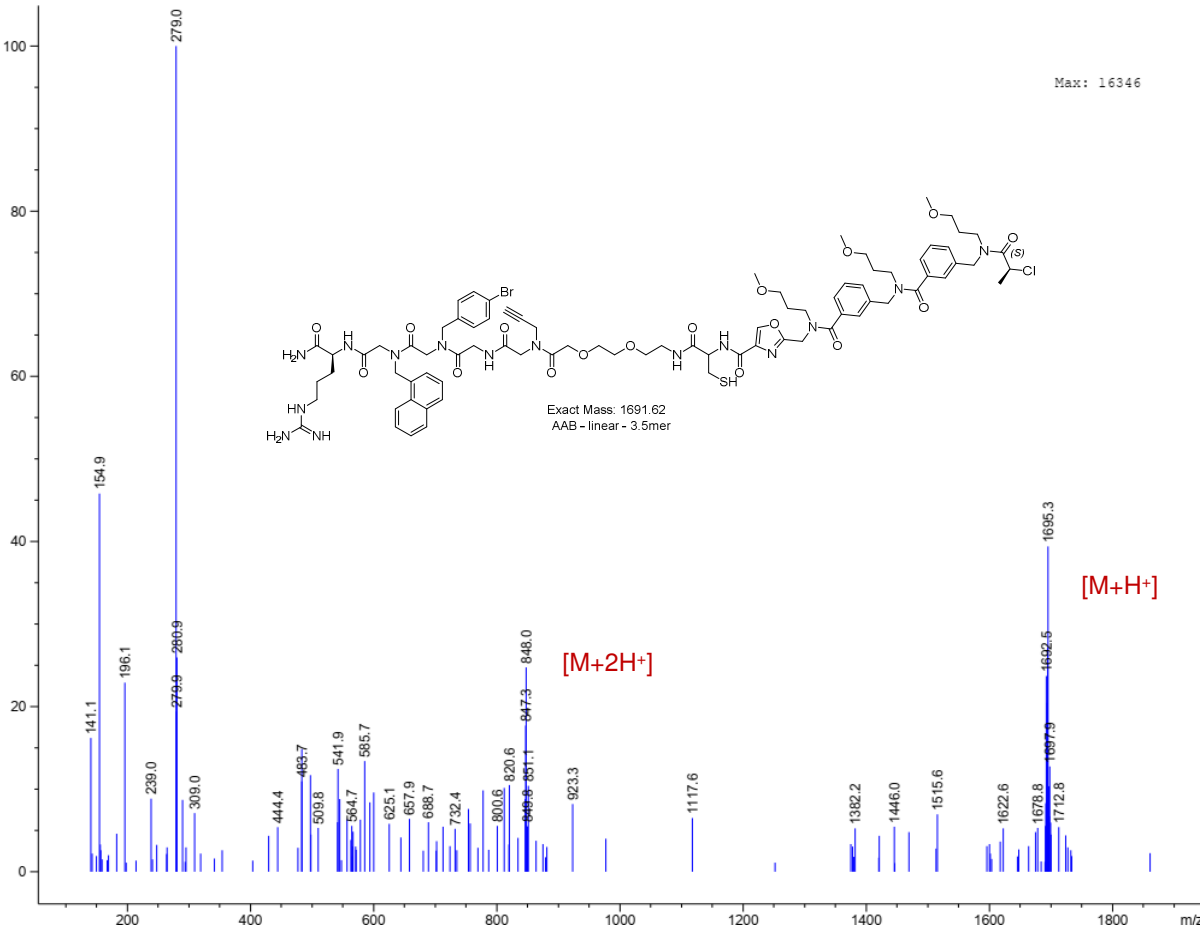


#	Time	Area	Height	Width	Area%
1	8.056	547.7	129.5	0.0705	58.580
2	8.473	387.3	97.1	0.0664	41.420

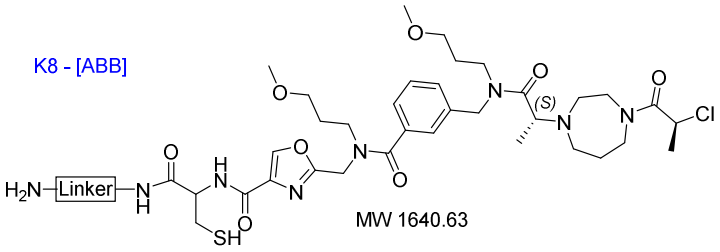
K7 - [AAB]

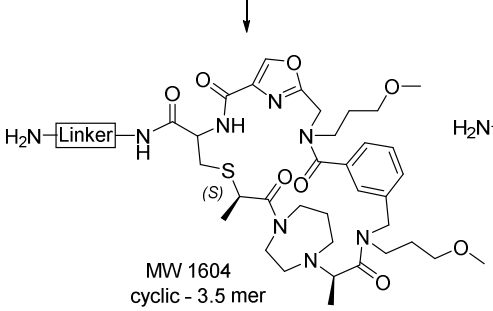
ions	size	MW	RT
cyclic	3.5	1655	8.056
linear	3.5	1691	8.473

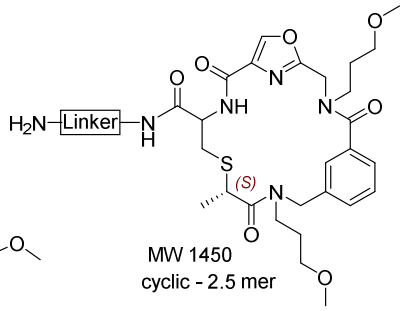

Max: 8825
[M+H+]
[M+2H+]
Exact Mass: 1655.65
AAB - cyclic - 3.5mer
m/z

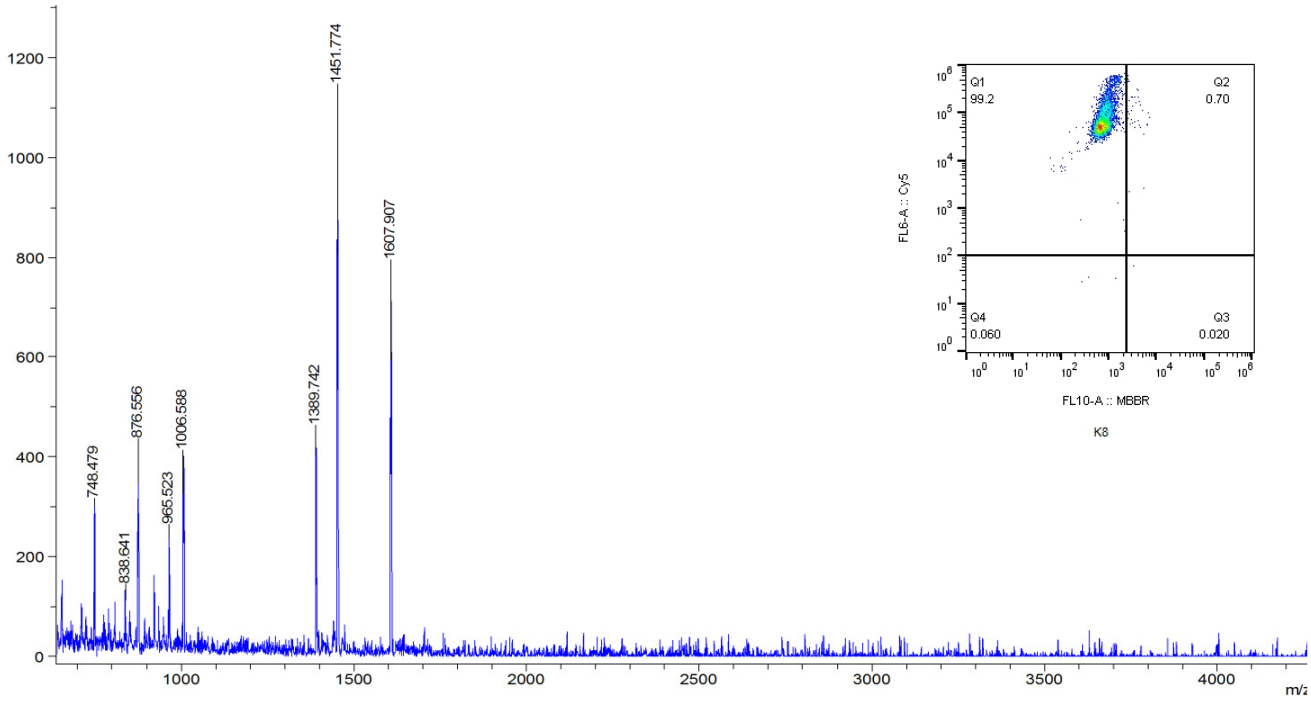

Max: 16346
[M+H+]
[M+2H+]
Exact Mass: 1691.62
AAB - linear - 3.5mer
m/z

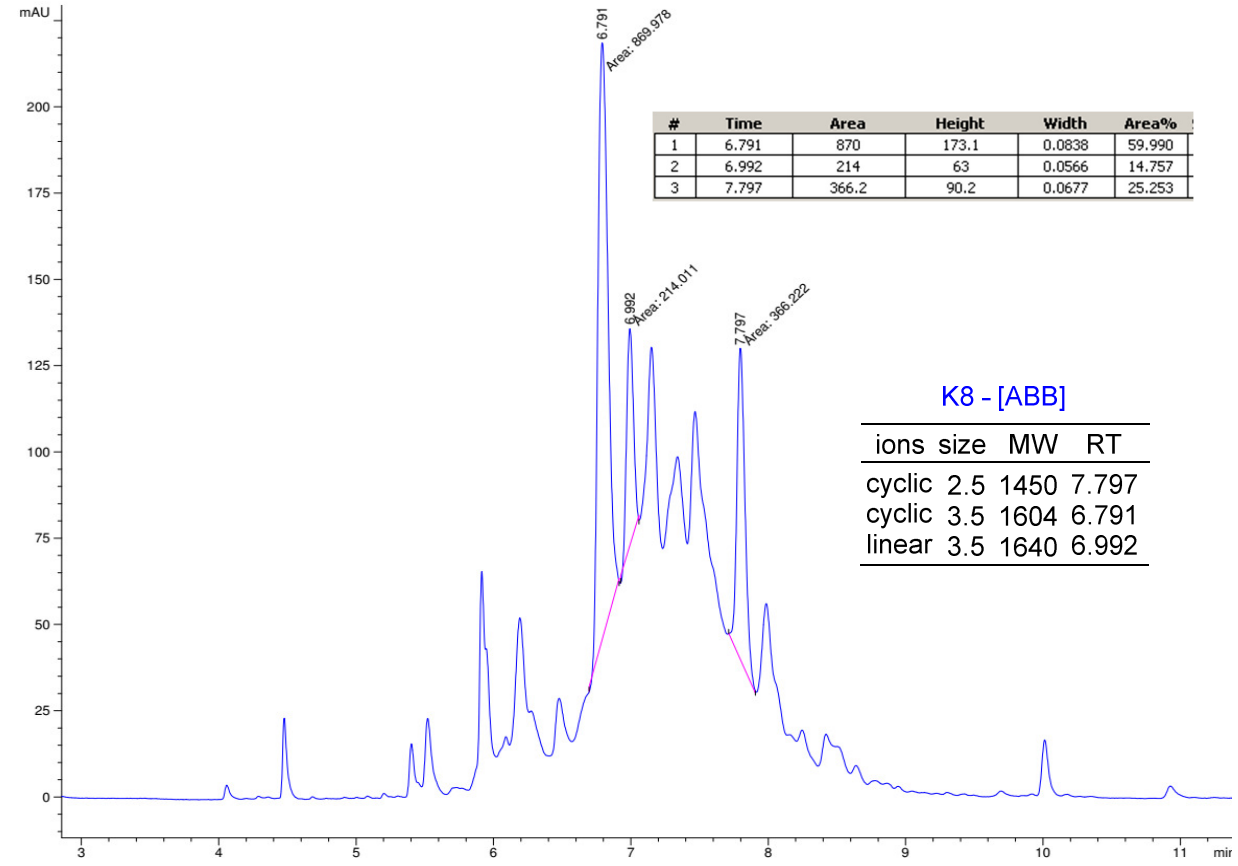
K8-[ABB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm beads.







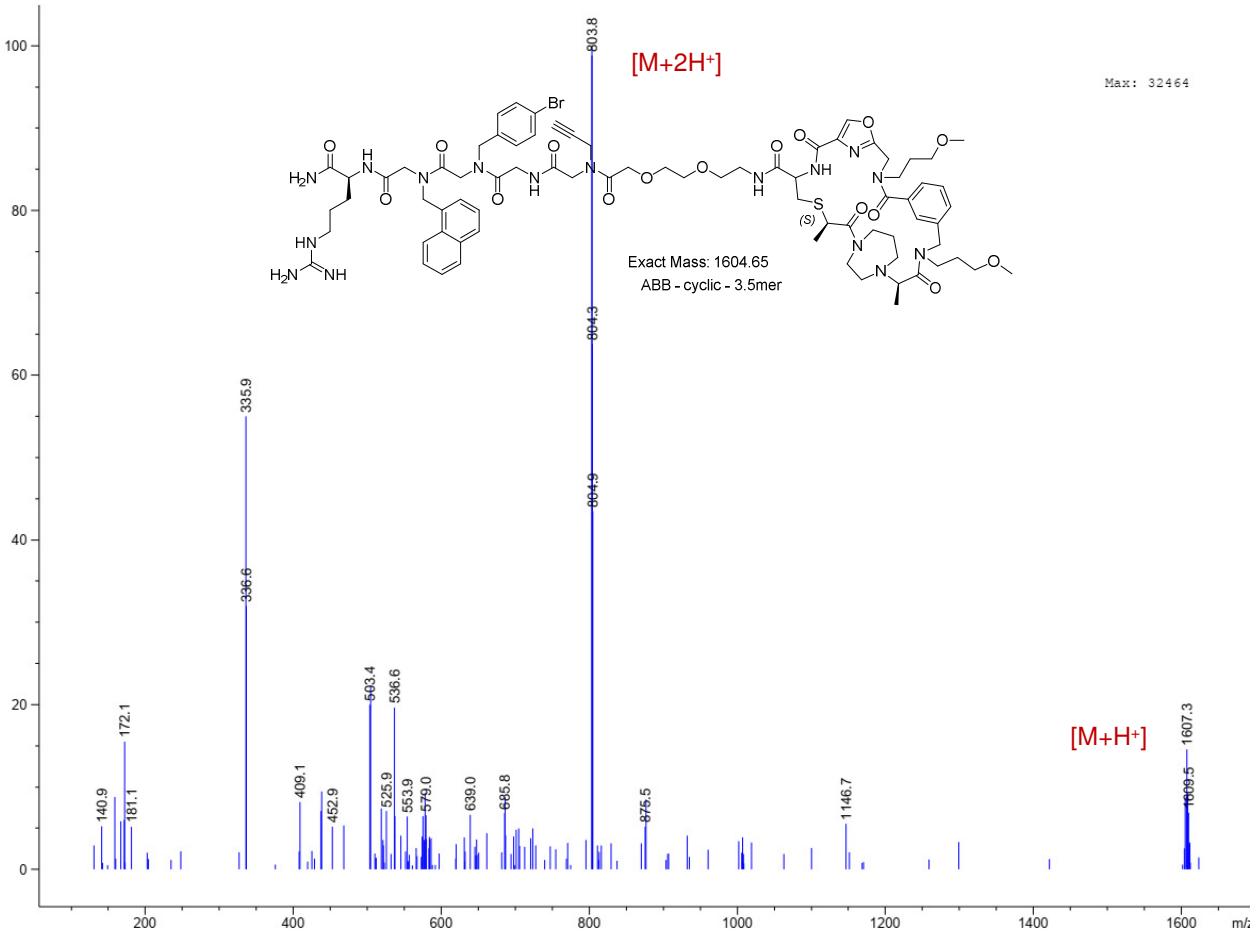


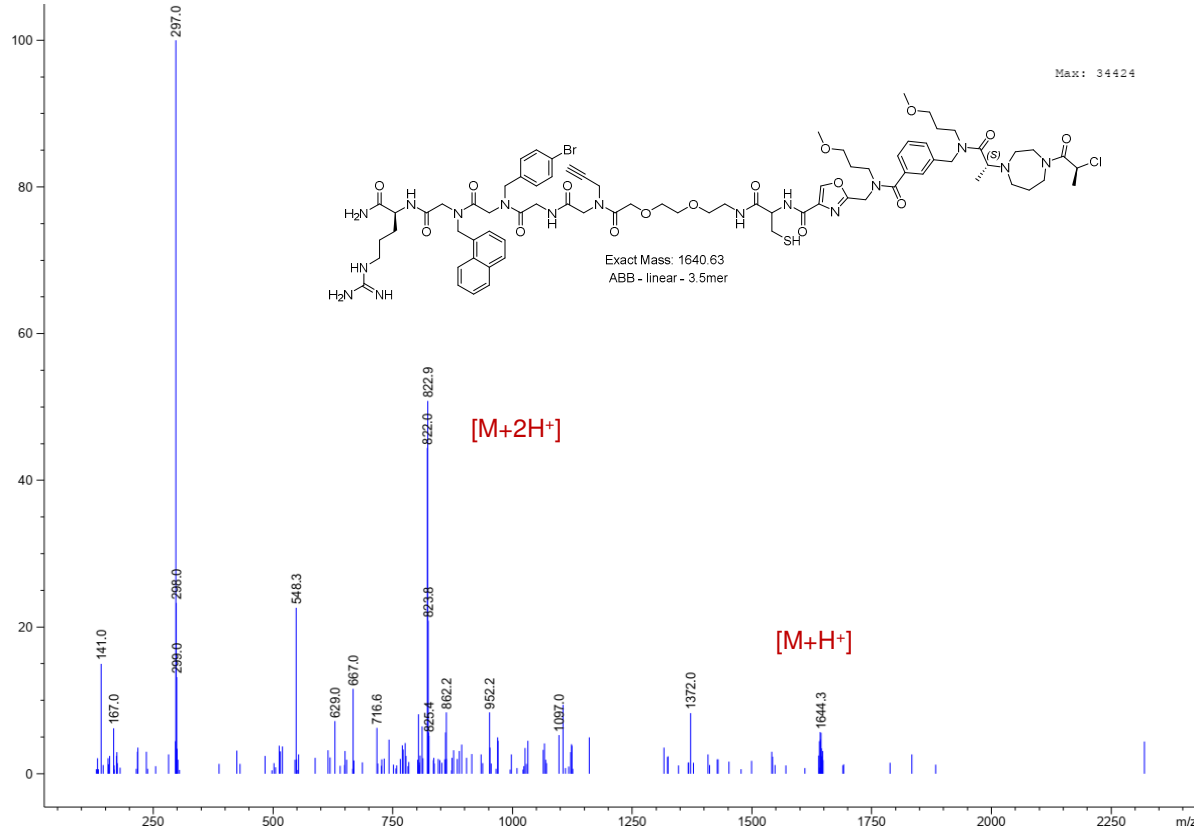


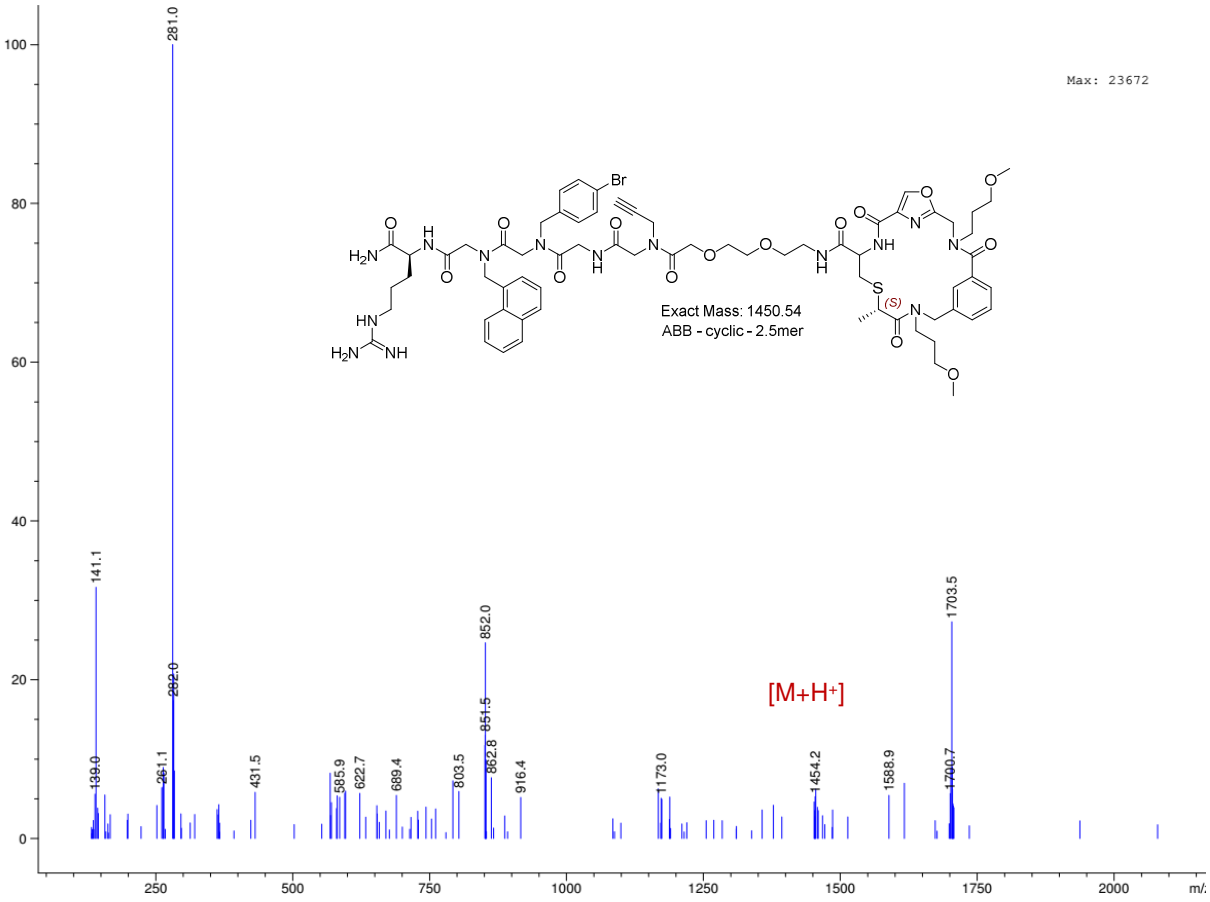
#	Time	Area	Height	Width	Area%
1	6.791	870	173.1	0.0838	59.990
2	6.992	214	63	0.0566	14.757
3	7.797	366.2	90.2	0.0677	25.253

K8 - [ABB]

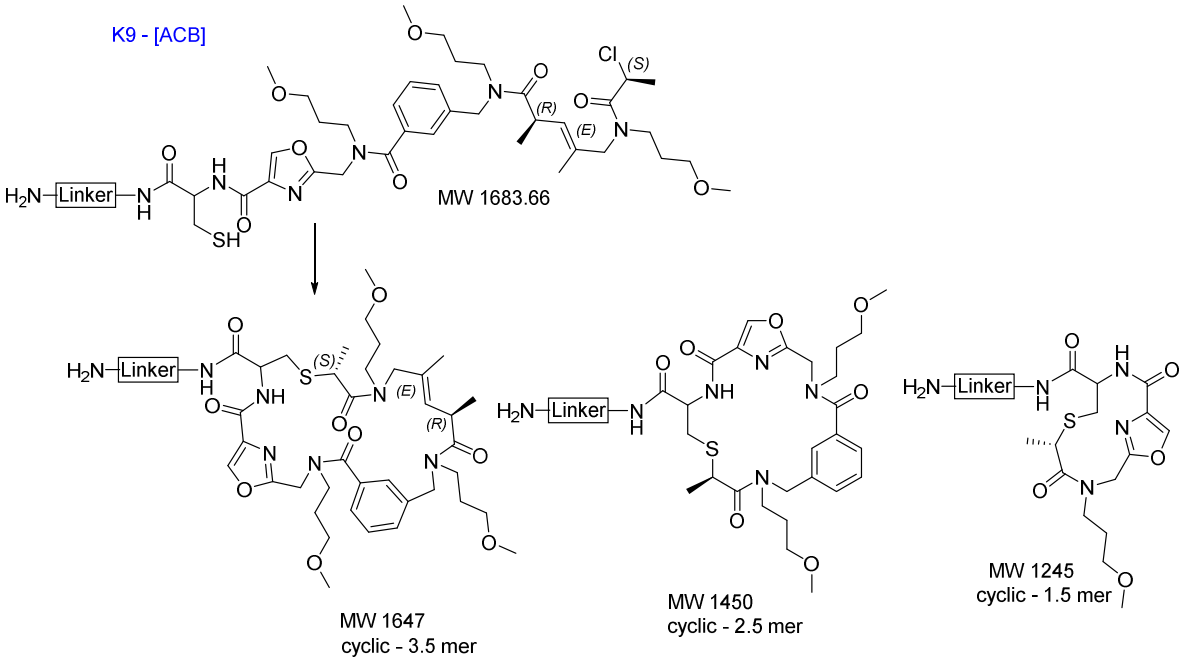
ions	size	MW	RT
cyclic	2.5	1450	7.797
cyclic	3.5	1604	6.791
linear	3.5	1640	6.992

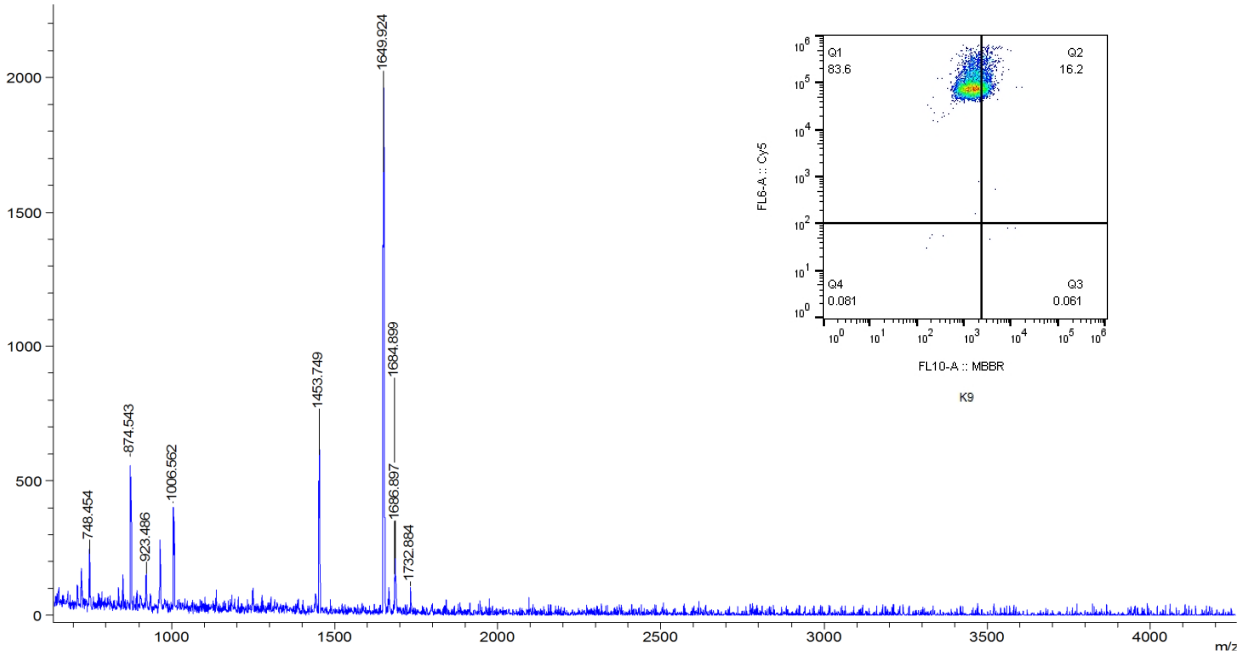


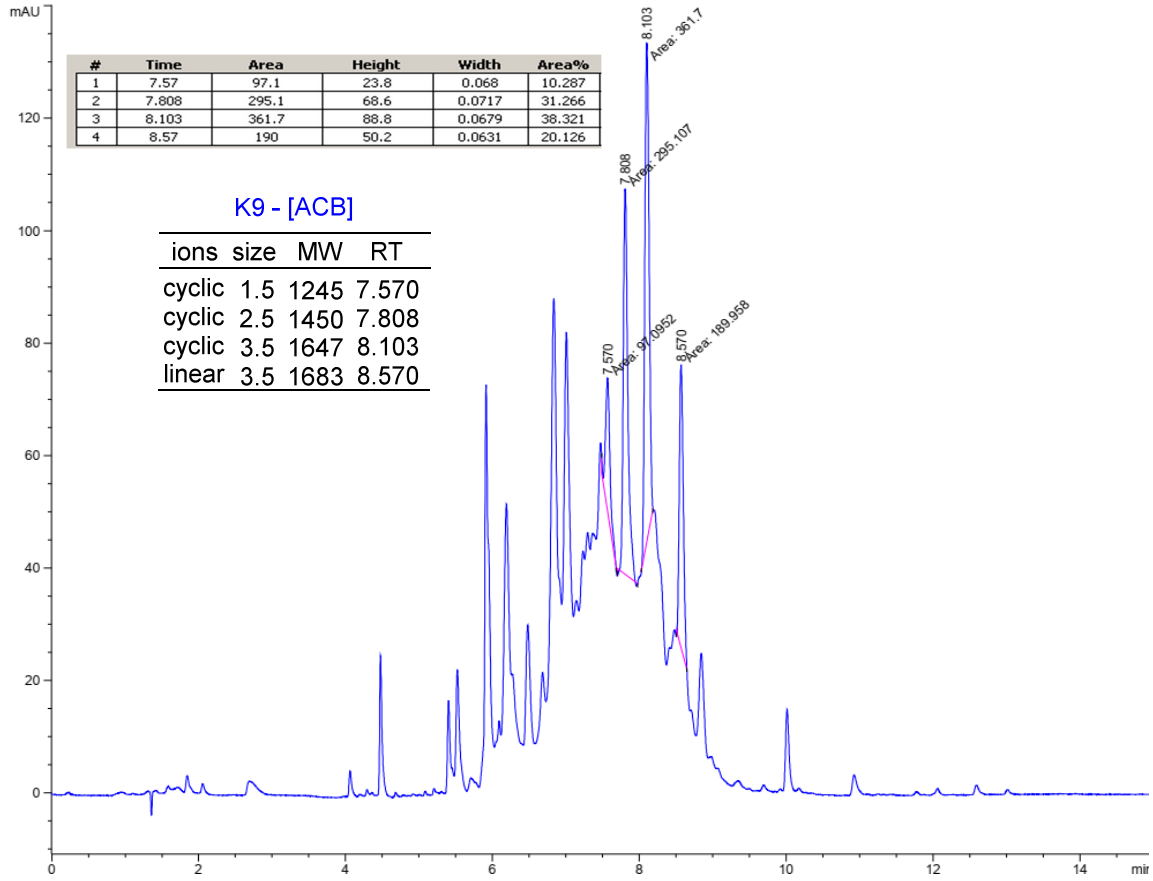

Max: 34424
Exact Mass: 1640.63
ABB - linear - 3.5mer
[M+2H+]
[M+H+]
297.0
822.9
822.0
548.3
141.0
298.0
299.0
823.0
667.0
629.0
716.6
862.2
952.2
1097.0
1372.0
1644.3
167.0


Max: 23672
Exact Mass: 1450.54
ABB - cyclic - 2.5mer
[M+H+]
281.0
141.1
852.0
851.5
862.8
1703.5
1700.7
139.0
261.1
431.5
585.9
622.7
689.4
803.5
916.4
1173.0
1454.2
1588.9

K9-[ACB]: Incomplete cyclization was observed on both 10 µm & 160 µm.



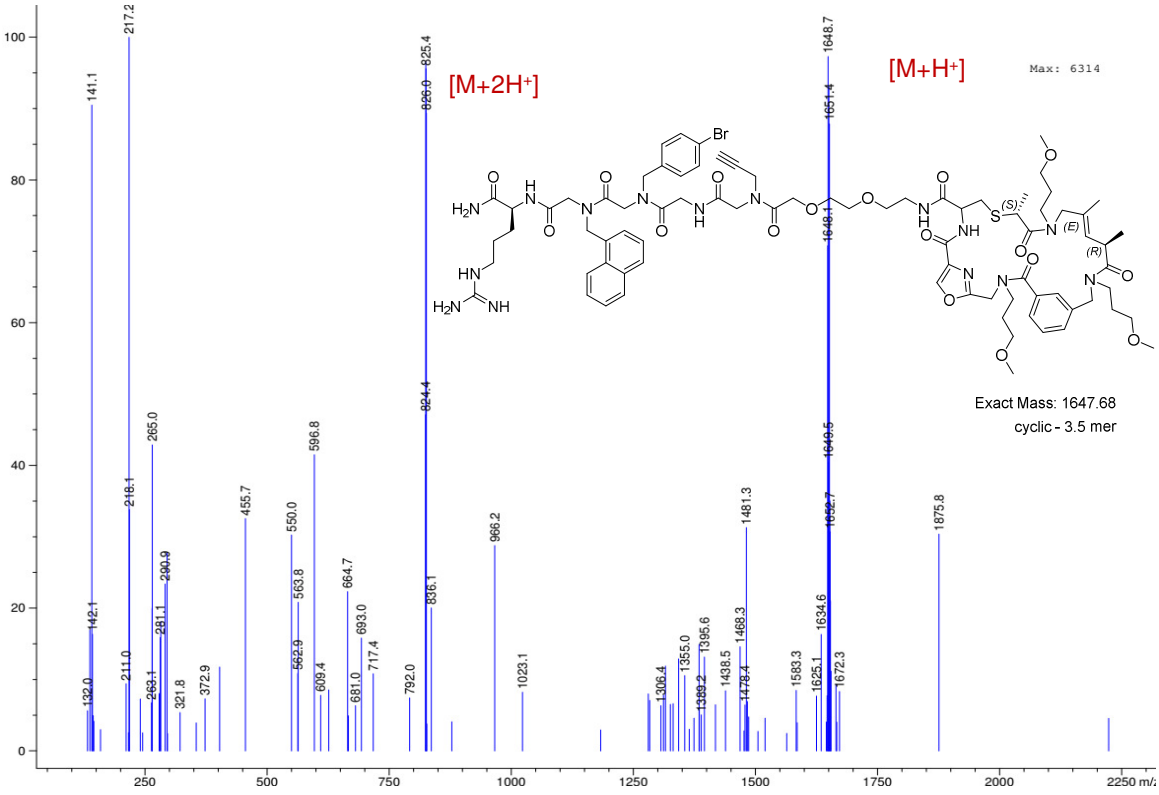


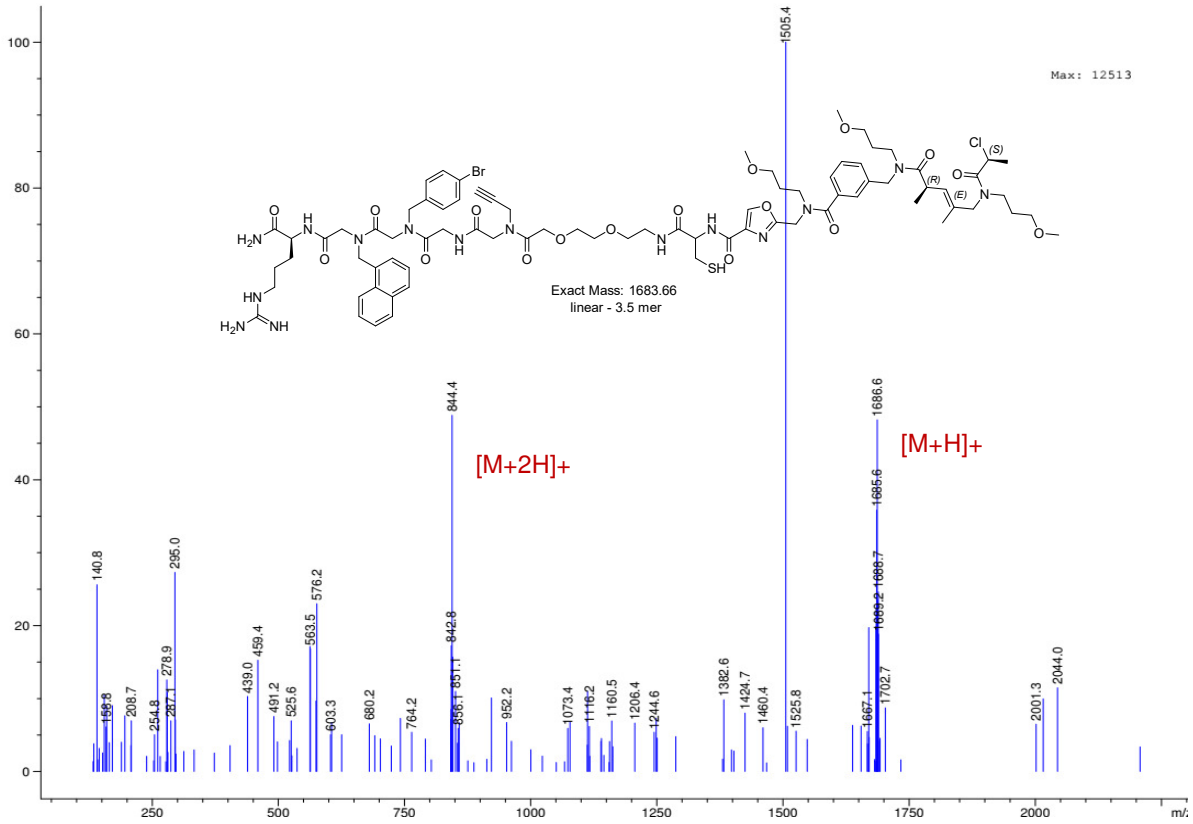


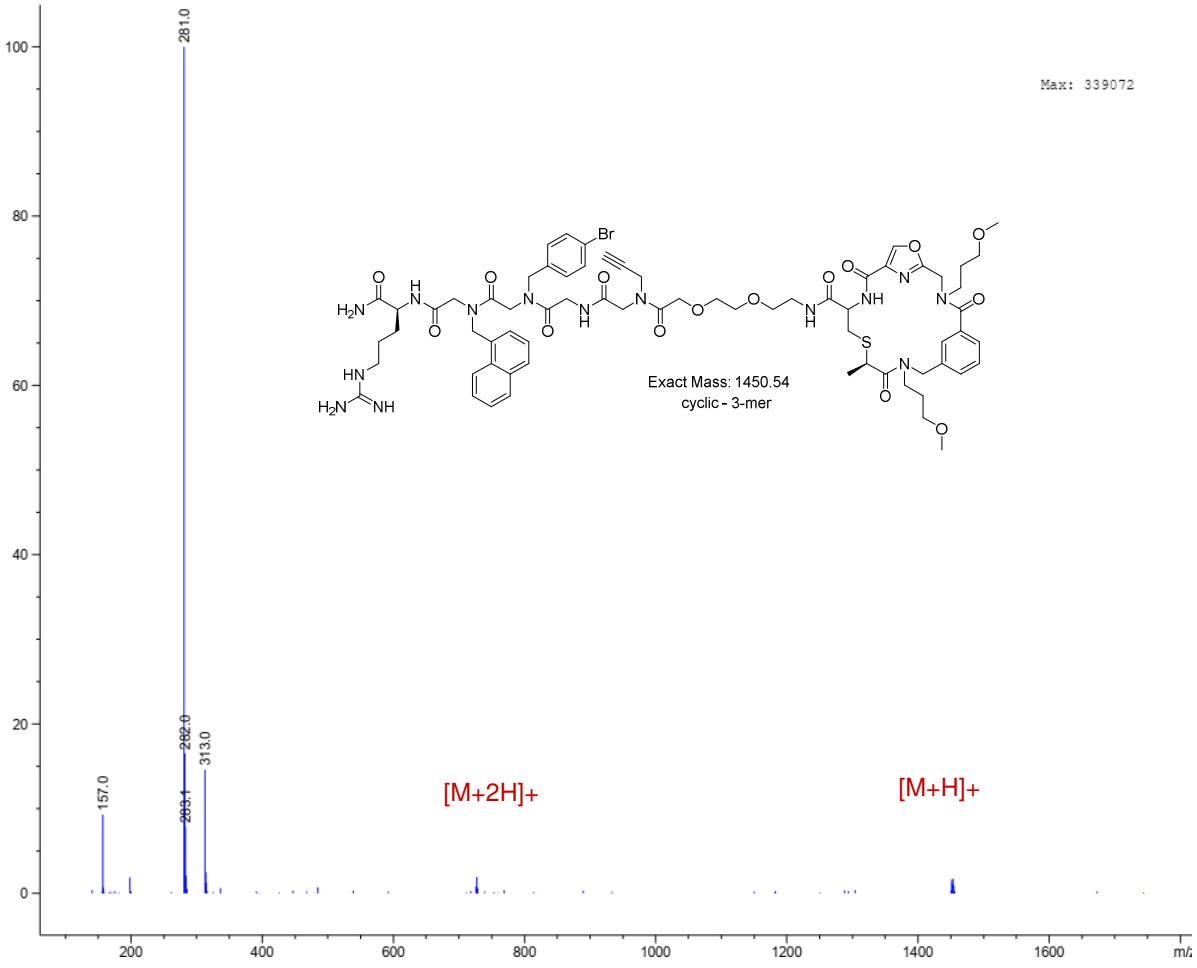
#	Time	Area	Height	Width	Area%
1	7.57	97.1	23.8	0.068	10.287
2	7.808	295.1	68.6	0.0717	31.266
3	8.103	361.7	88.8	0.0679	38.321
4	8.57	190	50.2	0.0631	20.126

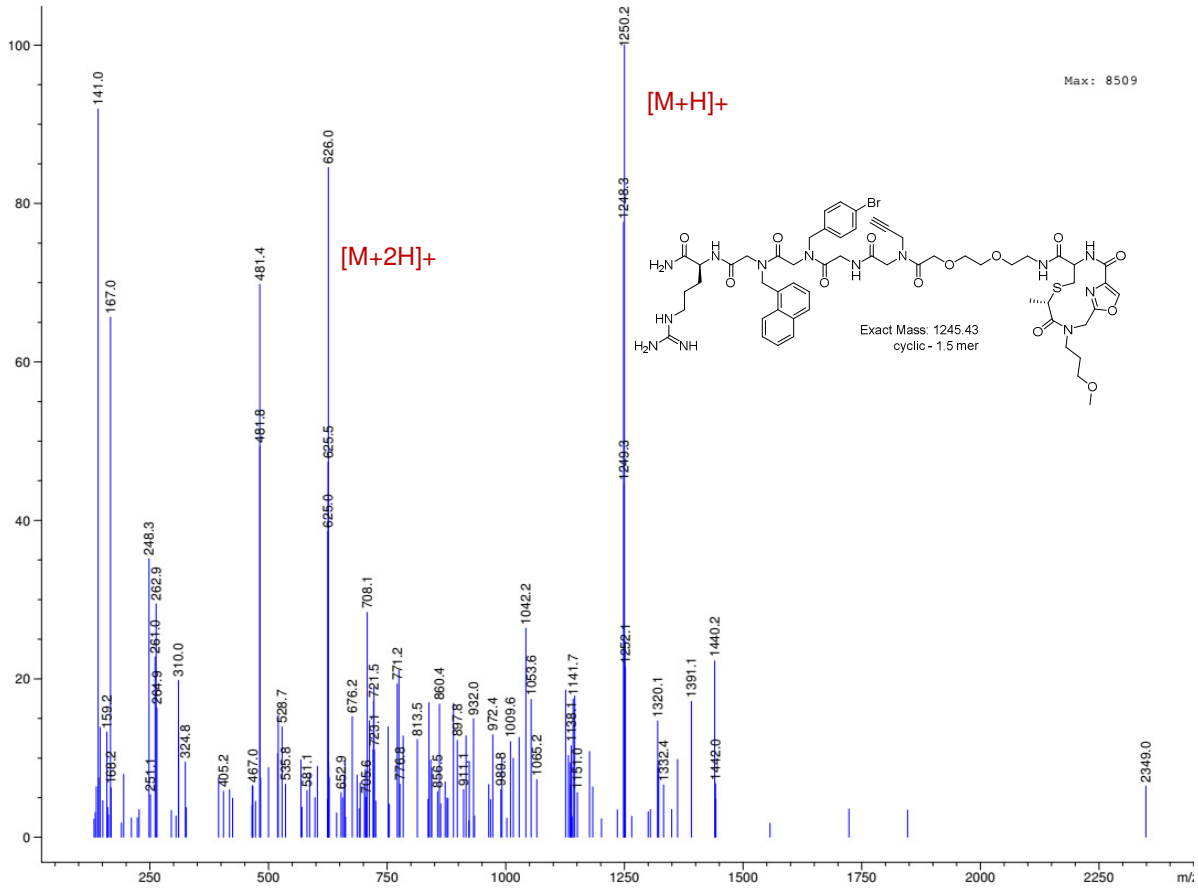
K9 - [ACB]

ions	size	MW	RT
cyclic	1.5	1245	7.570
cyclic	2.5	1450	7.808
cyclic	3.5	1647	8.103
linear	3.5	1683	8.570

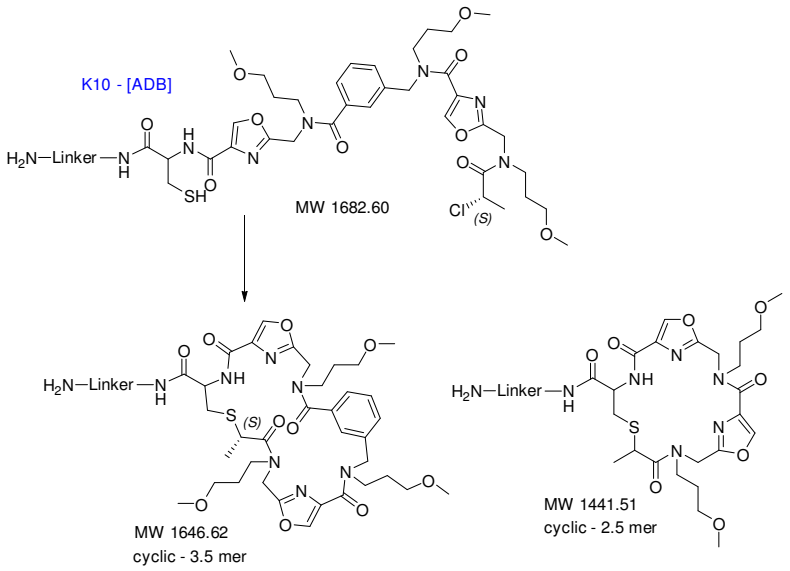


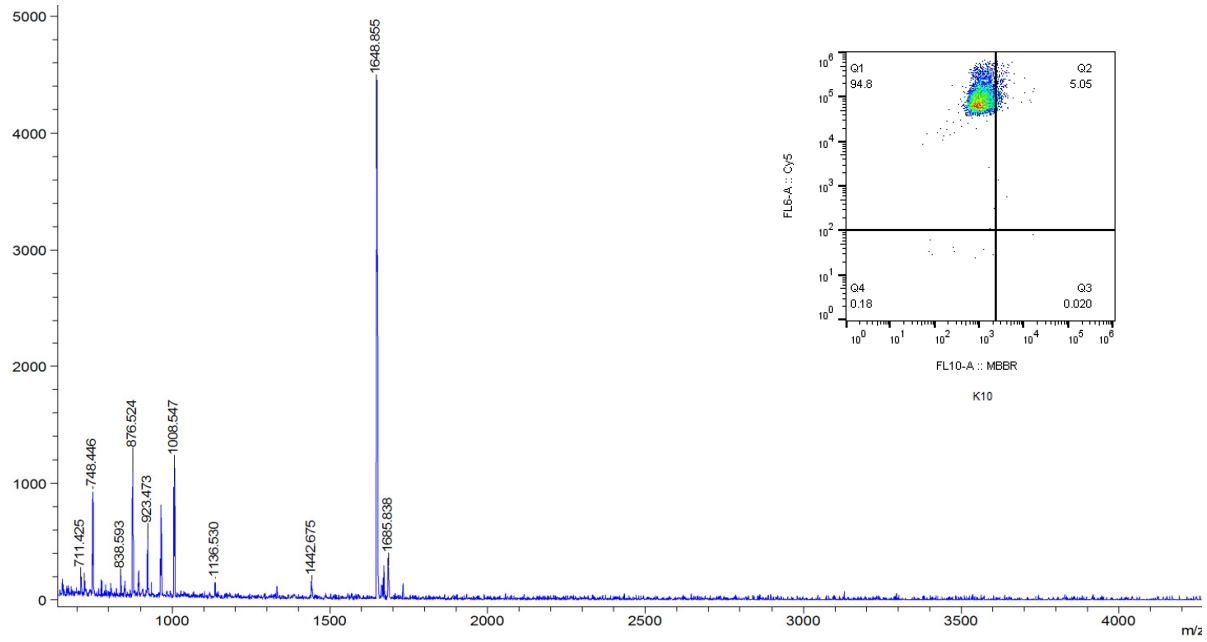

Max: 12513
Exact Mass: 1683.66
linear - 3.5 mer
[M+2H]+
[M+H]+
1505.4
844.4
1686.6
295.0
140.8
576.2
563.5
459.4
439.0
278.9
208.7
491.2
525.6
603.3
680.2
764.2
842.8
952.2
1073.4
1160.5
1206.4
1244.6
1382.6
1424.7
1460.4
1525.8
1685.6
1688.7
1702.7
2001.3
2044.0
m/z

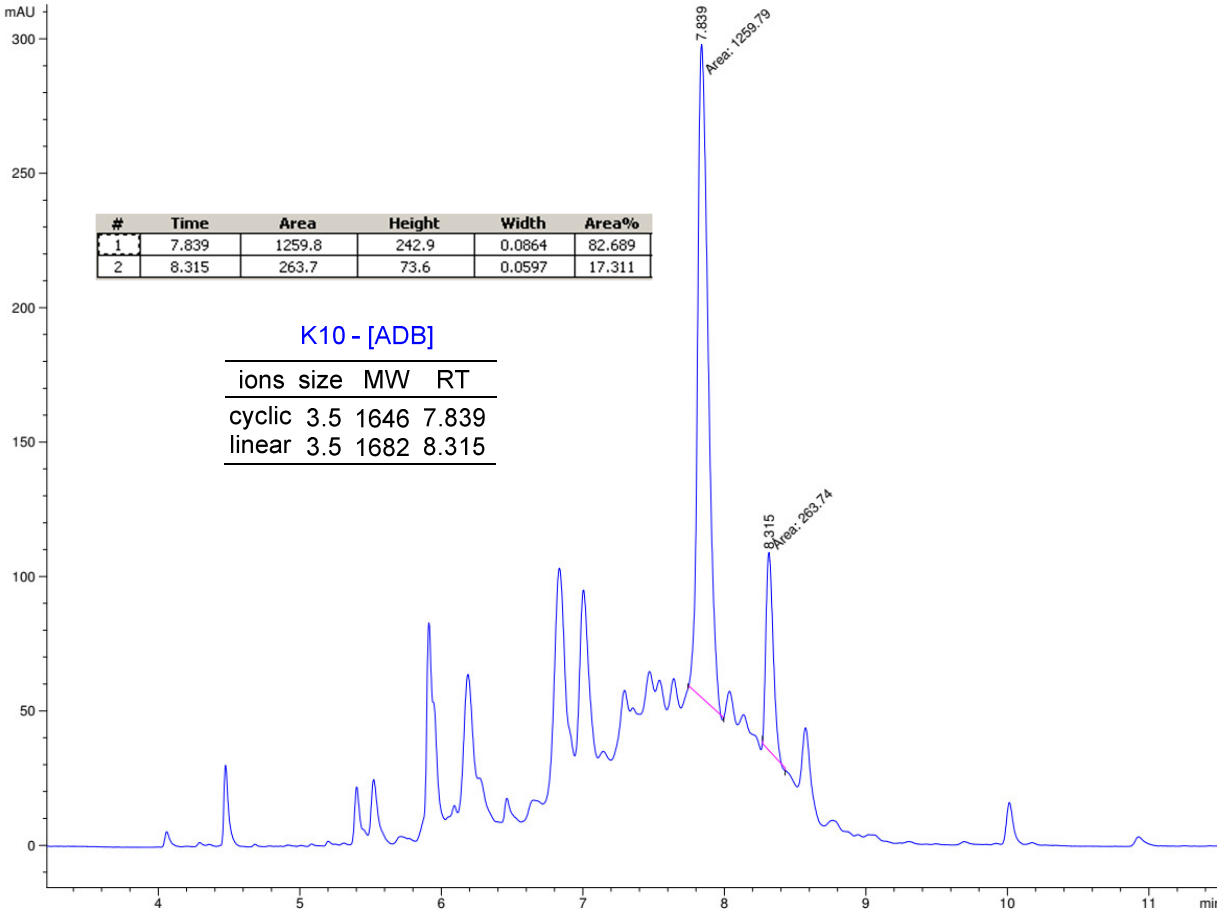

Max: 339072
Exact Mass: 1450.54
cyclic - 3-mer
[M+2H]+
[M+H]+
281.0
282.0
313.0
157.0
m/z



K10-[ADB]: Incomplete cyclization was observed on both 10 µm & 160 µm beads.



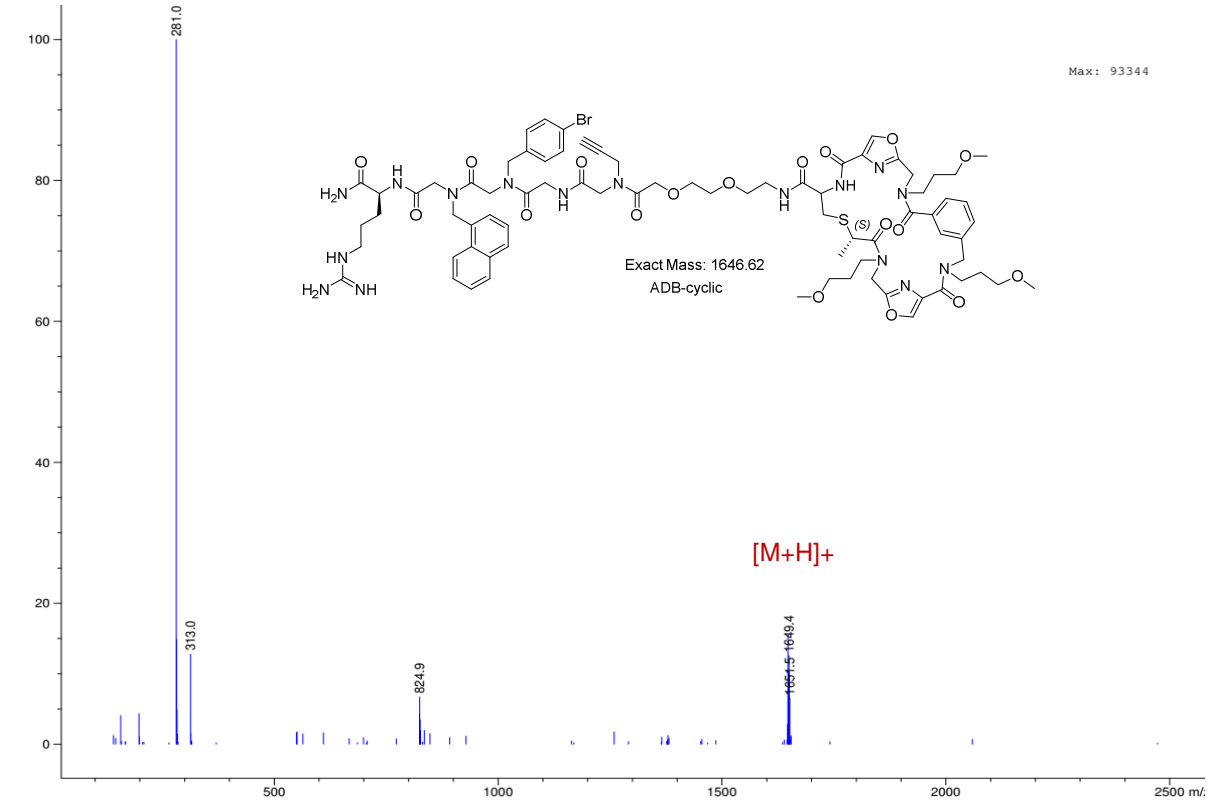


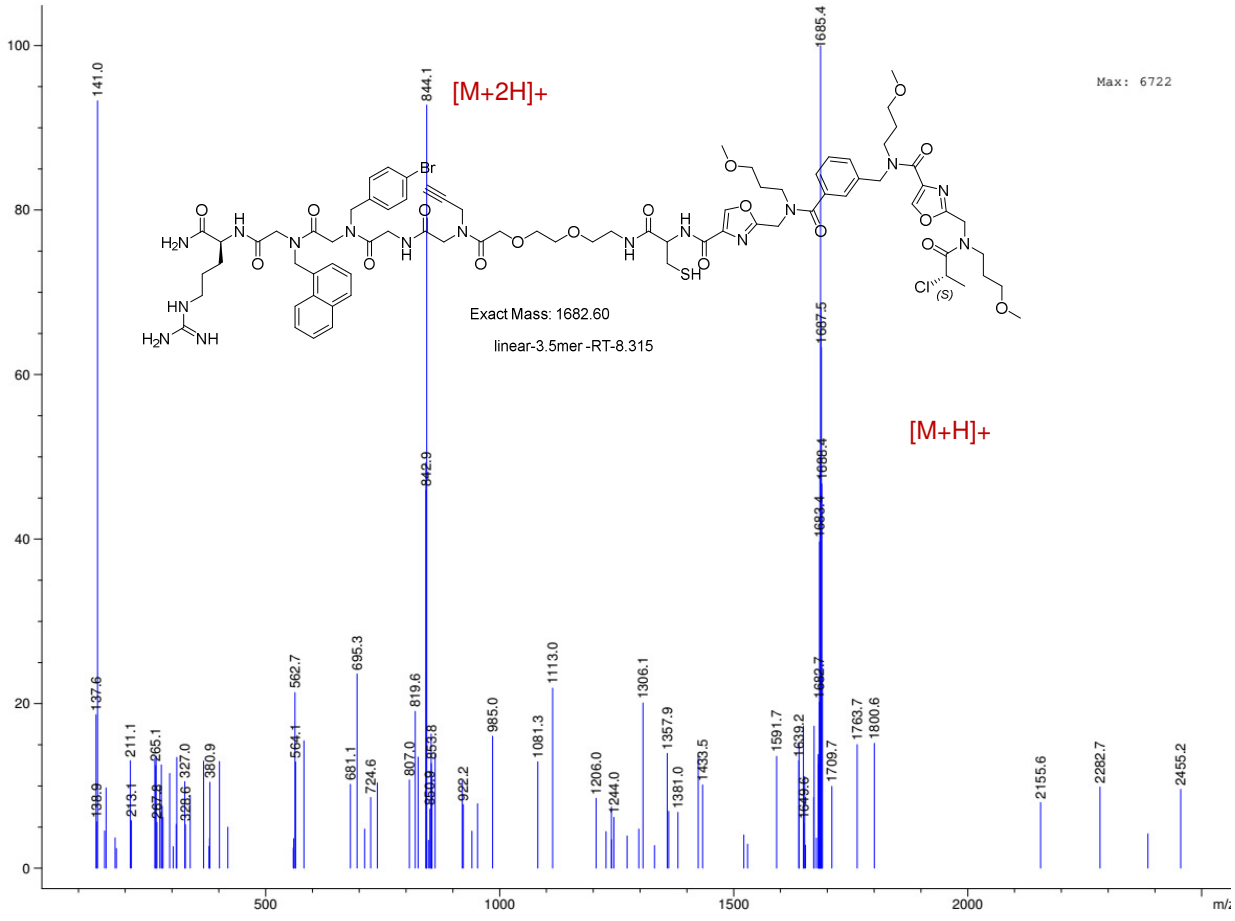


#	Time	Area	Height	Width	Area%
1	7.839	1259.8	242.9	0.0864	82.689
2	8.315	263.7	73.6	0.0597	17.311

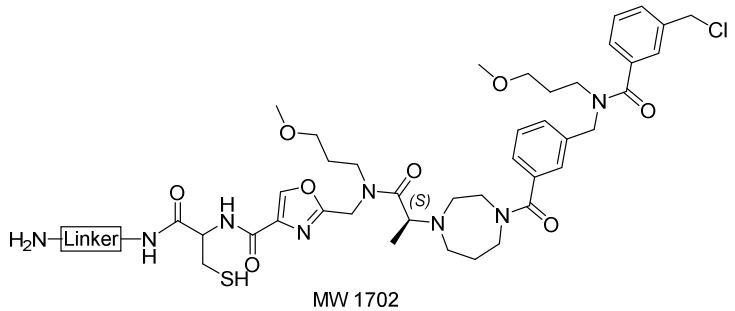
K10 - [ADB]

ions	size	MW	RT
cyclic	3.5	1646	7.839
linear	3.5	1682	8.315


Max: 93344
Exact Mass: 1646.62
ADB-cyclic
[M+H]+
281.0
313.0
824.9
1649.4
100
80
60
40
20
0
500
1000
1500
2000
2500 m/z

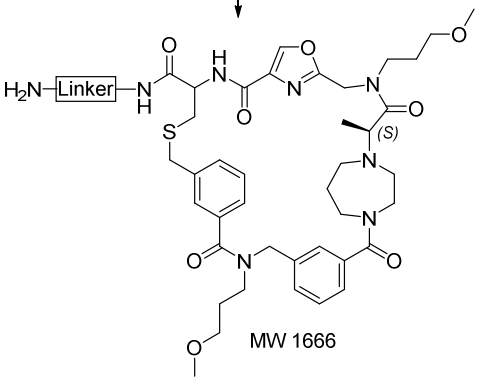

Max: 6722
[M+2H]+
[M+H]+
Exact Mass: 1682.60
linear-3.5mer -RT-8.315
141.0
844.1
1685.4
100
80
60
40
20
0
500
1000
1500
2000
m/z

L1-[BAA]: Cyclization was incomplete on 10 µm beads but was complete on 160 µm beads.

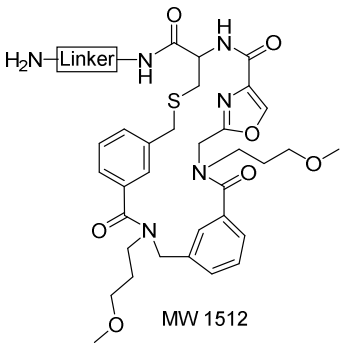


MW 1702

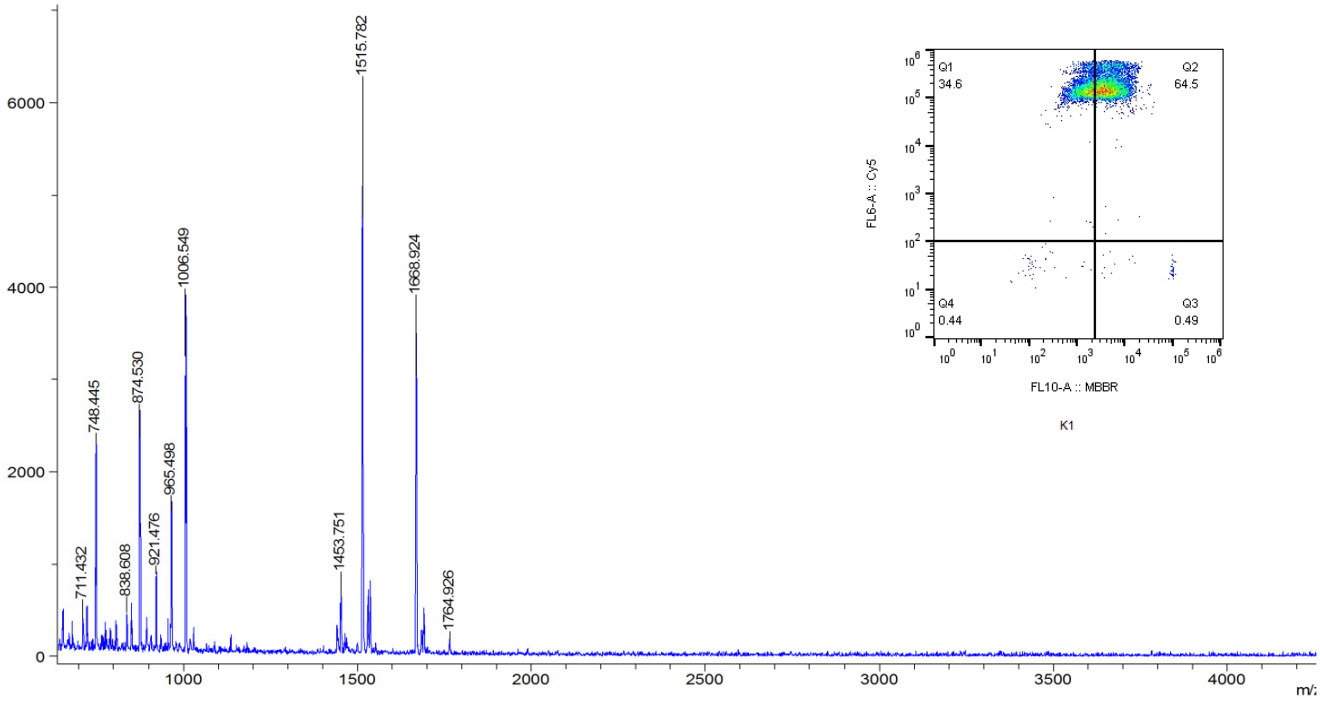
cyclization

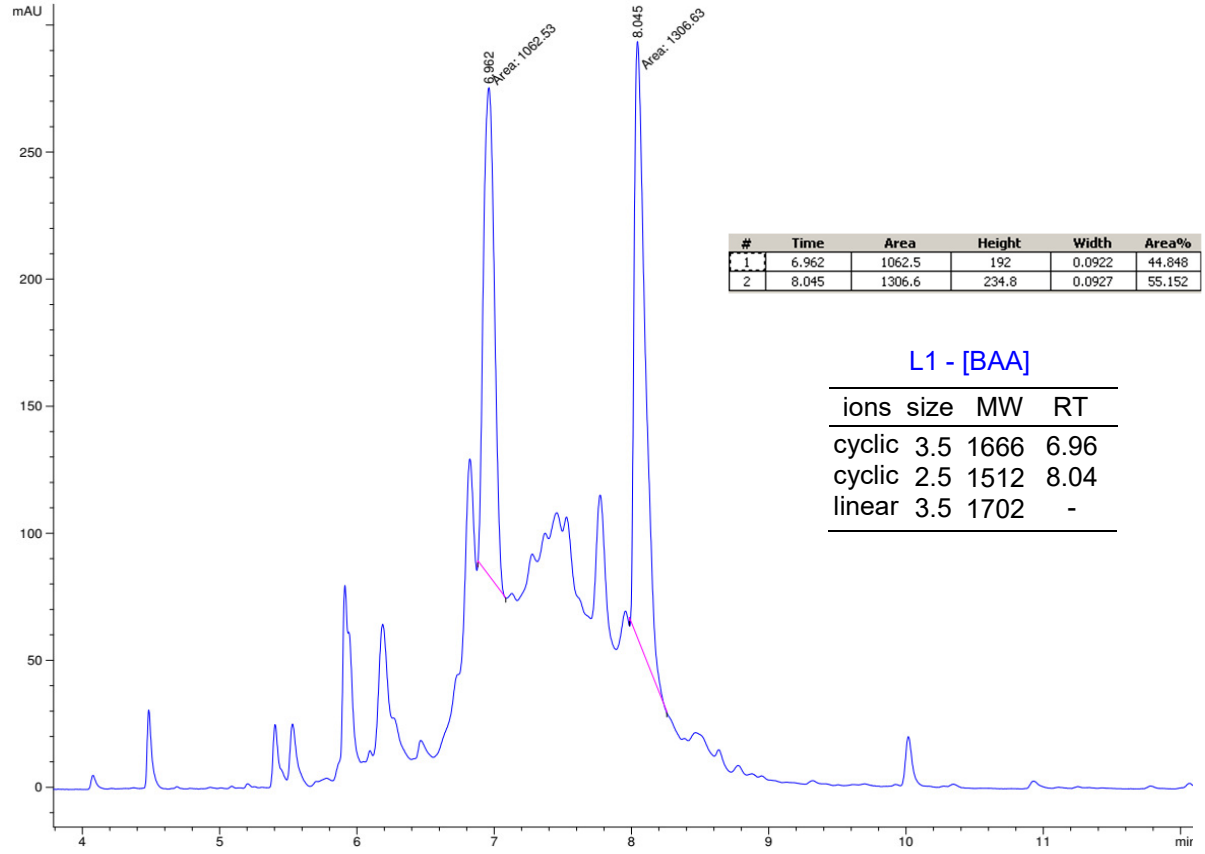


MW 1666



MW 1512

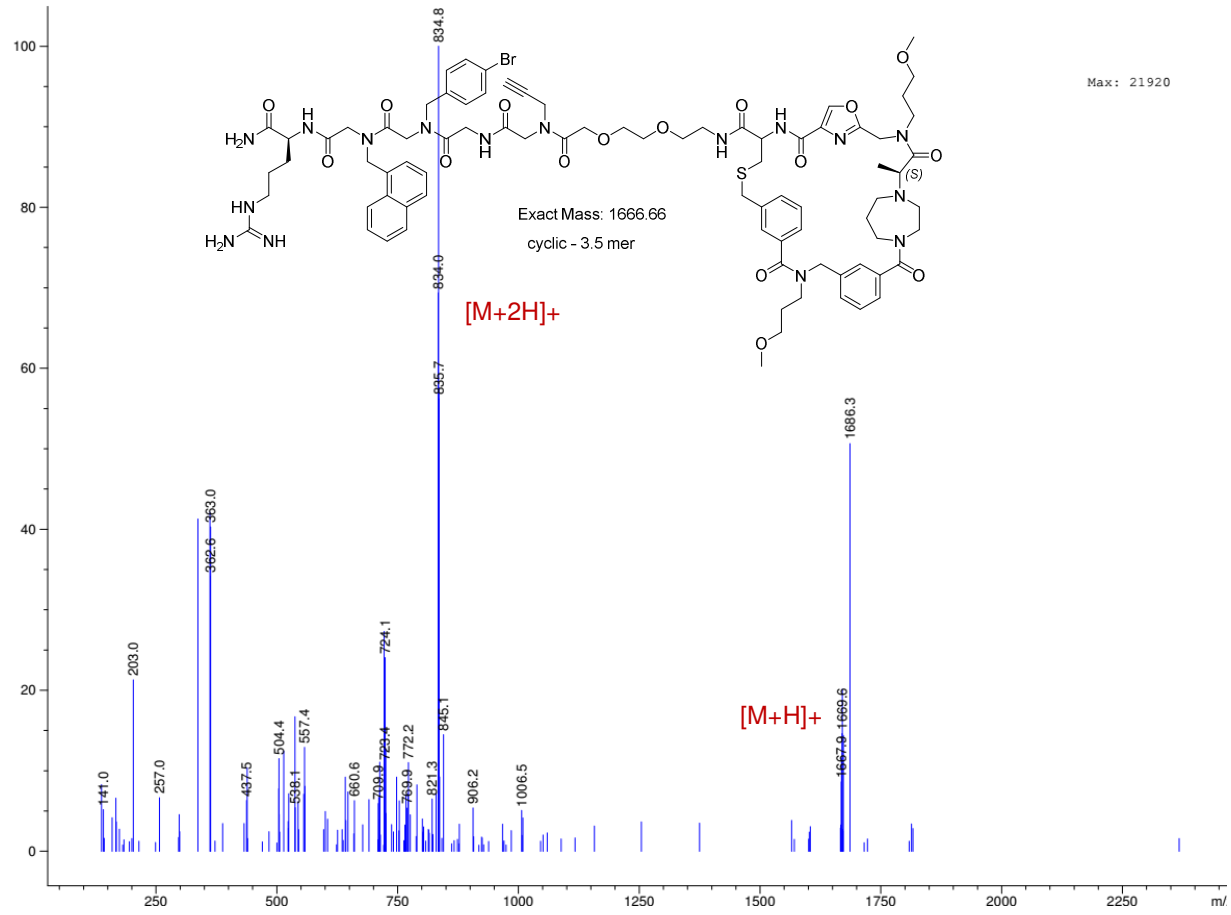


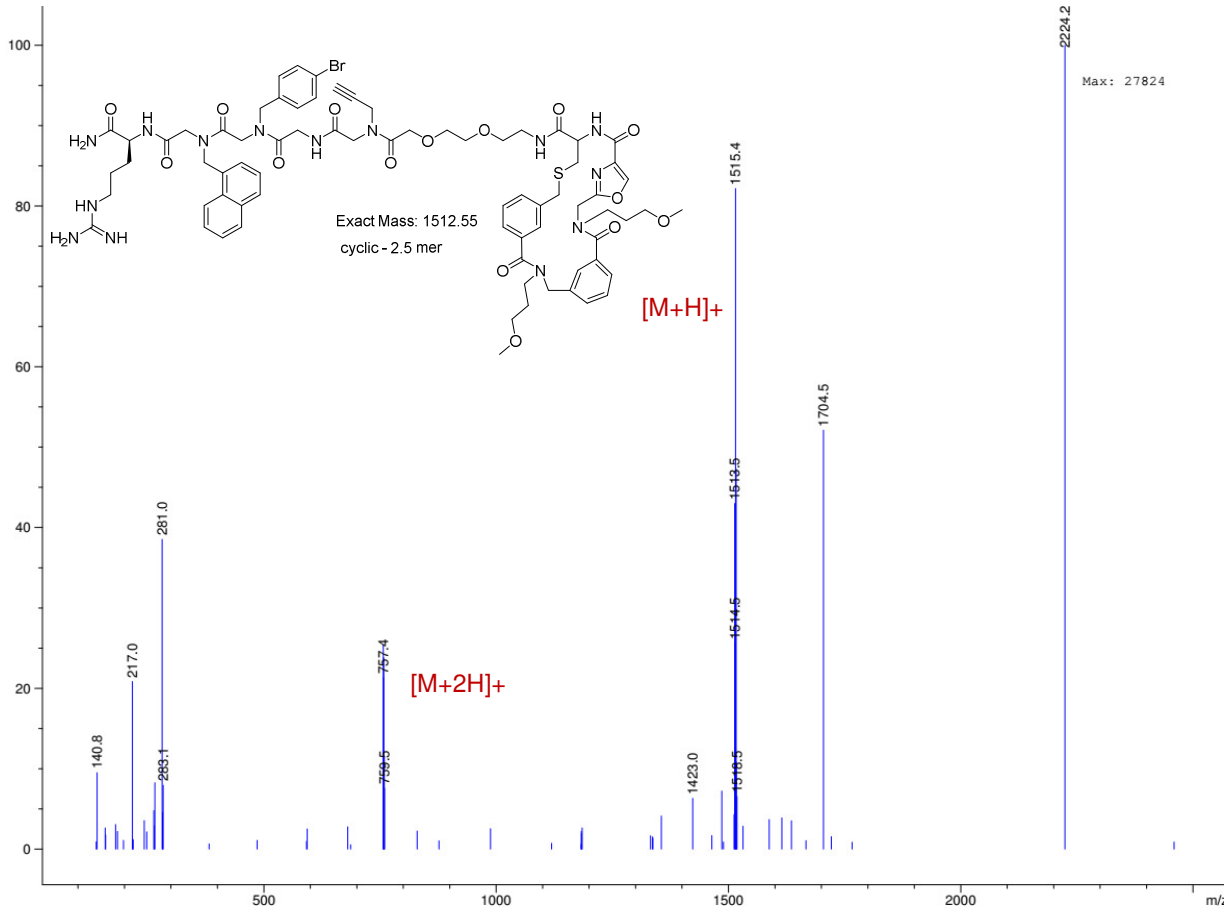


#	Time	Area	Height	Width	Area%
1	6.962	1062.5	192	0.0922	44.848
2	8.045	1306.6	234.8	0.0927	55.152

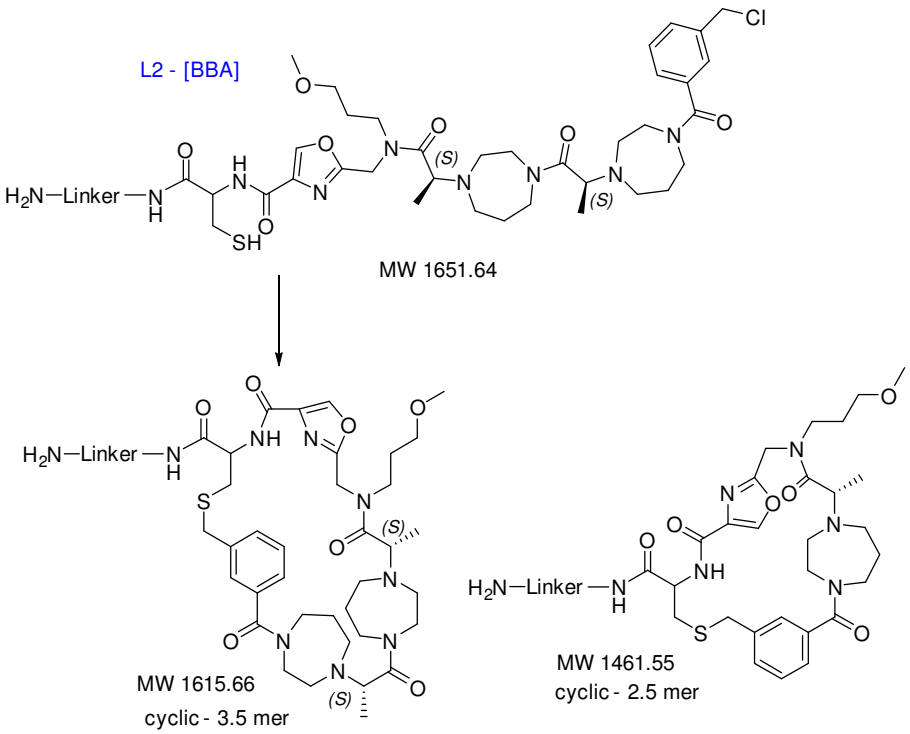
L1 - [BAA]

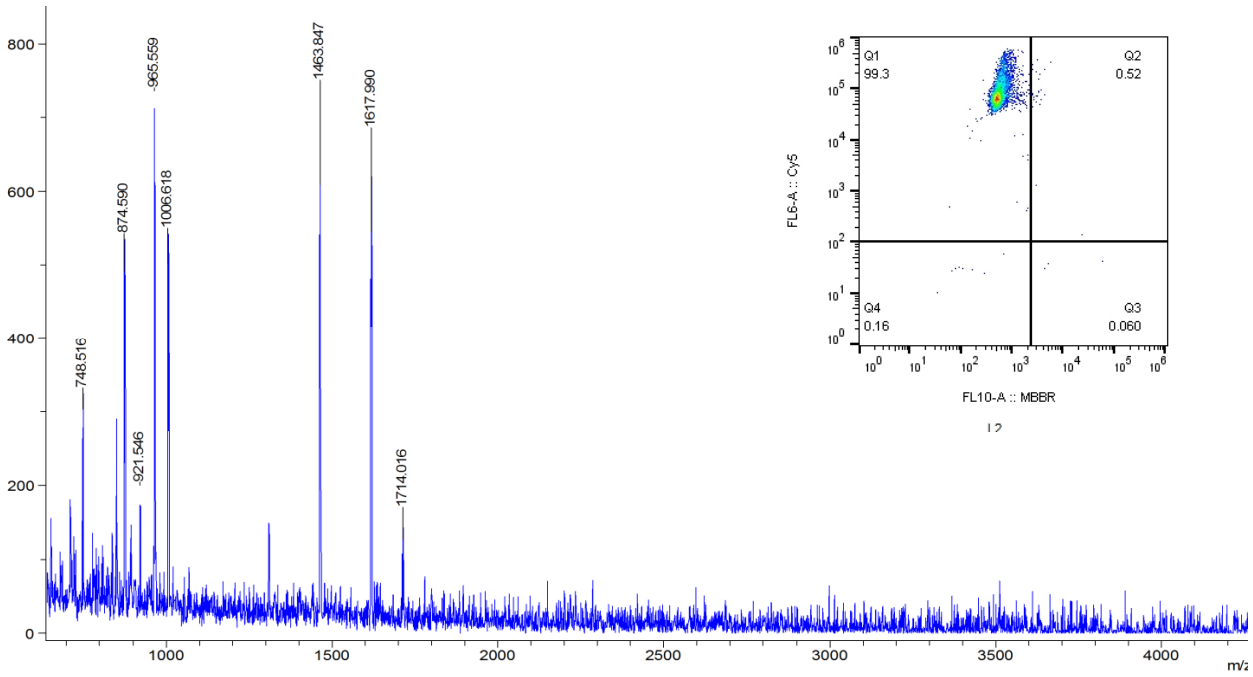
ions	size	MW	RT
cyclic	3.5	1666	6.96
cyclic	2.5	1512	8.04
linear	3.5	1702	-

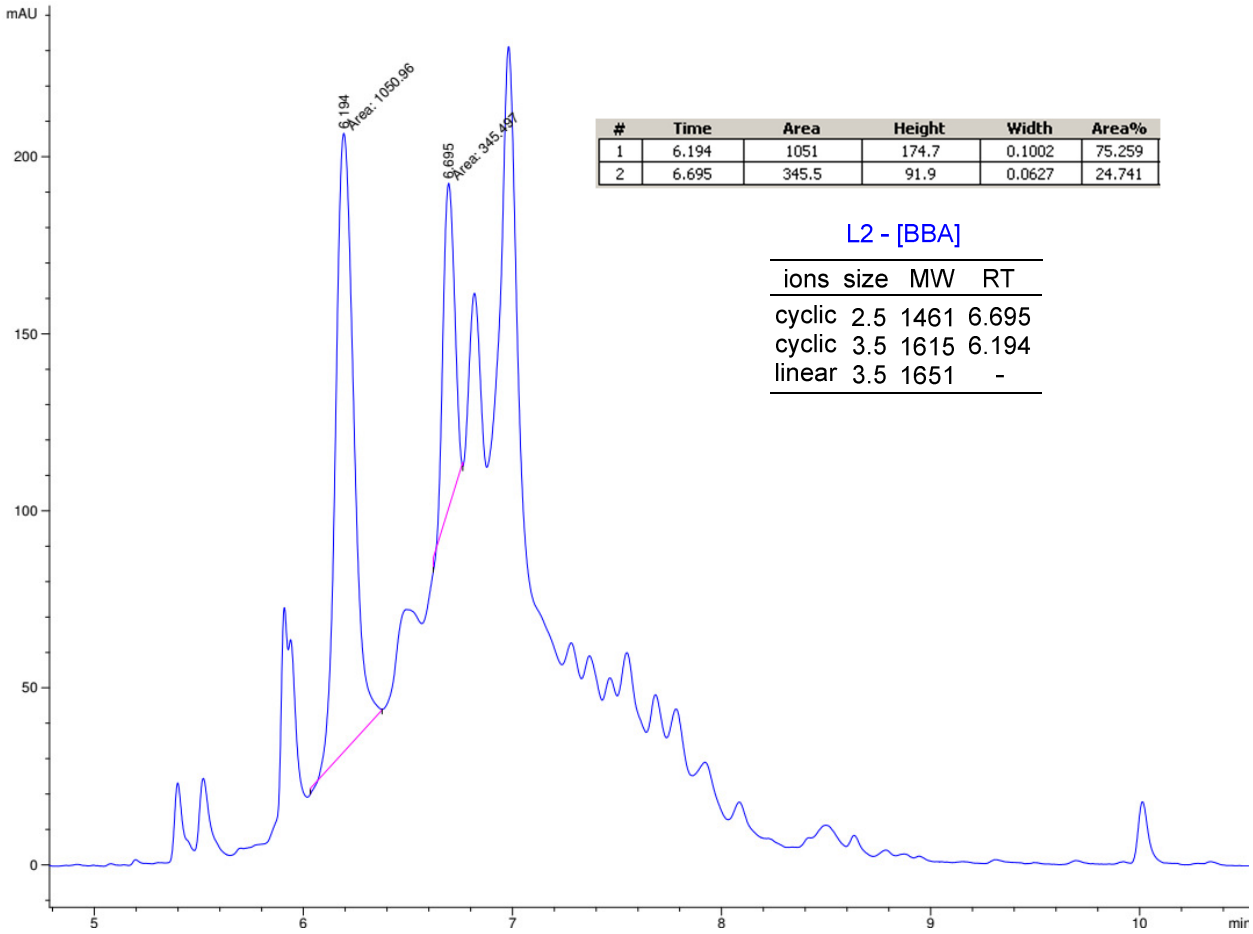




L2-[BBA]: Complete cyclization was observed on 10 µm & 160 µm beads.



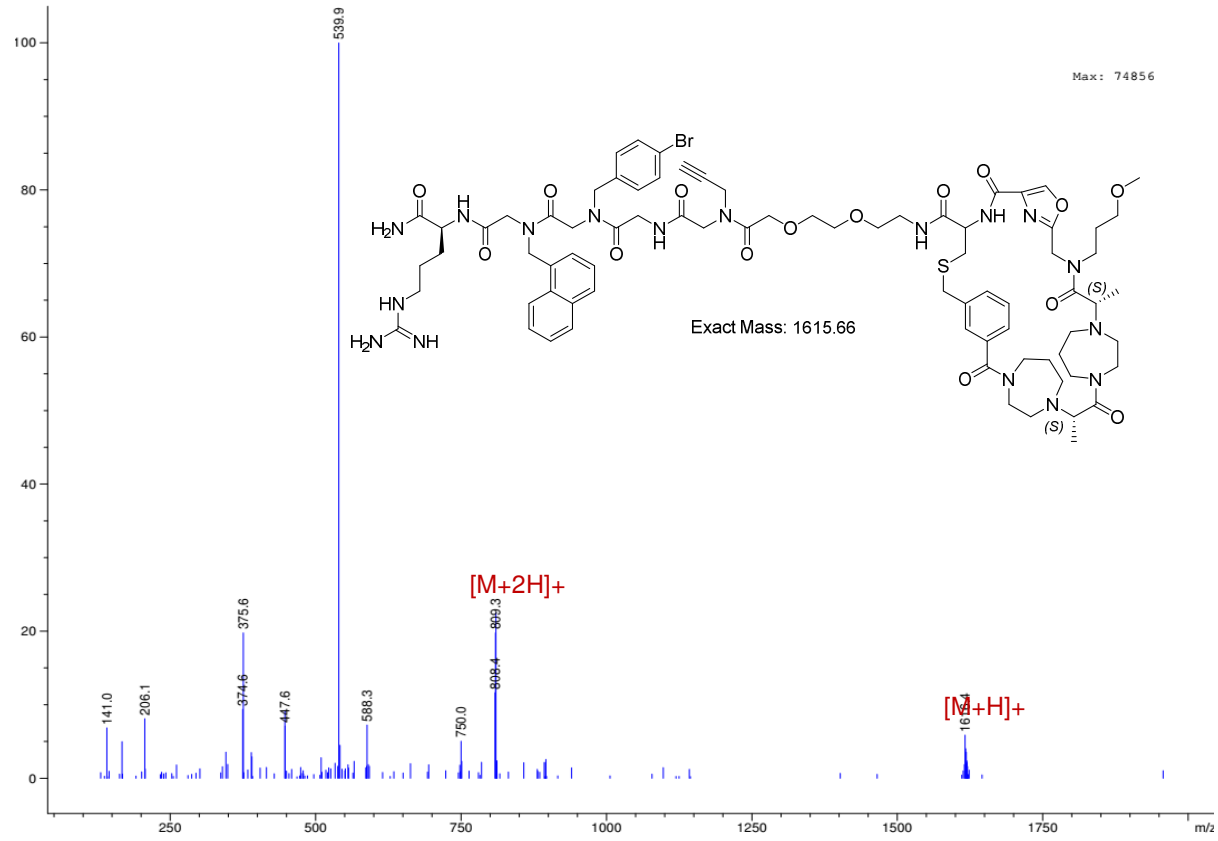


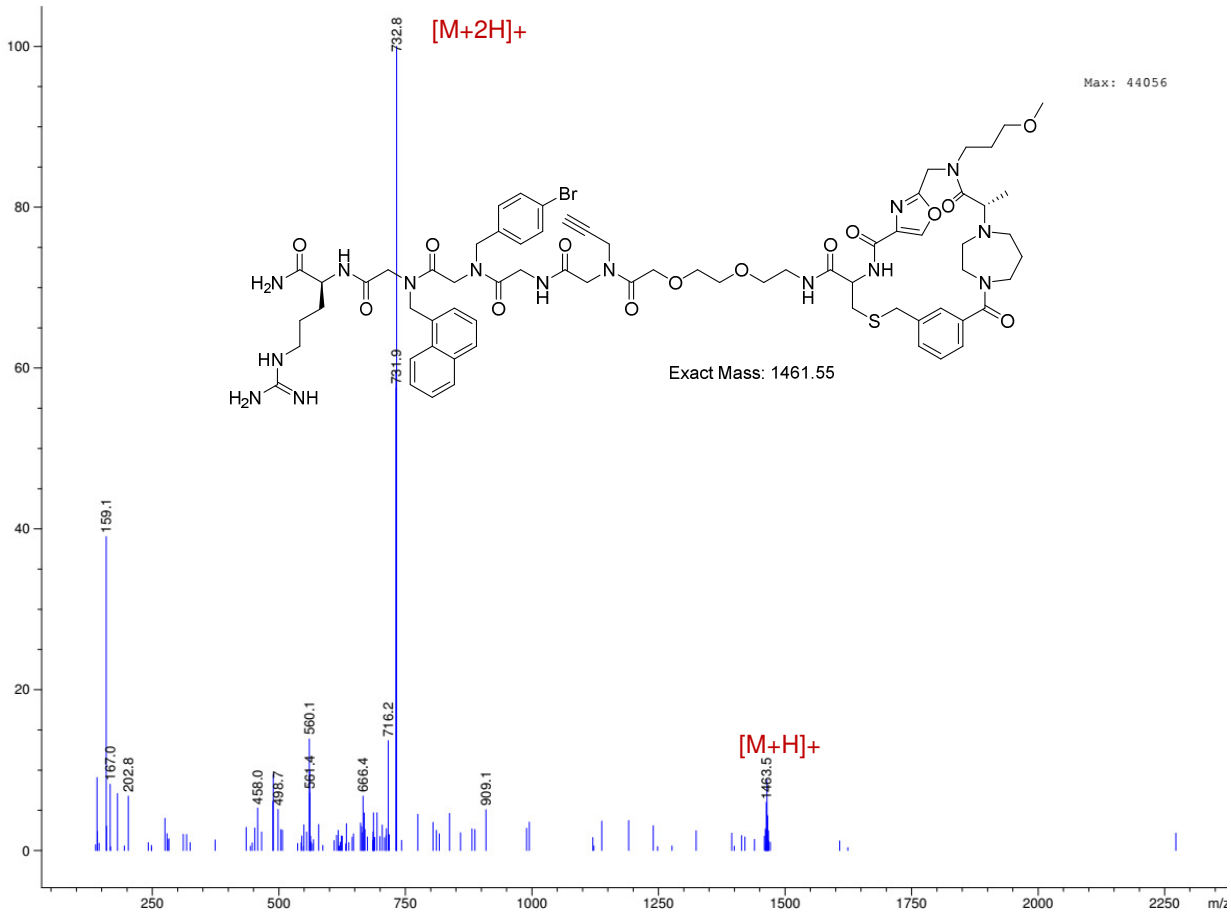


#	Time	Area	Height	Width	Area%
1	6.194	1051	174.7	0.1002	75.259
2	6.695	345.5	91.9	0.0627	24.741

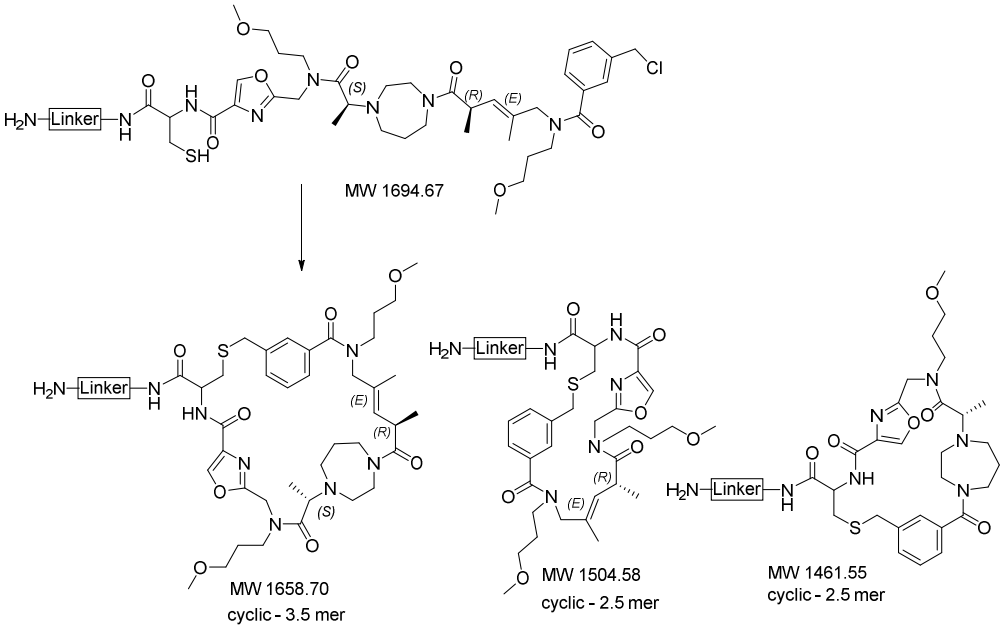
L2 - [BBA]

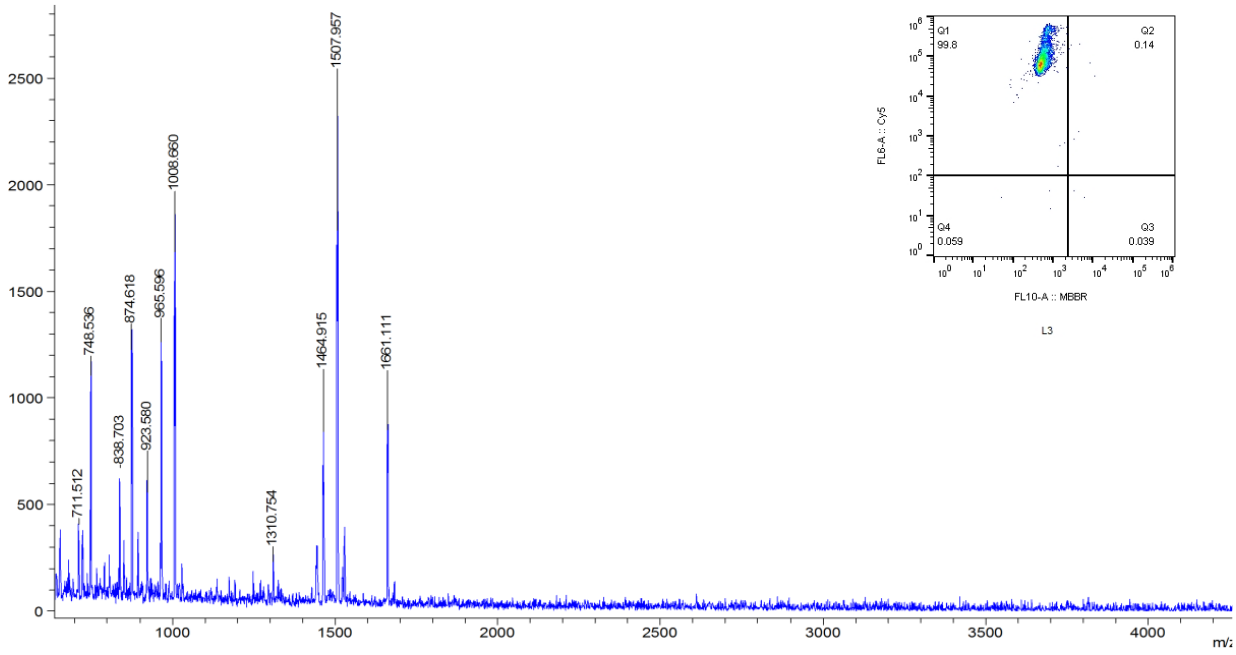
ions	size	MW	RT
cyclic	2.5	1461	6.695
cyclic	3.5	1615	6.194
linear	3.5	1651	-

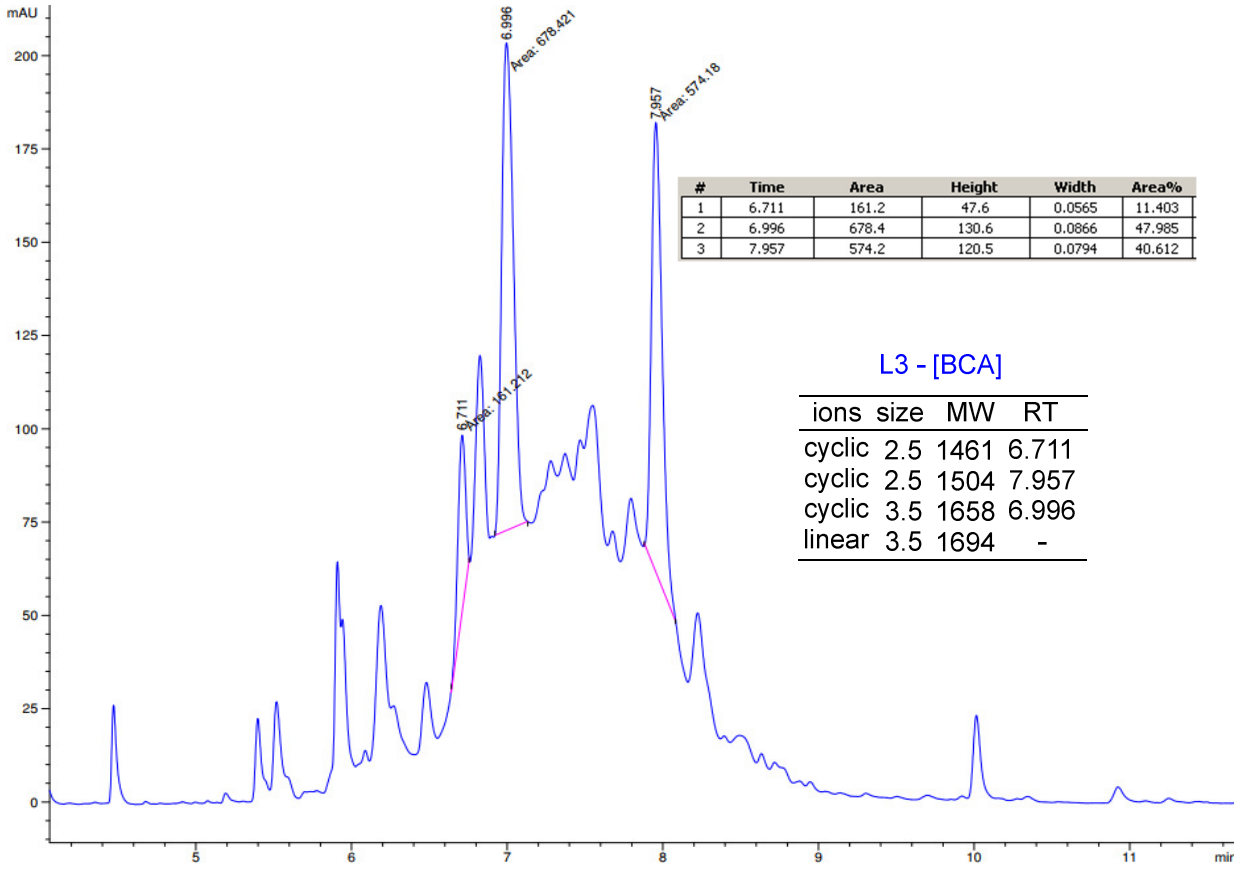

Max: 74856
539.9
[M+2H]+
[M+H]+
Exact Mass: 1615.66
Br
100
80
60
40
20
0
250
500
750
1000
1250
1500
1750
m/z


Max: 44056
732.8
[M+2H]+
[M+H]+
Exact Mass: 1461.55
Br
100
80
60
40
20
0
250
500
750
1000
1250
1500
1750
2000
2250
m/z

L3-[BCA]: Cyclization was complete on both 10 µm & 160 µm beads.



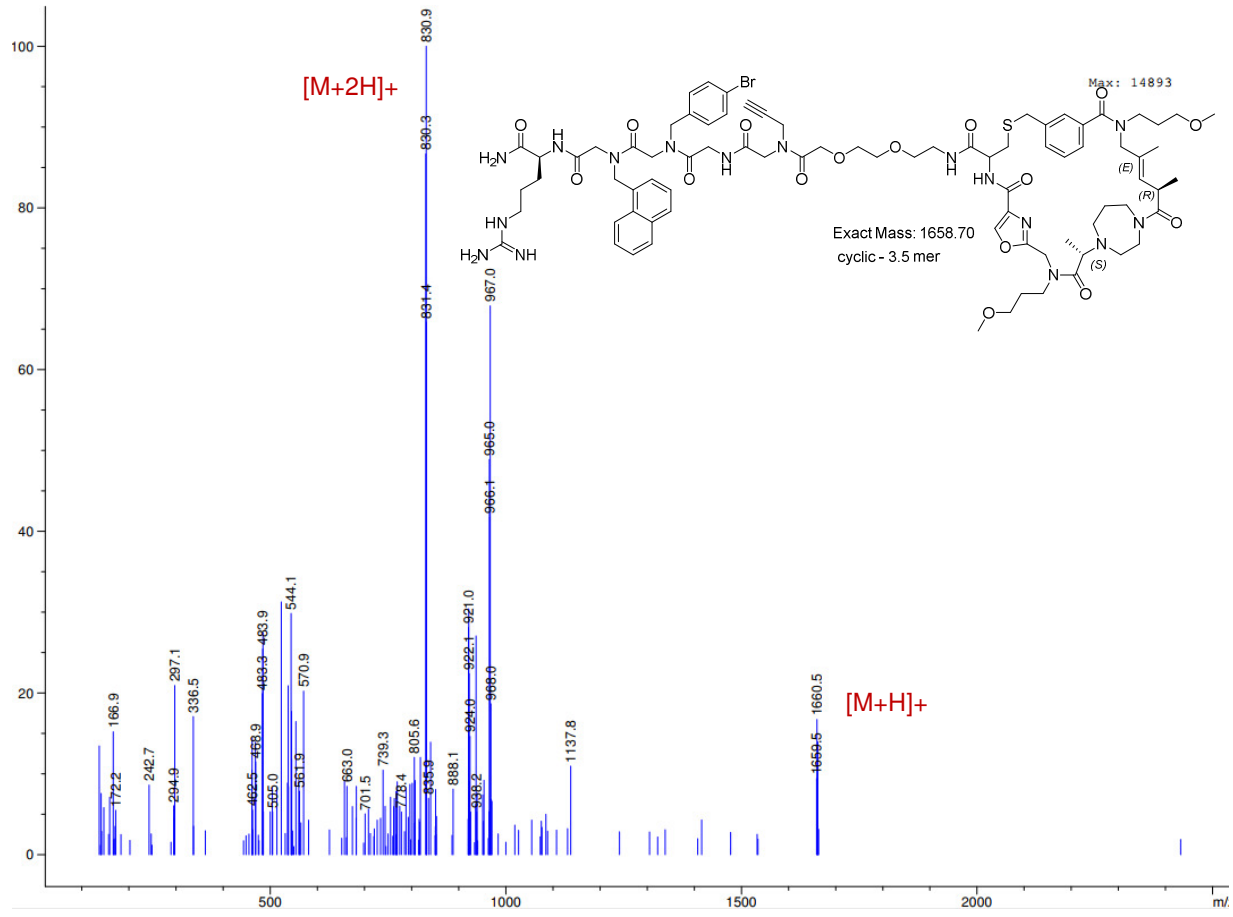


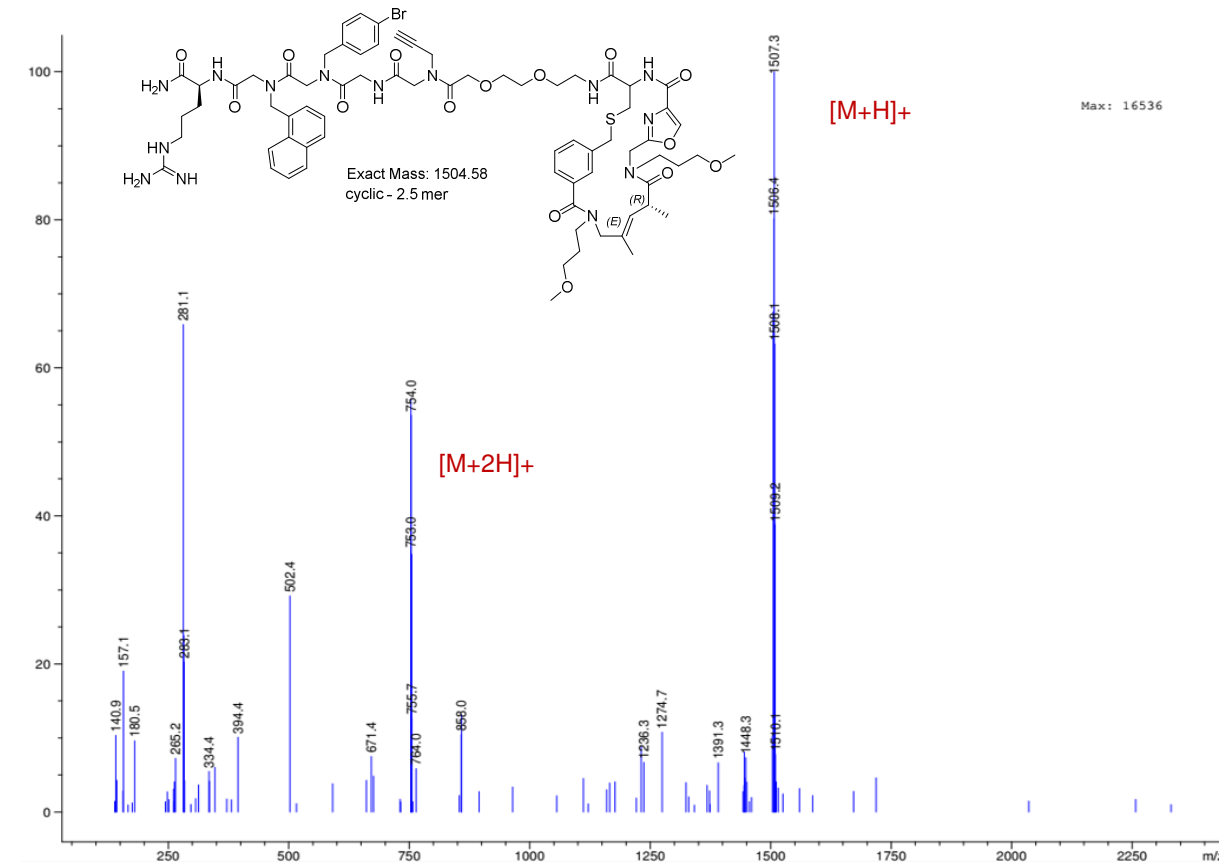


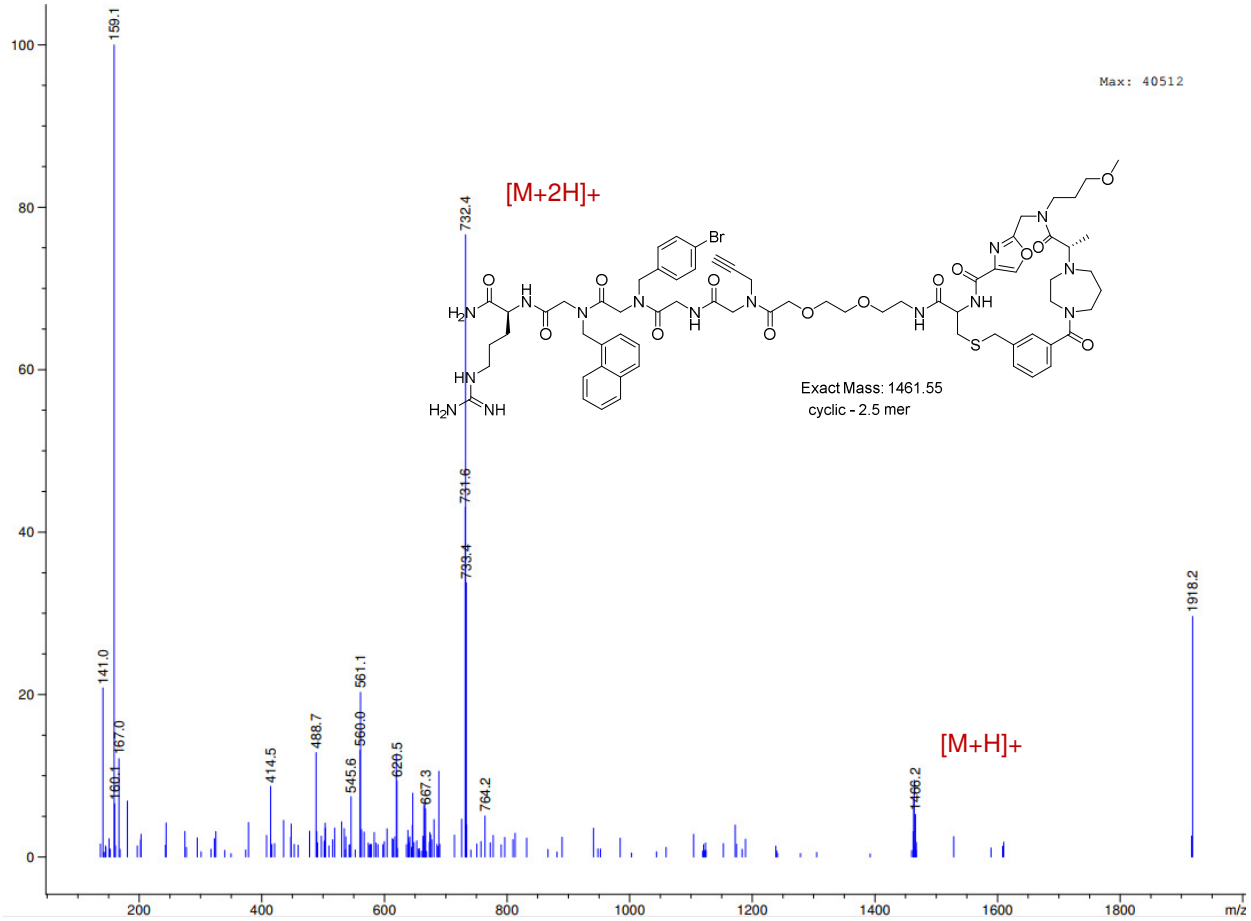
#	Time	Area	Height	Width	Area%
1	6.711	161.2	47.6	0.0565	11.403
2	6.996	678.4	130.6	0.0866	47.985
3	7.957	574.2	120.5	0.0794	40.612

L3 - [BCA]

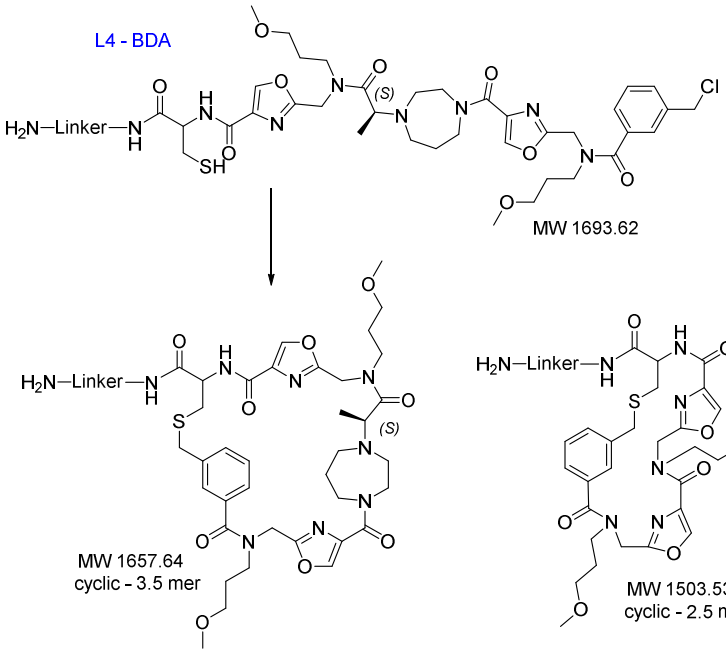
ions	size	MW	RT
cyclic	2.5	1461	6.711
cyclic	2.5	1504	7.957
cyclic	3.5	1658	6.996
linear	3.5	1694	-

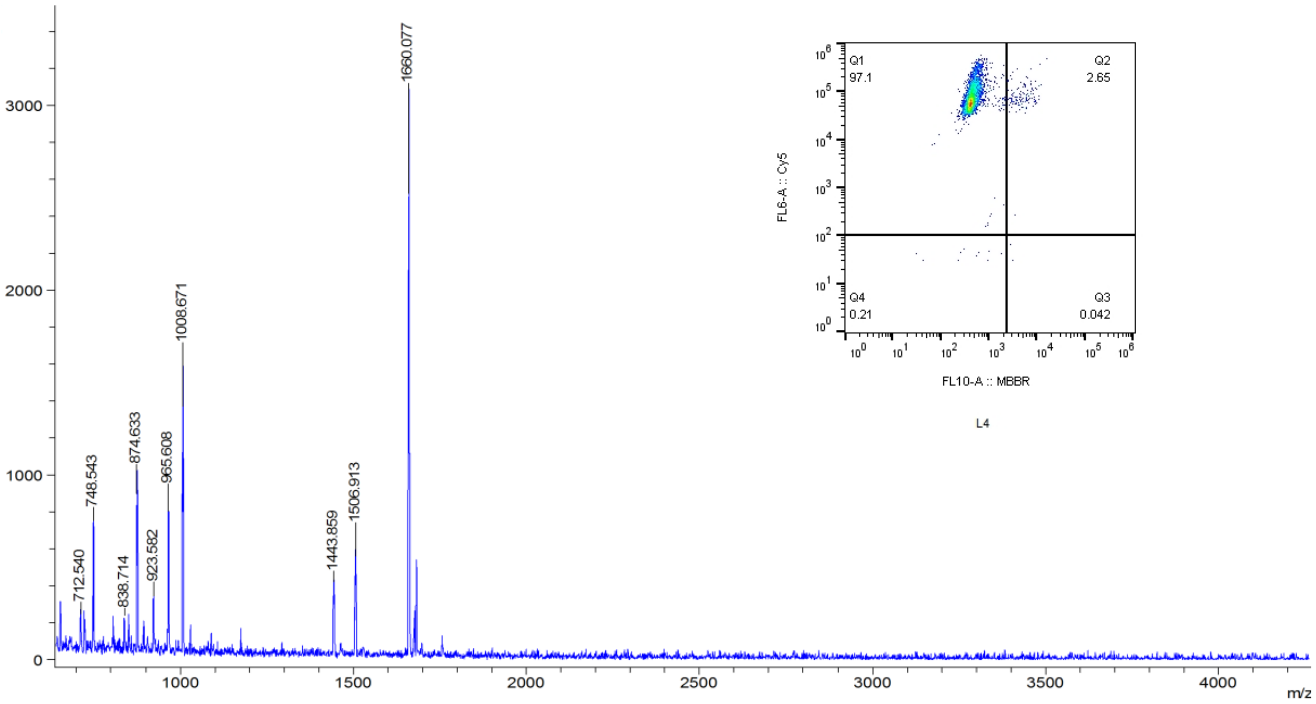


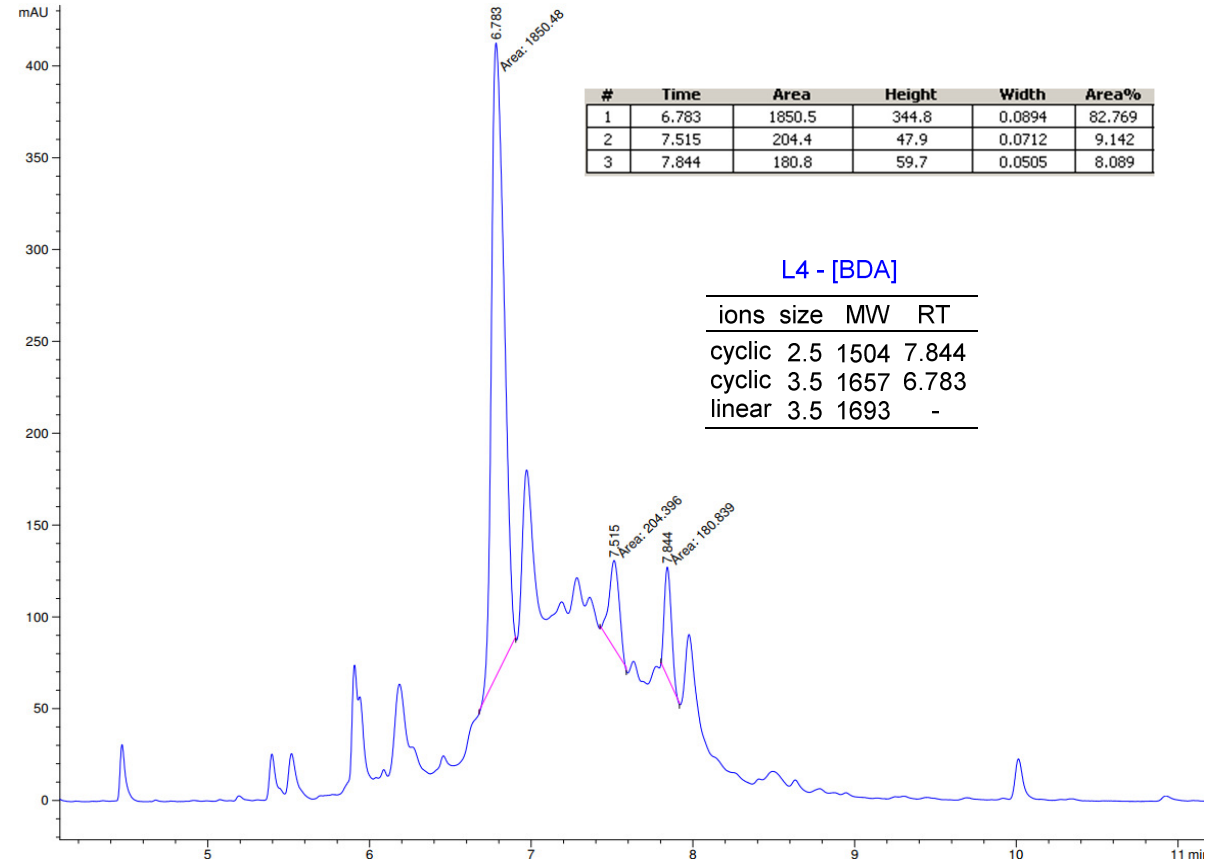

Exact Mass: 1504.58
cyclic - 2.5 mer
[M+H]+
[M+2H]+
Max: 16536
1507.3
1506.4
1508.1
1509.2
754.0
753.0
281.1
502.4
157.1
140.9
180.5
265.2
334.4
394.4
671.4
755.7
764.0
858.0
1236.3
1274.7
1391.3
1448.3
1910.1


Max: 40512
[M+2H]+
Exact Mass: 1461.55
cyclic - 2.5 mer
[M+H]+
159.1
732.4
731.6
733.4
1918.2
1466.2
141.0
167.0
160.1
414.5
488.7
545.6
560.0
561.1
620.5
667.3
764.2

L4-[BDA]: Complete cyclization was observed on 10 µm & 160 µm beads.



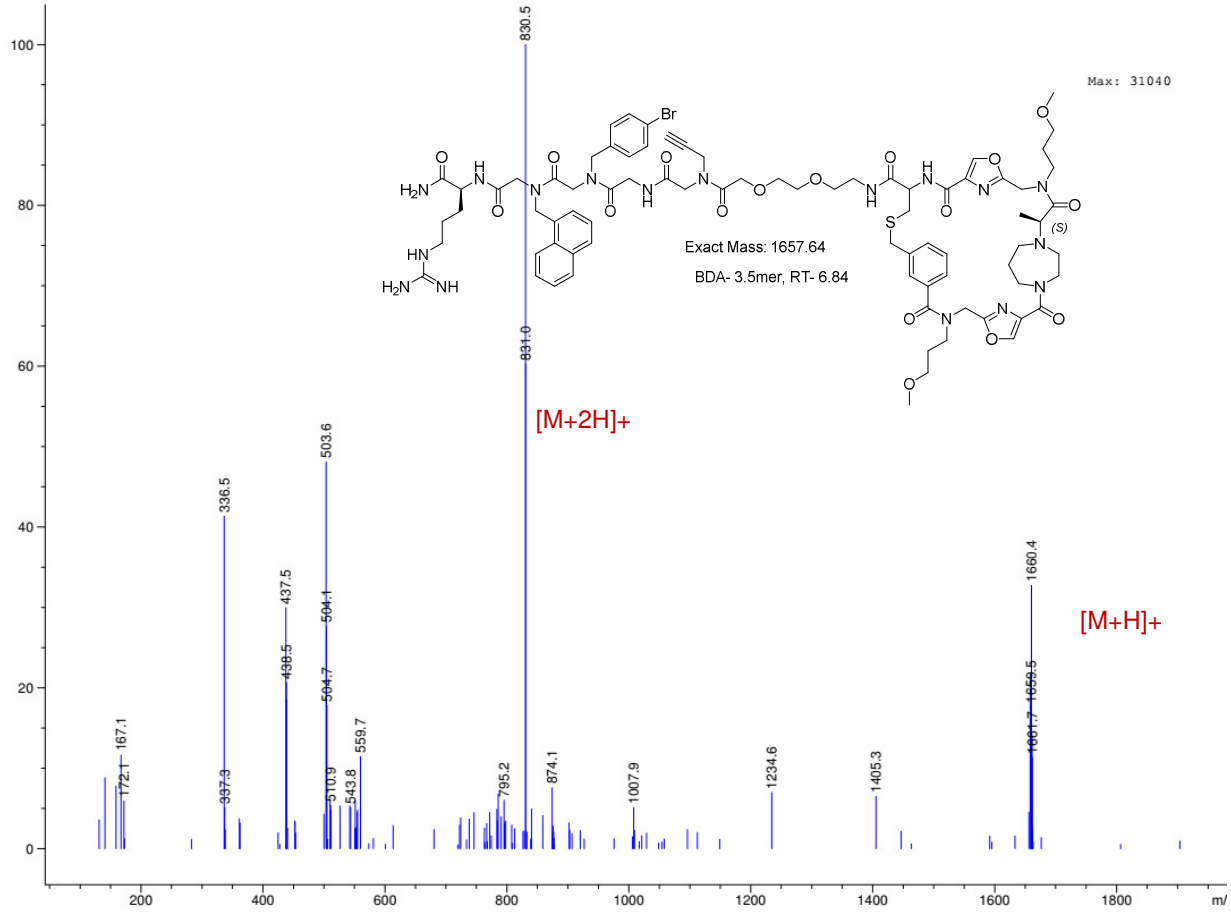


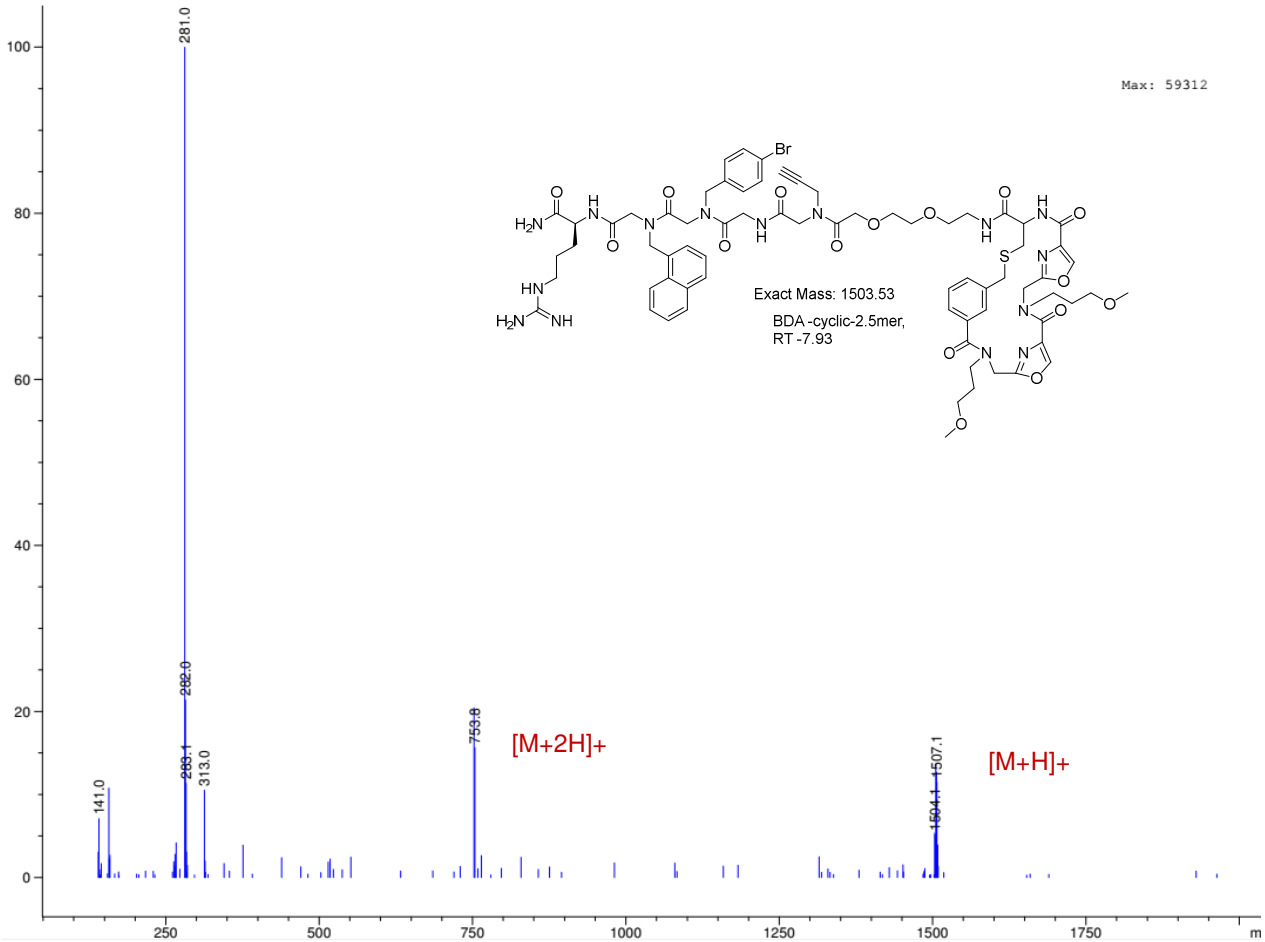


#	Time	Area	Height	Width	Area%
1	6.783	1850.5	344.8	0.0894	82.769
2	7.515	204.4	47.9	0.0712	9.142
3	7.844	180.8	59.7	0.0505	8.089

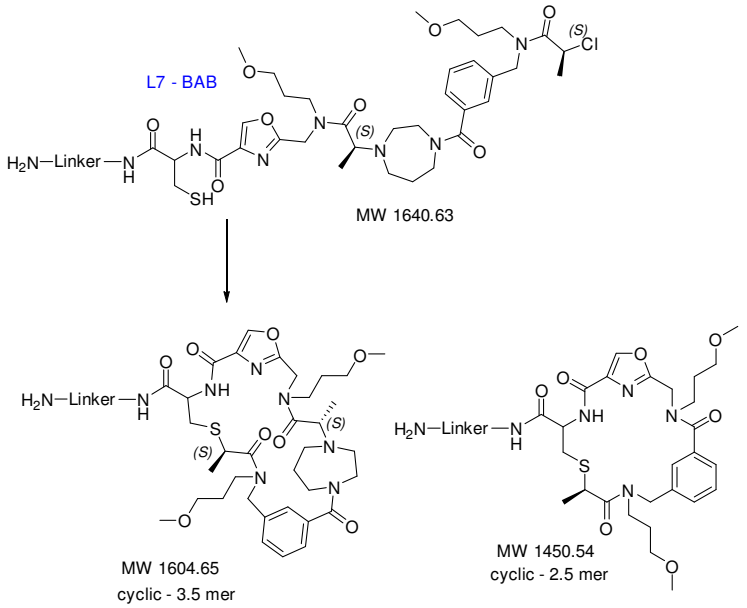
L4 - [BDA]

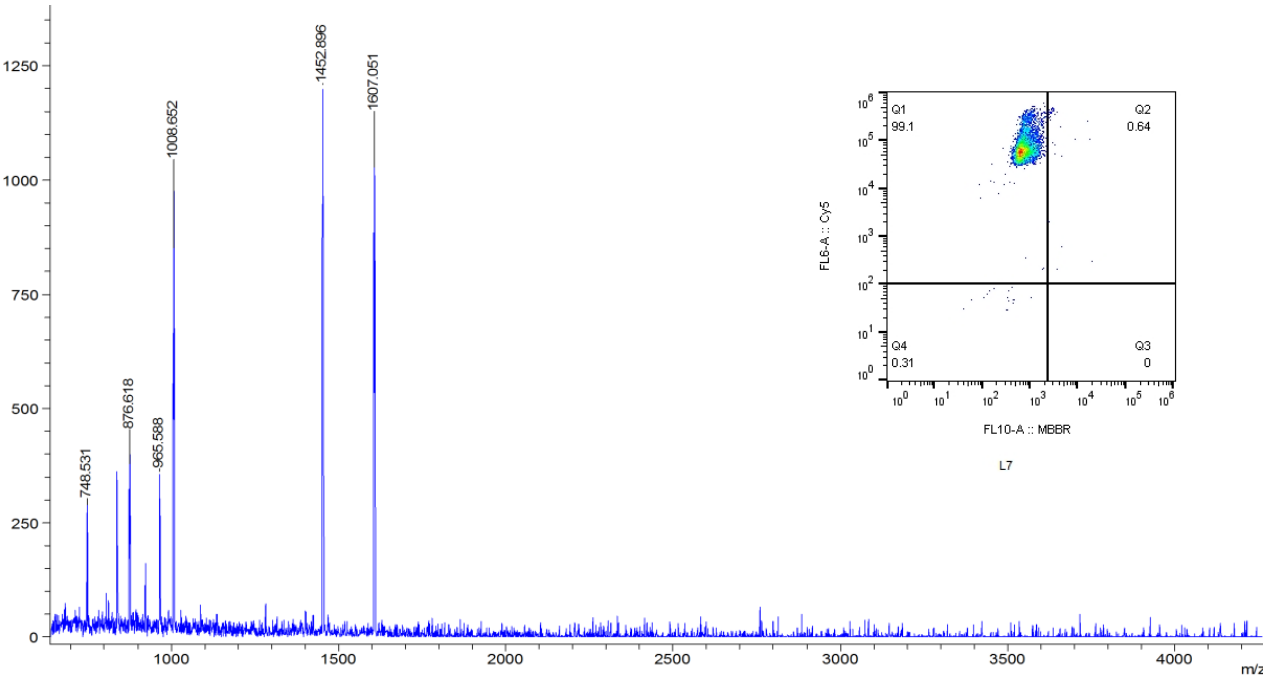
ions	size	MW	RT
cyclic	2.5	1504	7.844
cyclic	3.5	1657	6.783
linear	3.5	1693	-

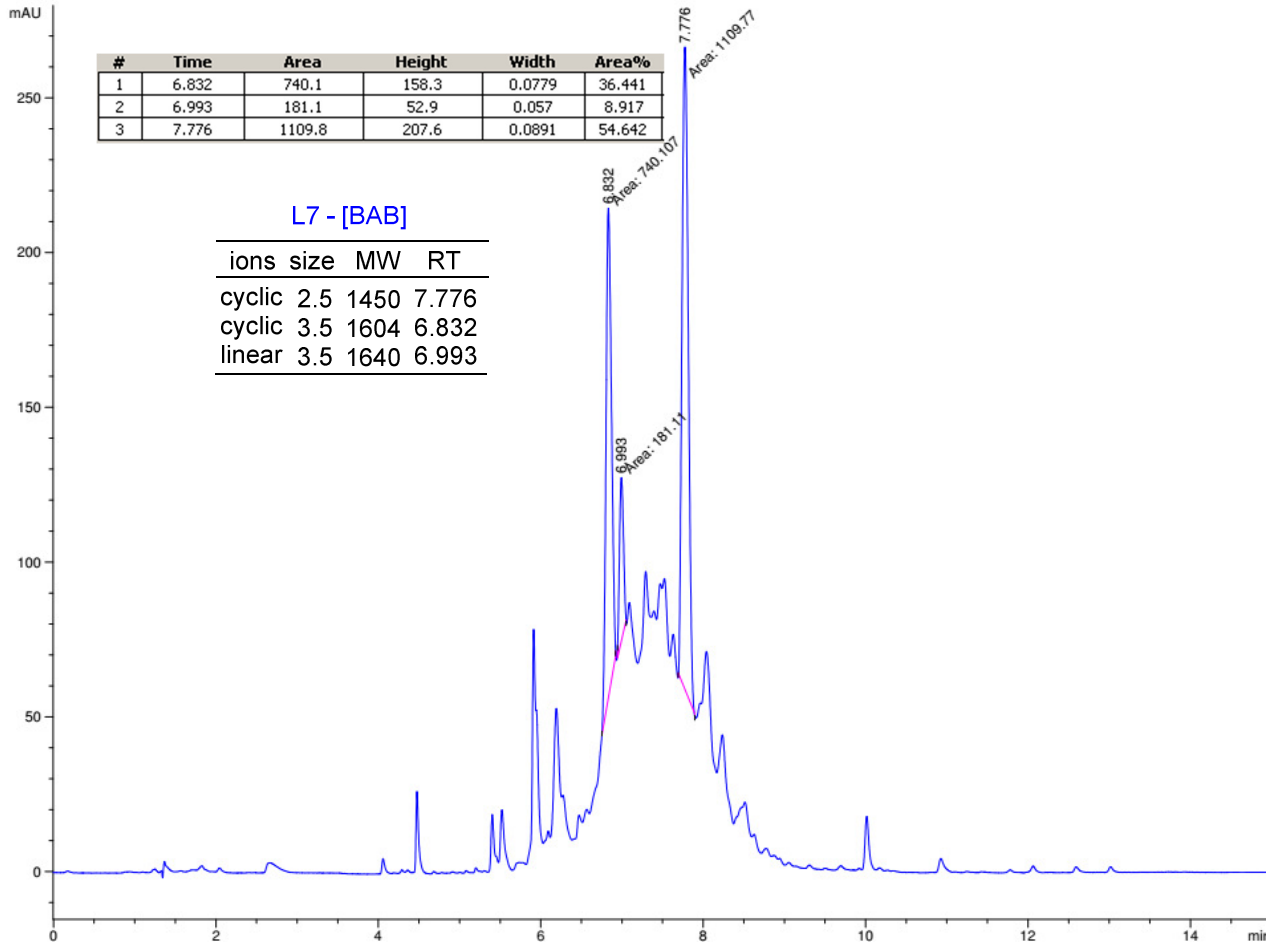




L7-[BAB]: Complete cyclization was observed on 10 µm & 160 µm beads have >90% cyclization complete.



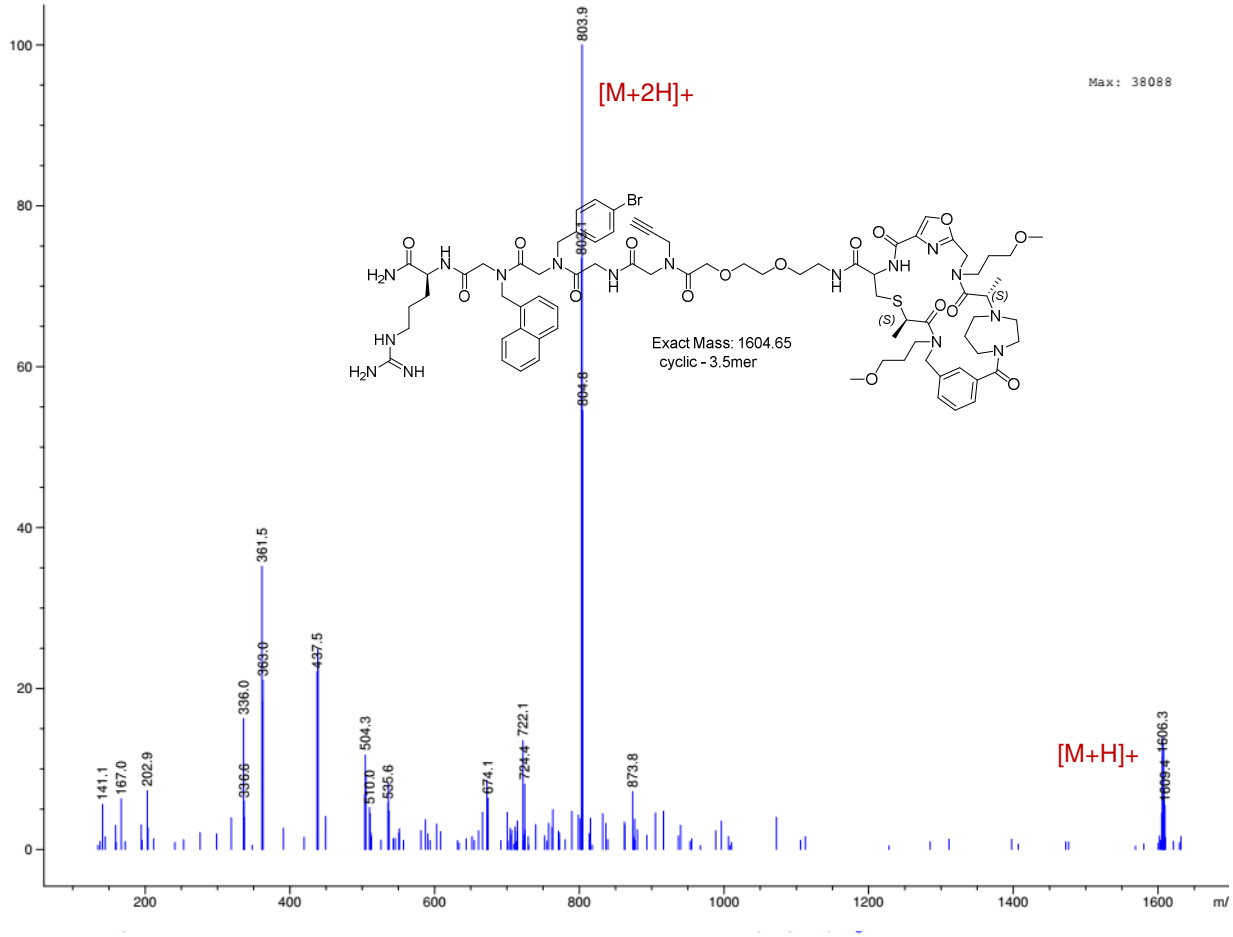


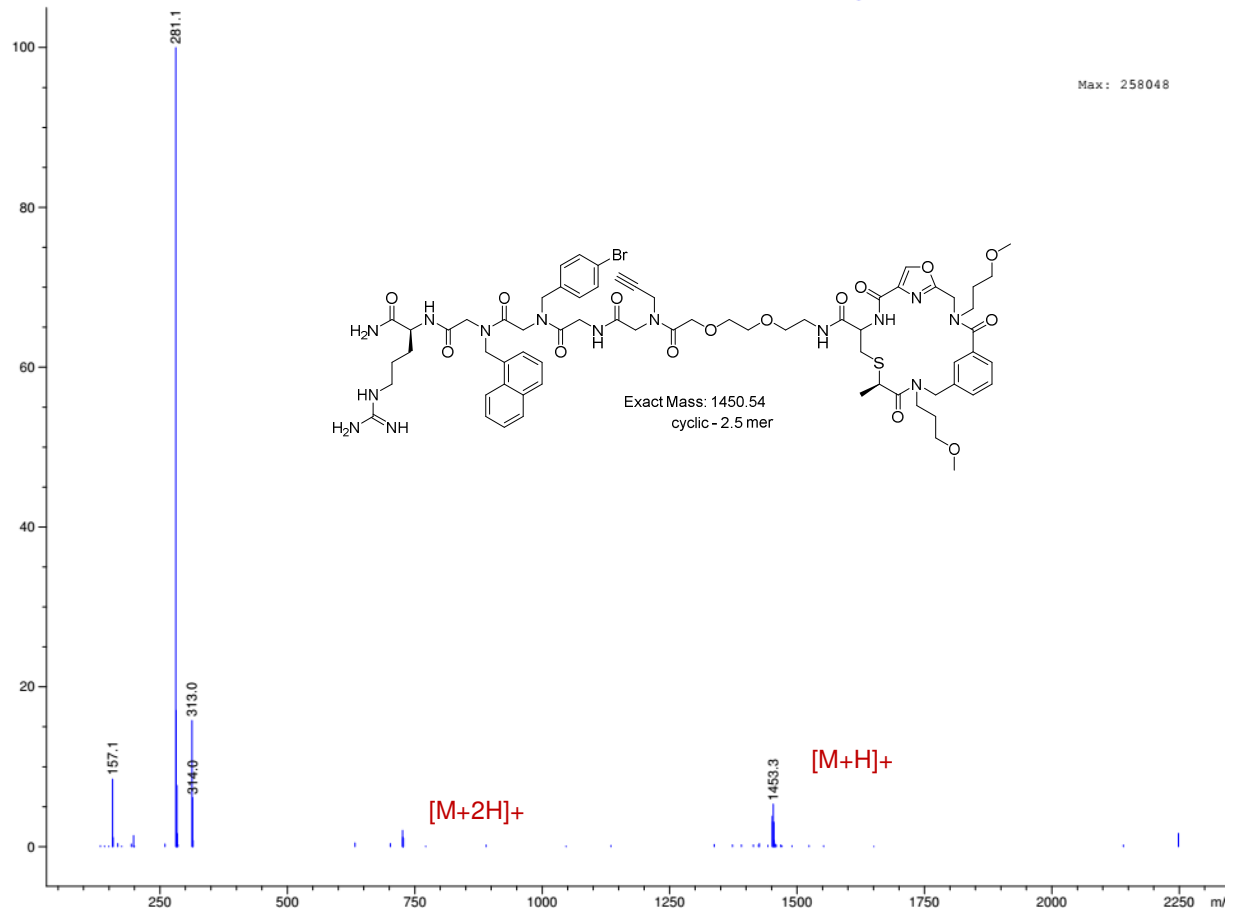


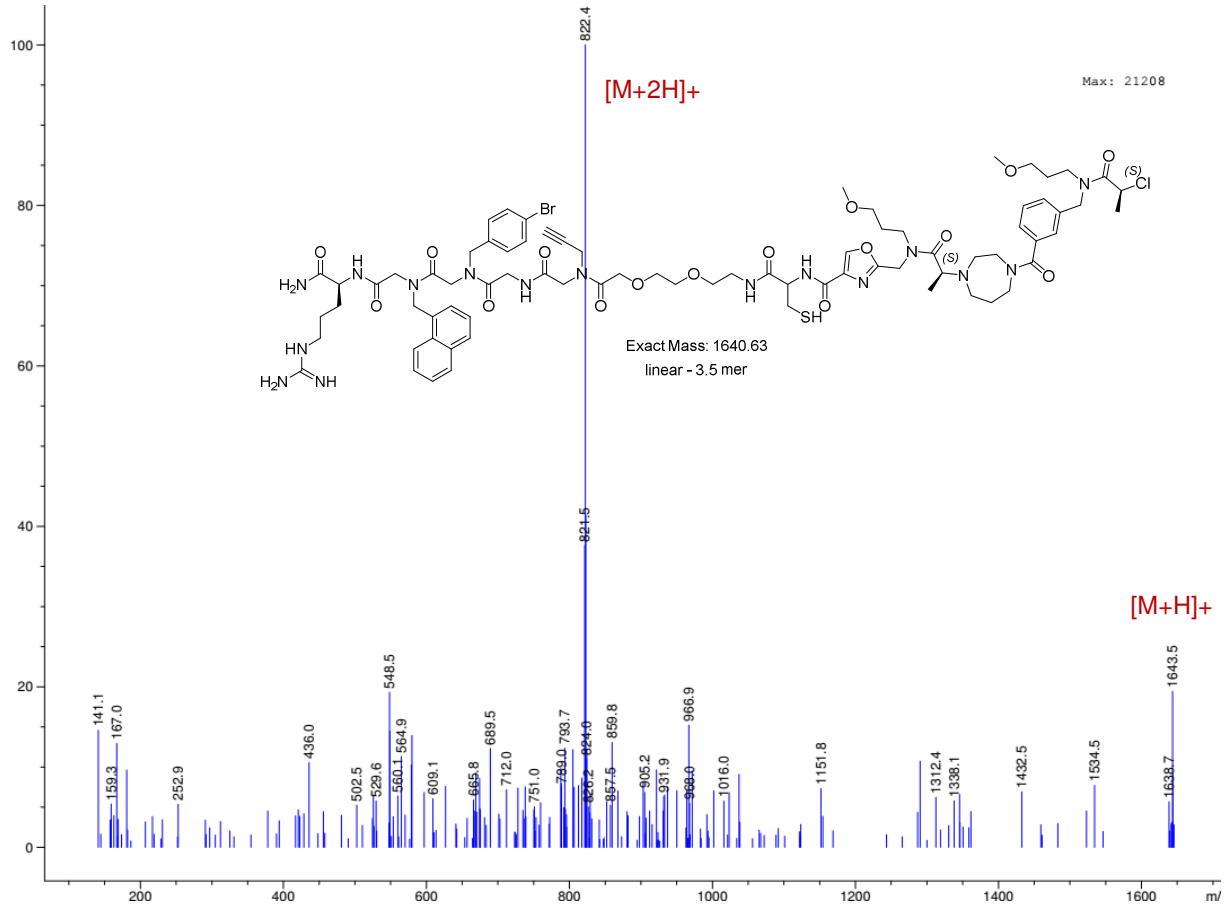
#	Time	Area	Height	Width	Area%
1	6.832	740.1	158.3	0.0779	36.441
2	6.993	181.1	52.9	0.057	8.917
3	7.776	1109.8	207.6	0.0891	54.642

L7 - [BAB]

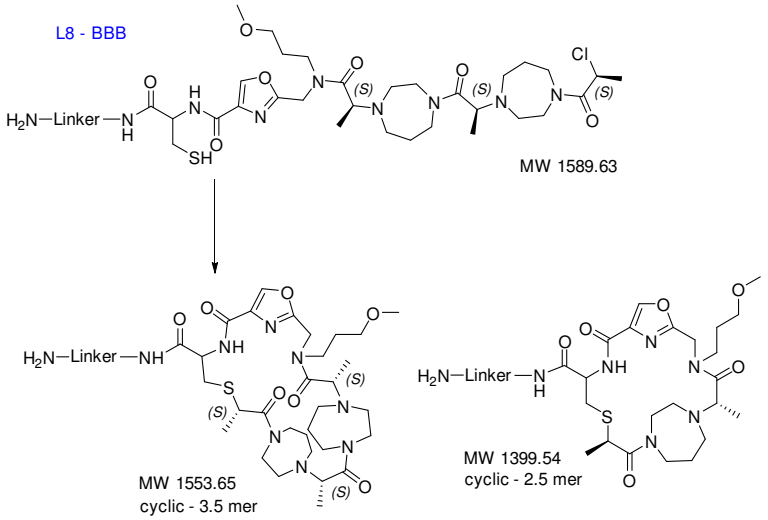
ions	size	MW	RT
cyclic	2.5	1450	7.776
cyclic	3.5	1604	6.832
linear	3.5	1640	6.993

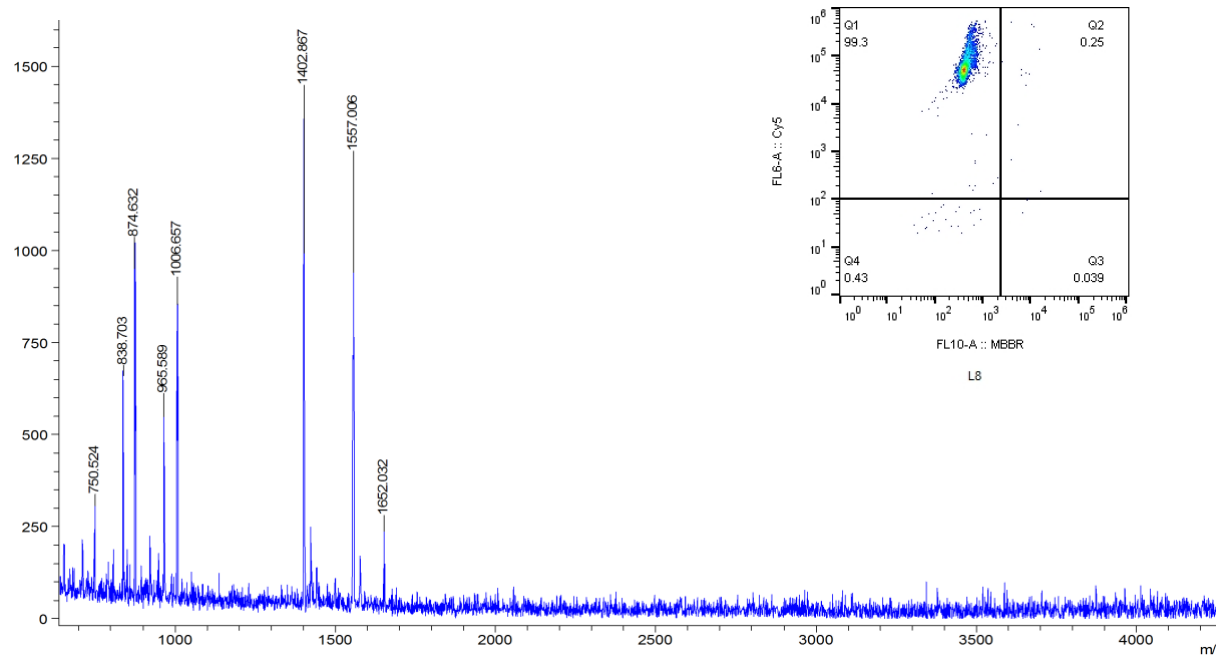

[M+2H]+
Max: 38088
Exact Mass: 1604.65
cyclic - 3.5mer
[M+H]+
803.9
804.8
361.5
336.0
396.6
363.0
437.5
504.3
510.0
595.6
674.1
722.1
724.4
873.8
141.1
167.0
202.9
1606.3
1609.4
m/

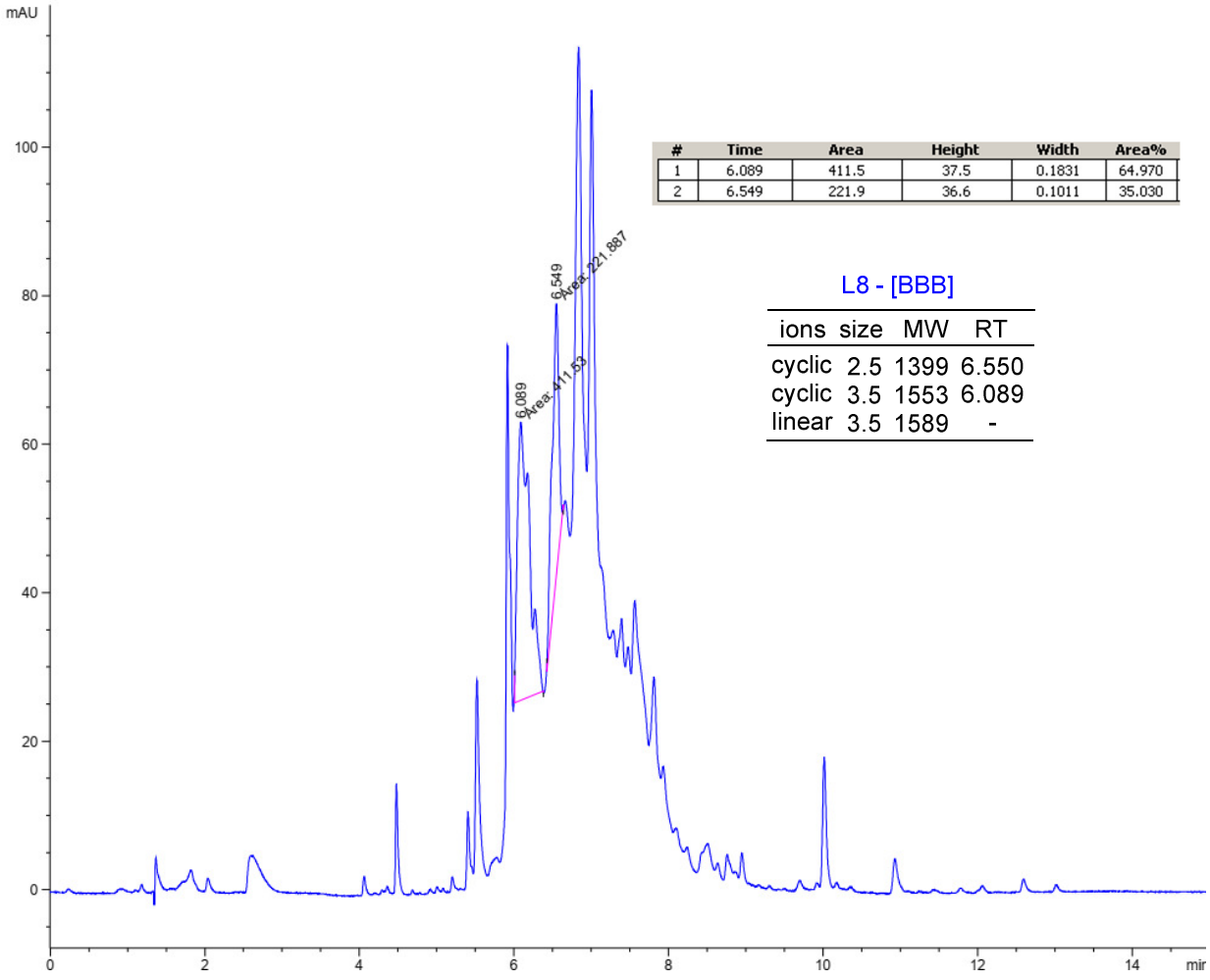

Max: 258048
Exact Mass: 1450.54
cyclic - 2.5 mer
[M+2H]+
[M+H]+
281.1
313.0
157.1
914.0
1453.3
m/



L8-[BBB]: Complete cyclization was observed on 10 µm & 160 µm beads.



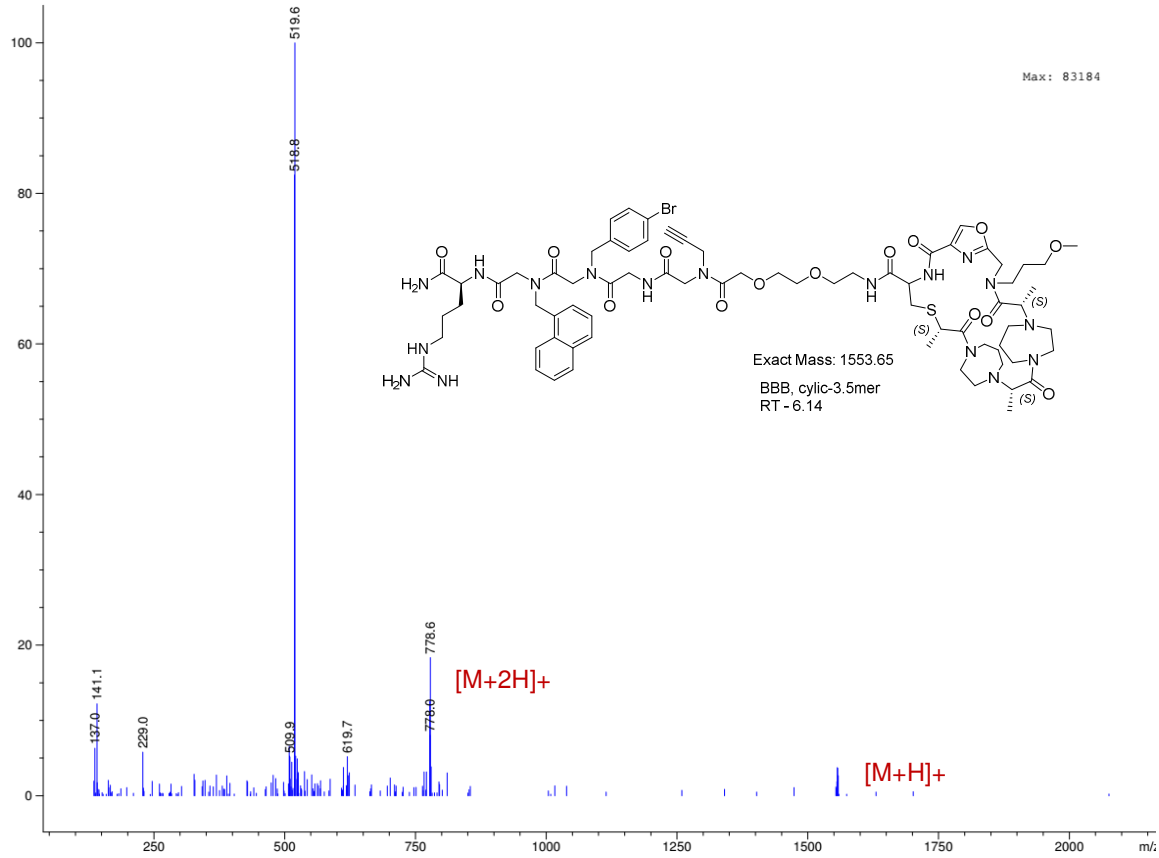


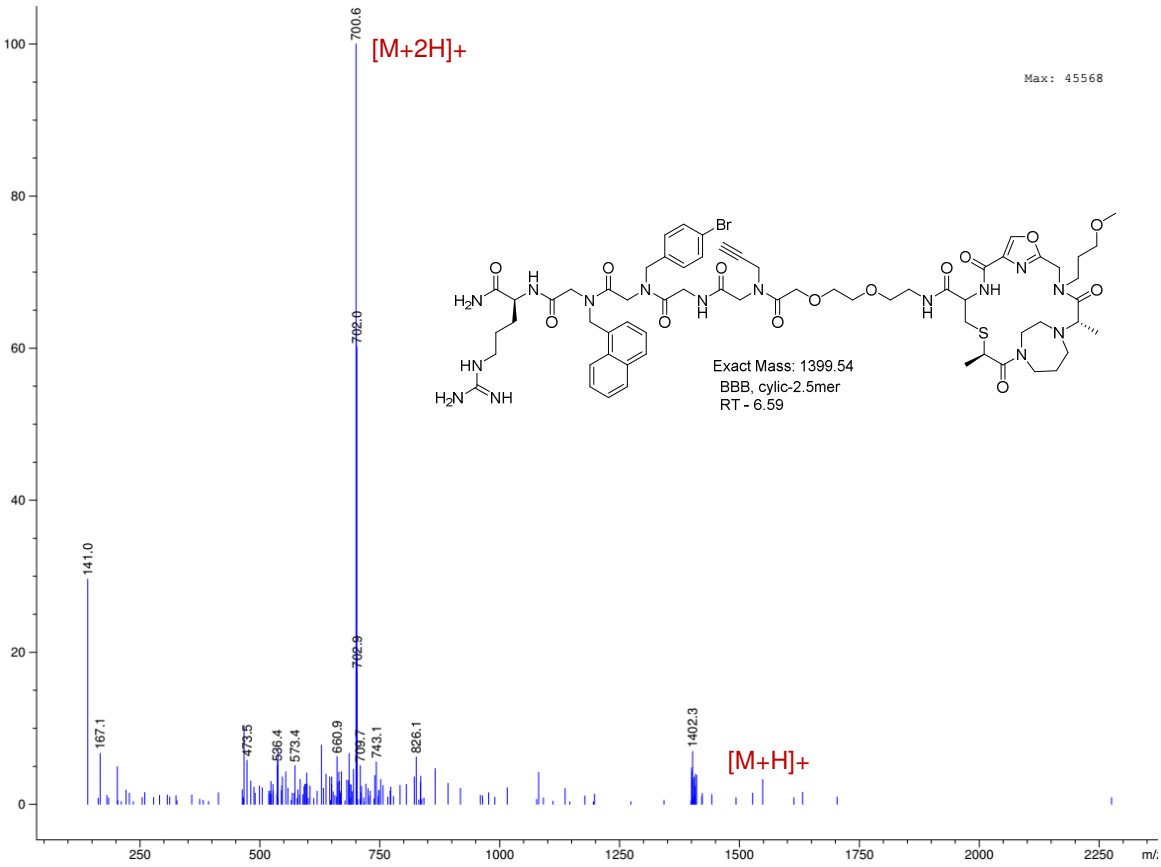


#	Time	Area	Height	Width	Area%
1	6.089	411.5	37.5	0.1831	64.970
2	6.549	221.9	36.6	0.1011	35.030

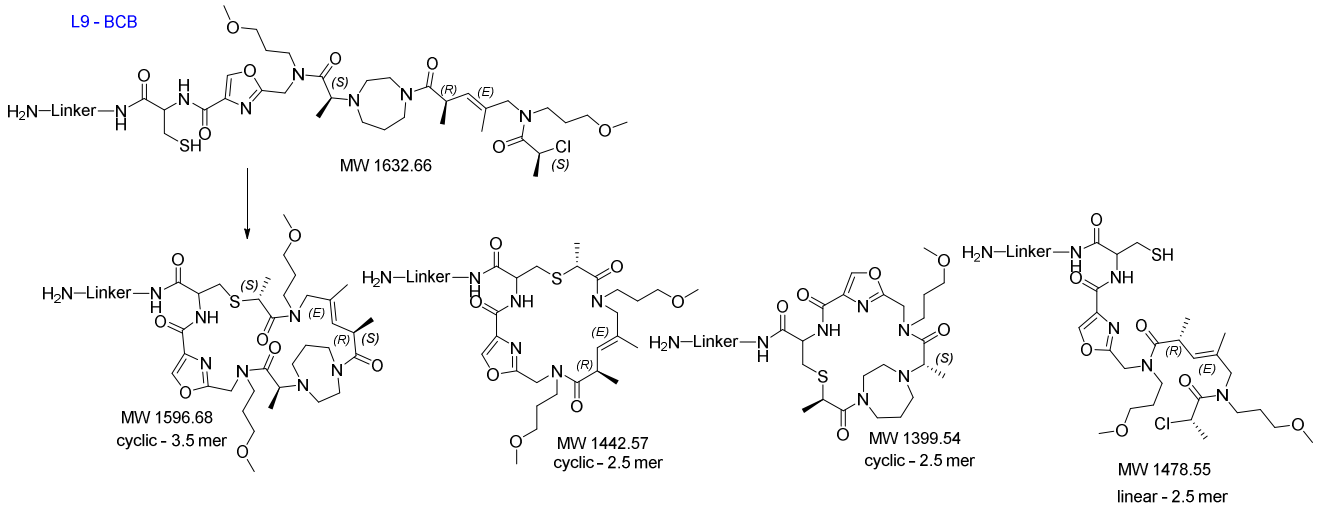
L8 - [BBB]

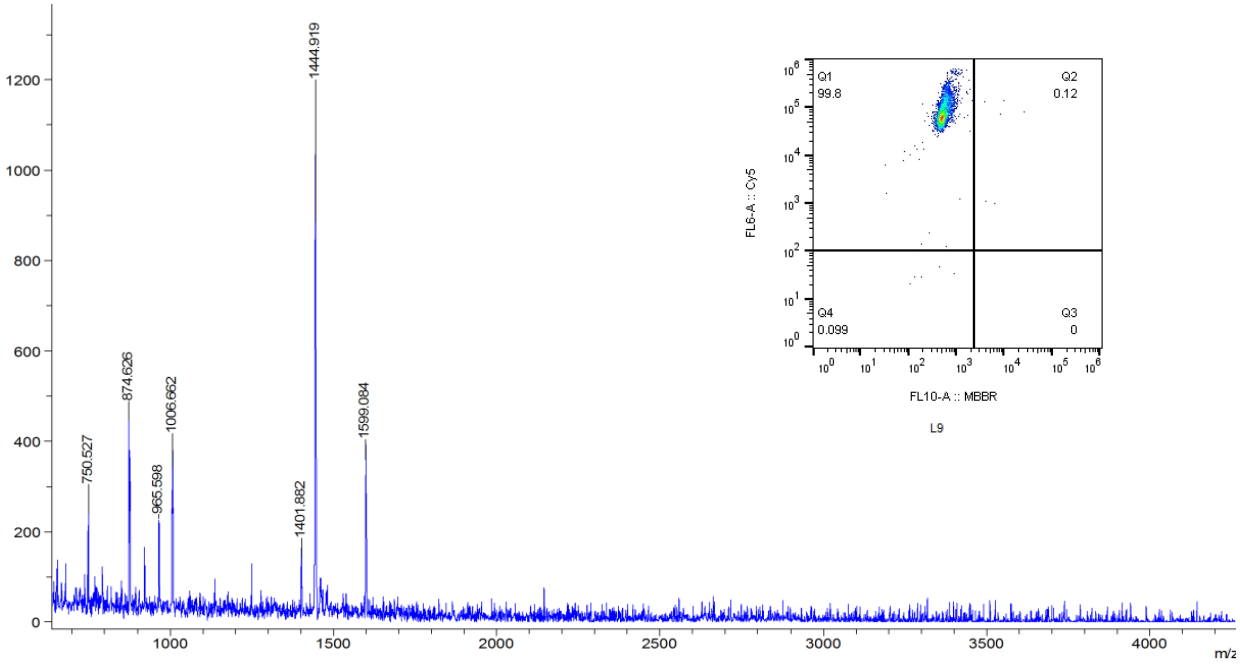
ions	size	MW	RT
cyclic	2.5	1399	6.550
cyclic	3.5	1553	6.089
linear	3.5	1589	-

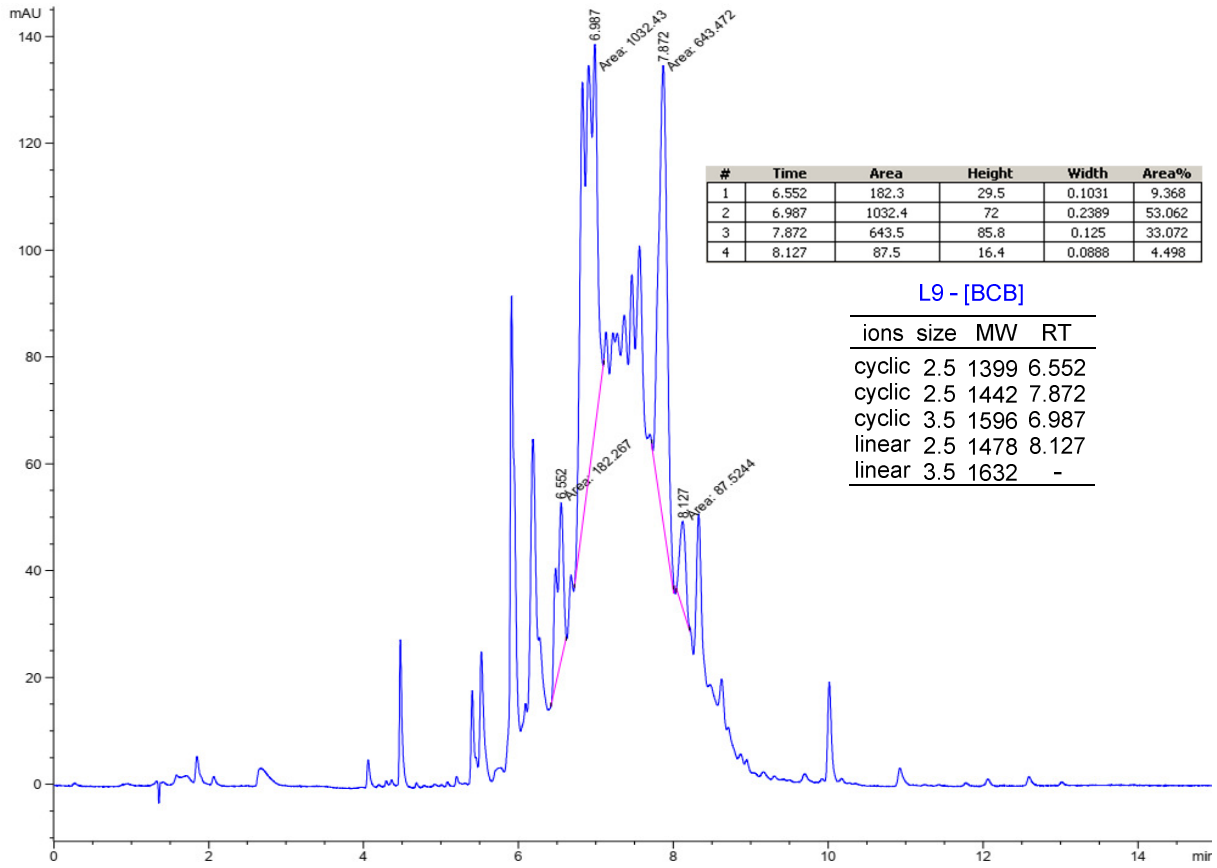

Max: 83184
519.6
518.8
778.6
778.0
141.1
137.0
229.0
509.9
619.7
[M+2H]+
[M+H]+
Exact Mass: 1553.65
BBB, cylic-3.5mer
RT - 6.14
Br
100
80
60
40
20
0
250
500
750
1000
1250
1500
1750
2000
m/z


Max: 45568
700.6
[M+2H]+
702.0
702.9
141.0
167.1
473.5
536.4
573.4
660.9
709.7
743.1
826.1
1402.3
[M+H]+
Exact Mass: 1399.54
BBB, cylic-2.5mer
RT - 6.59
Br
100
80
60
40
20
0
250
500
750
1000
1250
1500
1750
2000
2250
m/z

L9-[BCB]: Complete cyclization was observed on 10 µm & 160 µm beads. A linear (2.5mer) fragment could not cyclize (MW 1478, RT- 8.124). Other fragments (2.5mers) cyclized and identified.



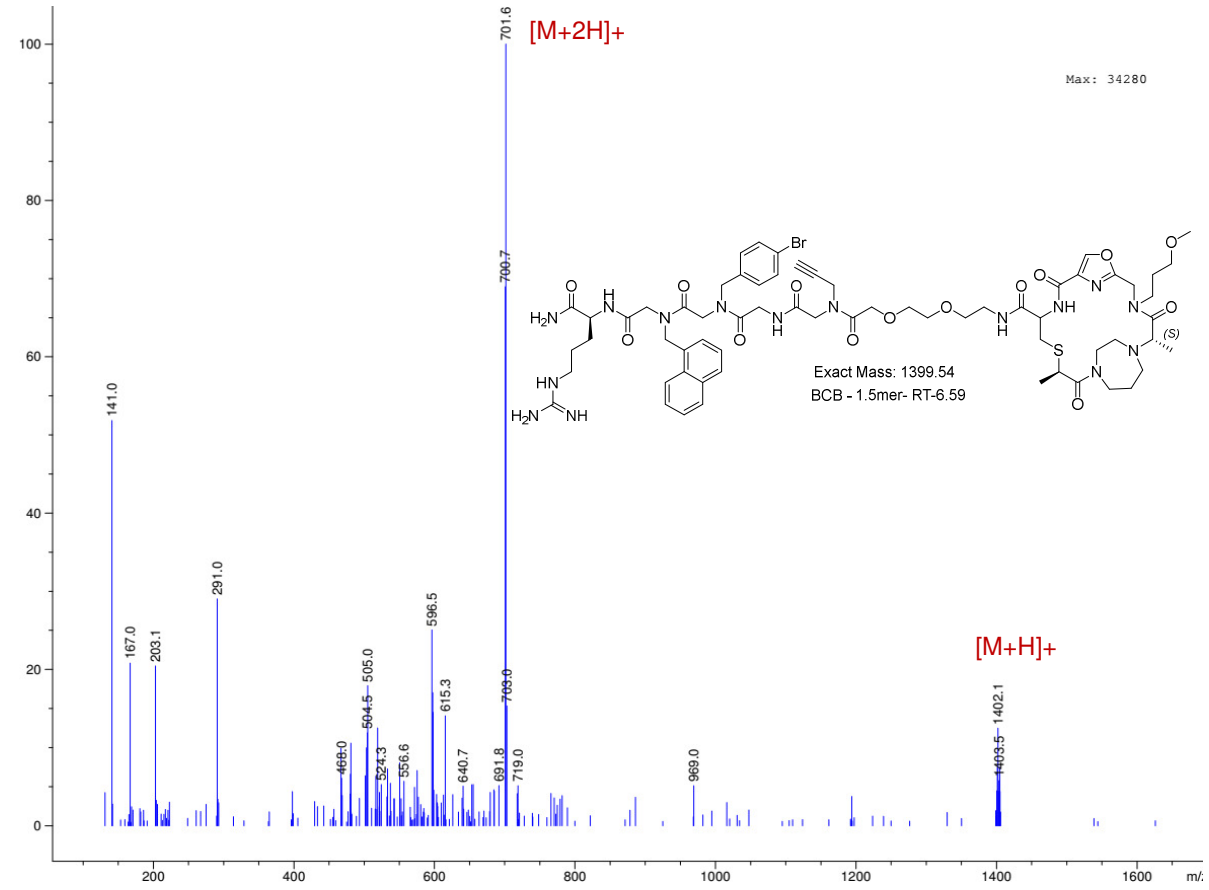


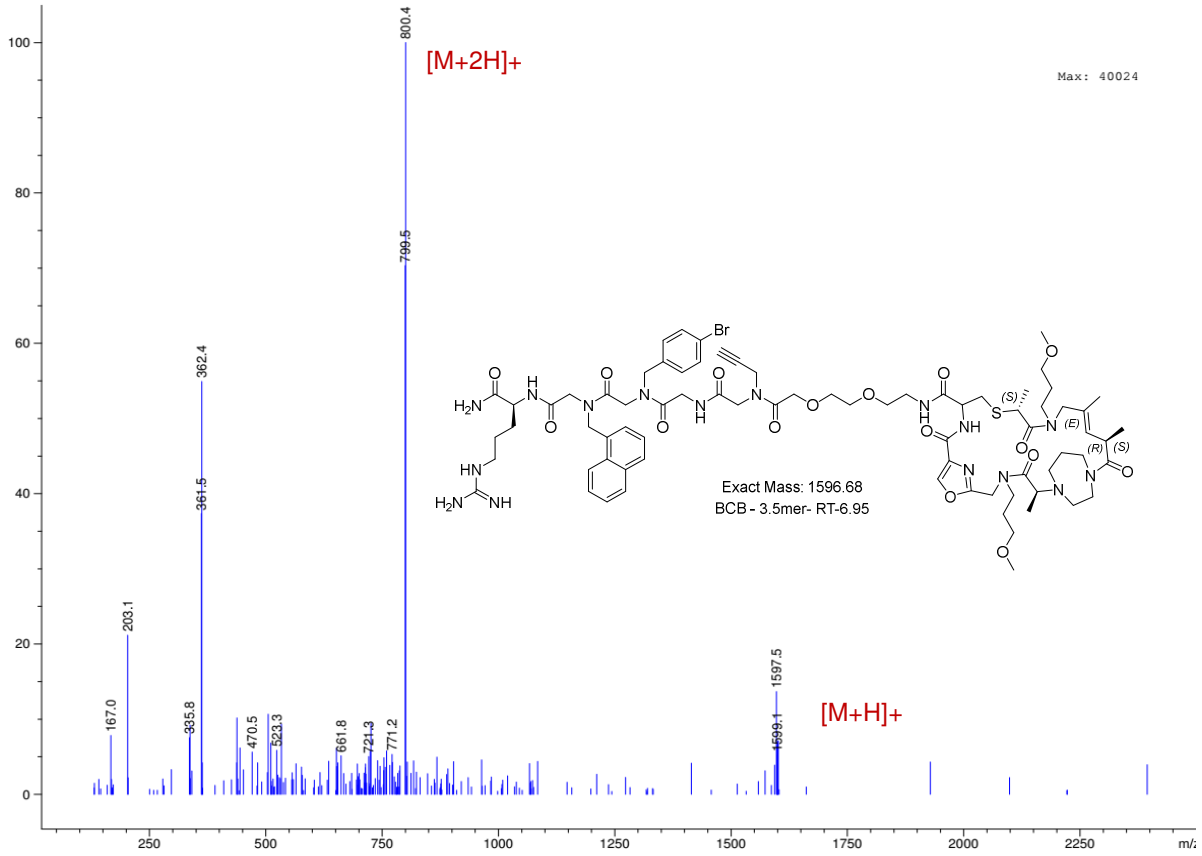


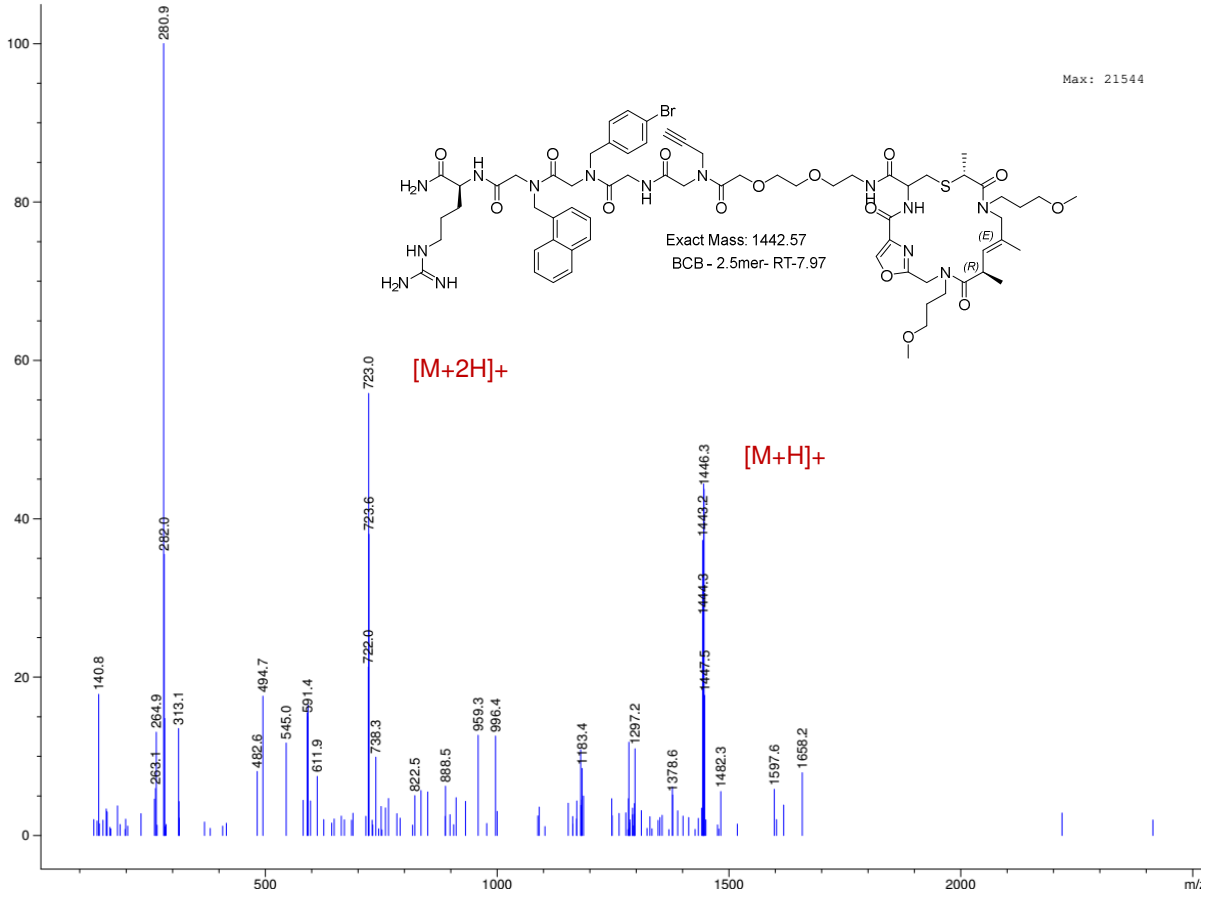
#	Time	Area	Height	Width	Area%
1	6.552	182.3	29.5	0.1031	9.368
2	6.987	1032.4	72	0.2389	53.062
3	7.872	643.5	85.8	0.125	33.072
4	8.127	87.5	16.4	0.0888	4.498

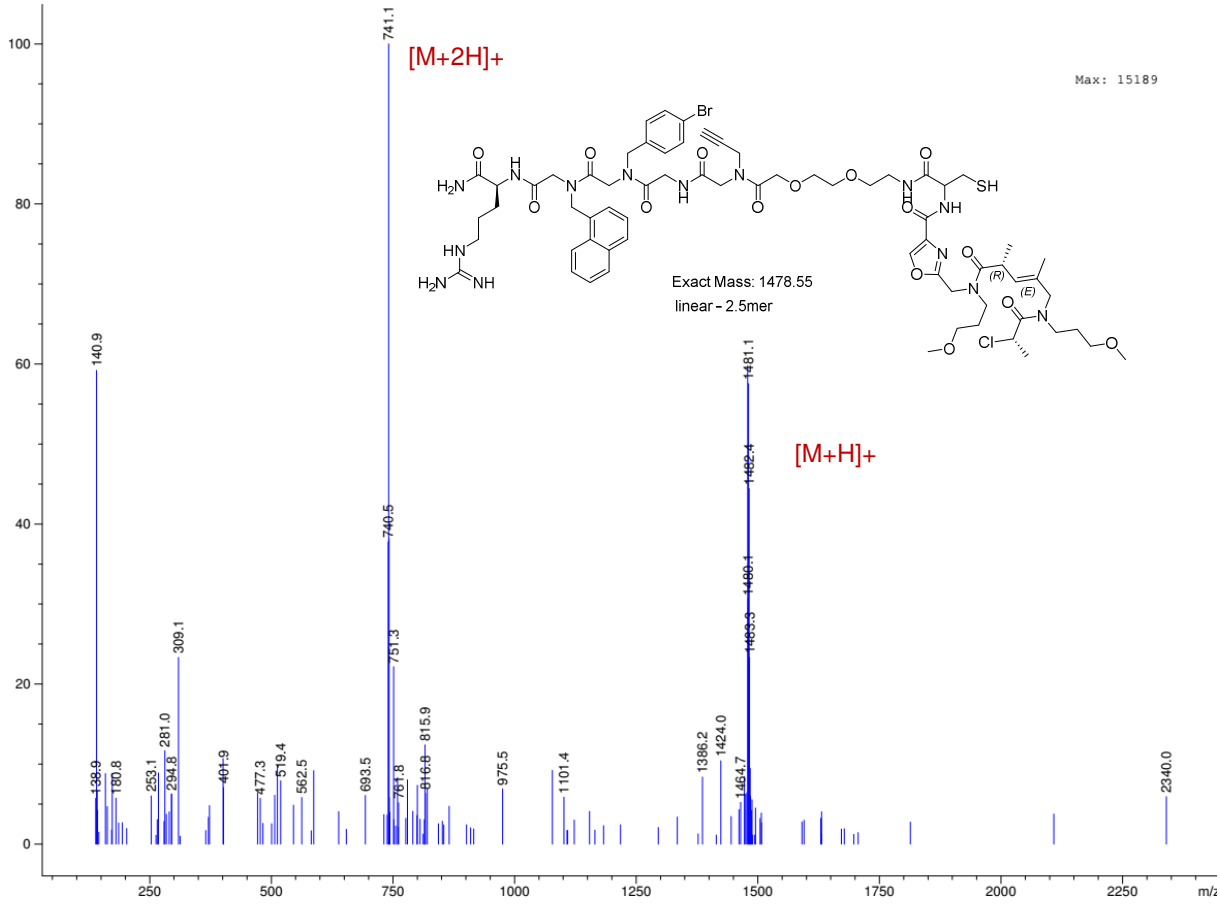
L9 - [BCB]

ions	size	MW	RT
cyclic	2.5	1399	6.552
cyclic	2.5	1442	7.872
cyclic	3.5	1596	6.987
linear	2.5	1478	8.127
linear	3.5	1632	-

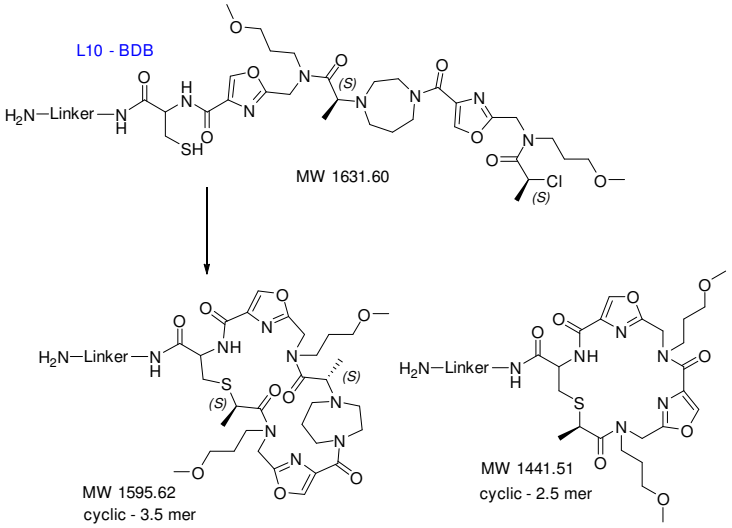


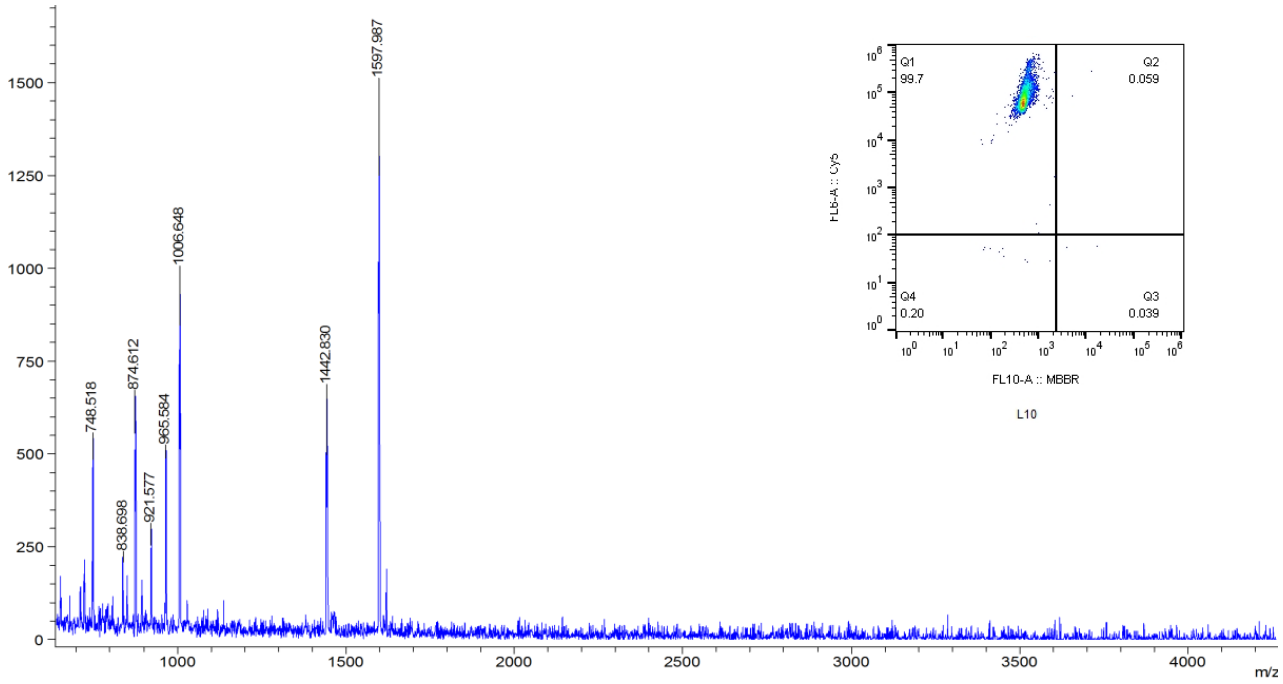

[M+2H]+
Max: 40024
800.4
799.5
362.4
361.5
203.1
167.0
385.8
470.5
523.3
661.8
721.3
771.2
1597.5
1599.1
[M+H]+
Exact Mass: 1596.68
BCB - 3.5mer- RT-6.95
Br
100
80
60
40
20
0
250
500
750
1000
1250
1500
1750
2000
2250

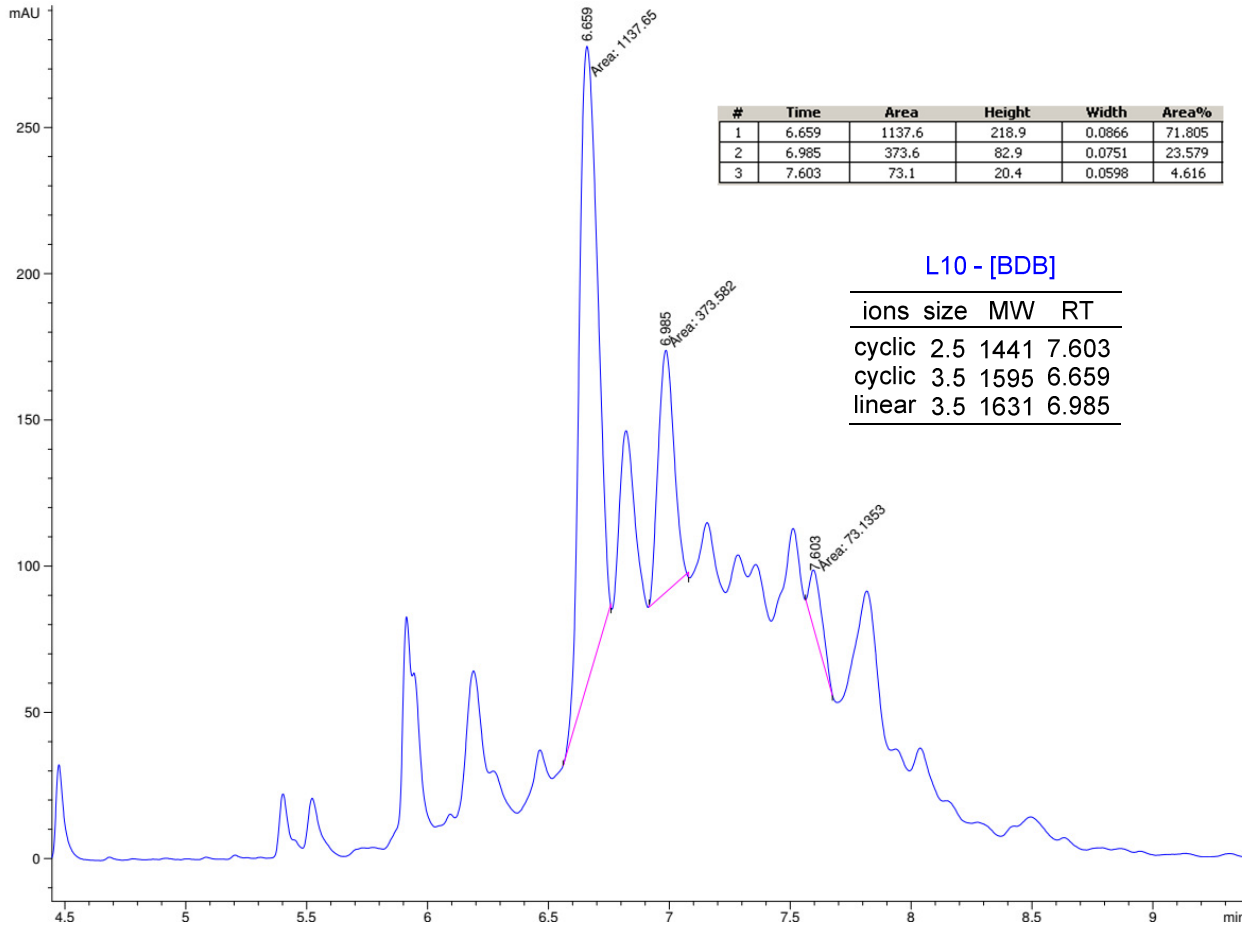

Max: 21544
280.9
282.0
140.8
264.9
263.1
313.1
482.6
494.7
545.0
591.4
611.9
723.0
722.0
738.3
822.5
888.5
959.3
996.4
1183.4
1297.2
1378.6
1446.3
1443.2
1444.3
1447.5
1482.3
1597.6
1658.2
[M+2H]+
[M+H]+
Exact Mass: 1442.57
BCB - 2.5mer- RT-7.97
Br
100
80
60
40
20
0
500
1000
1500
2000



L10-[BDB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm.



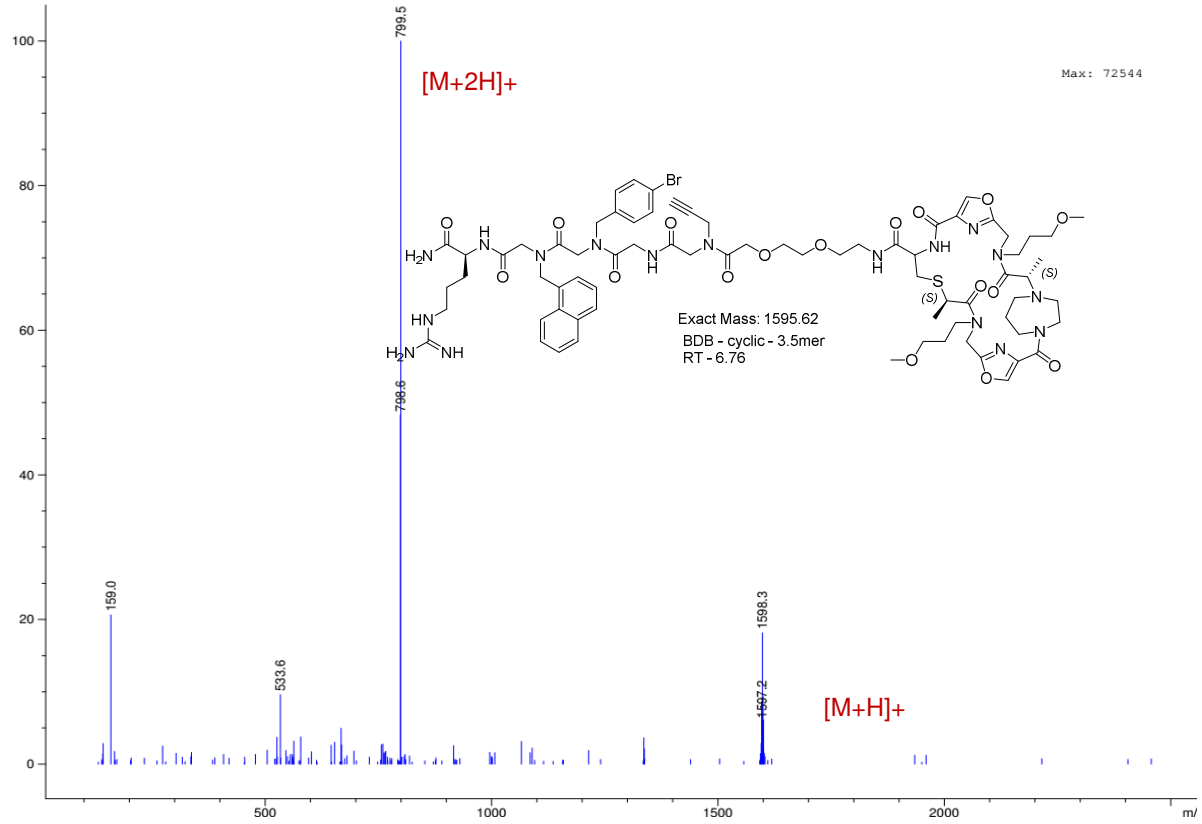


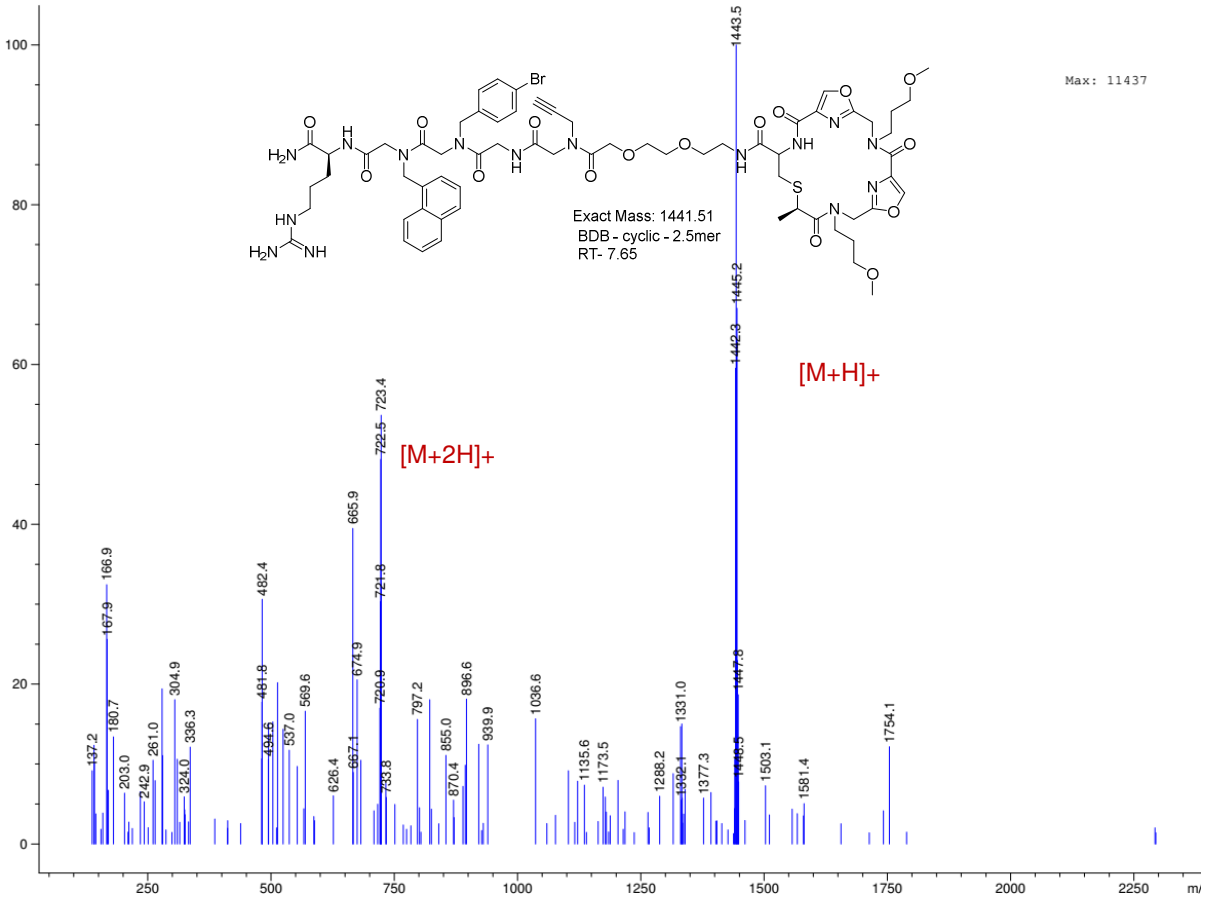


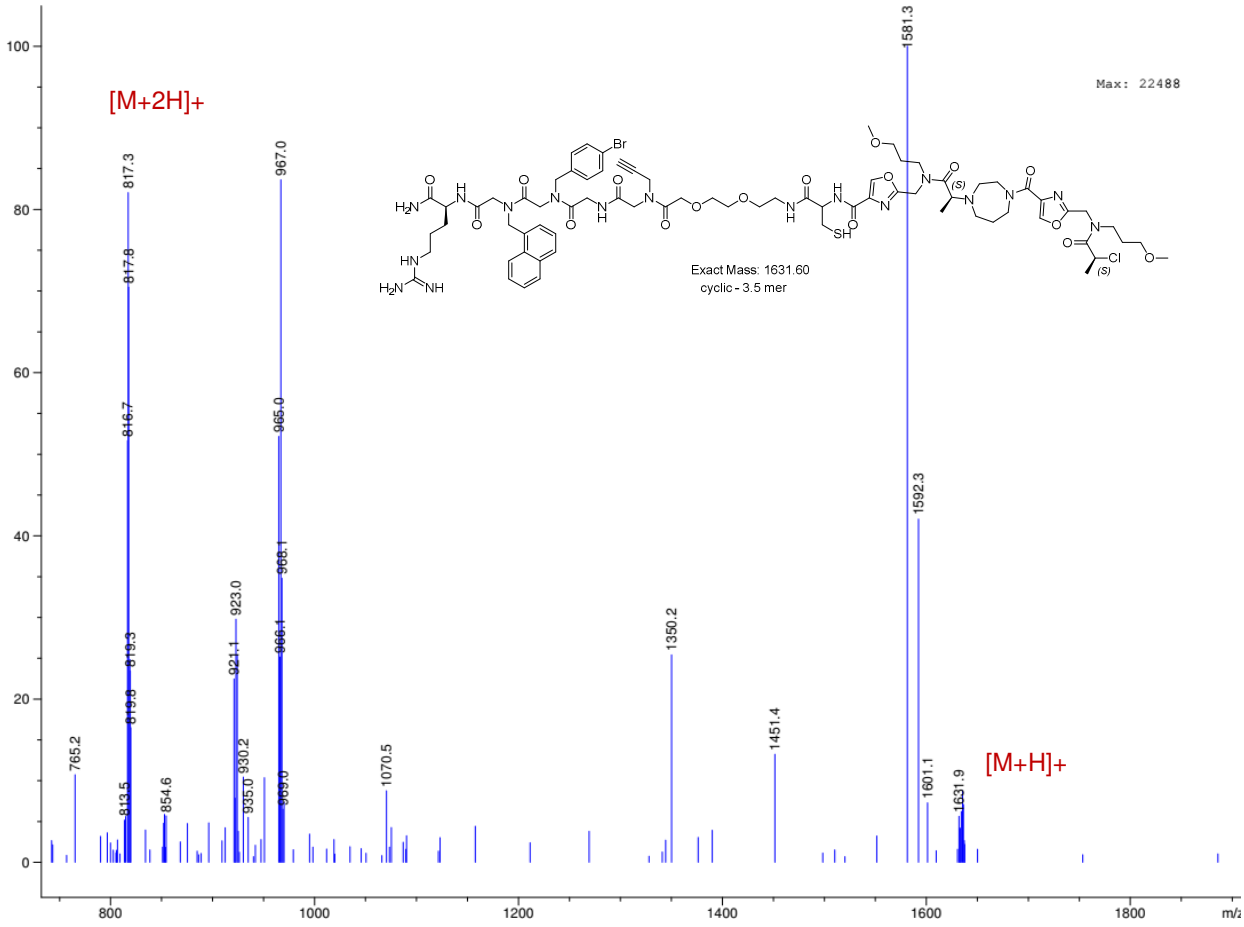
#	Time	Area	Height	Width	Area%
1	6.659	1137.6	218.9	0.0866	71.805
2	6.985	373.6	82.9	0.0751	23.579
3	7.603	73.1	20.4	0.0598	4.616

L10 - [BDB]

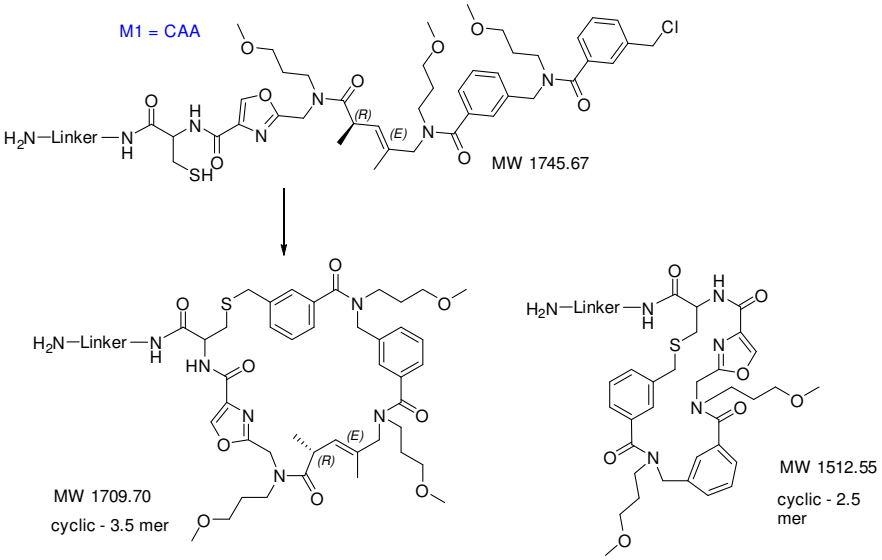
ions	size	MW	RT
cyclic	2.5	1441	7.603
cyclic	3.5	1595	6.659
linear	3.5	1631	6.985

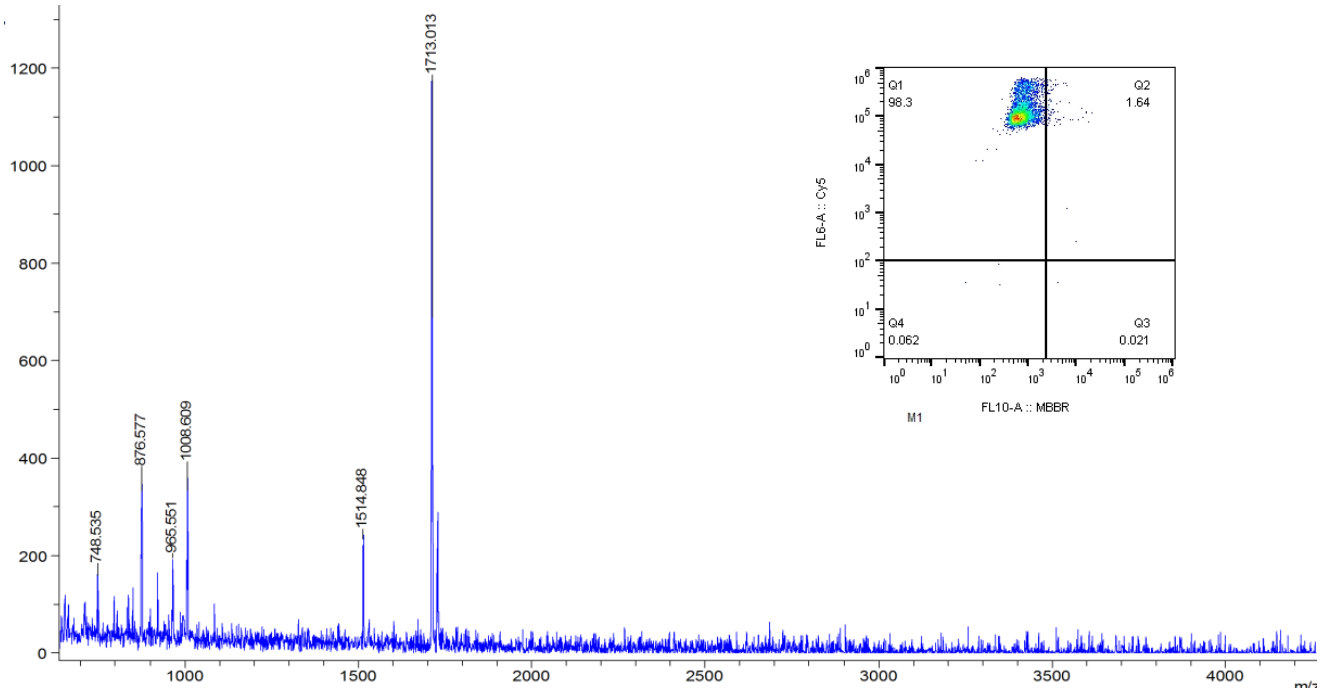

[M+2H]+
Max: 72544
Exact Mass: 1595.62
BDB - cyclic - 3.5mer
RT - 6.76
[M+H]+

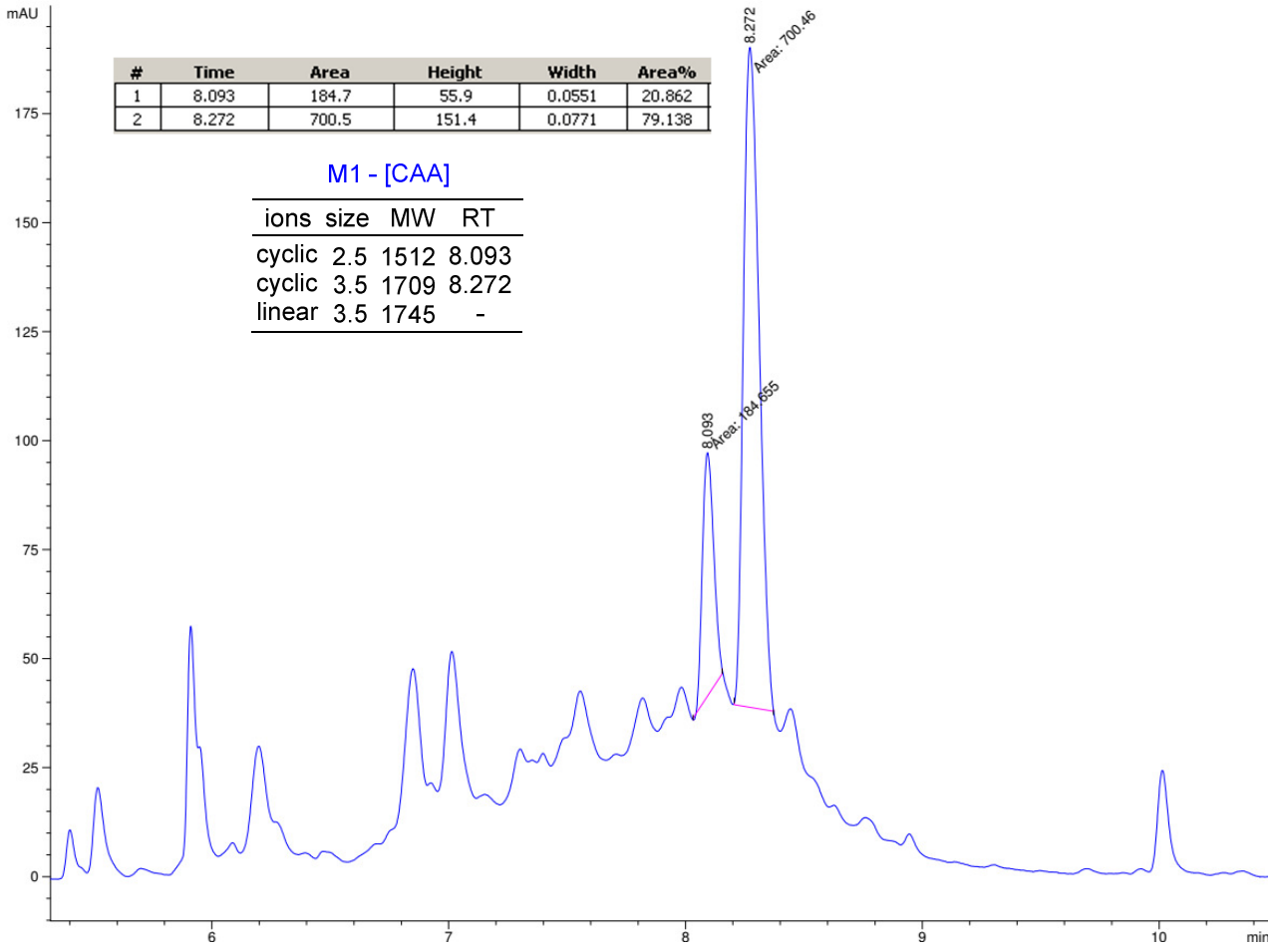

Max: 11437
Exact Mass: 1441.51
BDB - cyclic - 2.5mer
RT- 7.65
[M+H]+
[M+2H]+



M1-[CAA]: Complete cyclization was observed on 10 µm & 160 µm beads.



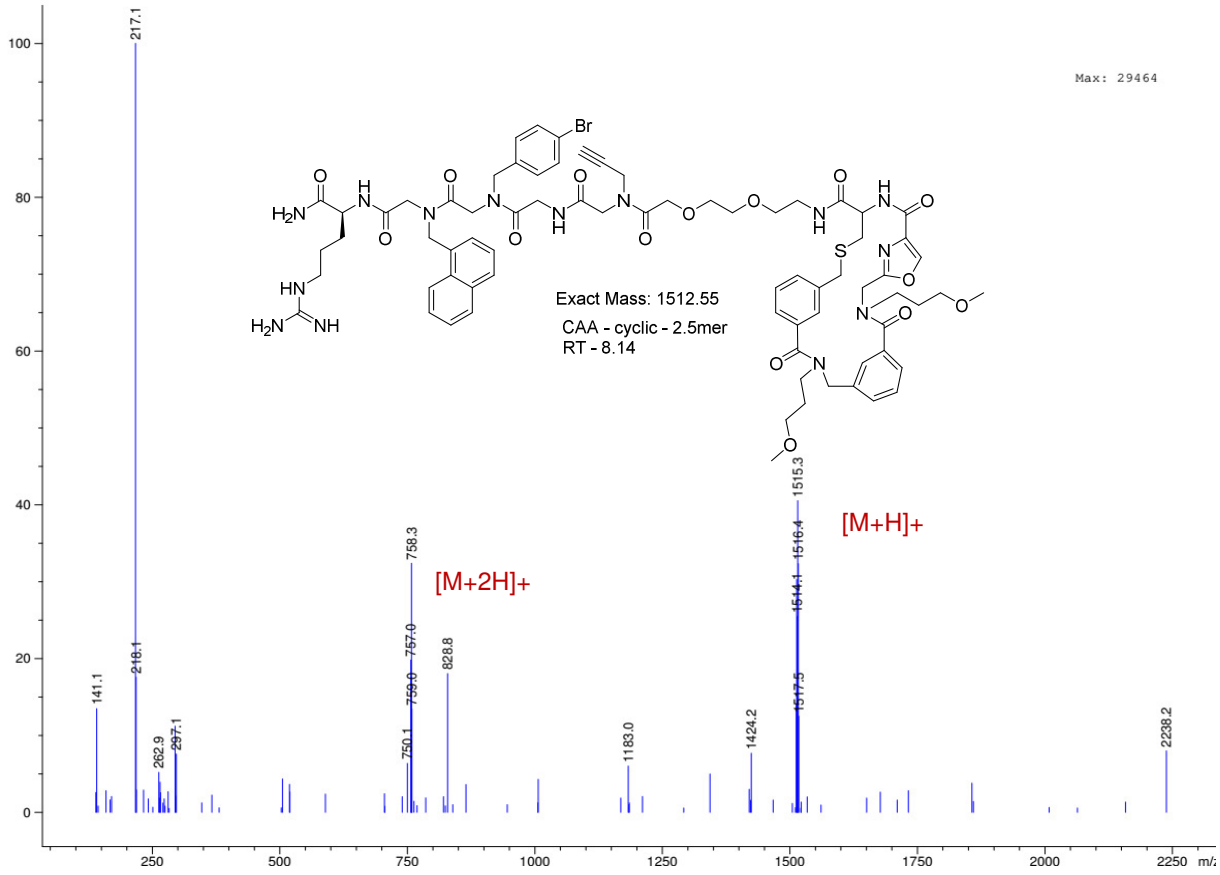


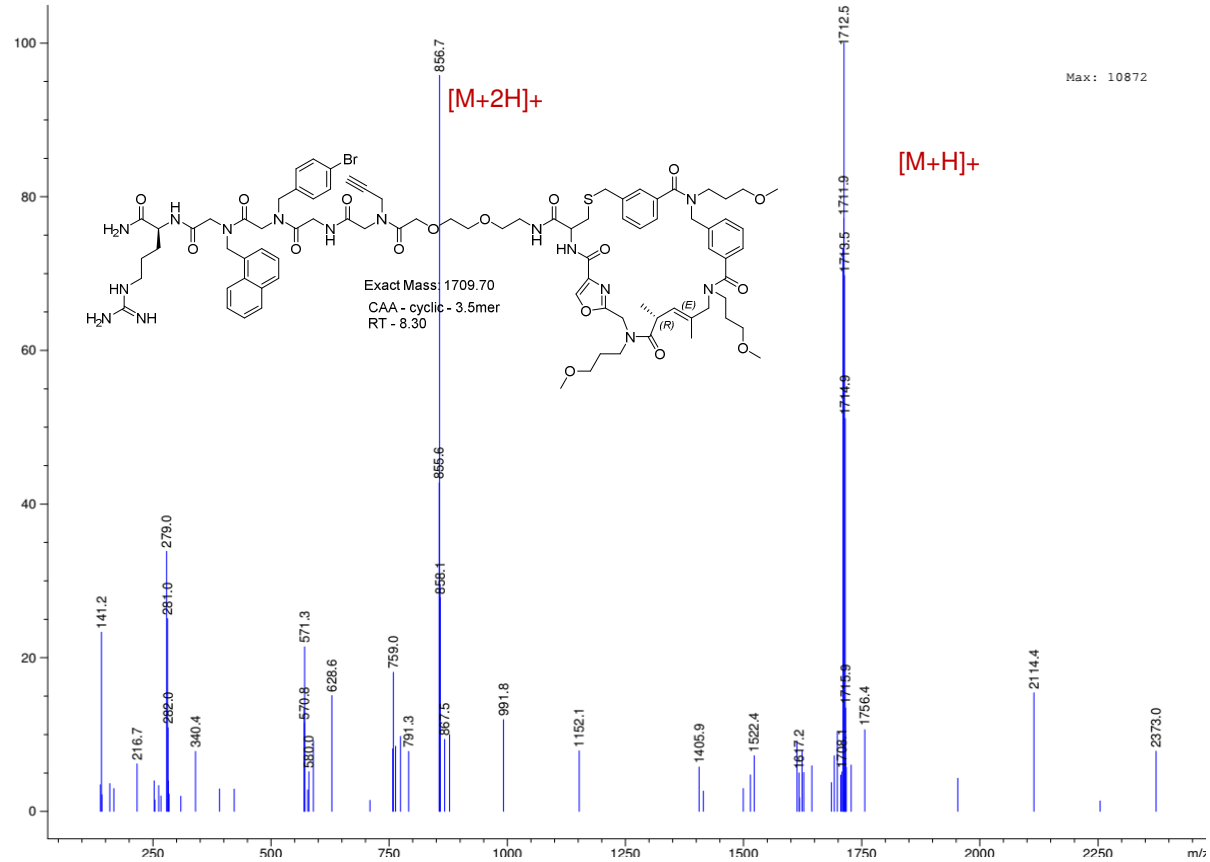


#	Time	Area	Height	Width	Area%
1	8.093	184.7	55.9	0.0551	20.862
2	8.272	700.5	151.4	0.0771	79.138

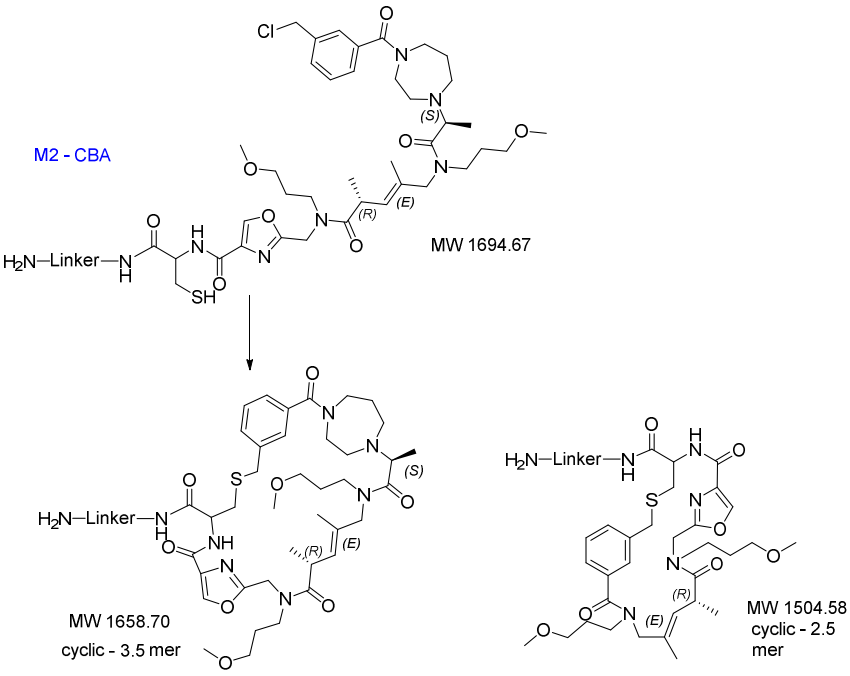
M1 - [CAA]

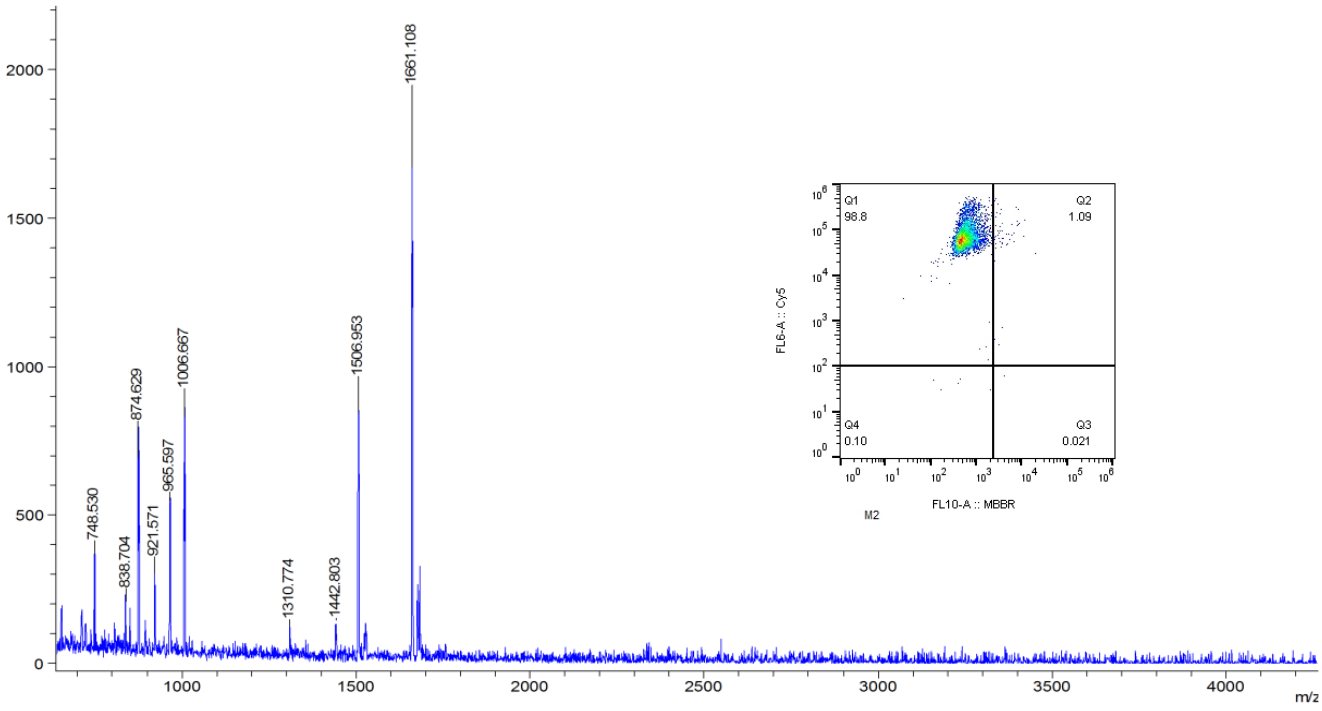
ions	size	MW	RT
cyclic	2.5	1512	8.093
cyclic	3.5	1709	8.272
linear	3.5	1745	-

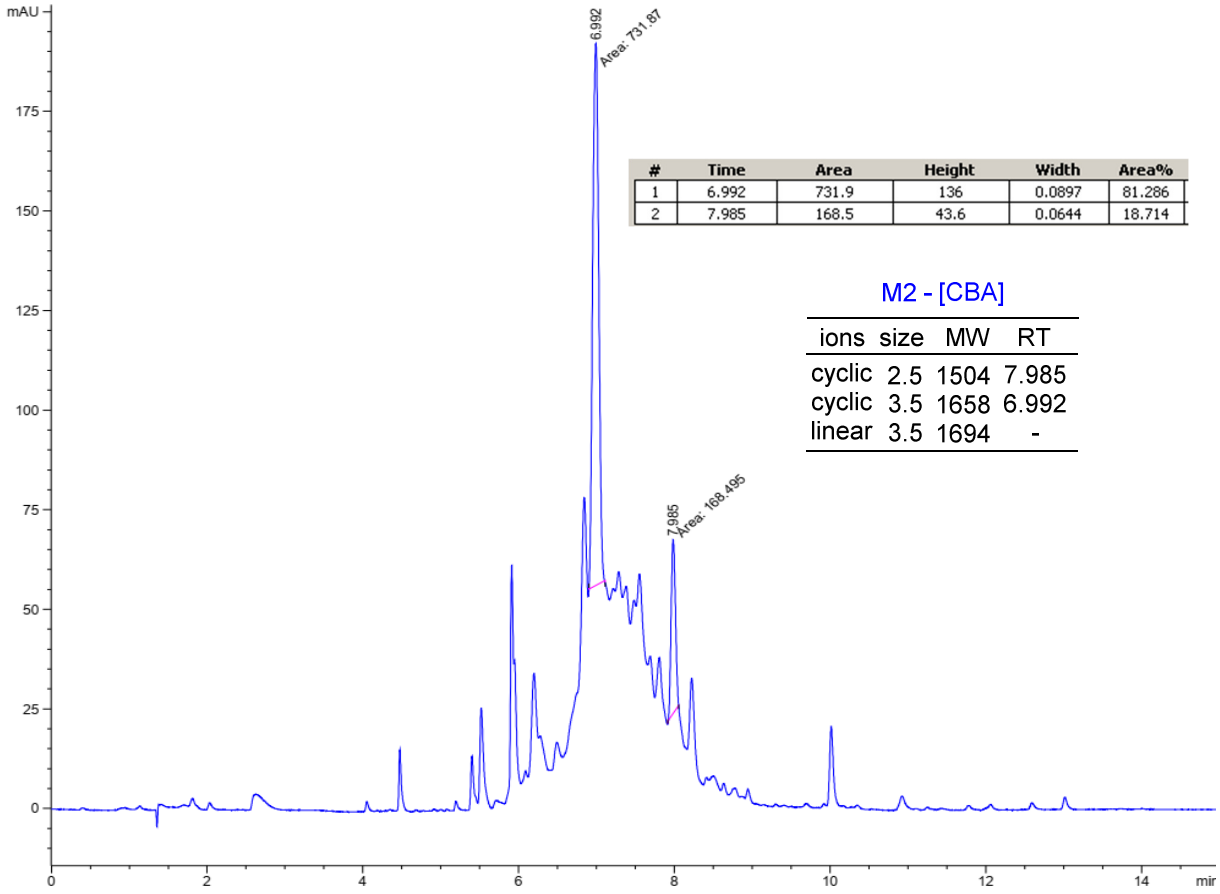

Max: 29464
Exact Mass: 1512.55
CAA - cyclic - 2.5mer
RT - 8.14
[M+2H]+
[M+H]+
217.1
758.3
1515.3
m/z


Max: 10872
Exact Mass: 1709.70
CAA - cyclic - 3.5mer
RT - 8.30
[M+2H]+
[M+H]+
856.7
1712.5
m/z

M2-[CBA]: Complete cyclization was observed on 10 µm & 160 µm beads.



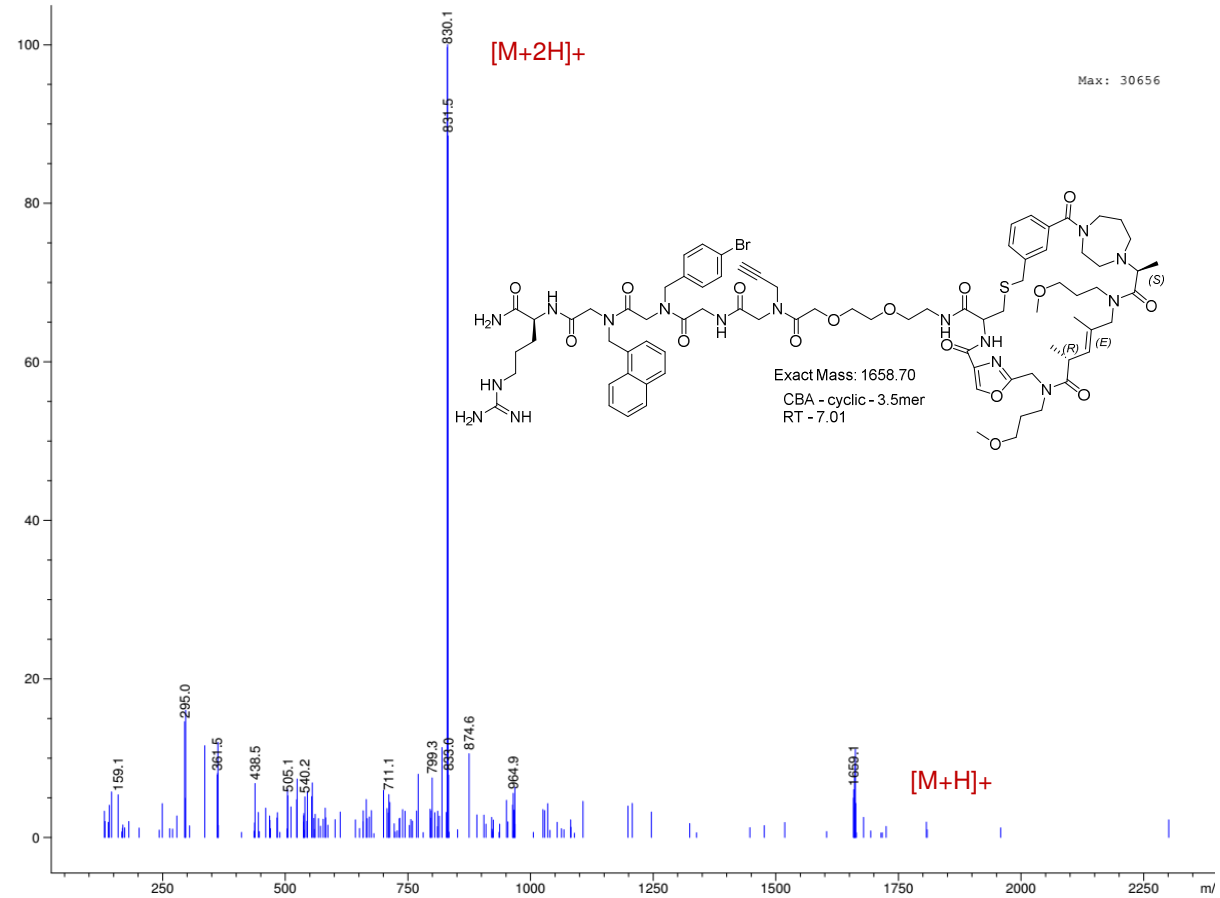


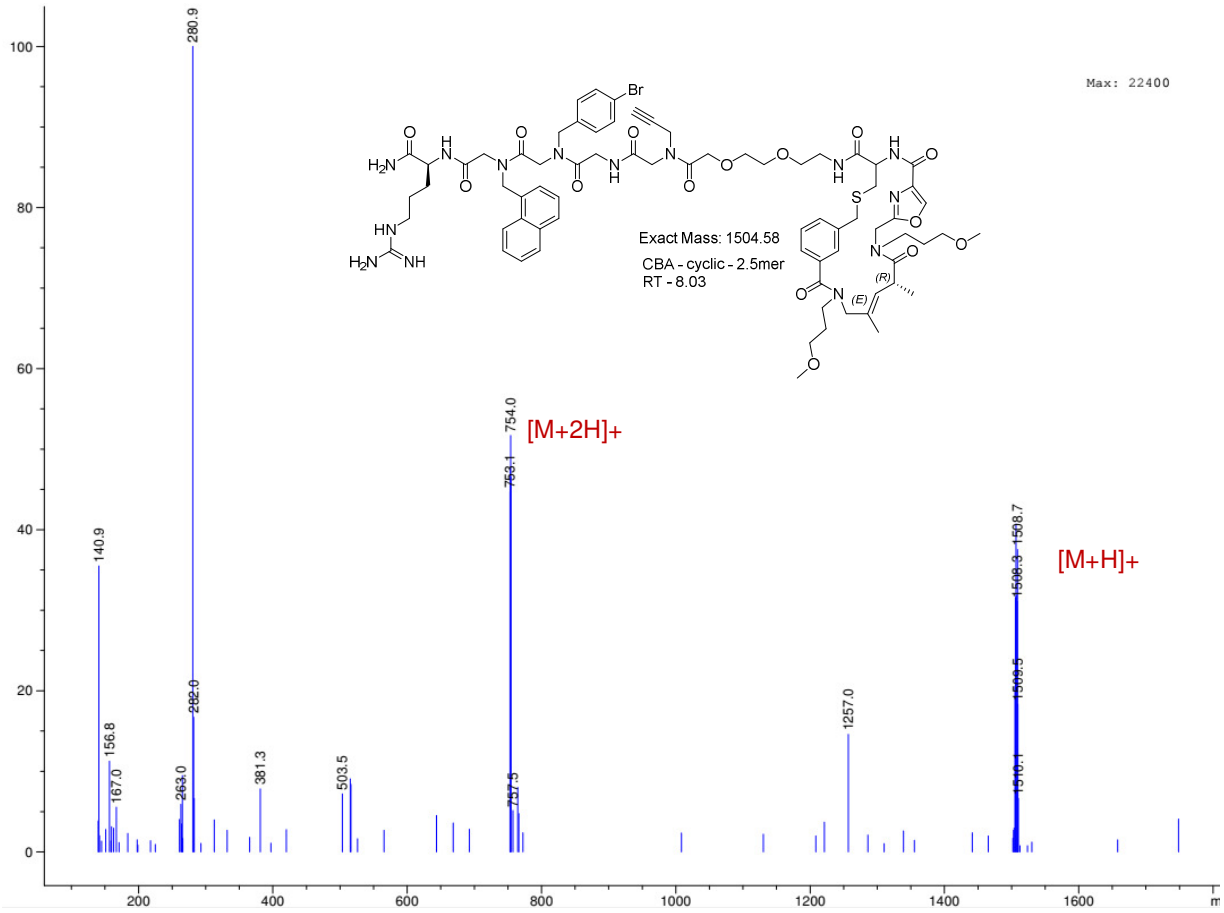


#	Time	Area	Height	Width	Area%
1	6.992	731.9	136	0.0897	81.286
2	7.985	168.5	43.6	0.0644	18.714

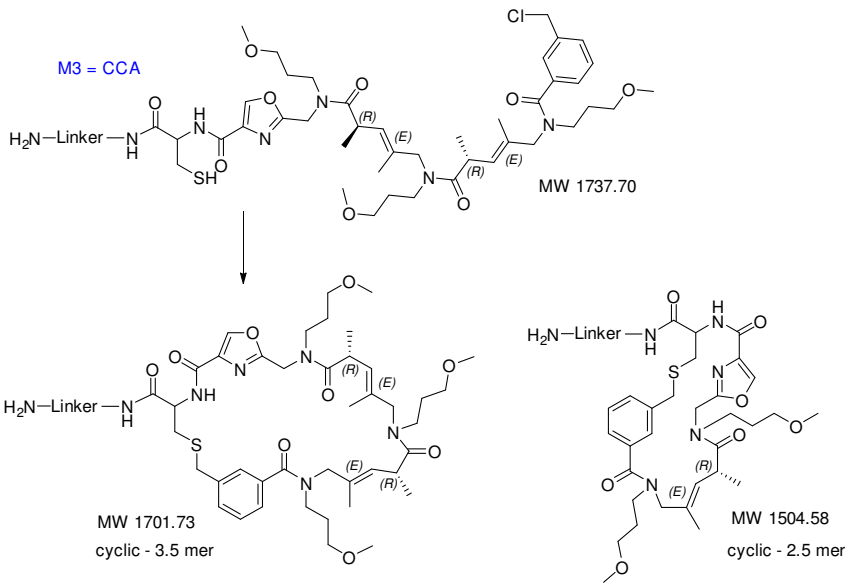
M2 - [CBA]

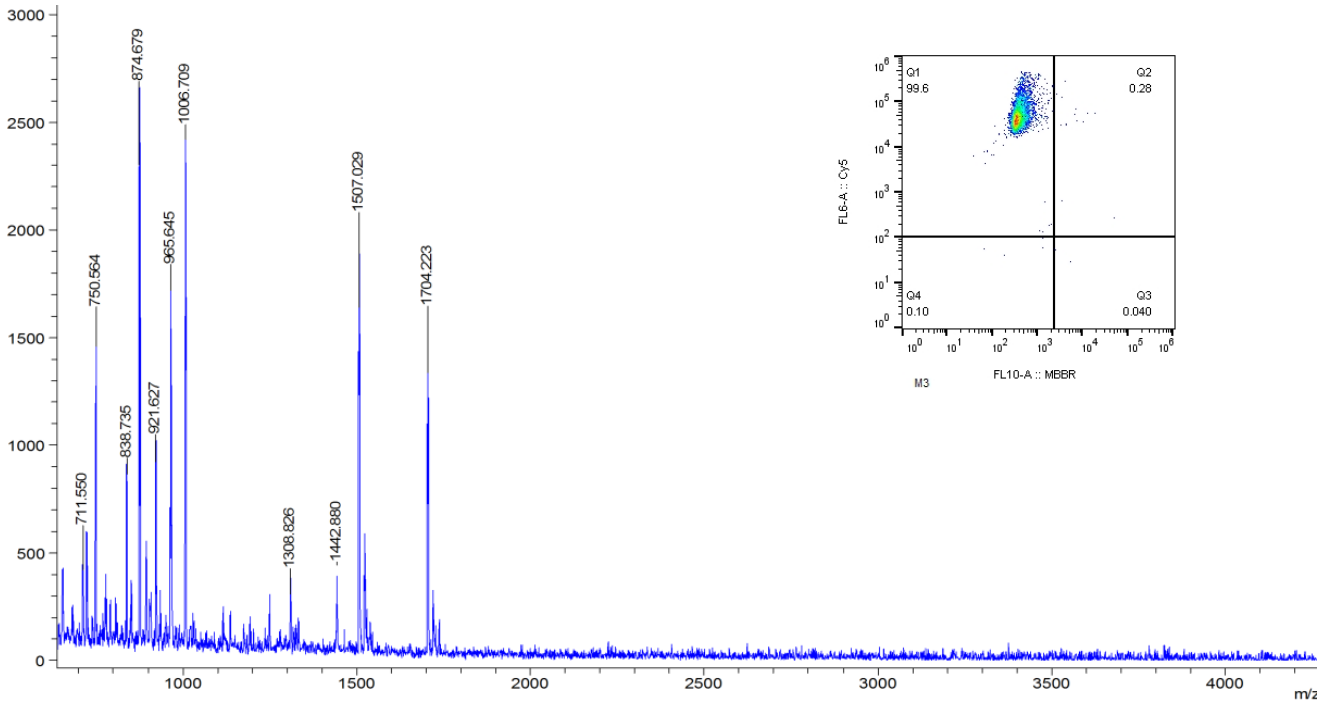
ions	size	MW	RT
cyclic	2.5	1504	7.985
cyclic	3.5	1658	6.992
linear	3.5	1694	-

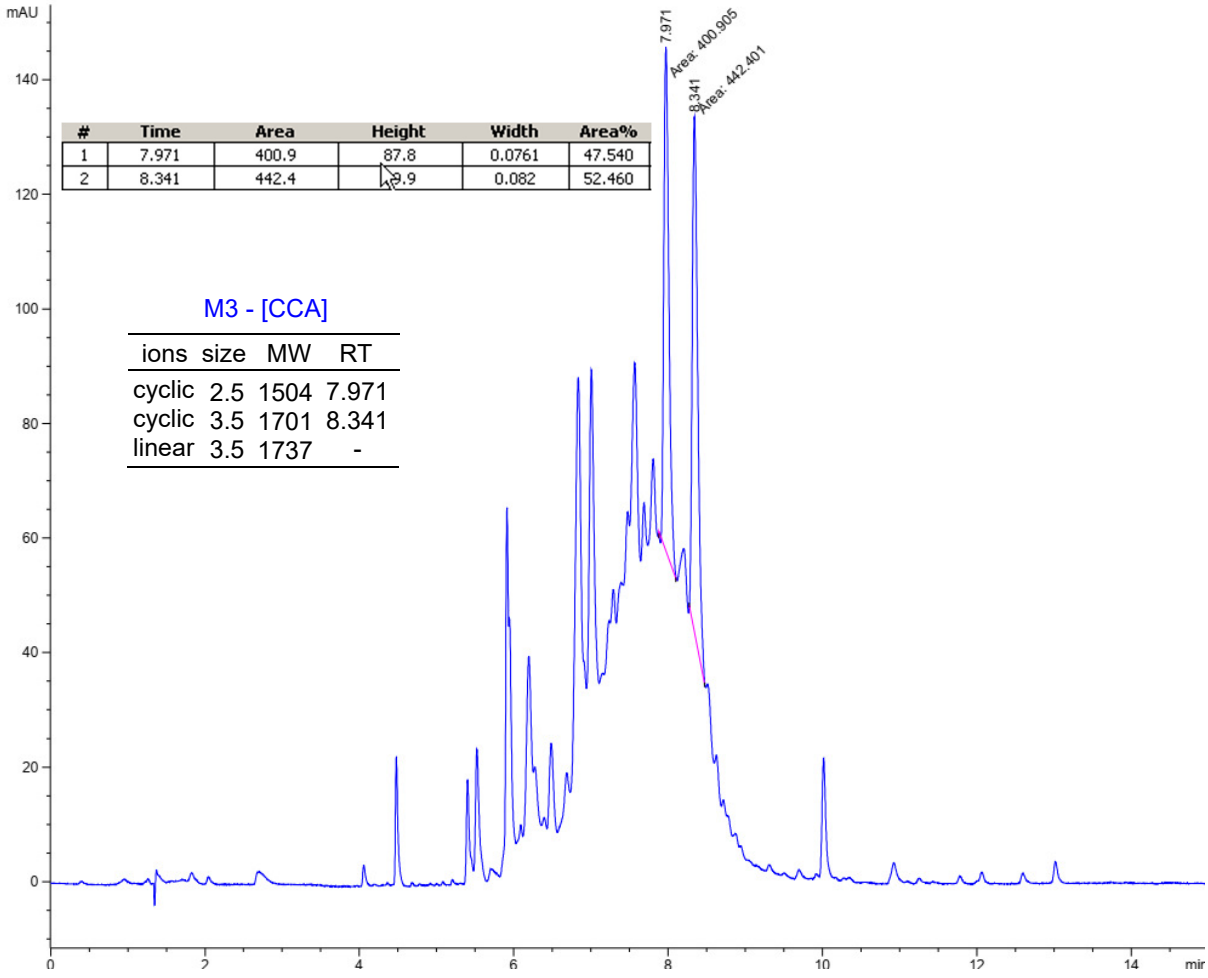




M3-[CCA]: Complete cyclization was observed on 10 µm & 160 µm beads.



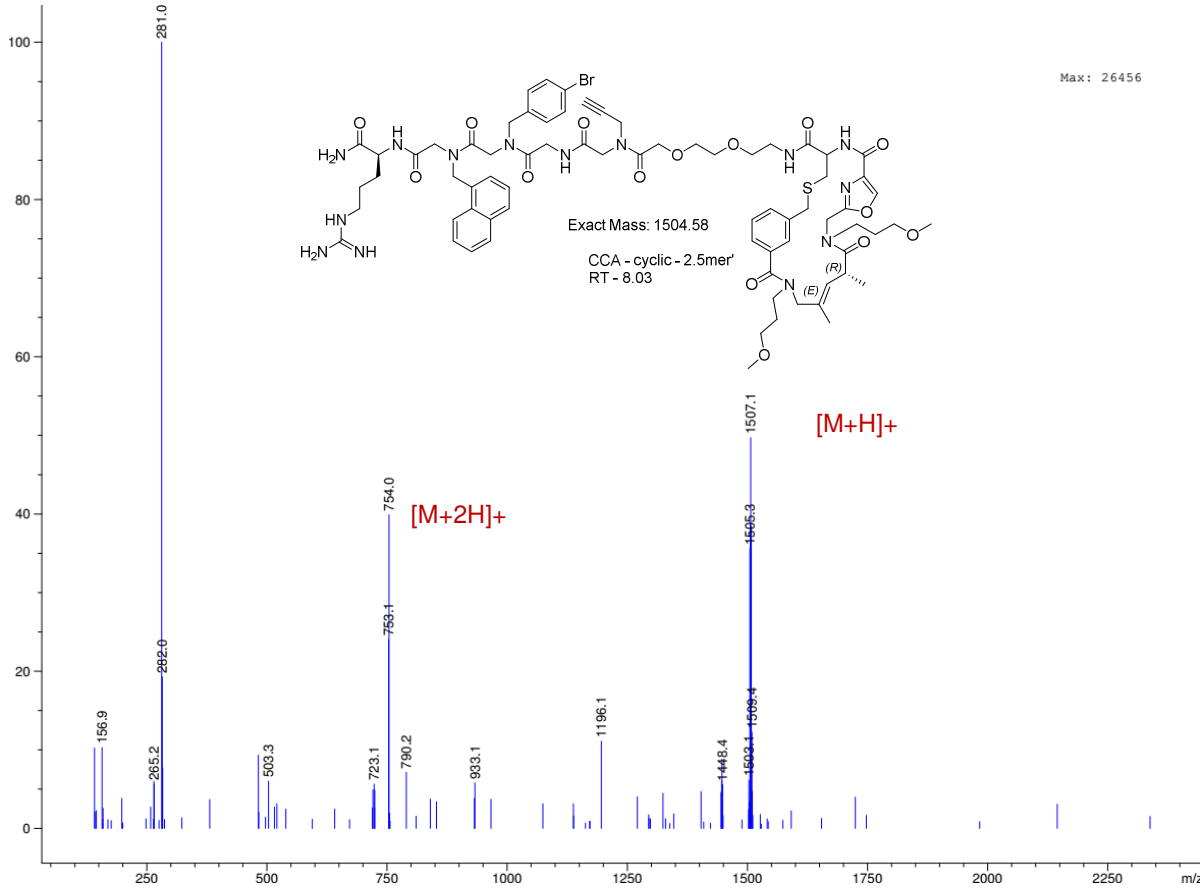


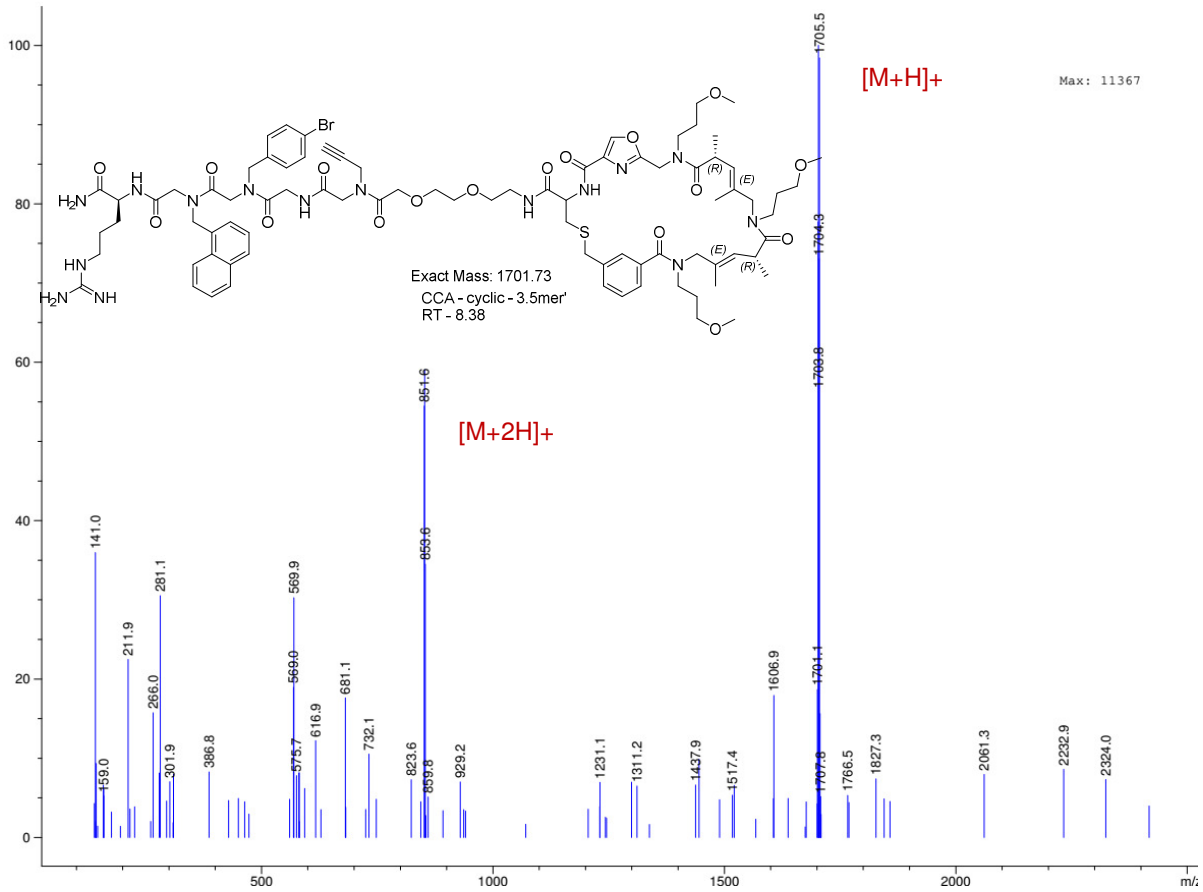


#	Time	Area	Height	Width	Area%
1	7.971	400.9	87.8	0.0761	47.540
2	8.341	442.4	89.9	0.082	52.460

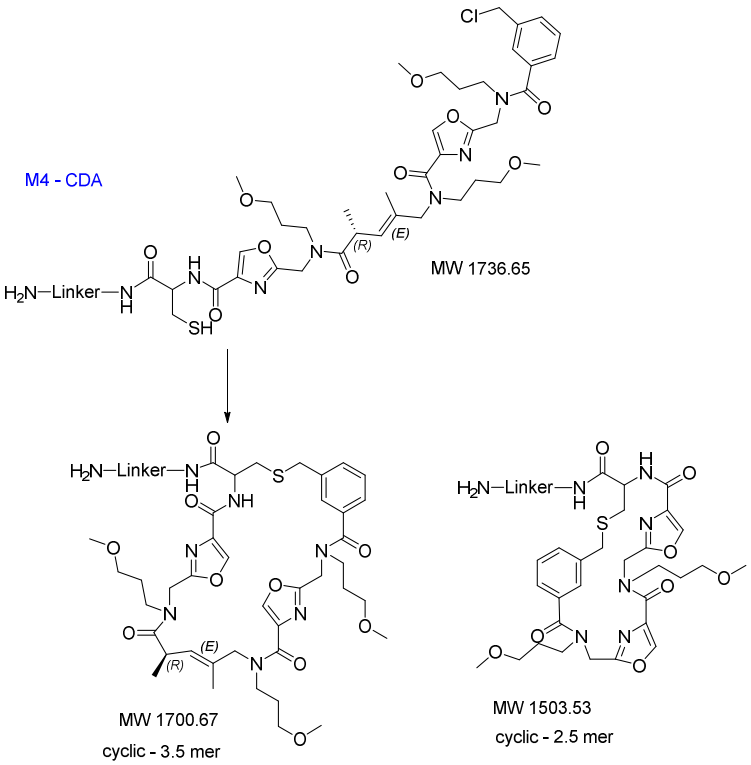
M3 - [CCA]

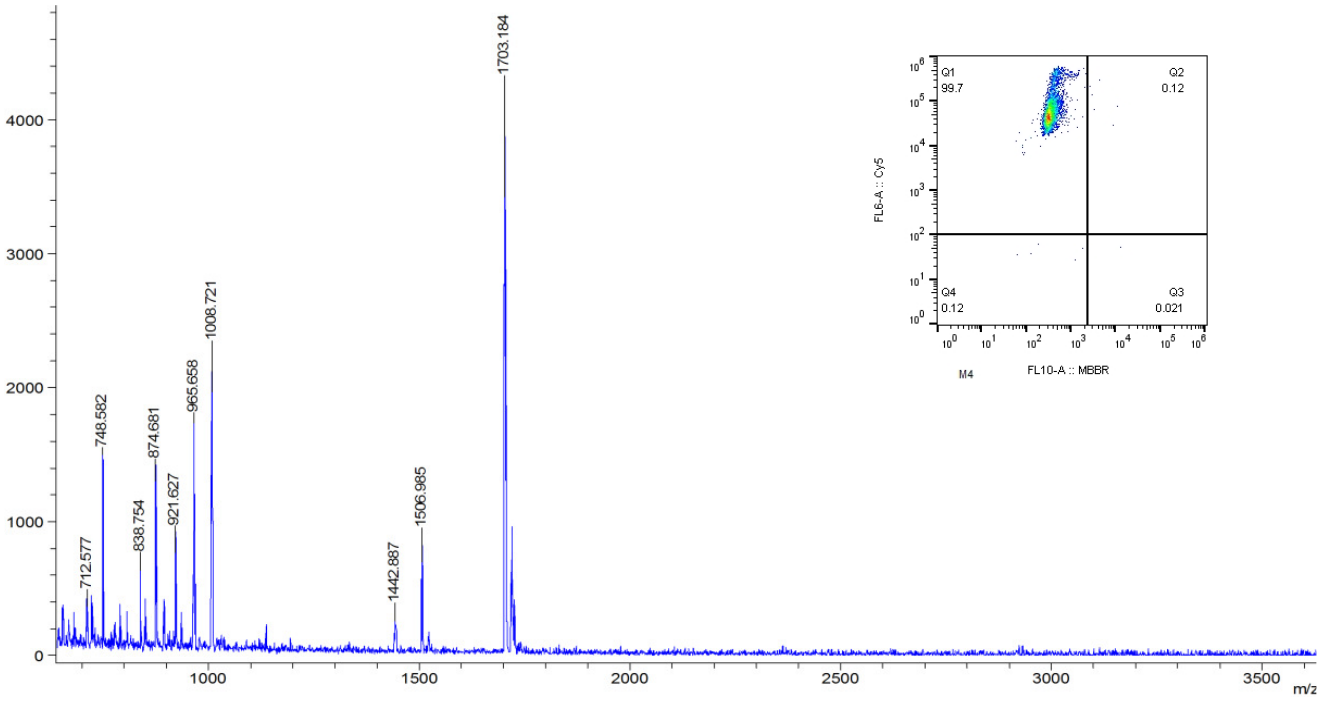
ions	size	MW	RT
cyclic	2.5	1504	7.971
cyclic	3.5	1701	8.341
linear	3.5	1737	-

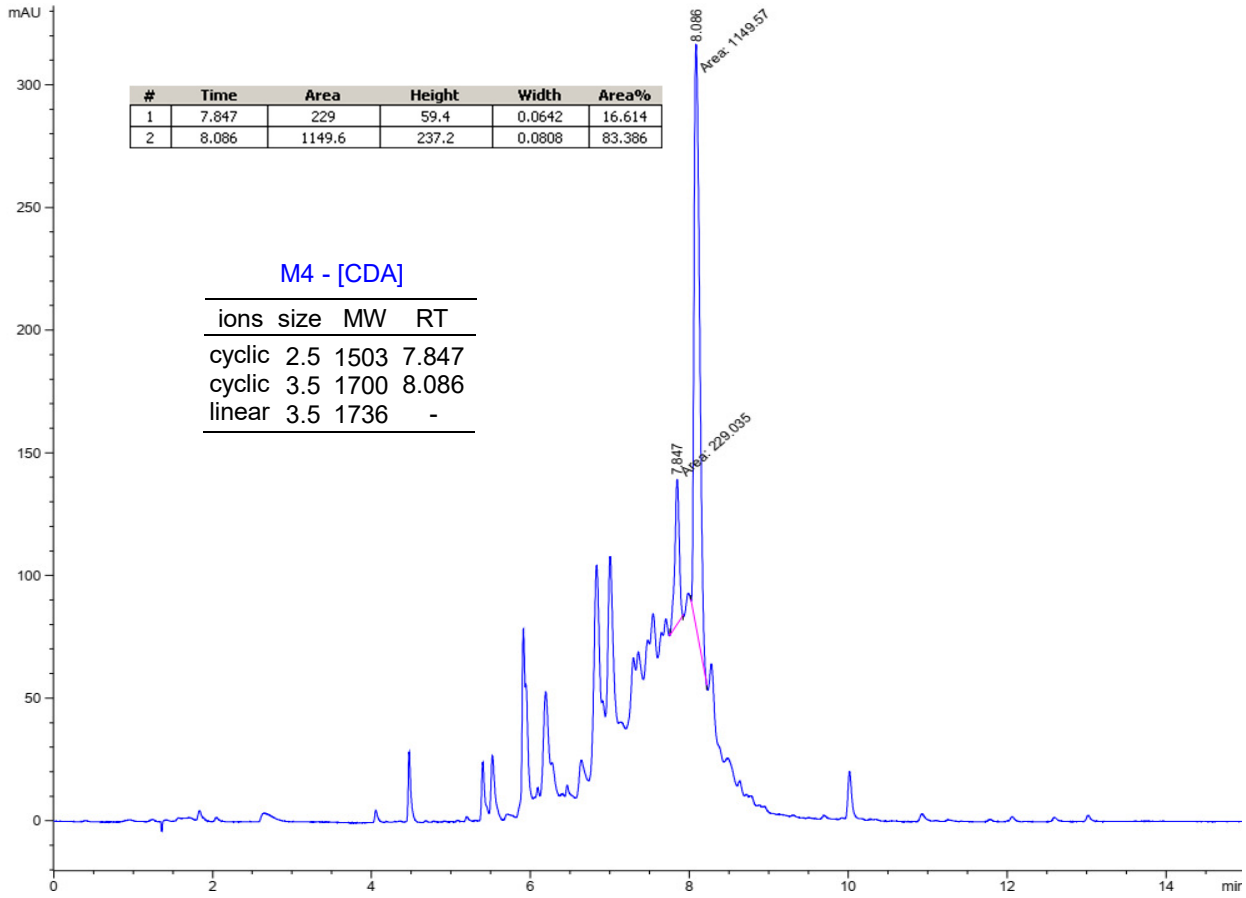

Max: 26456
Exact Mass: 1504.58
CCA - cyclic - 2.5mer'
RT - 8.03
[M+H]+
[M+2H]+
281.0
754.0
1507.1
282.0
753.1
1595.3
156.9
265.2
503.3
723.1
790.2
933.1
1196.1
1448.4
1603.1
1509.4


Max: 11367
Exact Mass: 1701.73
CCA - cyclic - 3.5mer'
RT - 8.38
[M+H]+
[M+2H]+
1705.5
851.6
853.6
141.0
281.1
211.9
569.9
266.0
569.0
681.1
616.9
732.1
386.8
301.9
575.7
823.6
859.8
929.2
1231.1
1311.2
1437.9
1517.4
1606.9
1701.1
1766.5
1827.3
2061.3
2232.9
2324.0
159.0

M4-[CDA]: Complete cyclization was observed on both 10 µm & 160 µm beads.



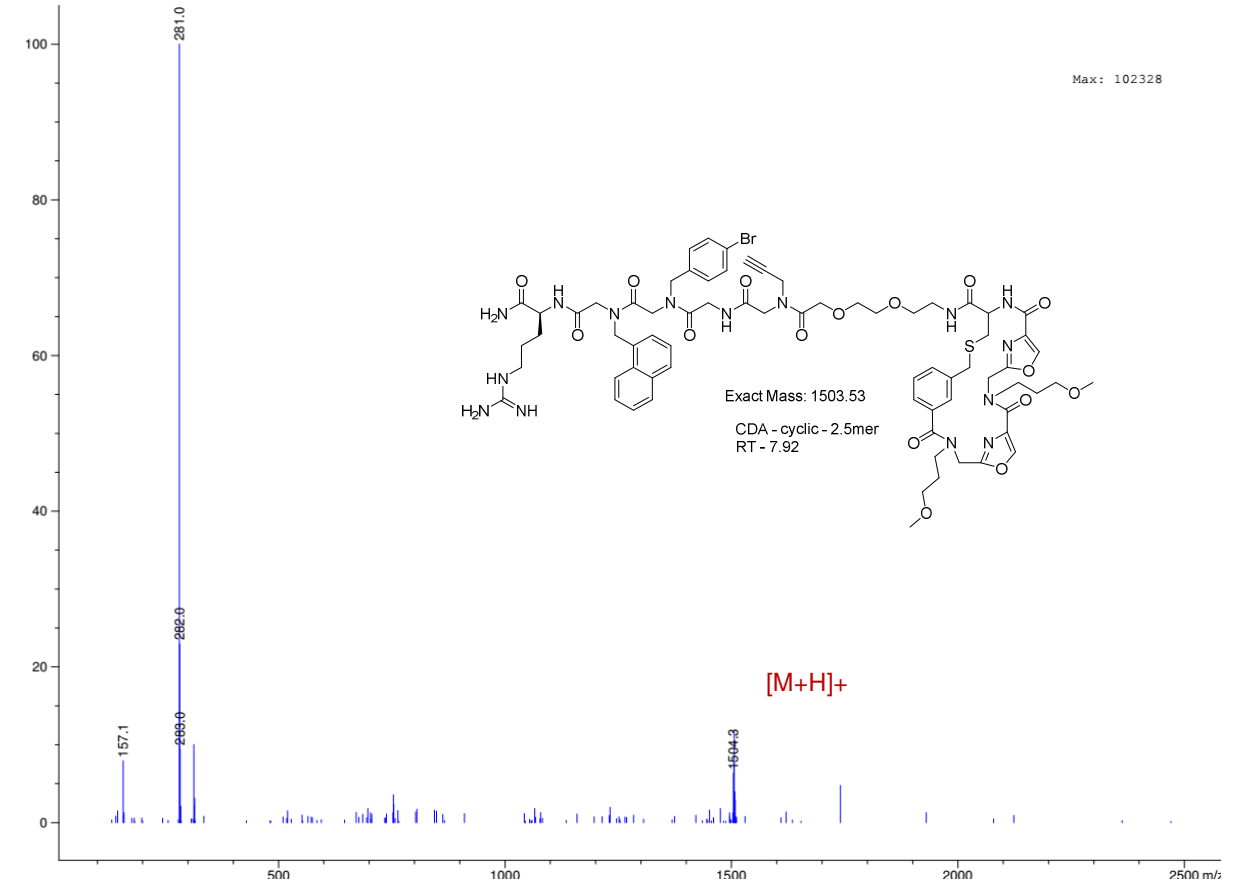


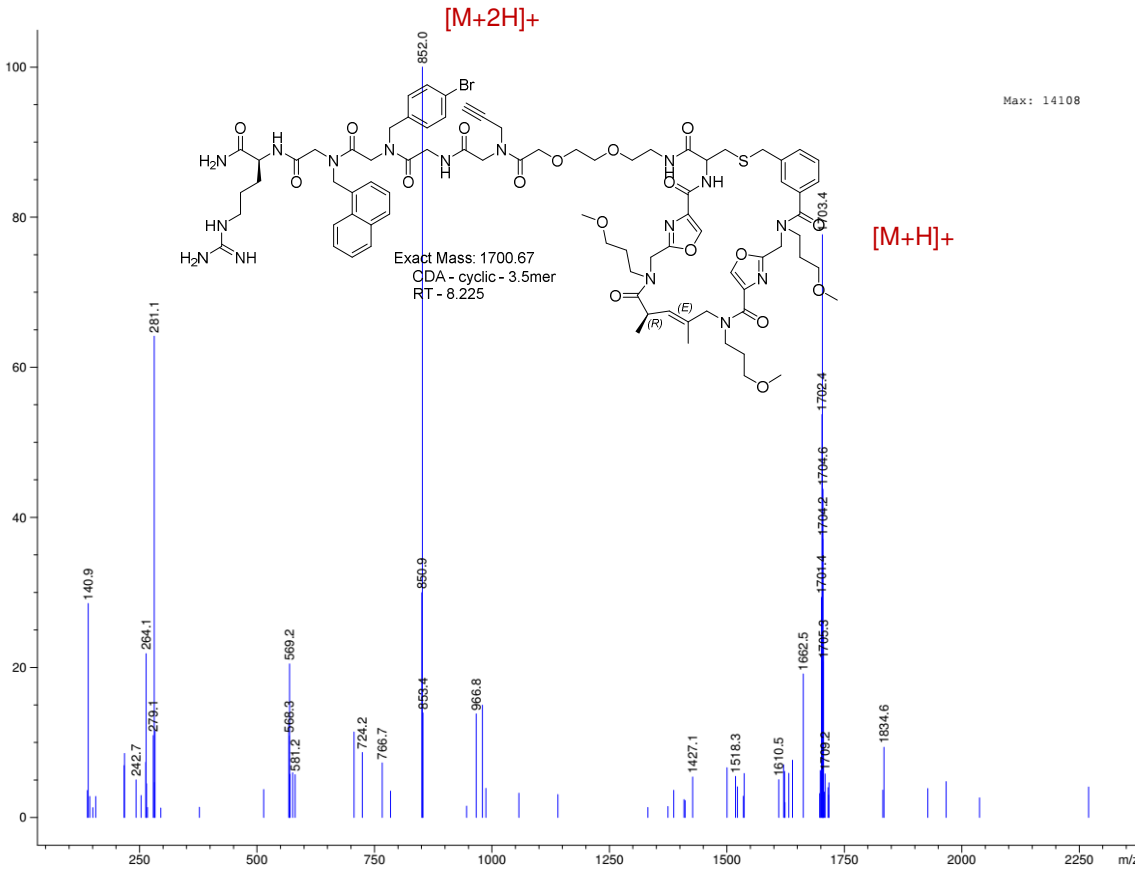


#	Time	Area	Height	Width	Area%
1	7.847	229	59.4	0.0642	16.614
2	8.086	1149.6	237.2	0.0808	83.386

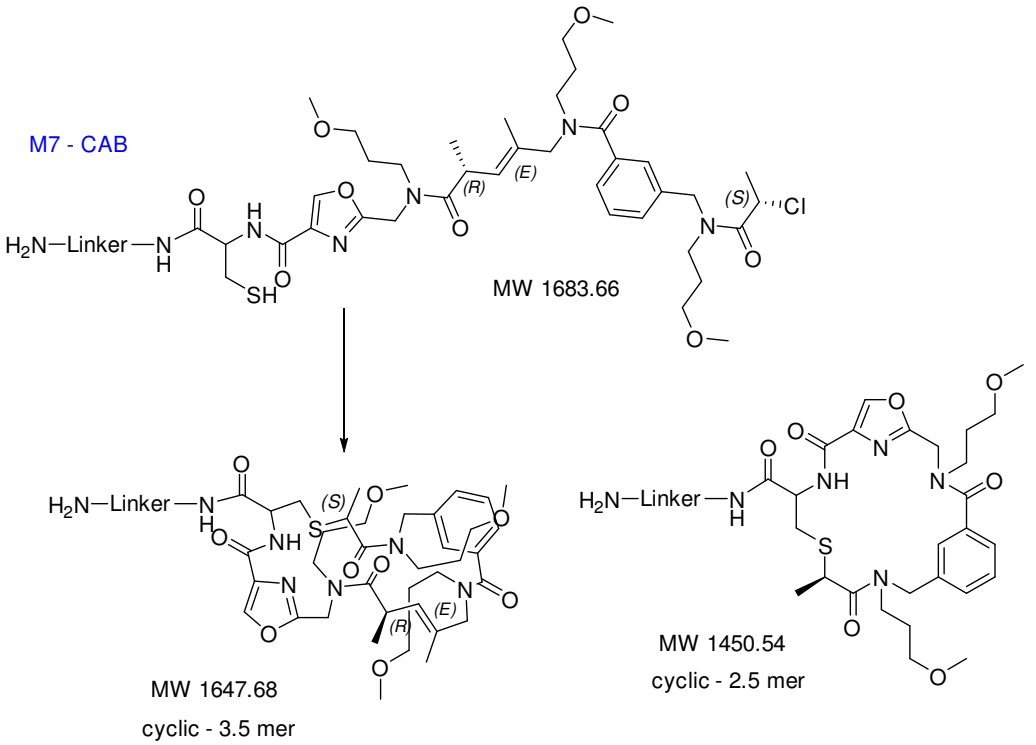
M4 - [CDA]

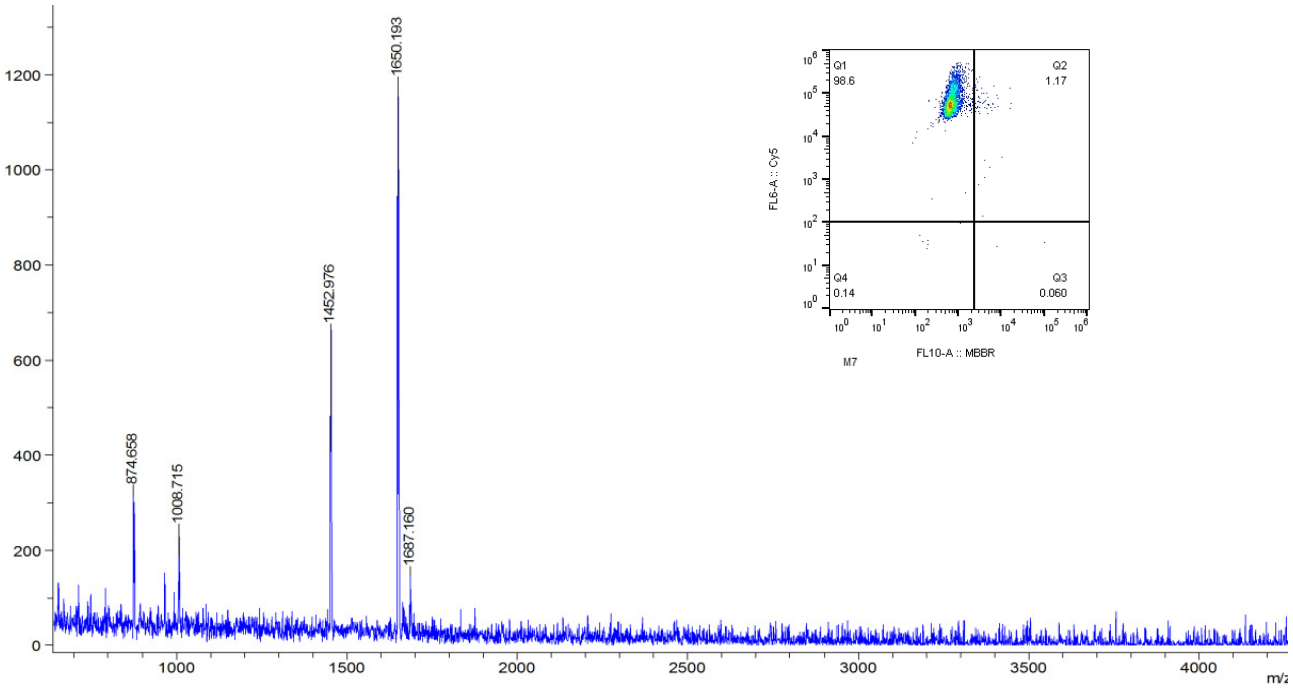
ions	size	MW	RT
cyclic	2.5	1503	7.847
cyclic	3.5	1700	8.086
linear	3.5	1736	-

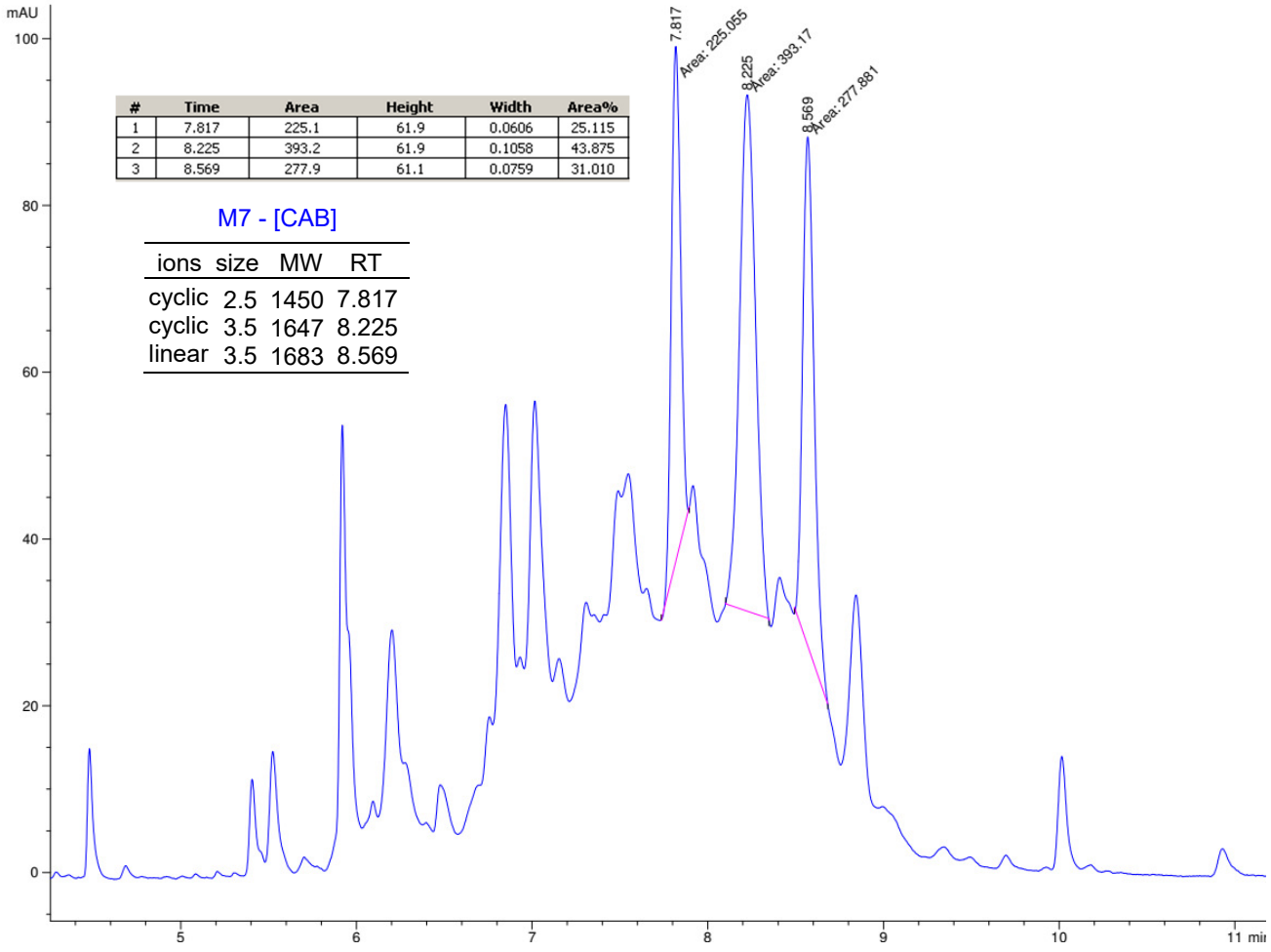




M7-[CAB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm beads.



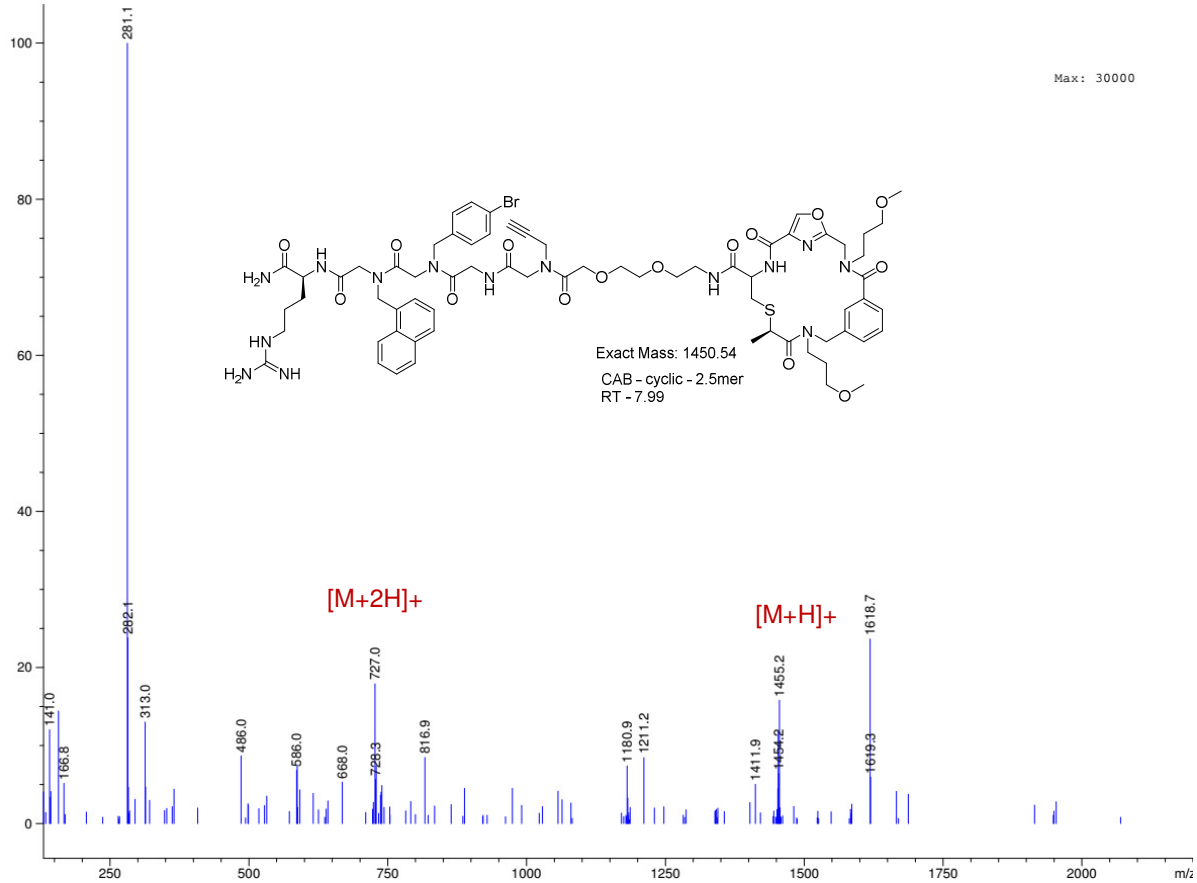


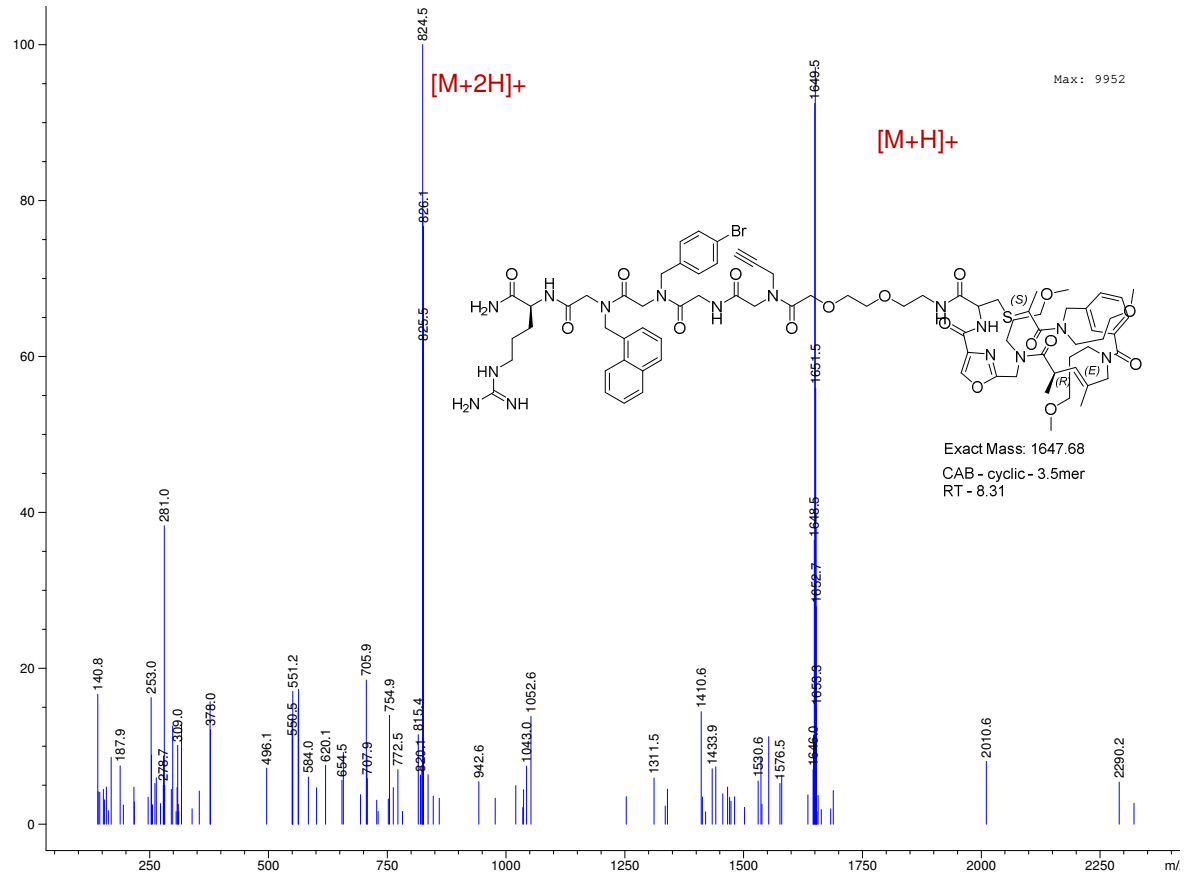


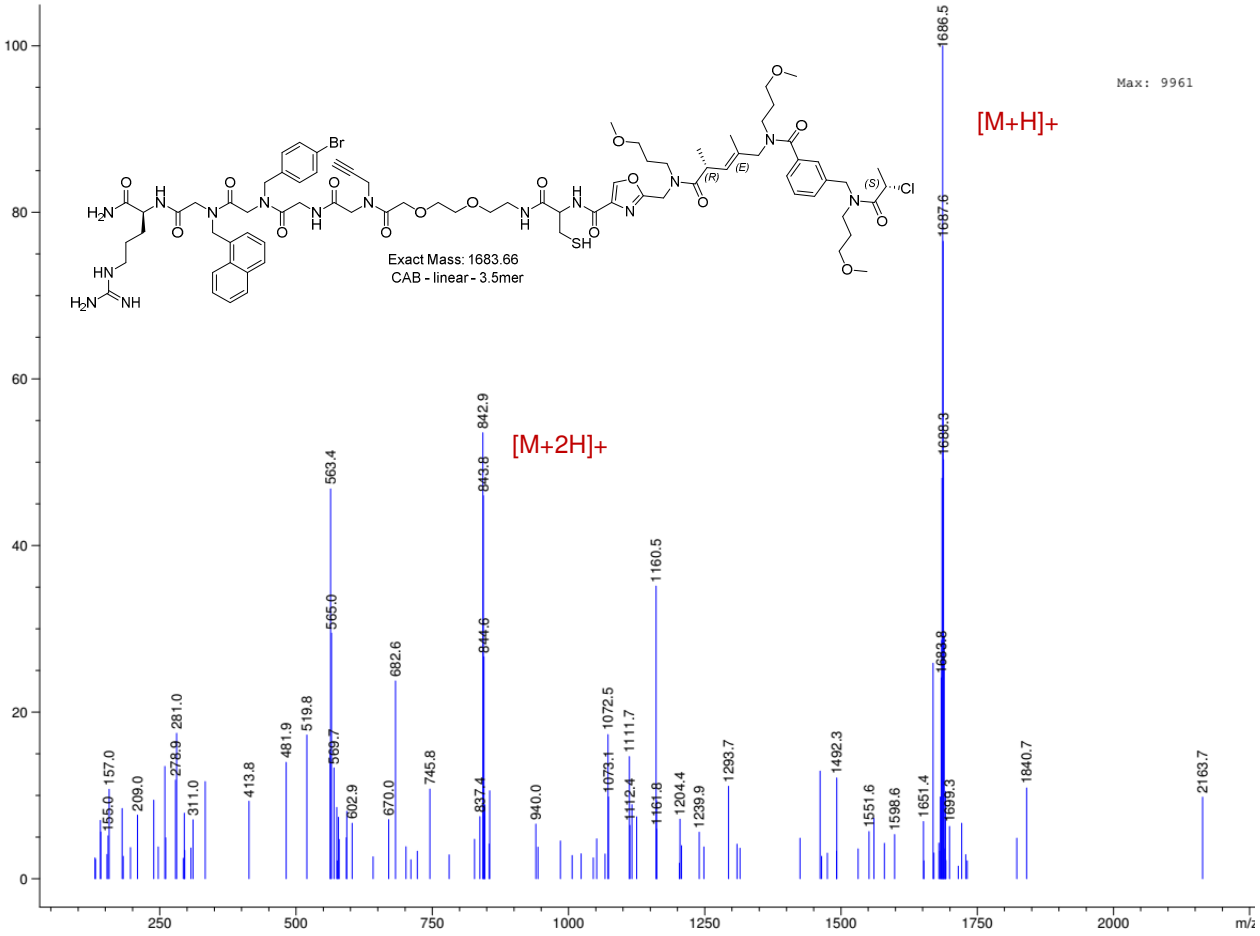
#	Time	Area	Height	Width	Area%
1	7.817	225.1	61.9	0.0606	25.115
2	8.225	393.2	61.9	0.1058	43.875
3	8.569	277.9	61.1	0.0759	31.010

M7 - [CAB]

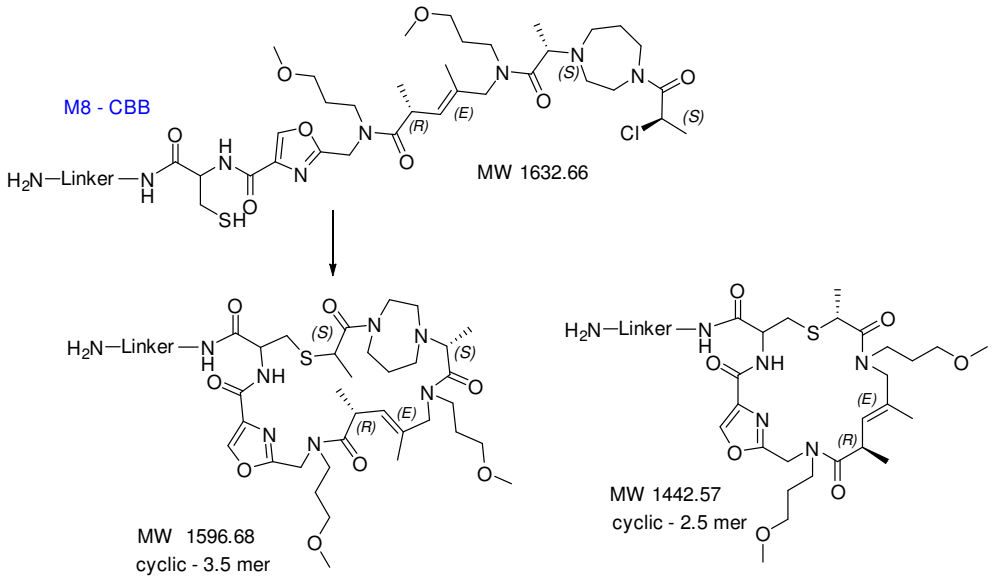
ions	size	MW	RT
cyclic	2.5	1450	7.817
cyclic	3.5	1647	8.225
linear	3.5	1683	8.569

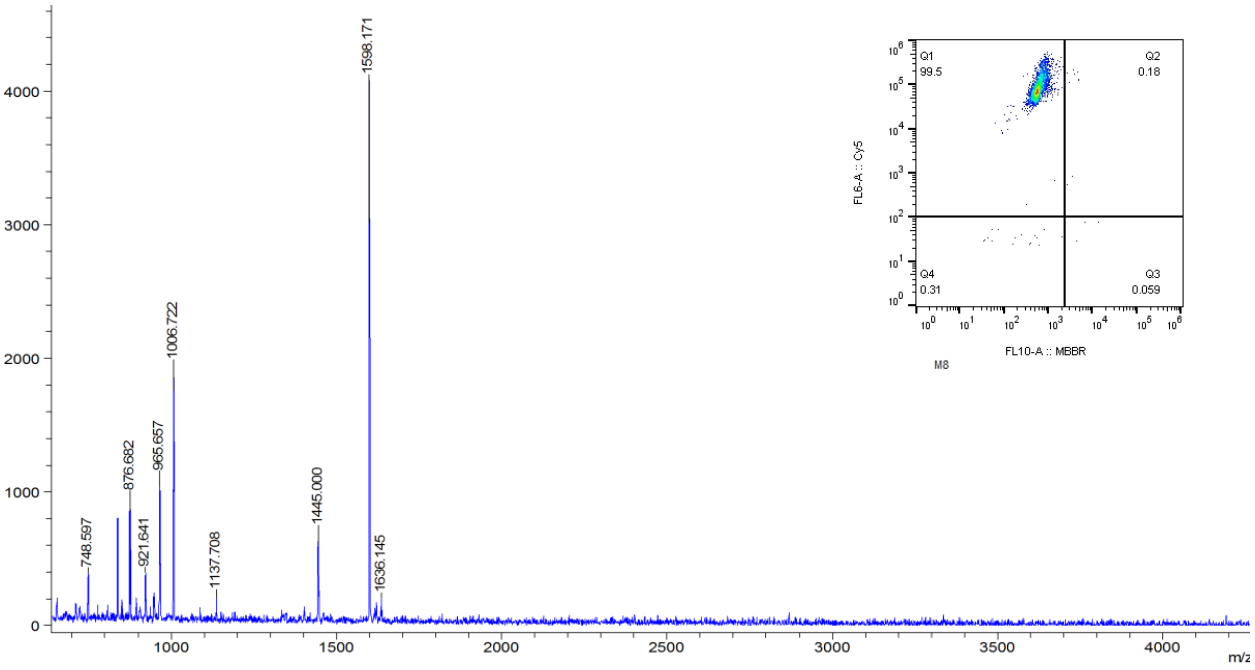

Max: 30000
[M+2H]+
[M+H]+
Exact Mass: 1450.54
CAB - cyclic - 2.5mer
RT - 7.99
281.1
282.1
313.0
141.0
166.8
486.0
586.0
668.0
727.0
728.3
816.9
1180.9
1211.2
1411.9
1454.2
1455.2
1618.7
1619.3
m/z

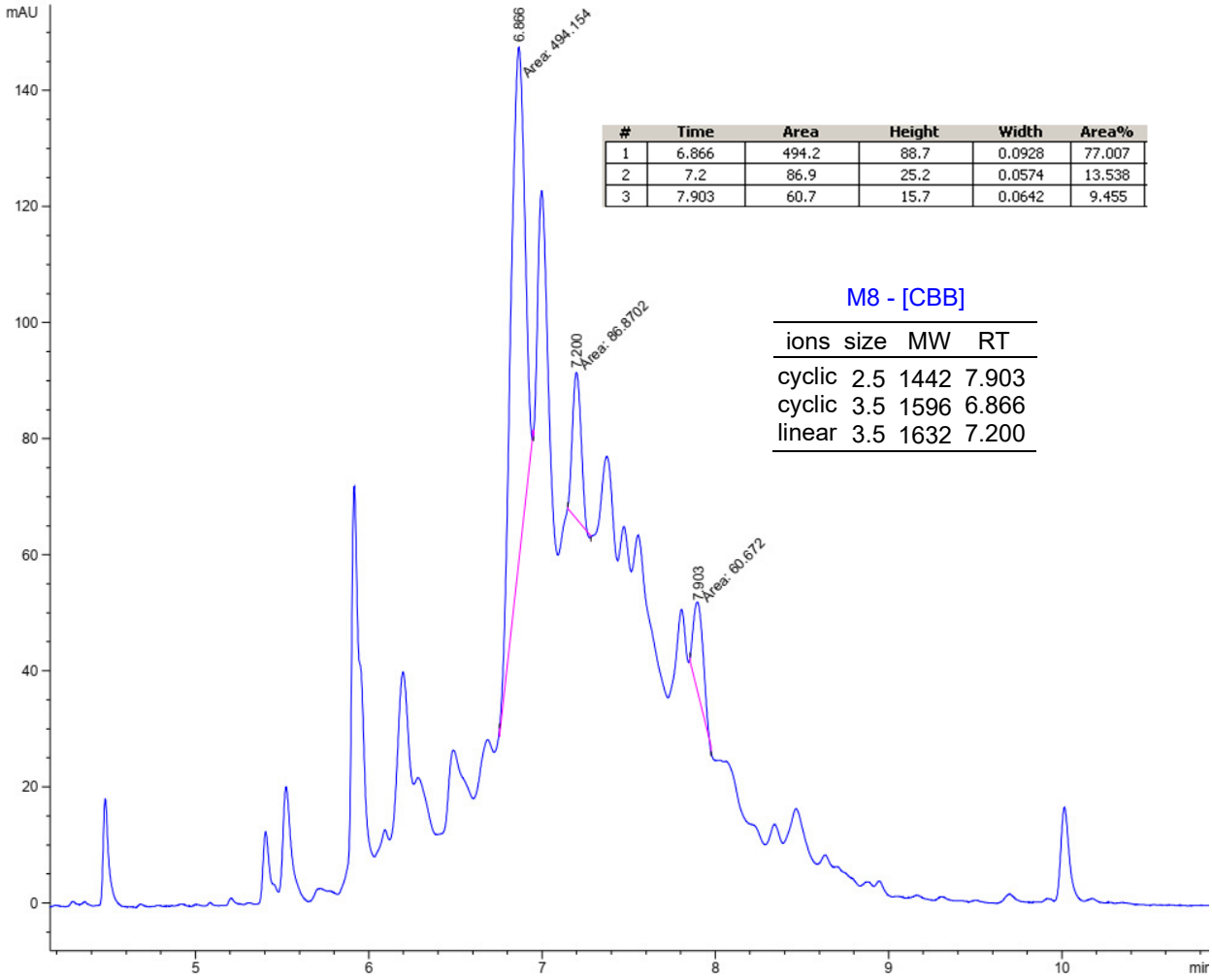

Max: 9952
[M+2H]+
[M+H]+
Exact Mass: 1647.68
CAB - cyclic - 3.5mer
RT - 8.31
824.5
826.1
825.5
1649.5
1651.5
281.0
140.8
187.9
253.0
278.7
309.0
378.0
496.1
550.5
551.2
584.0
620.1
654.5
705.9
707.9
754.9
772.5
815.4
820.1
942.6
1043.0
1052.6
1311.5
1410.6
1433.9
1530.6
1576.5
2010.6
2290.2
m/z



M8-[CBB]: Complete cyclization was observed on 10 µm but 160 µm had incomplete cyclization.



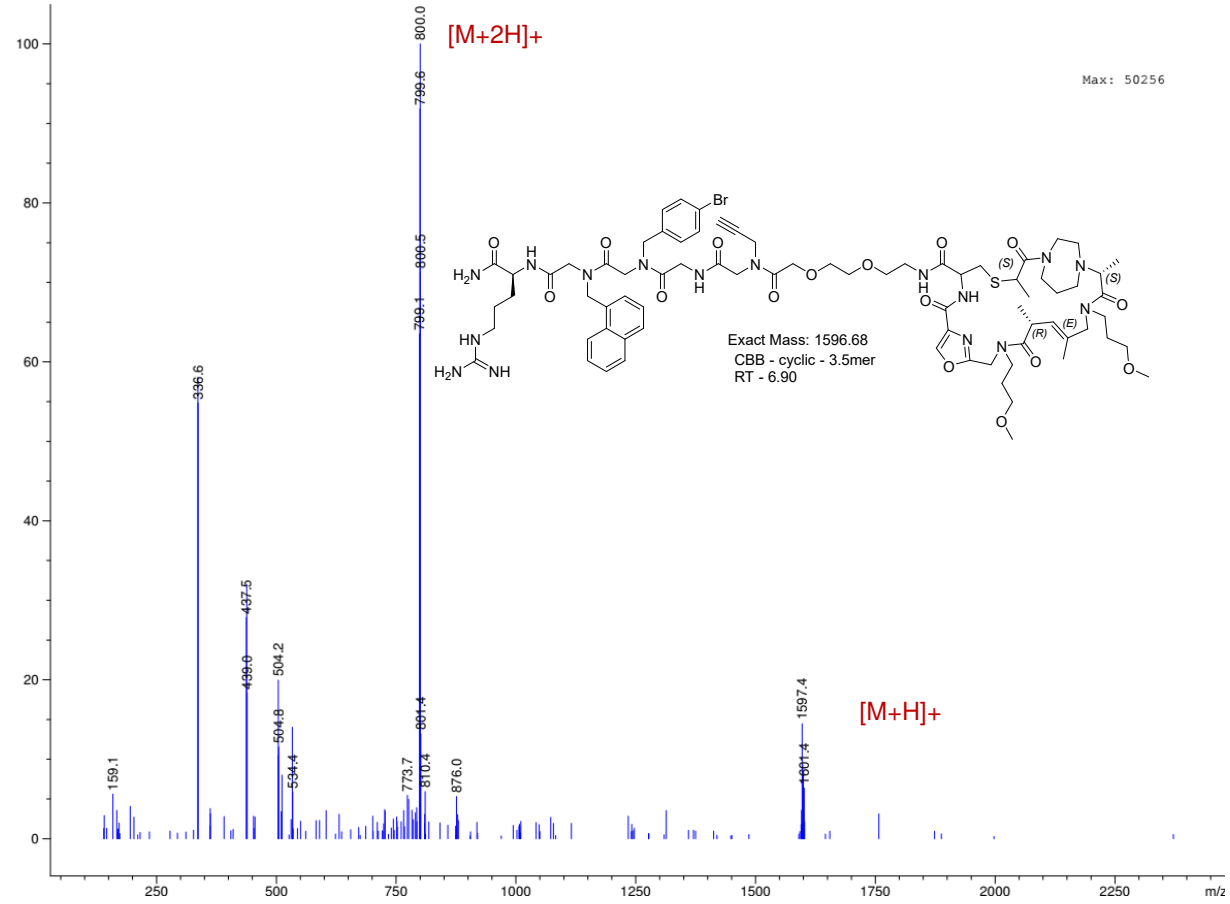


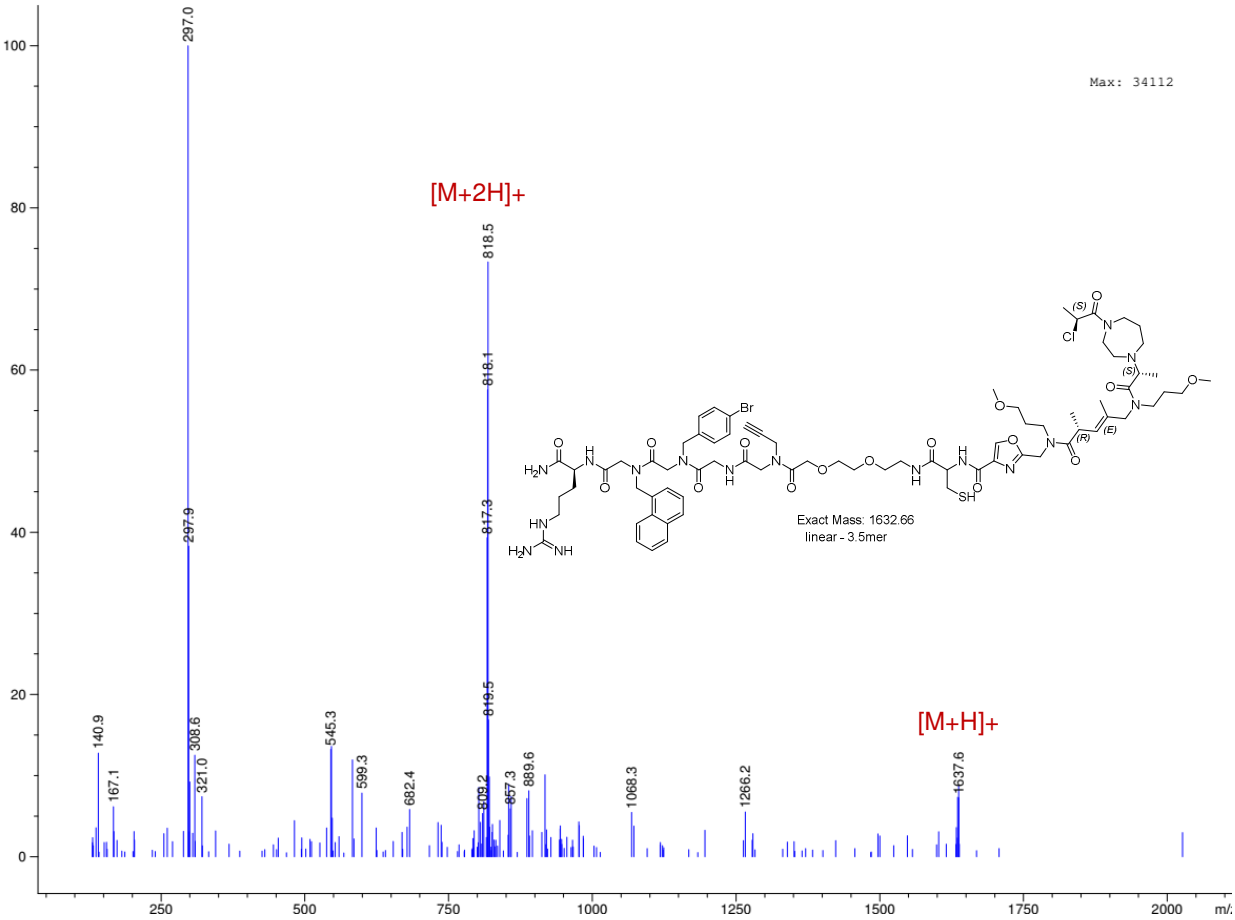


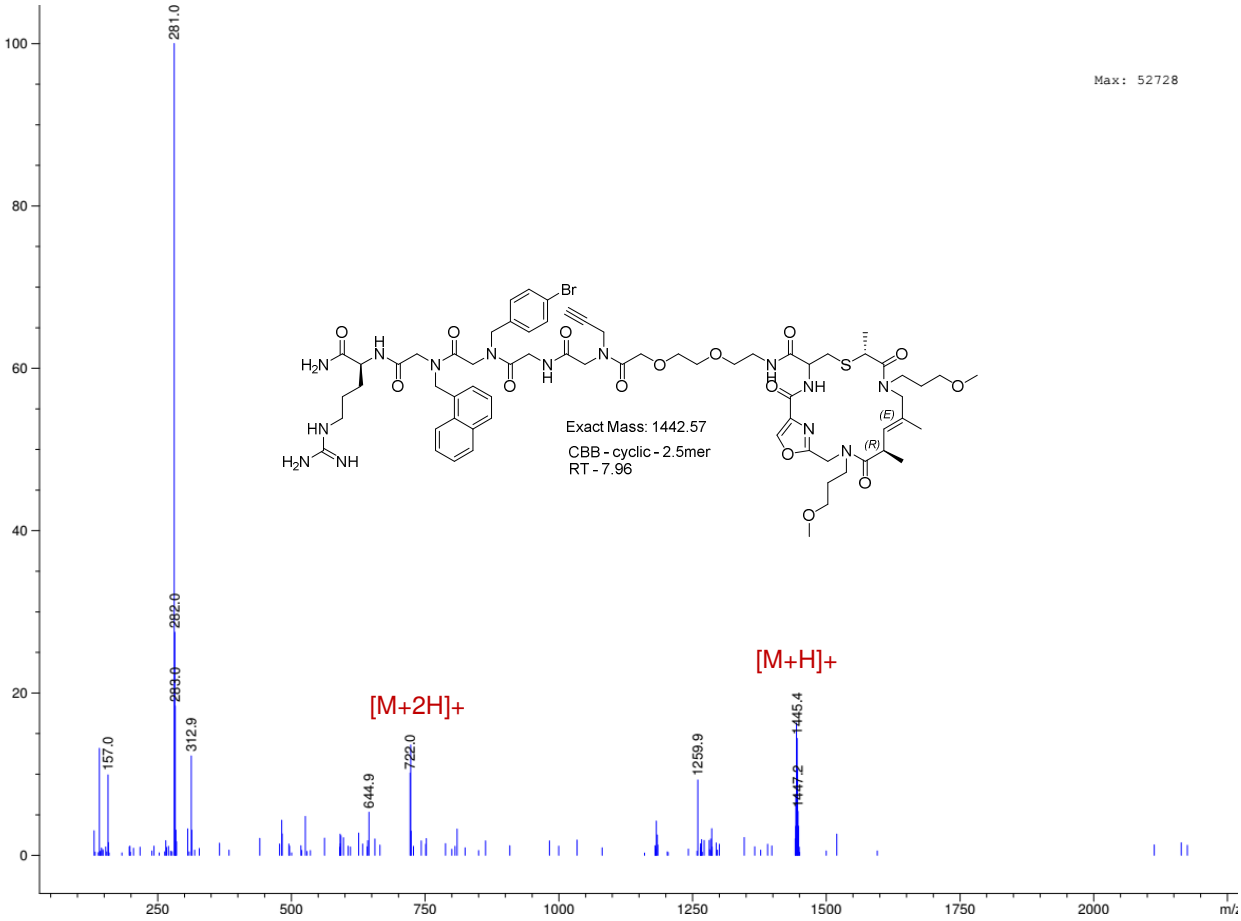
#	Time	Area	Height	Width	Area%
1	6.866	494.2	88.7	0.0928	77.007
2	7.2	86.9	25.2	0.0574	13.538
3	7.903	60.7	15.7	0.0642	9.455

M8 - [CBB]

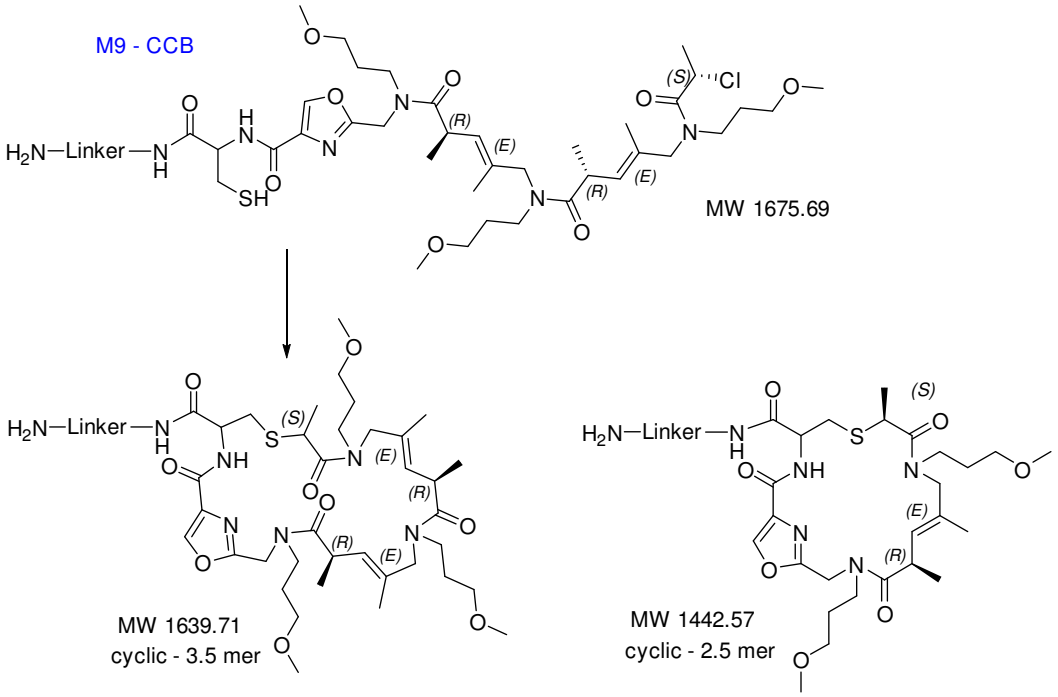
ions	size	MW	RT
cyclic	2.5	1442	7.903
cyclic	3.5	1596	6.866
linear	3.5	1632	7.200

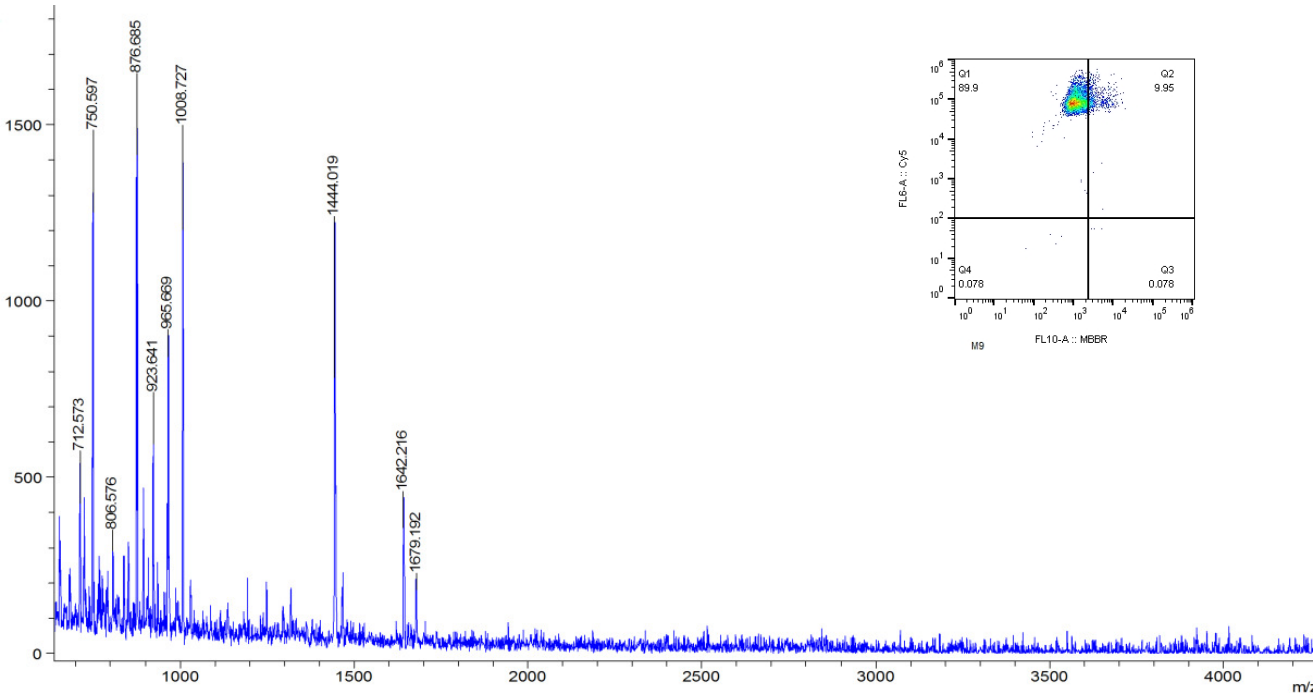

[M+2H]+
Max: 50256
800.0
799.6
800.5
799.1
396.6
437.5
439.0
504.2
504.8
534.4
801.4
773.7
810.4
876.0
159.1
1597.4
1601.4
[M+H]+
Exact Mass: 1596.68
CBB - cyclic - 3.5mer
RT - 6.90
m/z

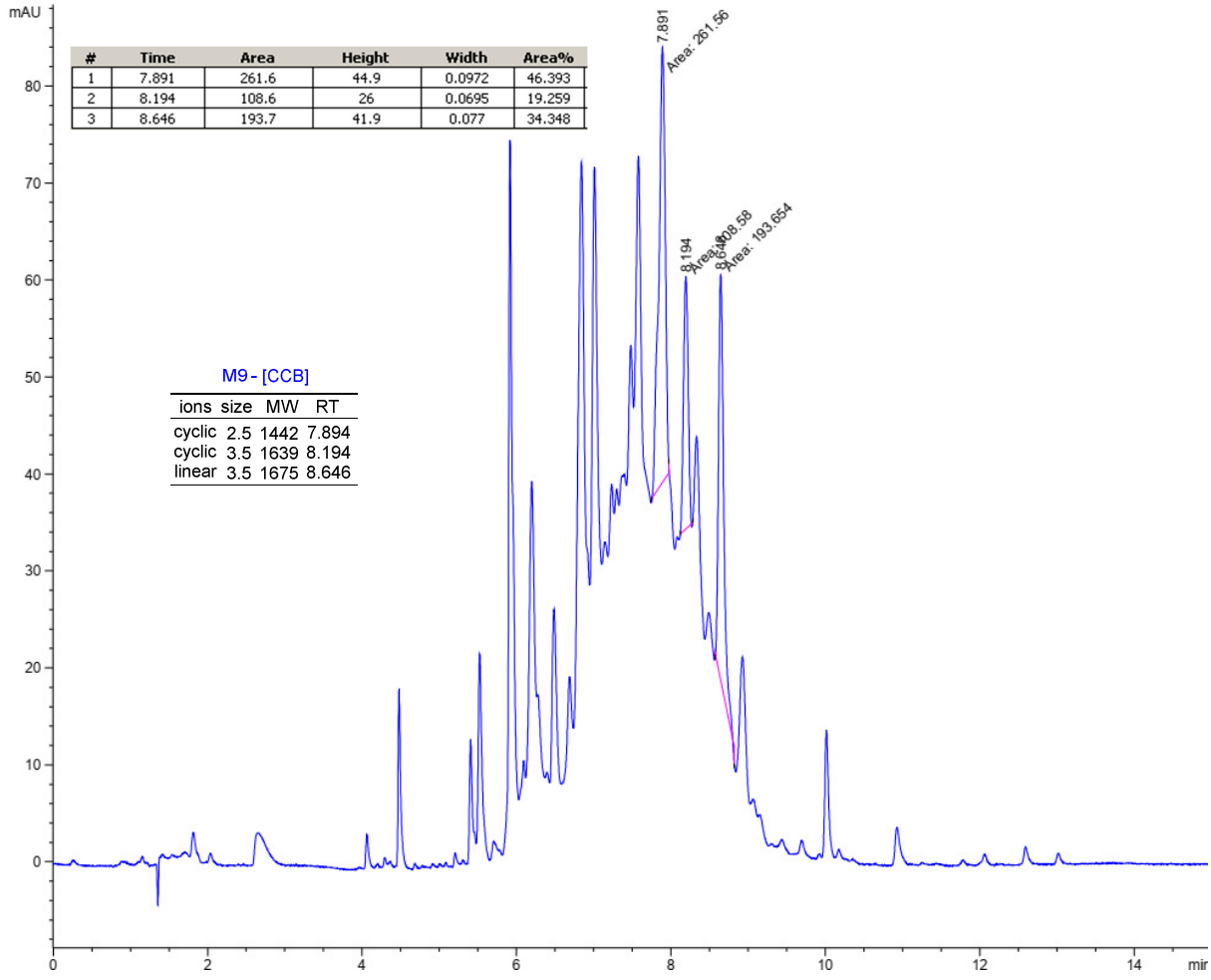

Max: 34112
297.0
[M+2H]+
818.5
818.1
817.3
297.9
819.5
140.9
308.6
321.0
167.1
545.3
599.3
682.4
809.2
857.3
889.6
1068.3
1266.2
1637.6
[M+H]+
Exact Mass: 1632.66
linear - 3.5mer
m/z



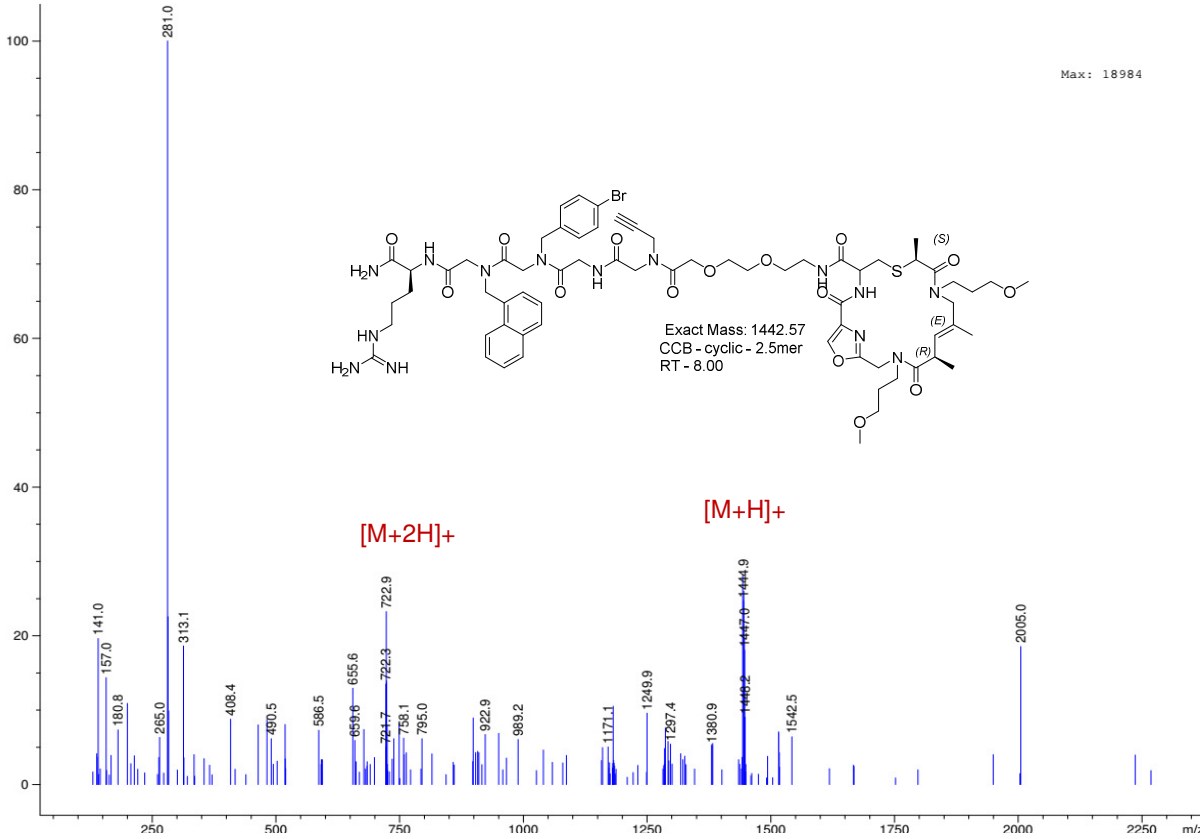
M9-[CCB]: Incomplete cyclization was observed on both 10 µm and 160 µm beads.

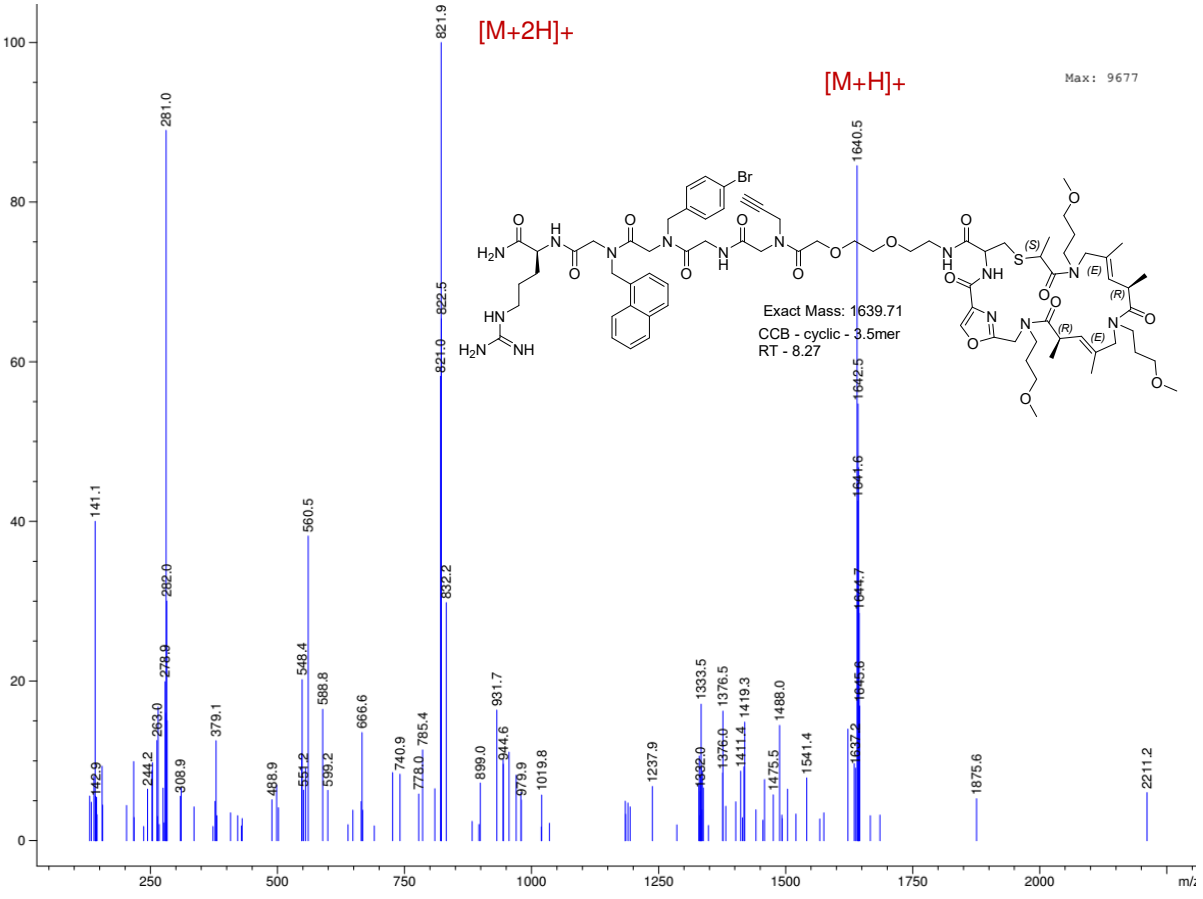


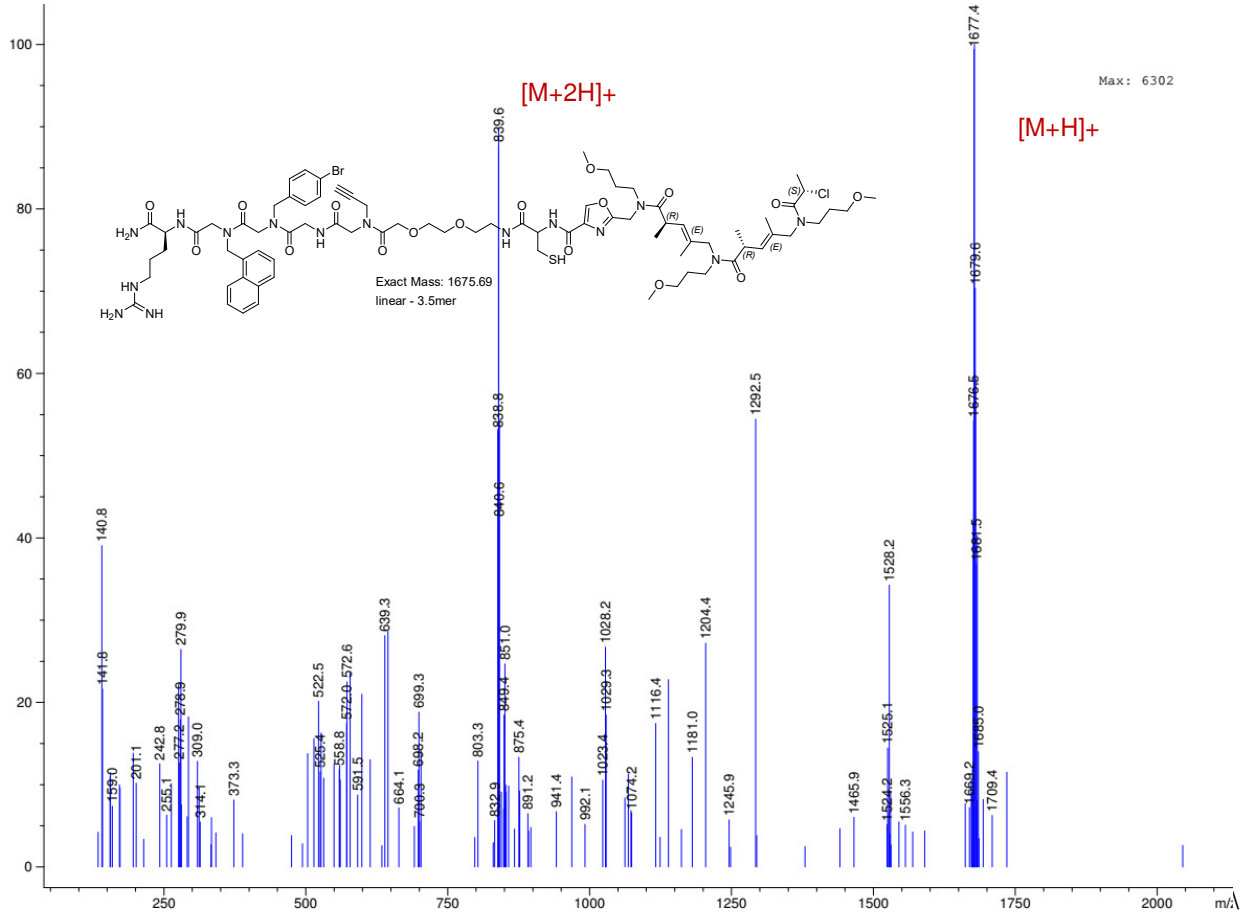




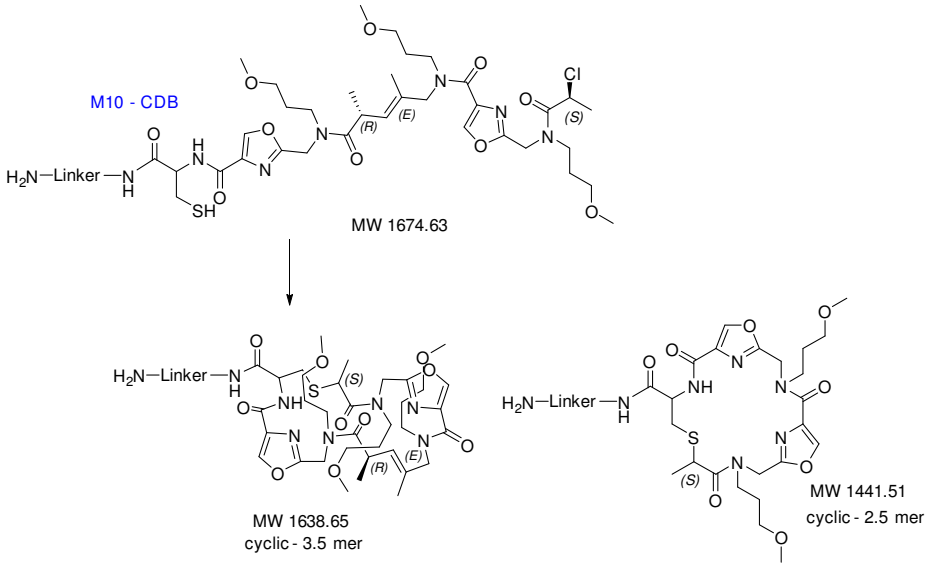
#	Time	Area	Height	Width	Area%
1	7.891	261.6	44.9	0.0972	46.393
2	8.194	108.6	26	0.0695	19.259
3	8.646	193.7	41.9	0.077	34.348

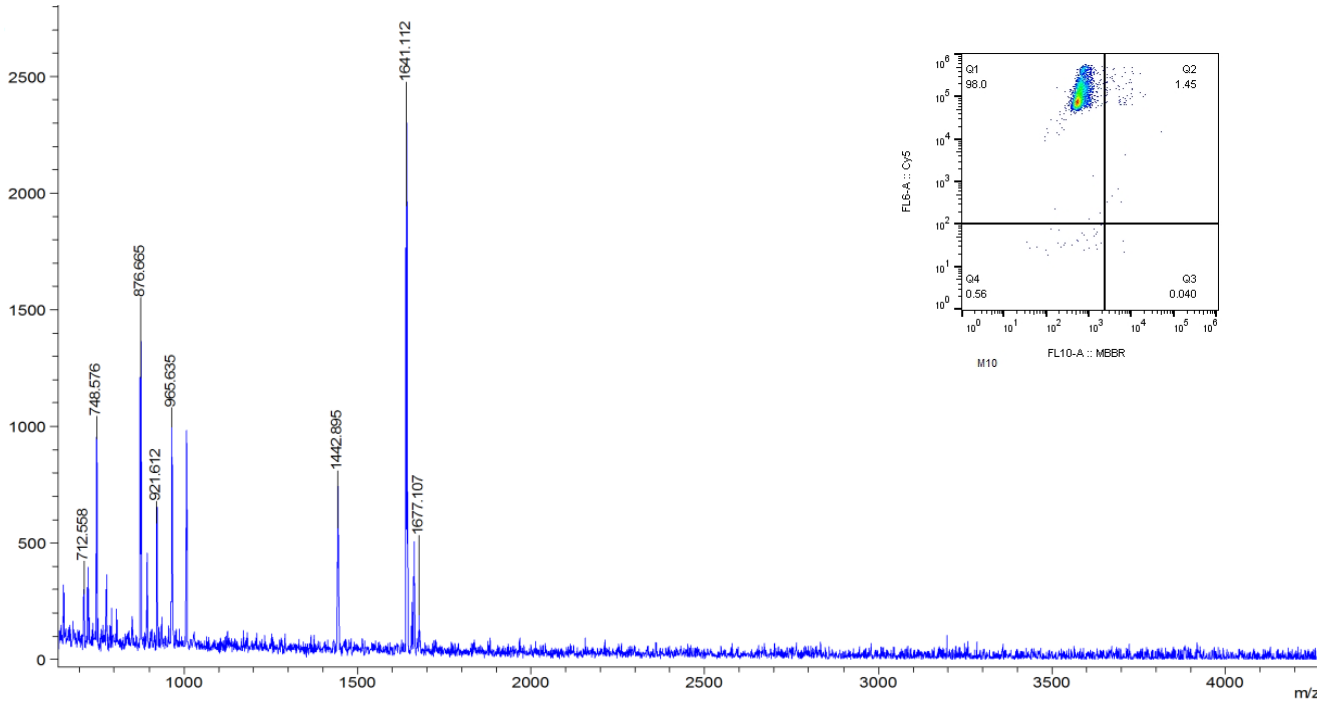

Max: 18984
Exact Mass: 1442.57
CCB - cyclic - 2.5mer
RT - 8.00
[M+2H]+
[M+H]+

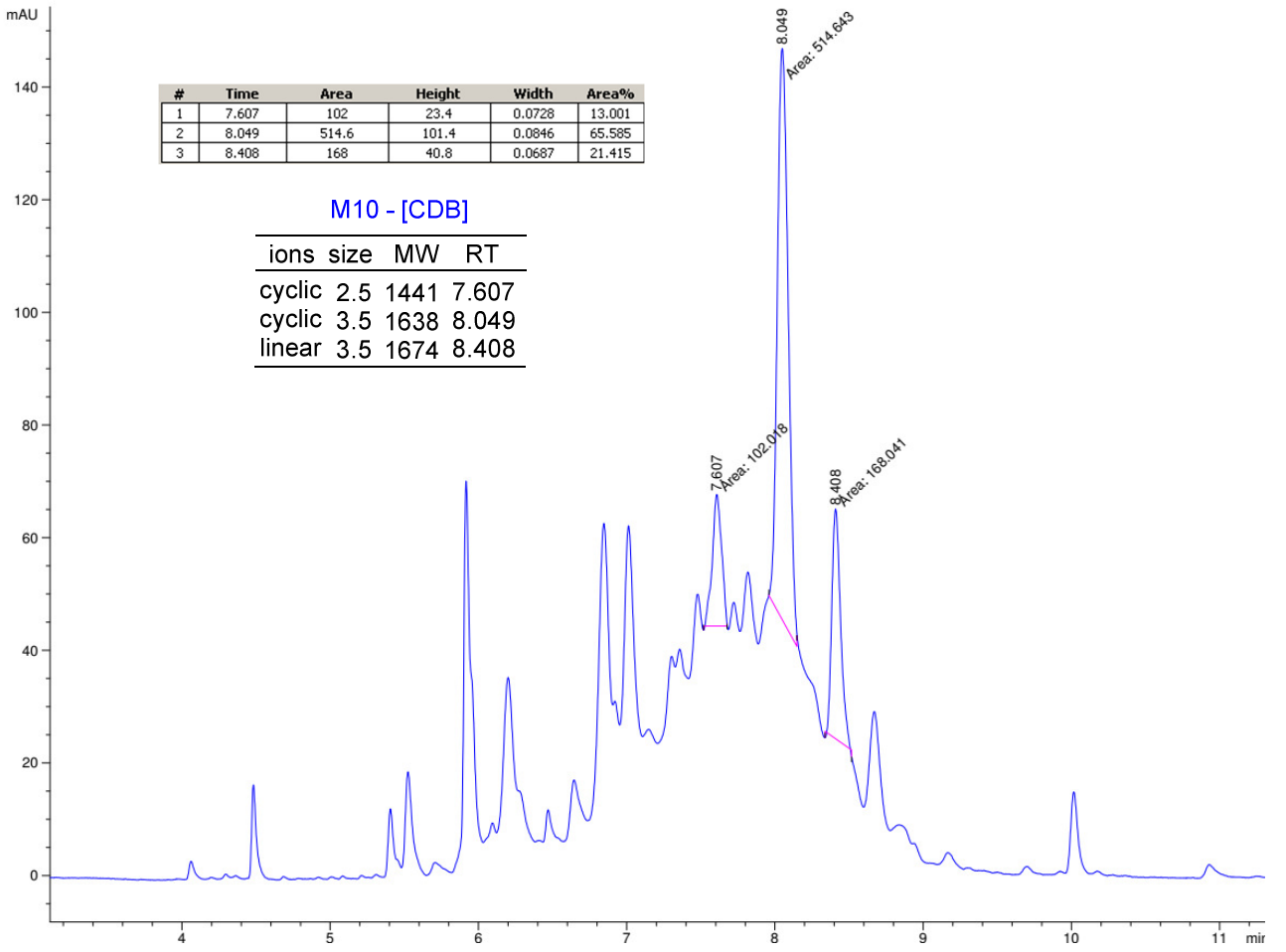

Max: 9677
Exact Mass: 1639.71
CCB - cyclic - 3.5mer
RT - 8.27
[M+2H]+
[M+H]+



M10-[CDB]: Complete cyclization was observed on 10 µm but 160 µm beads had incomplete cyclization. Linear precursor was detected (MW 1674, RT- 8.40).



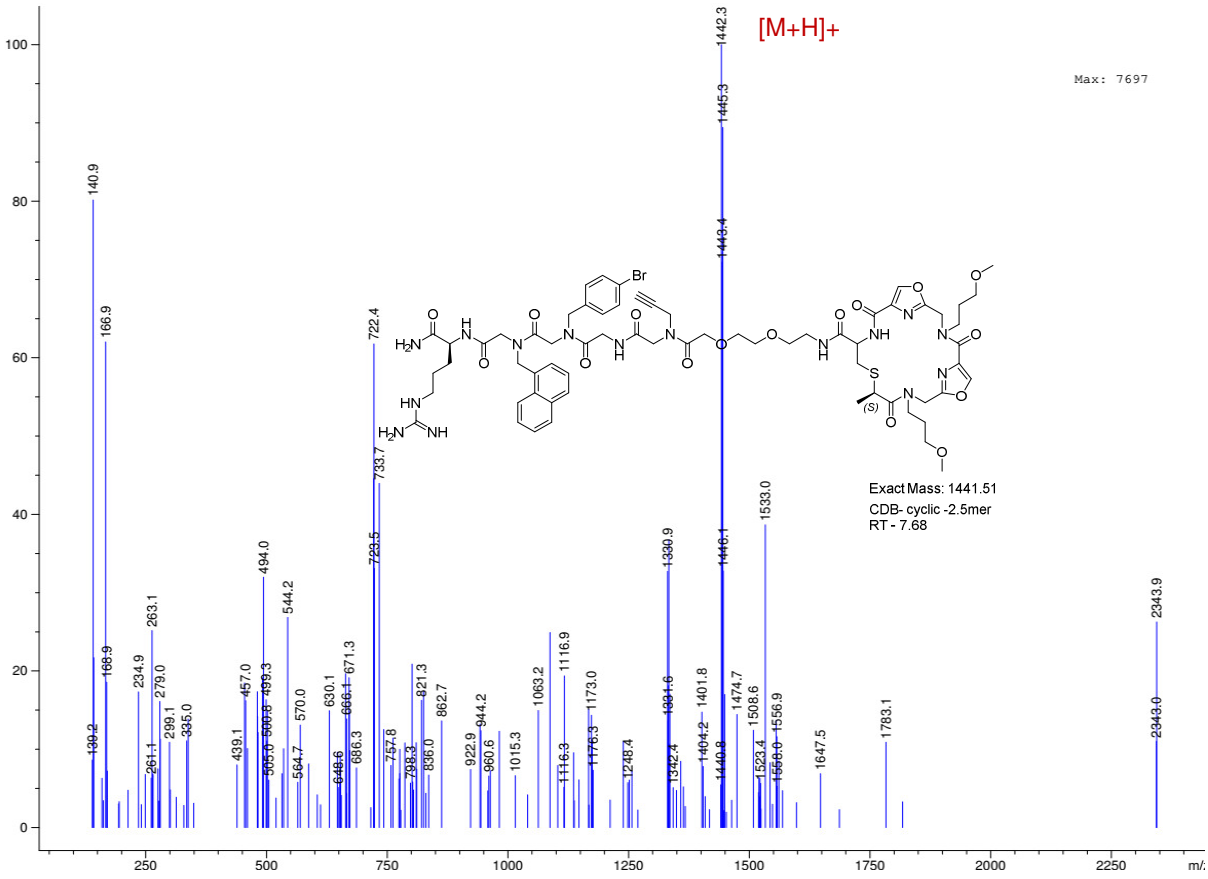


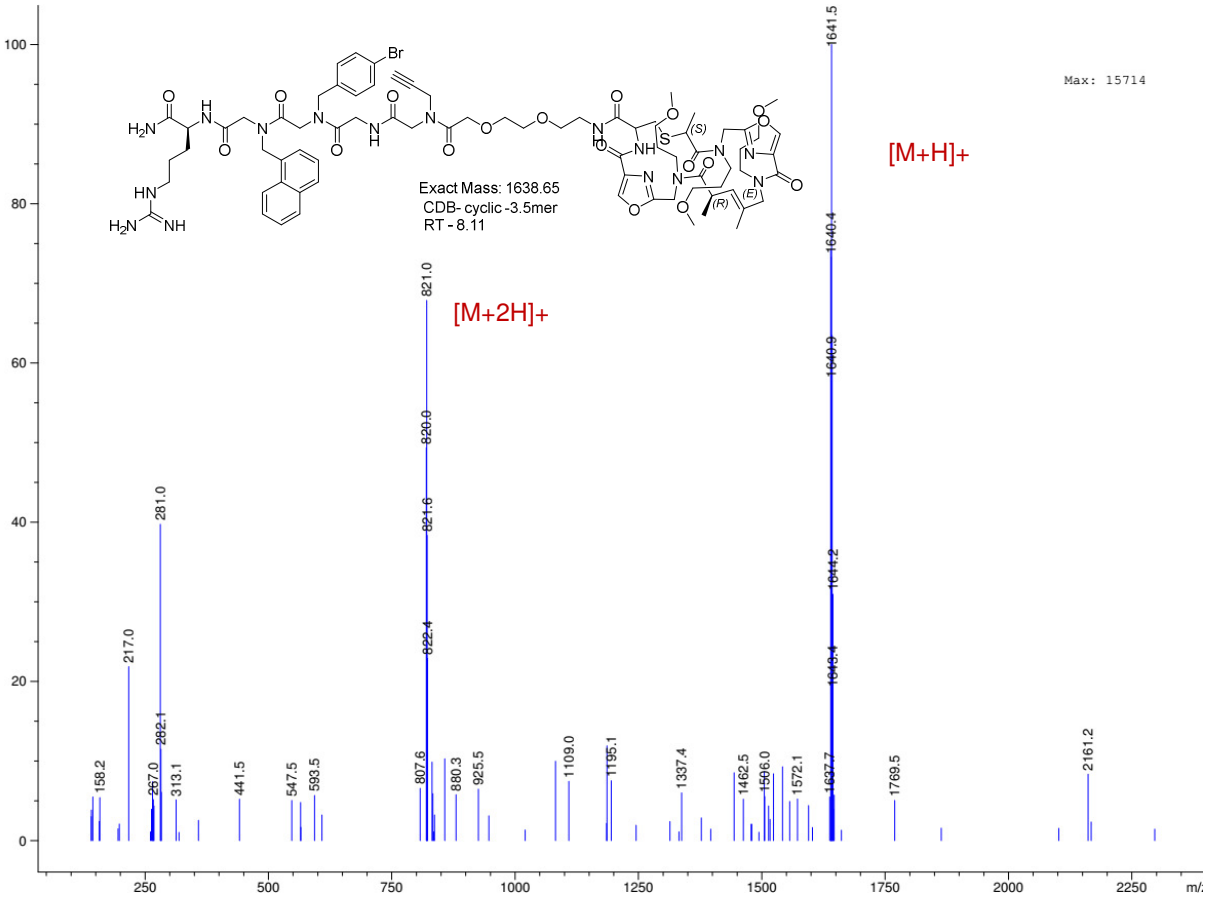


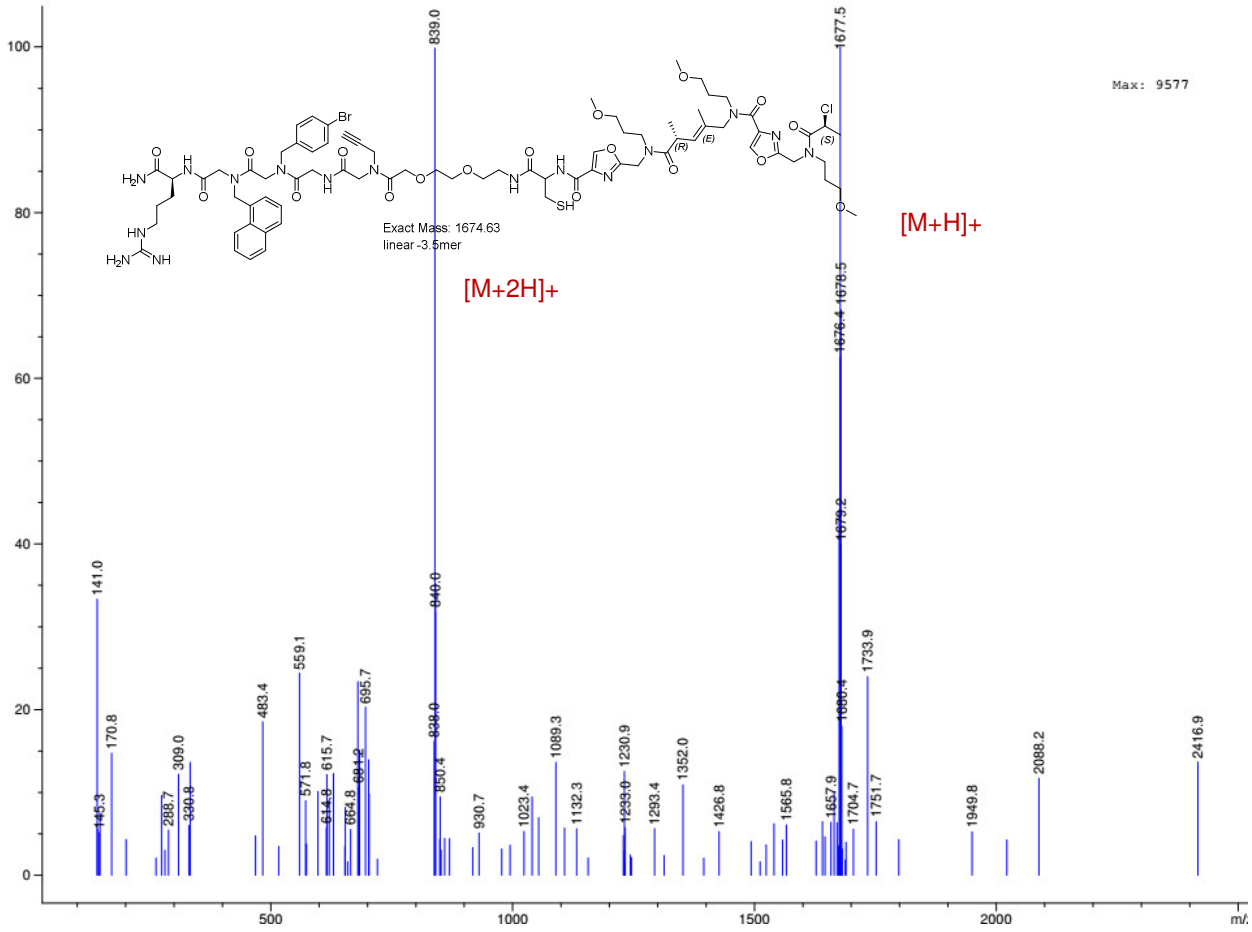
#	Time	Area	Height	Width	Area%
1	7.607	102	23.4	0.0728	13.001
2	8.049	514.6	101.4	0.0846	65.585
3	8.408	168	40.8	0.0687	21.415

M10 - [CDB]

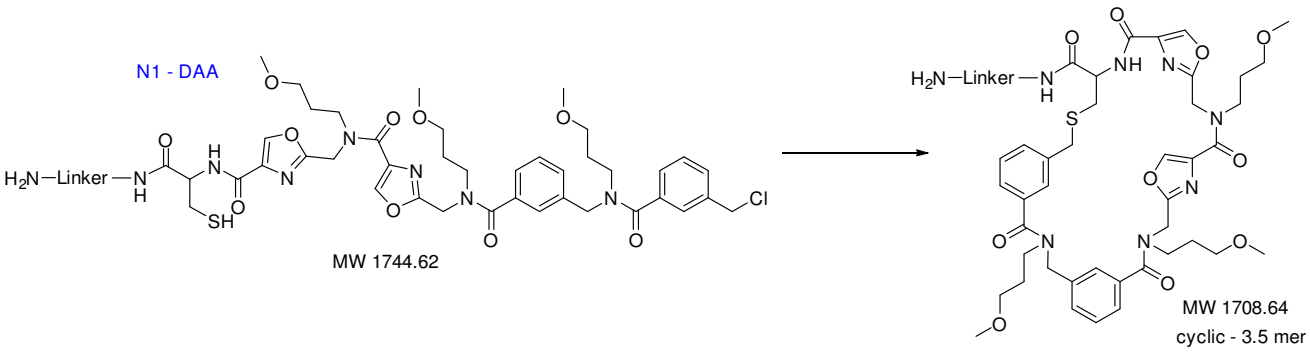
ions	size	MW	RT
cyclic	2.5	1441	7.607
cyclic	3.5	1638	8.049
linear	3.5	1674	8.408

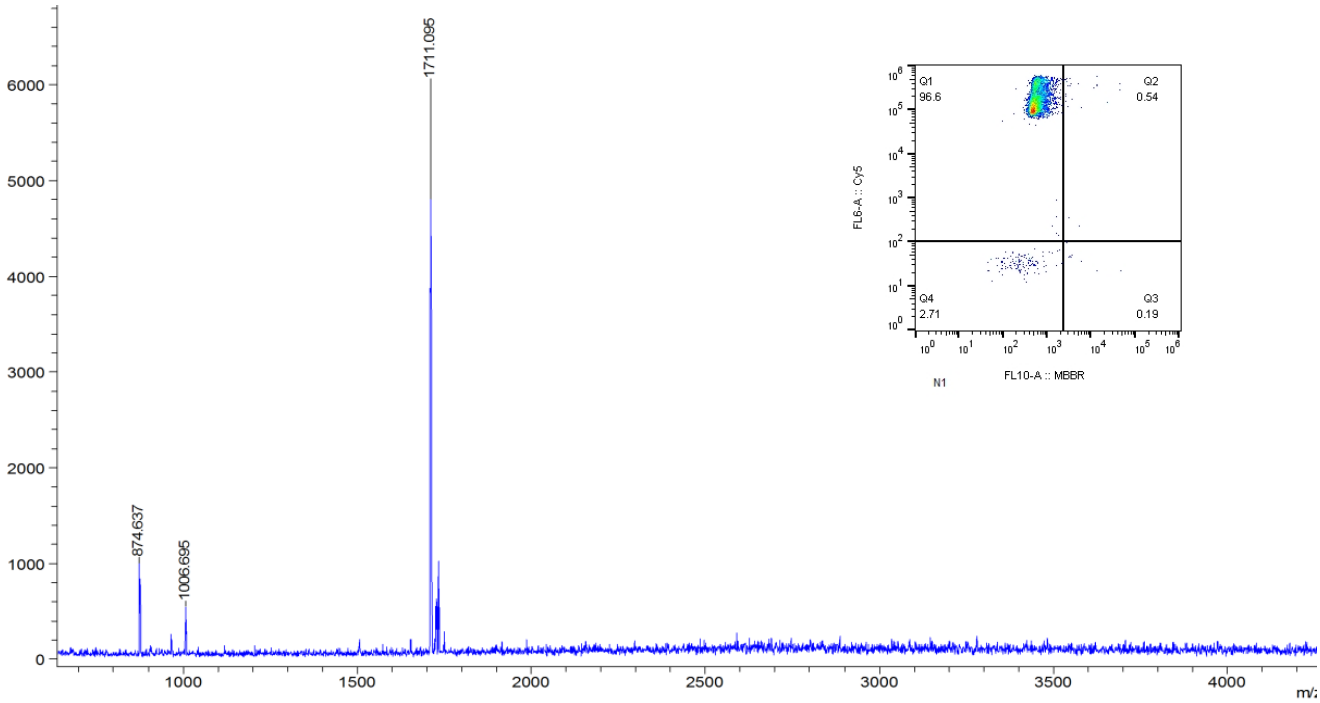

[M+H]+
Max: 7697
Exact Mass: 1441.51
CDB- cyclic -2.5mer
RT - 7.68

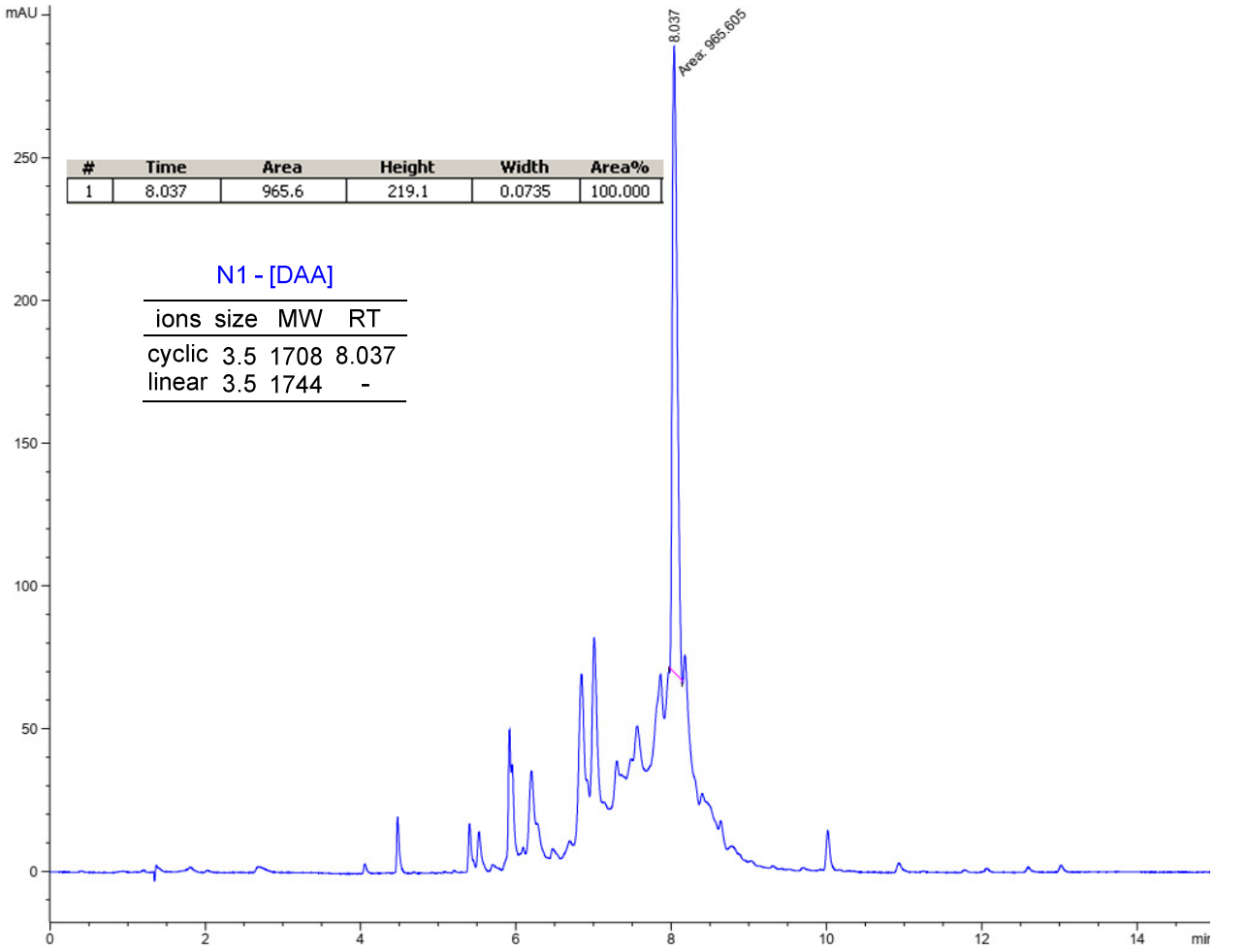

Max: 15714
[M+H]+
Exact Mass: 1638.65
CDB- cyclic -3.5mer
RT - 8.11
[M+2H]+



N1-[DAA]: Complete cyclization was observed on 10 µm &160 µm beads.



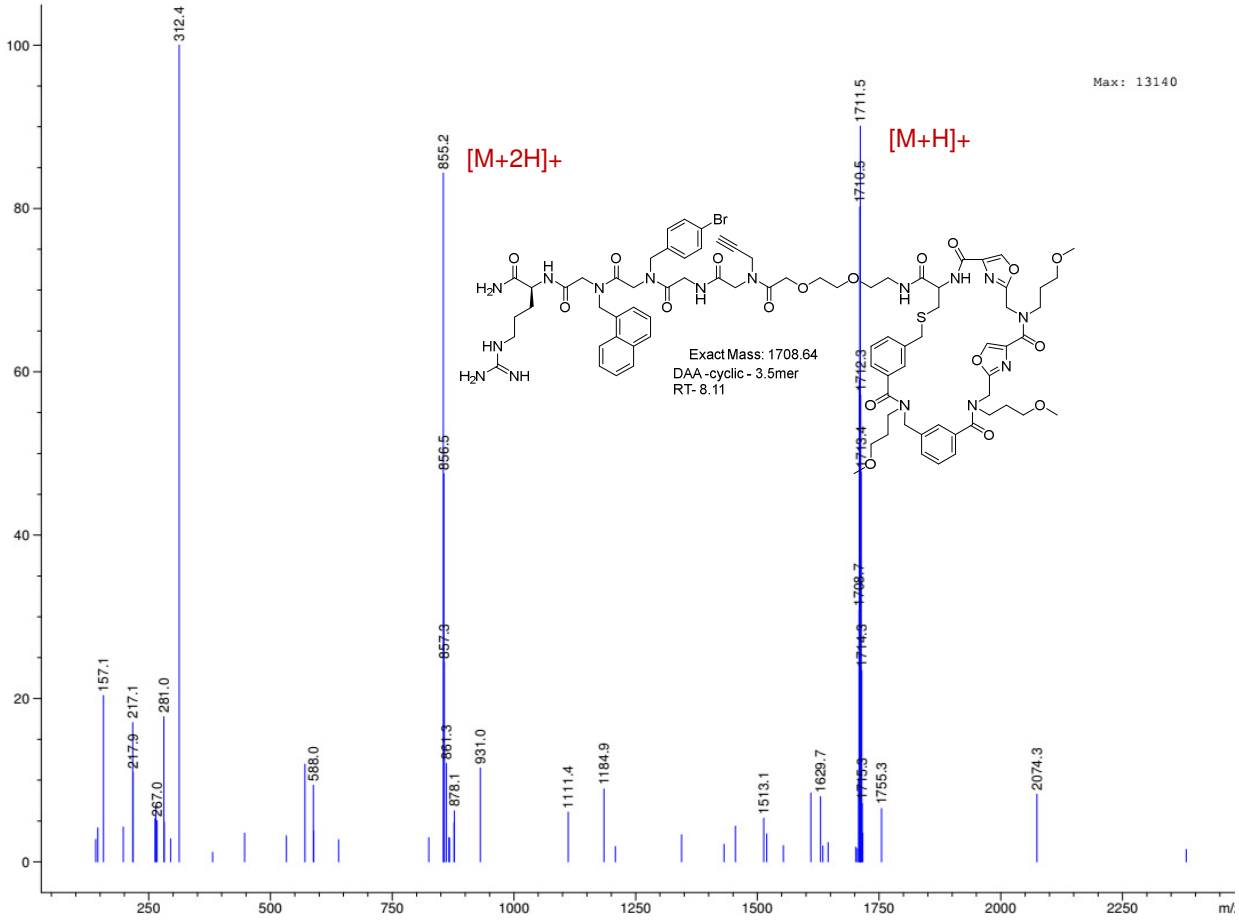




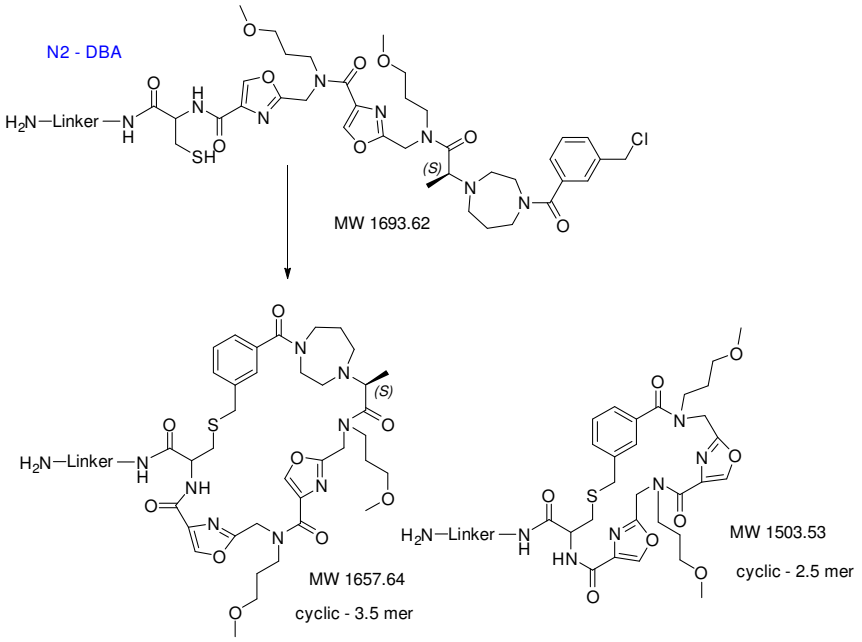
#	Time	Area	Height	Width	Area%
1	8.037	965.6	219.1	0.0735	100.000

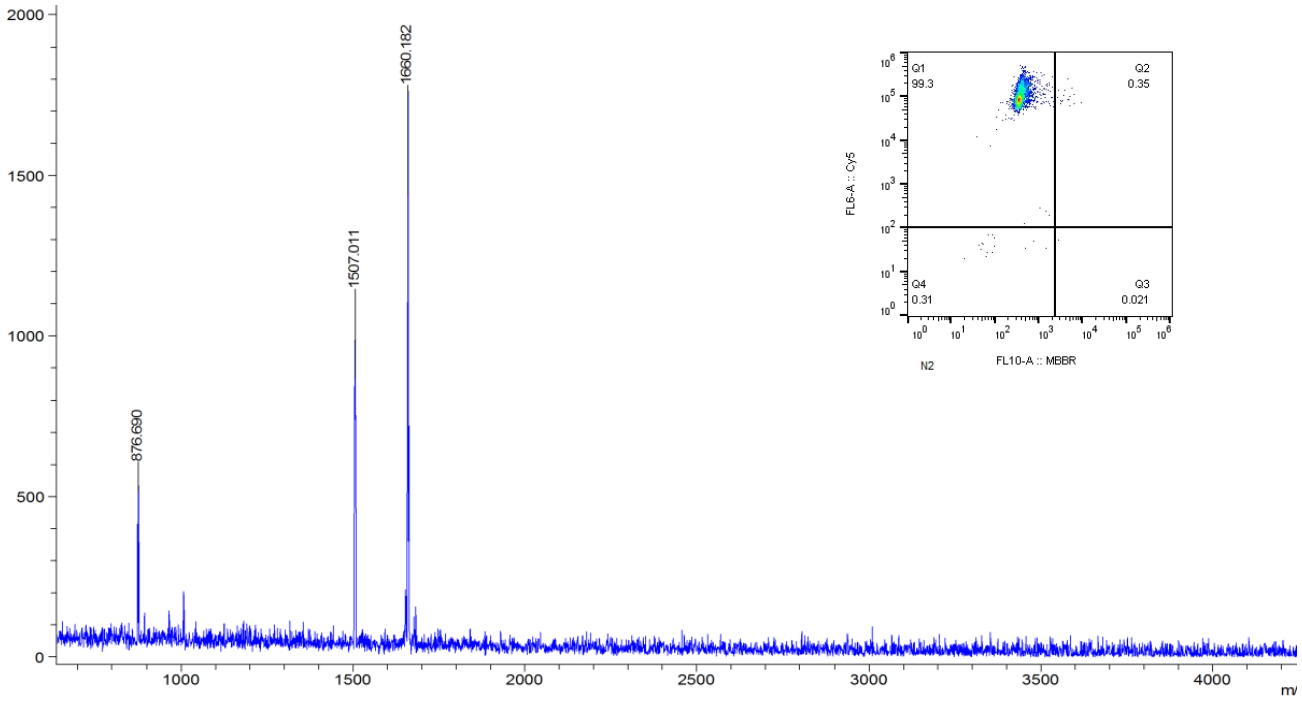
N1 - [DAA]

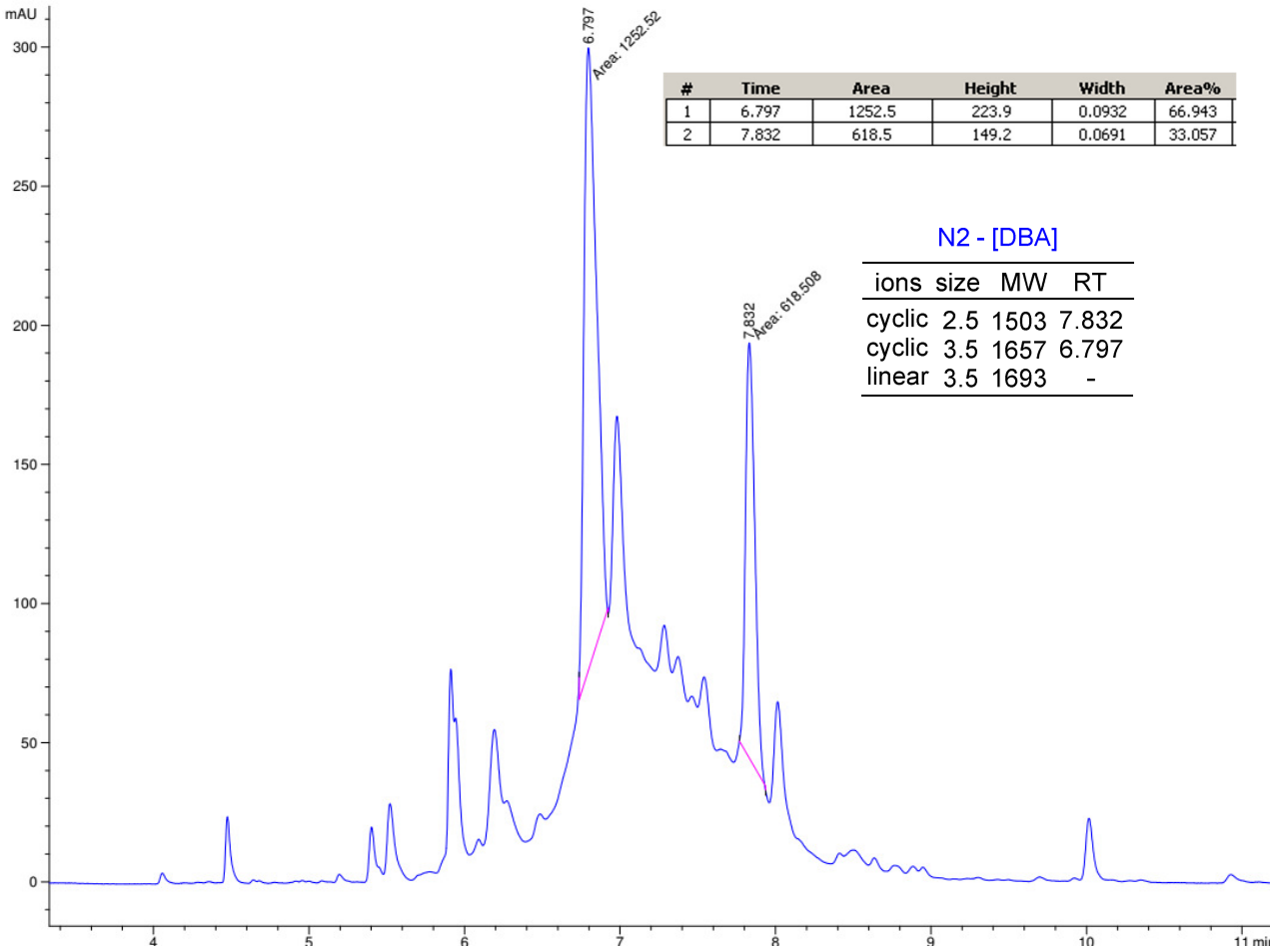
ions	size	MW	RT
cyclic	3.5	1708	8.037
linear	3.5	1744	-



N2-[DBA]: Complete cyclization was observed on 10 µm &160 µm beads.



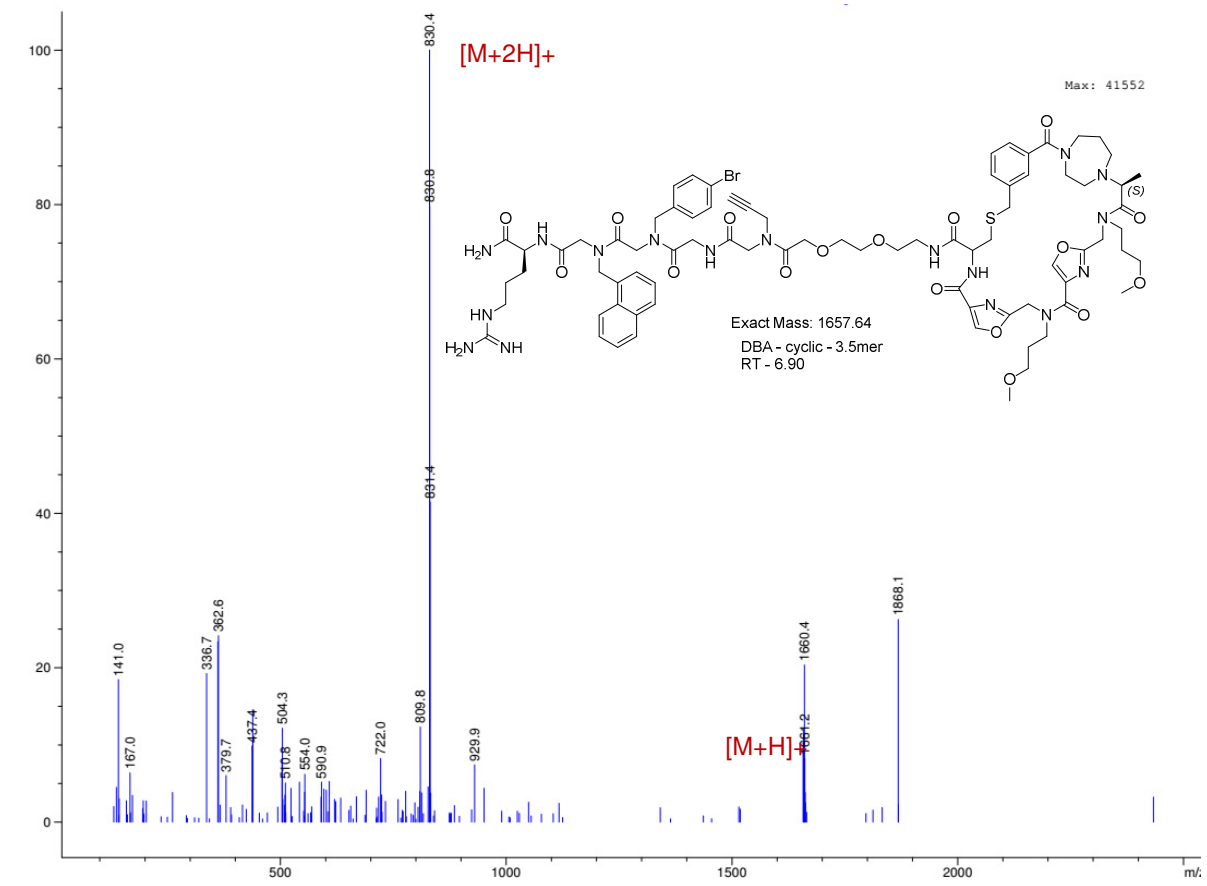


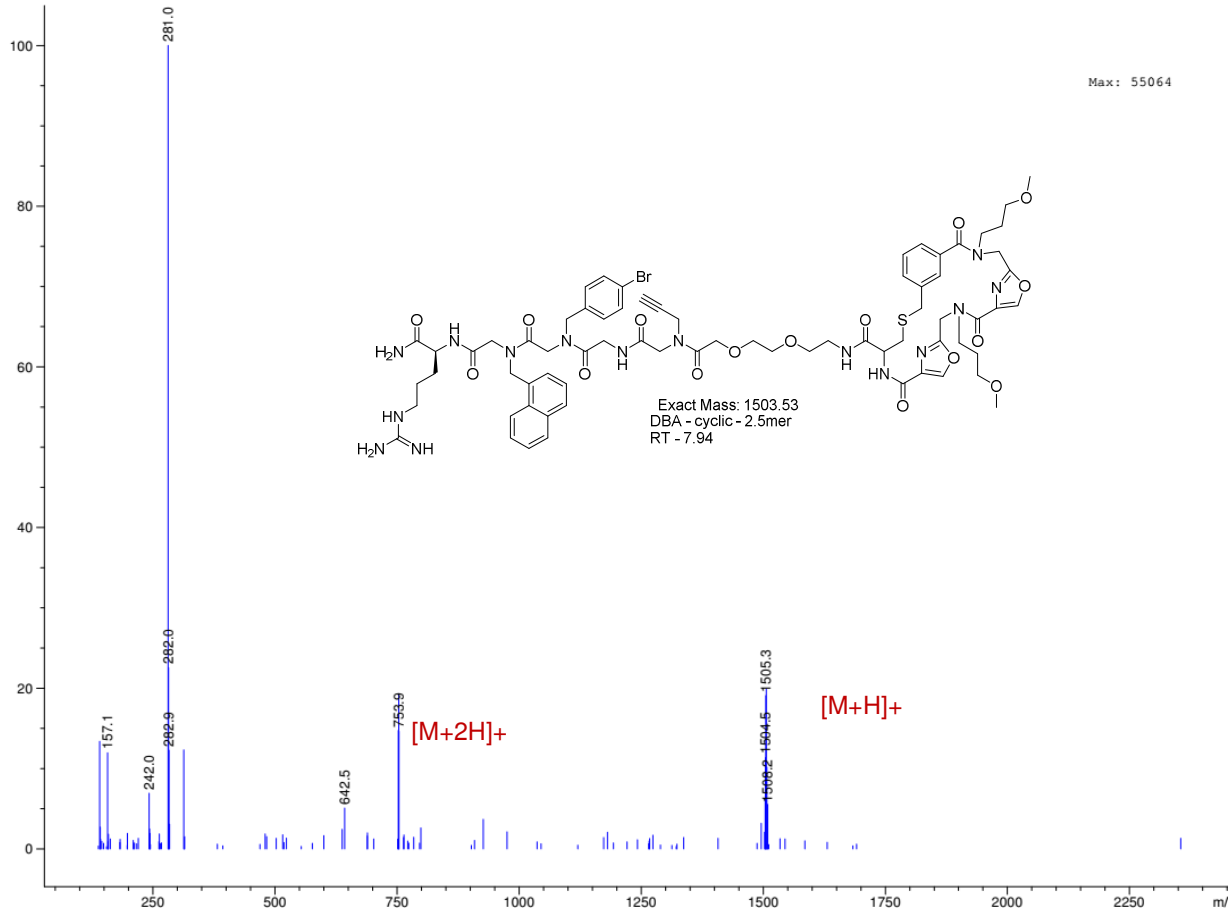


#	Time	Area	Height	Width	Area%
1	6.797	1252.5	223.9	0.0932	66.943
2	7.832	618.5	149.2	0.0691	33.057

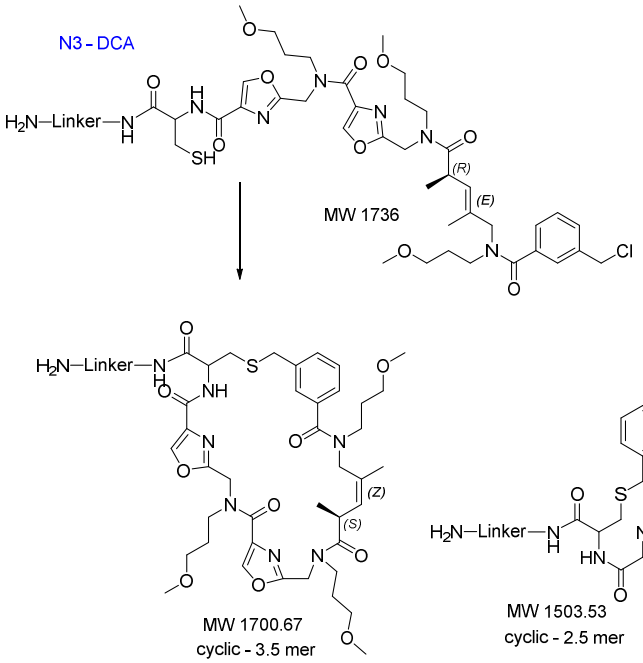
N2 - [DBA]

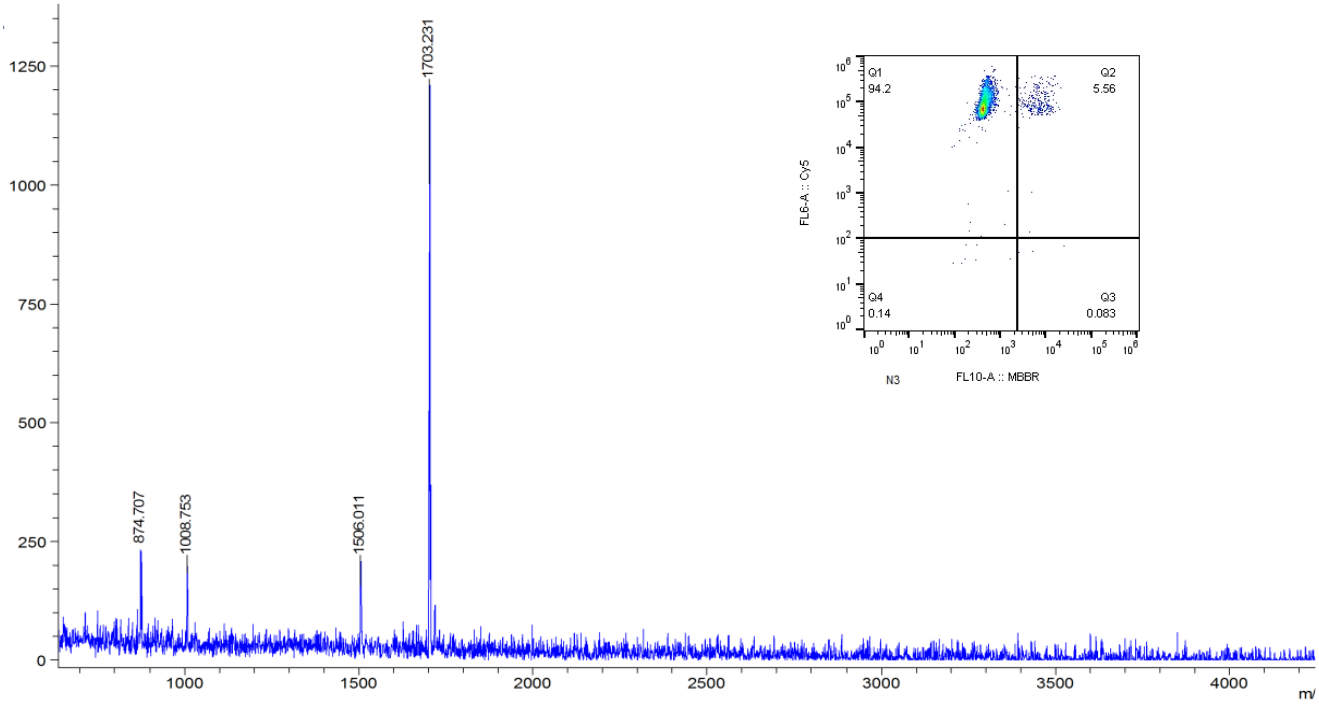
ions	size	MW	RT
cyclic	2.5	1503	7.832
cyclic	3.5	1657	6.797
linear	3.5	1693	-

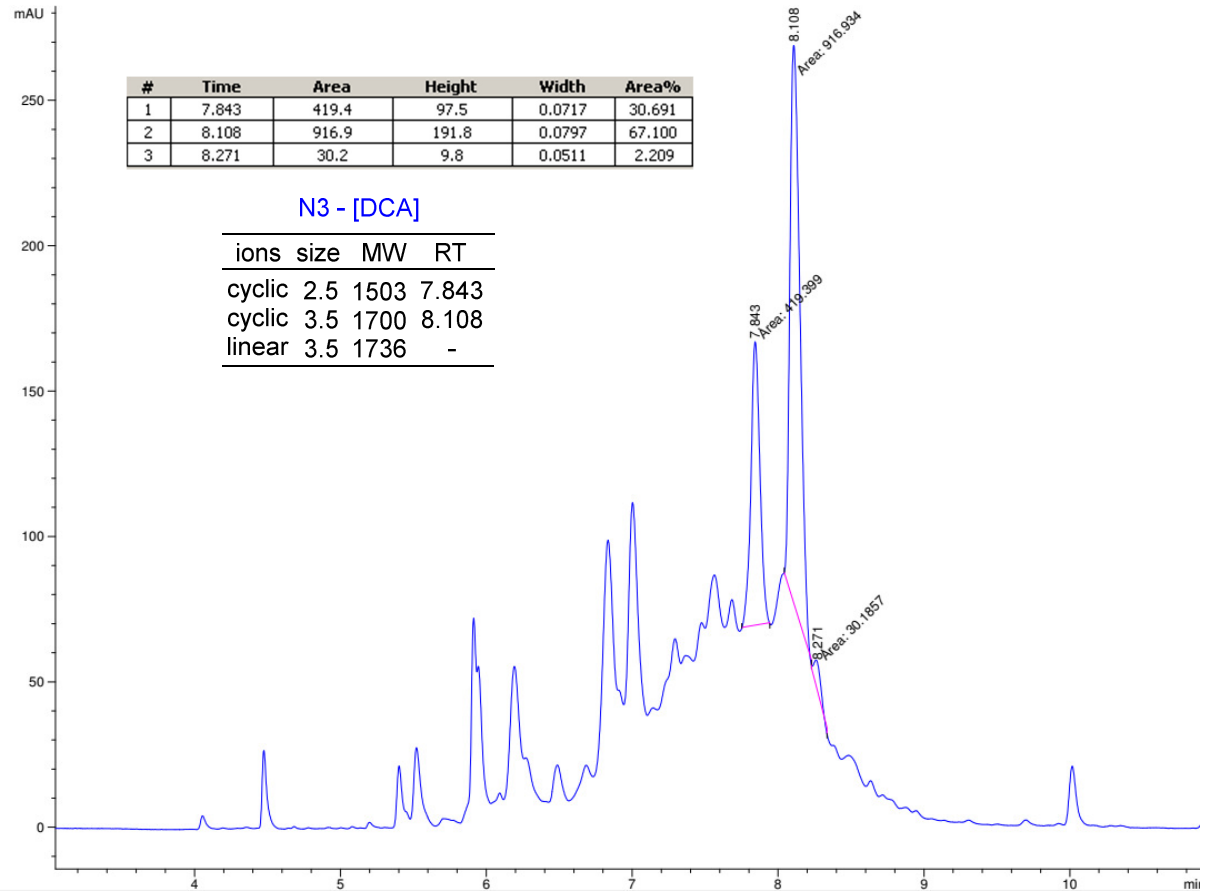

[M+2H]+
Max: 41552
Exact Mass: 1657.64
DBA - cyclic - 3.5mer
RT - 6.90
[M+H]+
830.4
830.8
831.4
1660.4
1661.2
1868.1
141.0
167.0
336.7
362.6
379.7
437.4
504.3
510.8
554.0
590.9
722.0
809.8
929.9


Max: 55064
Exact Mass: 1503.53
DBA - cyclic - 2.5mer
RT - 7.94
[M+2H]+
[M+H]+
281.0
282.0
282.9
753.9
1505.3
1504.5
1506.2
157.1
242.0
642.5

N3-[DCA]: Complete cyclization was observed on 10 µm &160 µm beads.



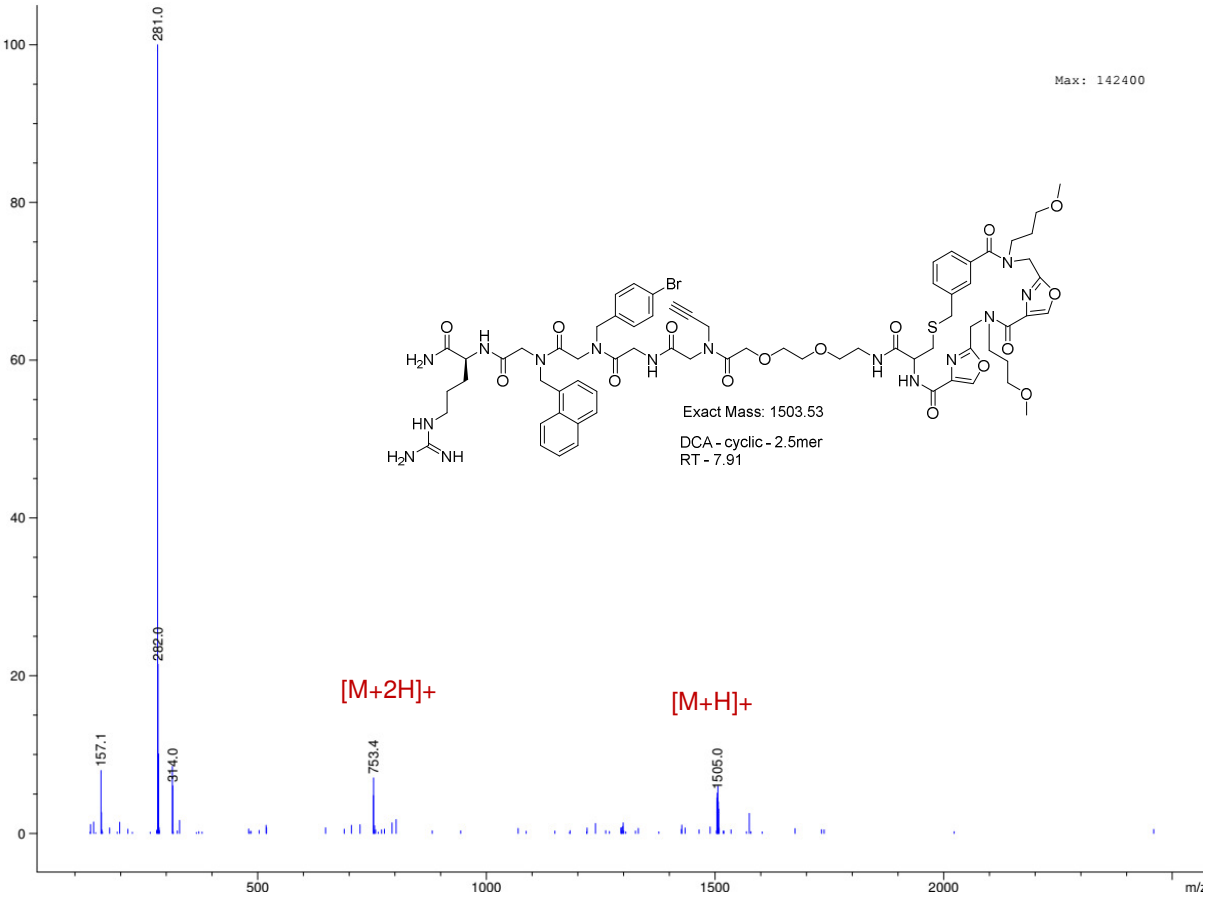


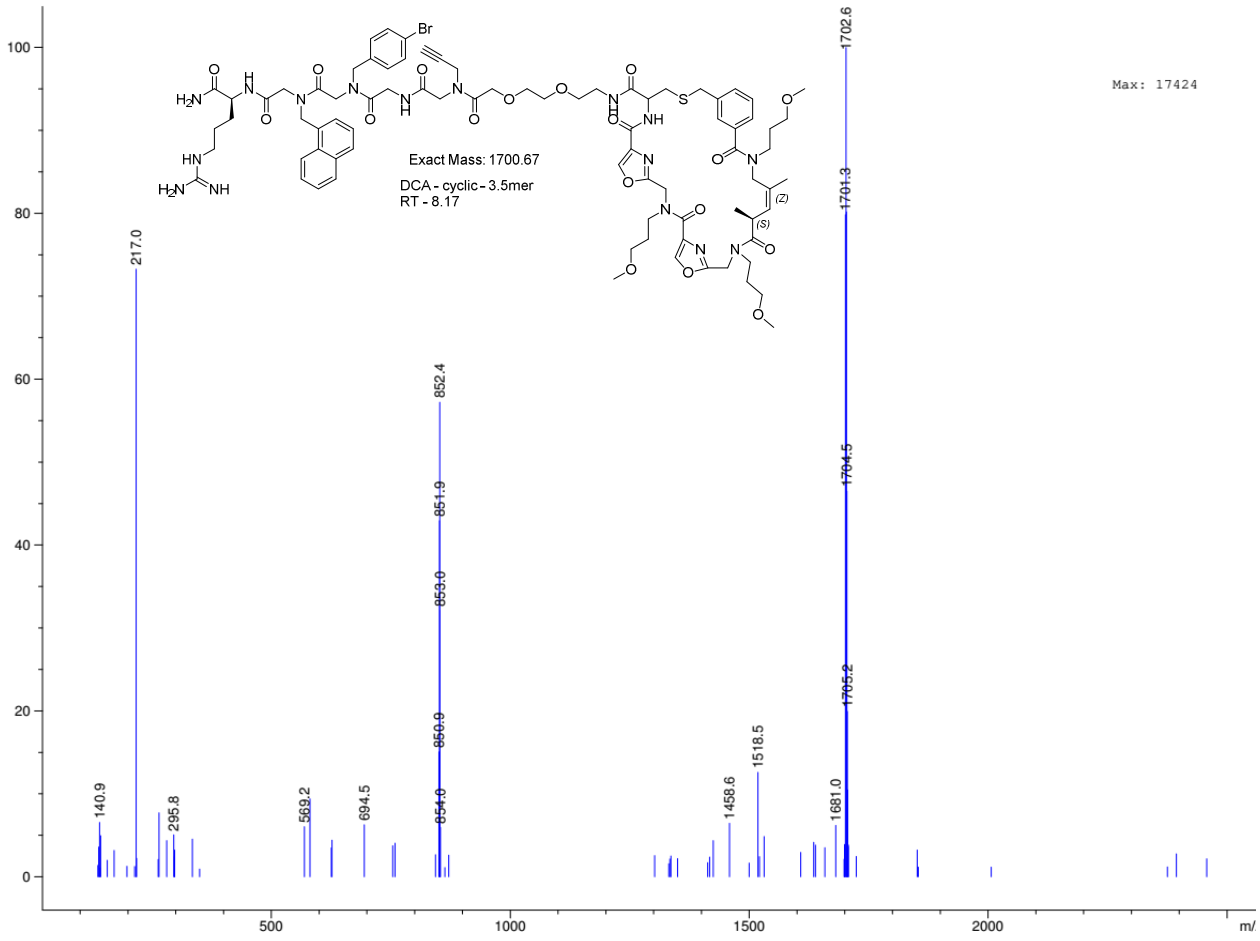


#	Time	Area	Height	Width	Area%
1	7.843	419.4	97.5	0.0717	30.691
2	8.108	916.9	191.8	0.0797	67.100
3	8.271	30.2	9.8	0.0511	2.209

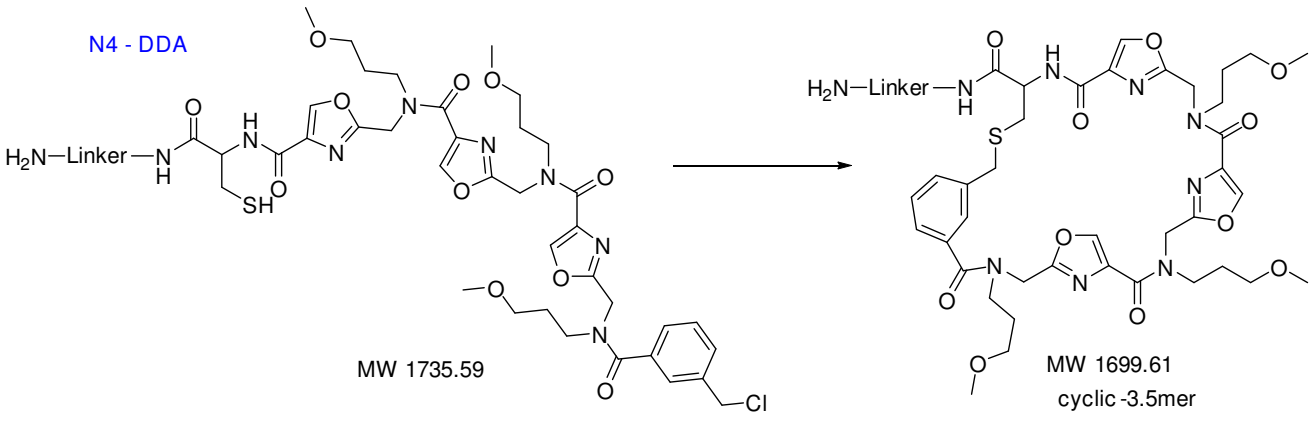
N3 - [DCA]

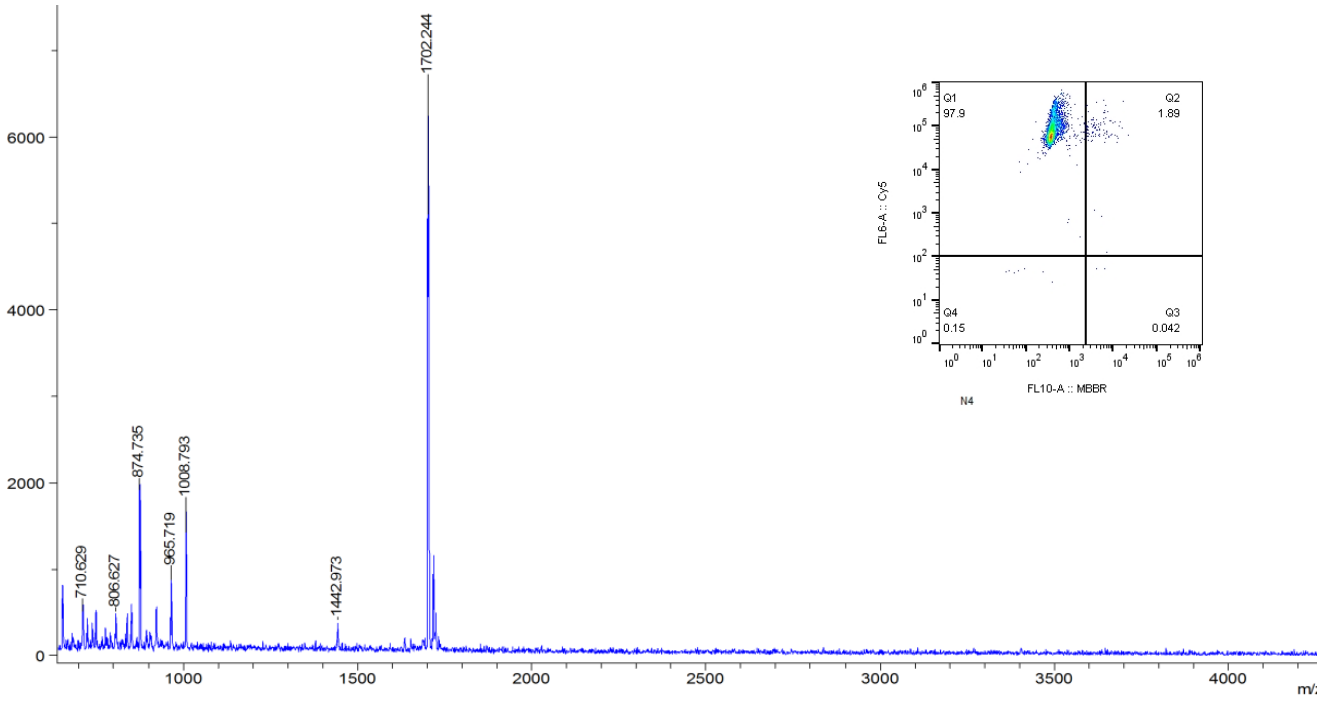
ions	size	MW	RT
cyclic	2.5	1503	7.843
cyclic	3.5	1700	8.108
linear	3.5	1736	-

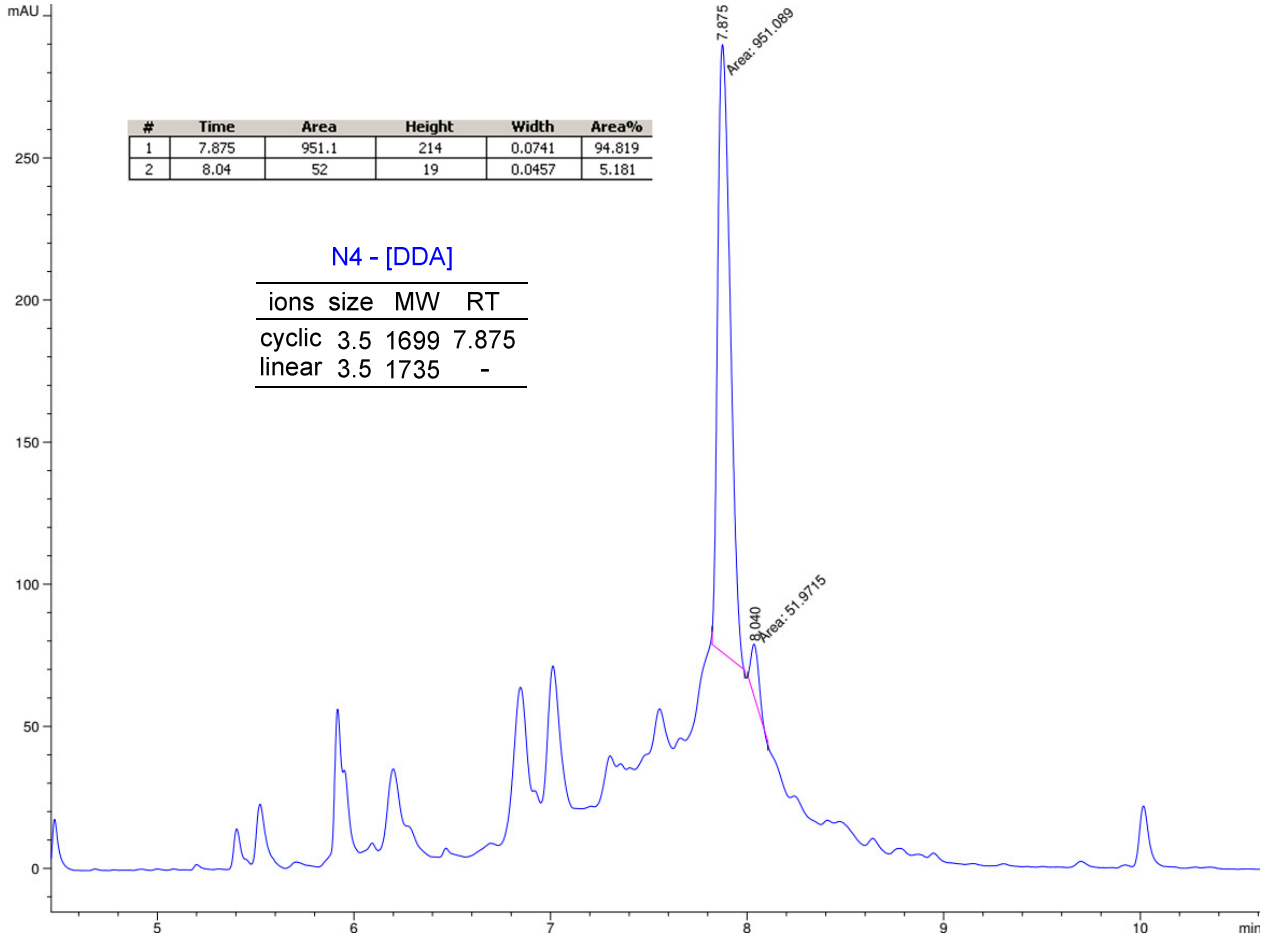




N4-[DDA]: Complete cyclization was observed on 10 µm &160 µm beads.



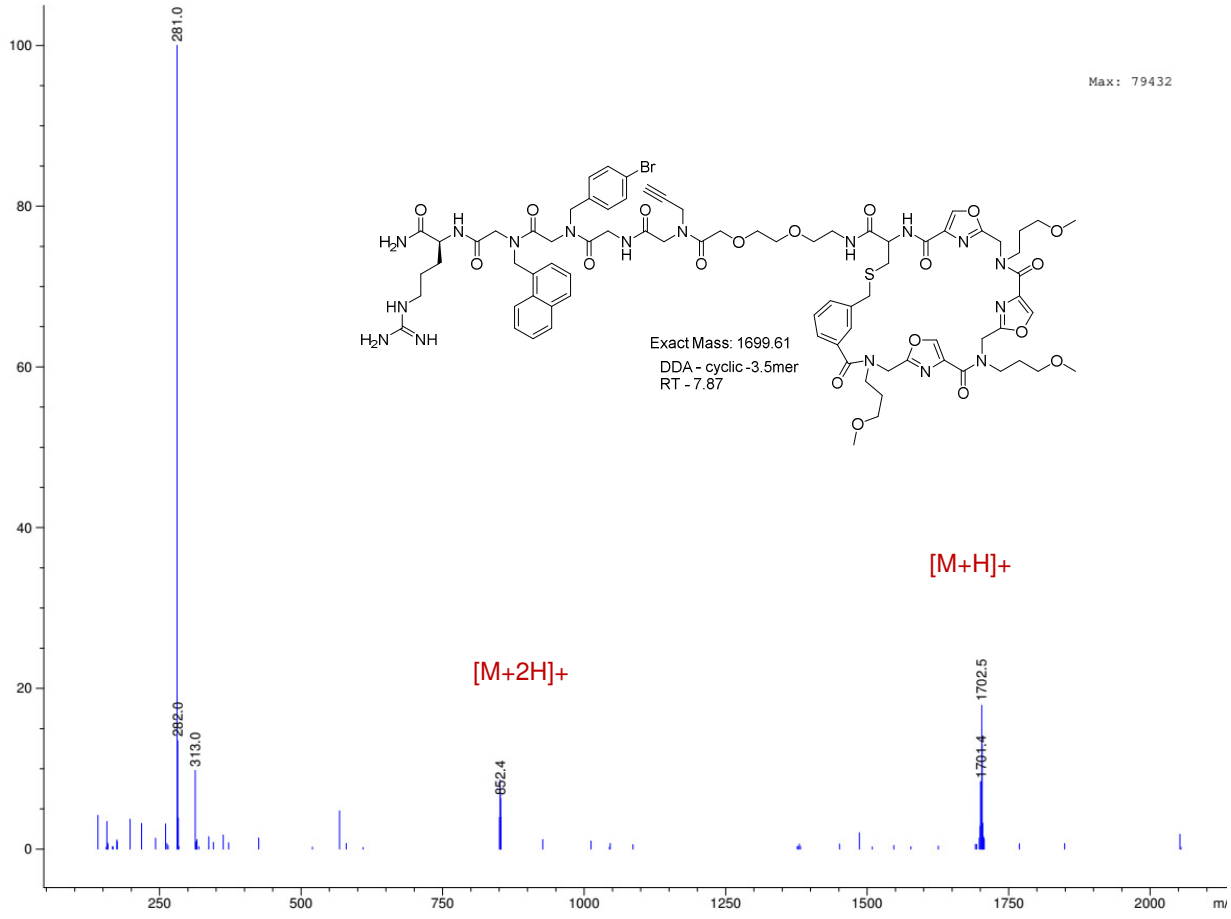




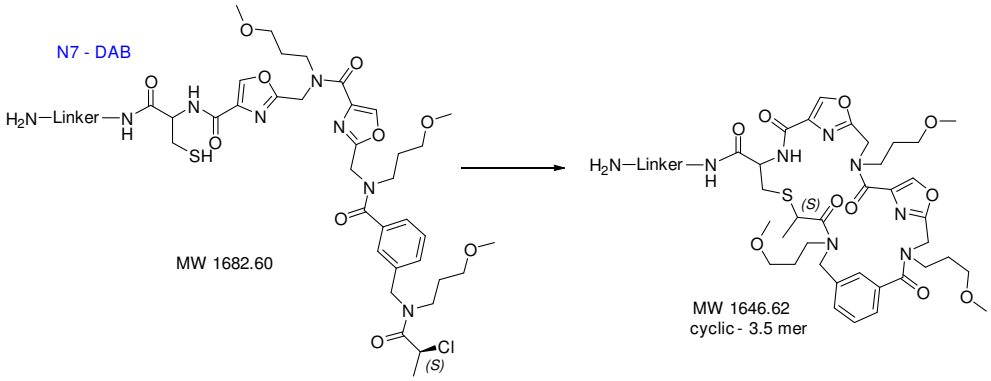
#	Time	Area	Height	Width	Area%
1	7.875	951.1	214	0.0741	94.819
2	8.04	52	19	0.0457	5.181

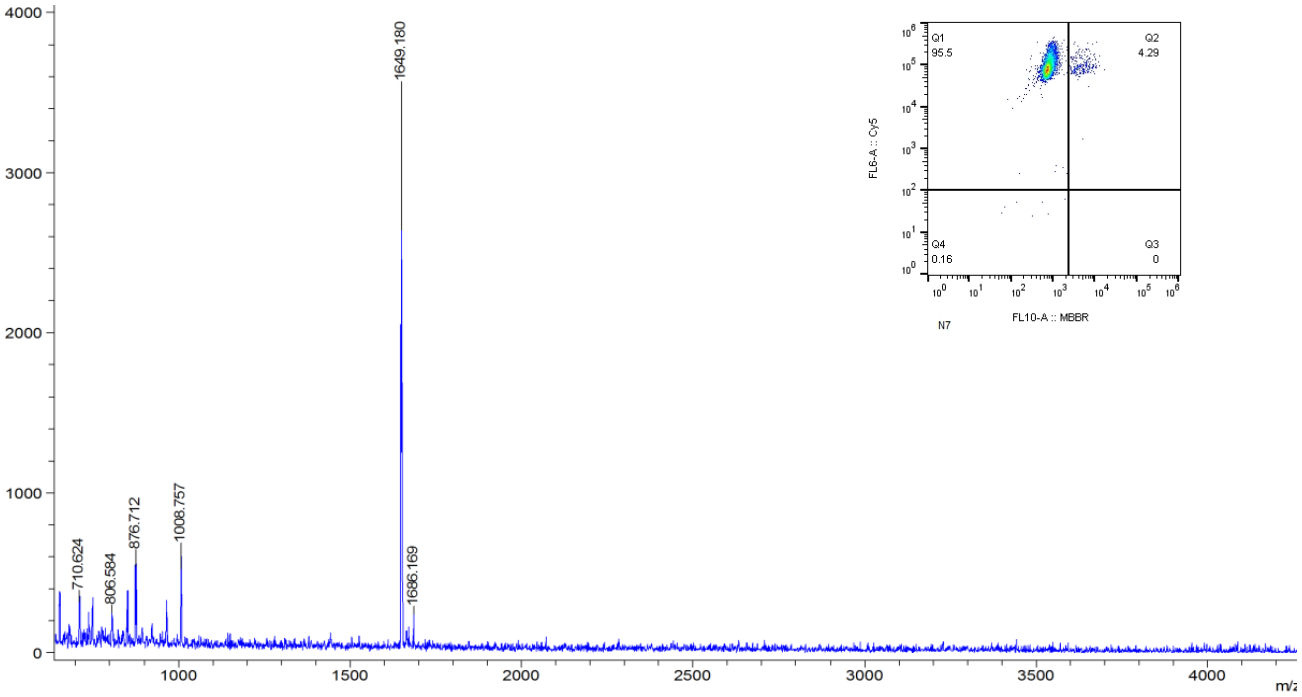
N4 - [DDA]

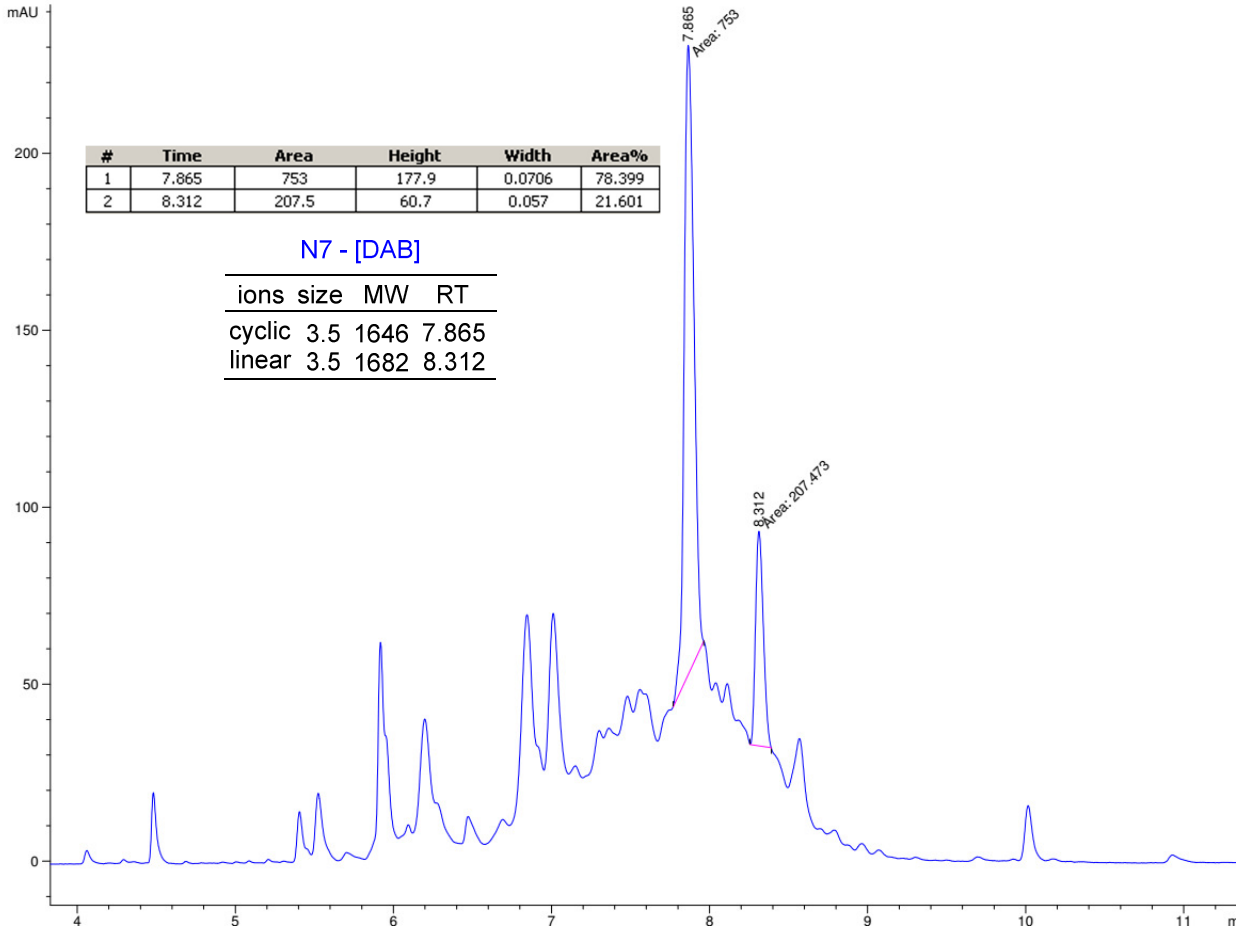
ions	size	MW	RT
cyclic	3.5	1699	7.875
linear	3.5	1735	-



N7-[DAB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm beads.



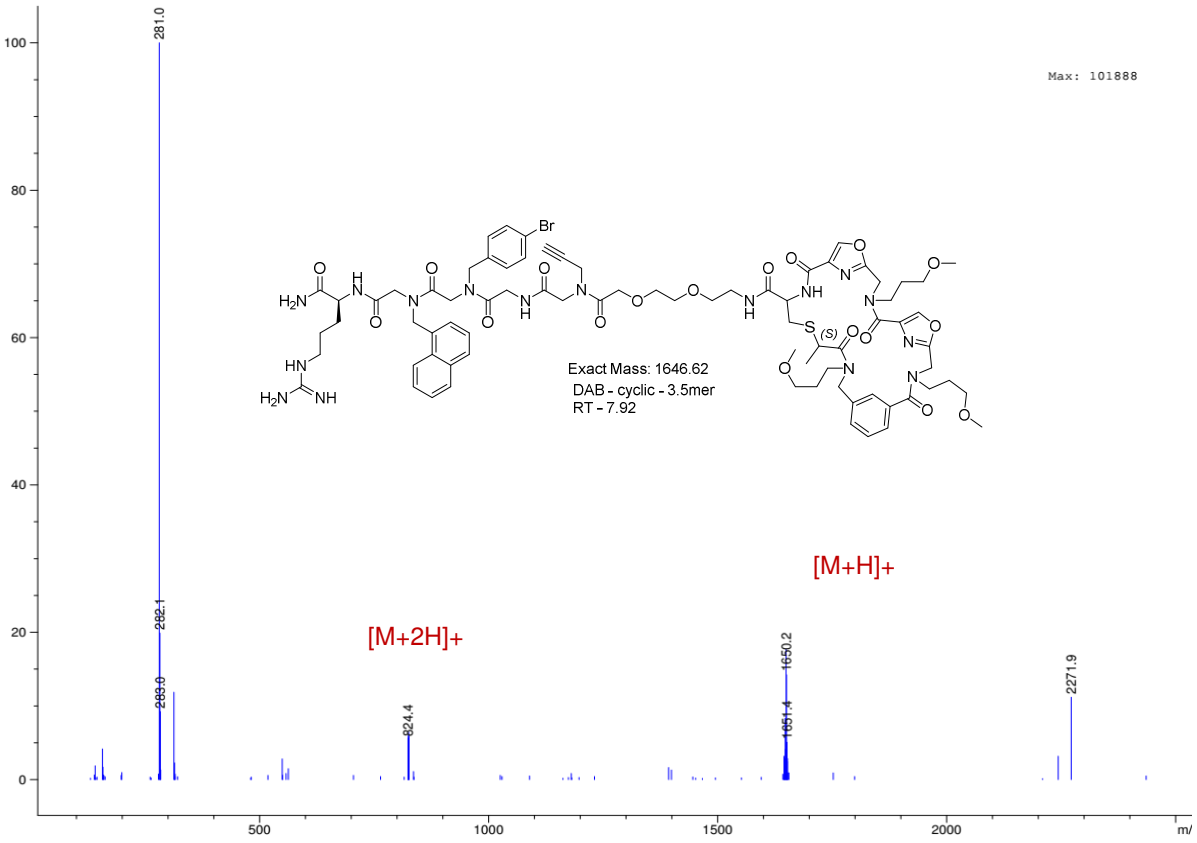


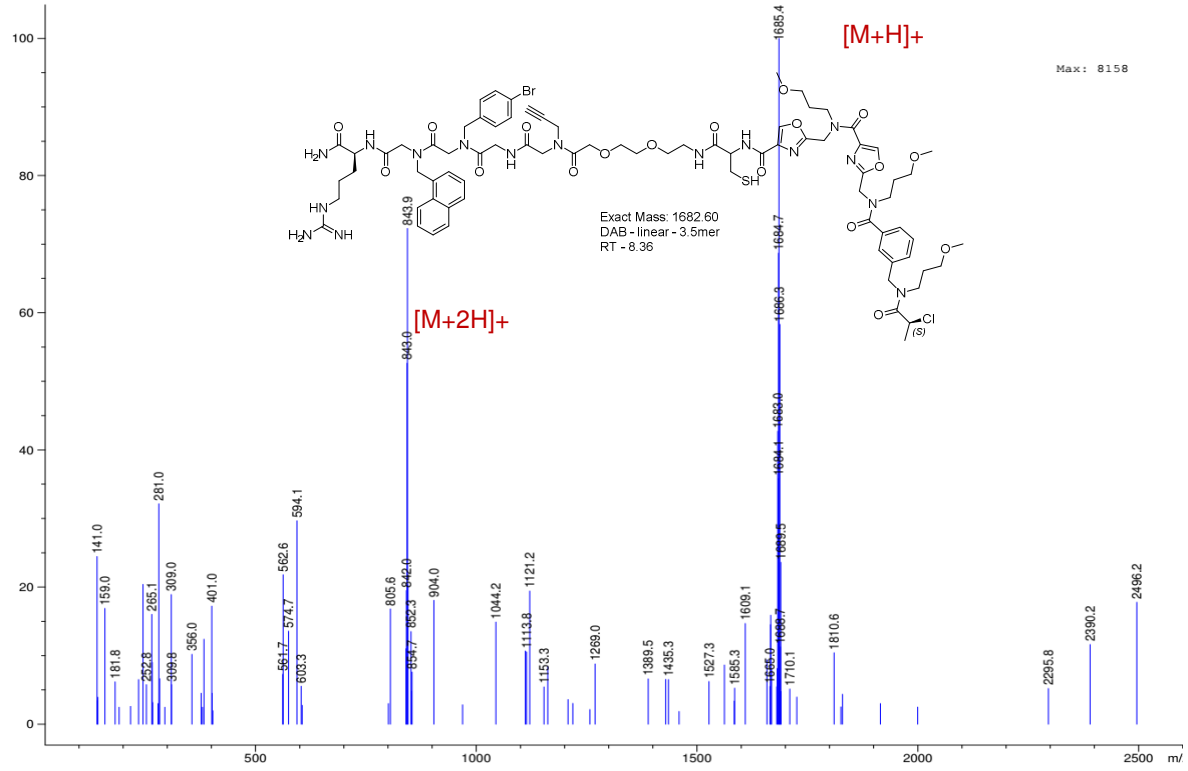


#	Time	Area	Height	Width	Area%
1	7.865	753	177.9	0.0706	78.399
2	8.312	207.5	60.7	0.057	21.601

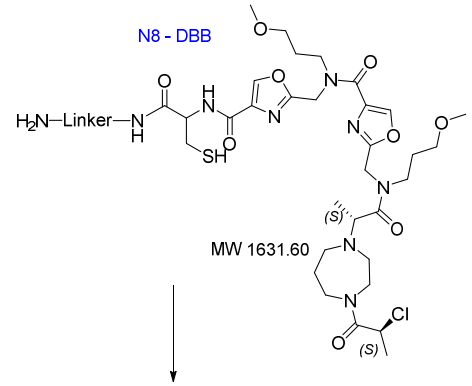
N7 - [DAB]

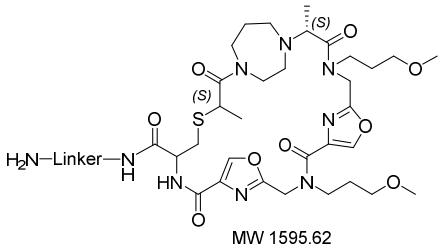
ions	size	MW	RT
cyclic	3.5	1646	7.865
linear	3.5	1682	8.312

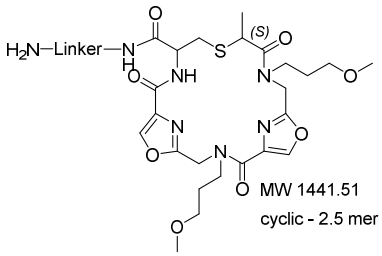

Max: 101888
Exact Mass: 1646.62
DAB - cyclic - 3.5mer
RT - 7.92
[M+H]+
[M+2H]+
281.0
282.1
283.0
824.4
1650.2
1651.4
2271.9
m/

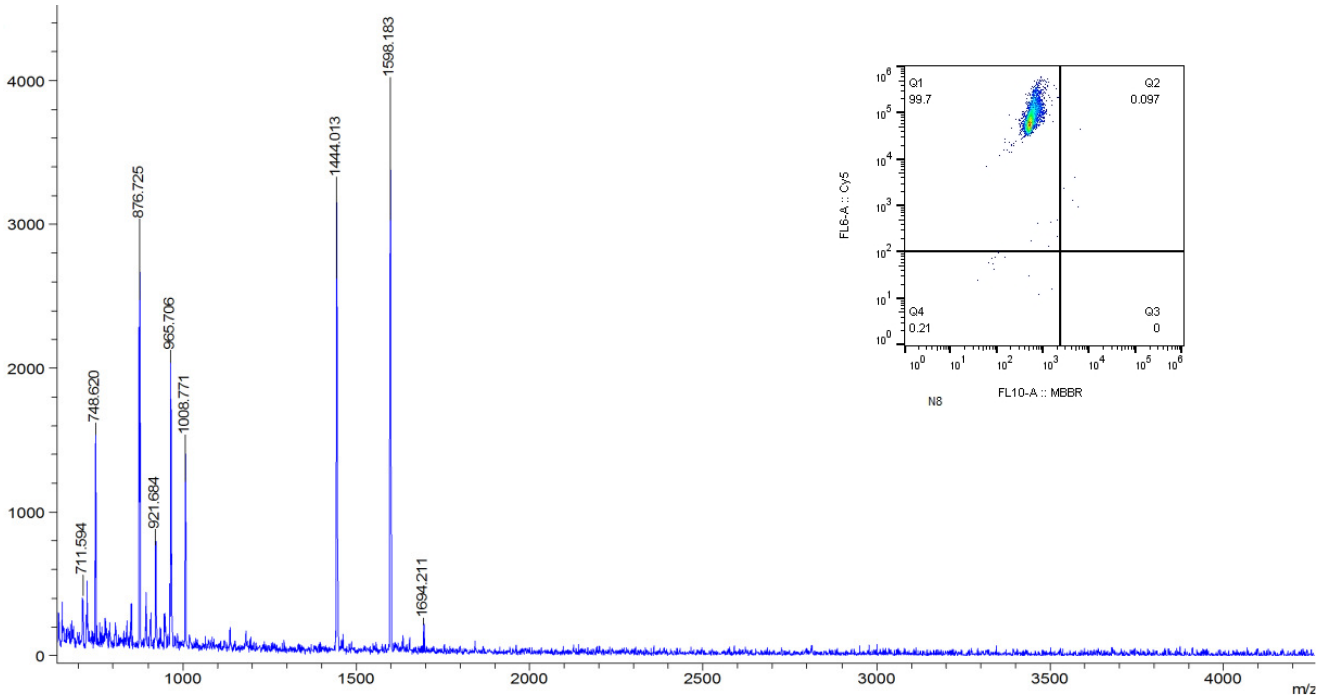

Max: 8158
Exact Mass: 1682.60
DAB - linear - 3.5mer
RT - 8.36
[M+H]+
[M+2H]+
m/

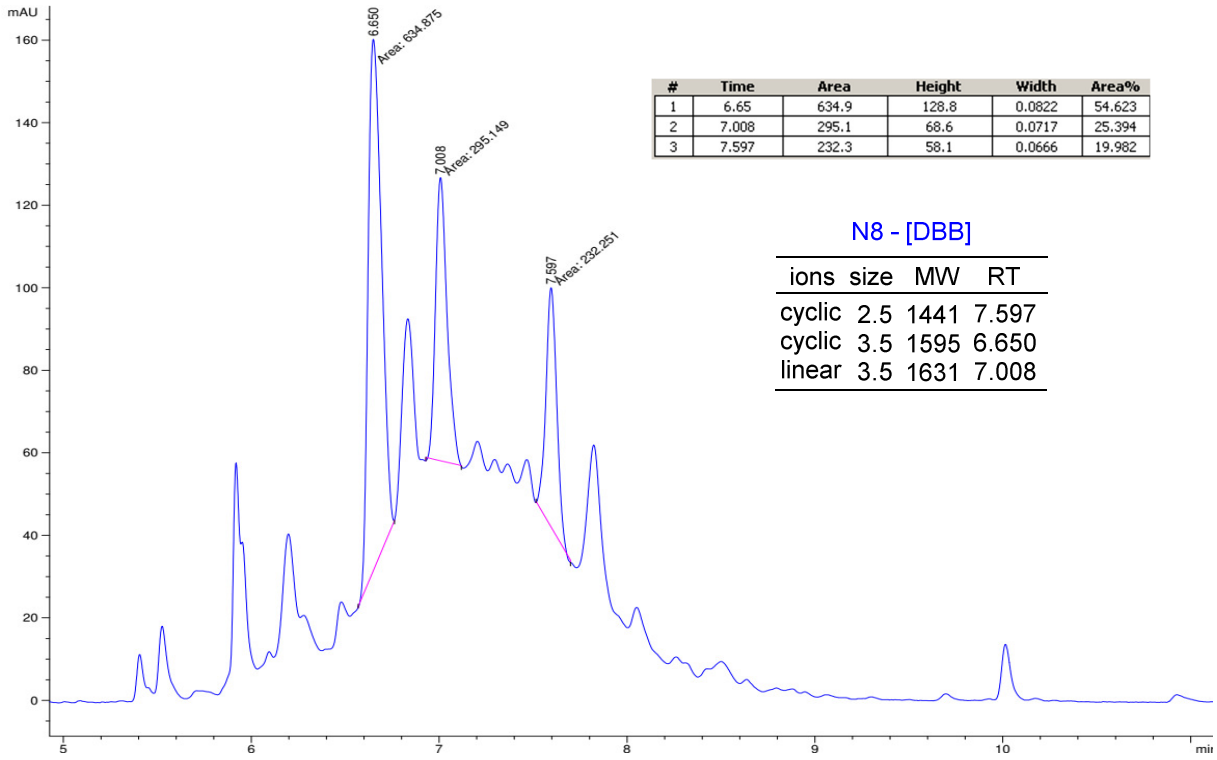
N8-[DBB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm beads.







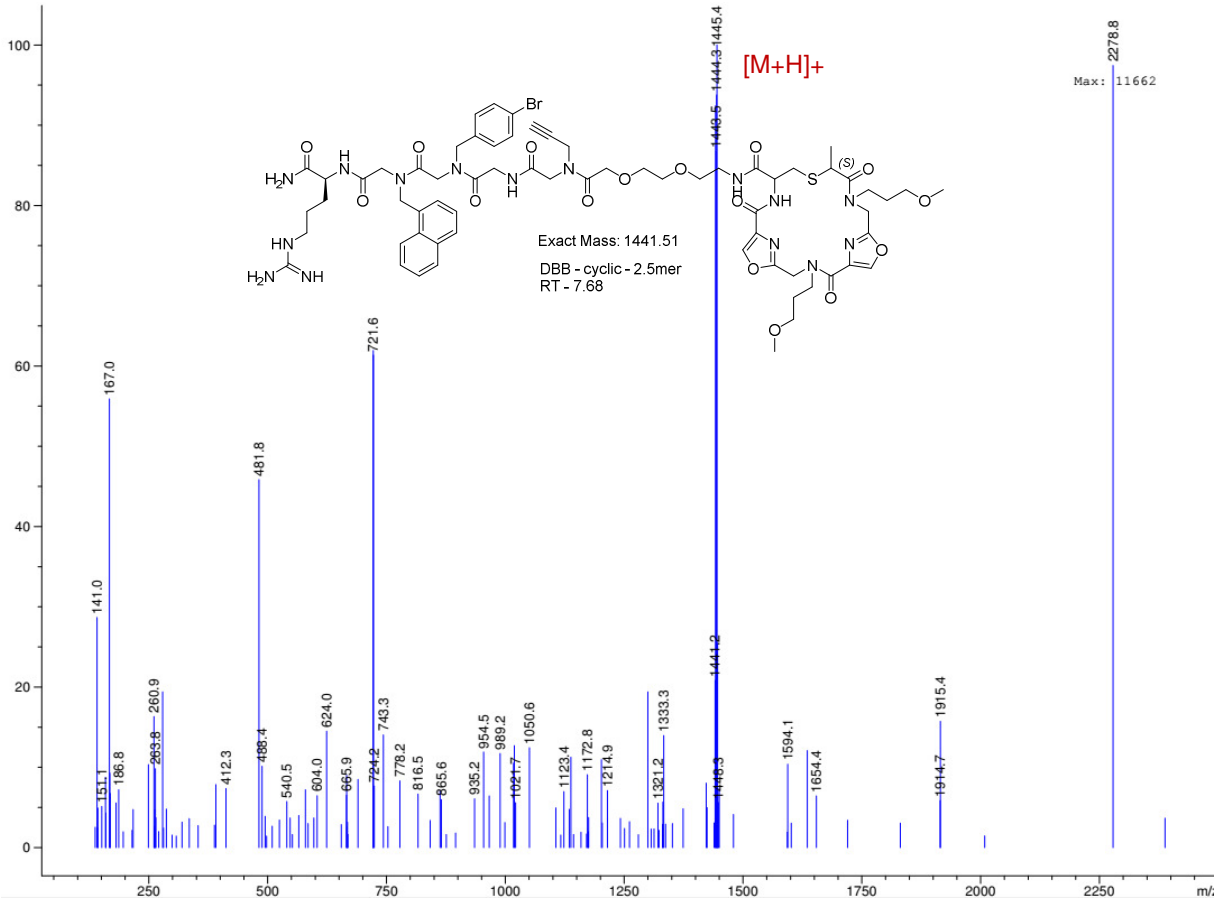


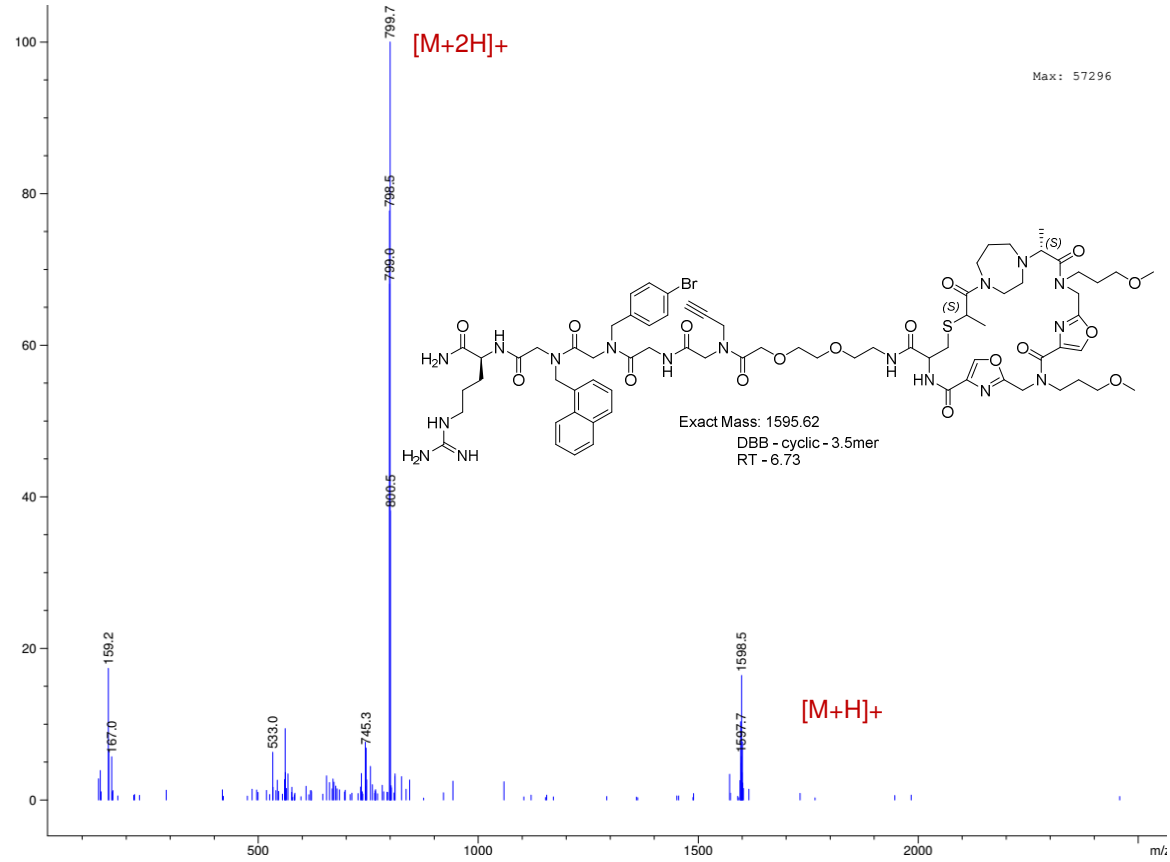


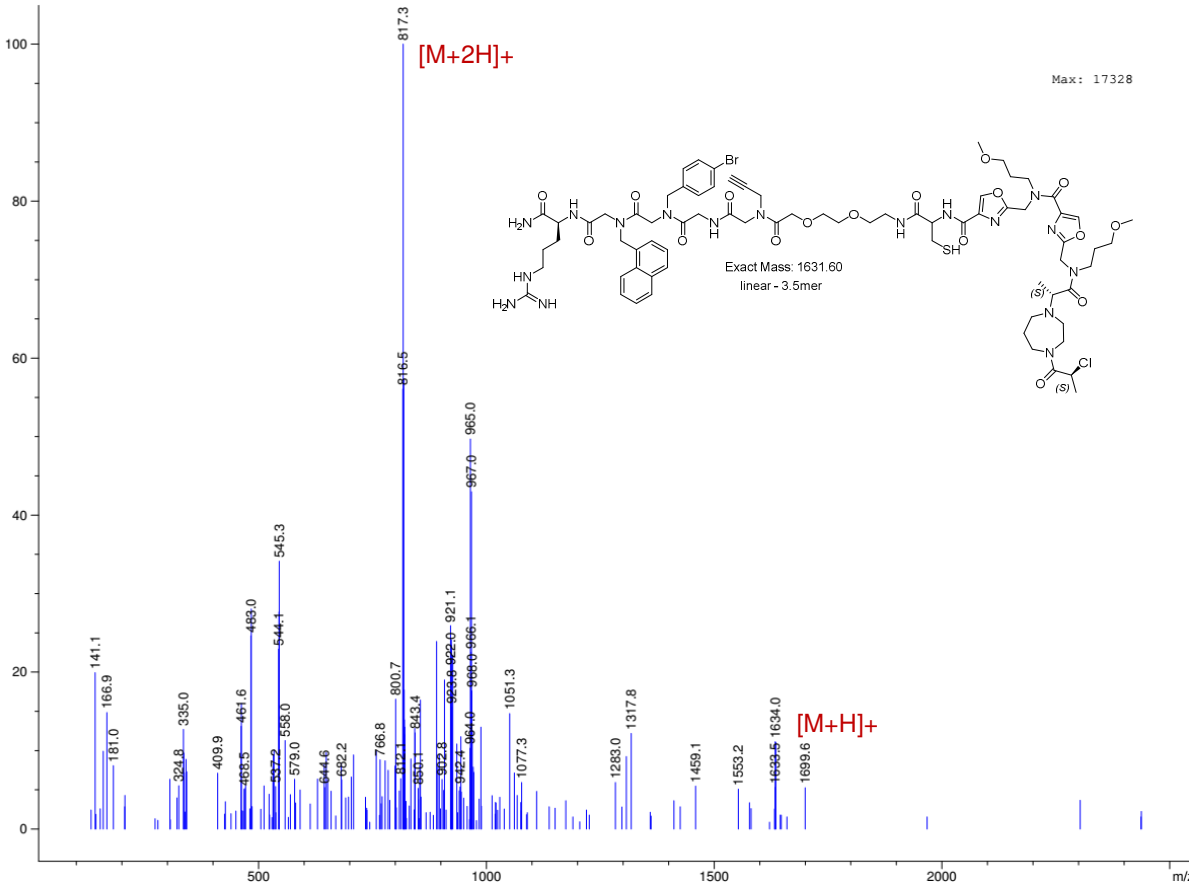
#	Time	Area	Height	Width	Area%
1	6.65	634.9	128.8	0.0822	54.623
2	7.008	295.1	68.6	0.0717	25.394
3	7.597	232.3	58.1	0.0666	19.982

N8 - [DBB]

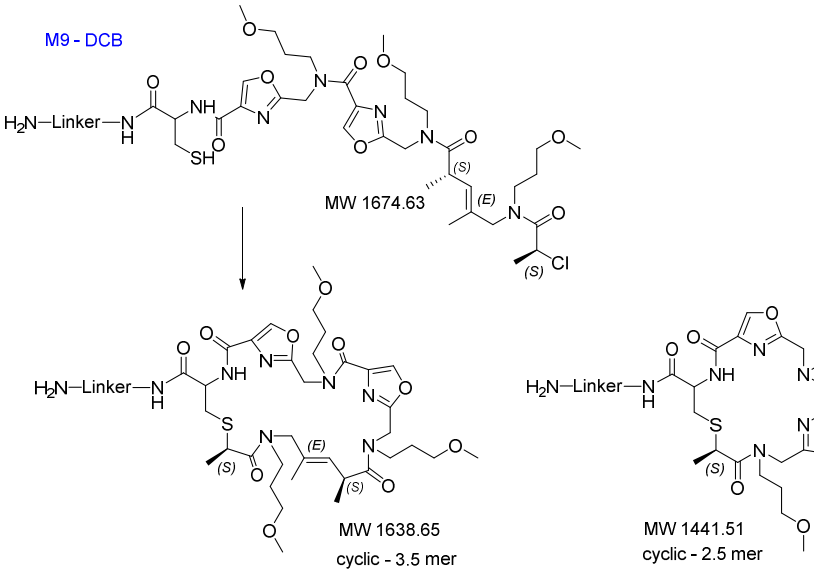
ions	size	MW	RT
cyclic	2.5	1441	7.597
cyclic	3.5	1595	6.650
linear	3.5	1631	7.008

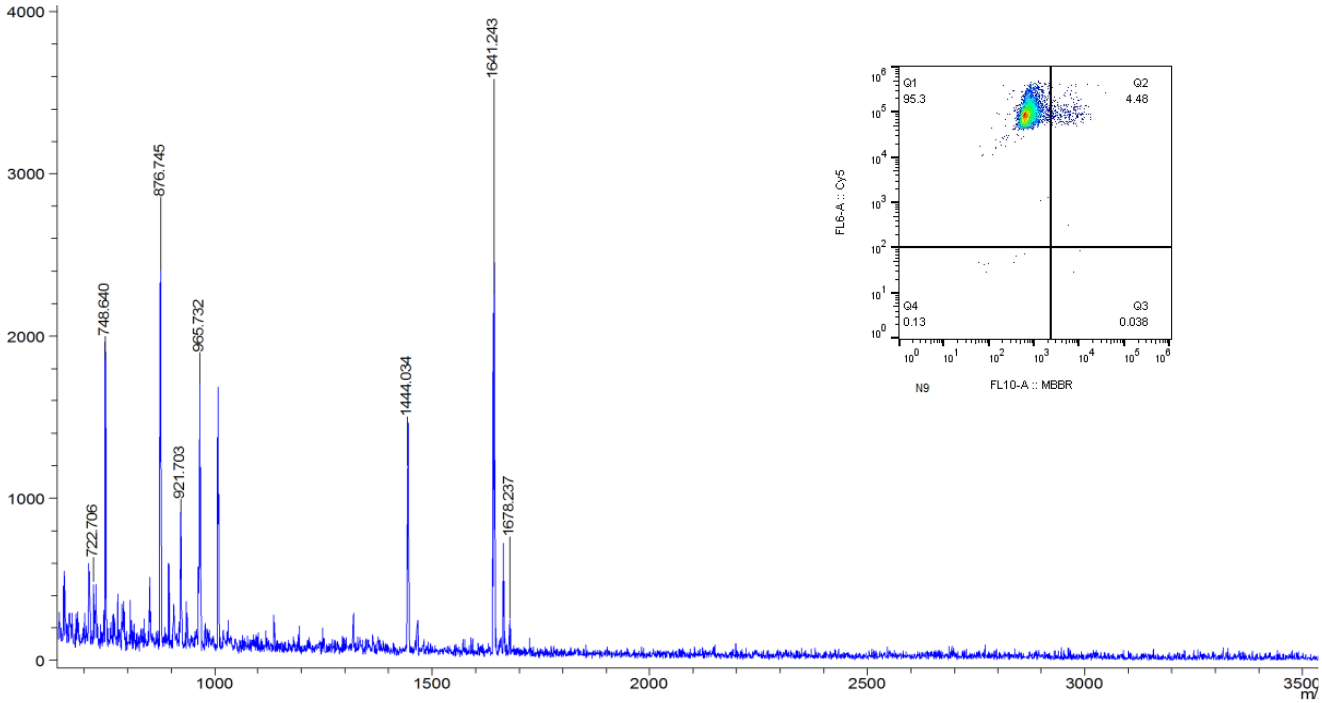


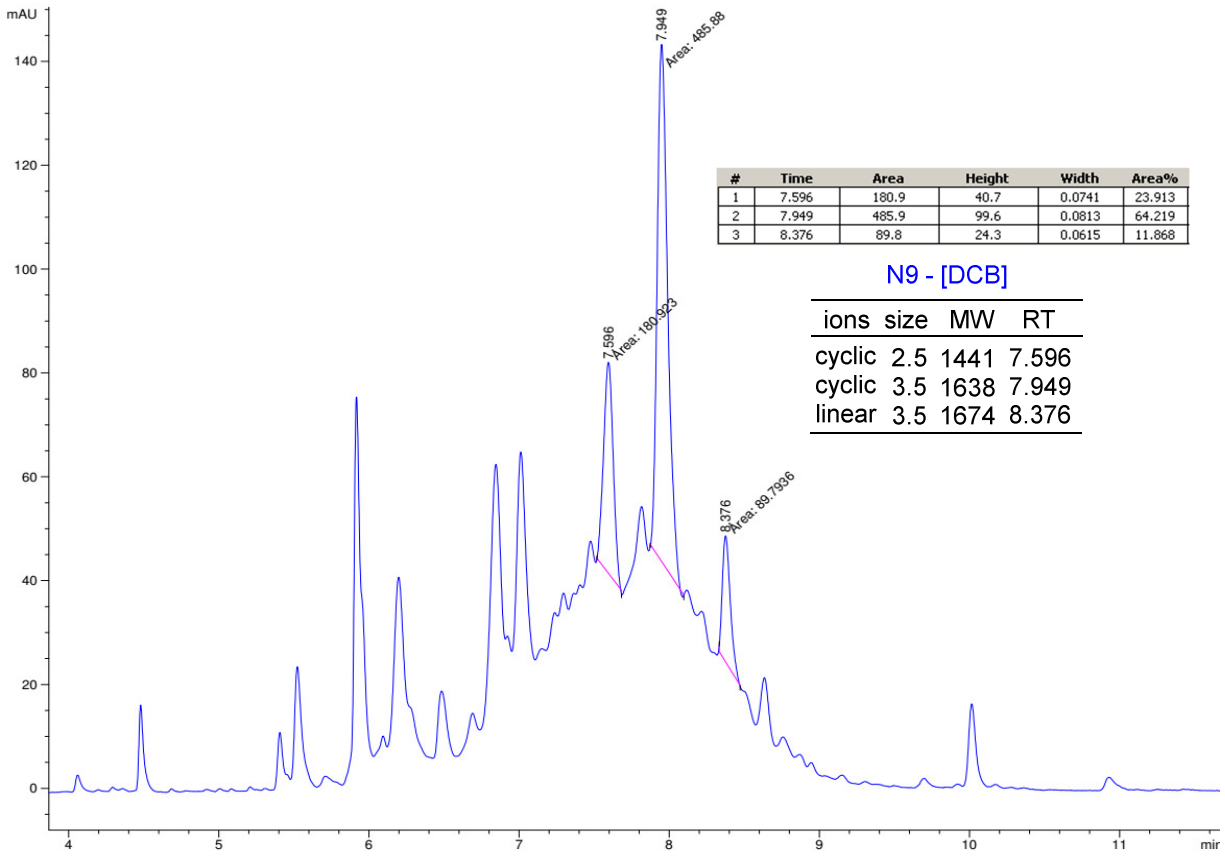

[M+2H]+
Max: 57296
799.7
798.5
799.0
800.5
159.2
167.0
533.0
745.3
1598.5
1597.7
[M+H]+
Exact Mass: 1595.62
DBB - cyclic - 3.5mer
RT - 6.73
100
80
60
40
20
0
500
1000
1500
2000


[M+2H]+
Max: 17328
817.3
816.5
965.0
967.0
545.3
544.1
489.0
921.1
966.1
800.7
843.4
766.8
1051.3
1317.8
1634.0
[M+H]+
Exact Mass: 1631.60
linear - 3.5mer
141.1
166.9
181.0
335.0
324.8
409.9
461.6
468.5
537.2
558.0
579.0
644.6
662.2
1077.3
1283.0
1459.1
1553.2
1699.6
100
80
60
40
20
0
500
1000
1500
2000

N9-[DCB]: Incomplete cyclization on both 10 µm and 160 µm beads, linear starting material was identified in small quantity (MW 1674, RT 8.376).



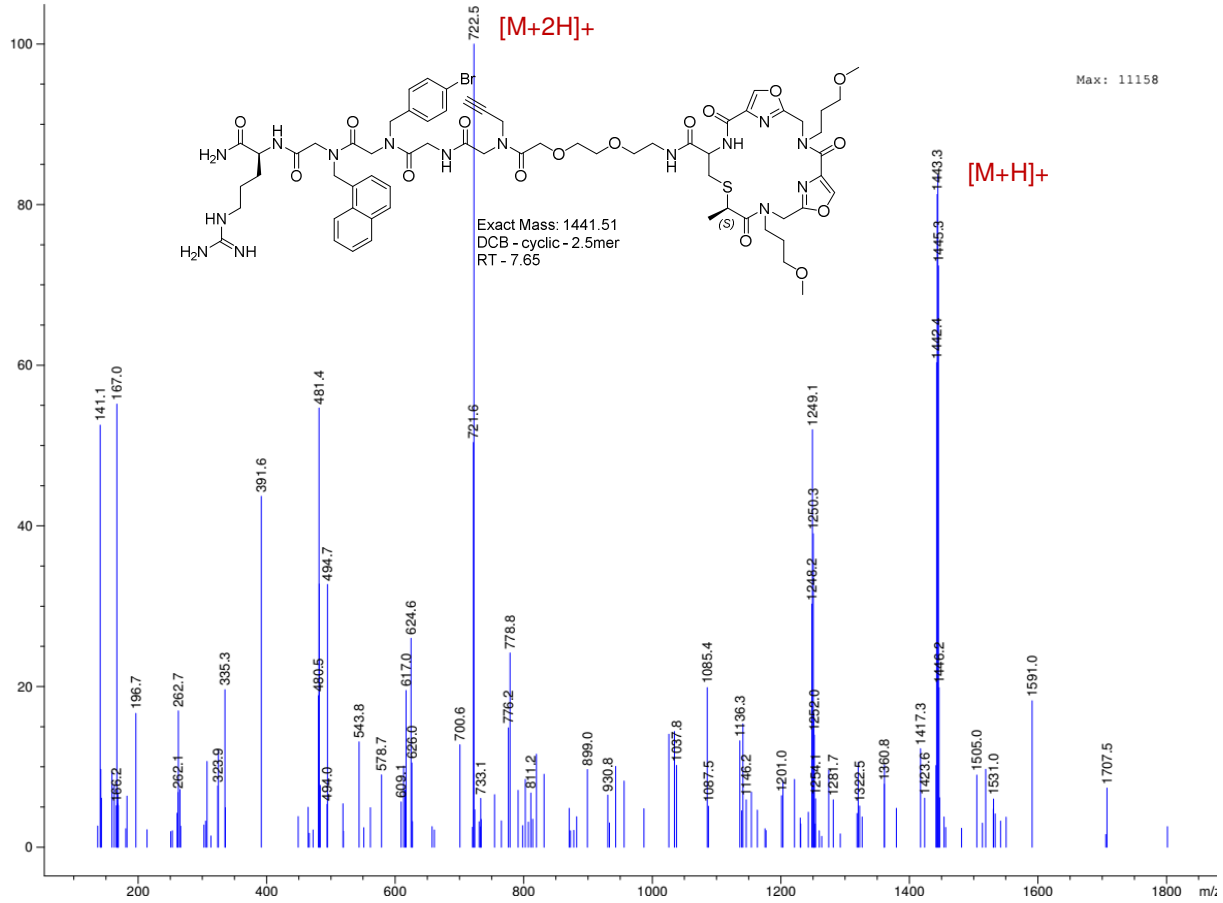


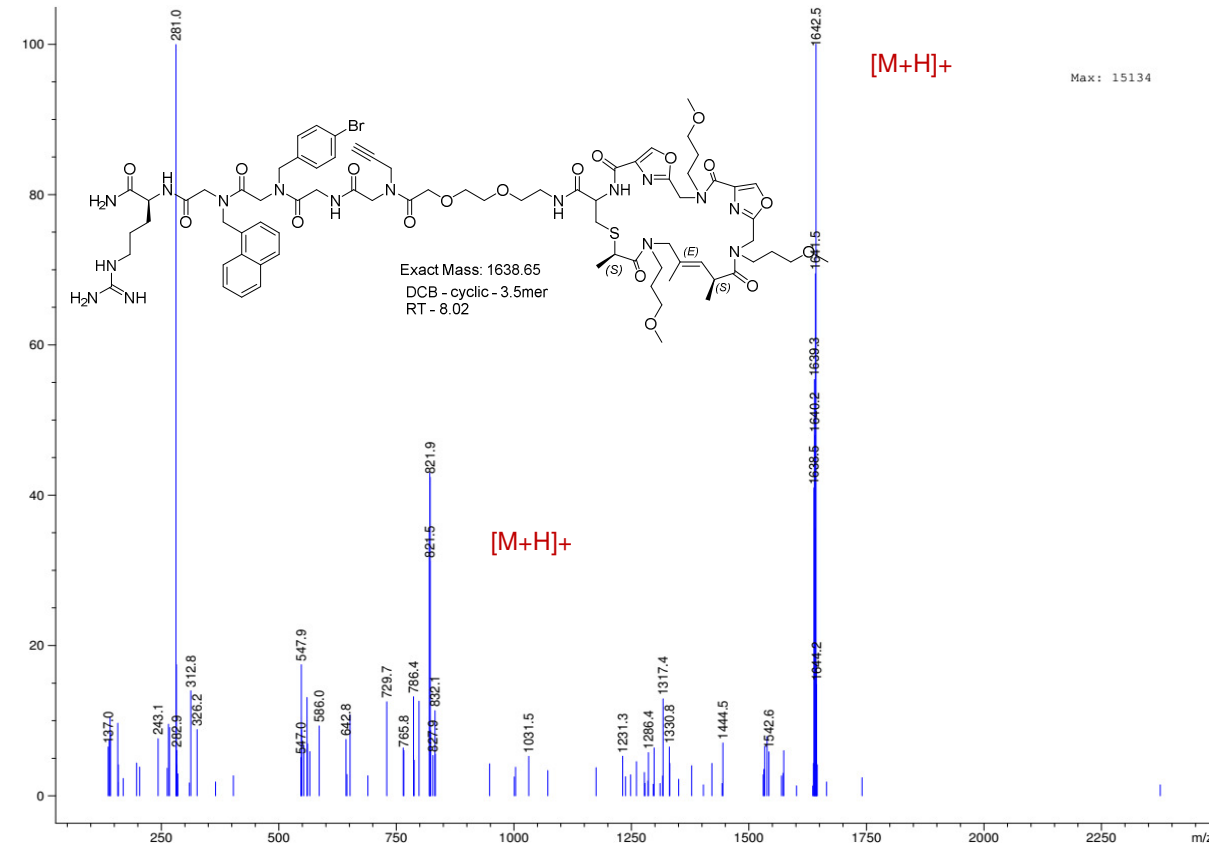


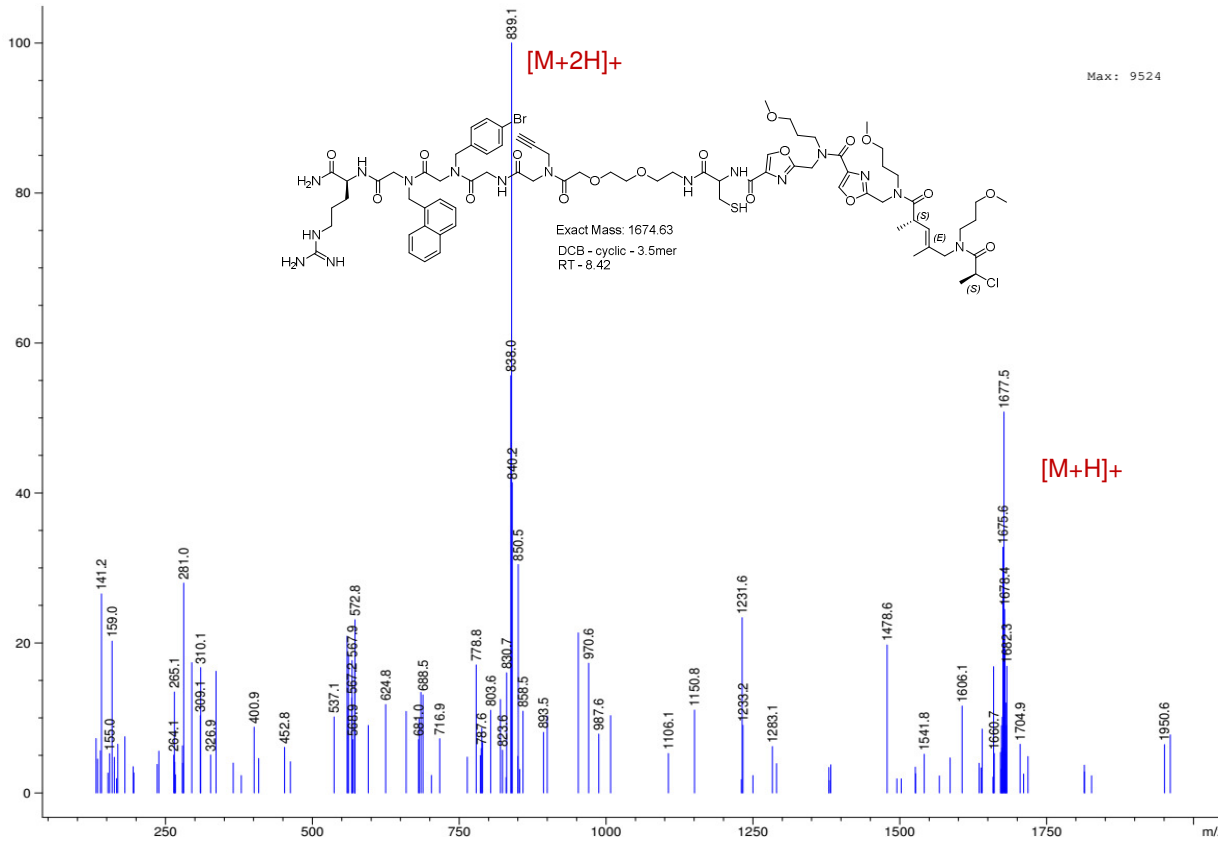
#	Time	Area	Height	Width	Area%
1	7.596	180.9	40.7	0.0741	23.913
2	7.949	485.9	99.6	0.0813	64.219
3	8.376	89.8	24.3	0.0615	11.868

N9 - [DCB]

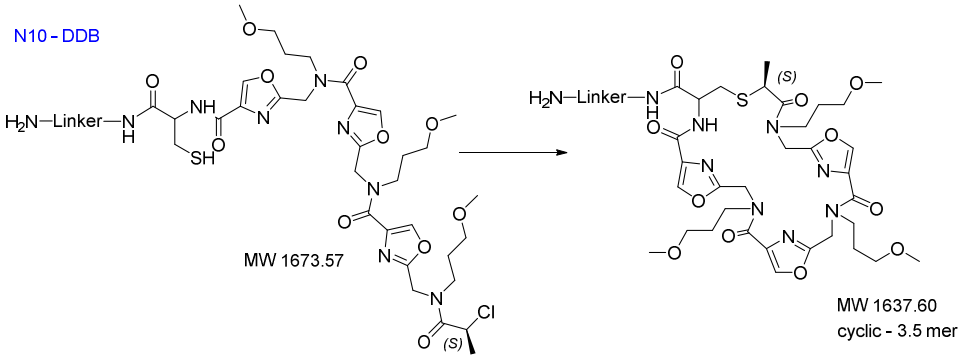
ions	size	MW	RT
cyclic	2.5	1441	7.596
cyclic	3.5	1638	7.949
linear	3.5	1674	8.376

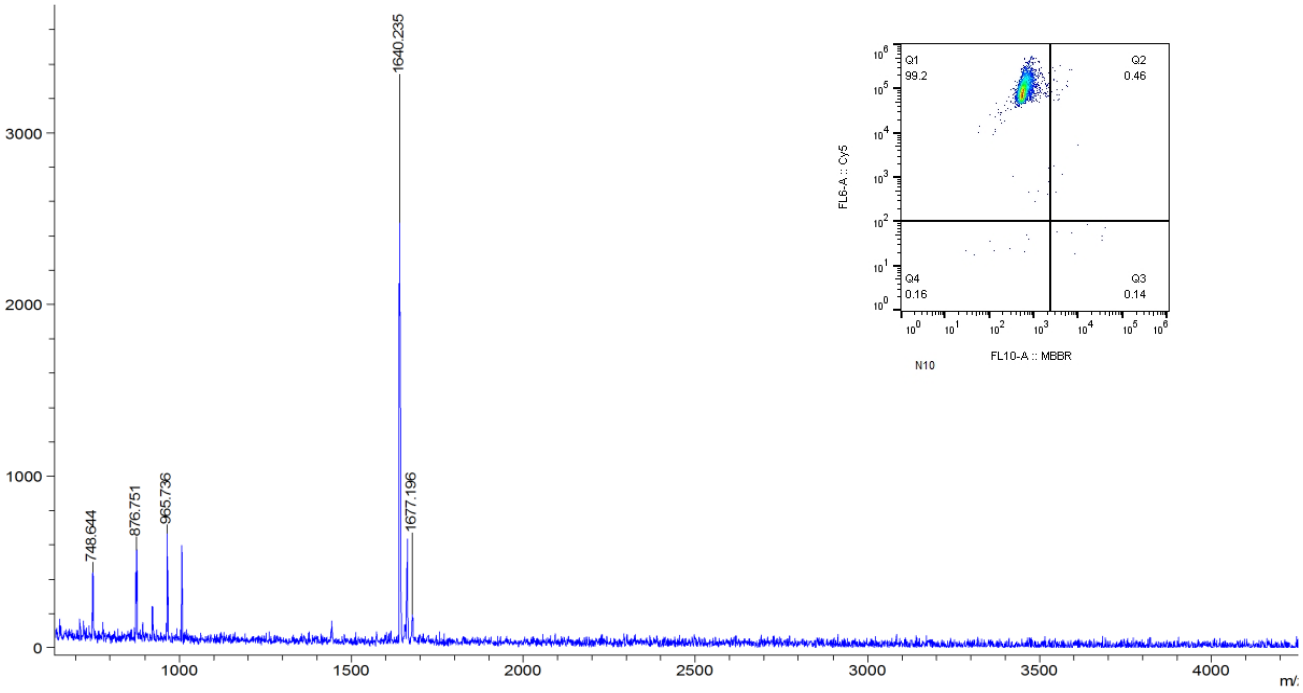


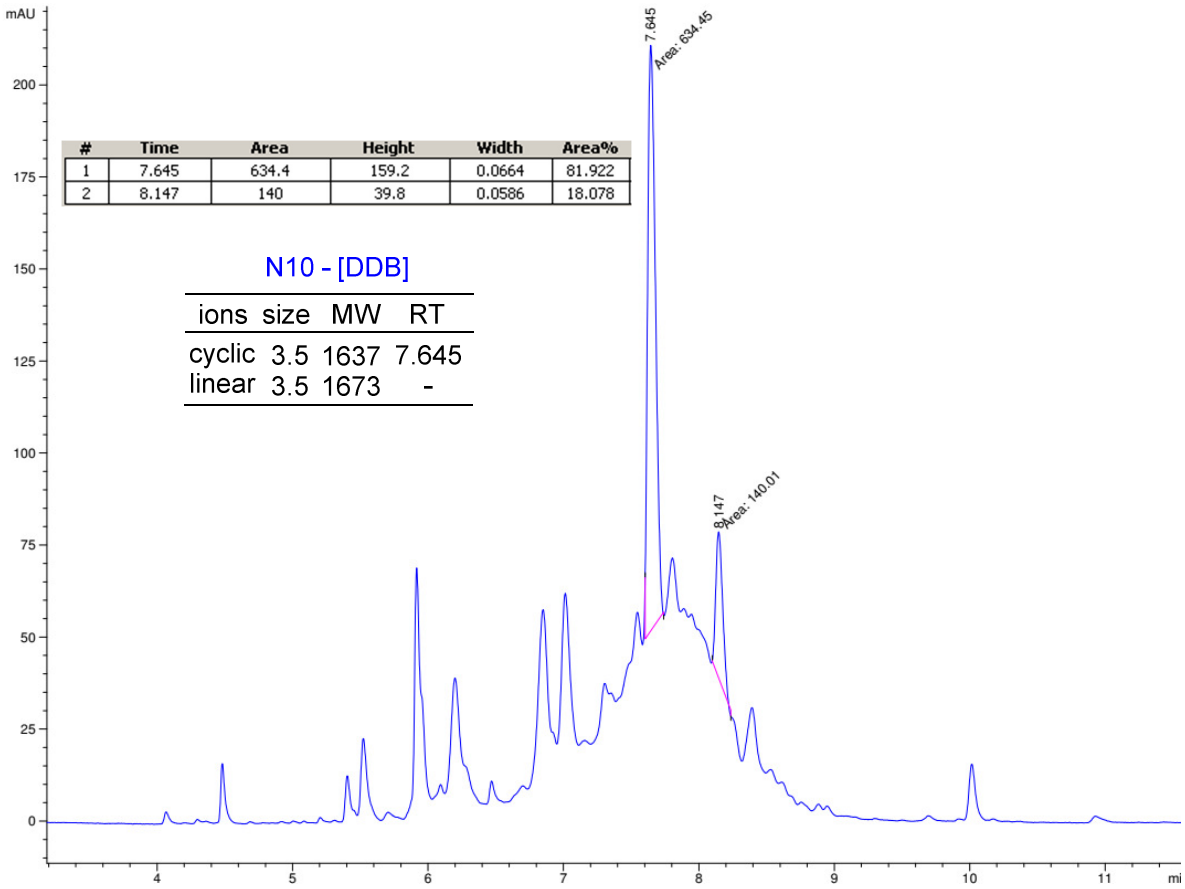

[M+H]+
Max: 15134
Exact Mass: 1638.65
DCB - cyclic - 3.5mer
RT - 8.02
[M+H]+
m/z


[M+2H]+
Max: 9524
Exact Mass: 1674.63
DCB - cyclic - 3.5mer
RT - 8.42
[M+H]+
m/z

N10-[DDB]: Cyclization was complete on both 10 µm & 160 µm beads.



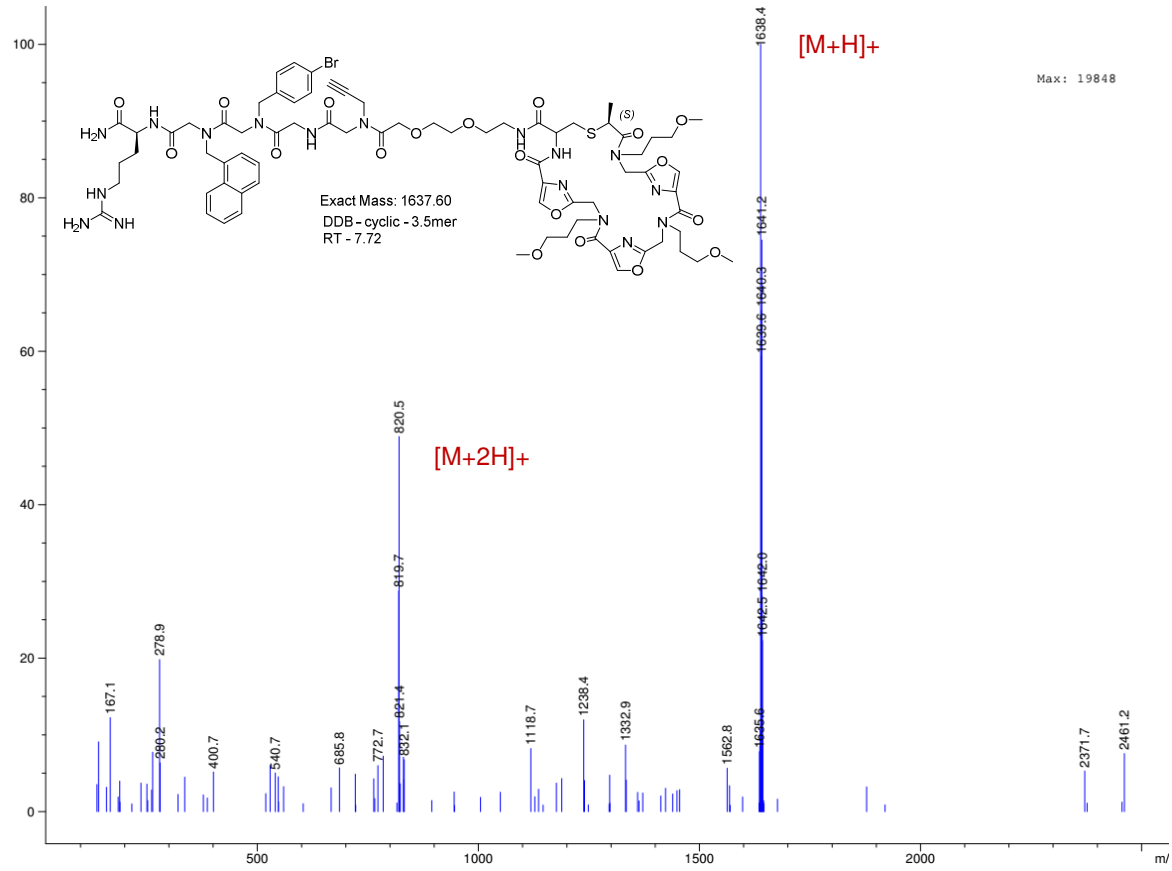




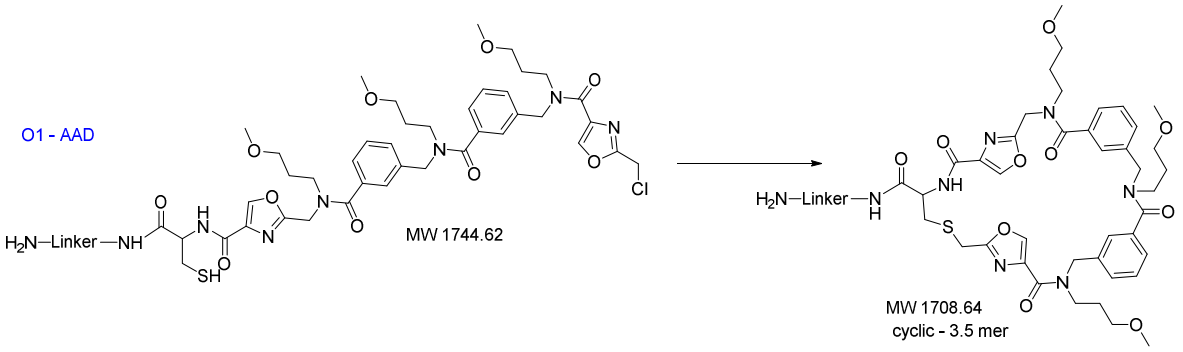
#	Time	Area	Height	Width	Area%
1	7.645	634.4	159.2	0.0664	81.922
2	8.147	140	39.8	0.0586	18.078

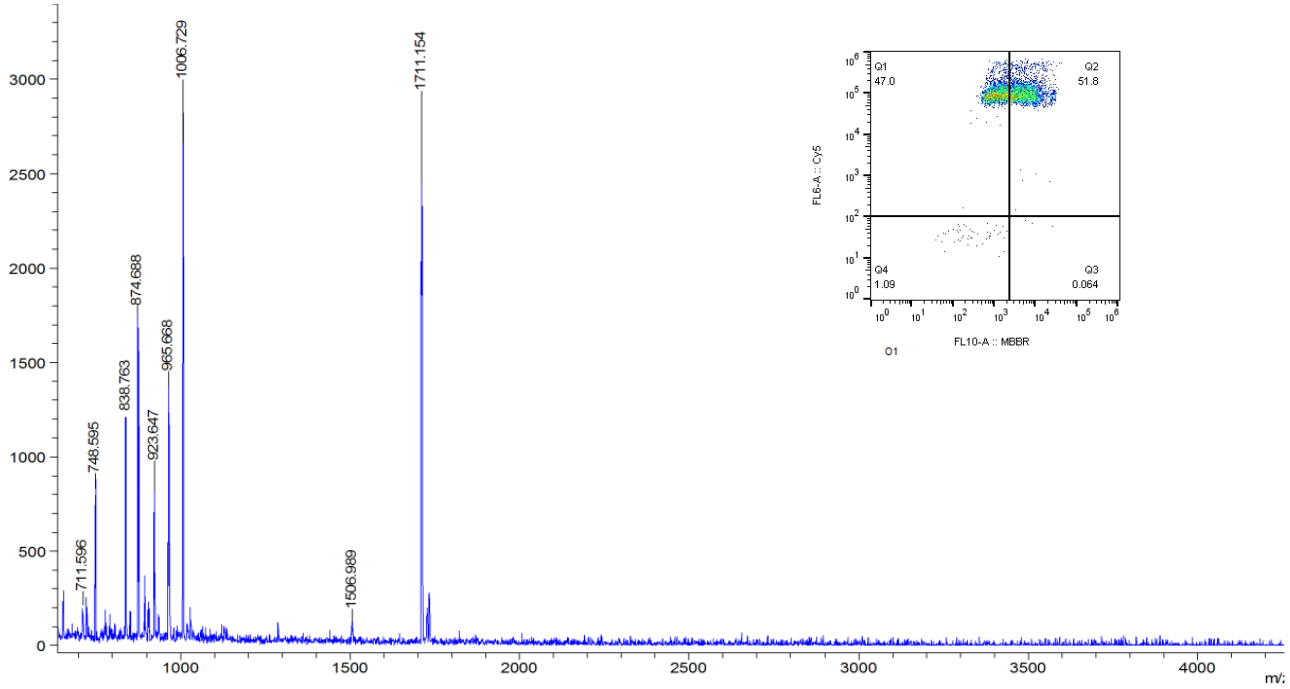
N10 - [DDB]

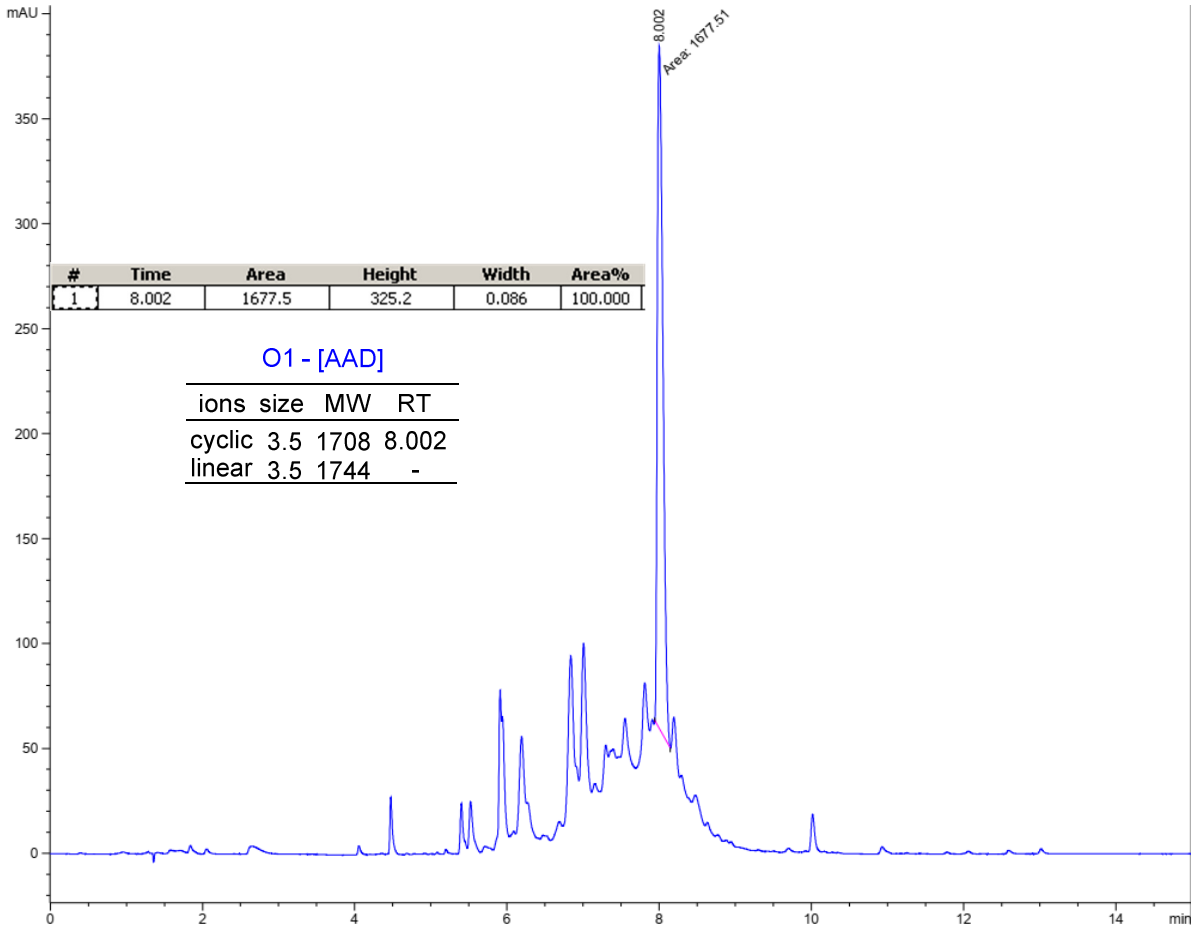
ions	size	MW	RT
cyclic	3.5	1637	7.645
linear	3.5	1673	-

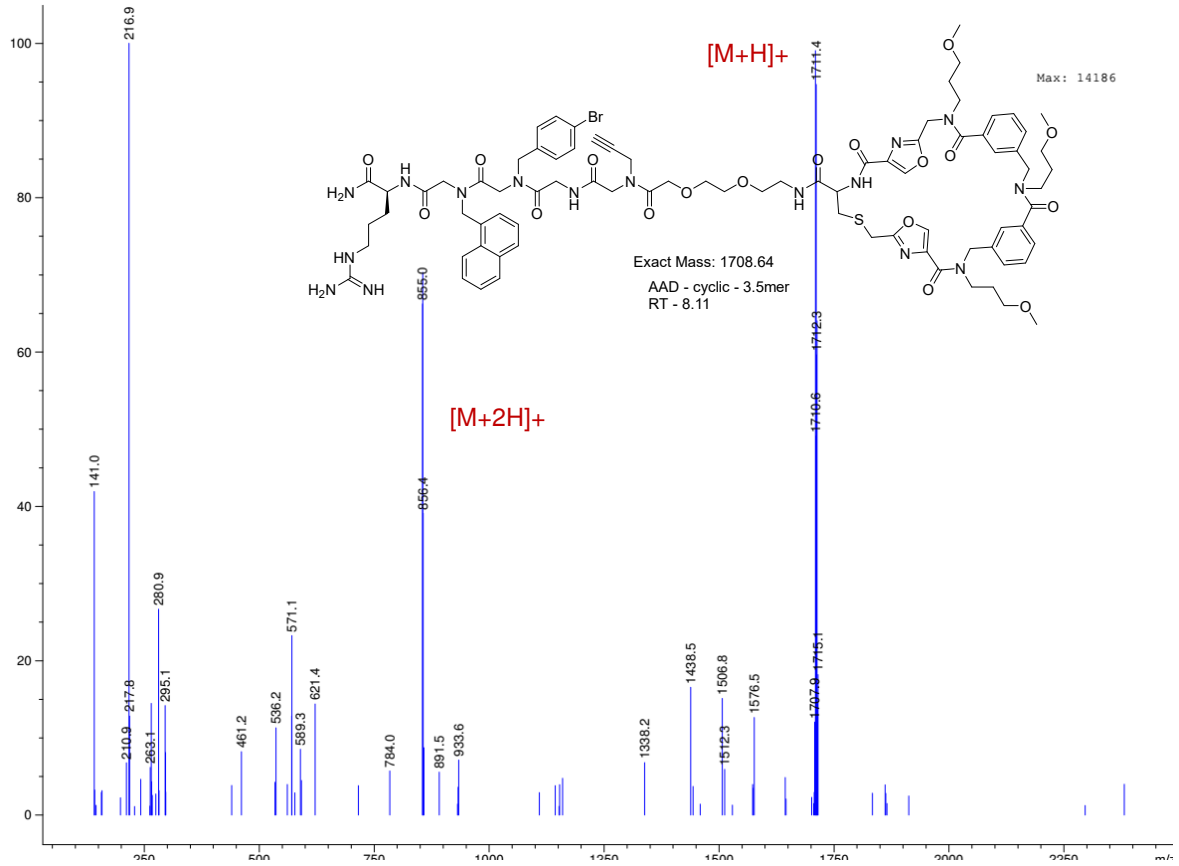


O1-[AAD]: Incomplete cyclization was detected on 10 µm but was complete on 160 µm beads.

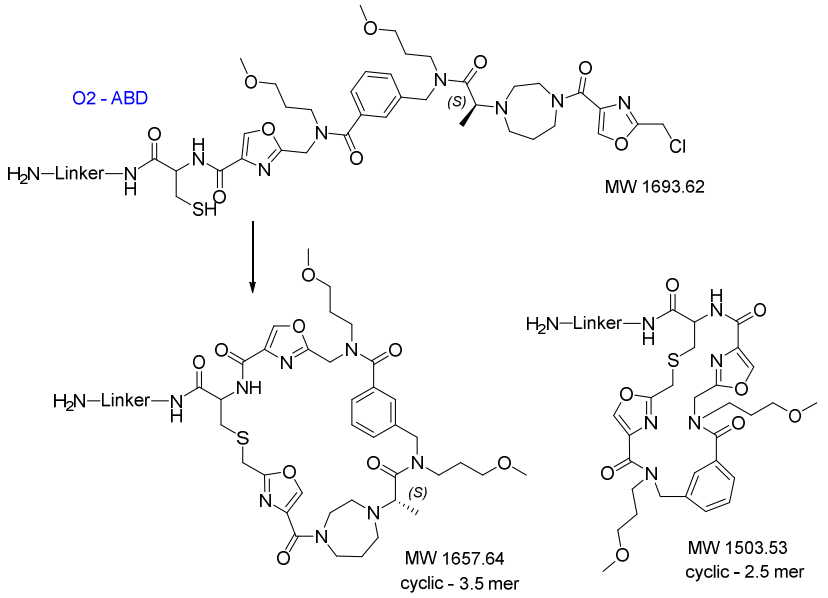


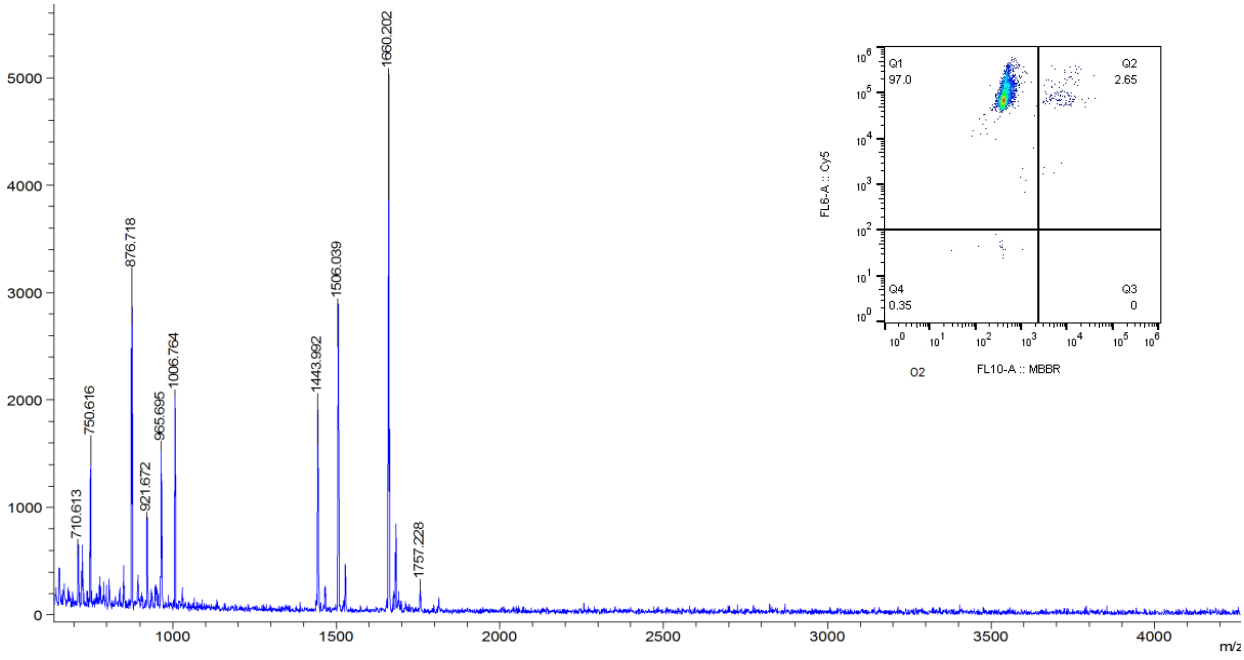


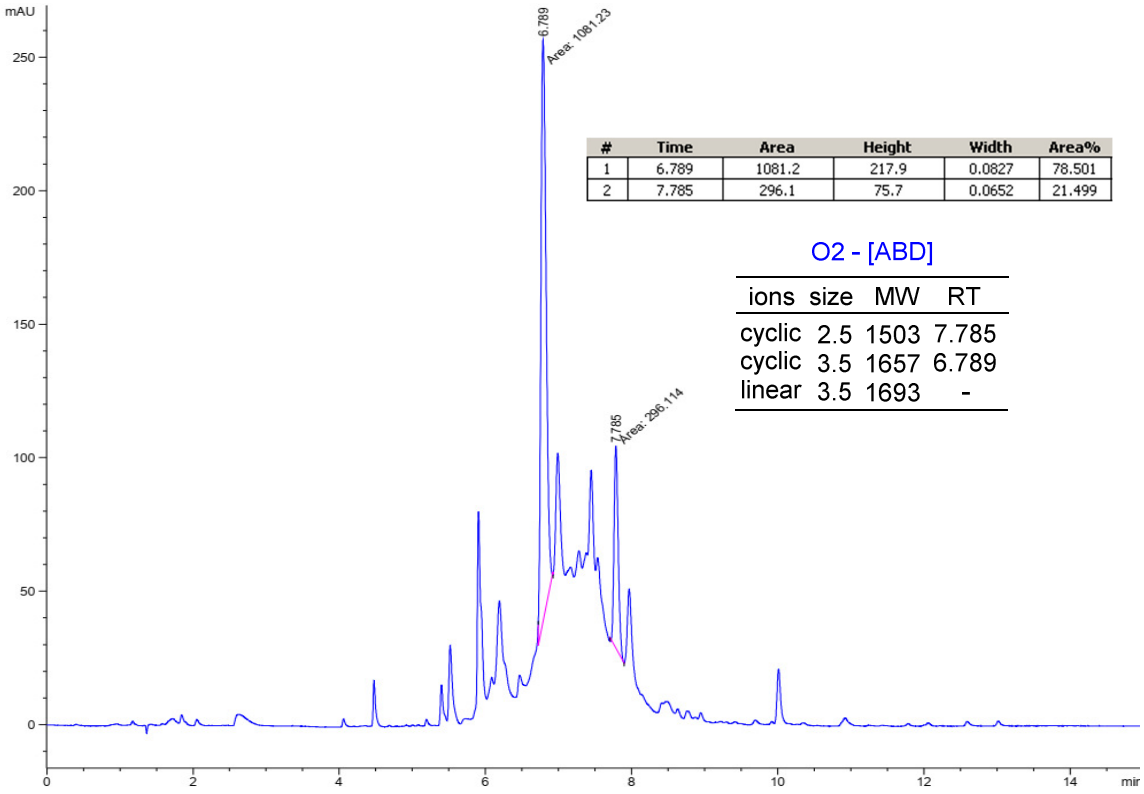

mAU
8.002
Area: 1677.51
Time Area Height Width Area%
1 8.002 1677.5 325.2 0.086 100.000
O1 - [AAD]
ions size MW RT
cyclic 3.5 1708 8.002
linear 3.5 1744 -
min


[M+H]+
[M+2H]+
Exact Mass: 1708.64
AAD - cyclic - 3.5mer
RT - 8.11
Max: 14186

O2-[ABD]: Cyclization was complete on both 10 µm & 160 µm.



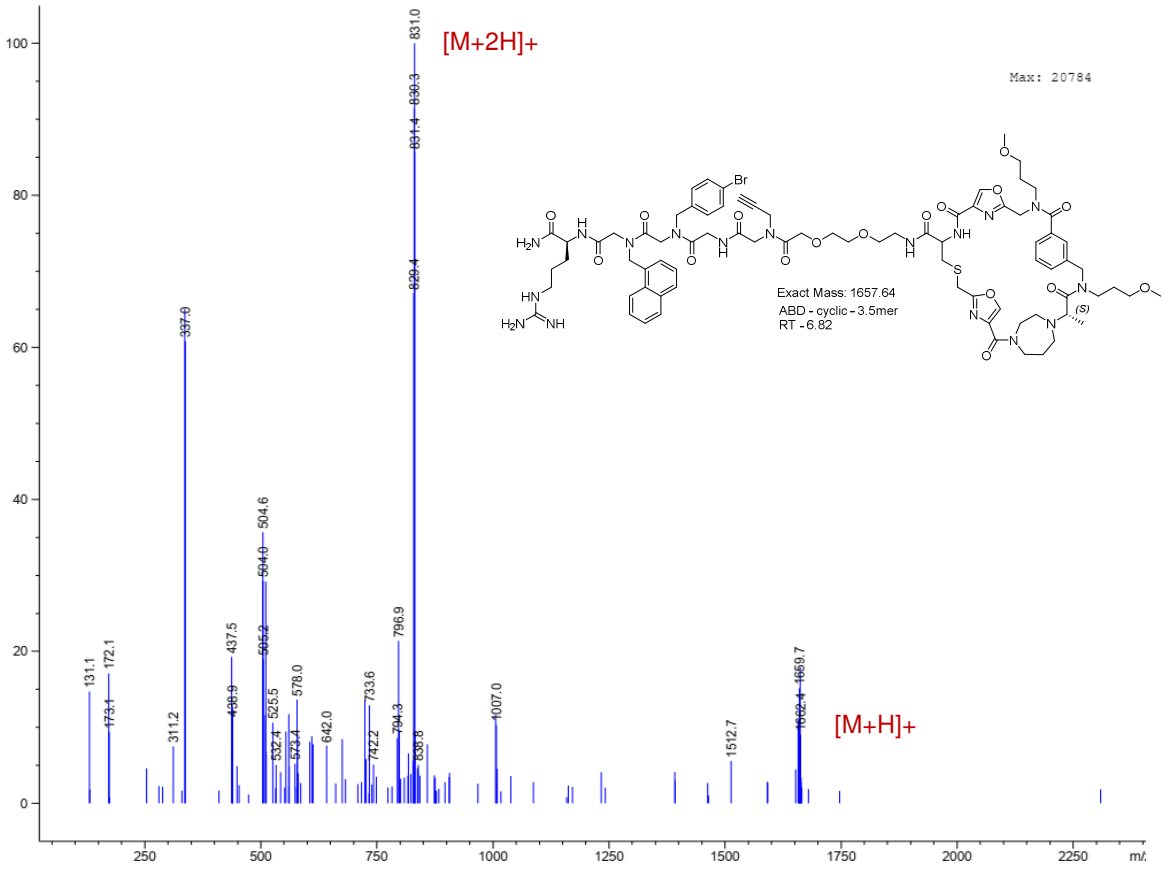


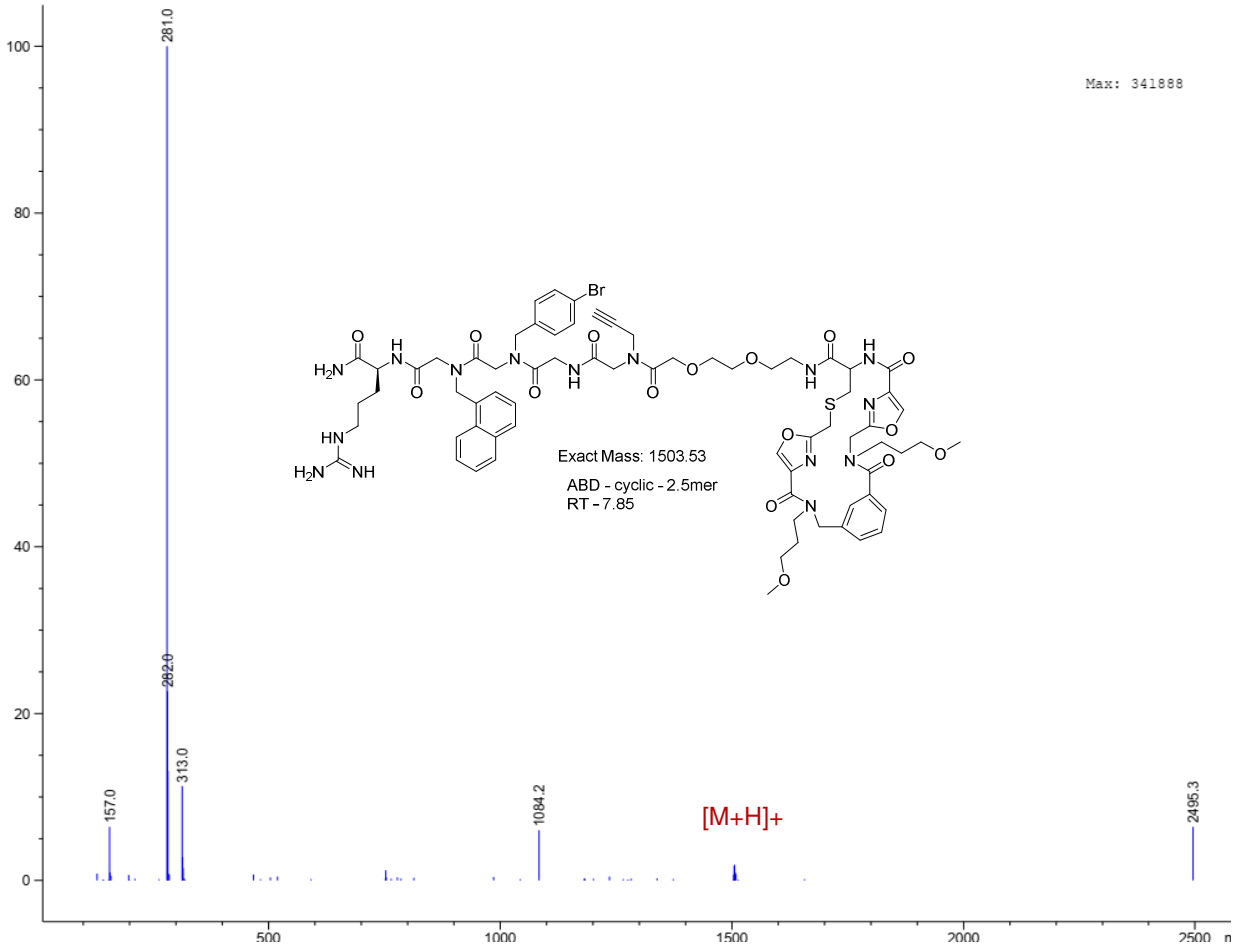


#	Time	Area	Height	Width	Area%
1	6.789	1081.2	217.9	0.0827	78.501
2	7.785	296.1	75.7	0.0652	21.499

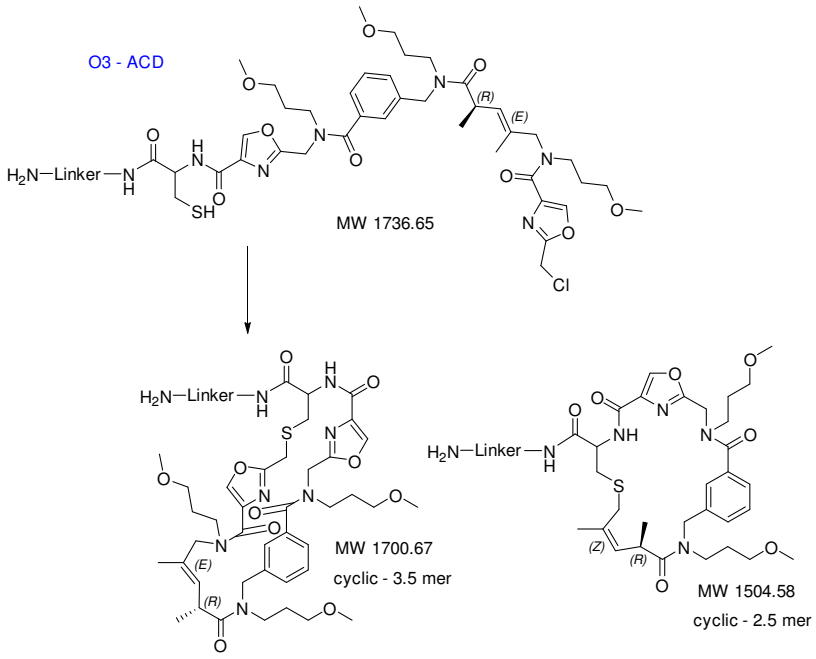
O2 - [ABD]

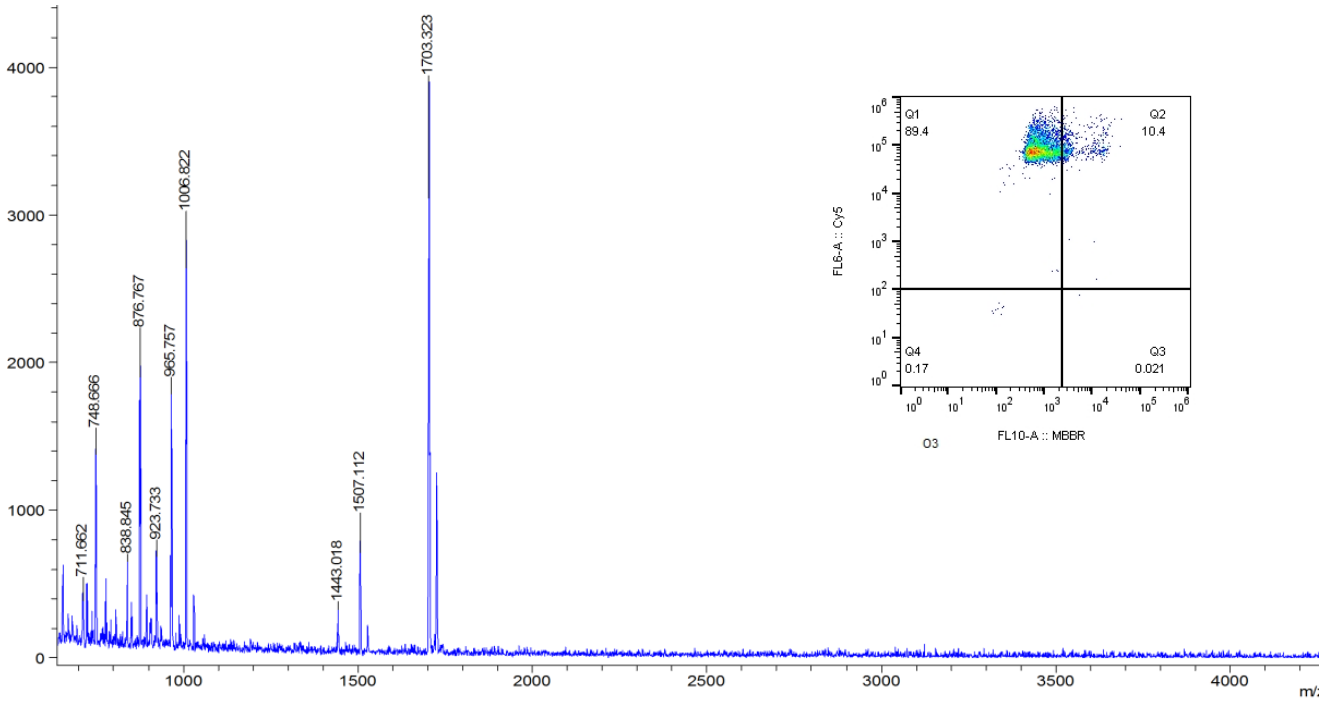
ions	size	MW	RT
cyclic	2.5	1503	7.785
cyclic	3.5	1657	6.789
linear	3.5	1693	-

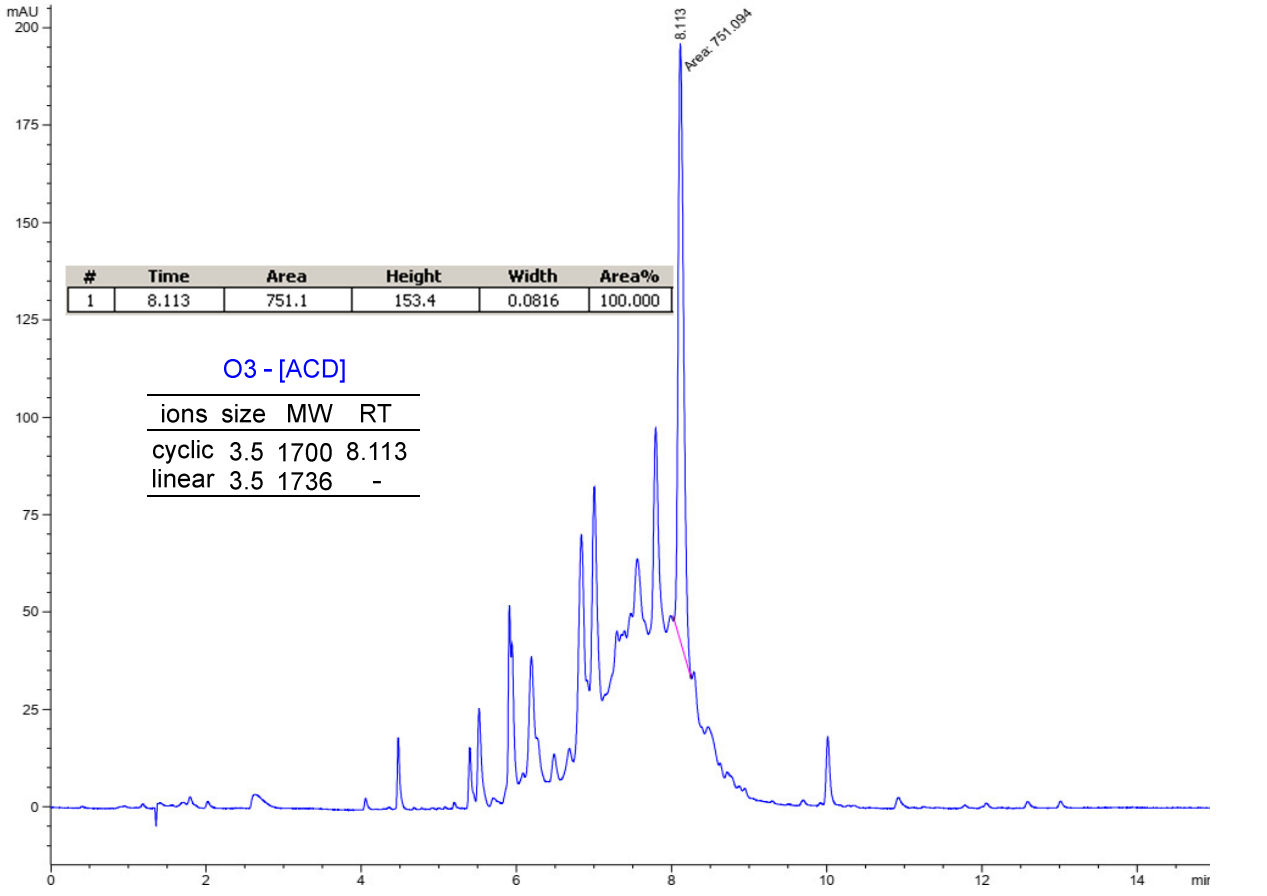




O3-[ACD]: Incomplete cyclization was detected on 10 µm but was complete on 160 µm beads.



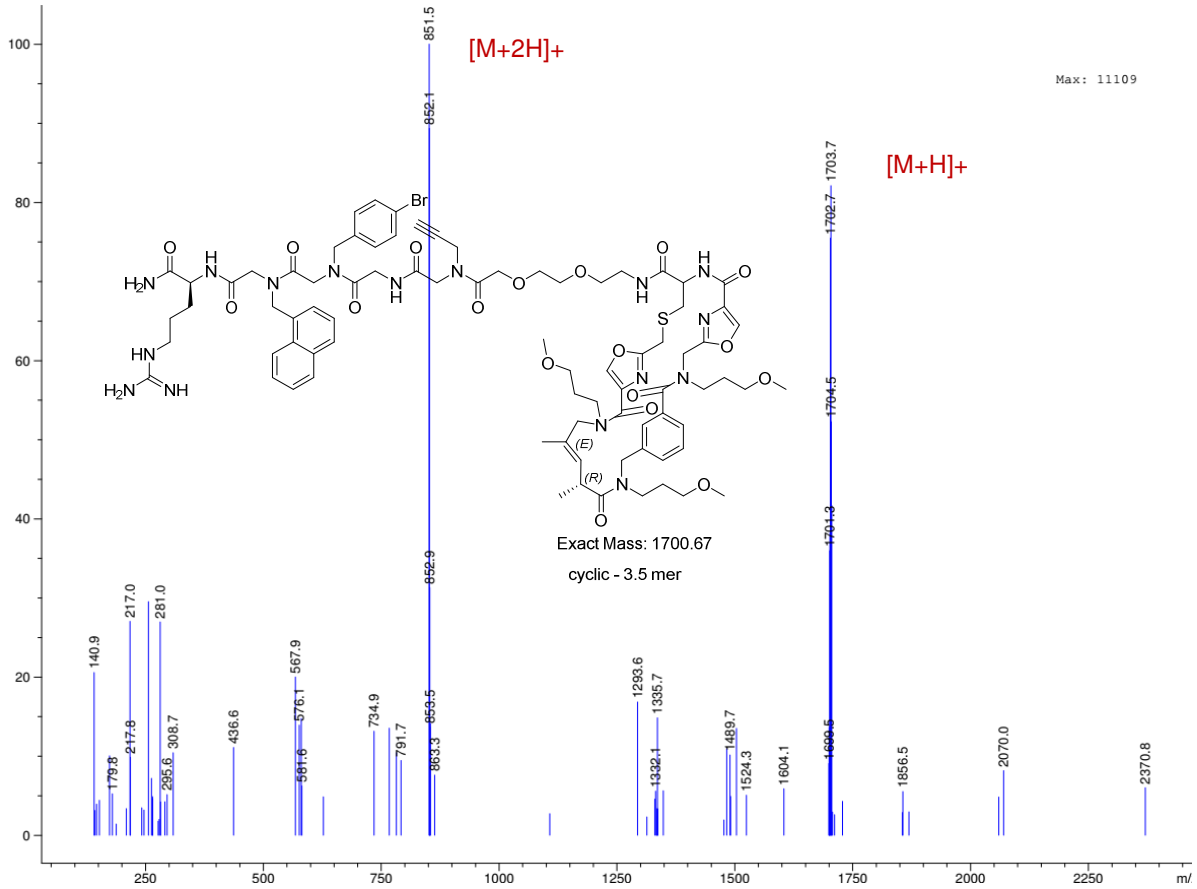




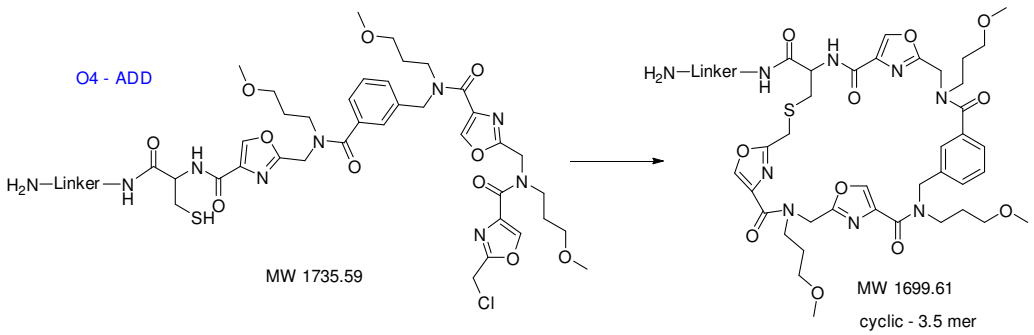
#	Time	Area	Height	Width	Area%
1	8.113	751.1	153.4	0.0816	100.000

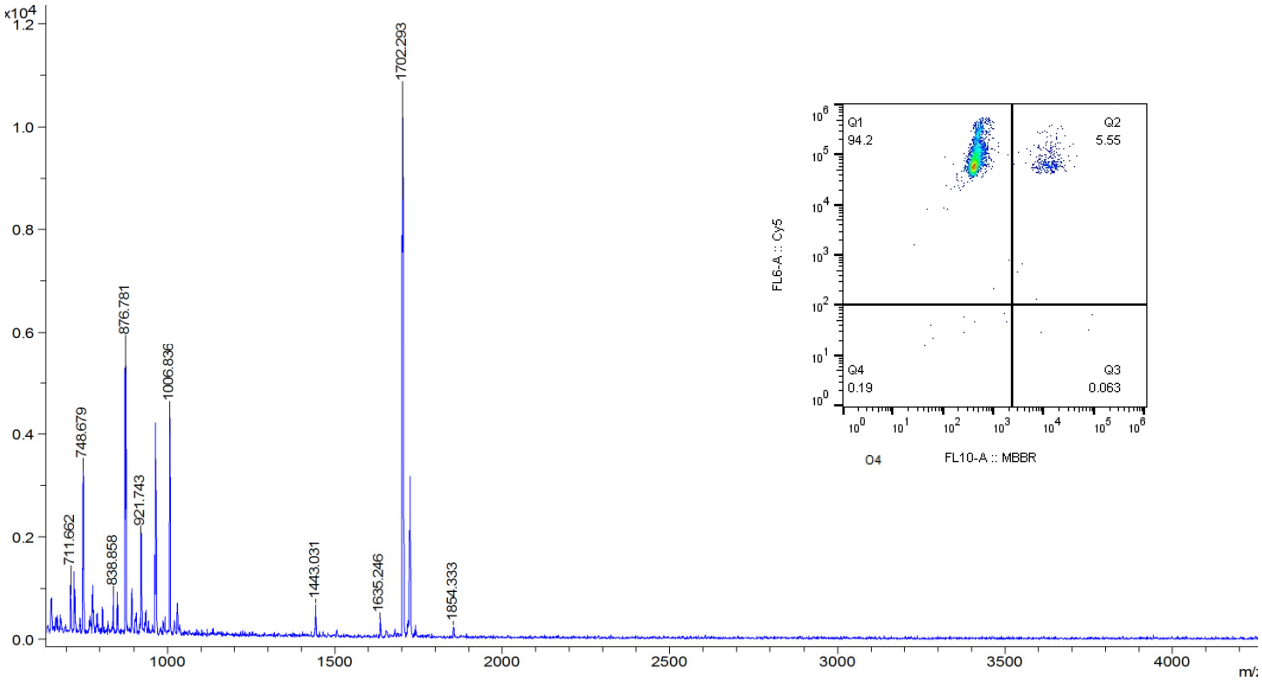
O3 - [ACD]

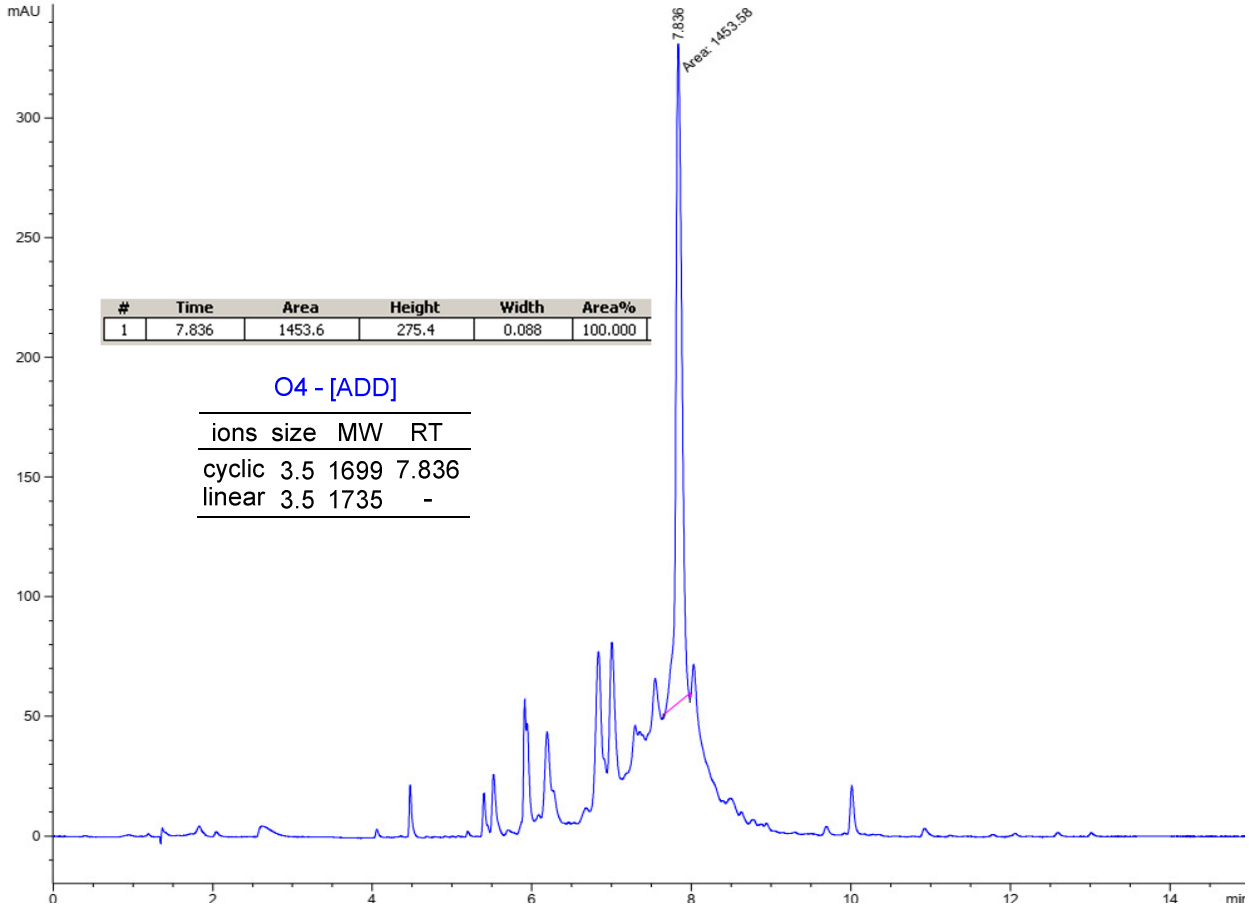
ions	size	MW	RT
cyclic	3.5	1700	8.113
linear	3.5	1736	-



O4-[ADD]: Cyclization was complete on both 10 µm & 160 µm beads.



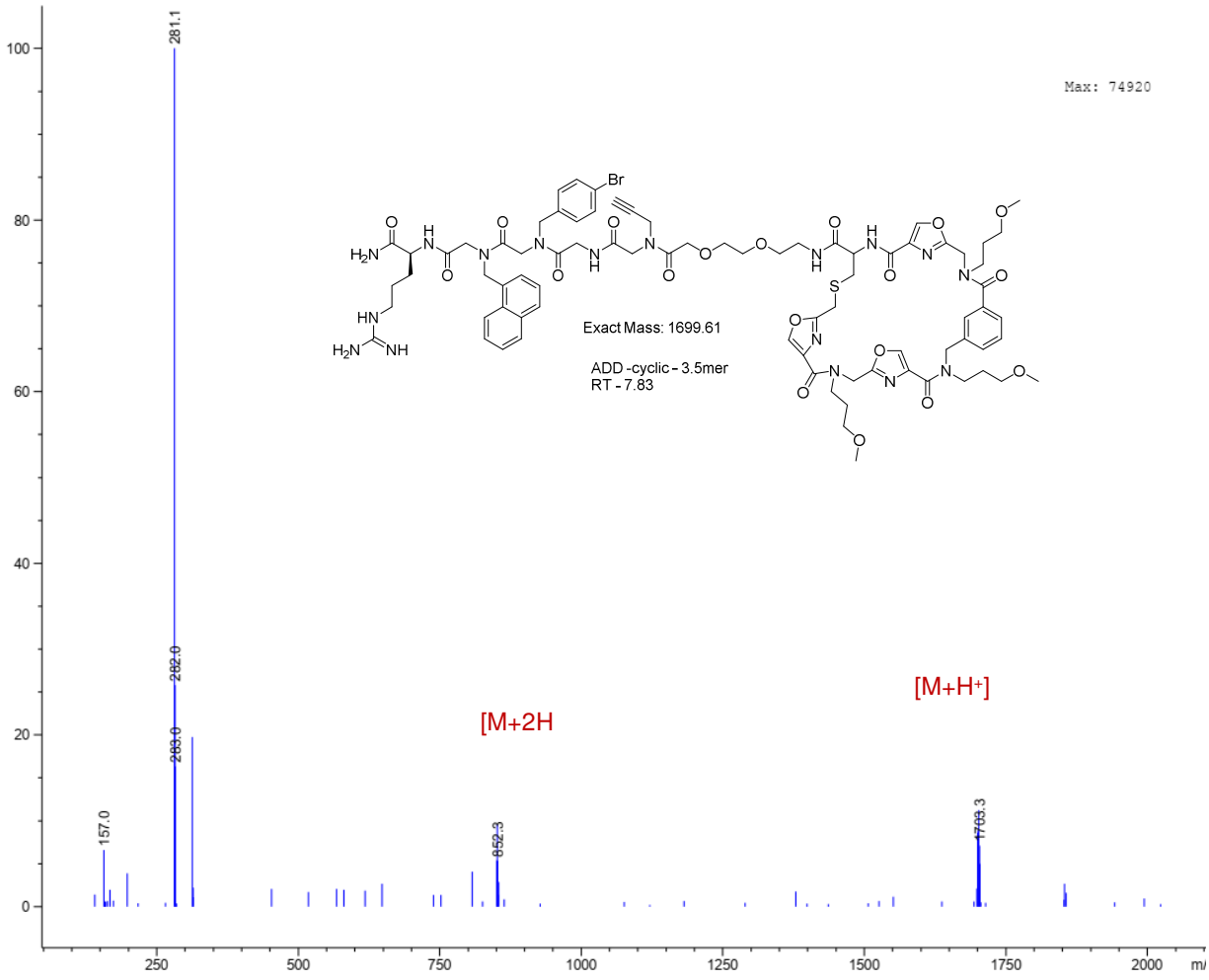




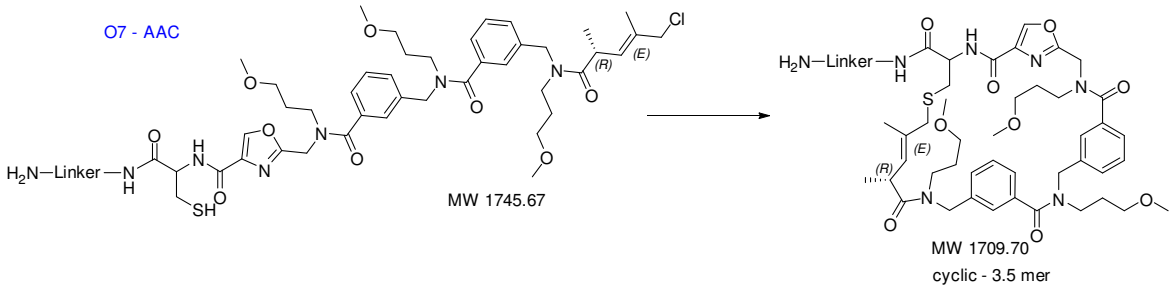
#	Time	Area	Height	Width	Area%
1	7.836	1453.6	275.4	0.088	100.000

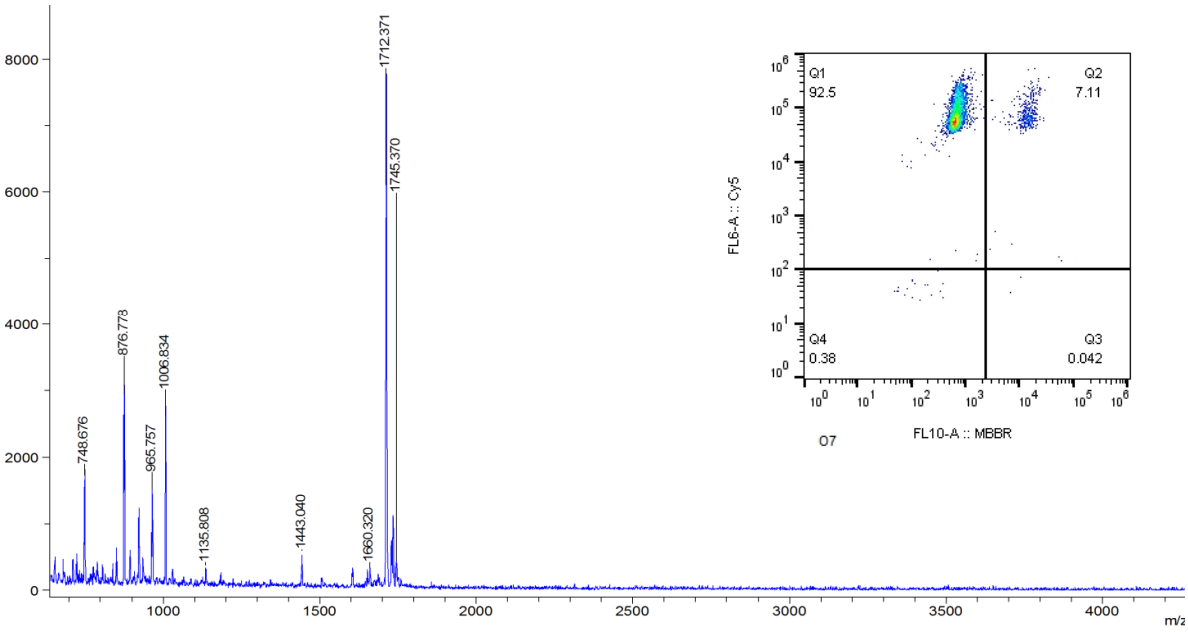
O4 - [ADD]

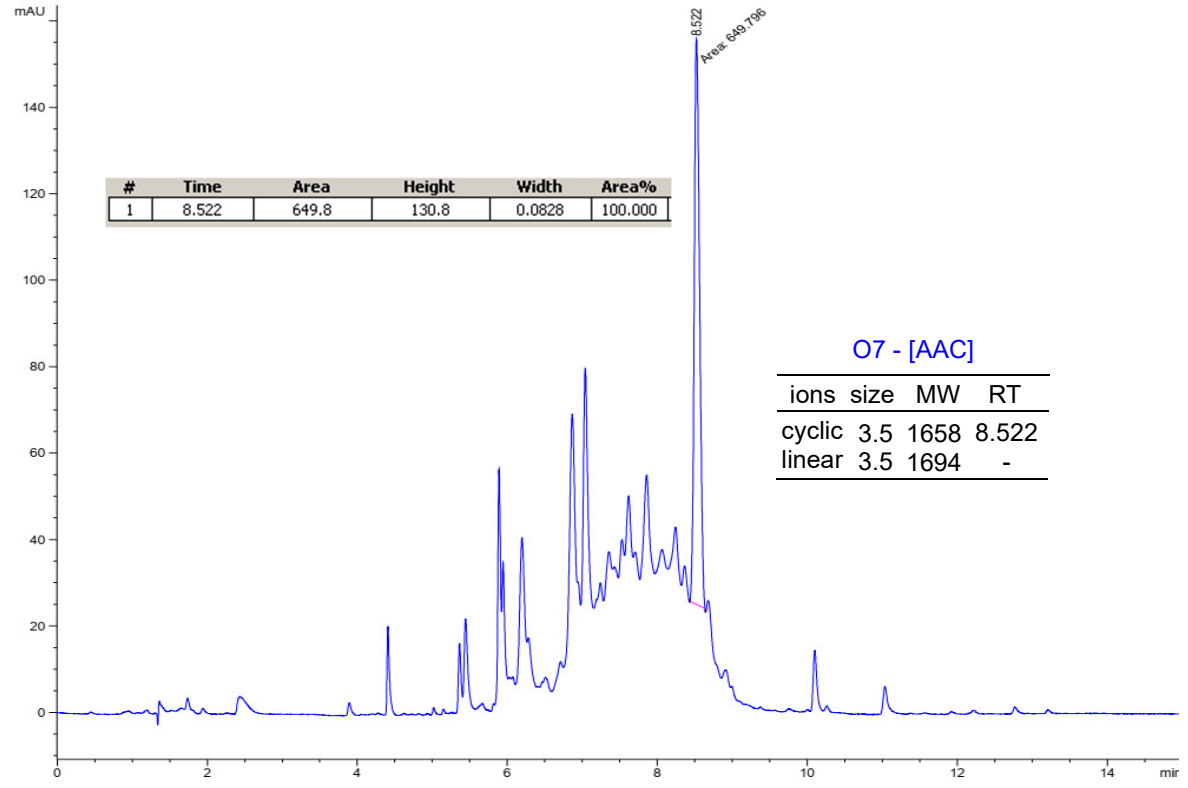
ions	size	MW	RT
cyclic	3.5	1699	7.836
linear	3.5	1735	-



O7-[AAC]: Cyclization was complete on both 10 µm & 160 µm beads.



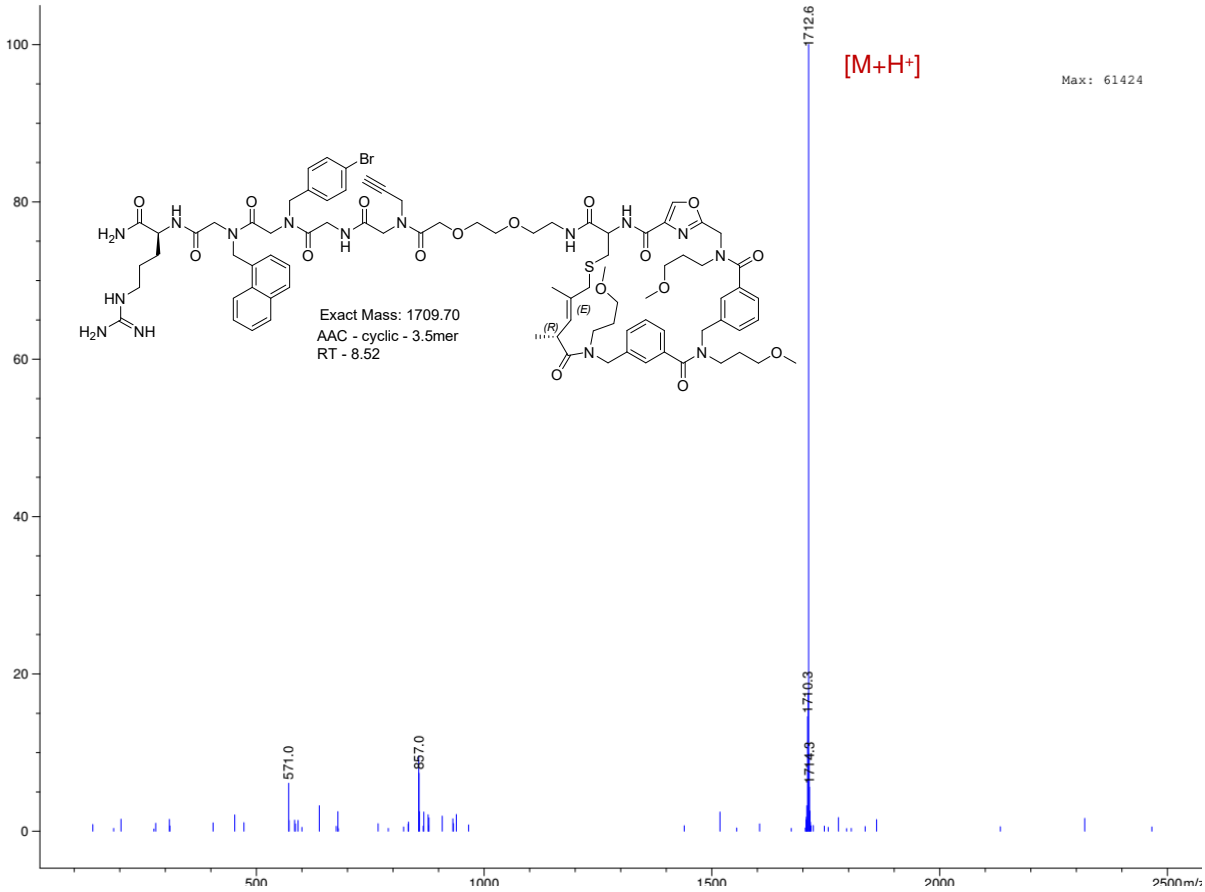




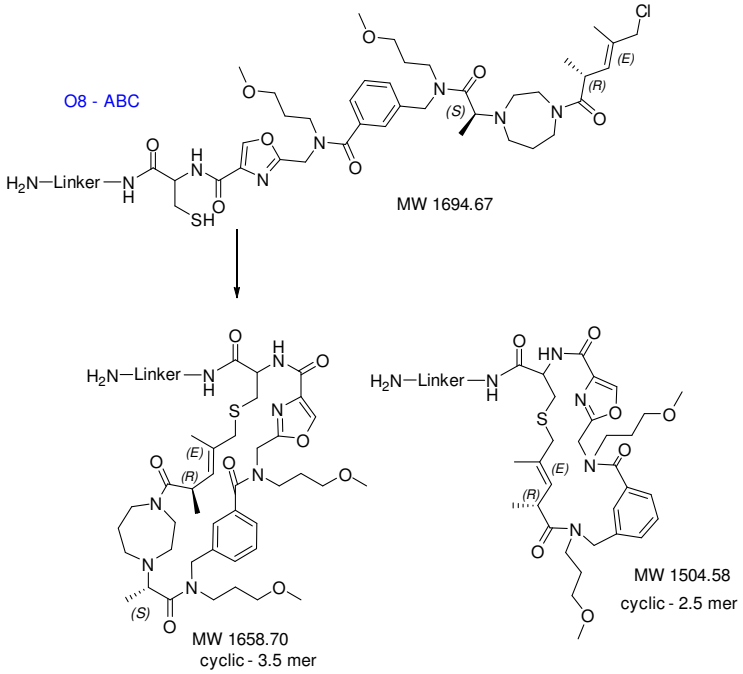
#	Time	Area	Height	Width	Area%
1	8.522	649.8	130.8	0.0828	100.000

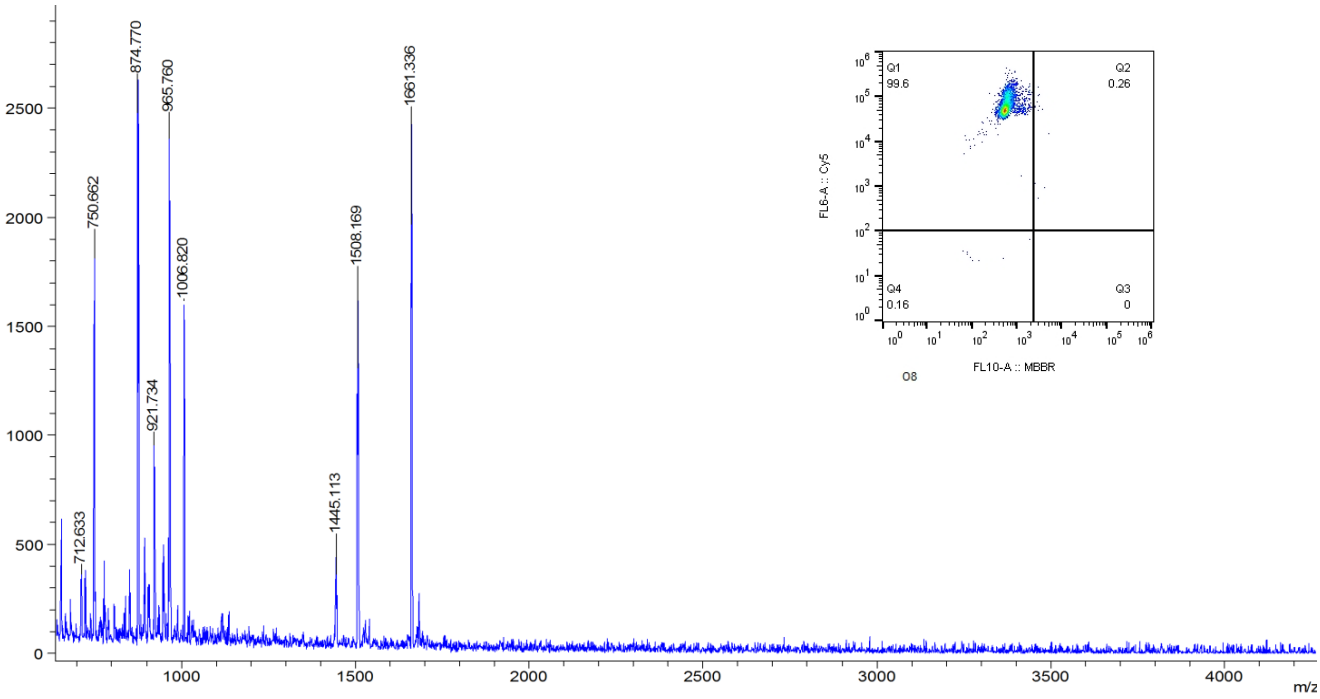
O7 - [AAC]

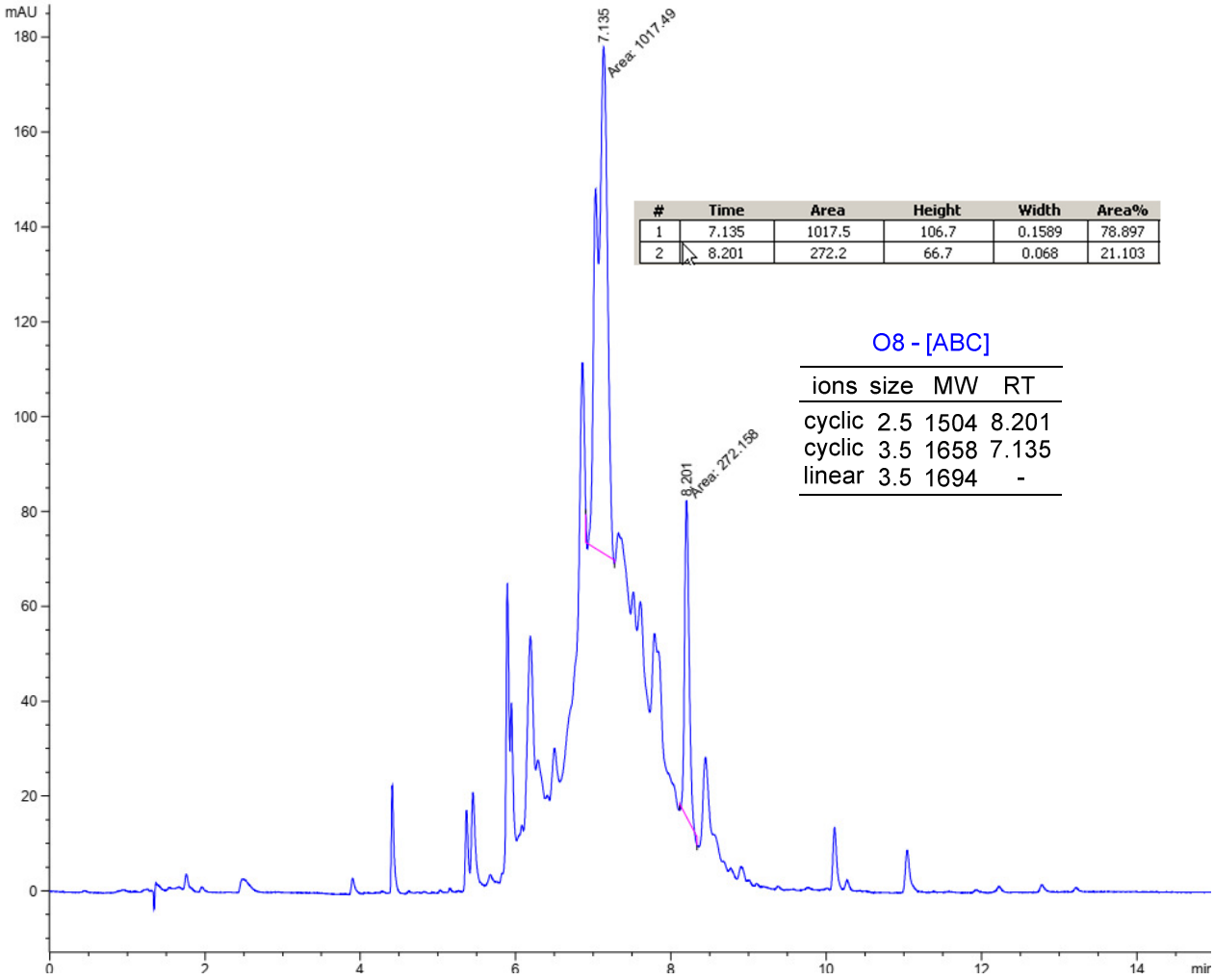
ions	size	MW	RT
cyclic	3.5	1658	8.522
linear	3.5	1694	-



O8-[ABC]: Cyclization was complete on both 10 µm & 160 µm beads.



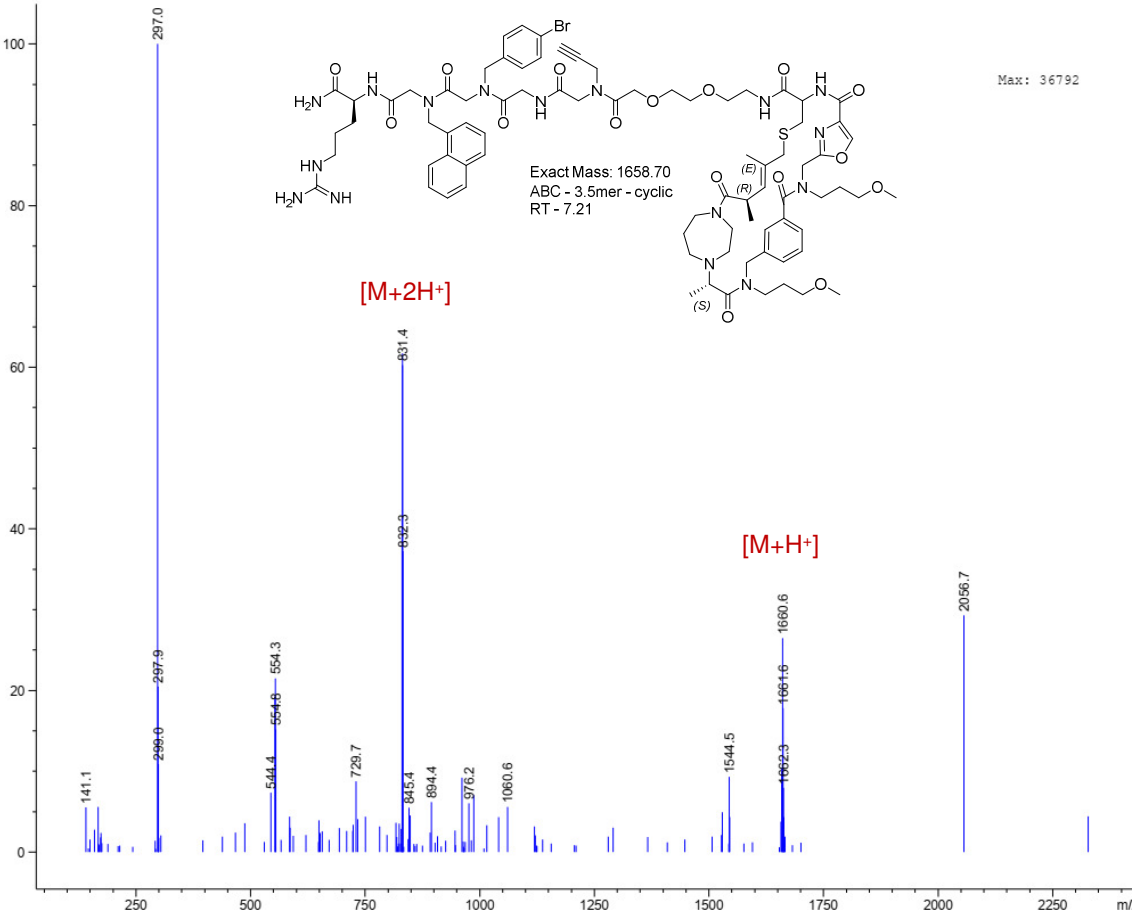


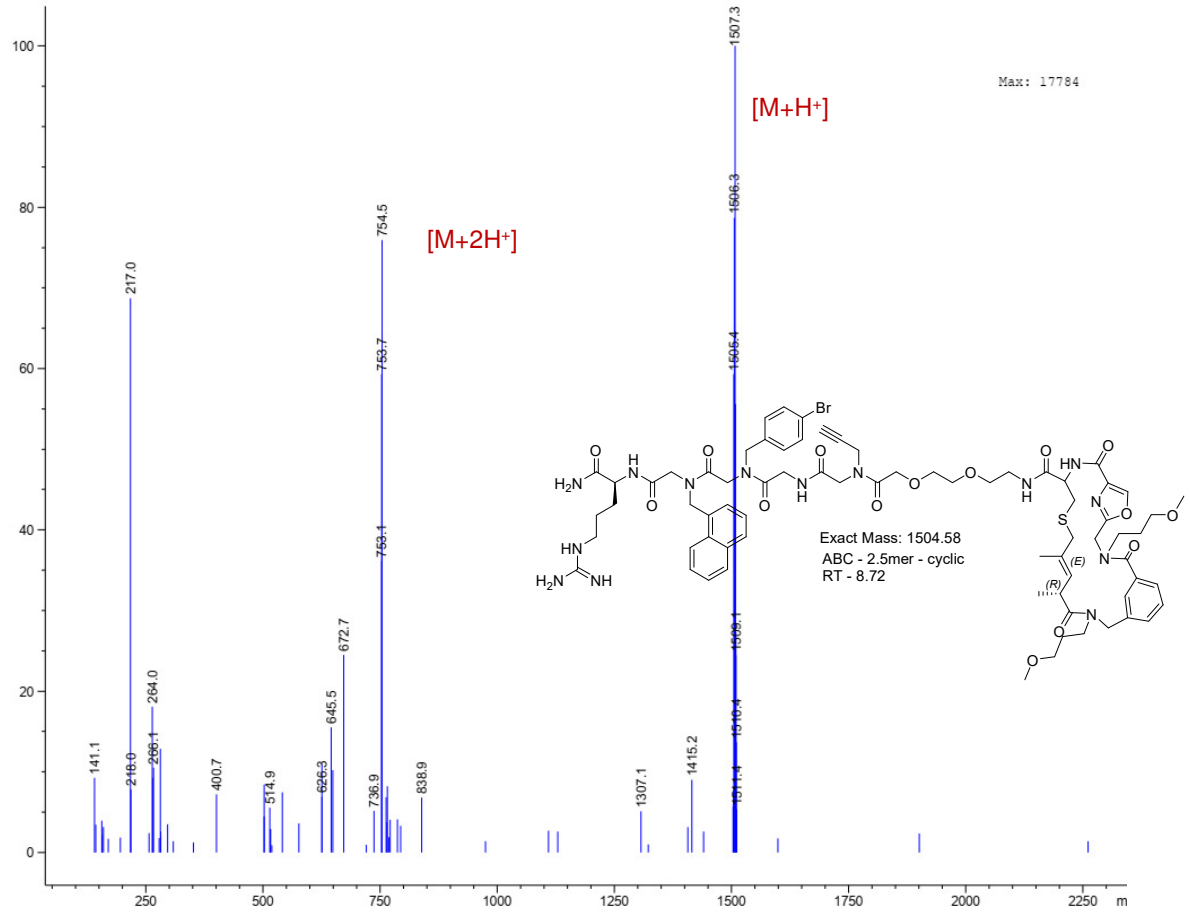


#	Time	Area	Height	Width	Area%
1	7.135	1017.5	106.7	0.1589	78.897
2	8.201	272.2	66.7	0.068	21.103

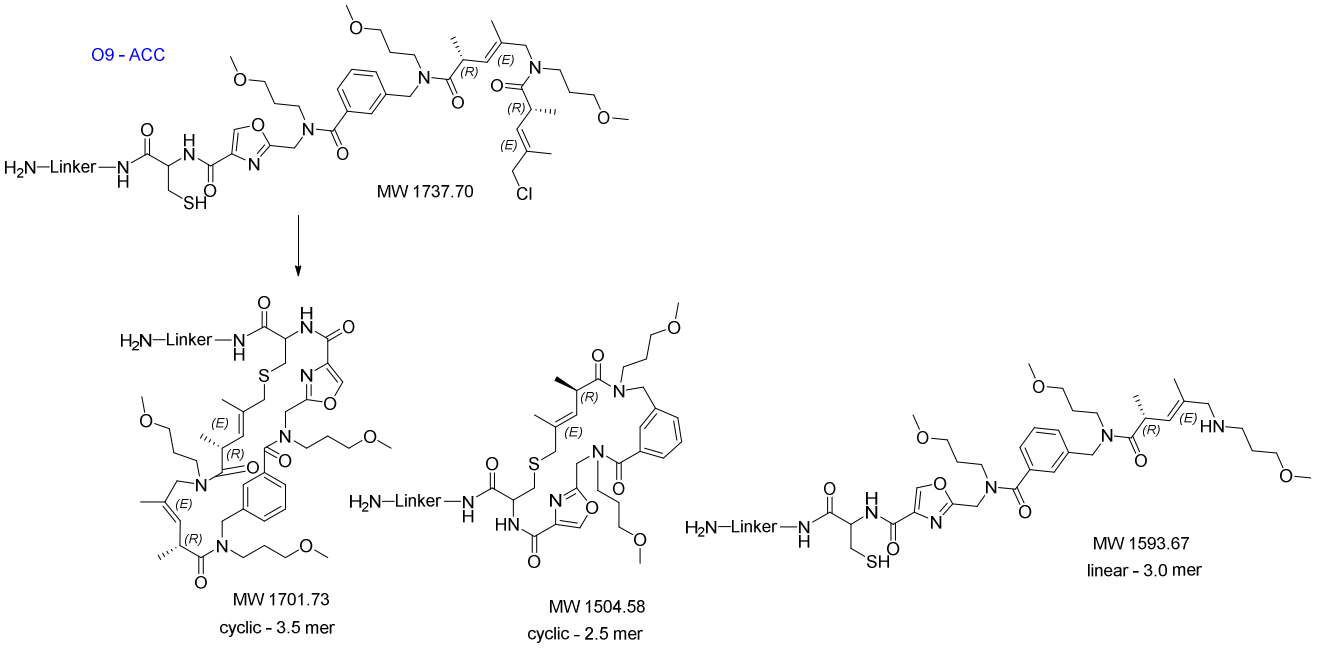
O8 - [ABC]

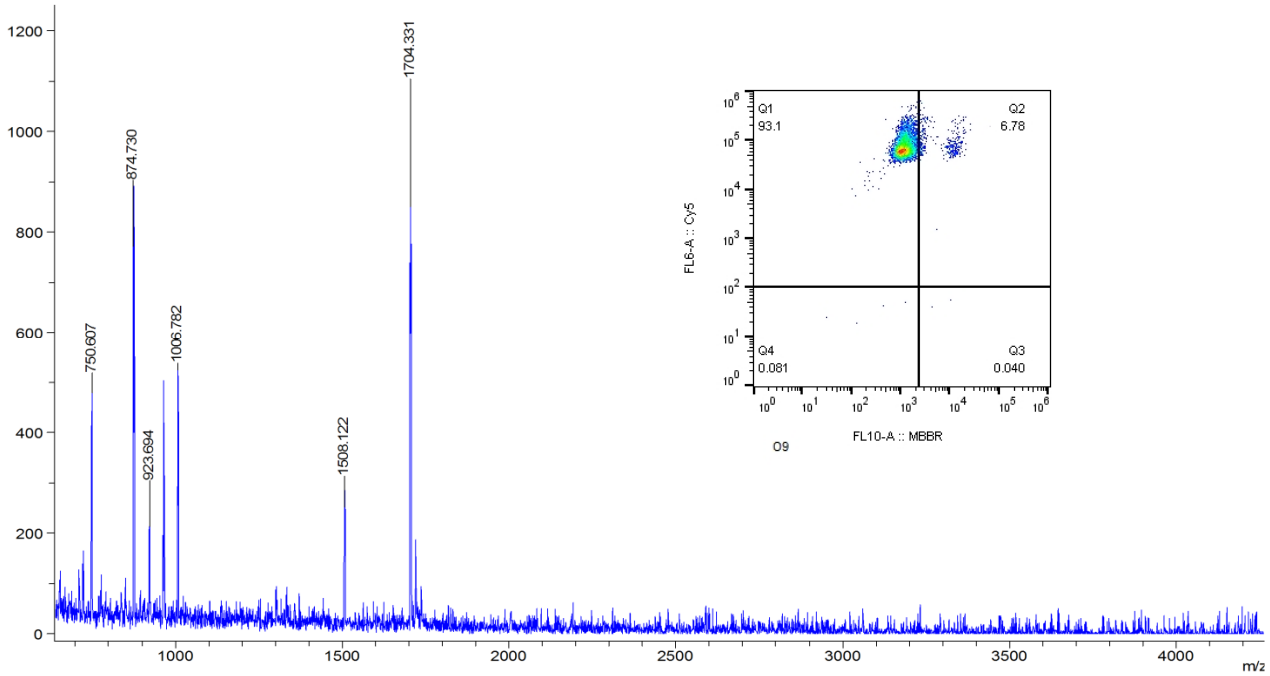
ions	size	MW	RT
cyclic	2.5	1504	8.201
cyclic	3.5	1658	7.135
linear	3.5	1694	-

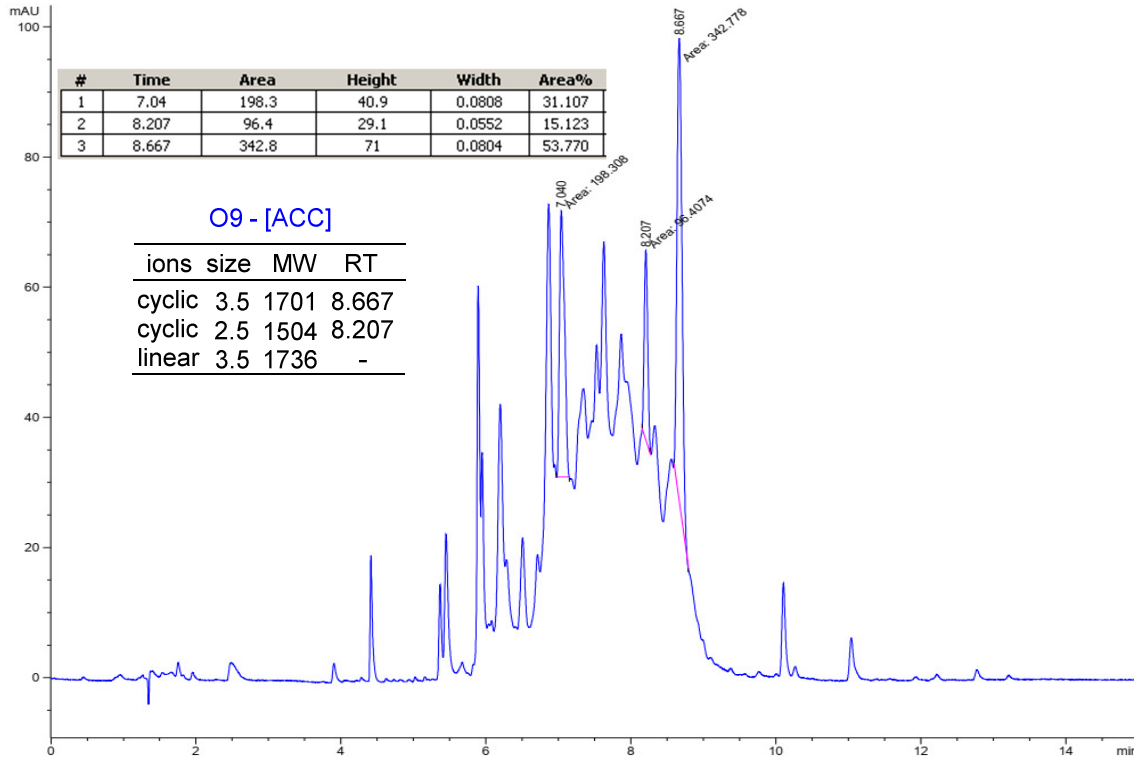

Max: 36792
Exact Mass: 1658.70
ABC - 3.5mer - cyclic
RT - 7.21
[M+2H+]
[M+H+]
297.0
631.4
832.3
554.3
1660.6
2056.7
297.9
1661.6
299.0
554.6
729.7
1544.5
141.1
544.4
845.4
894.4
976.2
1060.6
1662.3
m/


Max: 17784
[M+H+]
[M+2H+]
1507.3
754.5
1606.3
217.0
753.7
1606.4
769.1
Exact Mass: 1504.58
ABC - 2.5mer - cyclic
RT - 8.72
672.7
264.0
645.5
1508.1
141.1
1510.4
218.0
266.1
400.7
514.9
626.3
736.9
838.9
1307.1
1415.2
1511.4
m

O9-[ACC]: Cyclization was complete on both 10 µm & 160 µm beads.



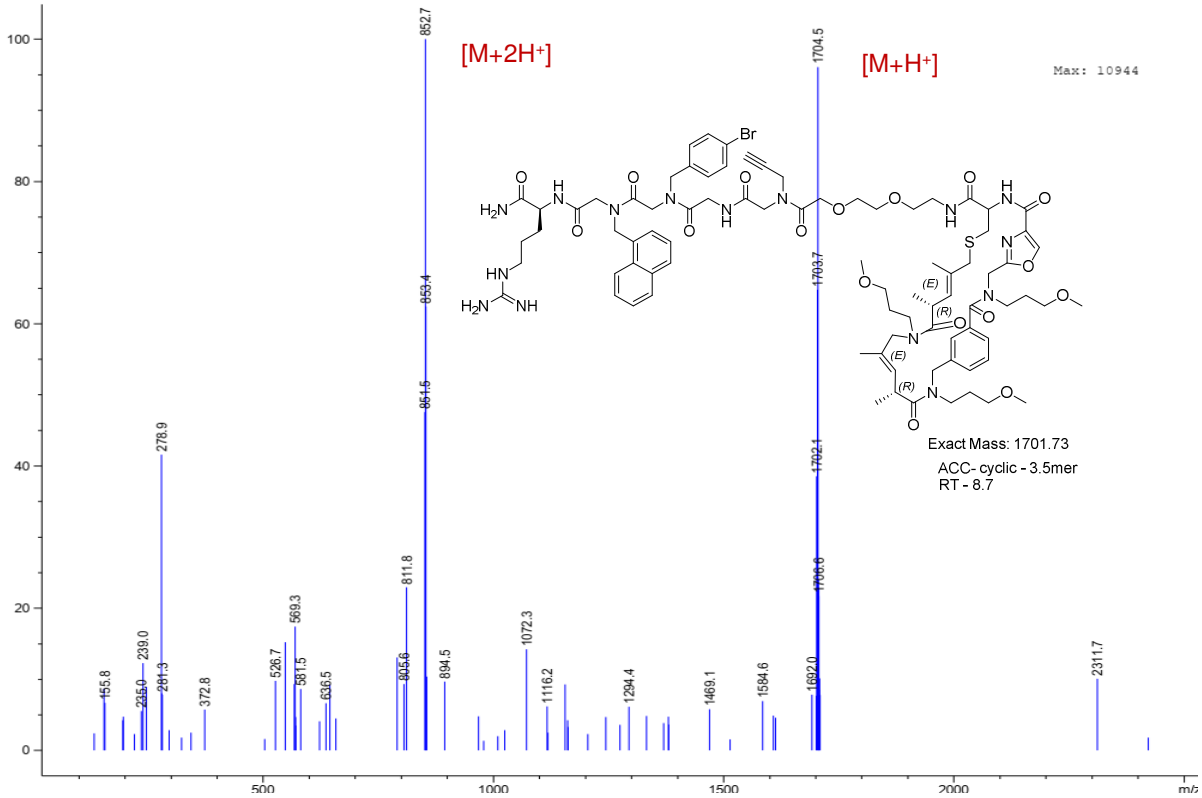




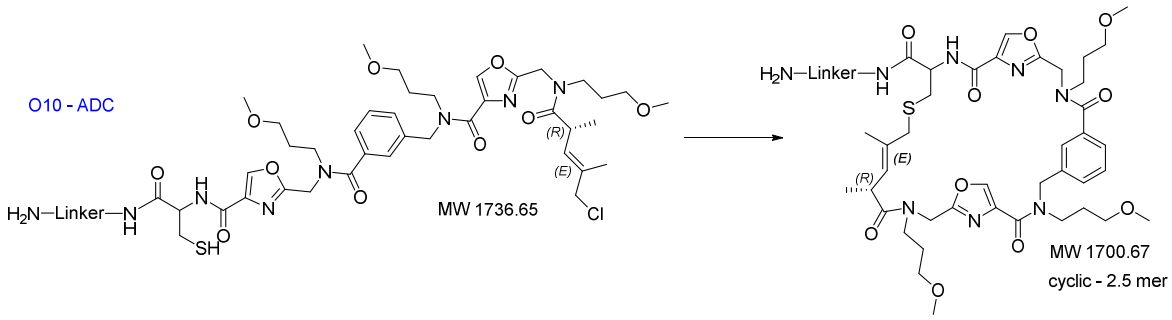
#	Time	Area	Height	Width	Area%
1	7.04	198.3	40.9	0.0808	31.107
2	8.207	96.4	29.1	0.0552	15.123
3	8.667	342.8	71	0.0804	53.770

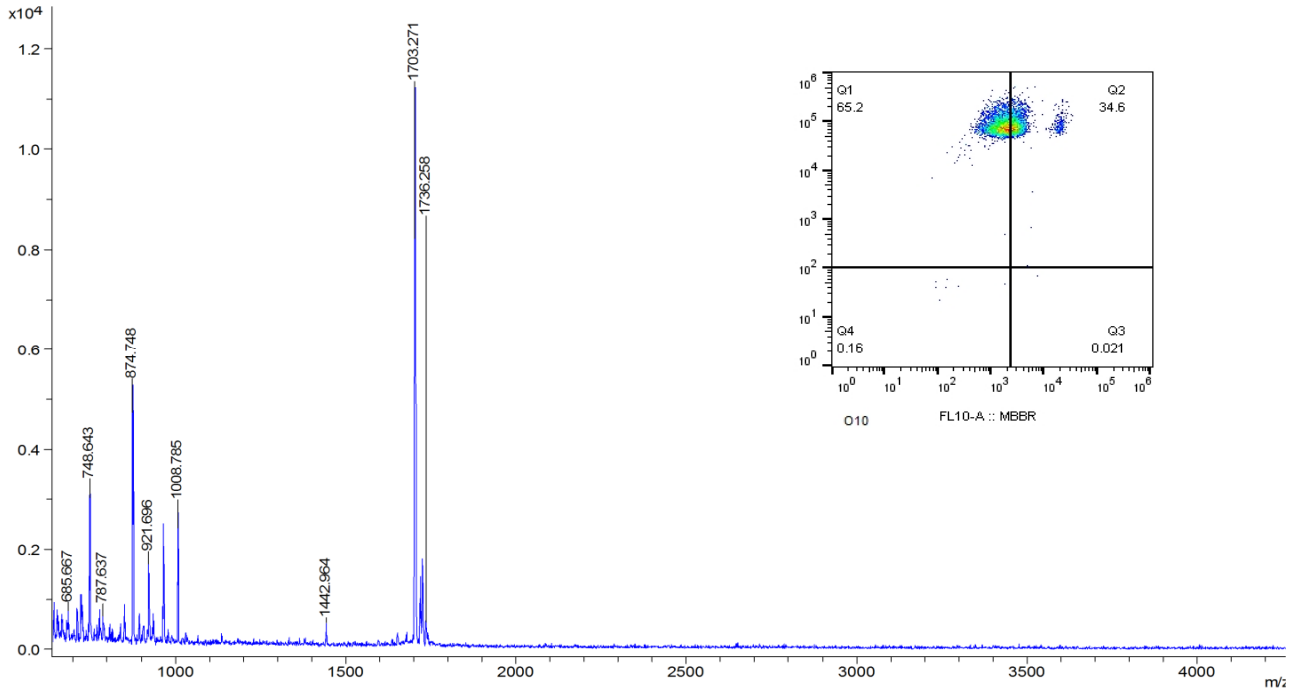
O9 - [ACC]

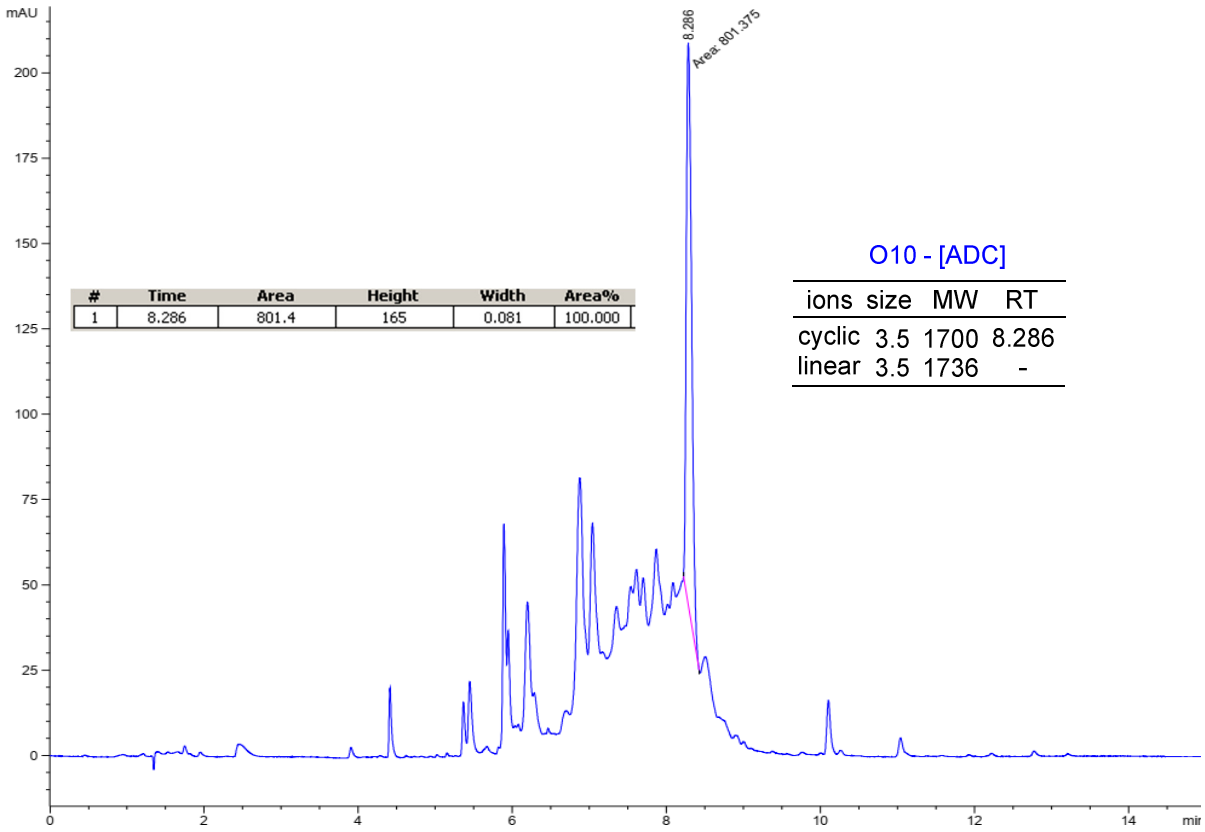
ions	size	MW	RT
cyclic	3.5	1701	8.667
cyclic	2.5	1504	8.207
linear	3.5	1736	-

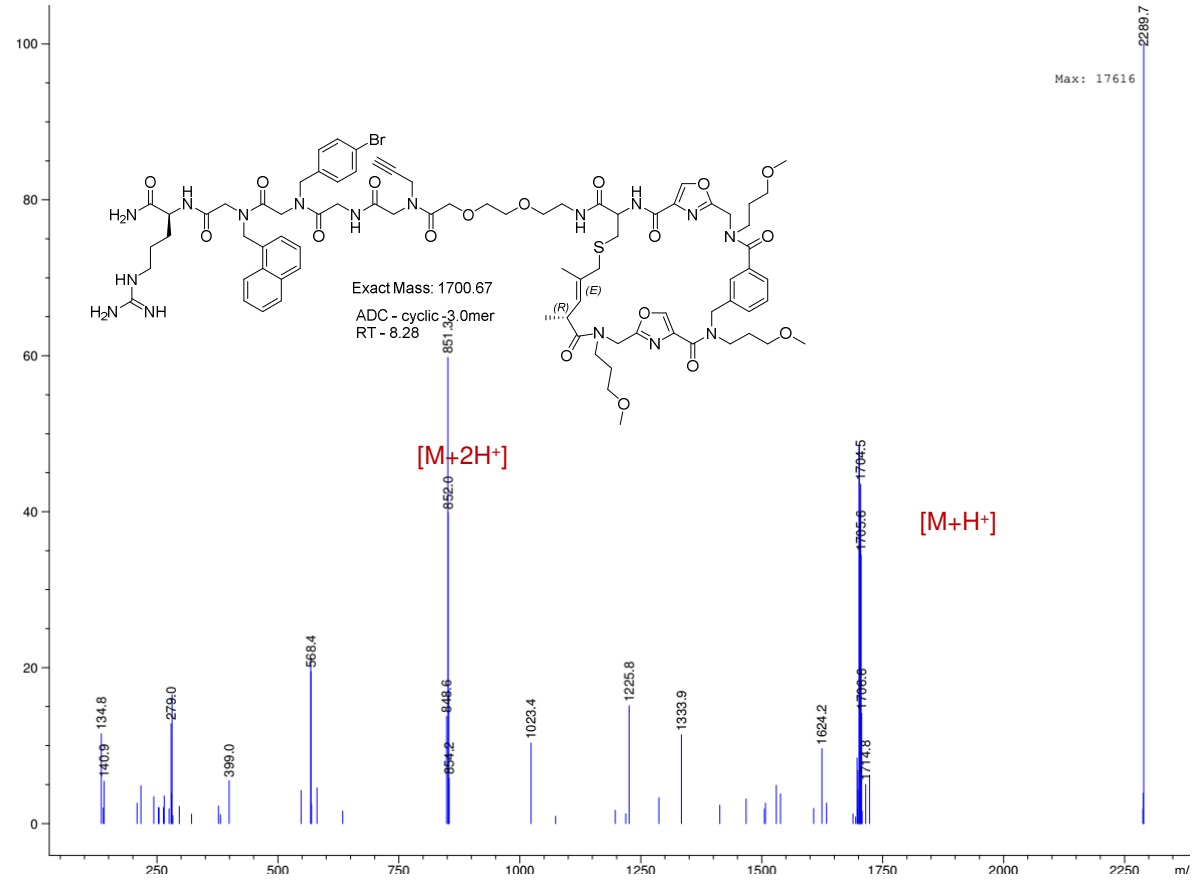


O10-[ADC]: Incomplete cyclization was detected on 10 µm but was completed on 160 µm beads.

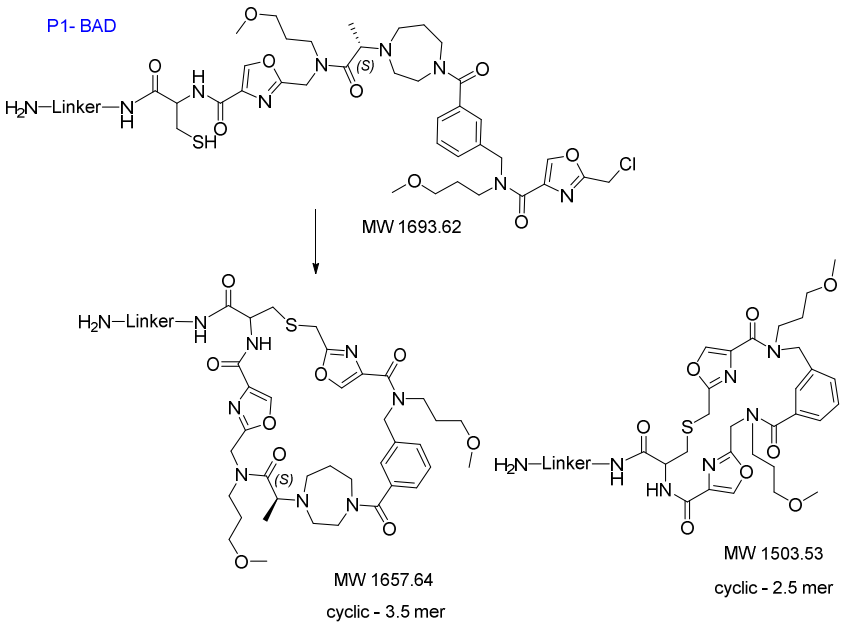


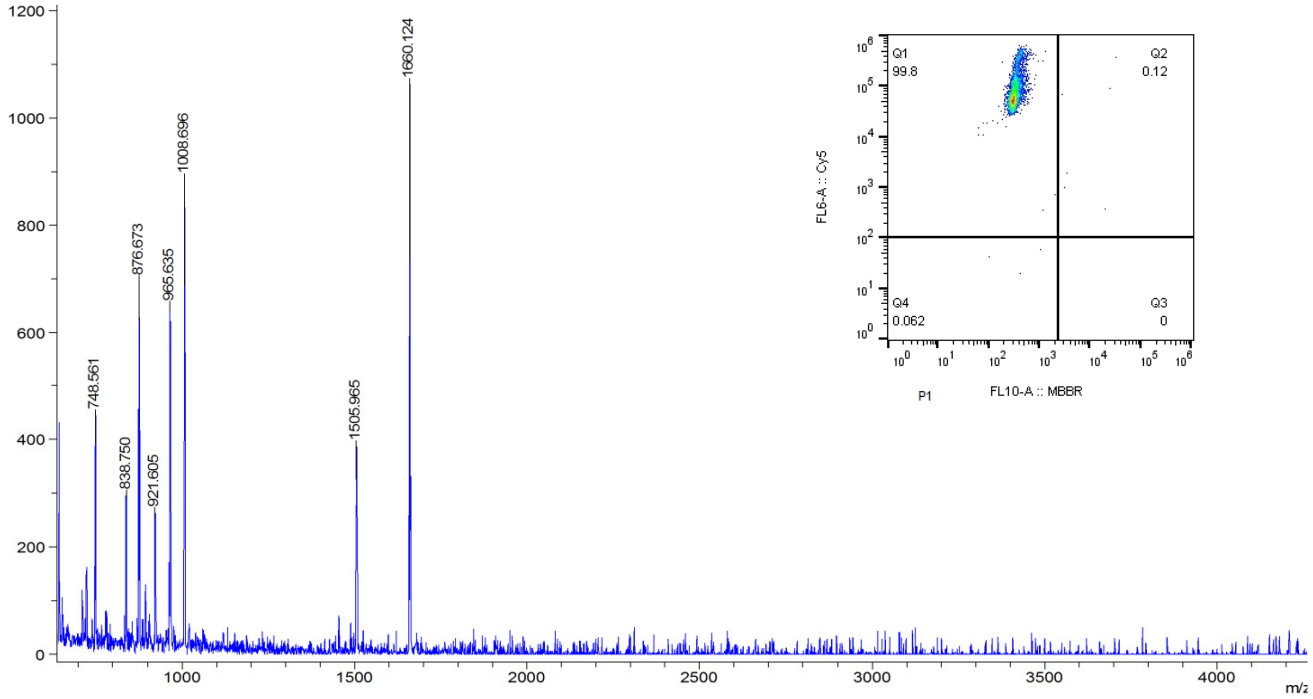


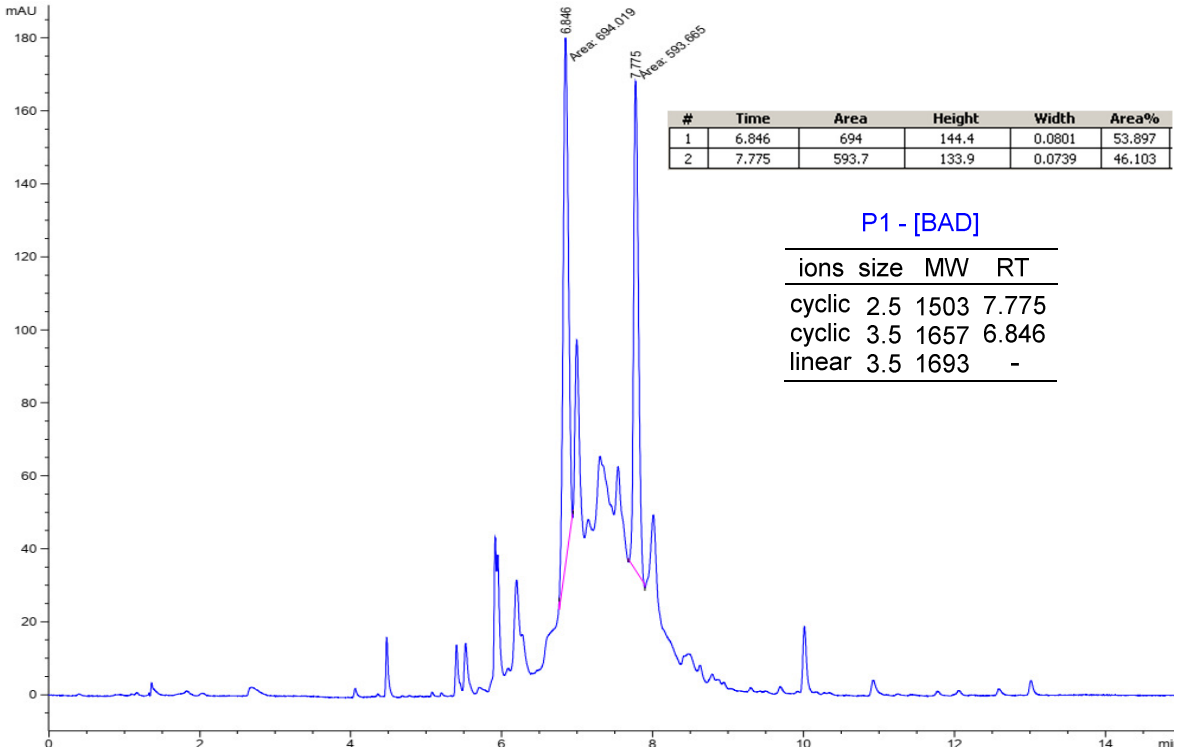

mAU
8.286
Area: 801.375
Time Area Height Width Area%
1 8.286 801.4 165 0.081 100.000
O10 - [ADC]
ions size MW RT
cyclic 3.5 1700 8.286
linear 3.5 1736 -
min


Exact Mass: 1700.67
ADC - cyclic -3.0mer
RT - 8.28
Max: 17616
[M+2H+]
[M+H+]
m/

P1-[BAD]: Cyclization was complete on both 10 µm & 160 µm beads.



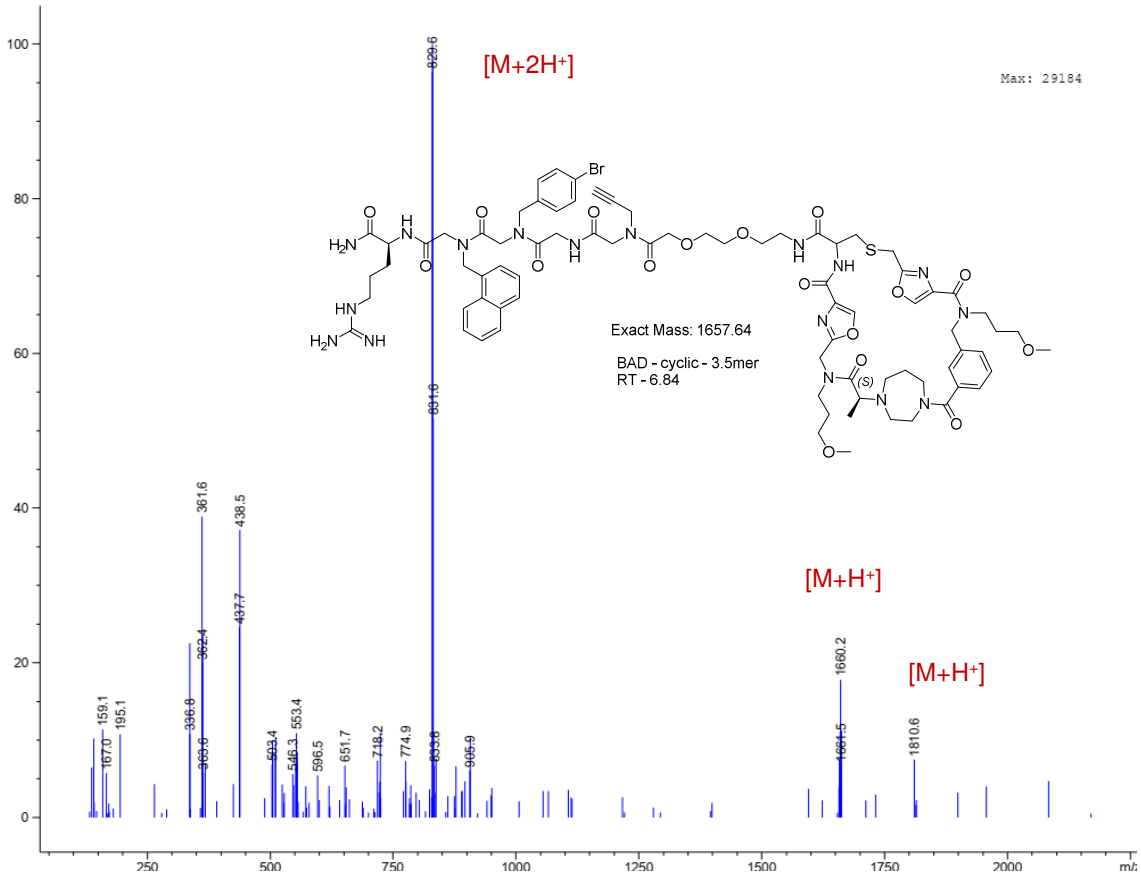


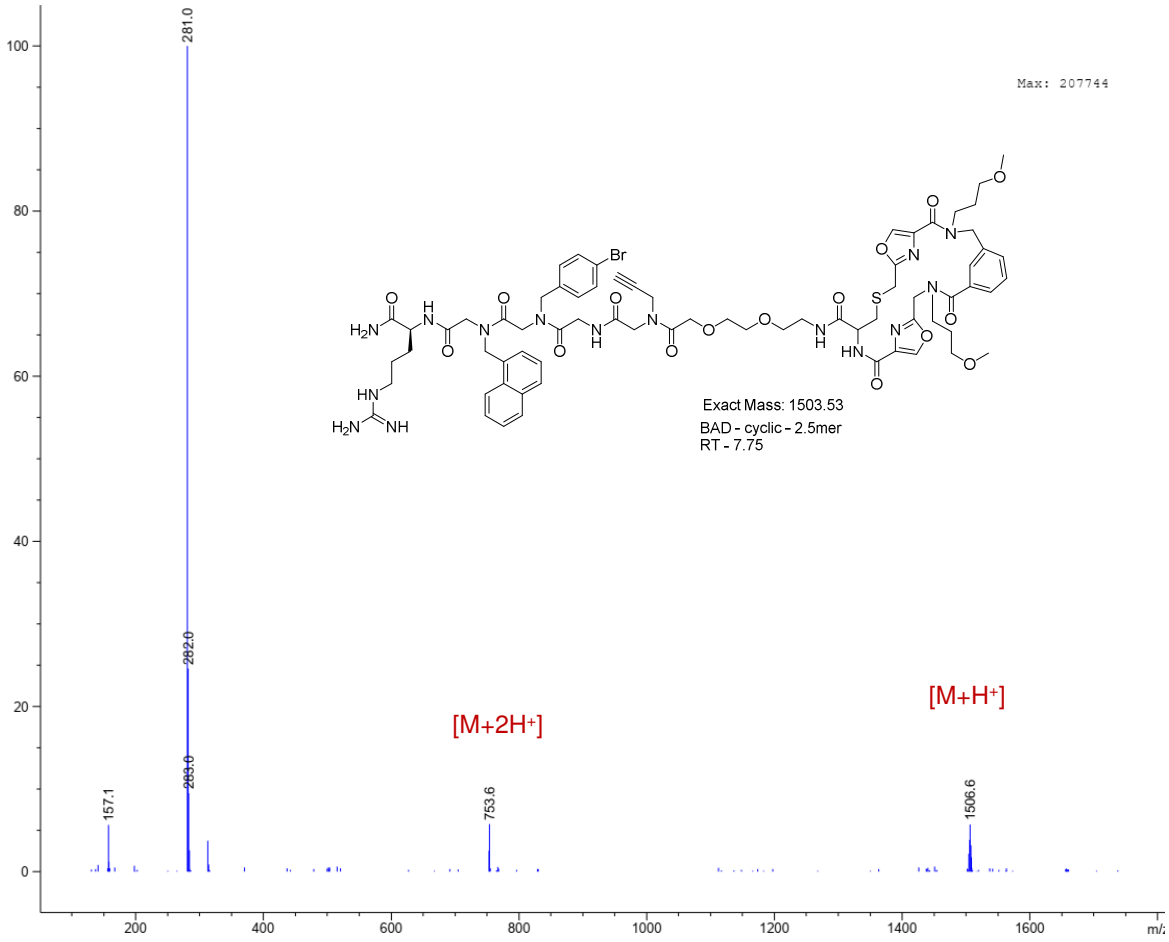


#	Time	Area	Height	Width	Area%
1	6.846	694	144.4	0.0801	53.897
2	7.775	593.7	133.9	0.0739	46.103

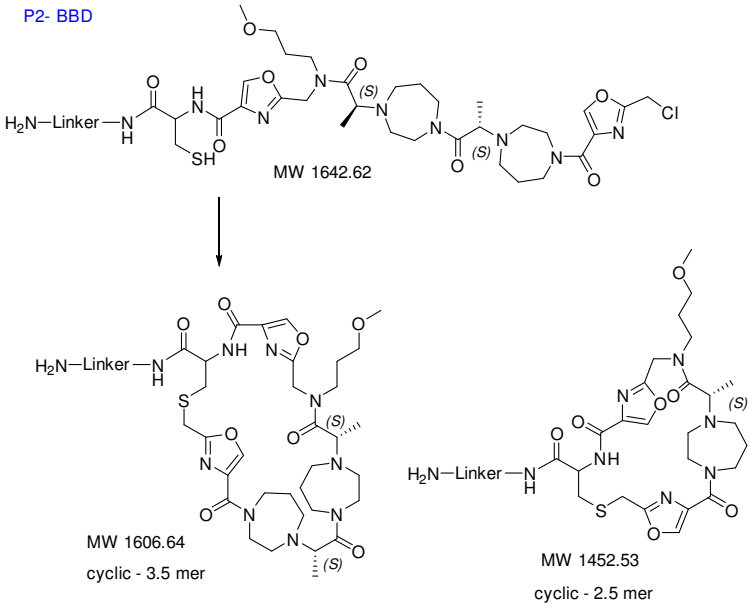
P1 - [BAD]

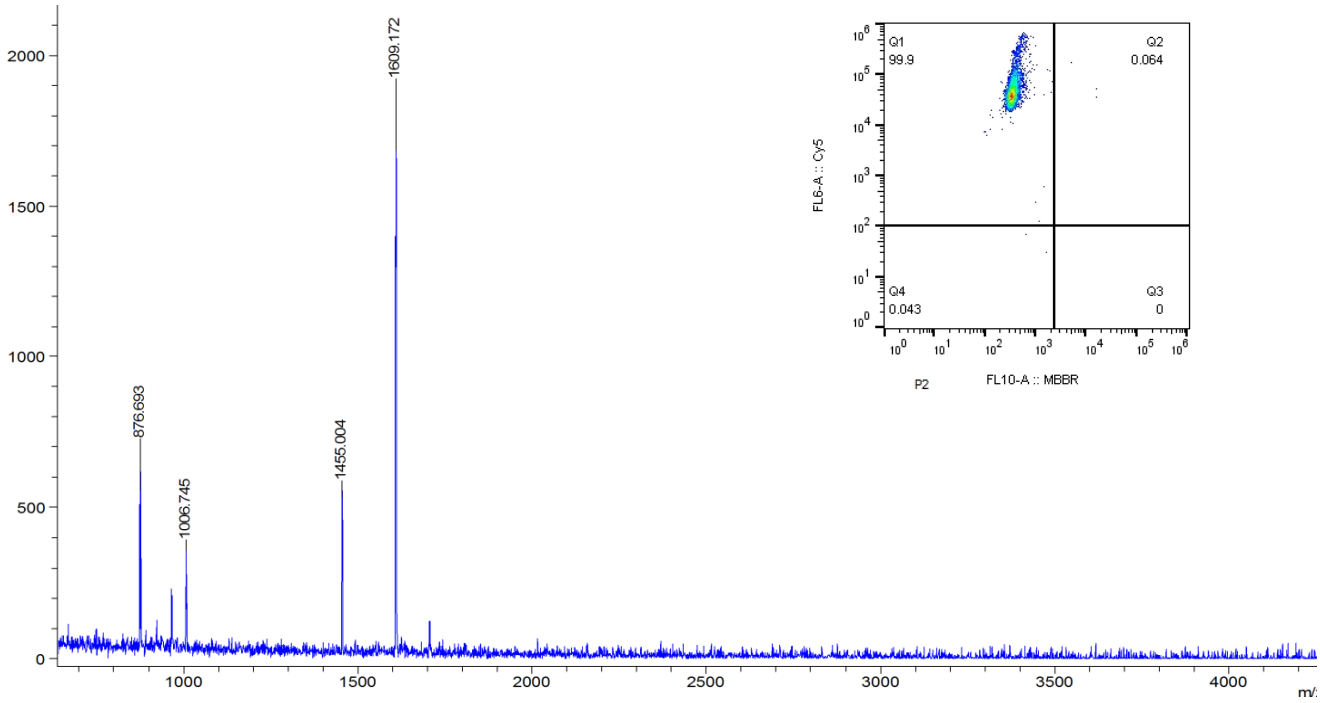
ions	size	MW	RT
cyclic	2.5	1503	7.775
cyclic	3.5	1657	6.846
linear	3.5	1693	-

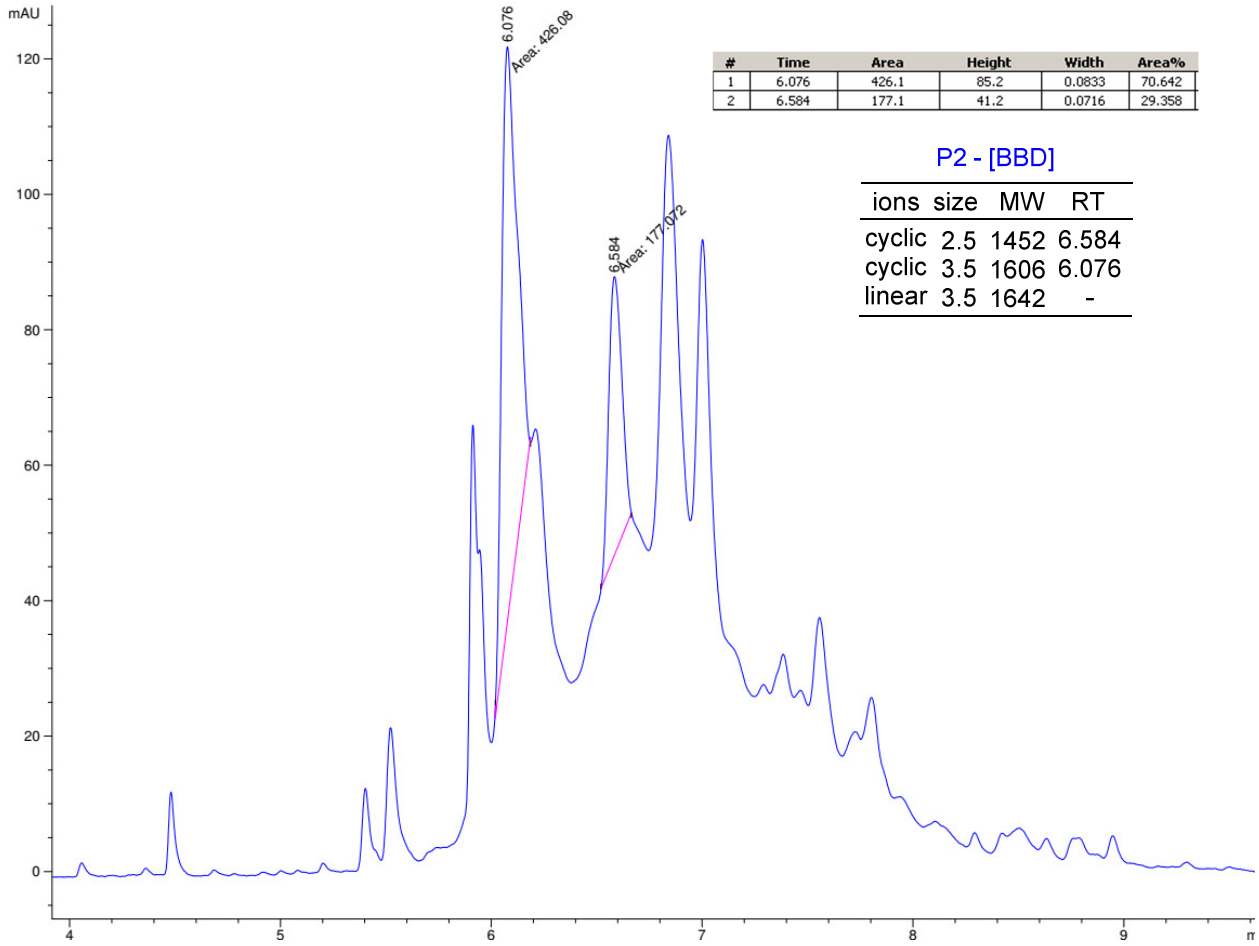




P2-[BBD]: Cyclization was complete on both 10 µm & 160 µm beads.



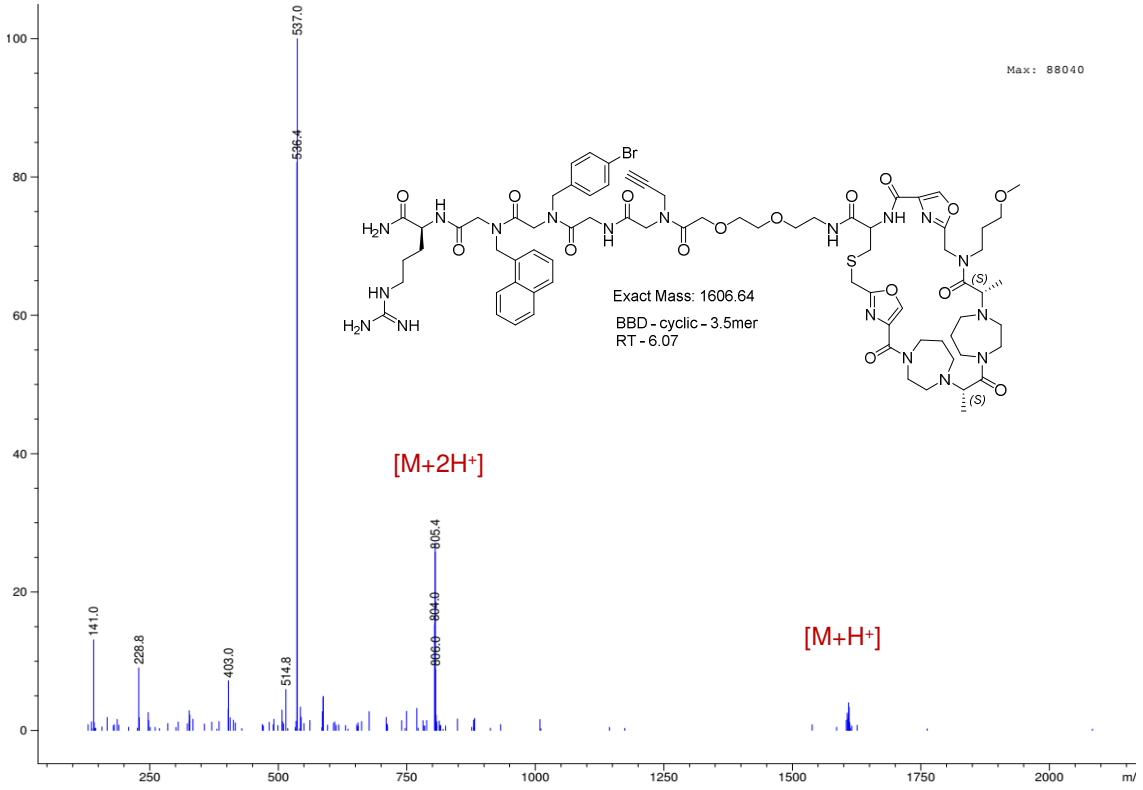


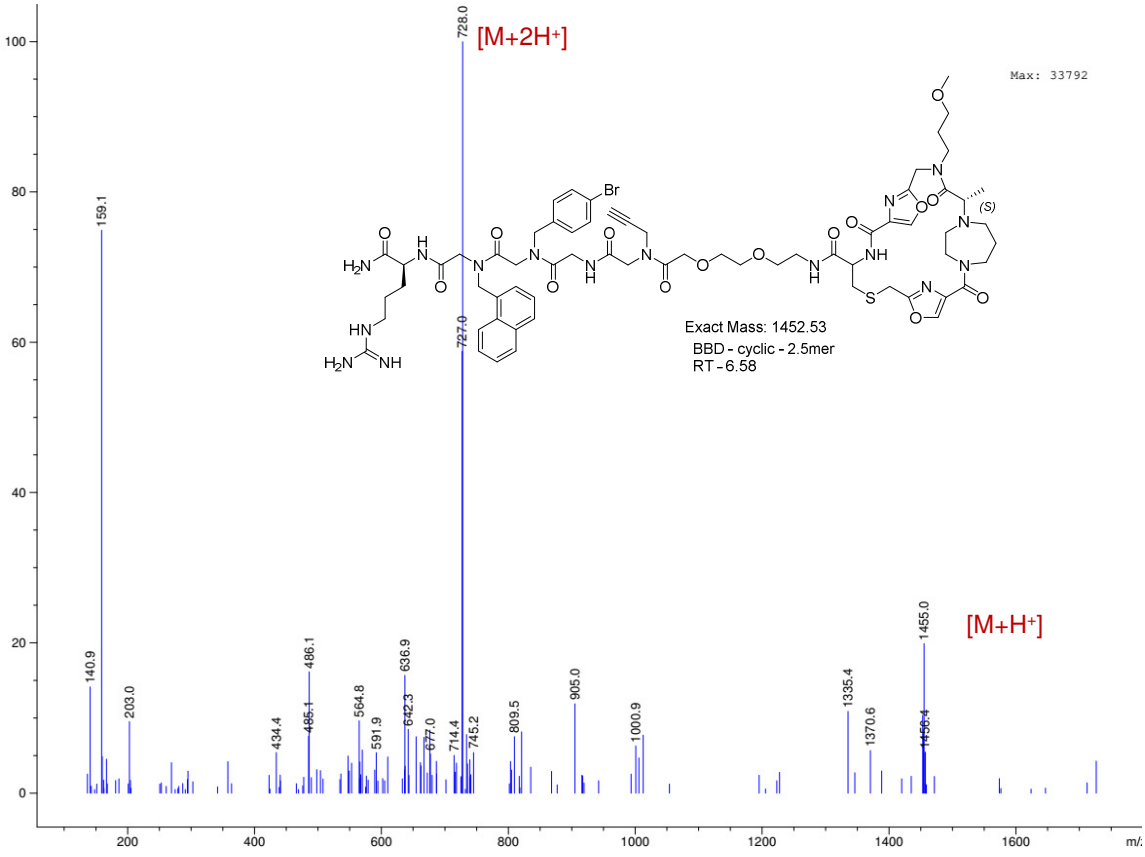


#	Time	Area	Height	Width	Area%
1	6.076	426.1	85.2	0.0833	70.642
2	6.584	177.1	41.2	0.0716	29.358

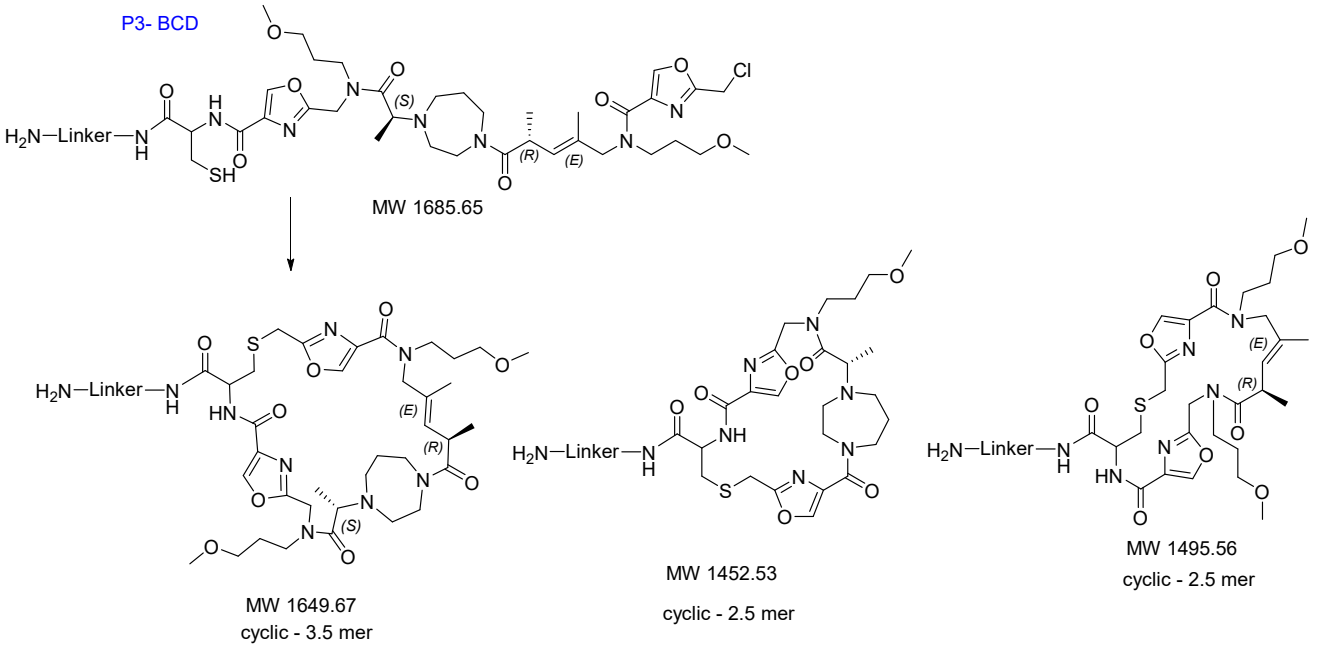
P2 - [BBD]

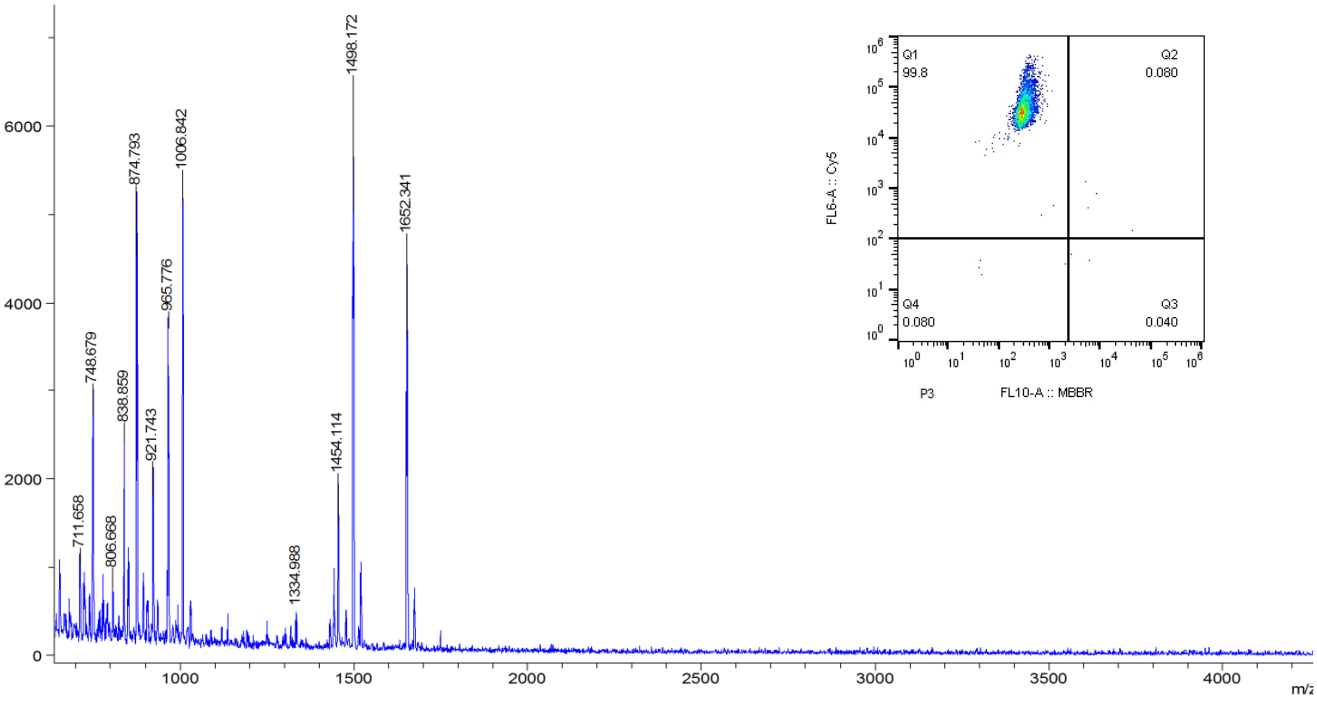
ions	size	MW	RT
cyclic	2.5	1452	6.584
cyclic	3.5	1606	6.076
linear	3.5	1642	-

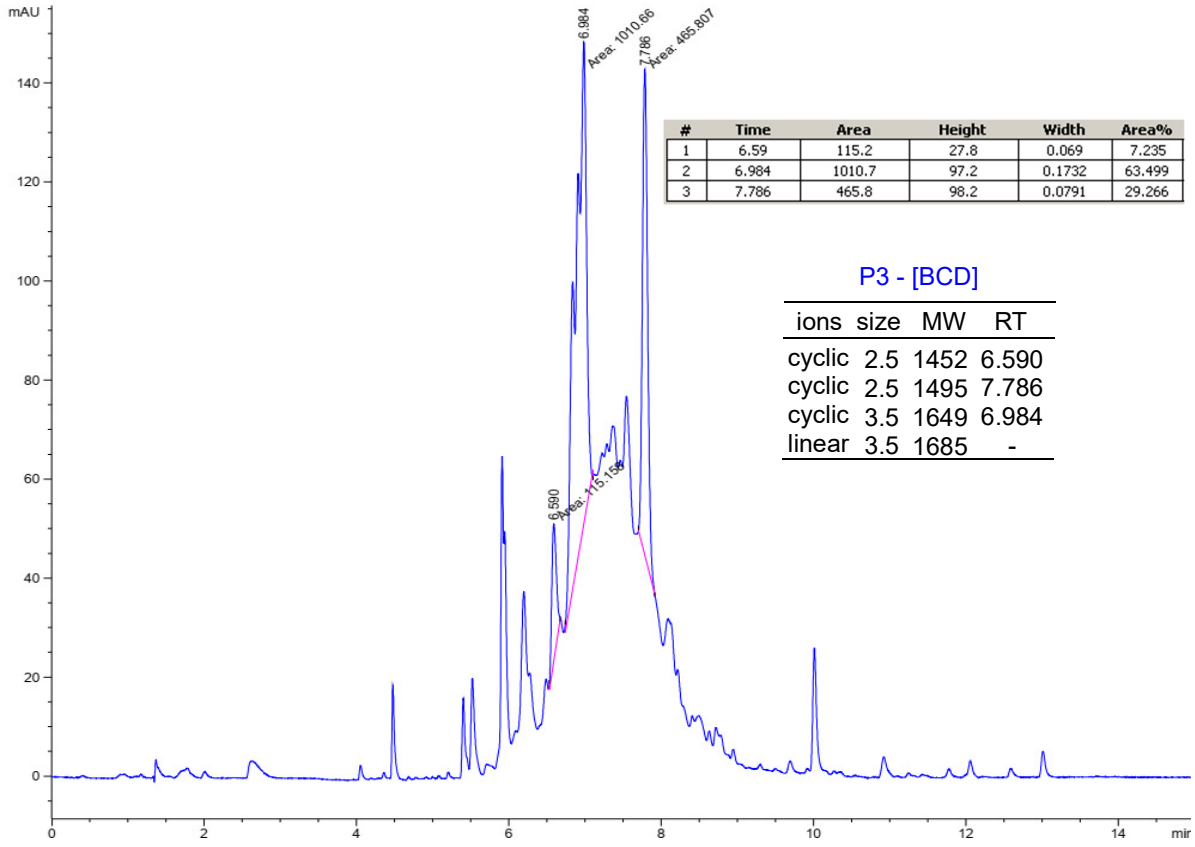

Max: 88040
537.0
536.4
805.4
804.0
806.0
141.0
228.8
403.0
514.8
Br
Exact Mass: 1606.64
BBD - cyclic - 3.5mer
RT - 6.07
[M+2H+]
[M+H+]
m/


Max: 33792
728.0
727.0
159.1
140.9
203.0
434.4
485.1
486.1
564.8
591.9
636.9
642.3
677.0
714.4
745.2
809.5
905.0
1000.9
1335.4
1370.6
1455.0
1456.4
Br
Exact Mass: 1452.53
BBD - cyclic - 2.5mer
RT - 6.58
[M+2H+]
[M+H+]
m/

P3-[BCD]: Cyclization was complete on both 10 µm & 160 µm beads.



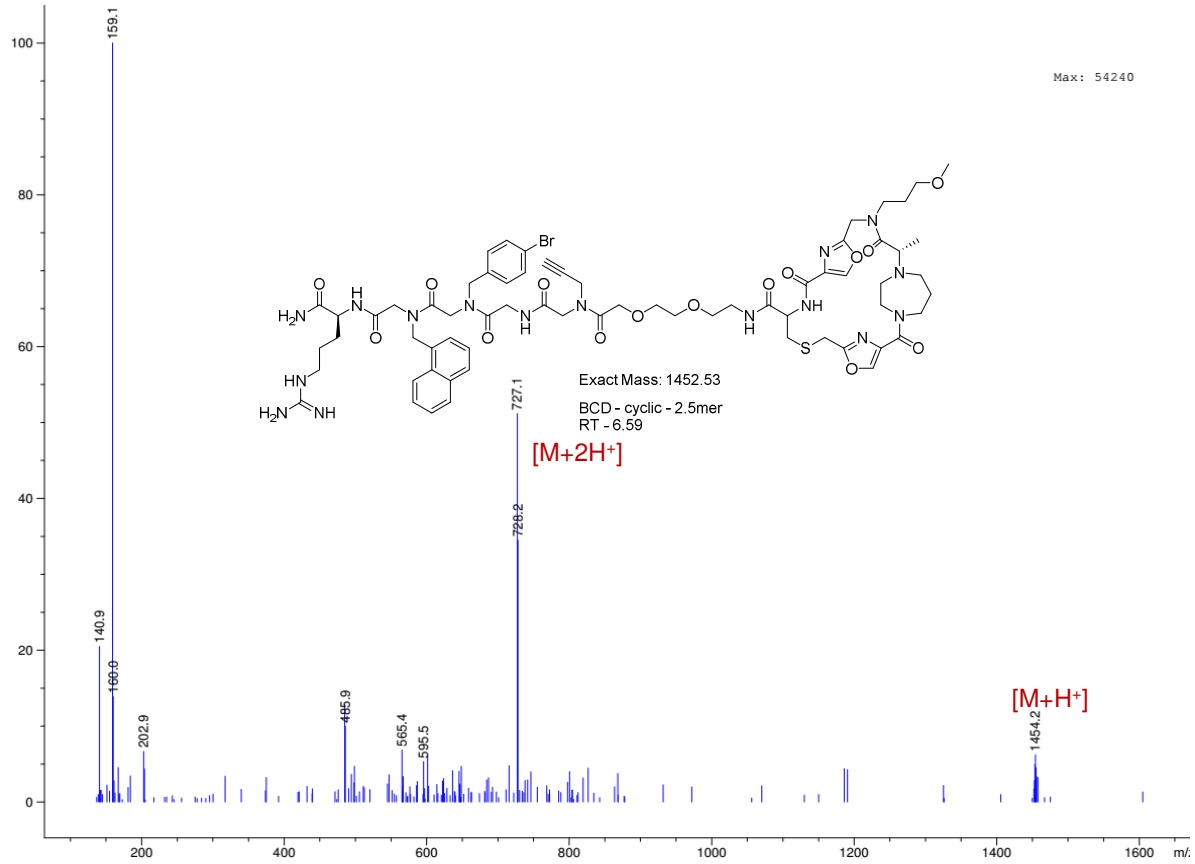


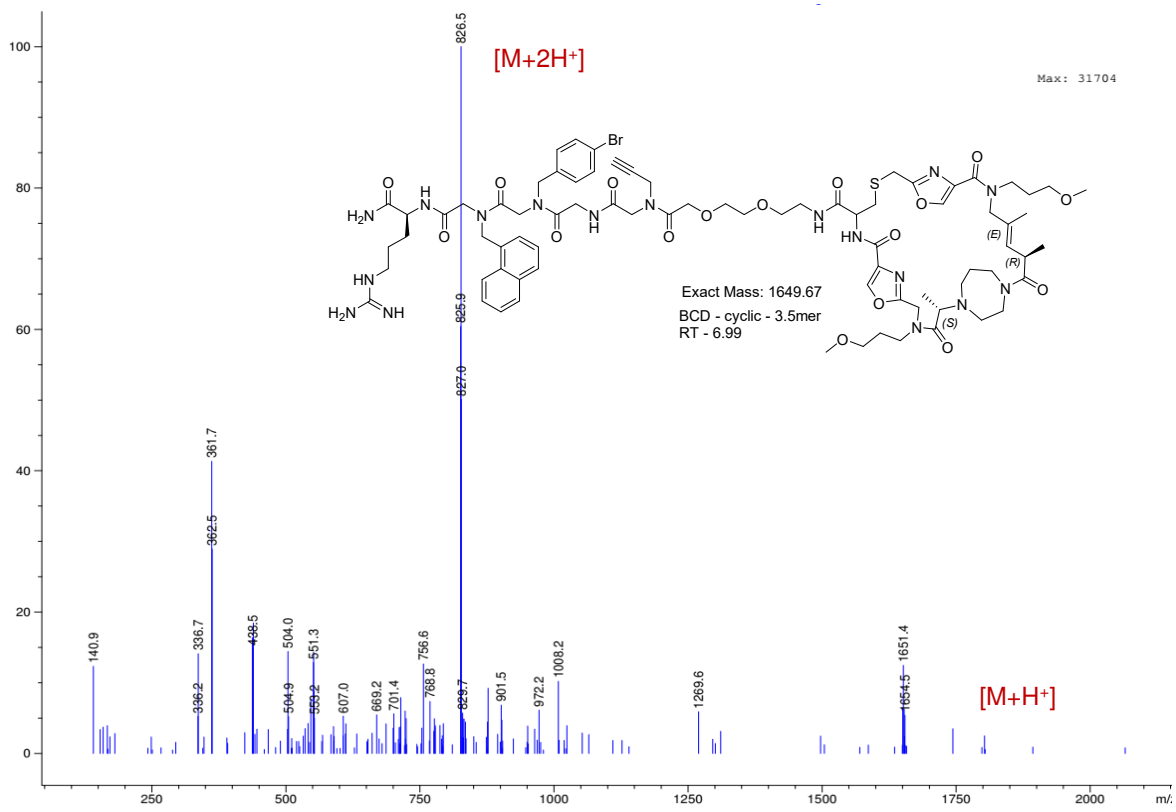


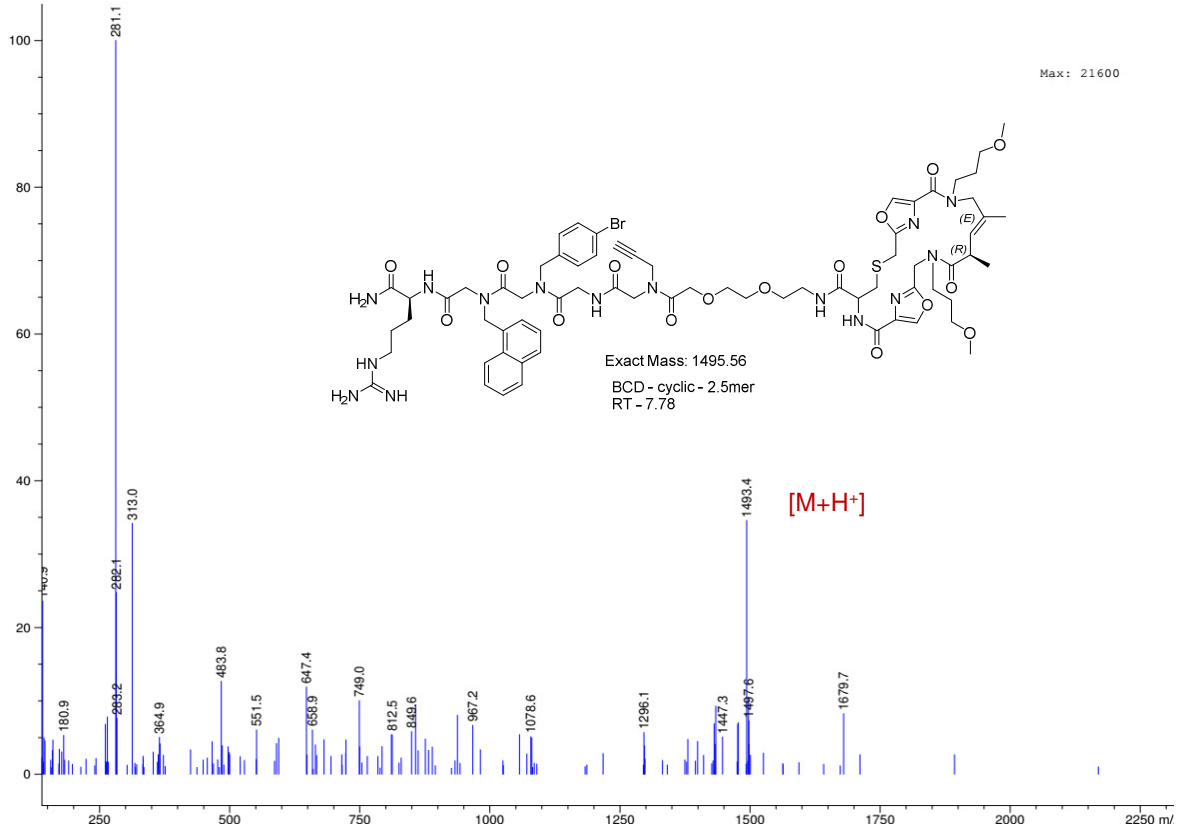
#	Time	Area	Height	Width	Area%
1	6.59	115.2	27.8	0.069	7.235
2	6.984	1010.7	97.2	0.1732	63.499
3	7.786	465.8	98.2	0.0791	29.266

P3 - [BCD]

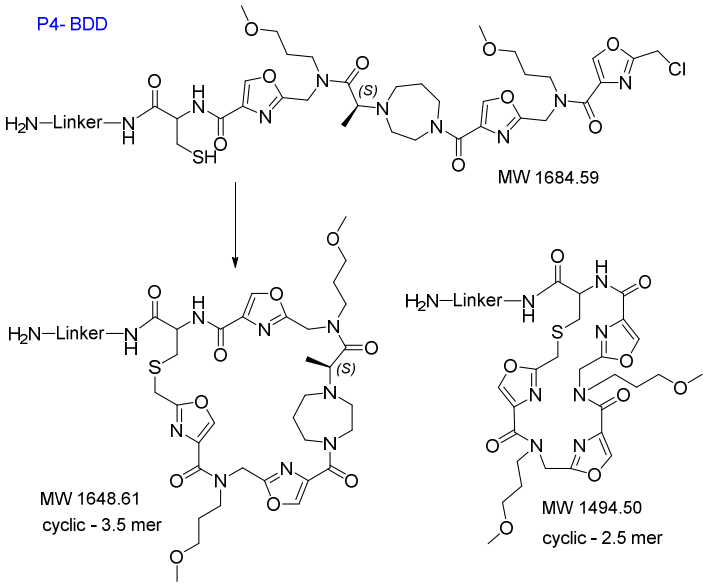
ions	size	MW	RT
cyclic	2.5	1452	6.590
cyclic	2.5	1495	7.786
cyclic	3.5	1649	6.984
linear	3.5	1685	-

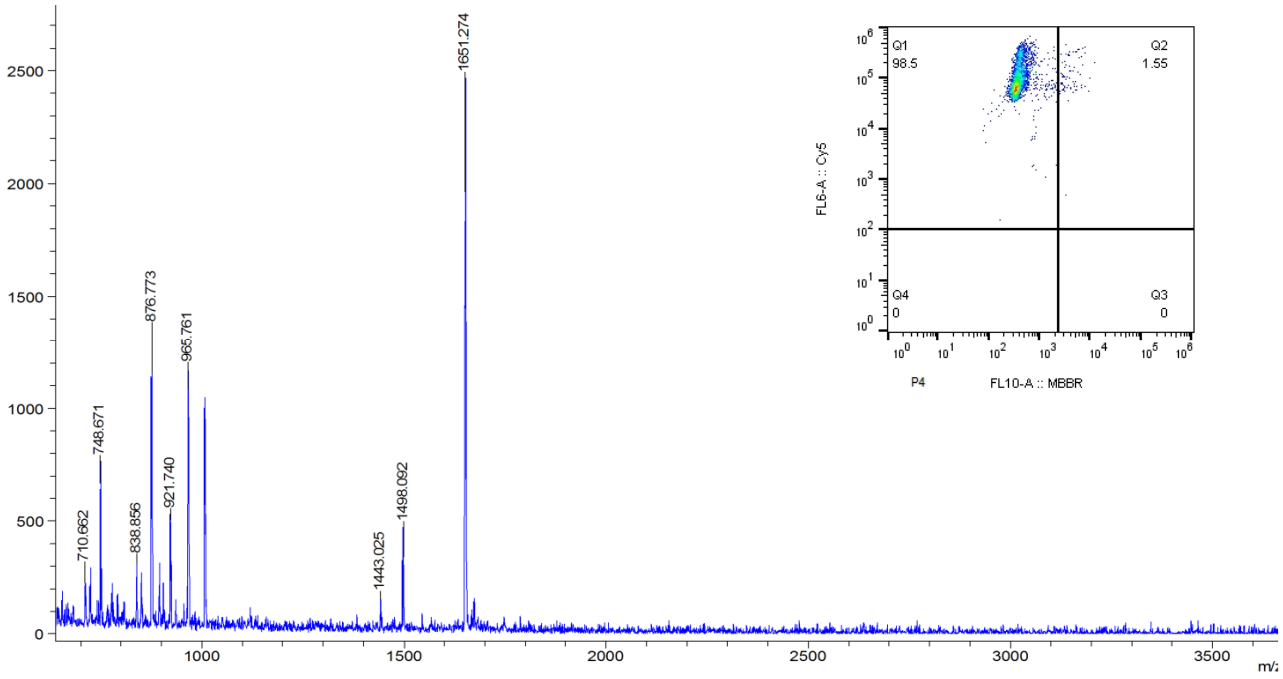


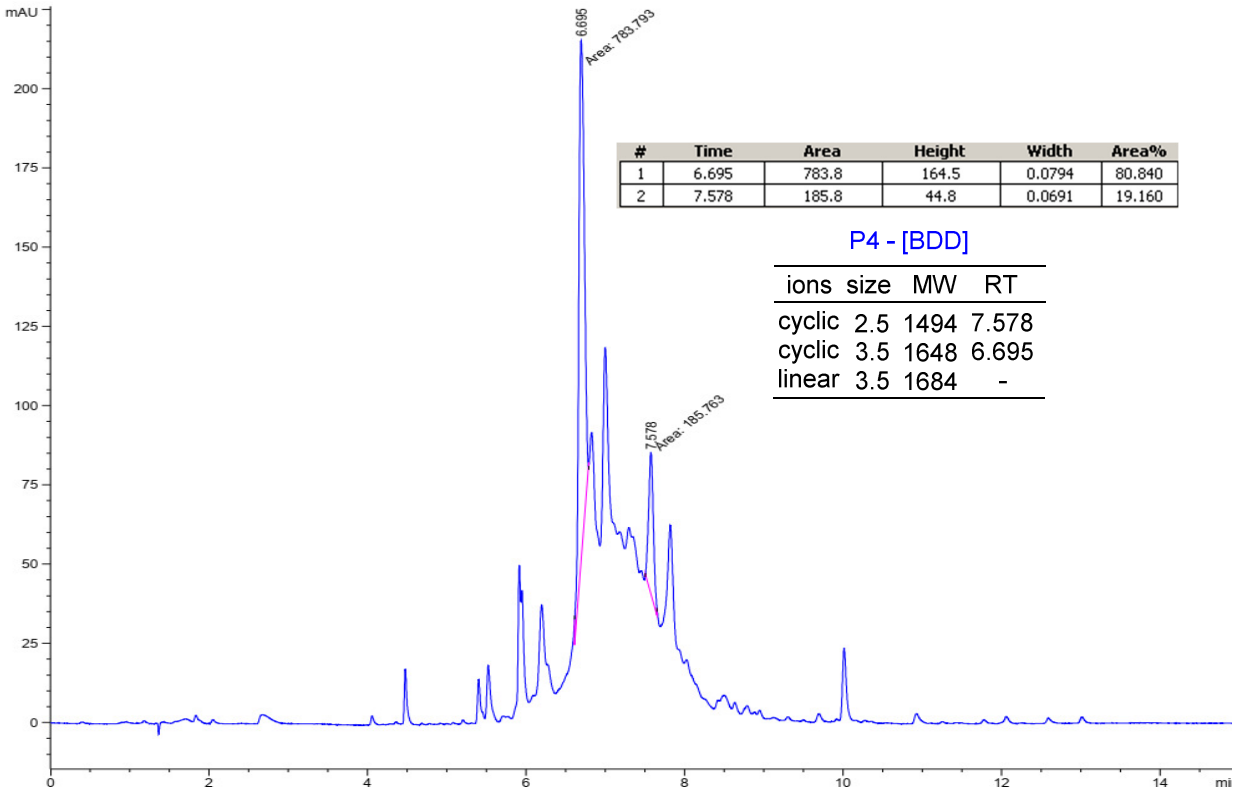

[M+2H+]
Max: 31704
Exact Mass: 1649.67
BCD - cyclic - 3.5mer
RT - 6.99
[M+H+]


Max: 21600
Exact Mass: 1495.56
BCD - cyclic - 2.5mer
RT - 7.78
[M+H+]

P4-[BDD]: Cyclization was complete on both 10 µm & 160 µm beads.



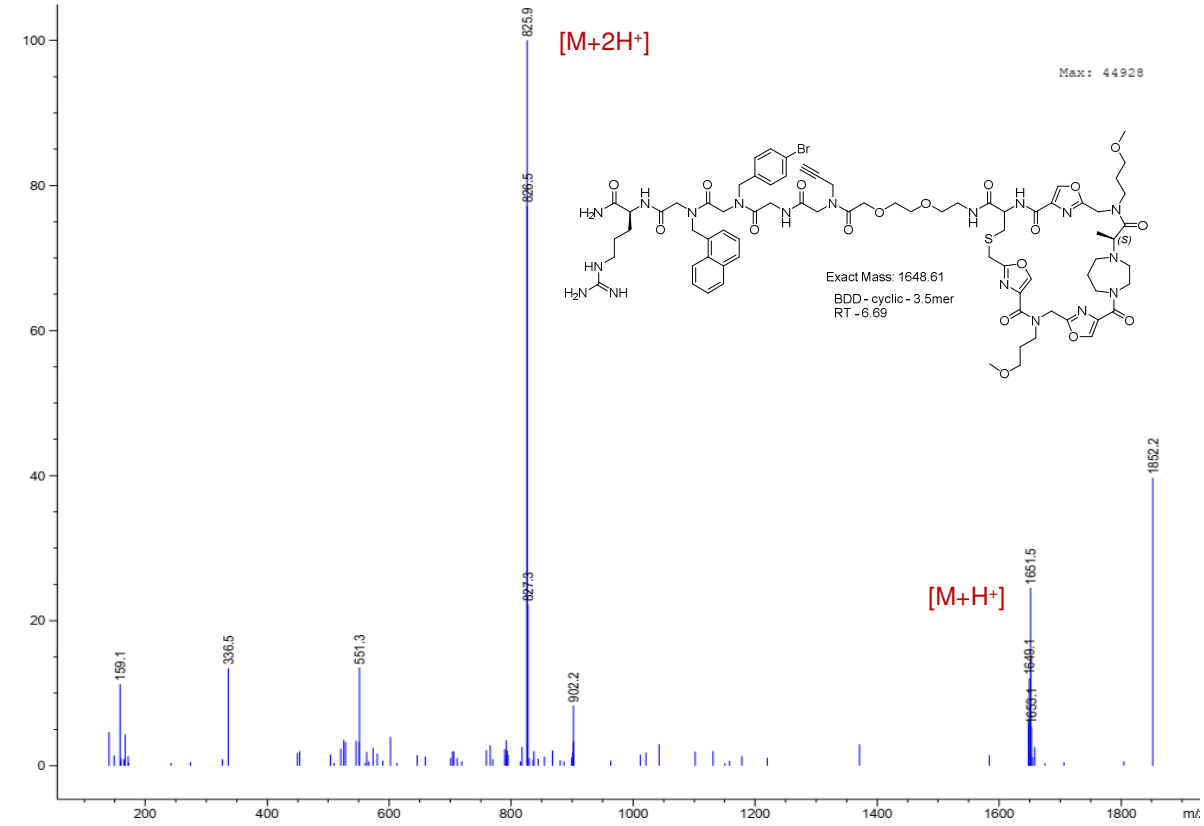


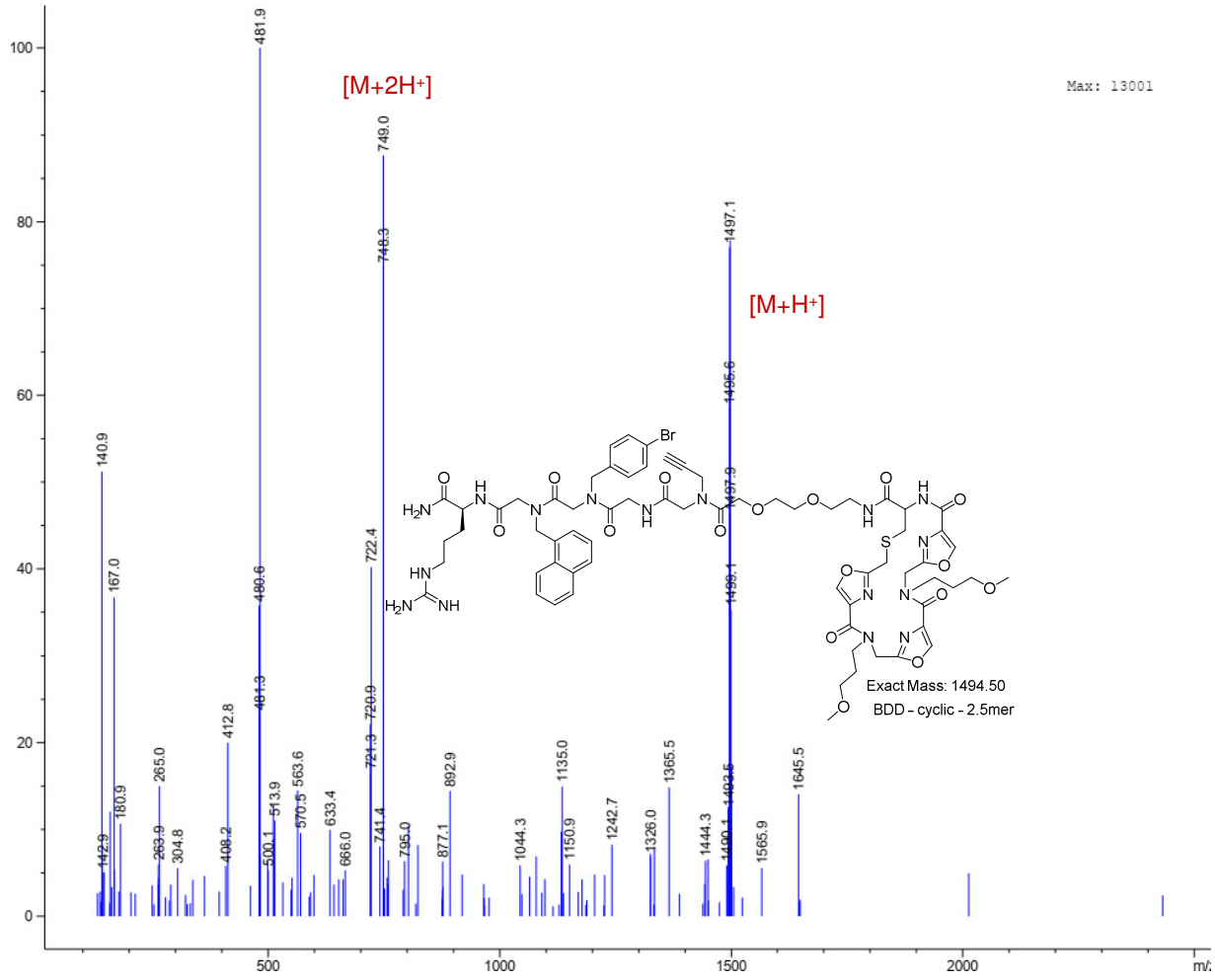


#	Time	Area	Height	Width	Area%
1	6.695	783.8	164.5	0.0794	80.840
2	7.578	185.8	44.8	0.0691	19.160

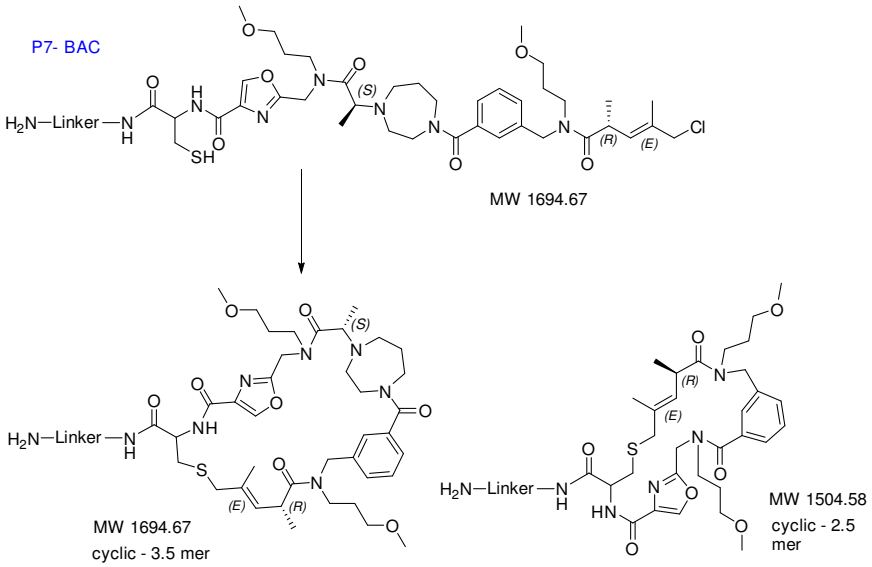
P4 - [BDD]

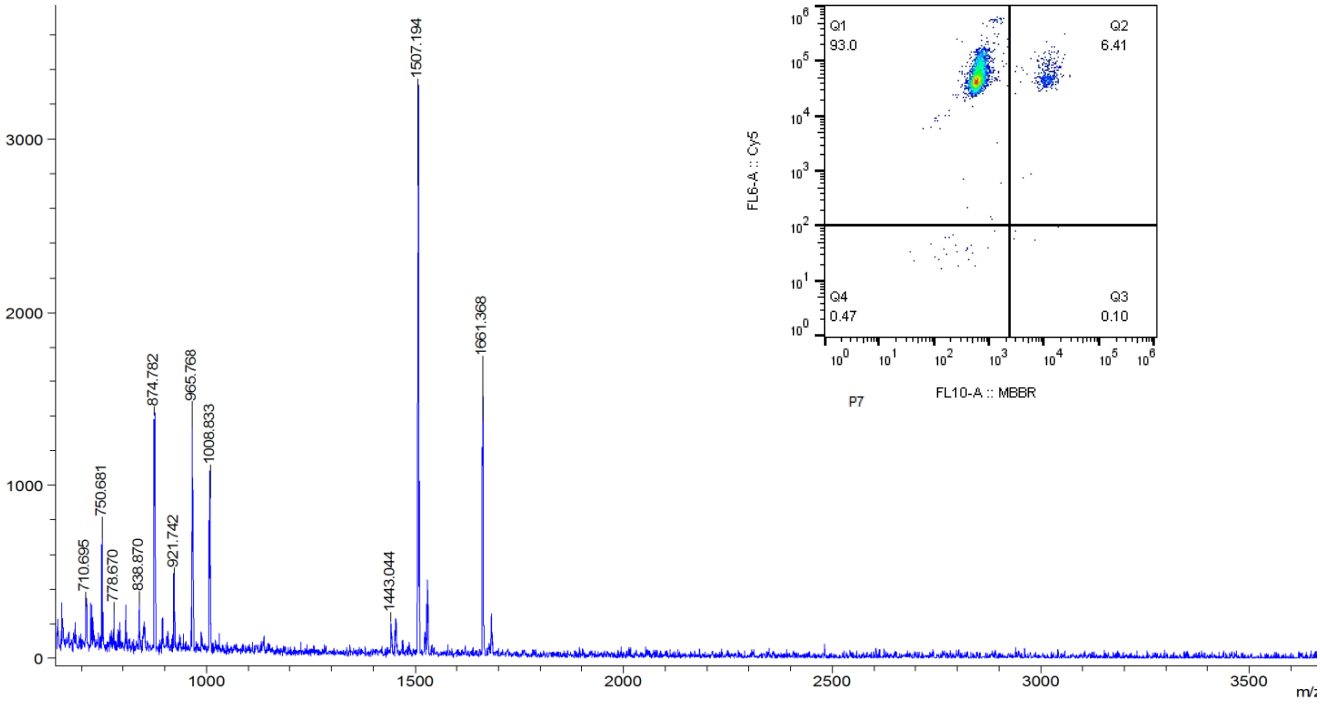
ions	size	MW	RT
cyclic	2.5	1494	7.578
cyclic	3.5	1648	6.695
linear	3.5	1684	-

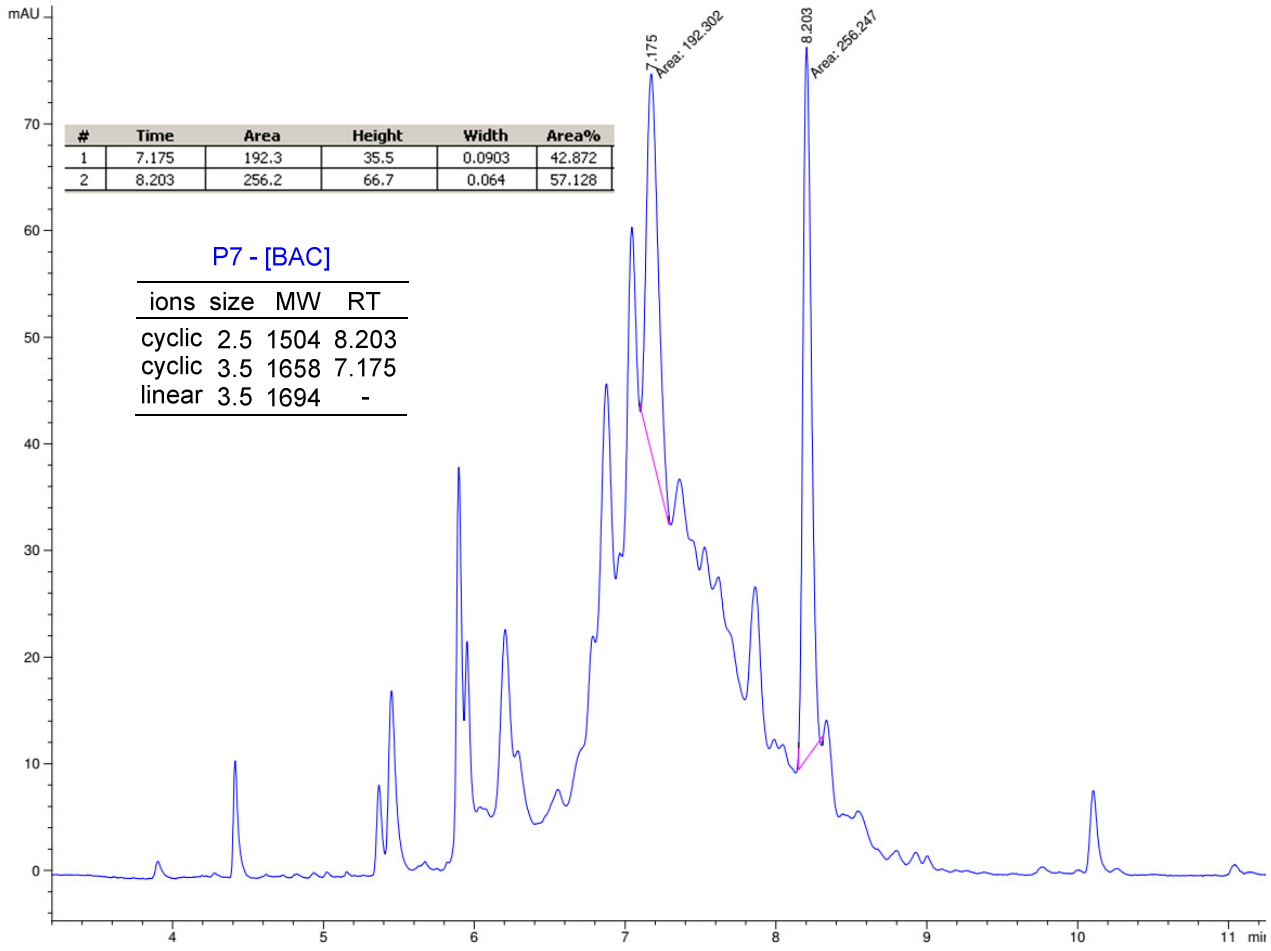




P7-[BAC]: Cyclization was complete on both 10 µm & 160 µm beads.



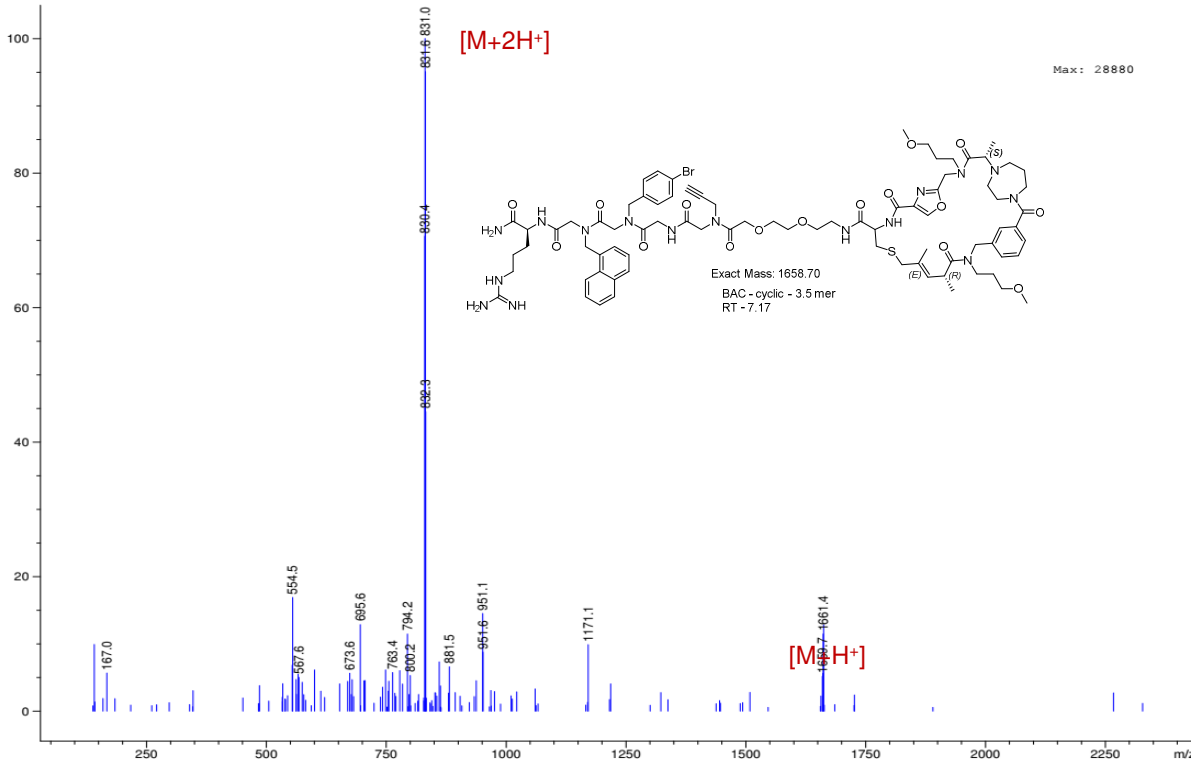


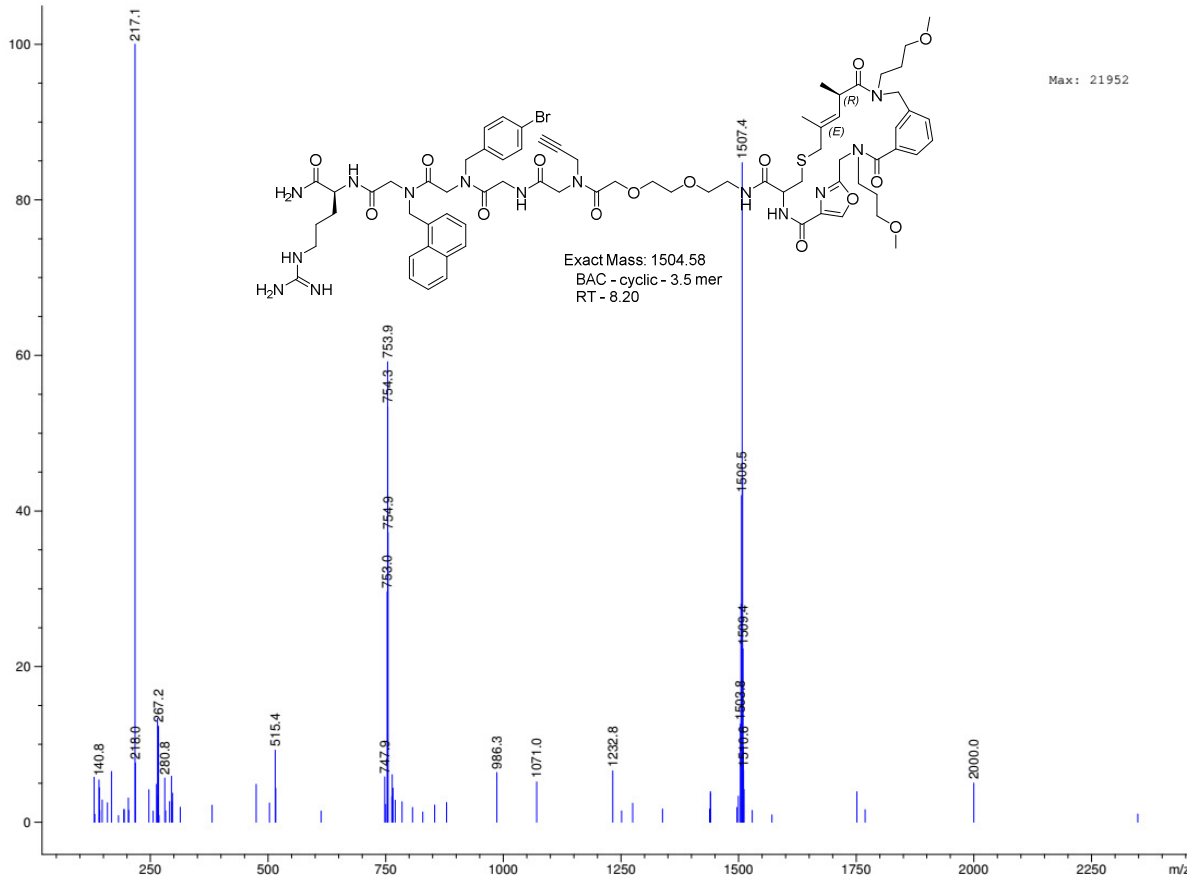


#	Time	Area	Height	Width	Area%
1	7.175	192.3	35.5	0.0903	42.872
2	8.203	256.2	66.7	0.064	57.128

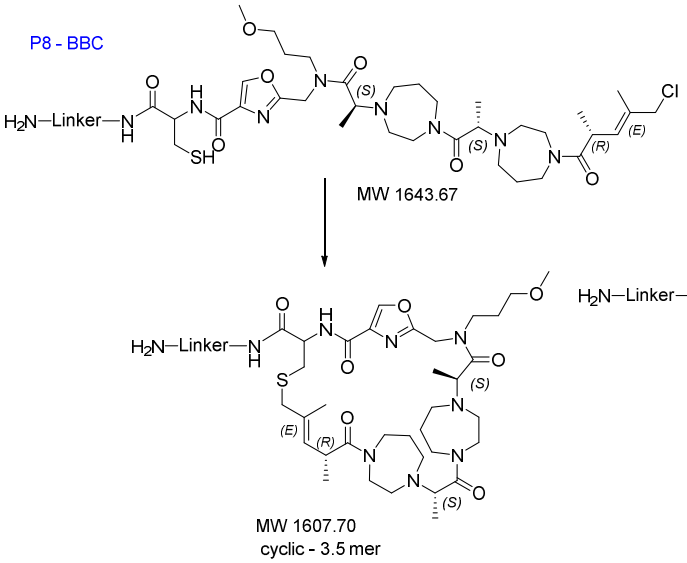
P7 - [BAC]

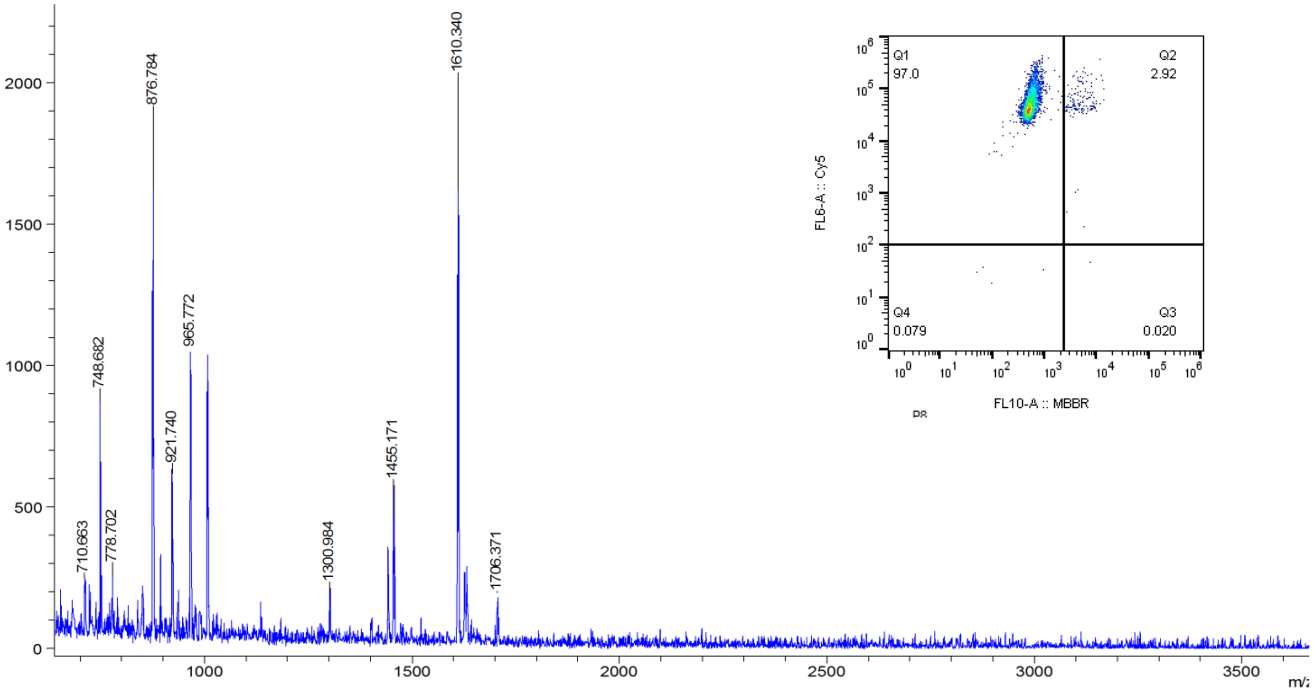
ions	size	MW	RT
cyclic	2.5	1504	8.203
cyclic	3.5	1658	7.175
linear	3.5	1694	-

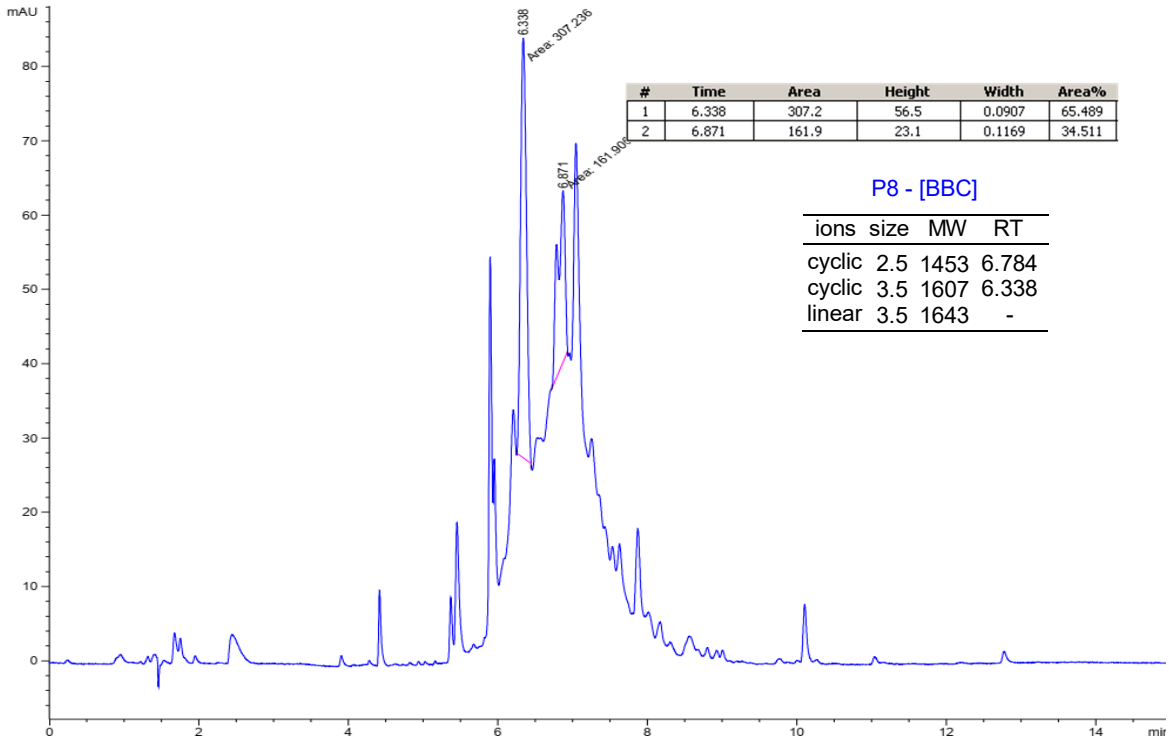

[M+2H+]
Max: 28880
Exact Mass: 1658.70
BAC - cyclic - 3.5 mer
RT - 7.17
[M+H+]
831.0
831.6
880.4
832.0
554.5
695.6
794.2
951.1
951.6
1171.1
1661.4
1660.7
167.0
567.6
673.6
763.4
800.2
881.5
m/z

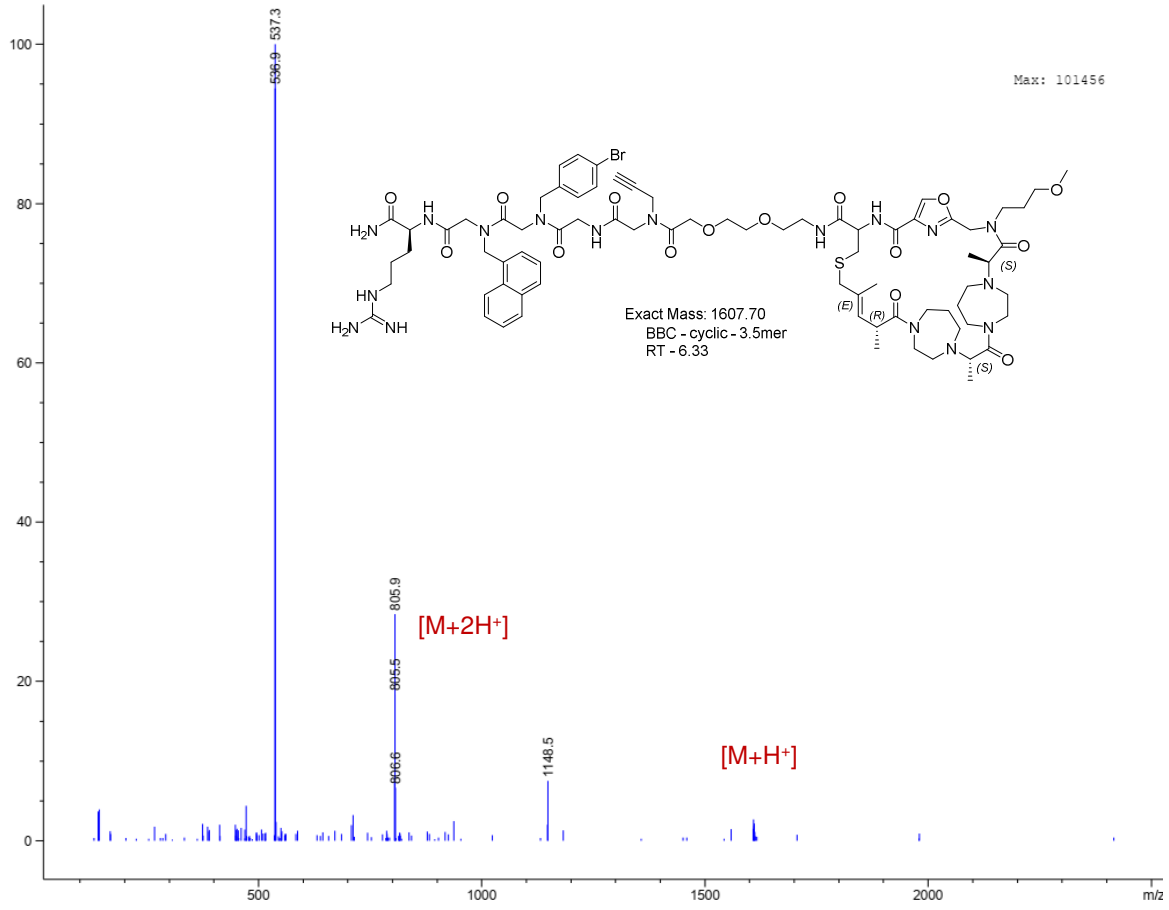

Max: 21952
Exact Mass: 1504.58
BAC - cyclic - 3.5 mer
RT - 8.20
217.1
753.9
754.3
754.9
763.0
1507.4
1506.5
1509.4
1503.8
1510.6
267.2
218.0
280.8
140.8
515.4
747.9
986.3
1071.0
1232.8
2000.0
m/z

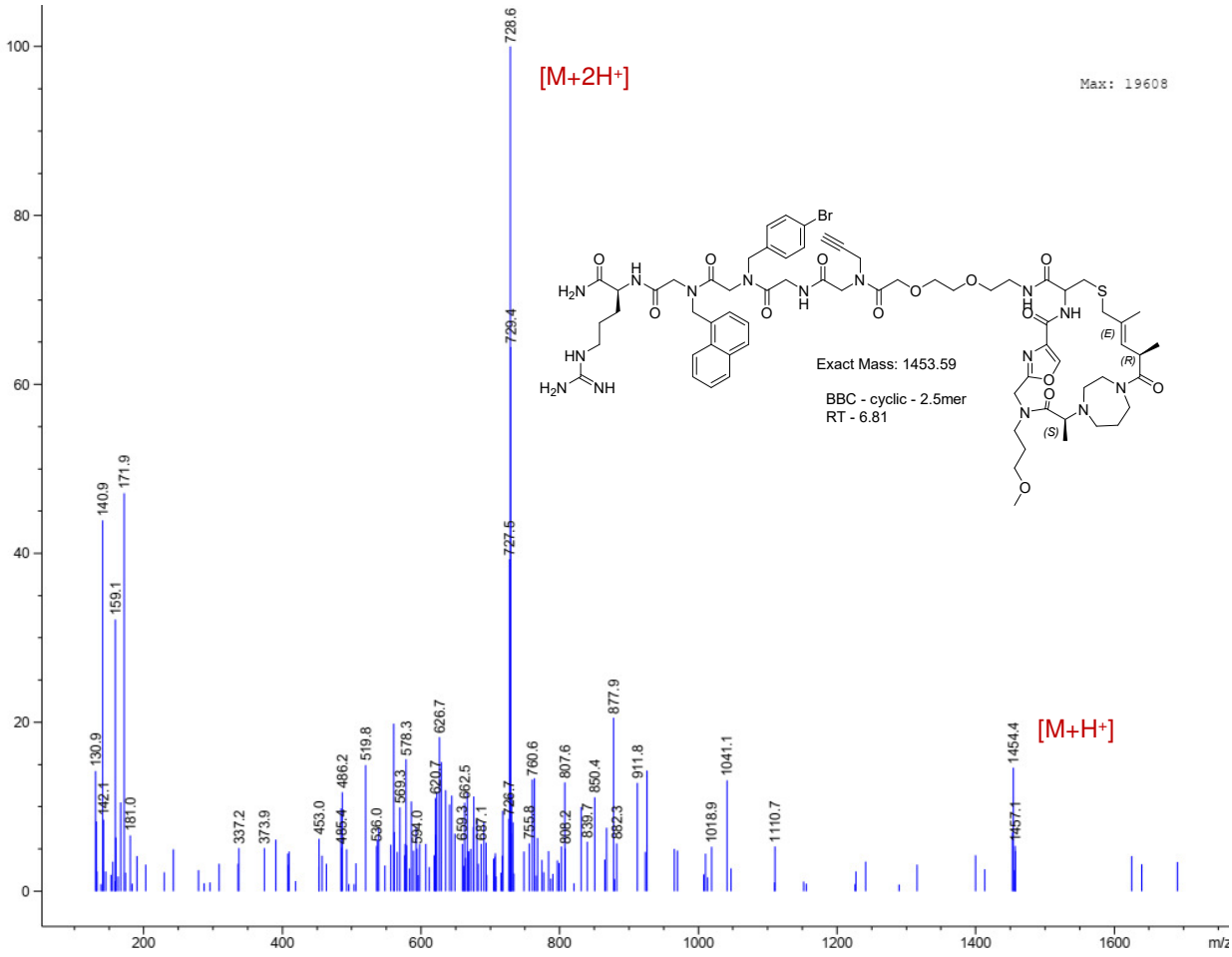
P8-[BBC]: Cyclization was complete on both 10 µm & 160 µm.



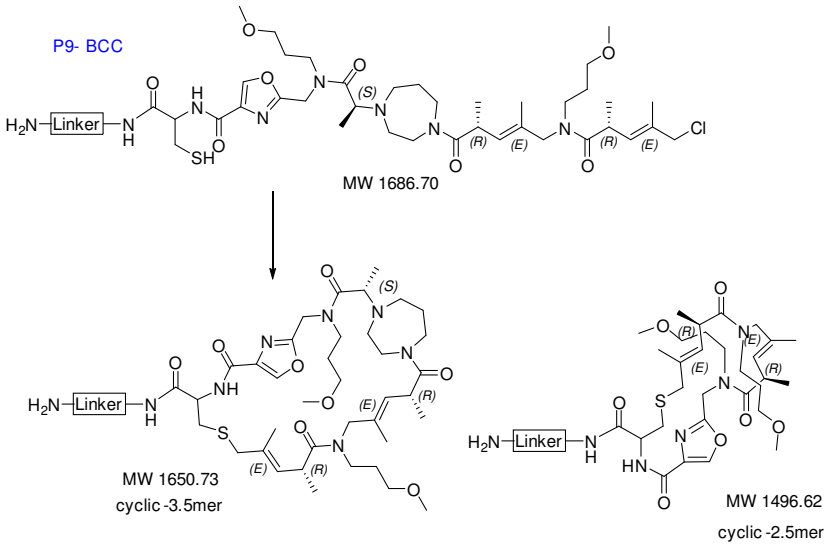


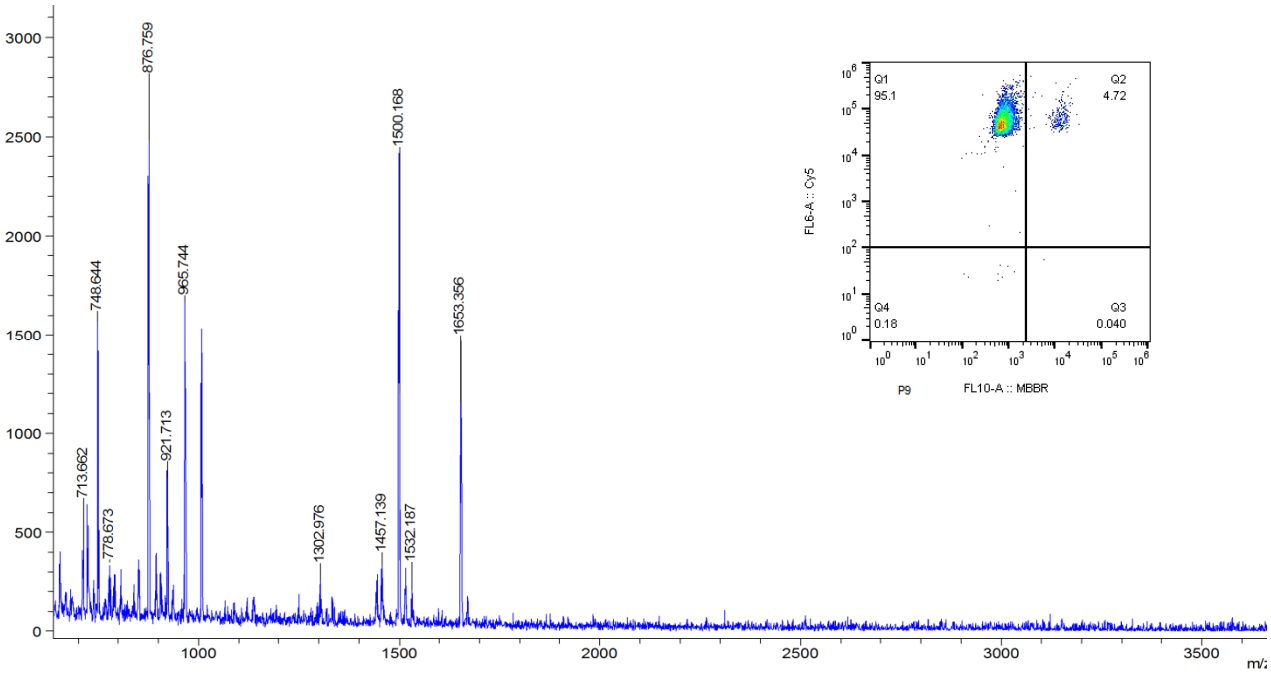

mAU
6.338
Area: 307.236
6.871
Area: 161.900
| Time | Area | Height | Width | Area%
1 | 6.338 | 307.2 | 56.5 | 0.0907 | 65.489
2 | 6.871 | 161.9 | 23.1 | 0.1169 | 34.511
P8 - [BBC]
ions size MW RT
cyclic 2.5 1453 6.784
cyclic 3.5 1607 6.338
linear 3.5 1643 -

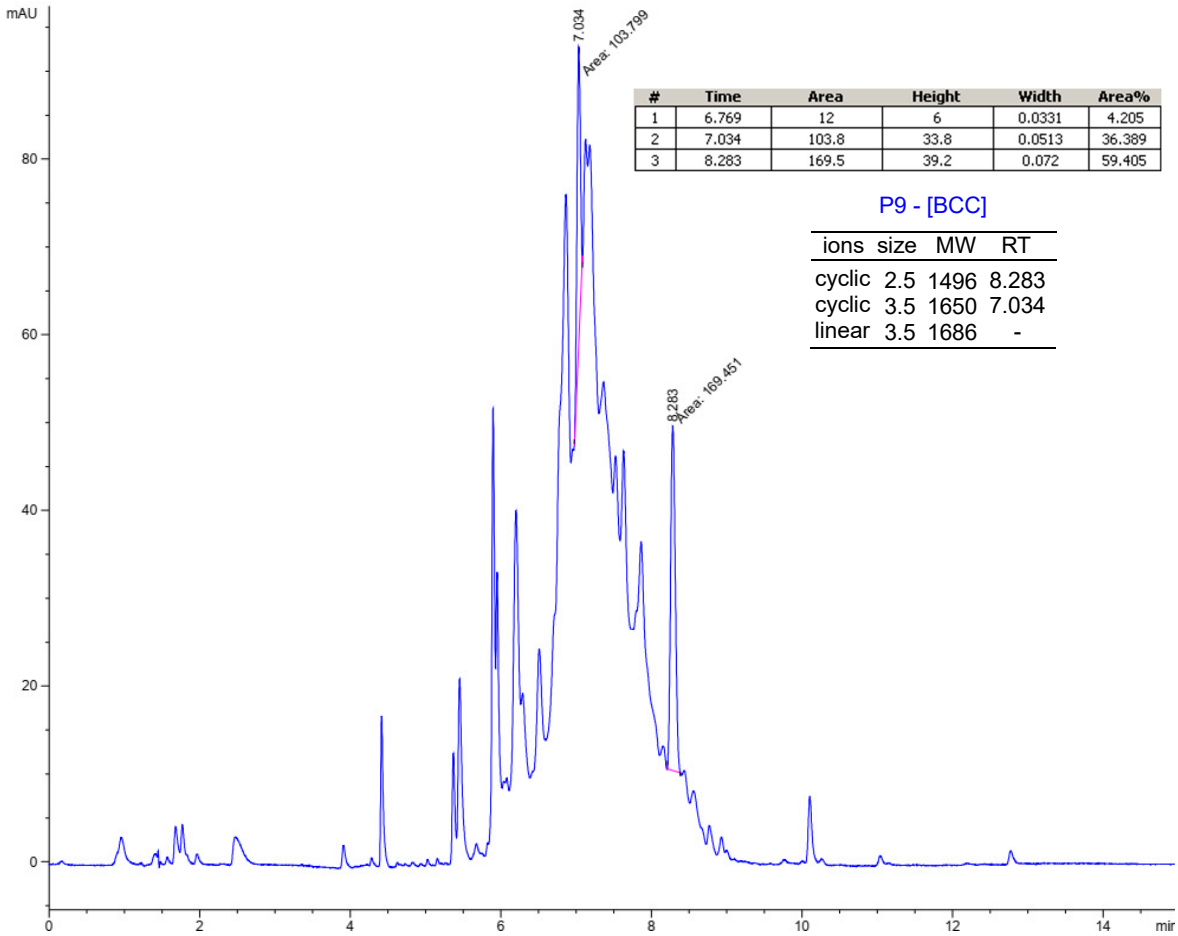

Max: 101456
537.3
805.9
805.5
806.6
1148.5
[M+2H+]
[M+H+]
Exact Mass: 1607.70
BBC - cyclic - 3.5mer
RT - 6.33
m/z



P9-[BCC]: Cyclization was complete on both 10 µm & 160 µm beads.



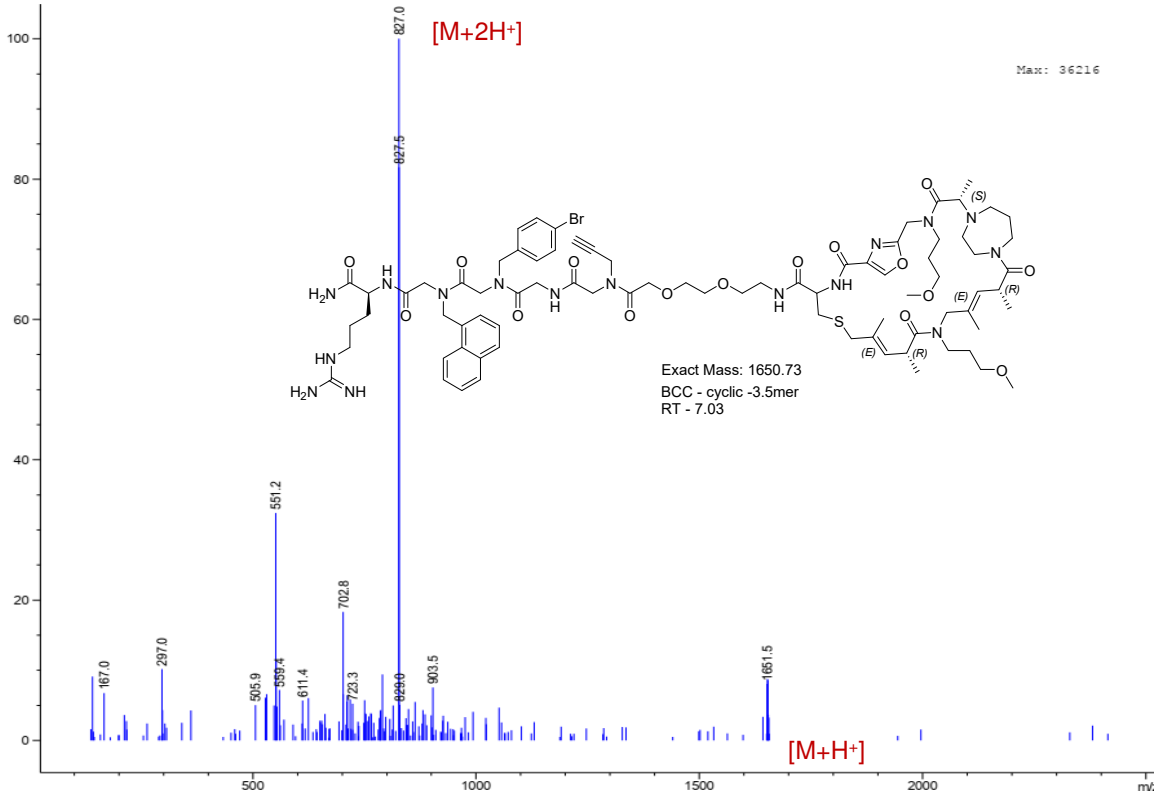


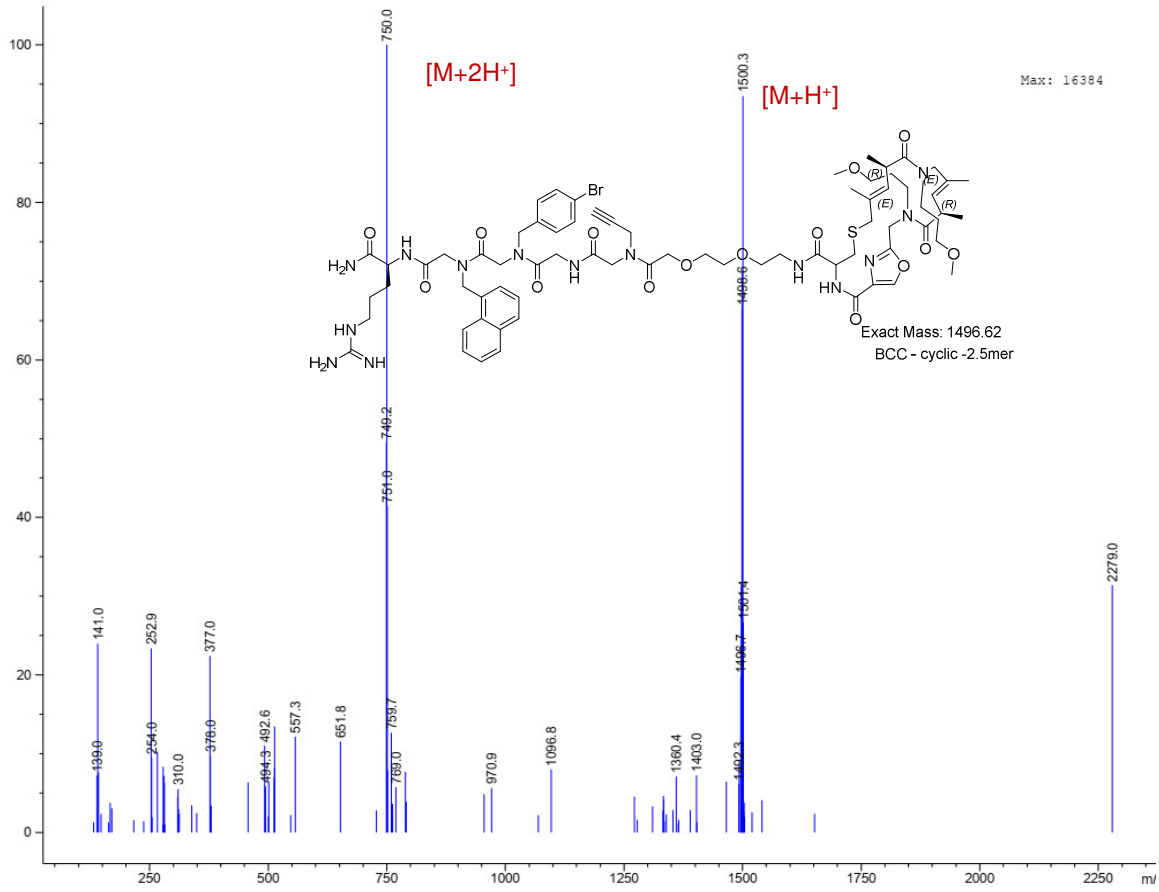


#	Time	Area	Height	Width	Area%
1	6.769	12	6	0.0331	4.205
2	7.034	103.8	33.8	0.0513	36.389
3	8.283	169.5	39.2	0.072	59.405

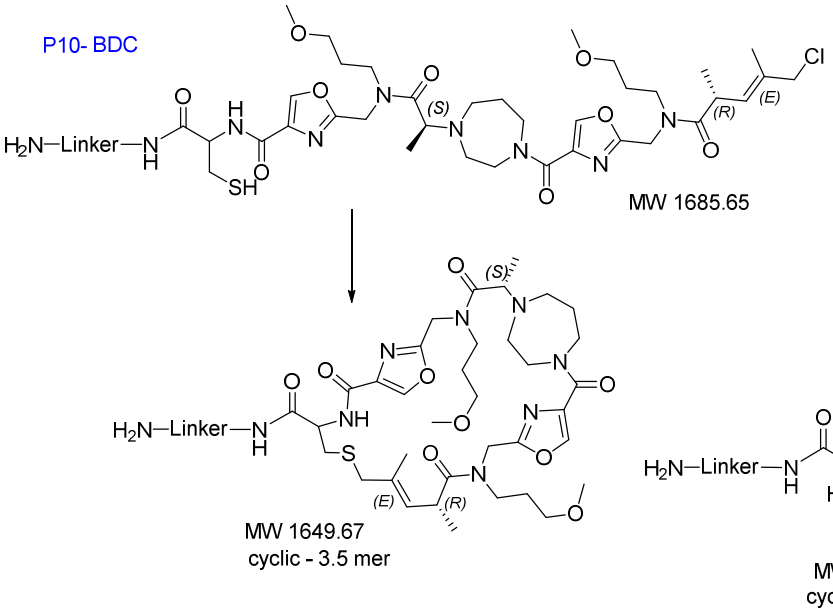
P9 - [BCC]

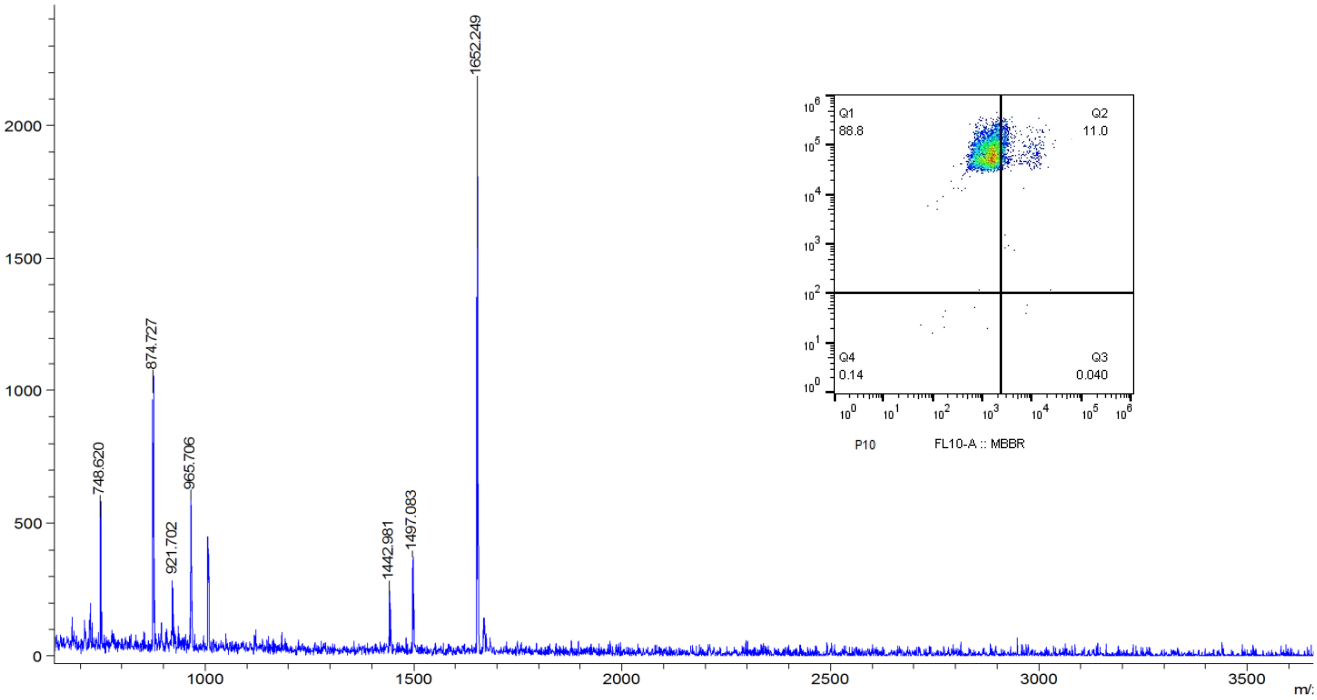
ions	size	MW	RT
cyclic	2.5	1496	8.283
cyclic	3.5	1650	7.034
linear	3.5	1686	-

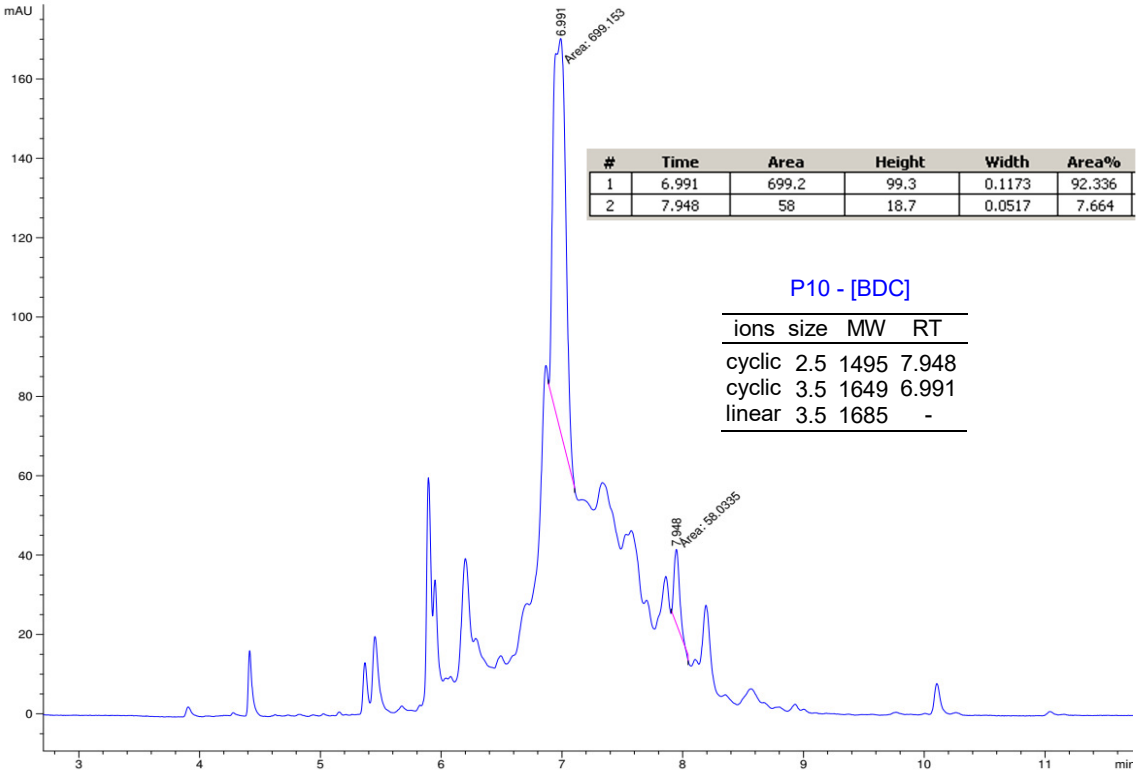

[M+2H+]
Max: 36216
827.0
827.5
551.2
702.8
297.0
167.0
505.9
559.4
611.4
723.3
829.0
903.5
1651.5
[M+H+]
Exact Mass: 1650.73
BCC - cyclic -3.5mer
RT - 7.03
100
80
60
40
20
0
500
1000
1500
2000
m/


[M+2H+]
[M+H+]
Max: 16384
750.0
1500.3
749.2
751.0
141.0
252.9
377.0
651.8
759.7
557.3
492.6
1096.8
970.9
1360.4
1403.0
2279.0
Exact Mass: 1496.62
BCC - cyclic -2.5mer
100
80
60
40
20
0
250
500
750
1000
1250
1500
1750
2000
2250
m/

P10-[BDC]: Incomplete cyclization was detected on 10 µm but was complete on 160 µm beads.



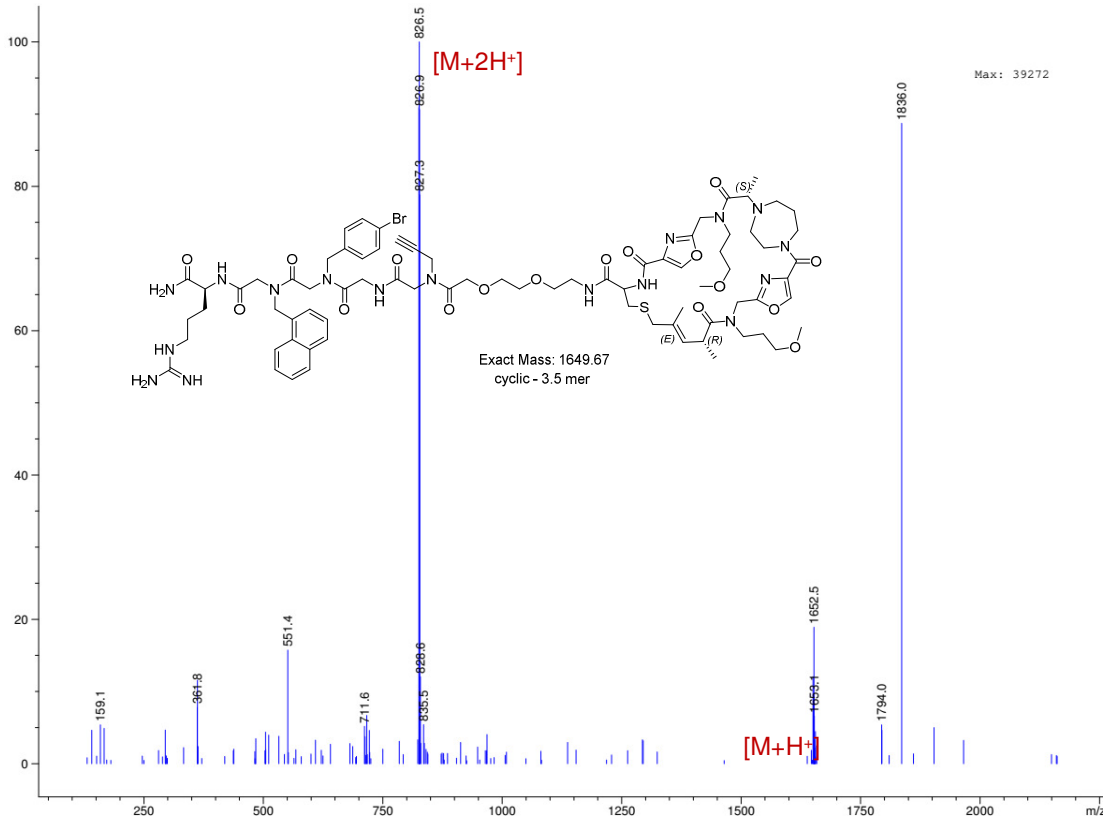


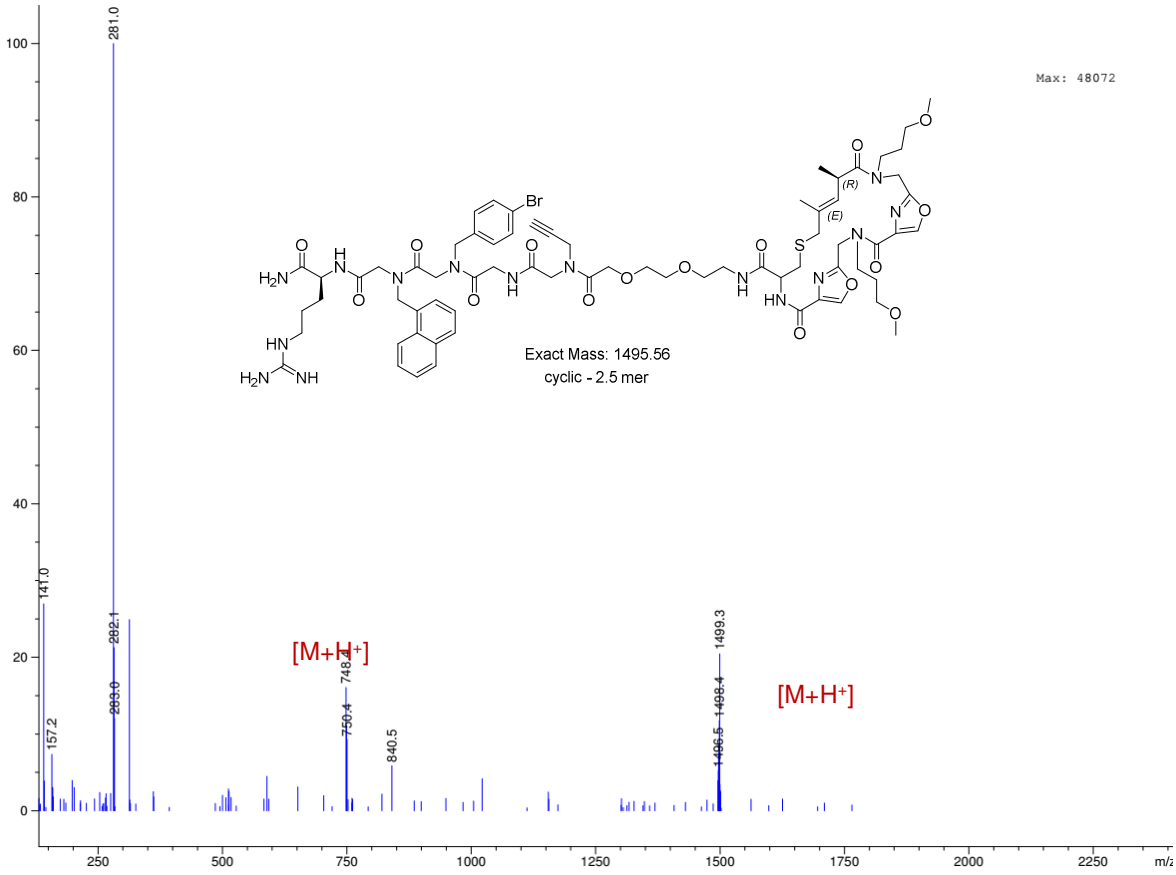


#	Time	Area	Height	Width	Area%
1	6.991	699.2	99.3	0.1173	92.336
2	7.948	58	18.7	0.0517	7.664

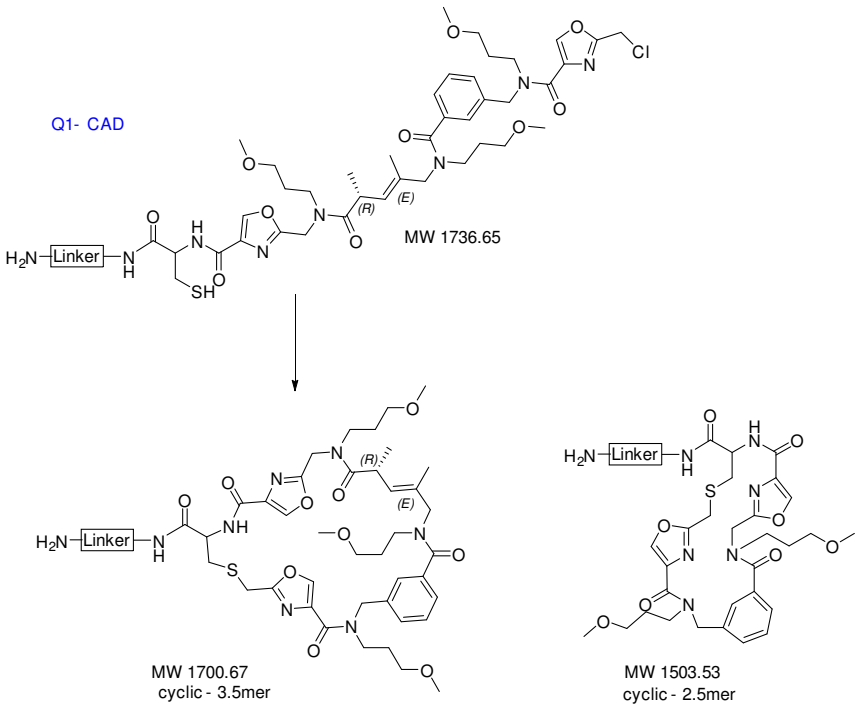
P10 - [BDC]

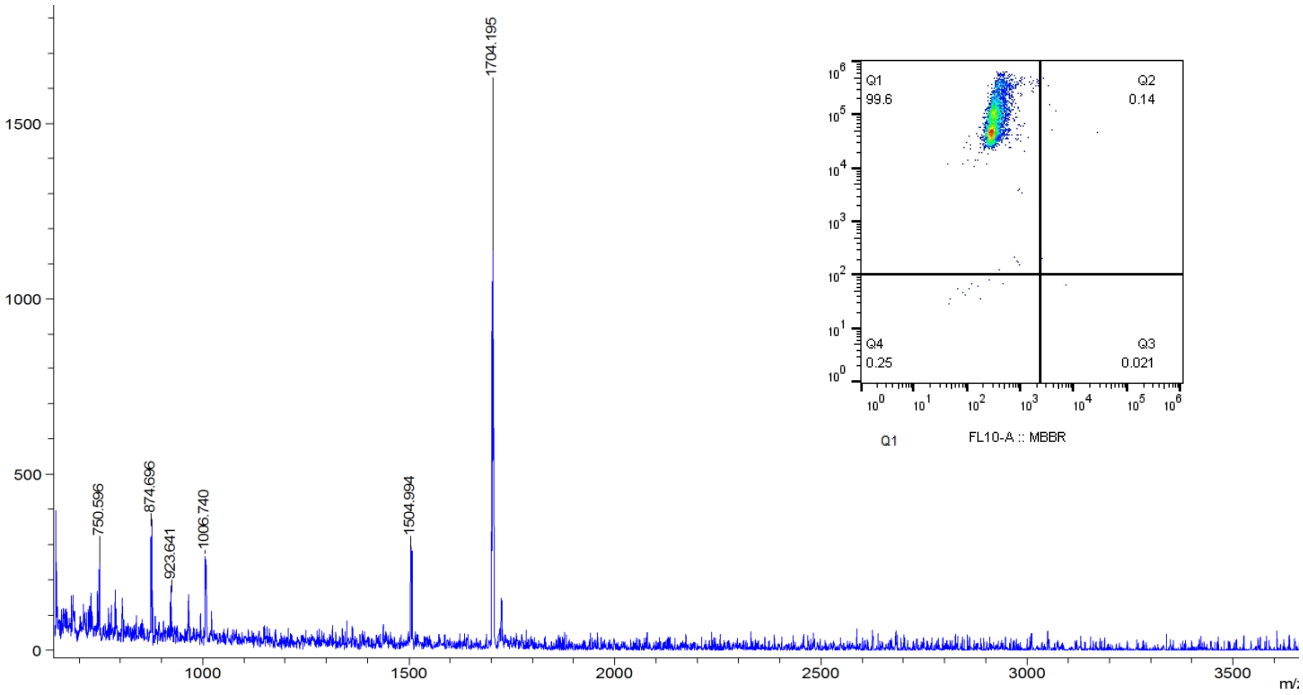
ions	size	MW	RT
cyclic	2.5	1495	7.948
cyclic	3.5	1649	6.991
linear	3.5	1685	-

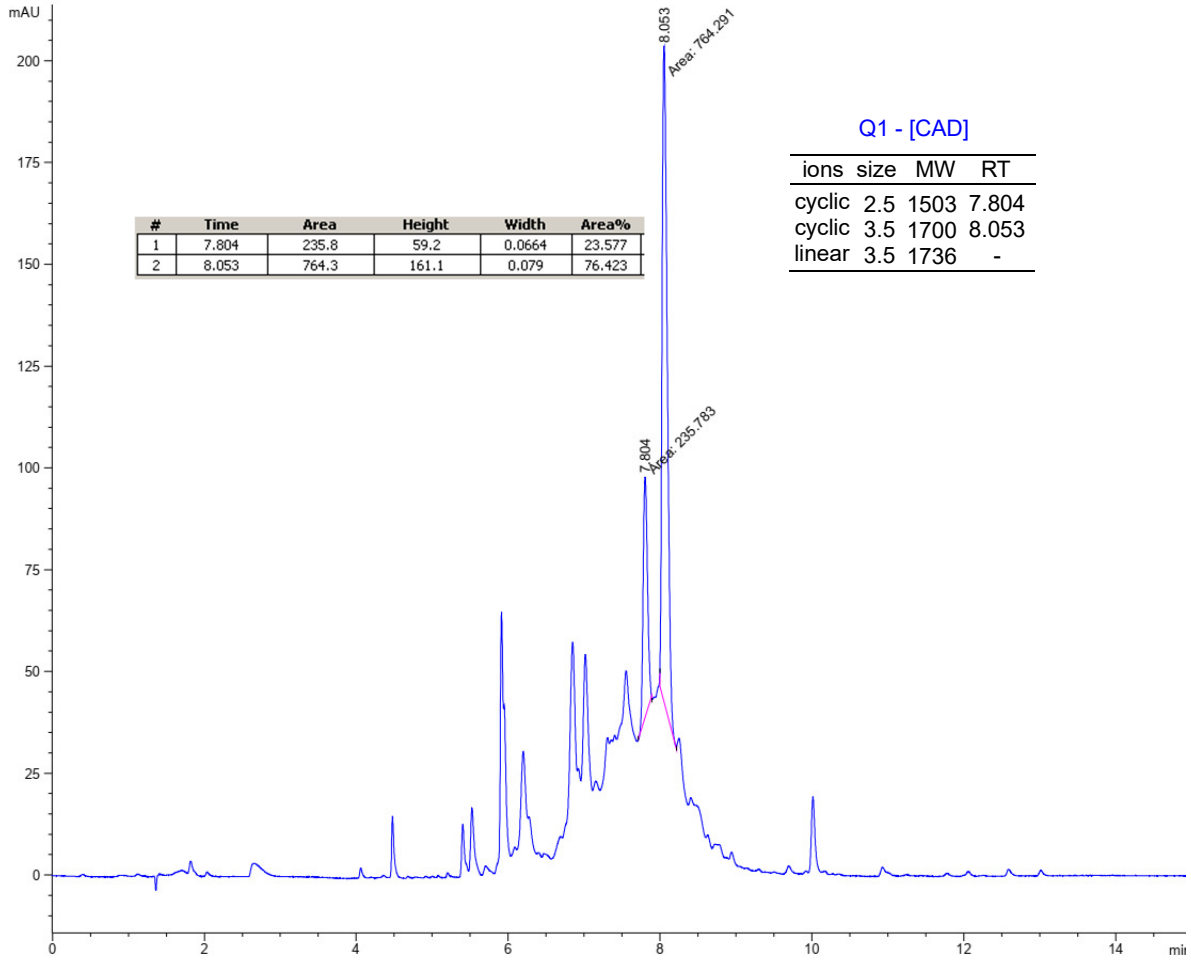




Q1-[CAD]: Cyclization was complete on both 10 µm & 160 µm beads.



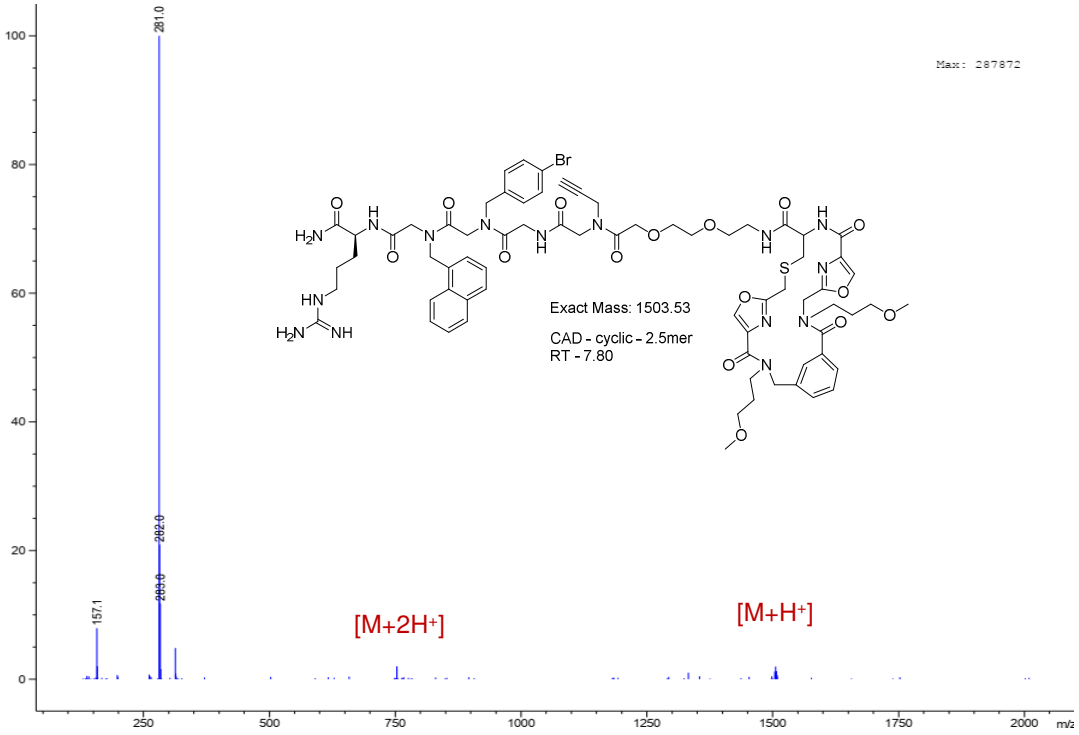


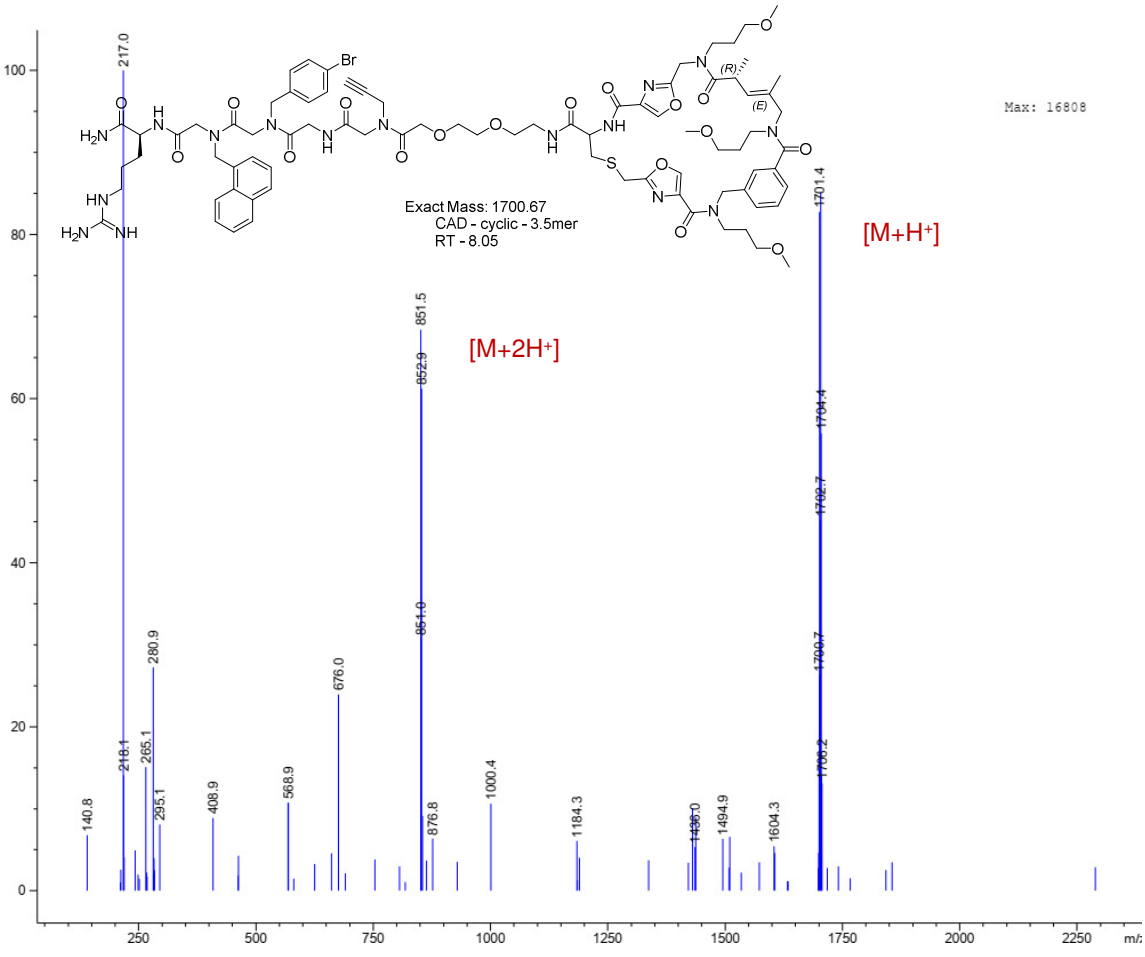


#	Time	Area	Height	Width	Area%
1	7.804	235.8	59.2	0.0664	23.577
2	8.053	764.3	161.1	0.079	76.423

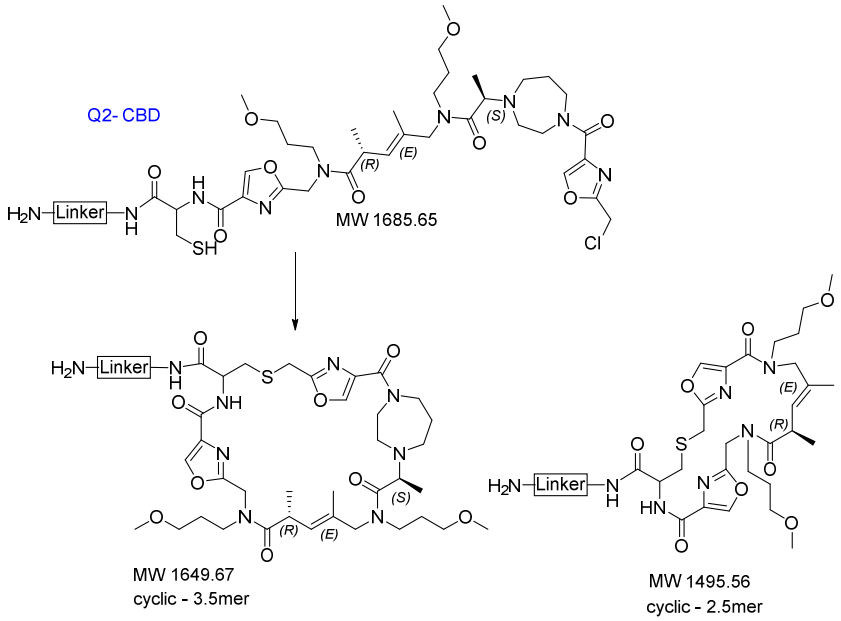
Q1 - [CAD]

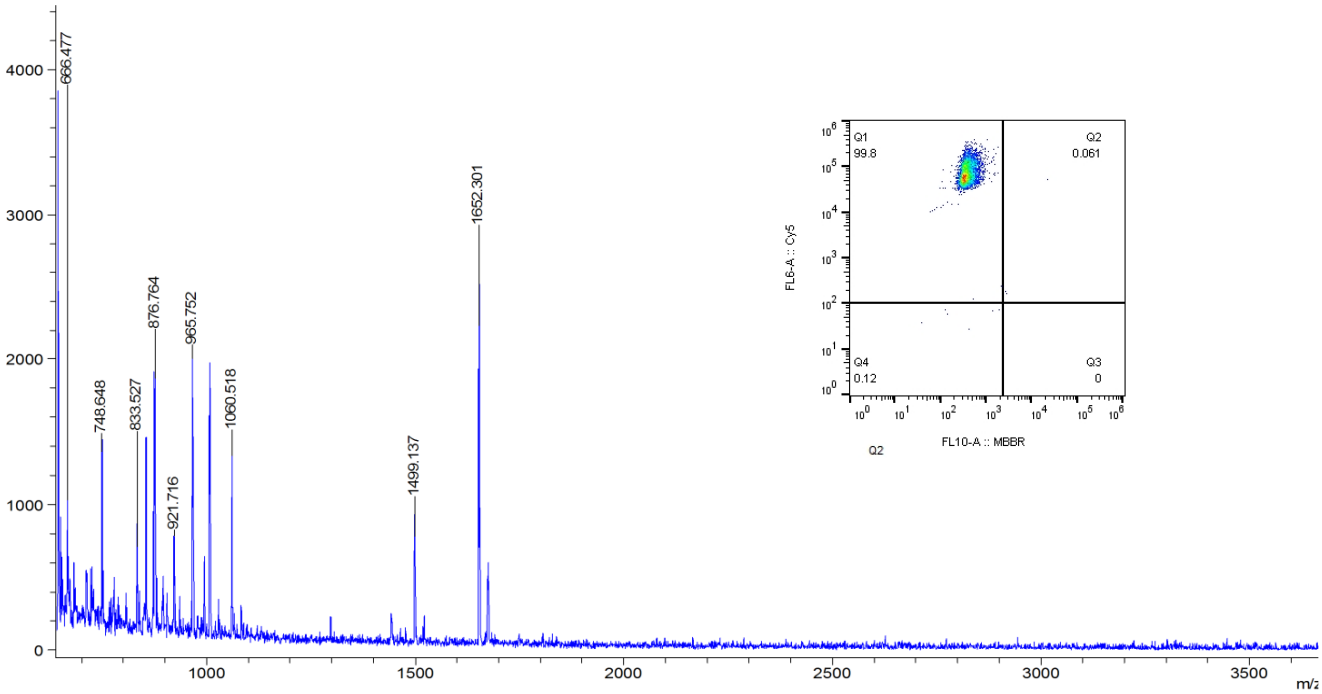
ions	size	MW	RT
cyclic	2.5	1503	7.804
cyclic	3.5	1700	8.053
linear	3.5	1736	-

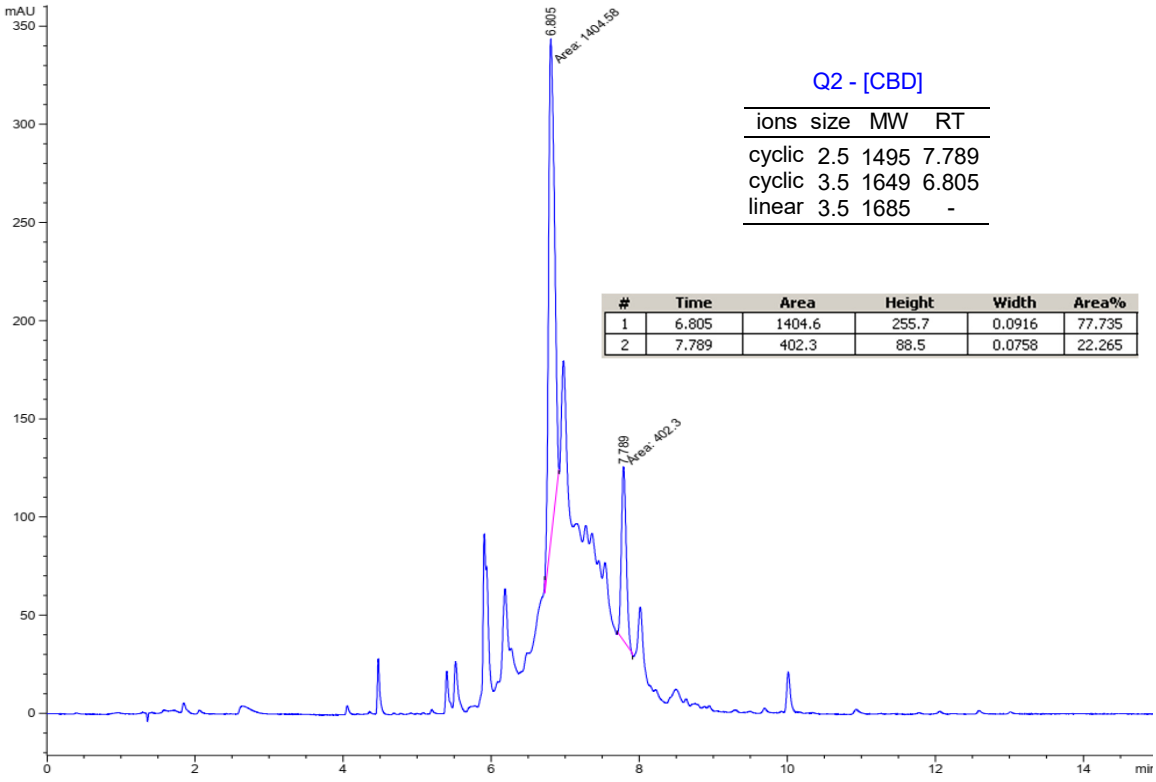

Max: 287872
Exact Mass: 1503.53
CAD - cyclic - 2.5mer
RT - 7.80
[M+2H+]
[M+H+]


Max: 16808
Exact Mass: 1700.67
CAD - cyclic - 3.5mer
RT - 8.05
[M+2H+]
[M+H+]

Q2-[CBD]: Cyclization was complete on both 10 µm & 160 µm beads.



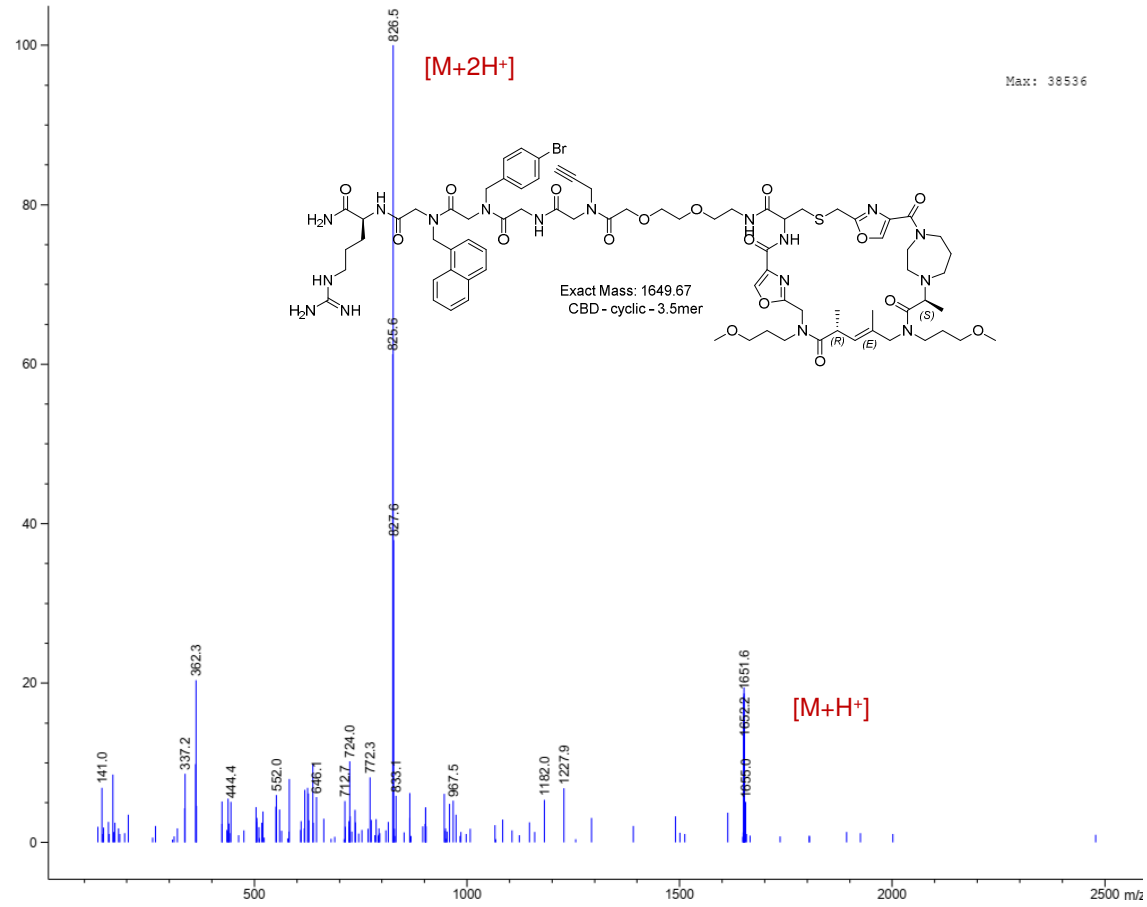


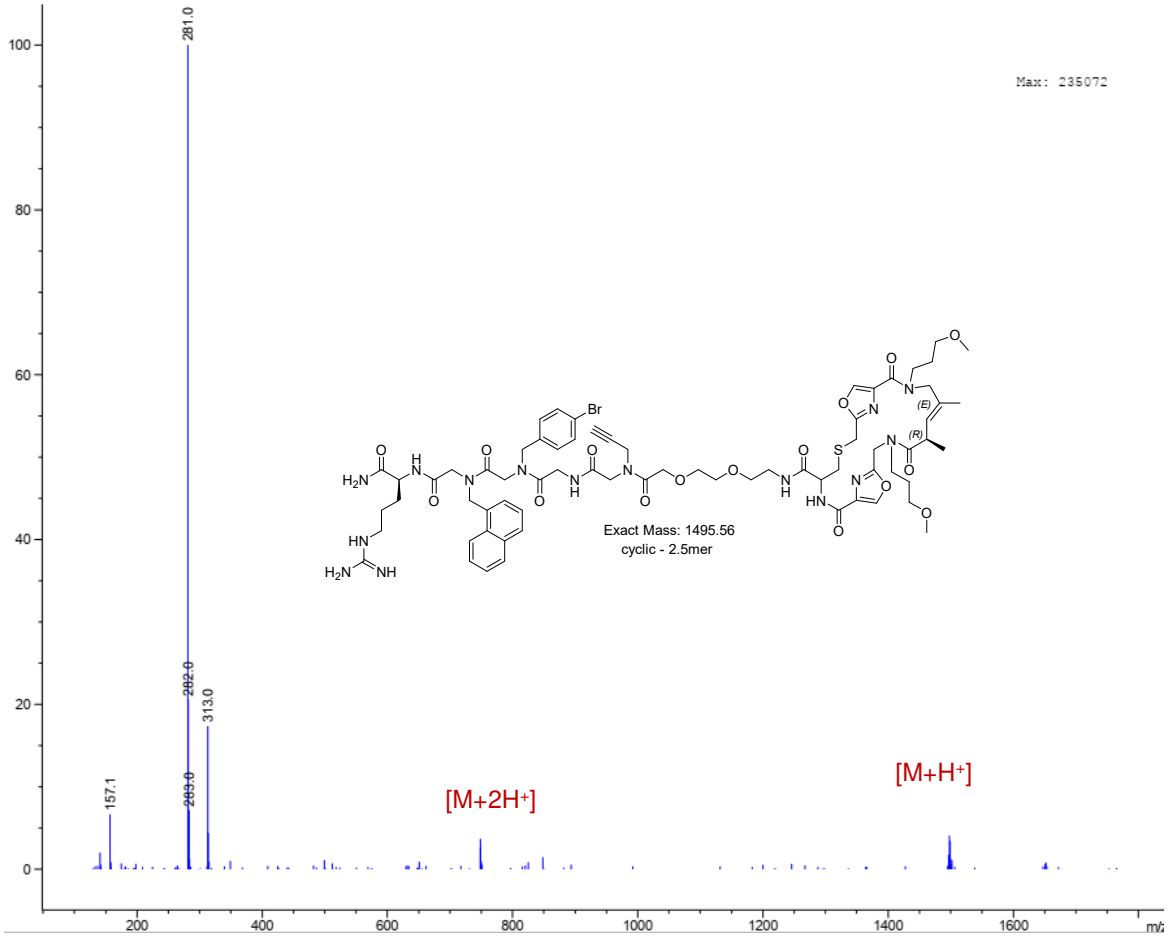


Q2 - [CBD]

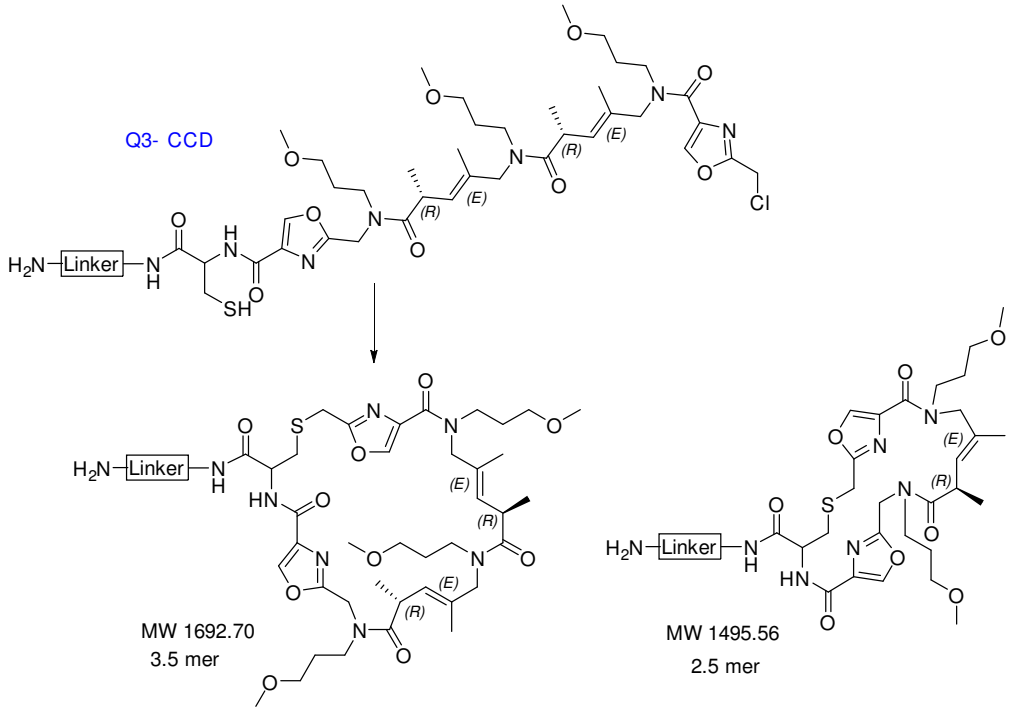
ions	size	MW	RT
cyclic	2.5	1495	7.789
cyclic	3.5	1649	6.805
linear	3.5	1685	-

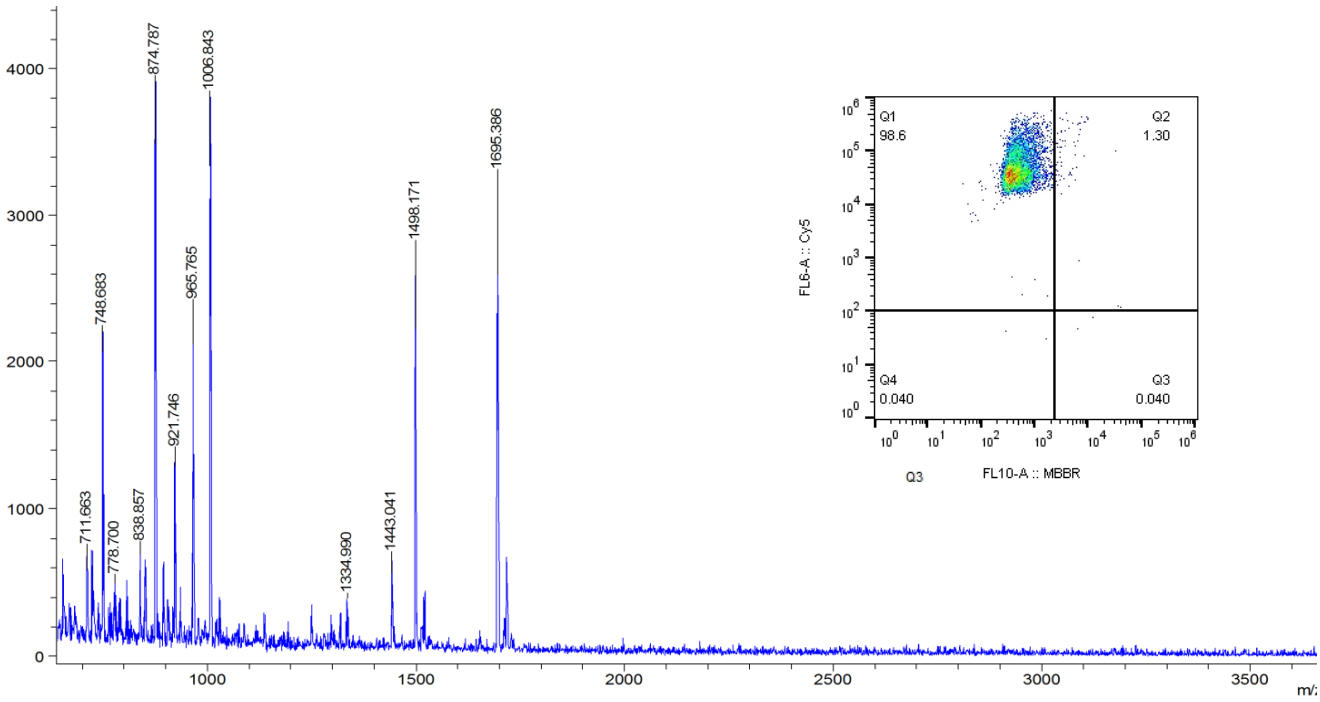
#	Time	Area	Height	Width	Area%
1	6.805	1404.6	255.7	0.0916	77.735
2	7.789	402.3	88.5	0.0758	22.265

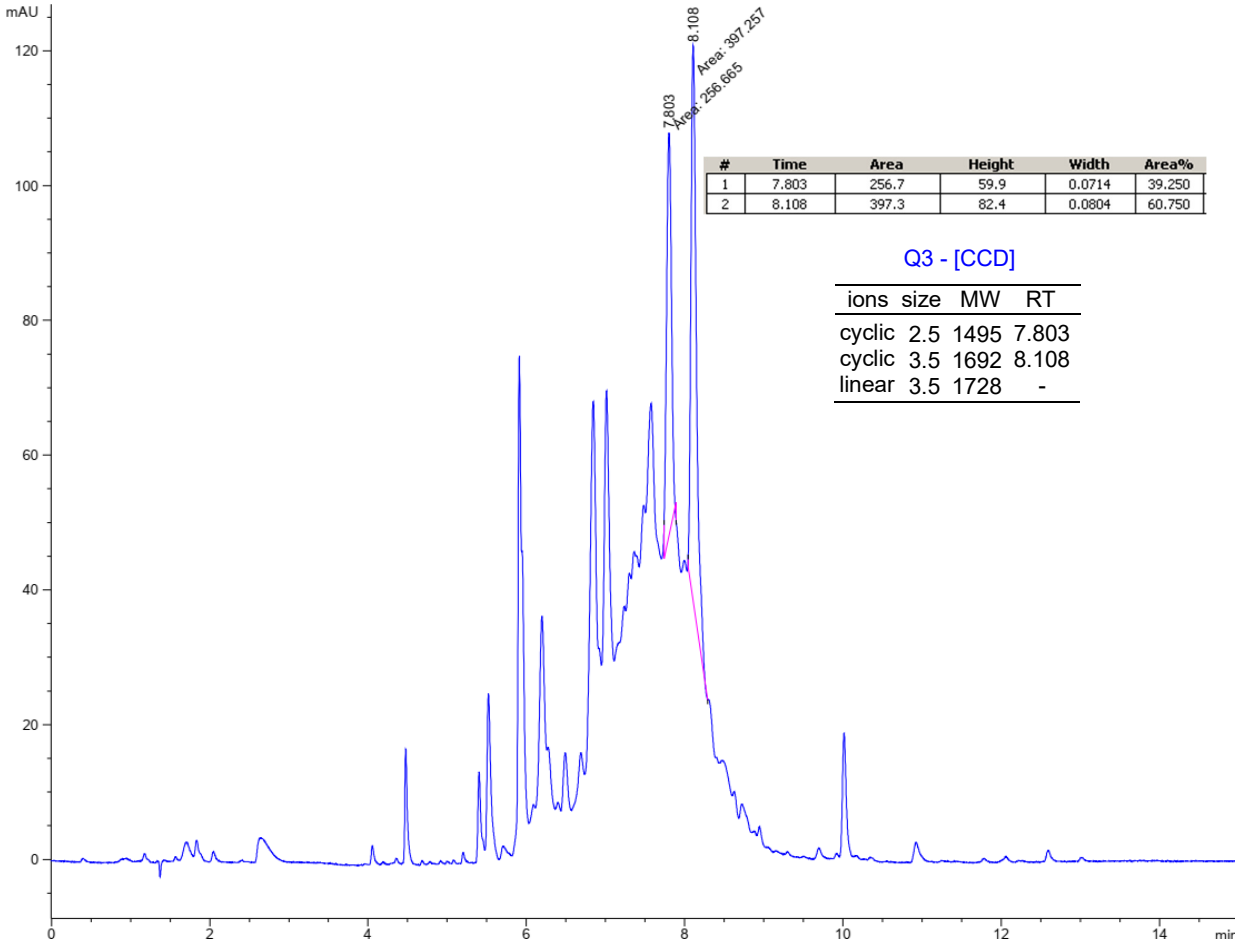




Q3-[CCD]: Cyclization was complete on both 10 µm & 160 µm beads.



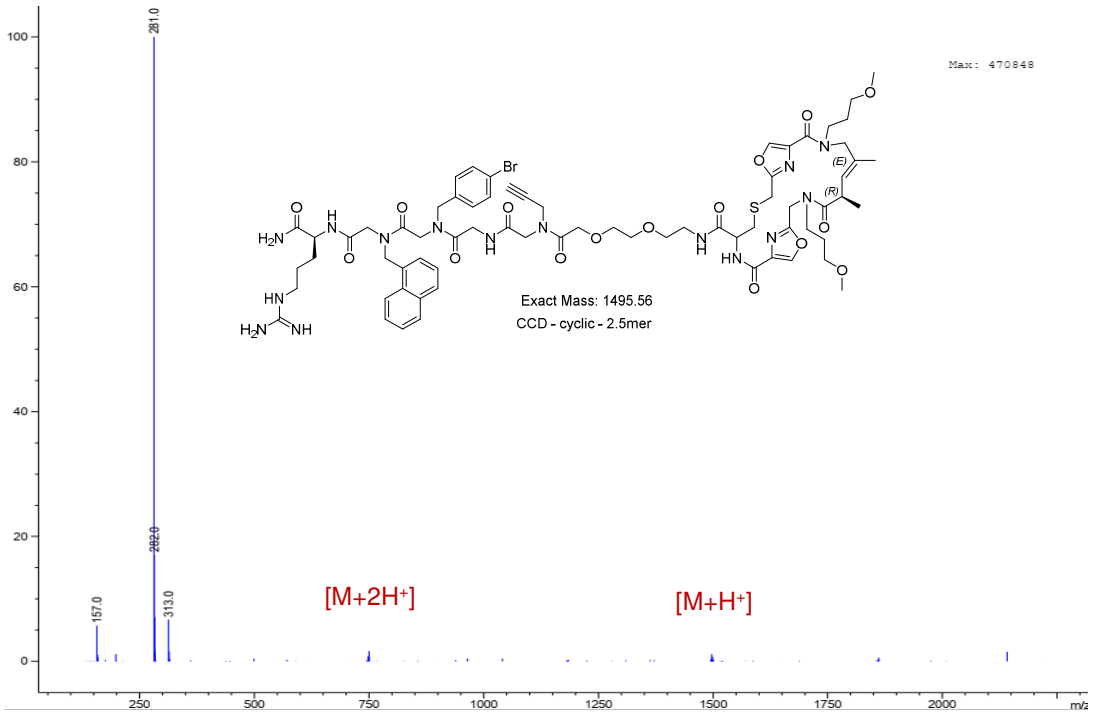


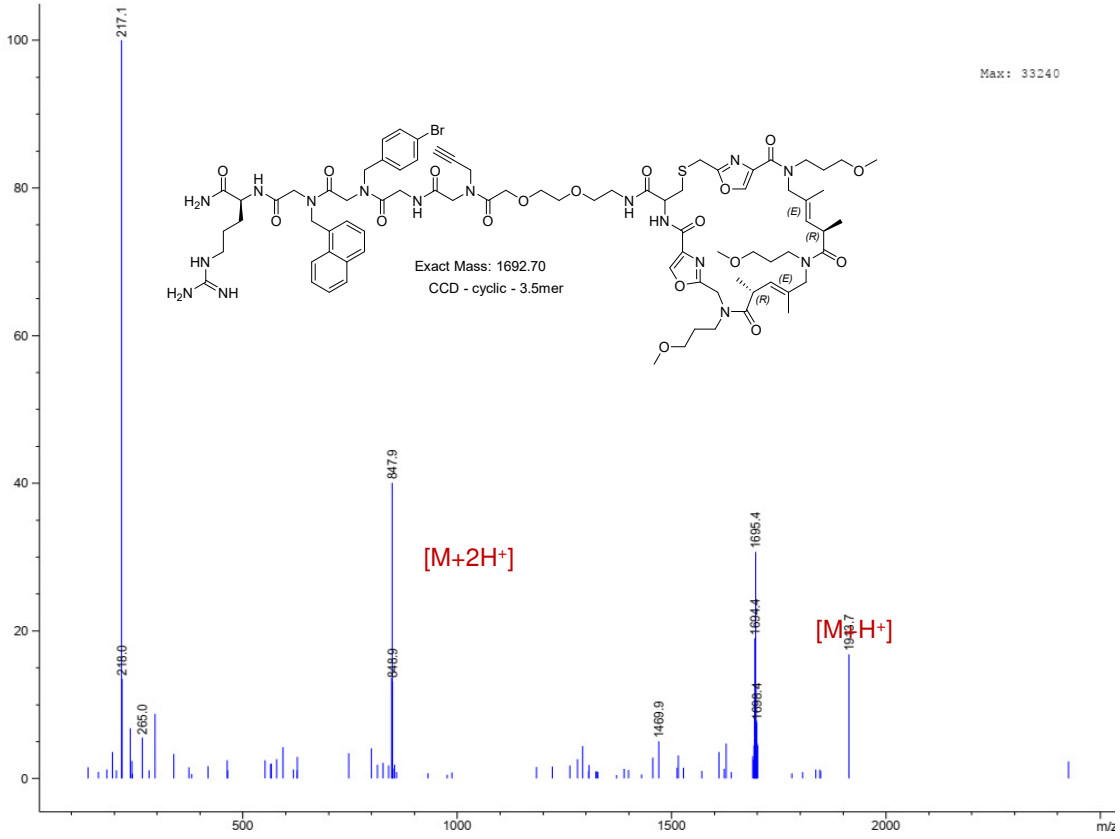


#	Time	Area	Height	Width	Area%
1	7.803	256.7	59.9	0.0714	39.250
2	8.108	397.3	82.4	0.0804	60.750

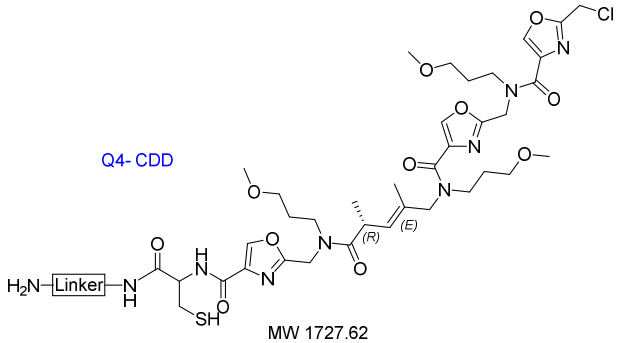
Q3 - [CCD]

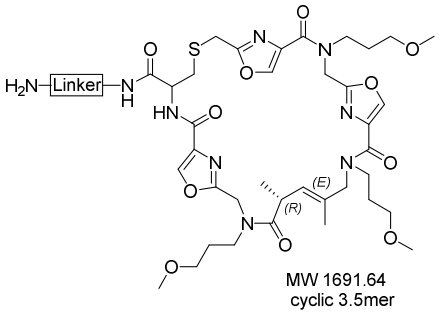
ions	size	MW	RT
cyclic	2.5	1495	7.803
cyclic	3.5	1692	8.108
linear	3.5	1728	-

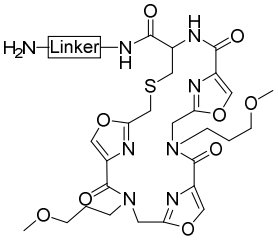

Max: 470848
Exact Mass: 1495.56
CCD - cyclic - 2.5mer
[M+2H+]
[M+H+]
281.0
282.0
313.0
157.0

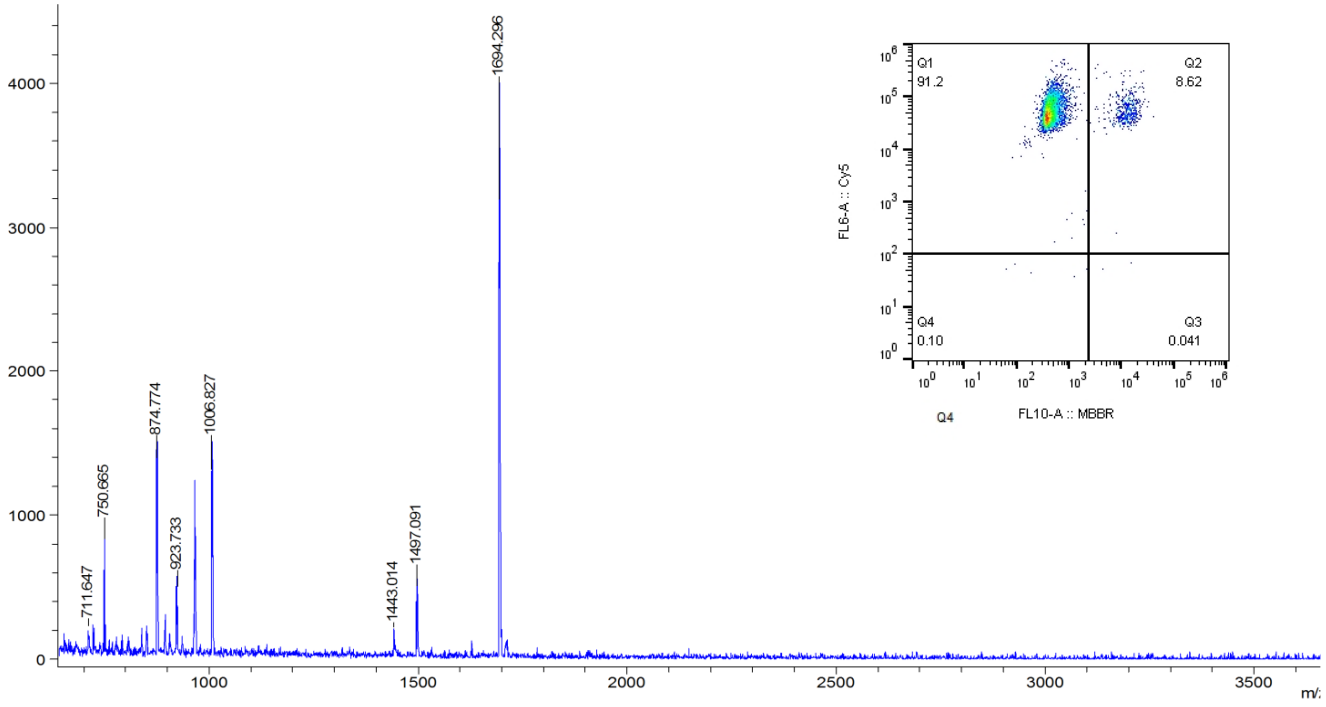

Max: 33240
Exact Mass: 1692.70
CCD - cyclic - 3.5mer
[M+2H+]
[M+H+]
217.1
847.9
1695.4
1694.4
1938.7
216.0
265.0
848.9
1469.9
1696.4

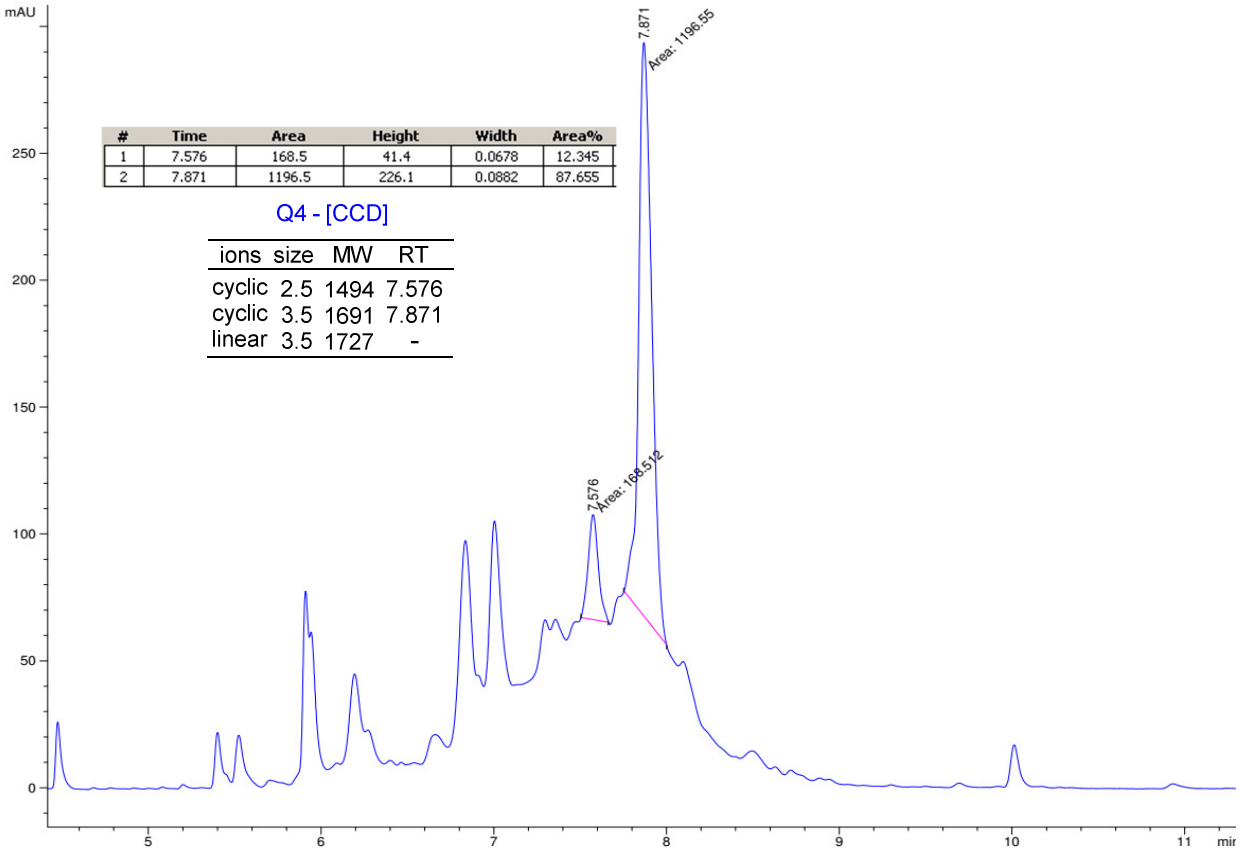
Q4-[CDD]: Cyclization was complete on both 10 µm & 160 µm beads.







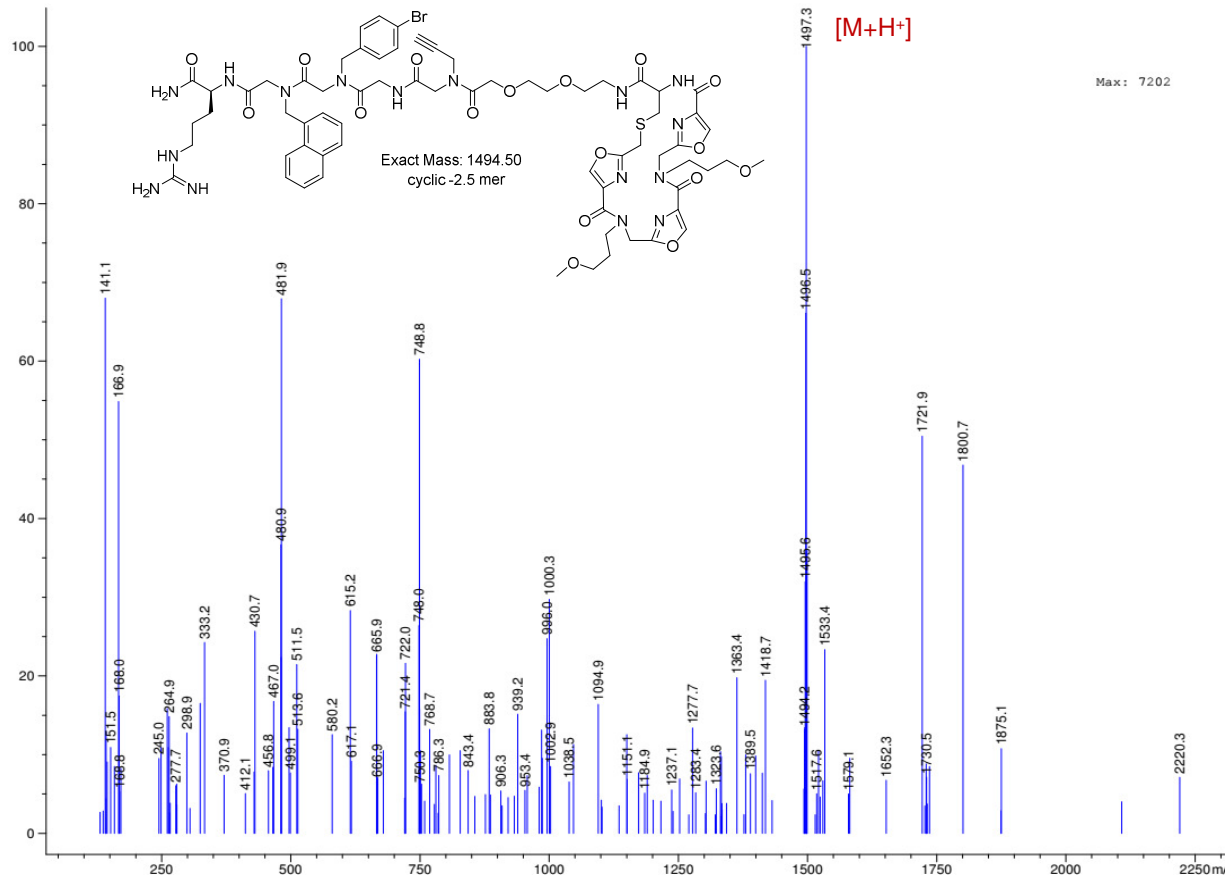


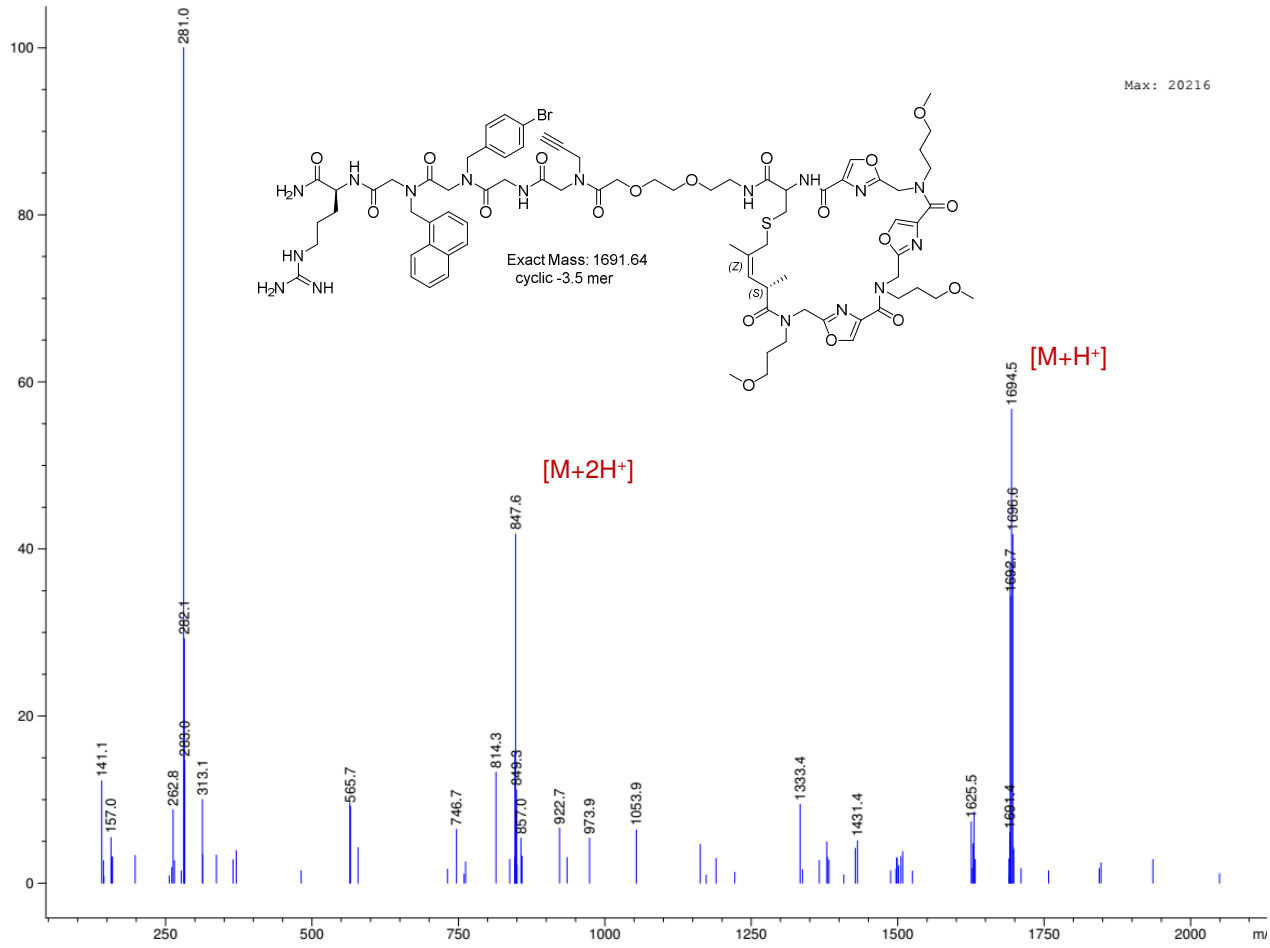


#	Time	Area	Height	Width	Area%
1	7.576	168.5	41.4	0.0678	12.345
2	7.871	1196.5	226.1	0.0882	87.655

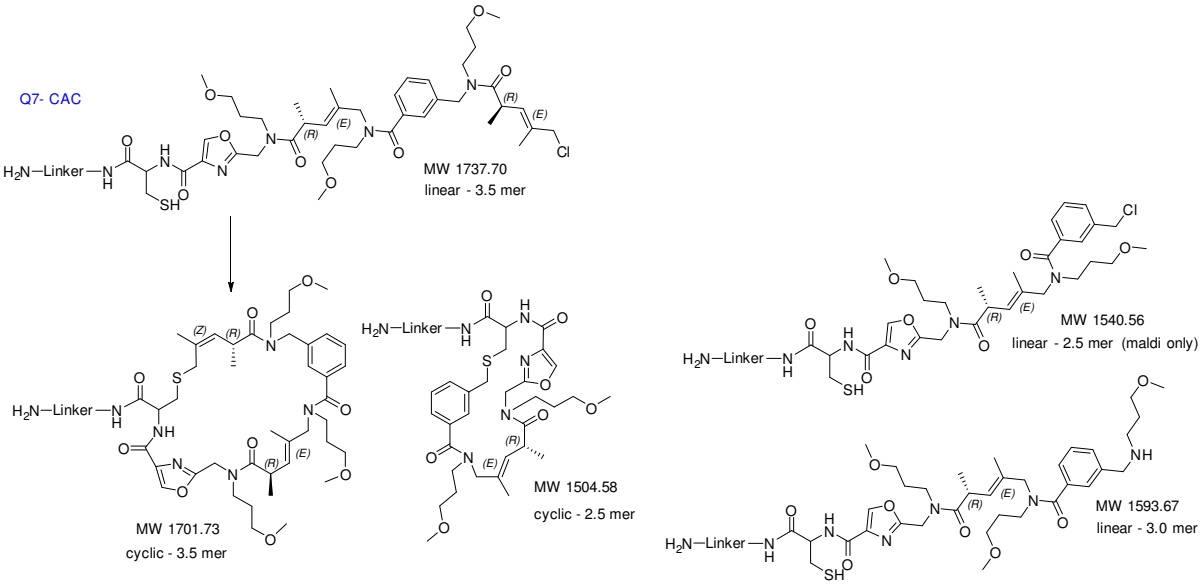
Q4 - [CCD]

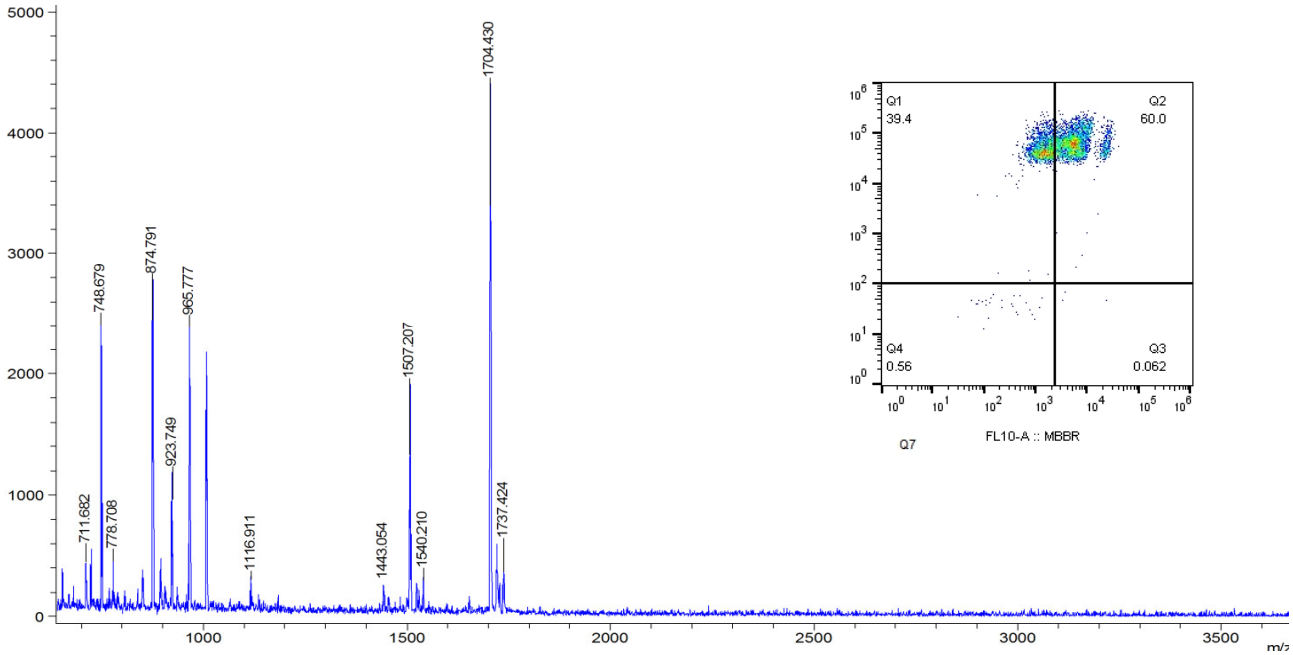
ions	size	MW	RT
cyclic	2.5	1494	7.576
cyclic	3.5	1691	7.871
linear	3.5	1727	-

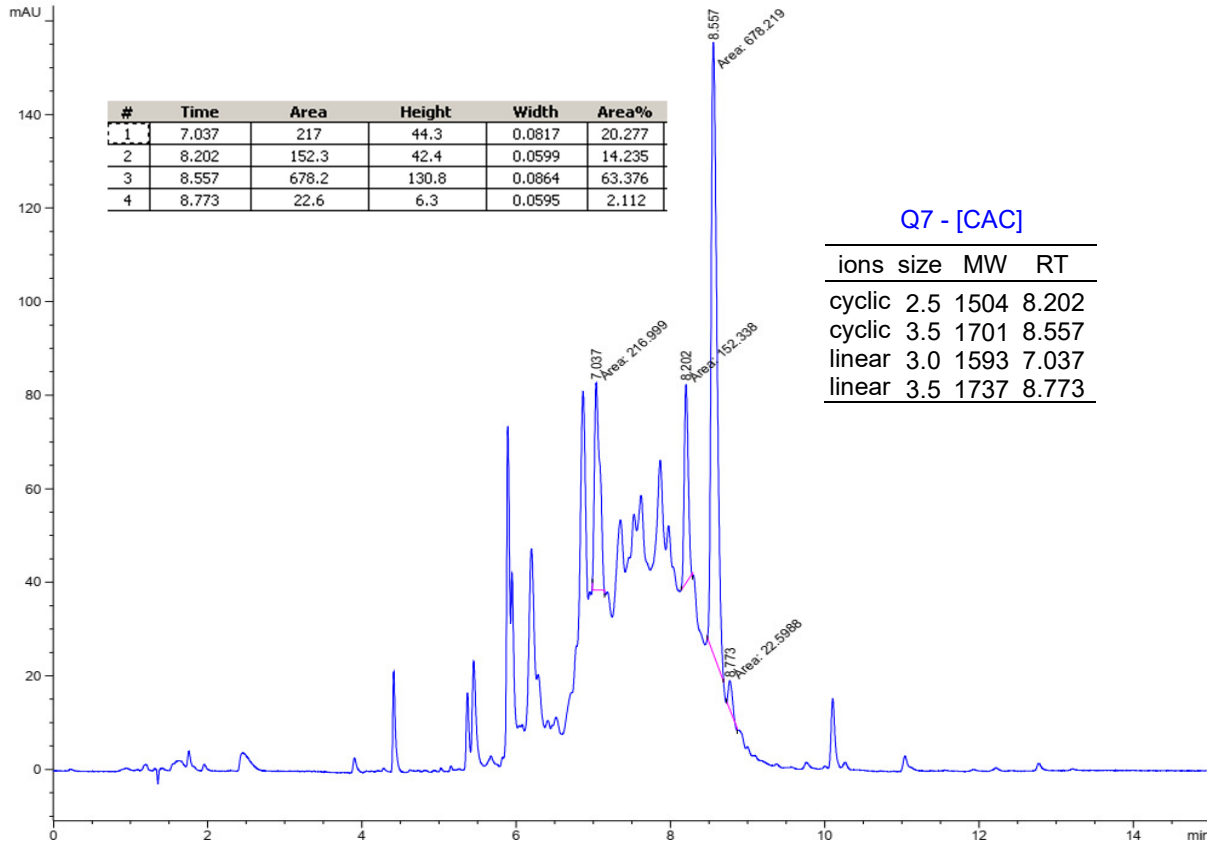




Q7-[CAC]: Incomplete cyclization was detected on 10 µm but completed >90% on 160 µm. A linear fragment (3.0-mer, MW 1593) were detected.



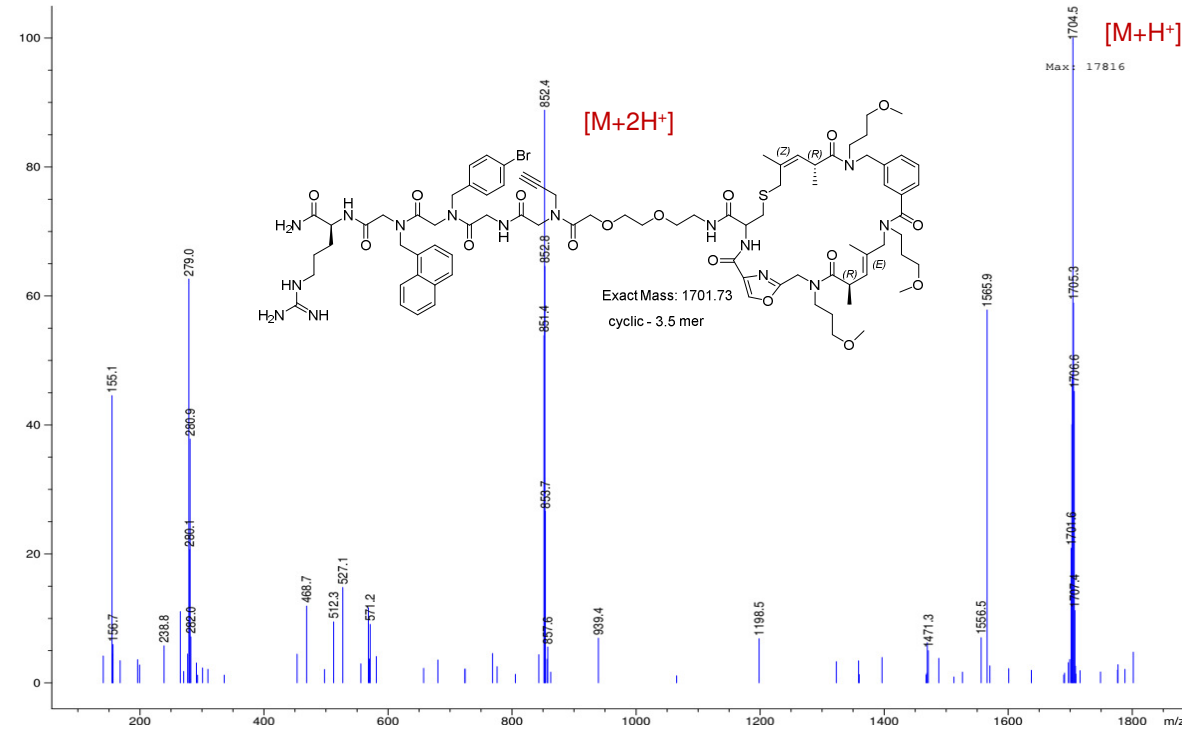


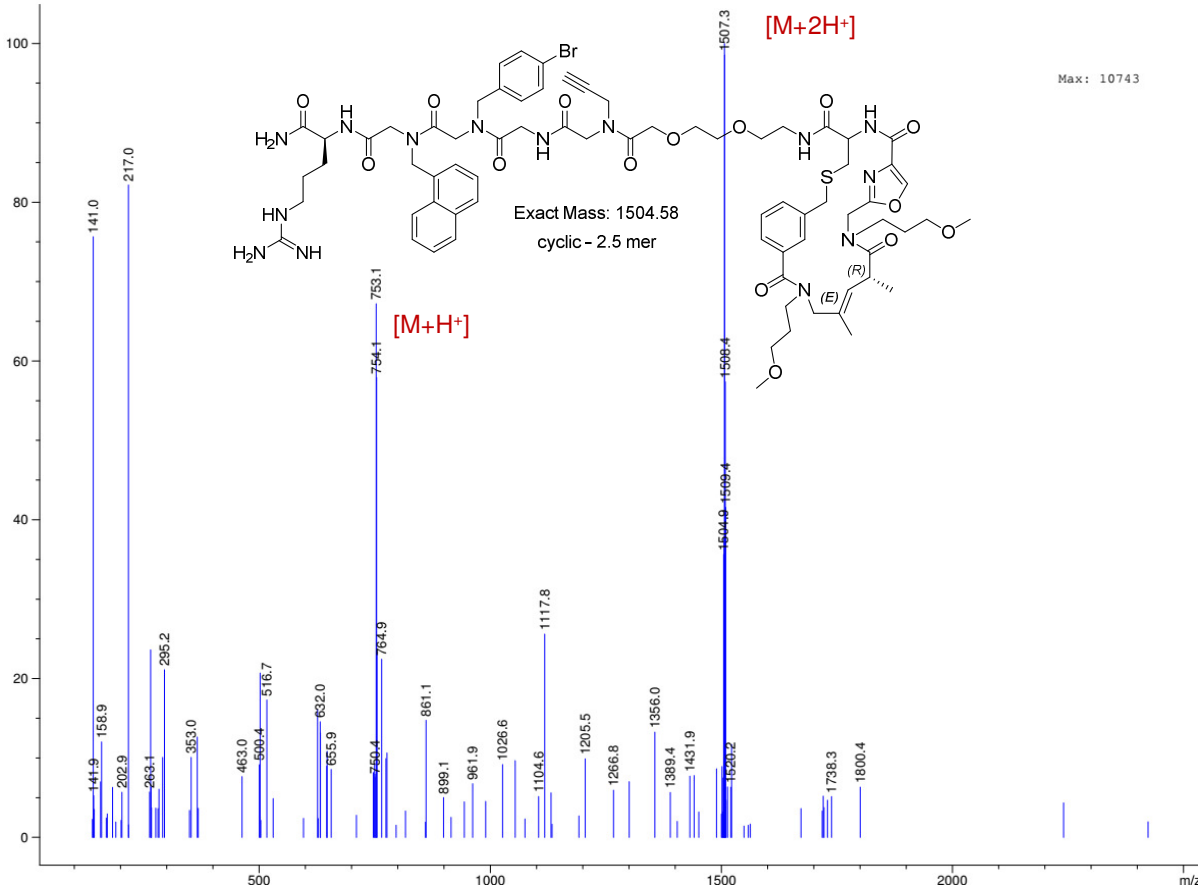


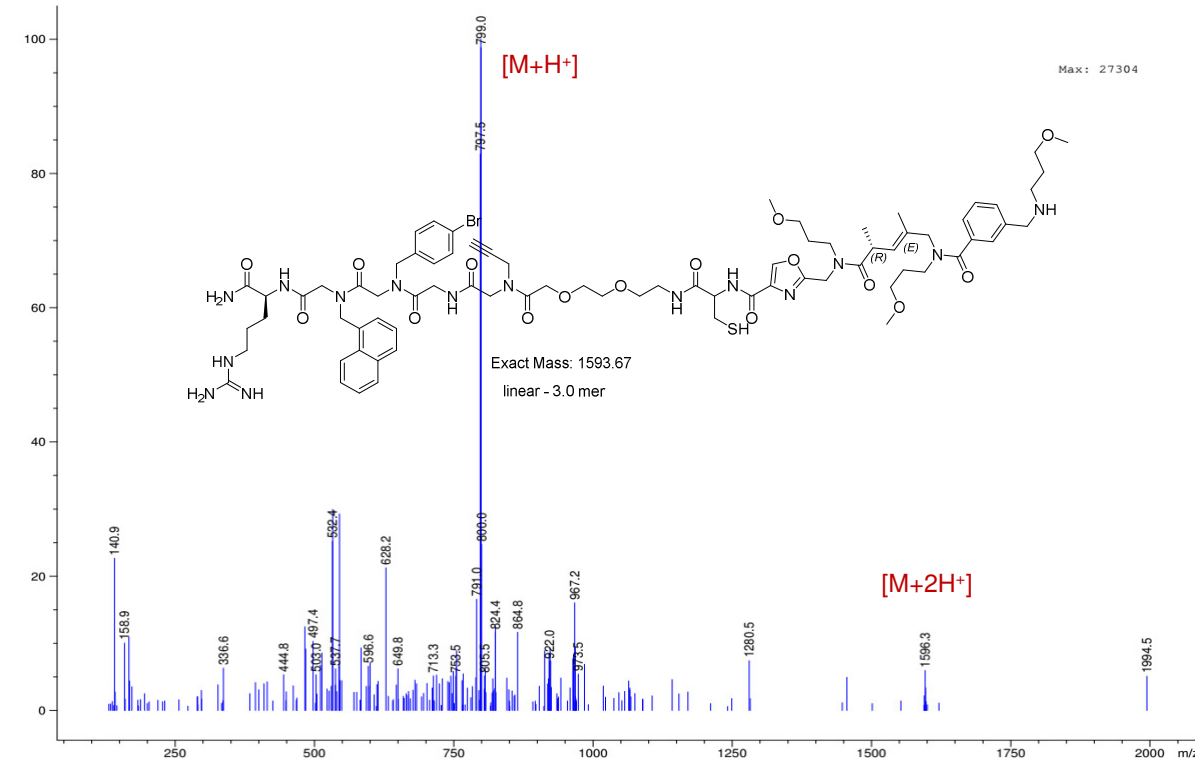
#	Time	Area	Height	Width	Area%
1	7.037	217	44.3	0.0817	20.277
2	8.202	152.3	42.4	0.0599	14.235
3	8.557	678.2	130.8	0.0864	63.376
4	8.773	22.6	6.3	0.0595	2.112

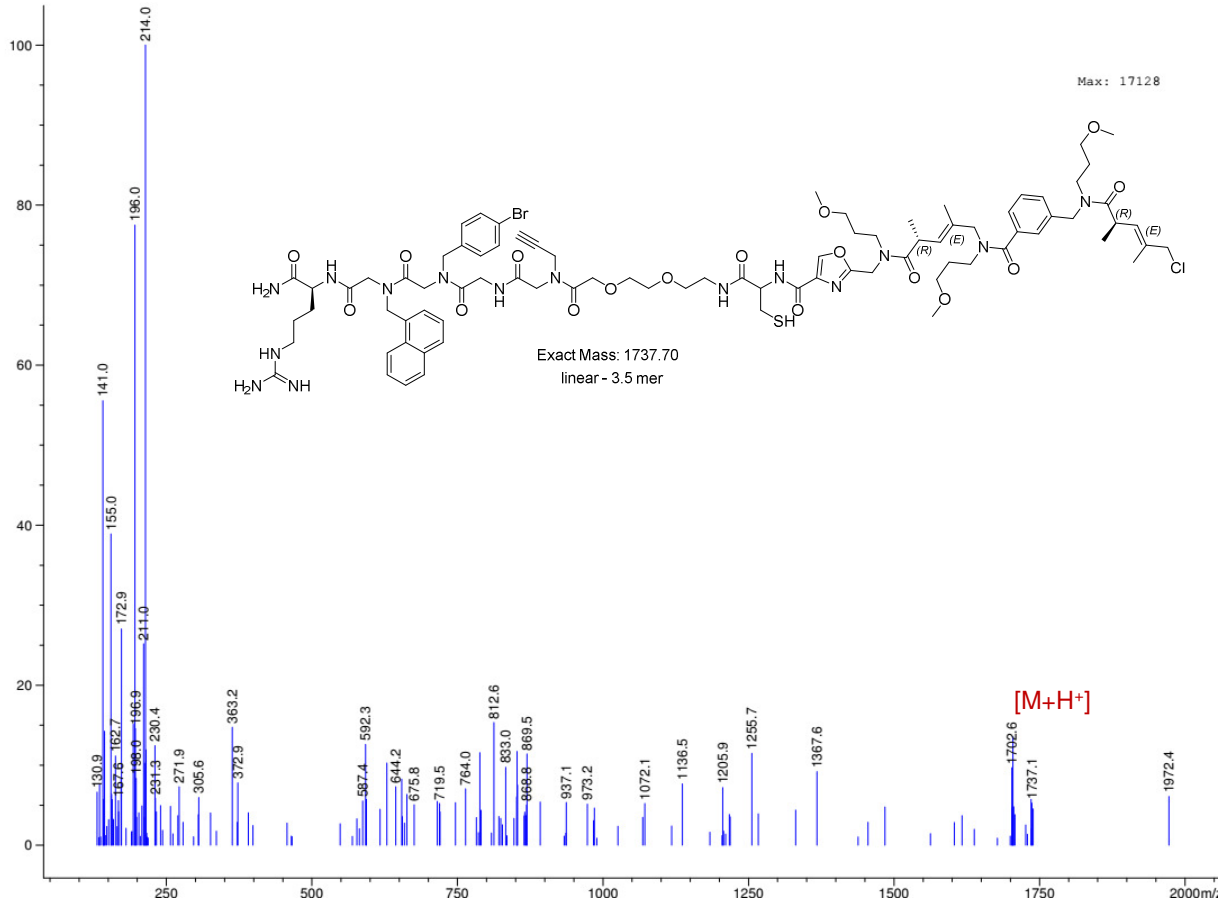
Q7 - [CAC]

ions	size	MW	RT
cyclic	2.5	1504	8.202
cyclic	3.5	1701	8.557
linear	3.0	1593	7.037
linear	3.5	1737	8.773

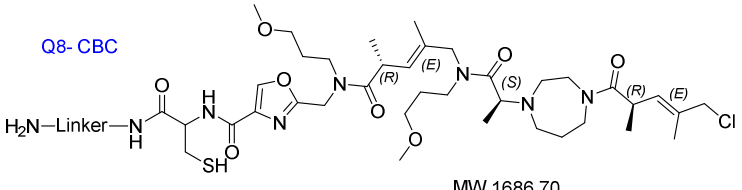

[M+H+]
Max: 17816
[M+2H+]
Exact Mass: 1701.73
cyclic - 3.5 mer
m/z

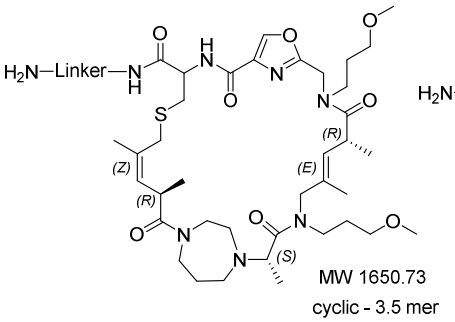

[M+2H+]
Max: 10743
Exact Mass: 1504.58
cyclic - 2.5 mer
[M+H+]
m/z

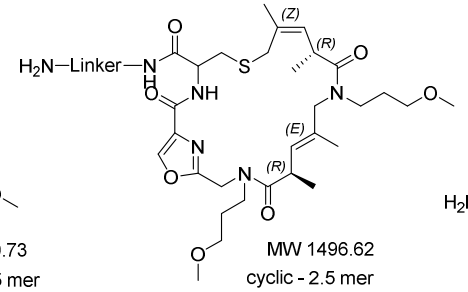

[M+H+]
Max: 27304
Exact Mass: 1593.67
linear - 3.0 mer
[M+2H+]

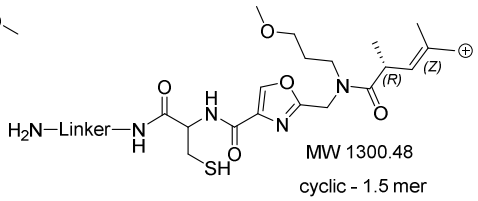

Max: 17128
Exact Mass: 1737.70
linear - 3.5 mer
[M+H+]

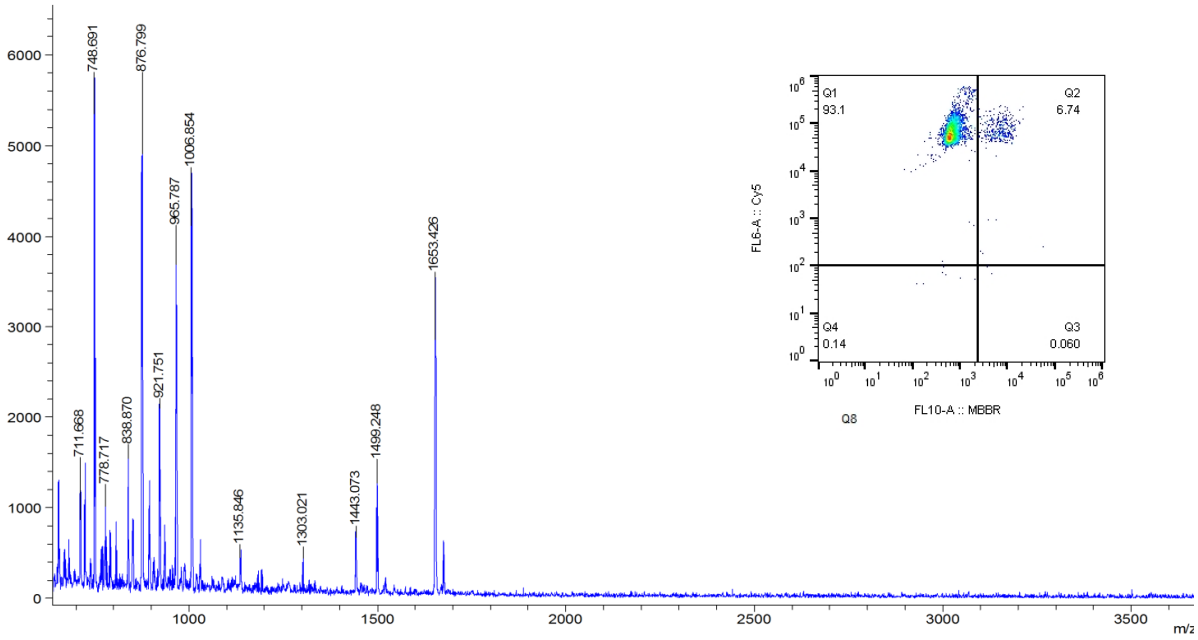
Q8-[CBC]: Cyclization was complete on both 10um & 160um. Dead beads could be due to 1.5mer linear fragments (MW 1300).

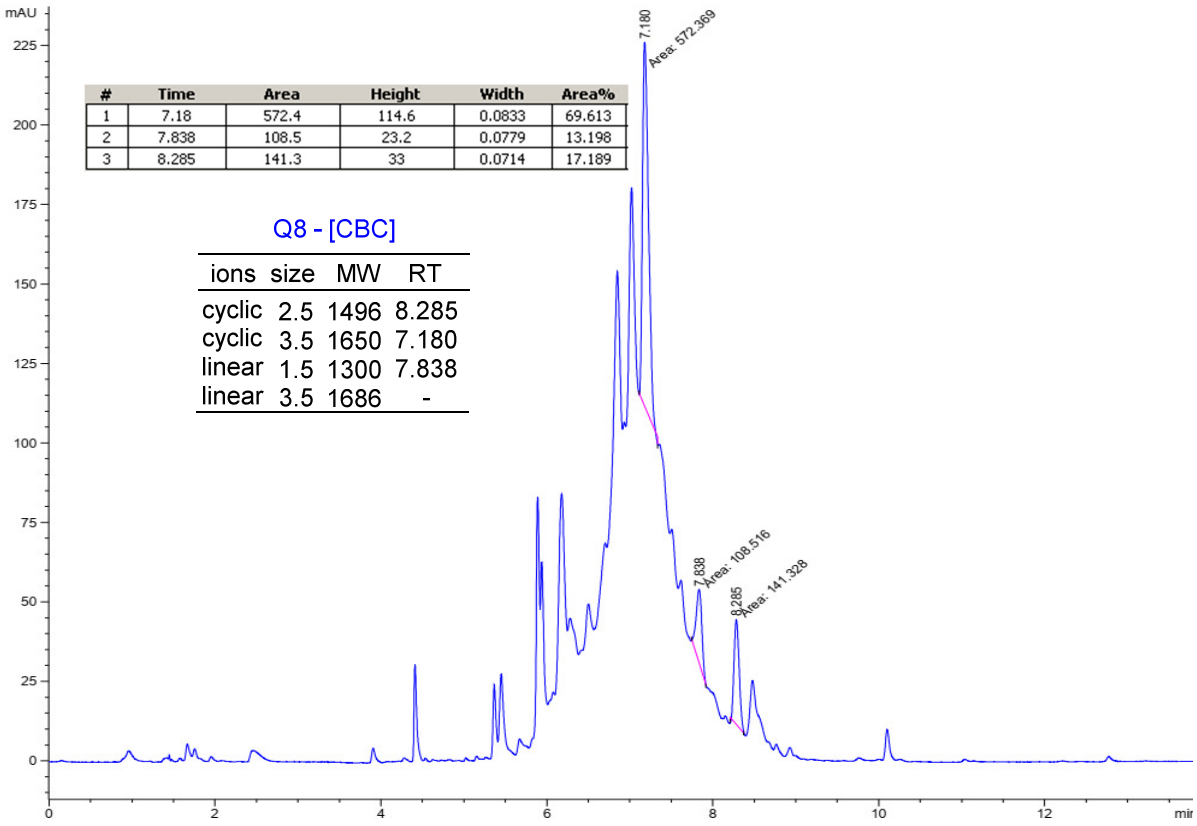








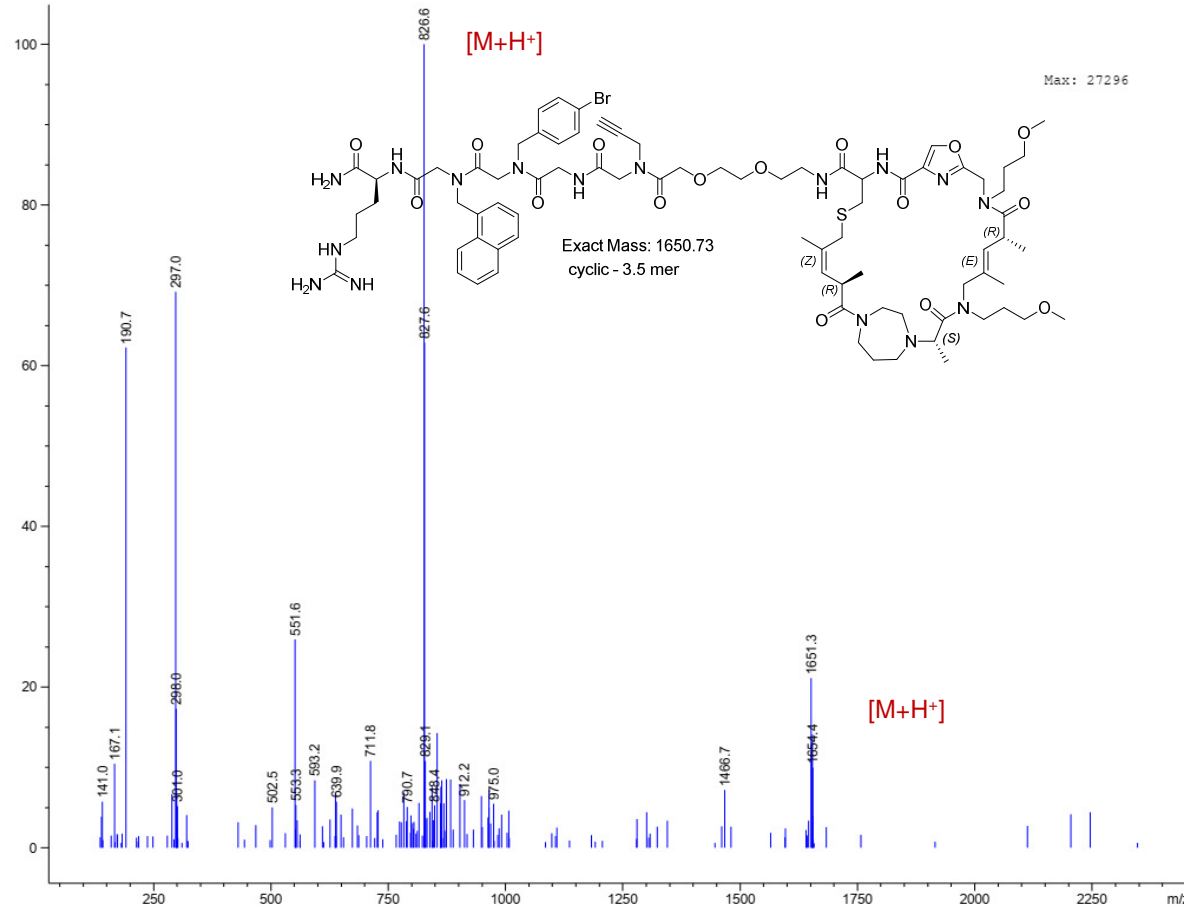


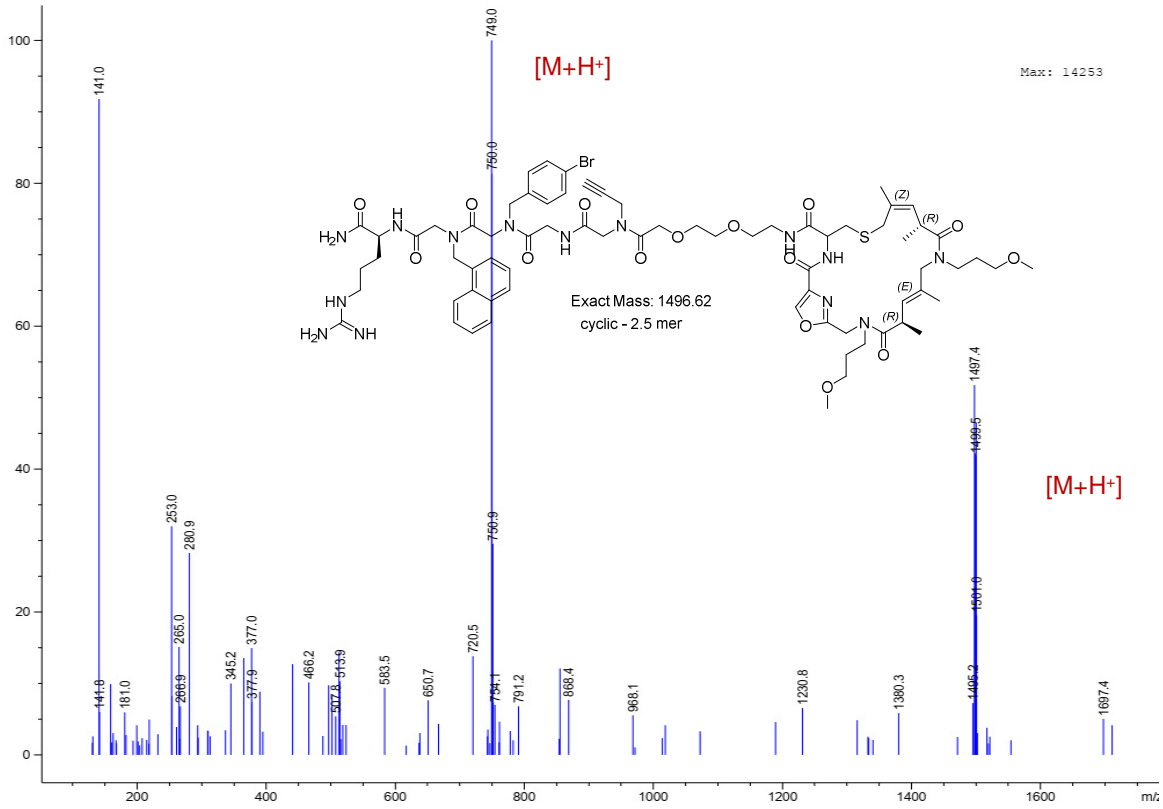


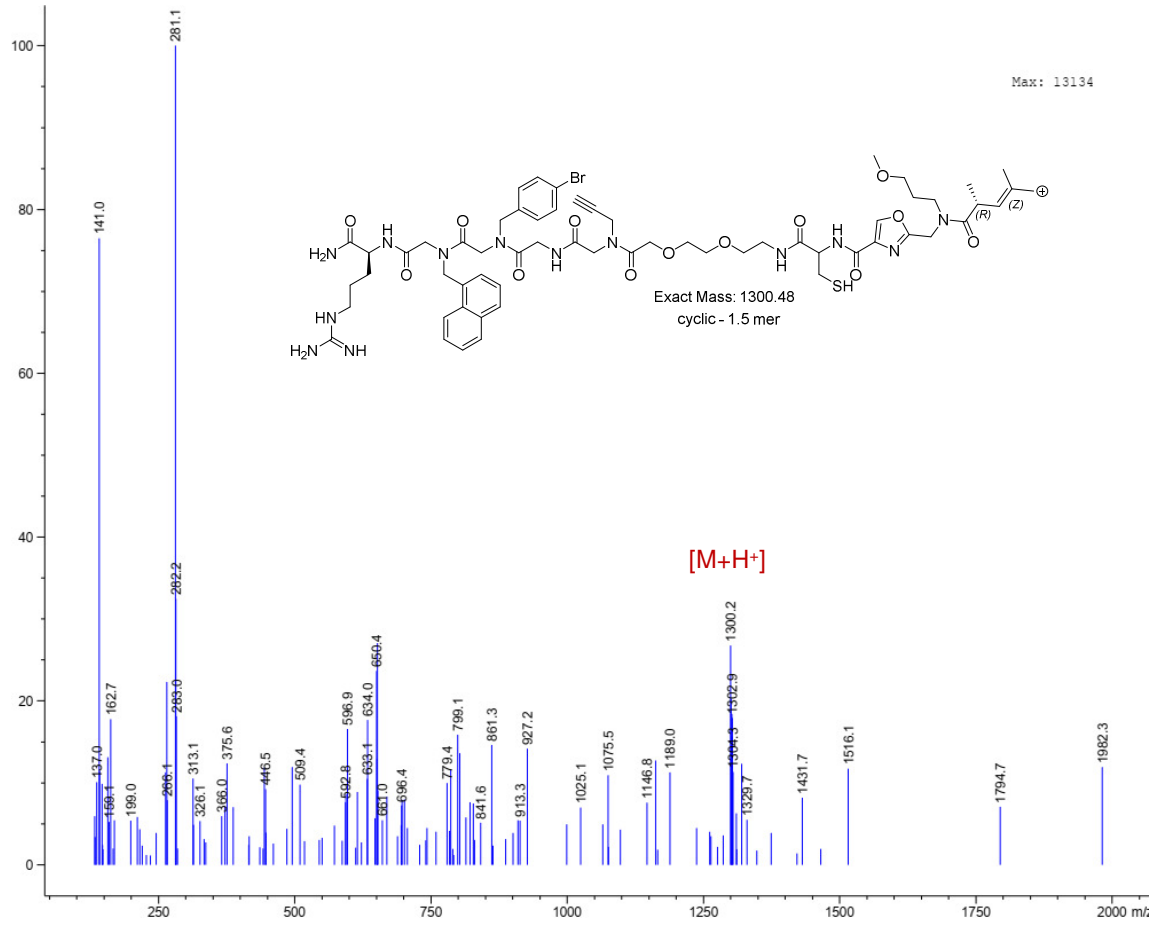
#	Time	Area	Height	Width	Area%
1	7.18	572.4	114.6	0.0833	69.613
2	7.838	108.5	23.2	0.0779	13.198
3	8.285	141.3	33	0.0714	17.189

Q8 - [CBC]

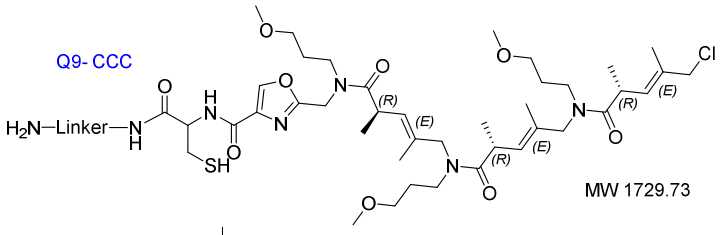
ions	size	MW	RT
cyclic	2.5	1496	8.285
cyclic	3.5	1650	7.180
linear	1.5	1300	7.838
linear	3.5	1686	-

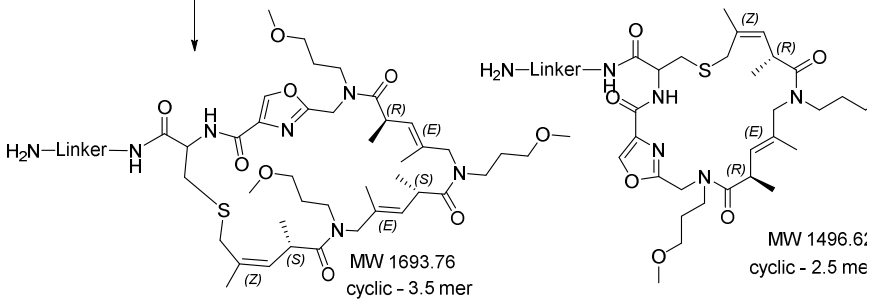


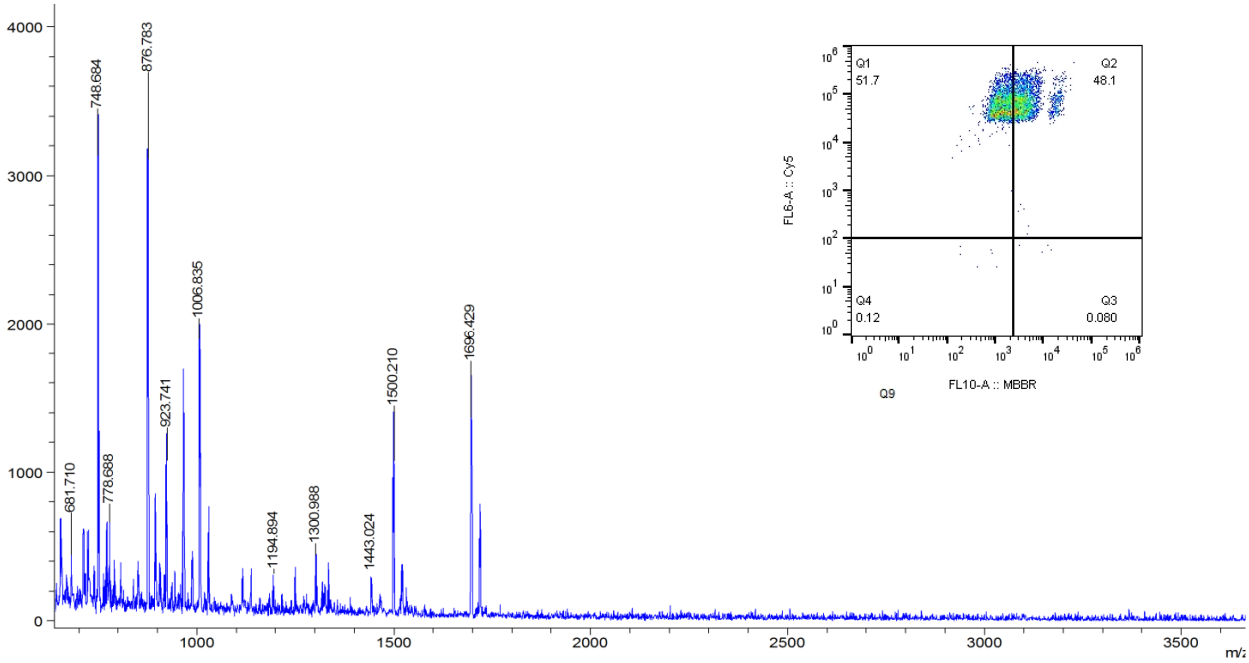

[M+H+]
Max: 14253
Exact Mass: 1496.62
cyclic - 2.5 mer
[M+H+]

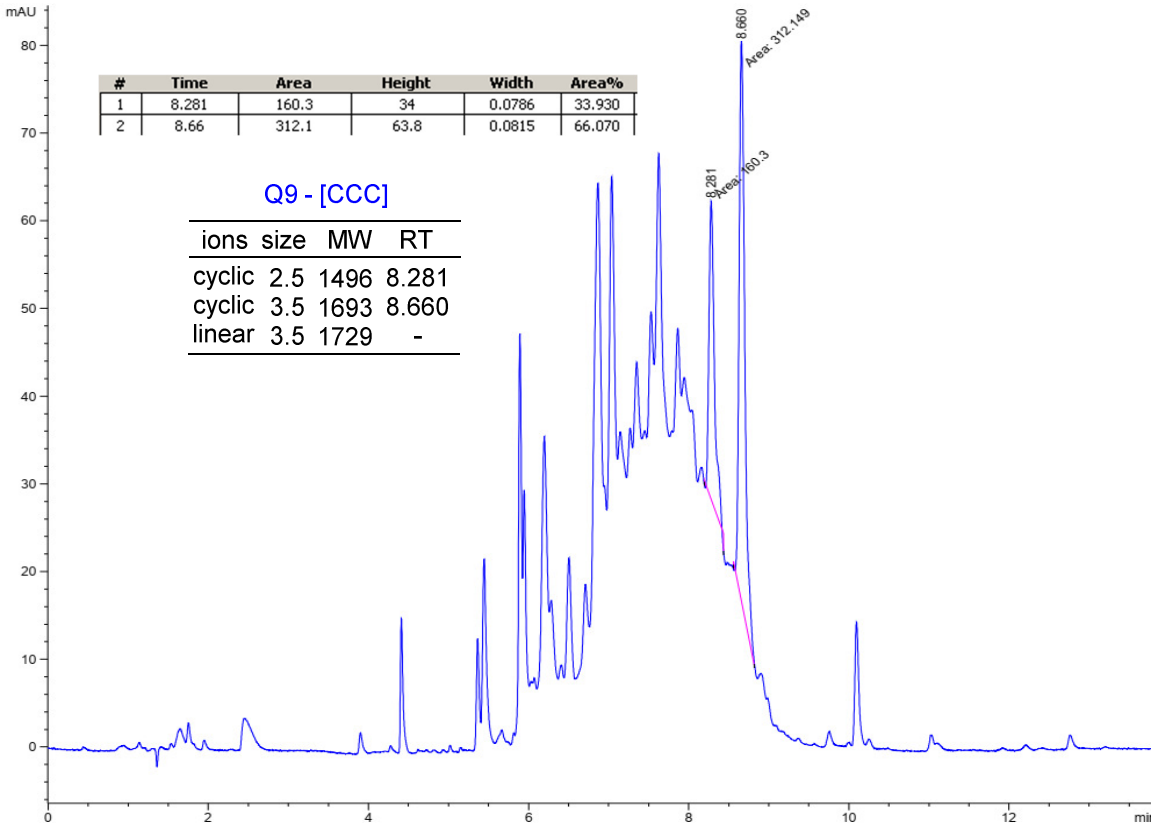

Max: 13134
Exact Mass: 1300.48
cyclic - 1.5 mer
[M+H+]

Q9-[CCC]: Incomplete cyclization was detected on 10um but was complete on 160um.





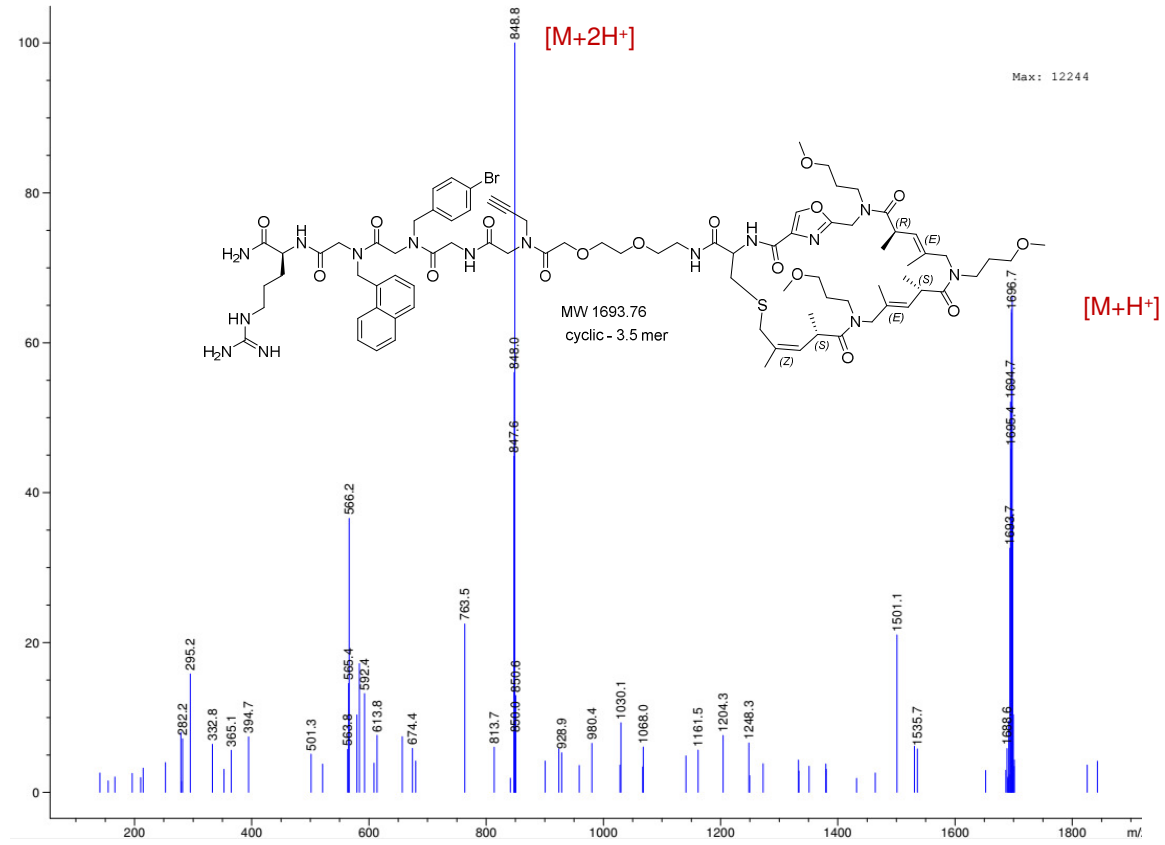


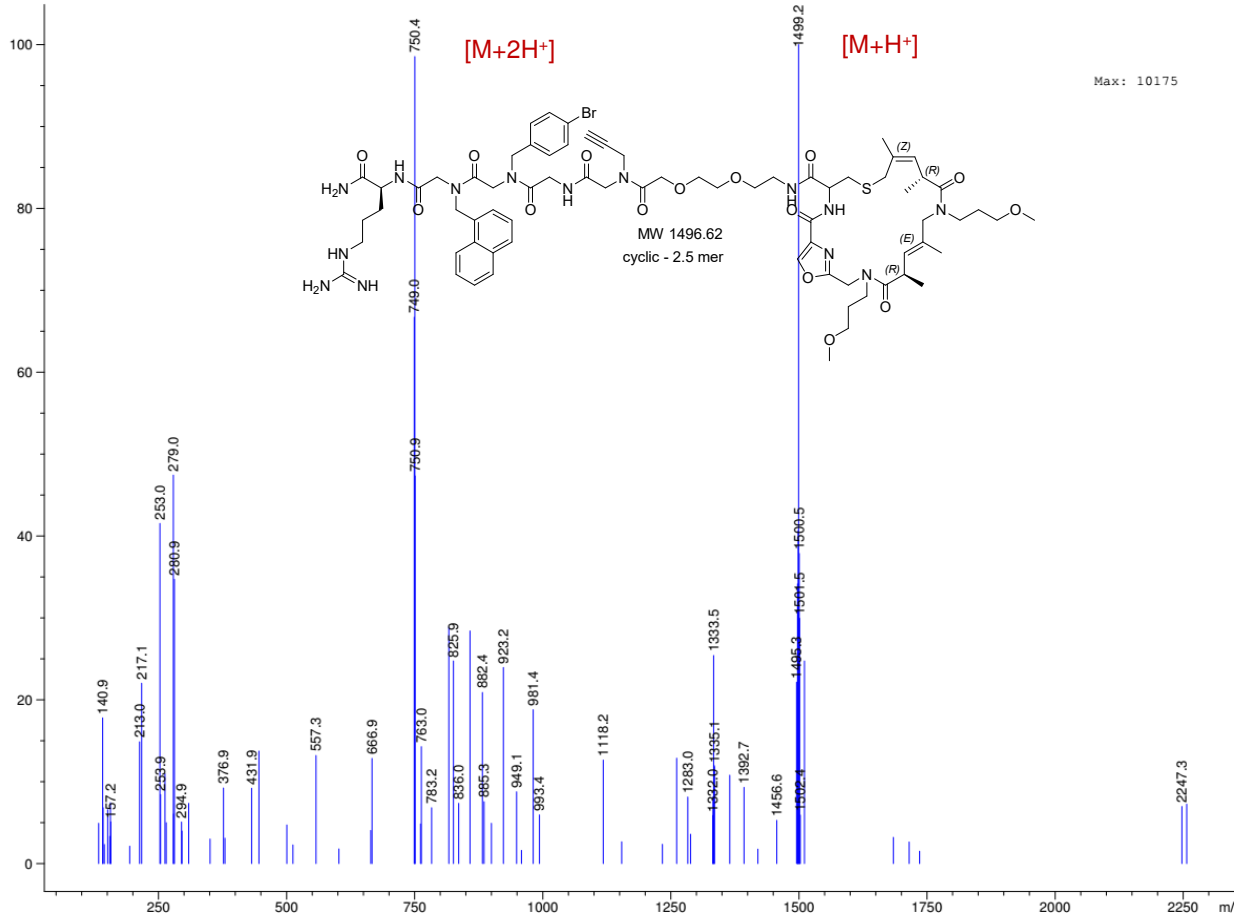


#	Time	Area	Height	Width	Area%
1	8.281	160.3	34	0.0786	33.930
2	8.66	312.1	63.8	0.0815	66.070

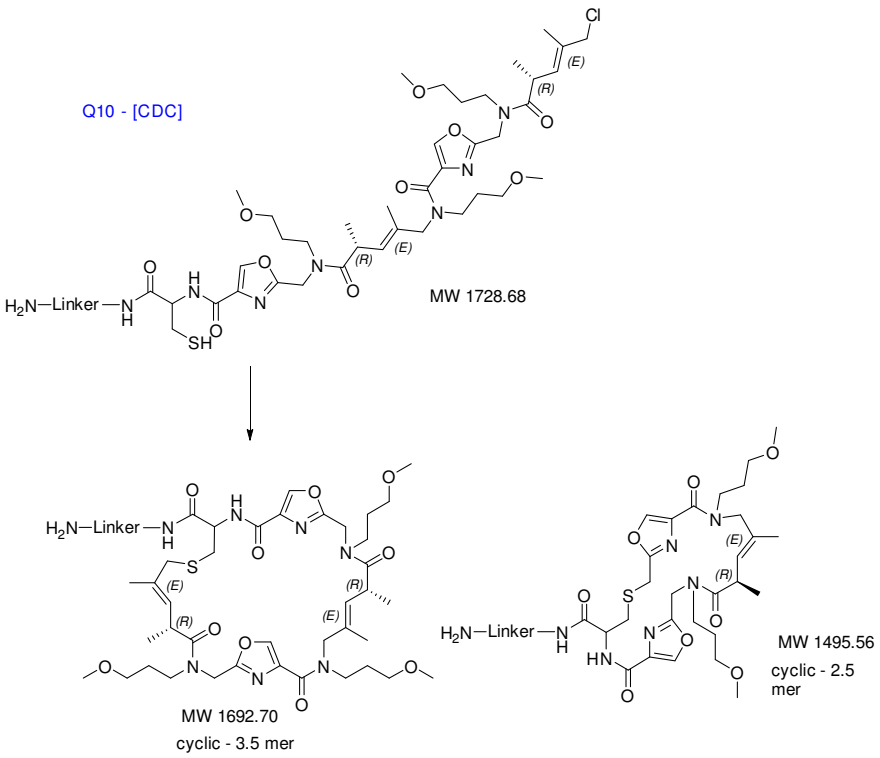
Q9 - [CCC]

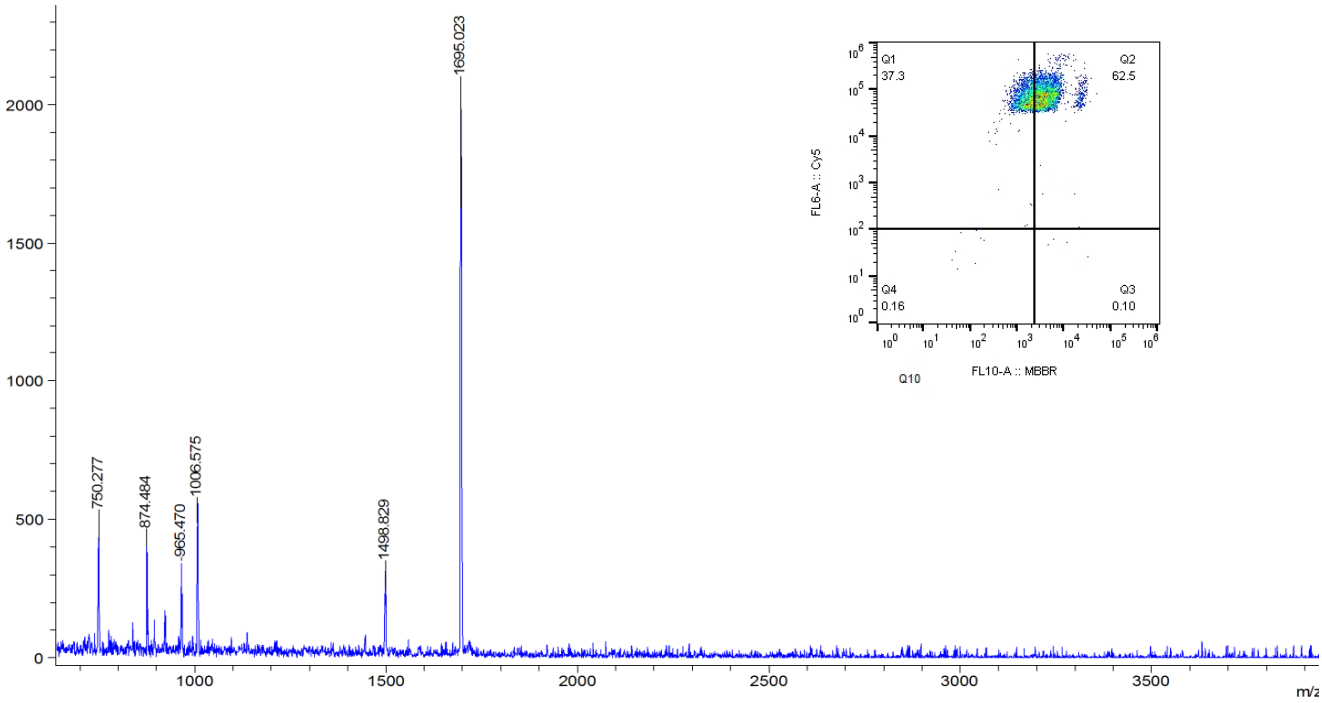
ions	size	MW	RT
cyclic	2.5	1496	8.281
cyclic	3.5	1693	8.660
linear	3.5	1729	-

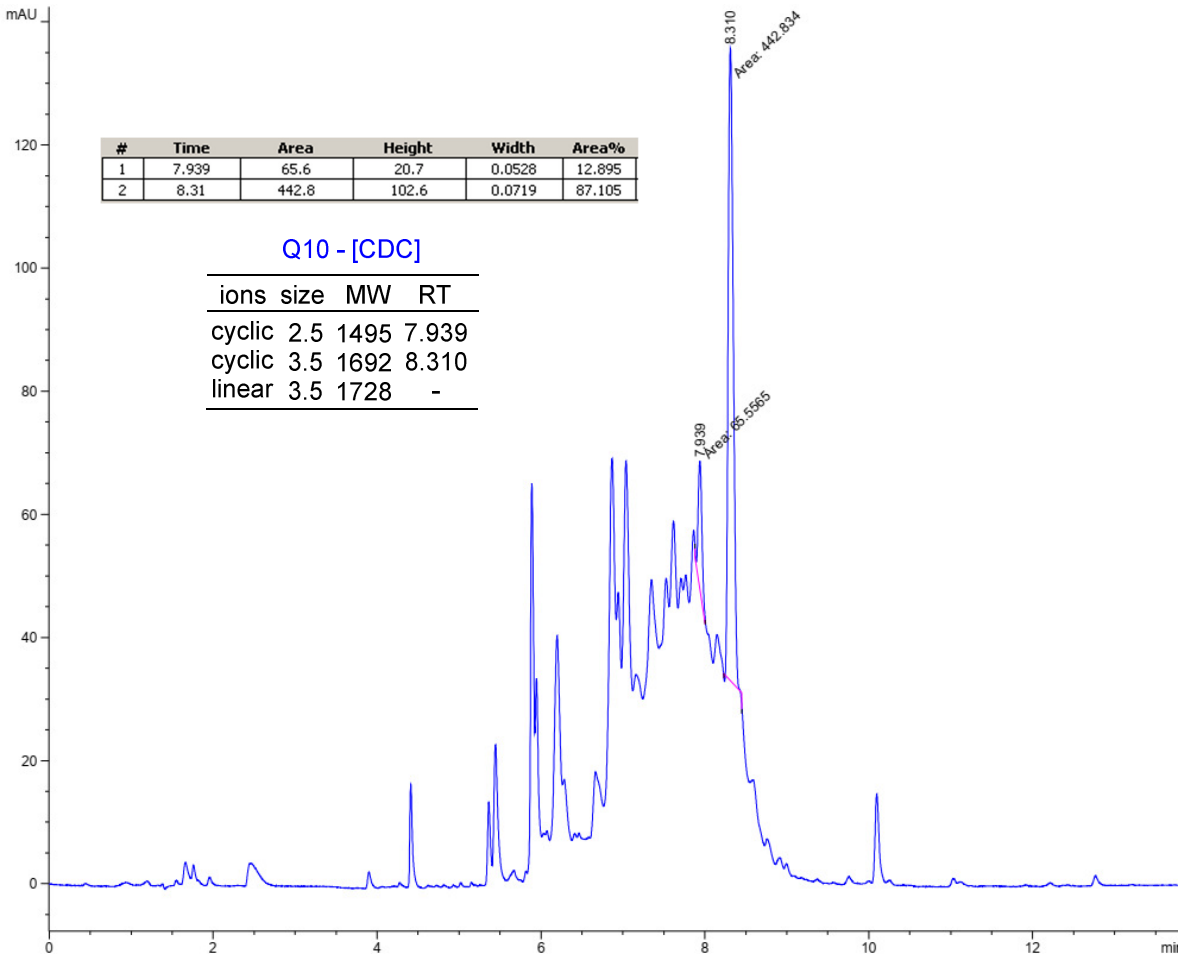




Q10-[CDC]: Incomplete cyclization was detected on 10um but was complete on 160um.



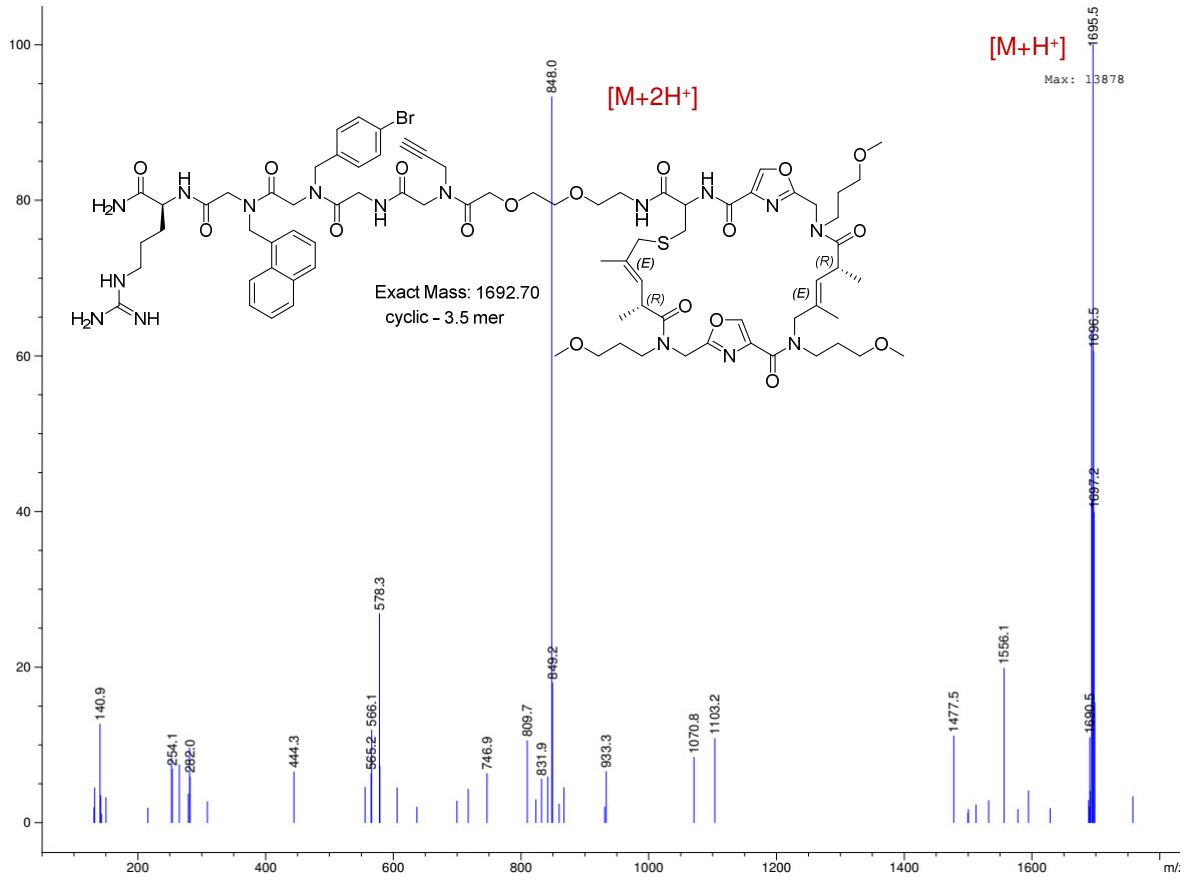


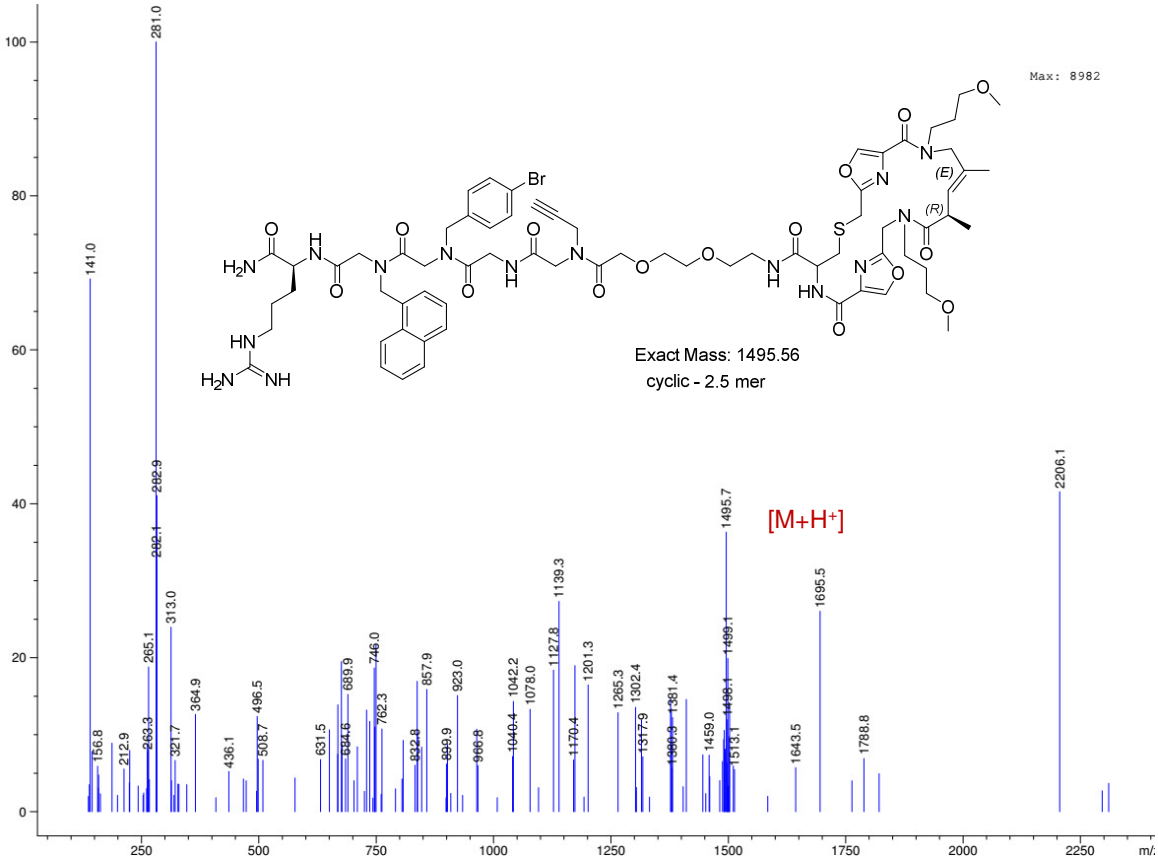


#	Time	Area	Height	Width	Area%
1	7.939	65.6	20.7	0.0528	12.895
2	8.31	442.8	102.6	0.0719	87.105

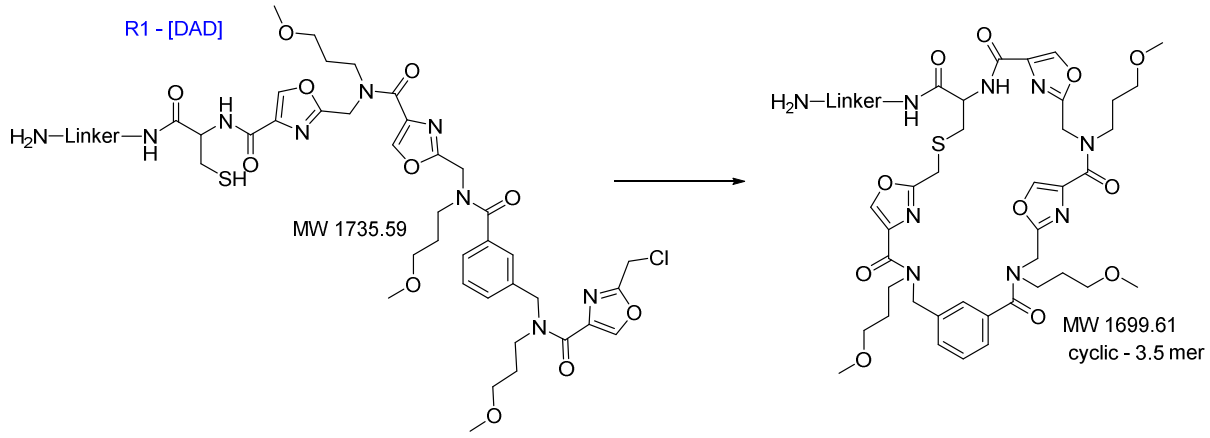
Q10 - [CDC]

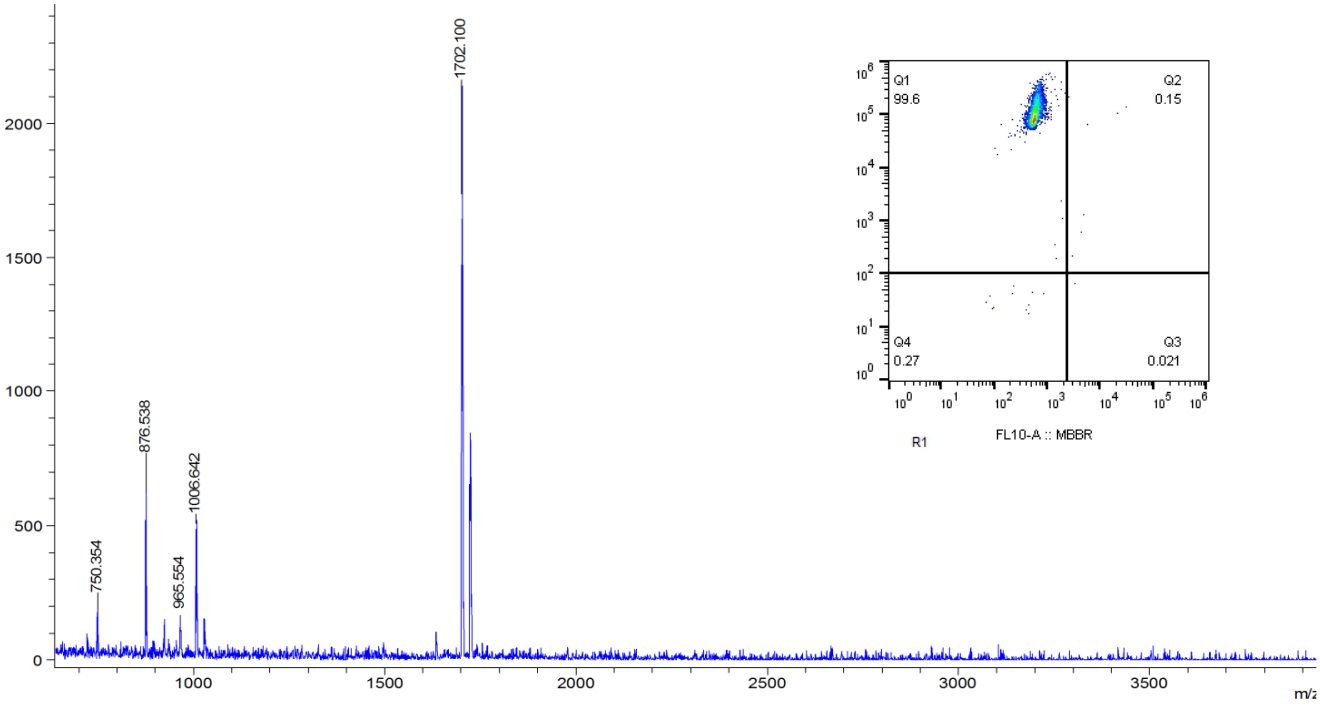
ions	size	MW	RT
cyclic	2.5	1495	7.939
cyclic	3.5	1692	8.310
linear	3.5	1728	-

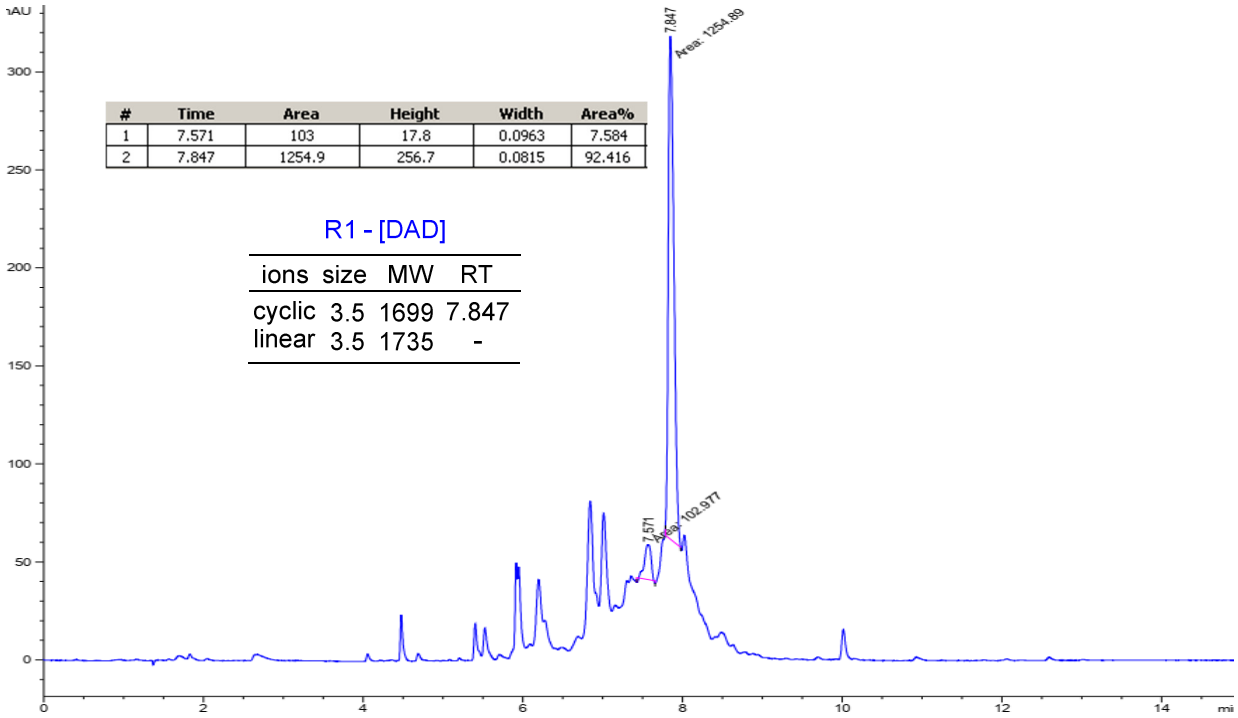

[M+H+]
Max: 13878
[M+2H+]
Exact Mass: 1692.70
cyclic - 3.5 mer
m/z


Max: 8982
Exact Mass: 1495.56
cyclic - 2.5 mer
[M+H+]
m/z

R1-[DAD]: Cyclization was complete on both 10um & 160um.



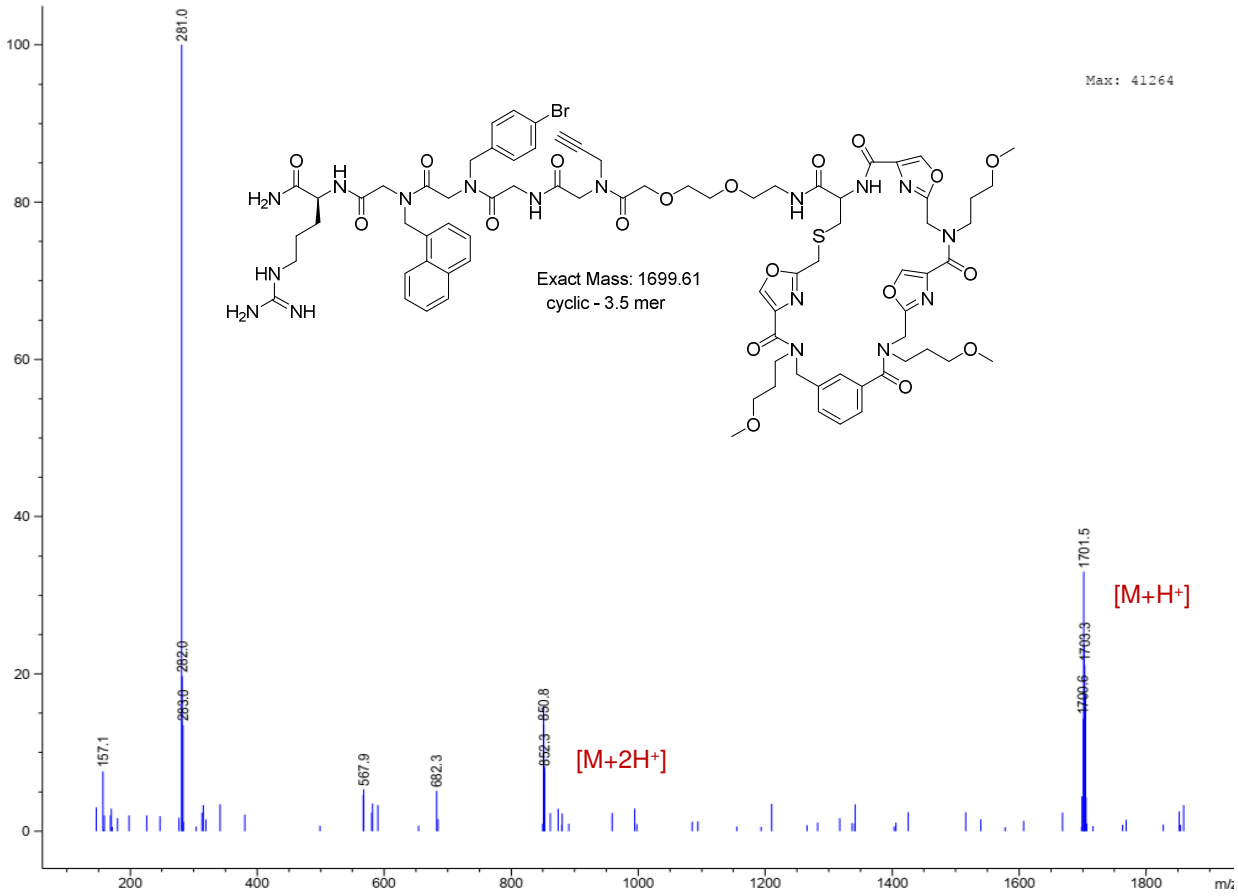




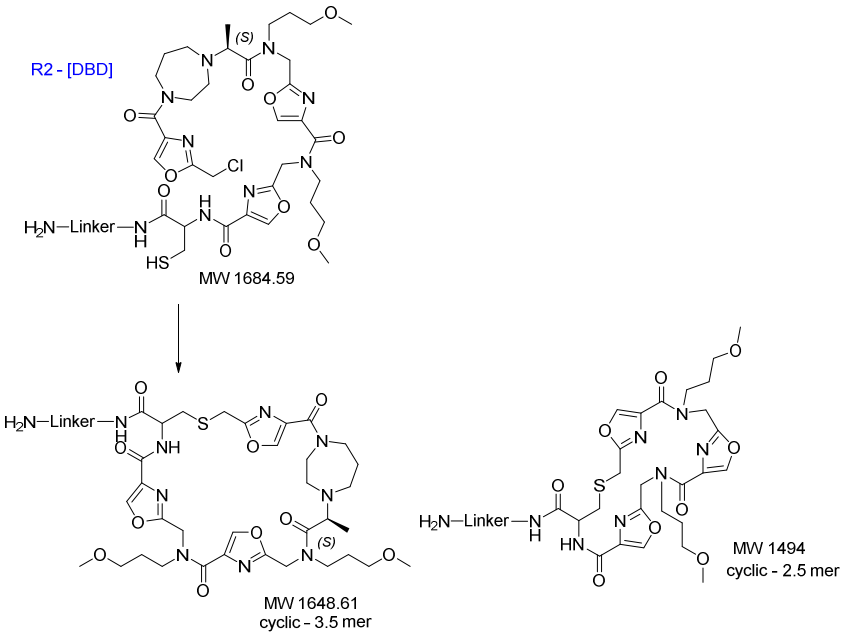
#	Time	Area	Height	Width	Area%
1	7.571	103	17.8	0.0963	7.584
2	7.847	1254.9	256.7	0.0815	92.416

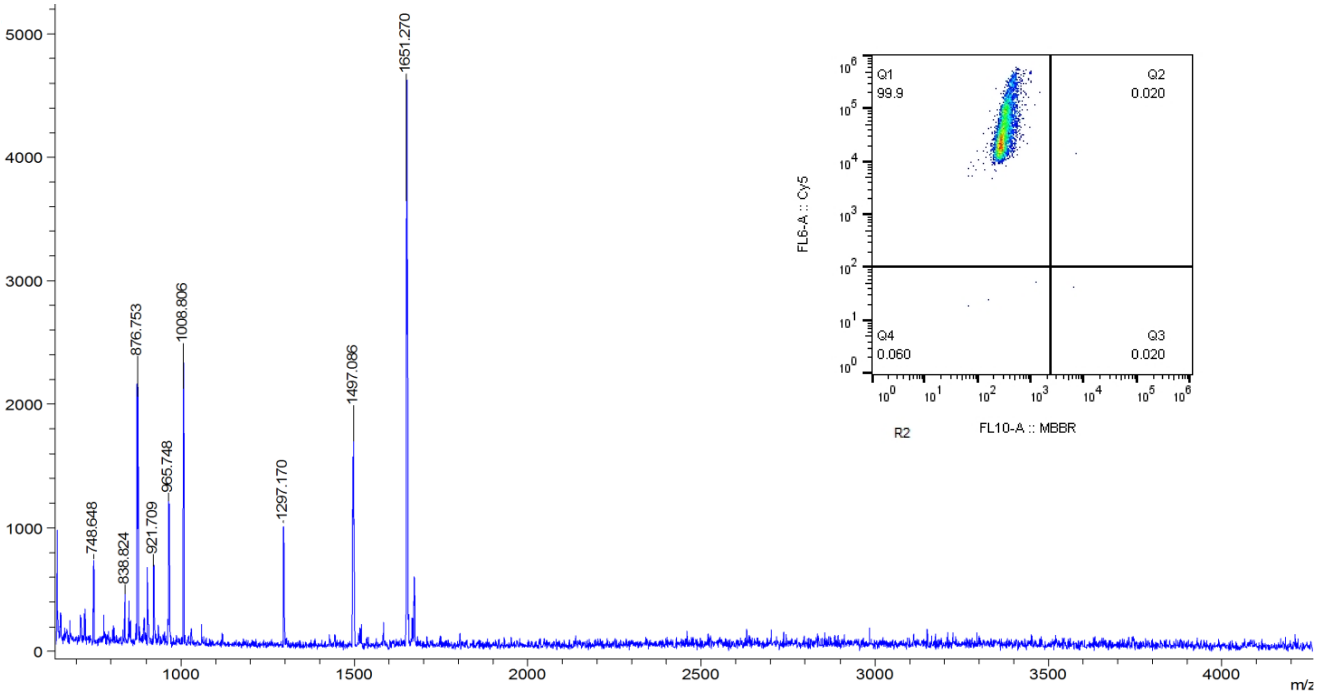
R1 - [DAD]

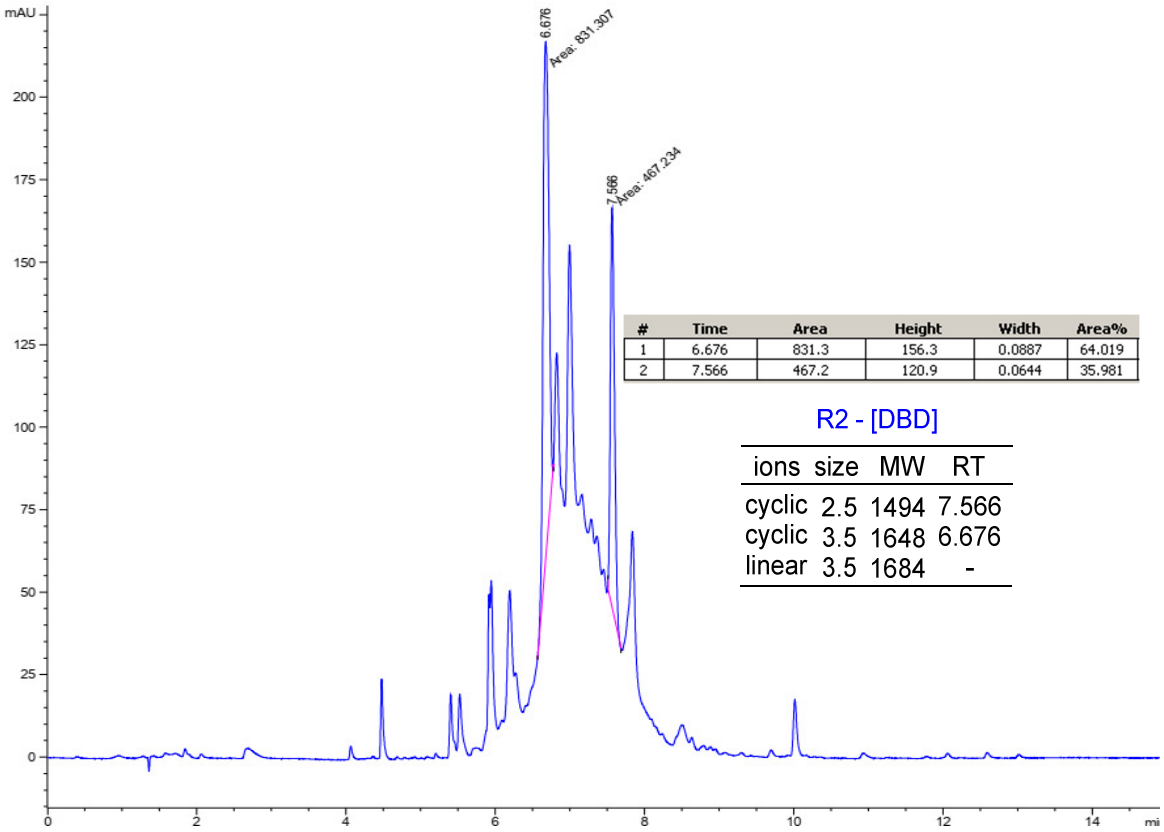
ions	size	MW	RT
cyclic	3.5	1699	7.847
linear	3.5	1735	-



R2-[DBD]: Cyclization was complete on both 10um & 160um.



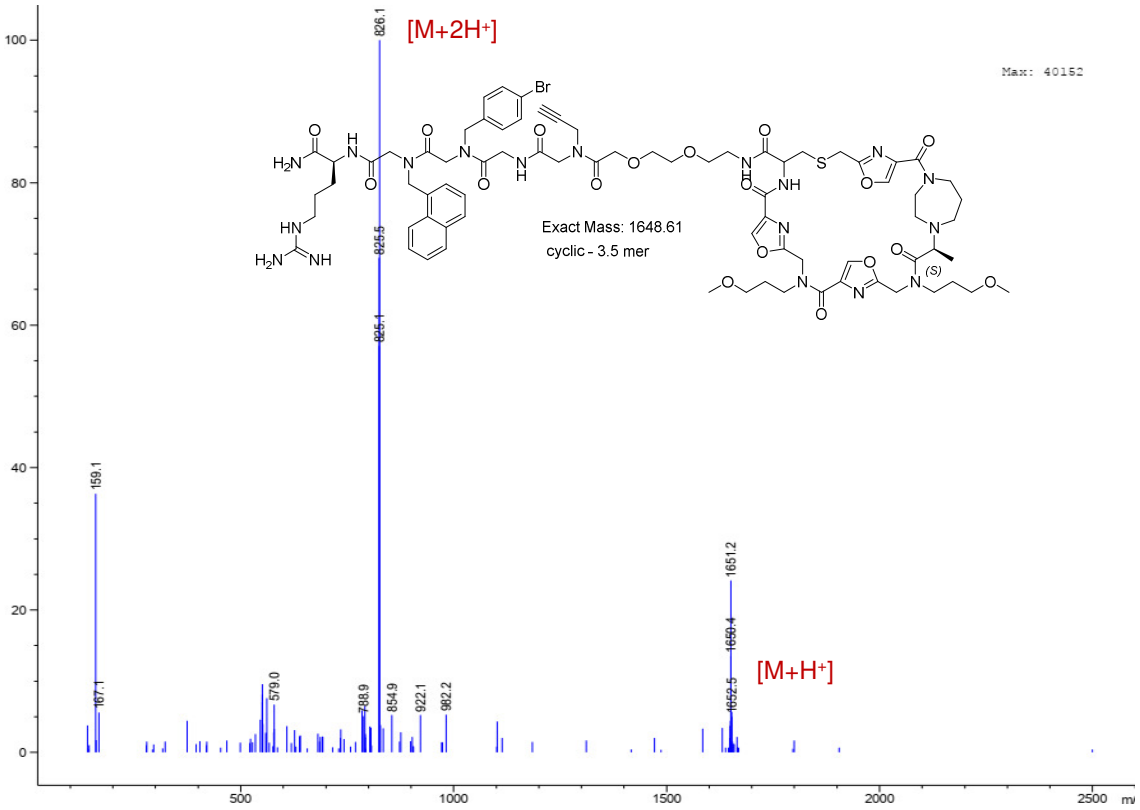


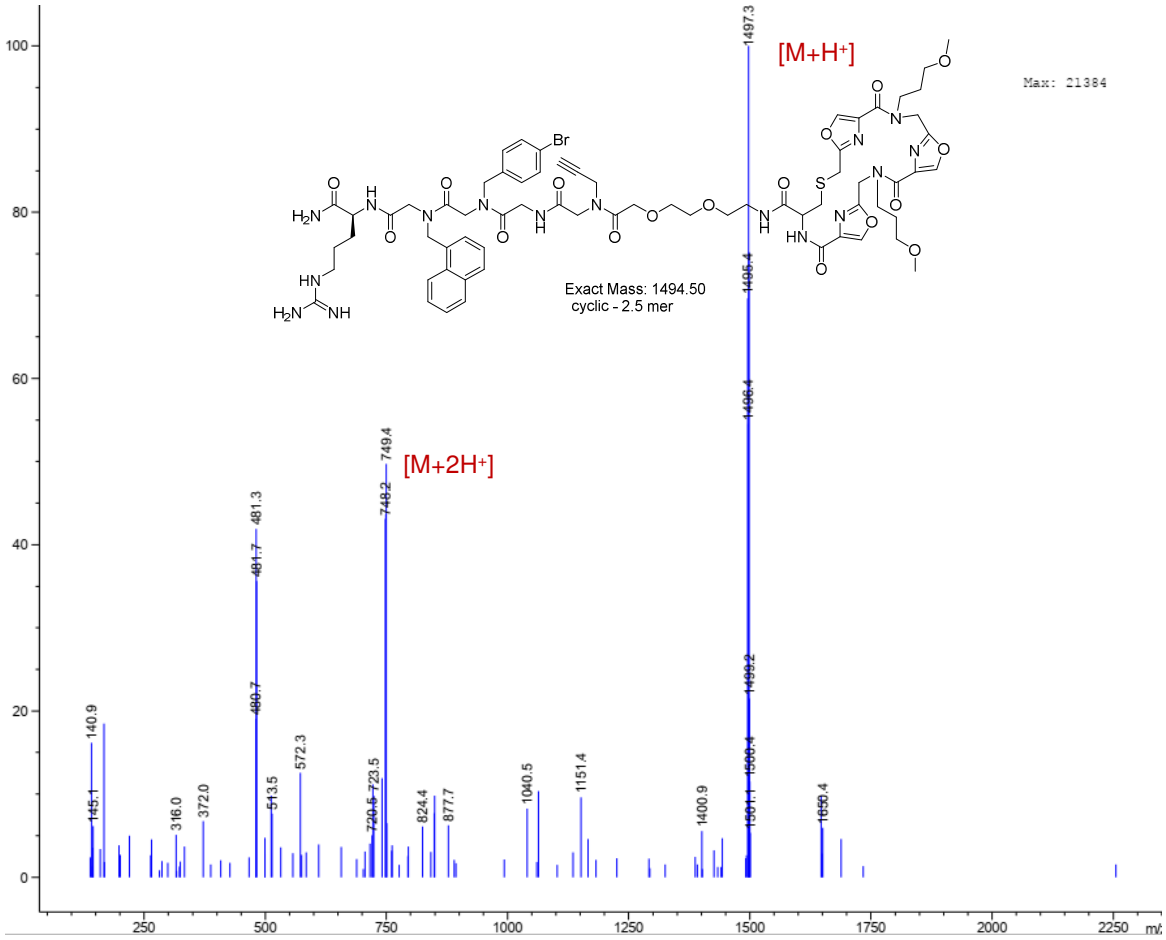


#	Time	Area	Height	Width	Area%
1	6.676	831.3	156.3	0.0887	64.019
2	7.566	467.2	120.9	0.0644	35.981

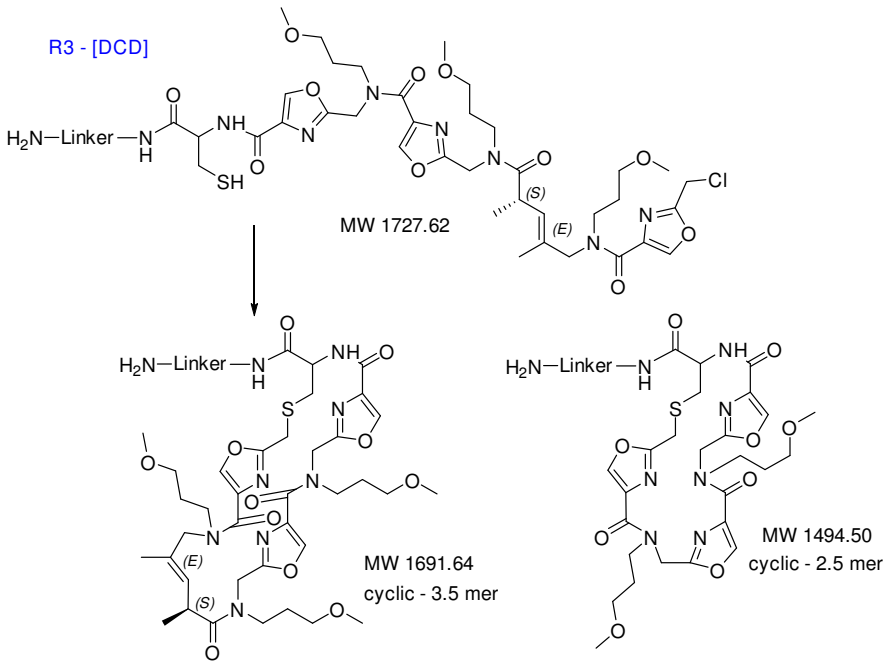
R2 - [DBD]

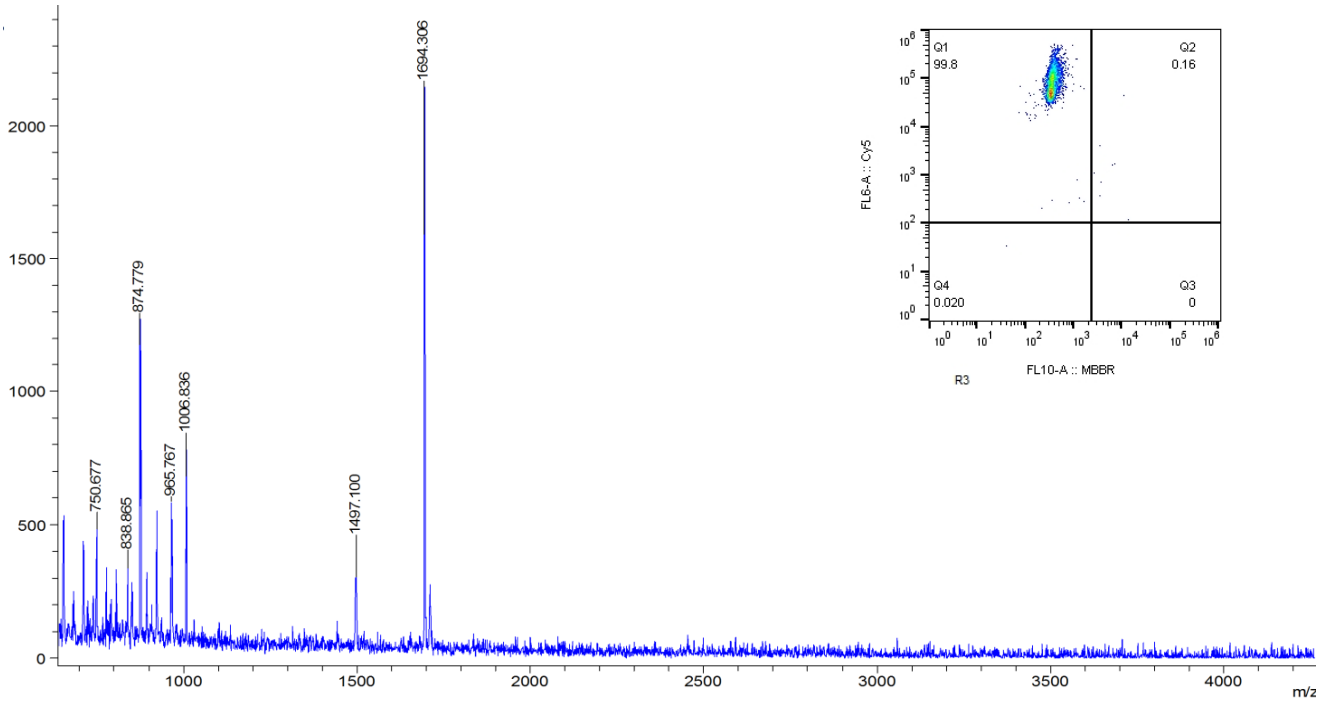
ions	size	MW	RT
cyclic	2.5	1494	7.566
cyclic	3.5	1648	6.676
linear	3.5	1684	-

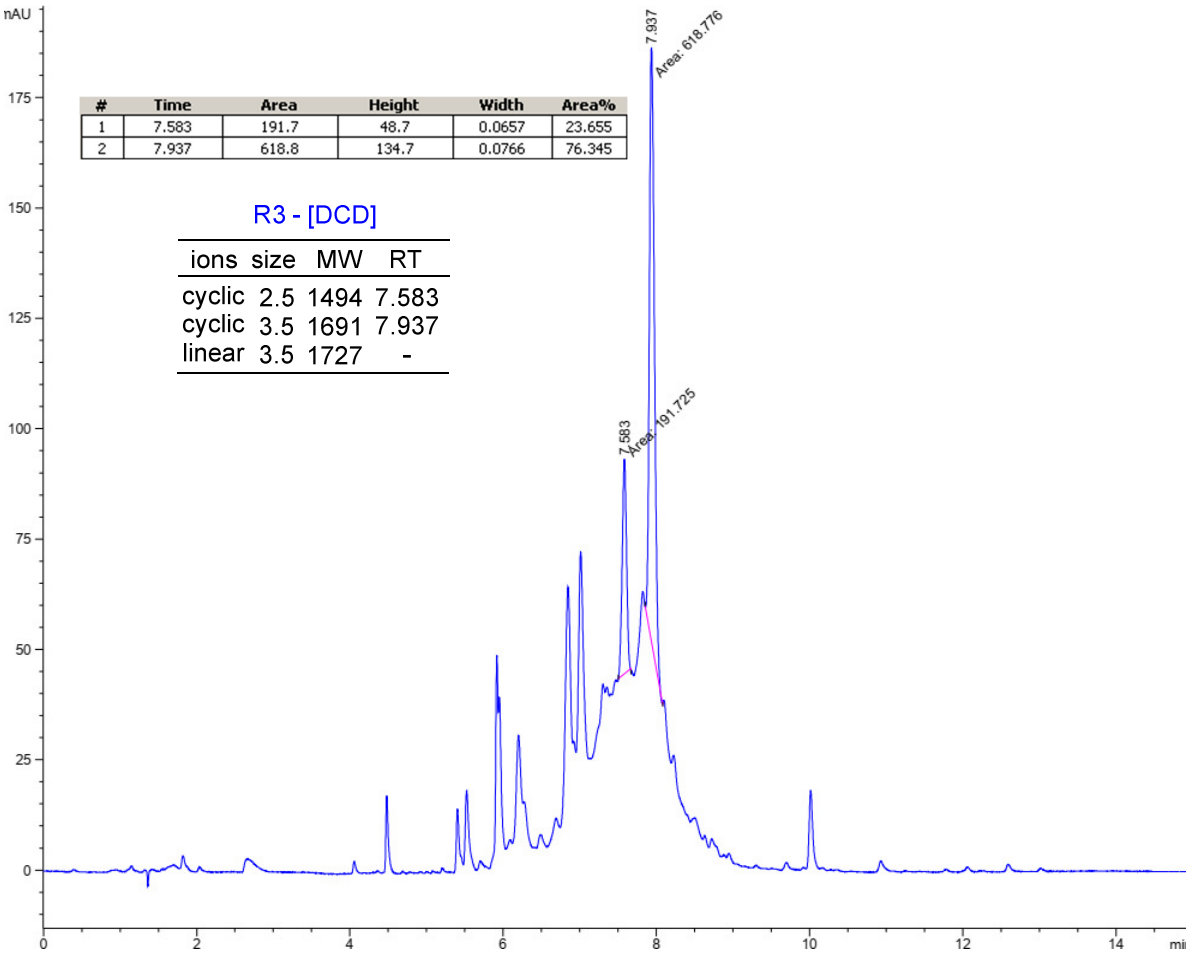


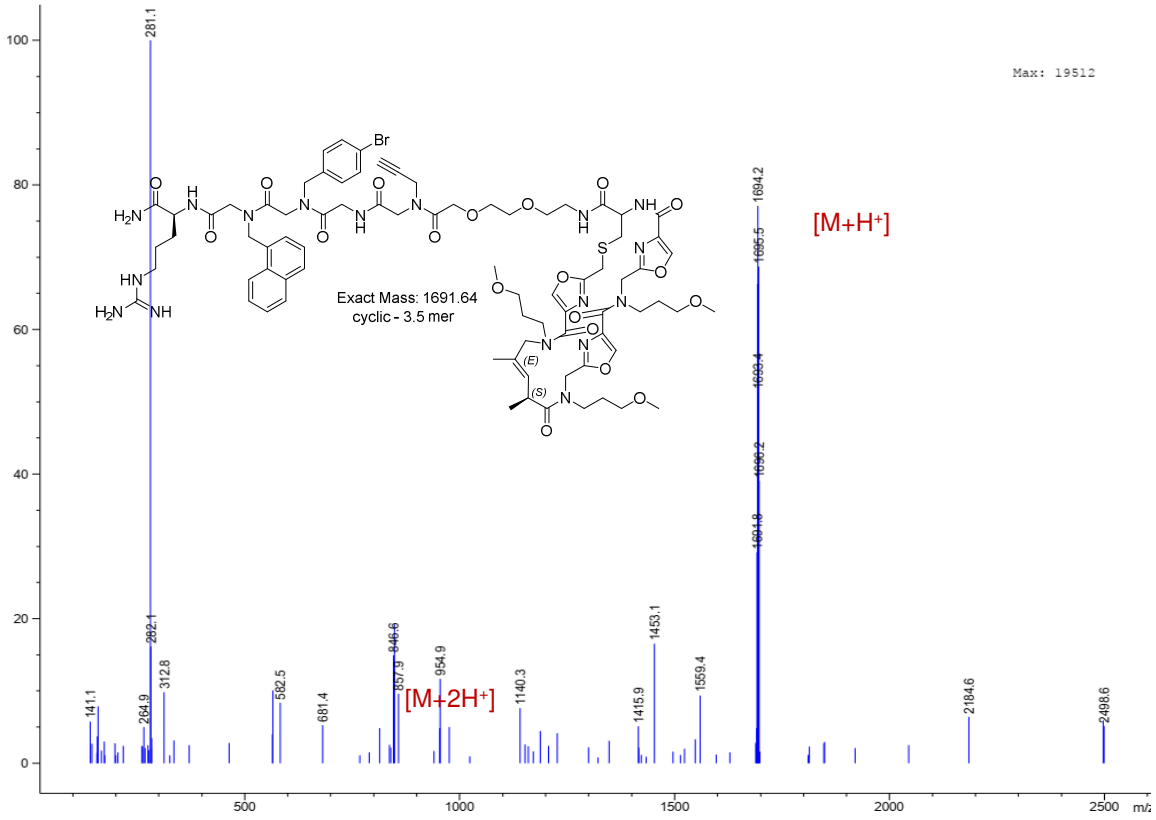


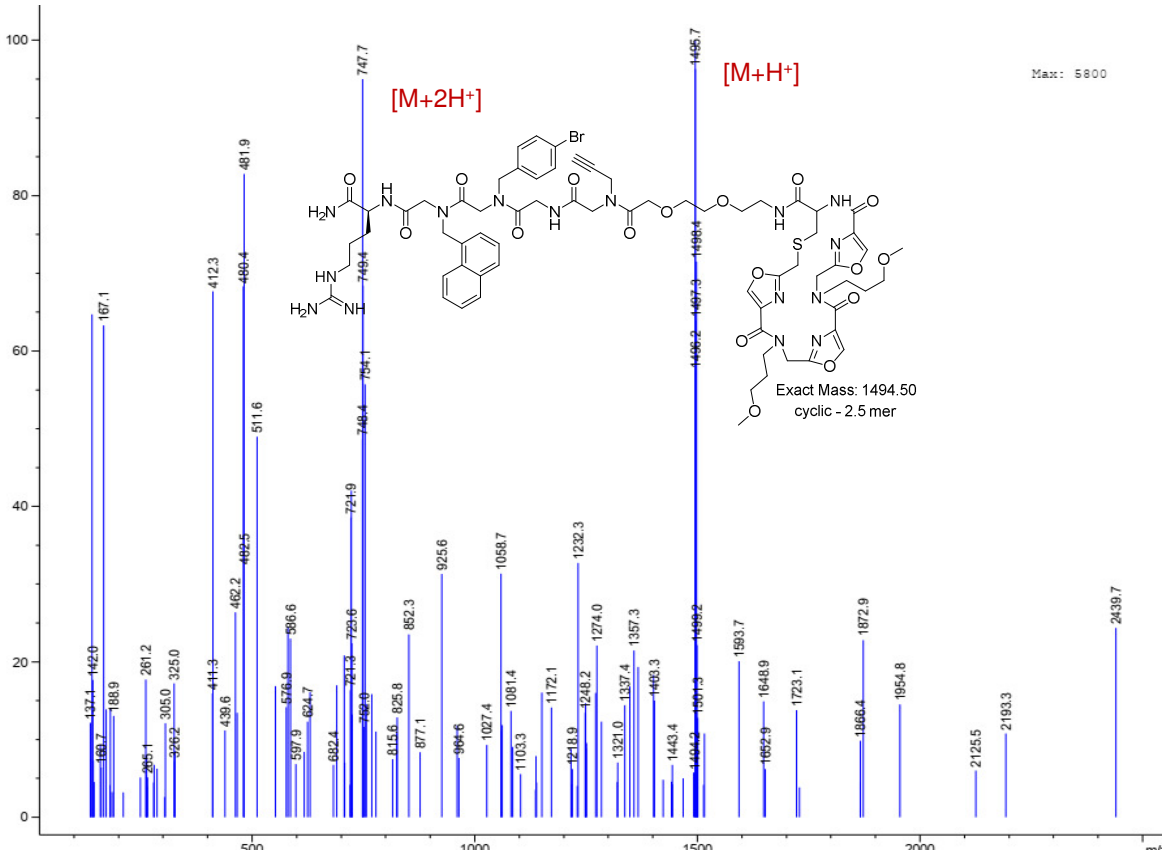
R3-[DCD]: Cyclization was complete on both 10um & 160um.



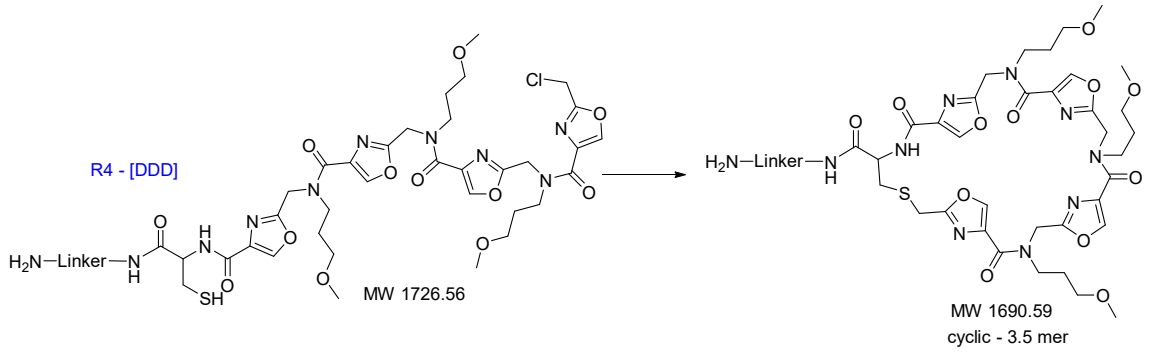

1694.306
874.779
1006.836
965.767
750.677
838.865
1497.100
2000
1500
1000
500
0
1000
1500
2000
2500
3000
3500
4000
m/z
Q1
99.8
Q2
0.16
Q4
0.020
Q3
0
FL6-A :: Cy5
FL10-A :: MBBR
R3

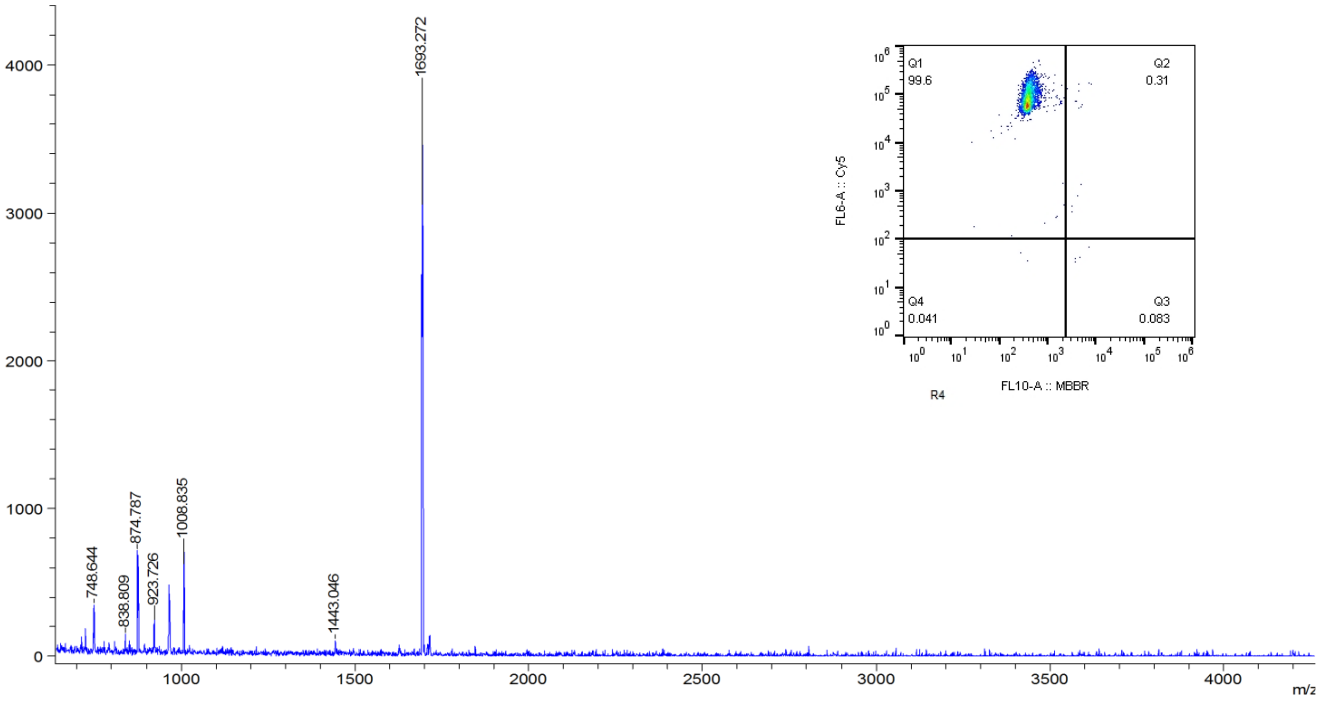

nAU
175
150
125
100
75
50
25
0
0
2
4
6
8
10
12
14
7.937
Area: 618.776
7.583
Area: 191.725
Time Area Height Width Area%
1 7.583 191.7 48.7 0.0657 23.655
2 7.937 618.8 134.7 0.0766 76.345
R3 - [DCD]
ions size MW RT
cyclic 2.5 1494 7.583
cyclic 3.5 1691 7.937
linear 3.5 1727 -

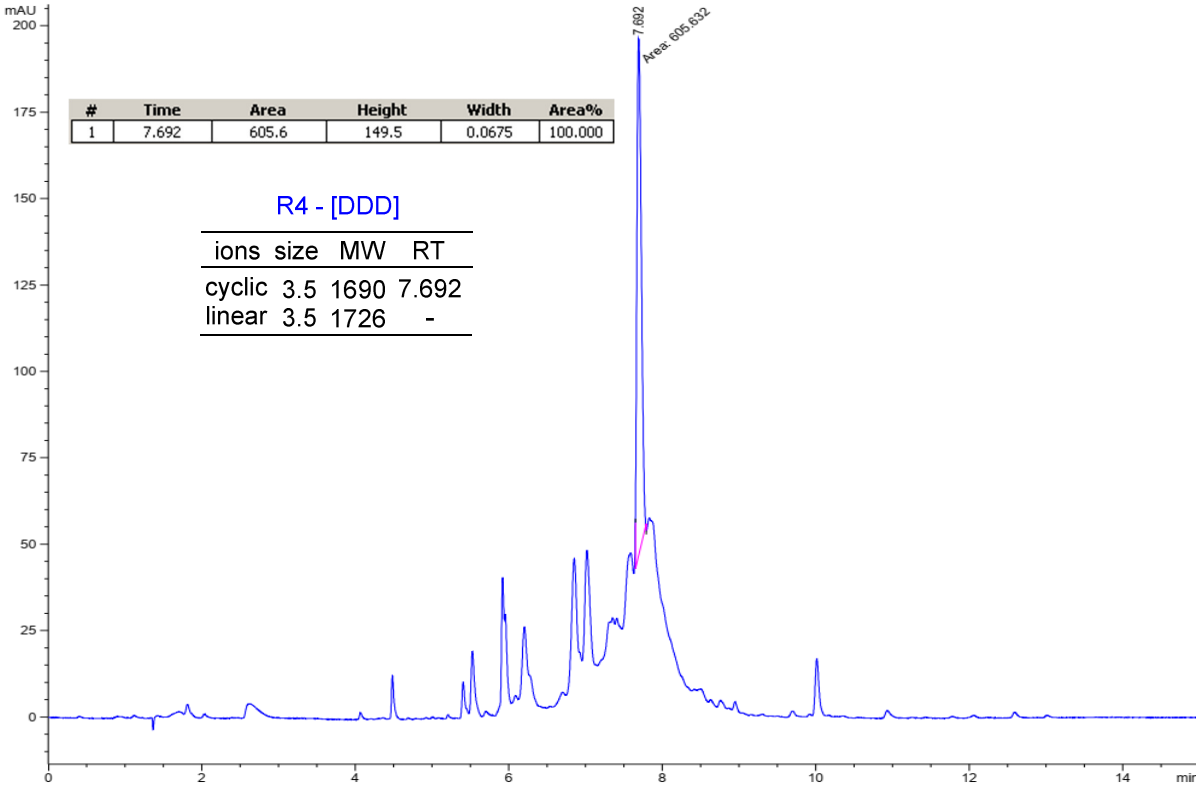

Max: 19512
[M+H+]
[M+2H+]
Exact Mass: 1691.64
cyclic - 3.5 mer
281.1
1694.2
1695.5
1693.4
1690.2
1691.8
292.1
312.8
264.9
141.1
582.5
681.4
846.6
857.9
954.9
1140.3
1453.1
1415.9
1559.4
2184.6
2498.6
m/z

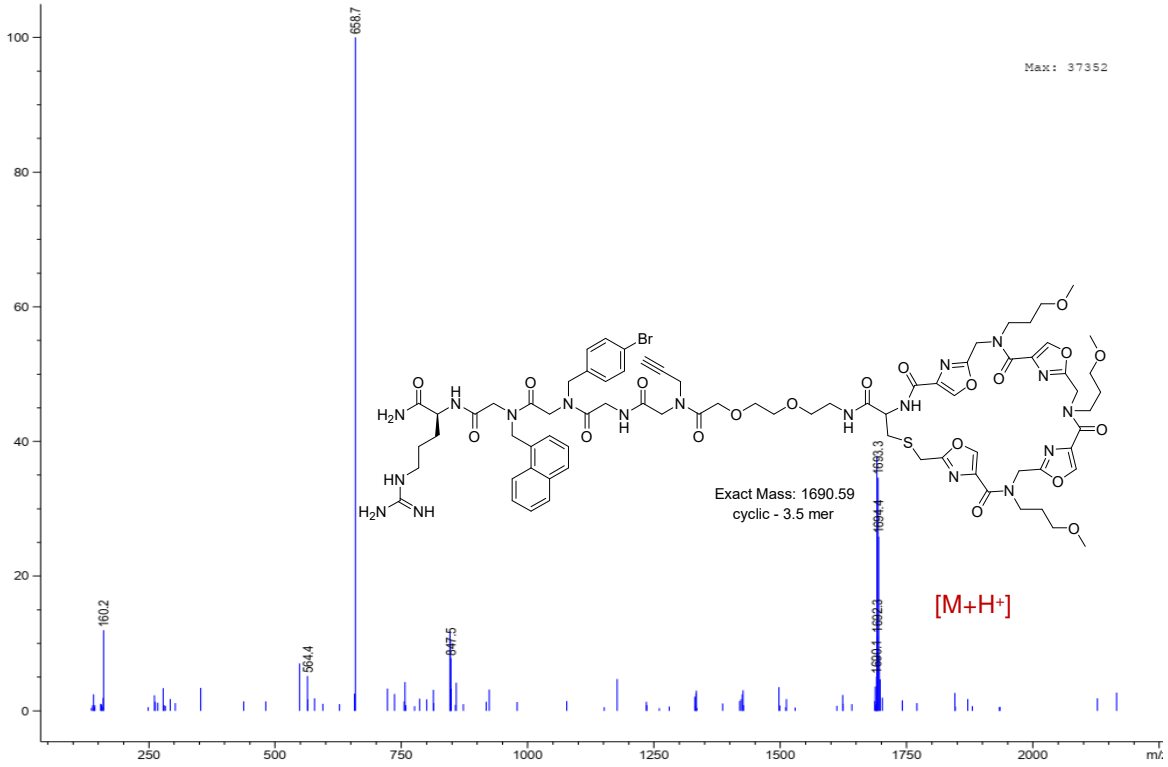

Max: 5800
[M+H+]
[M+2H+]
Exact Mass: 1494.50
cyclic - 2.5 mer
1496.7
747.7
481.9
412.3
480.4
167.1
511.6
462.2
482.5
586.6
721.9
925.6
1058.7
1232.3
852.3
1274.0
1357.3
1593.7
1872.9
2439.7
1648.9
1723.1
1954.8
2193.3
2125.5

R4-[DDD]: Cyclization was complete on both 10um & 160um.

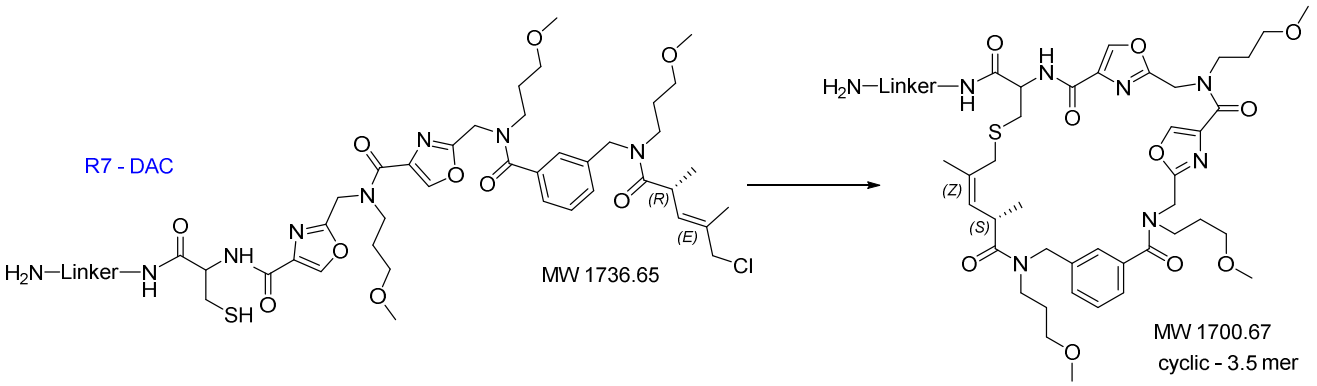


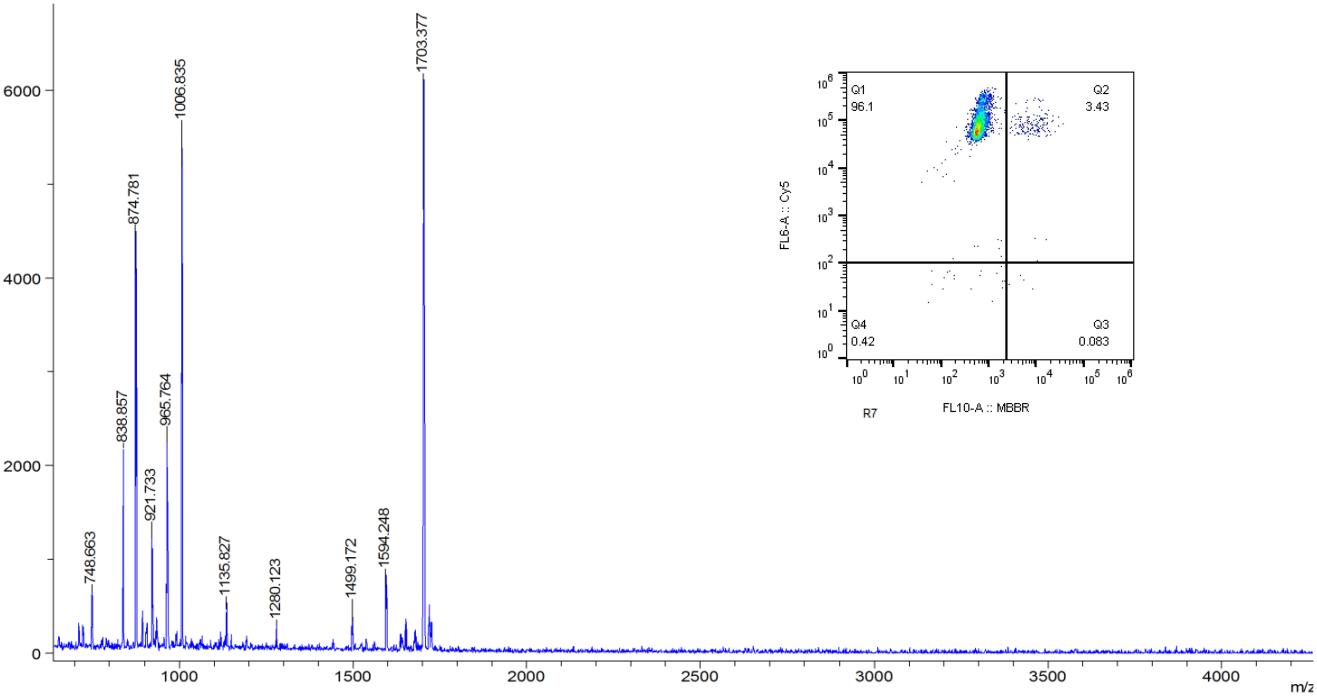


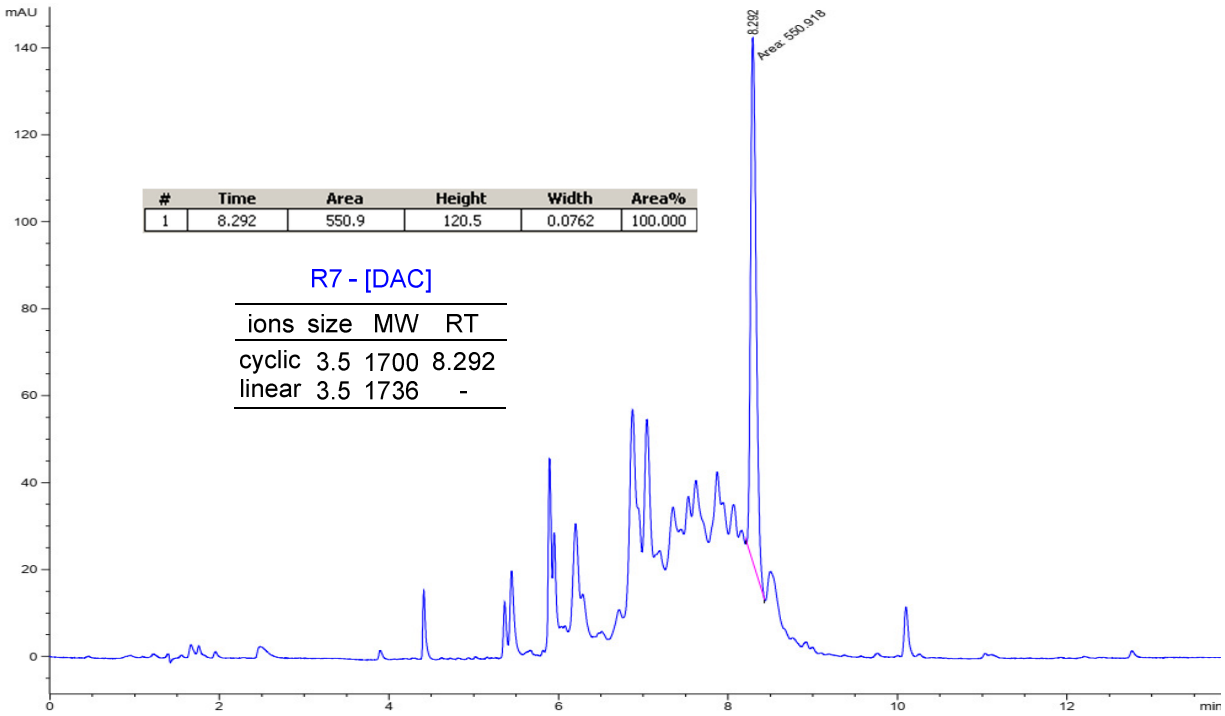

mAU
7.692
Area: 605.632
Time Area Height Width Area%
1 7.692 605.6 149.5 0.0675 100.000
R4 - [DDD]
ions size MW RT
cyclic 3.5 1690 7.692
linear 3.5 1726 -
min

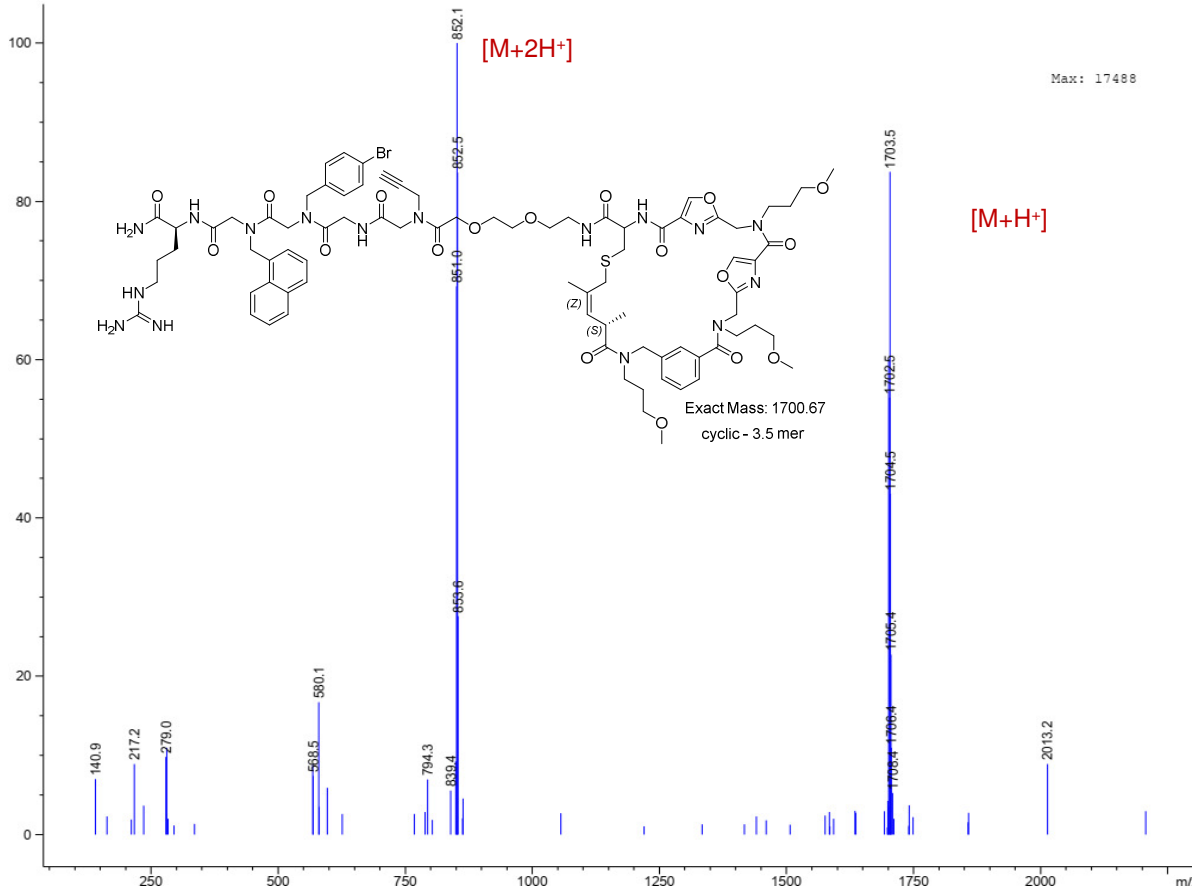

658.7
Max: 37352
Exact Mass: 1690.59
cyclic - 3.5 mer
[M+H+]
160.2
564.4
847.5
1691.4
1693.3
m/z

R7-[DAC]: Cyclization was complete on both 10um & 160um.

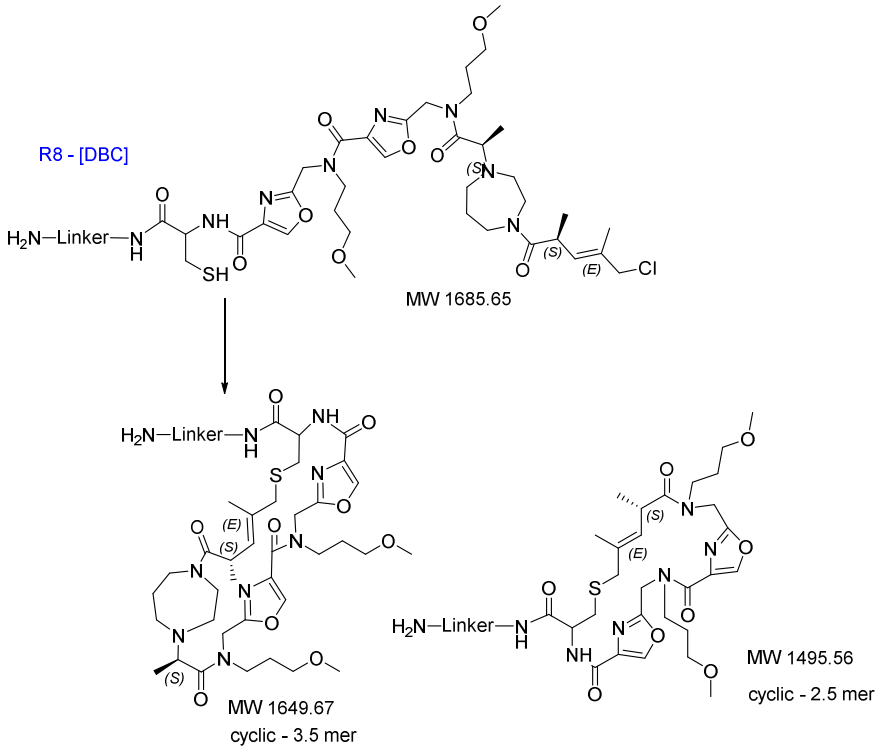


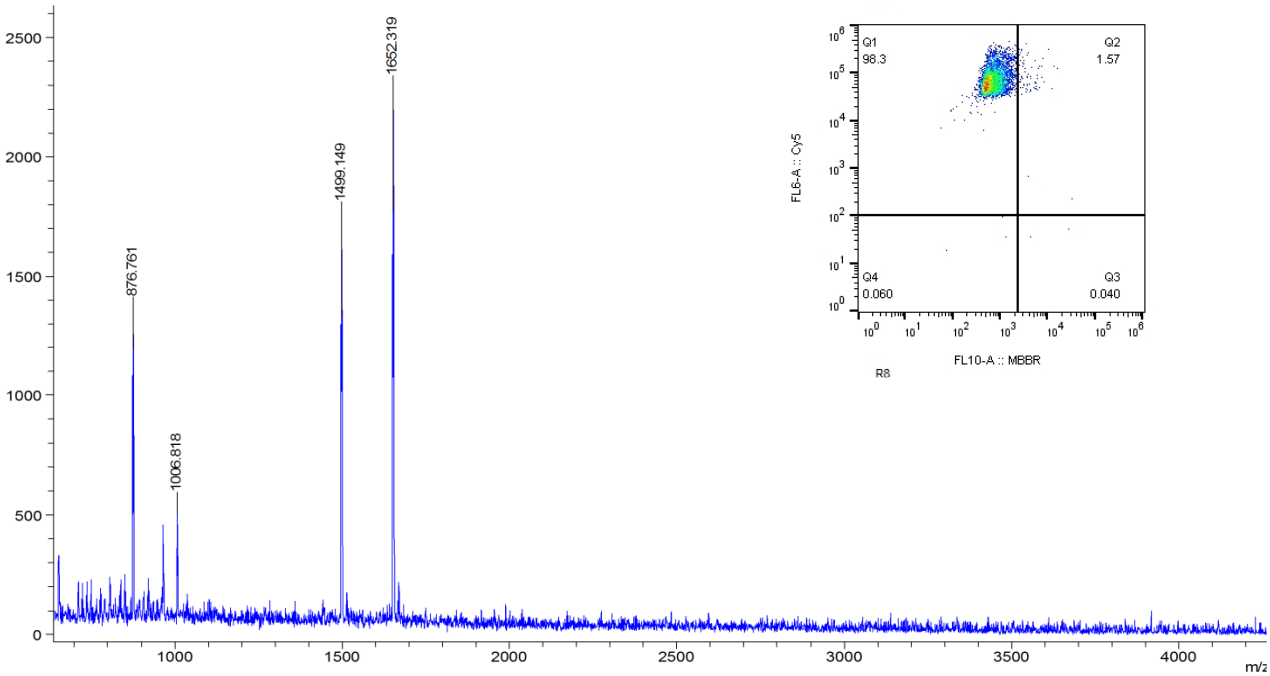


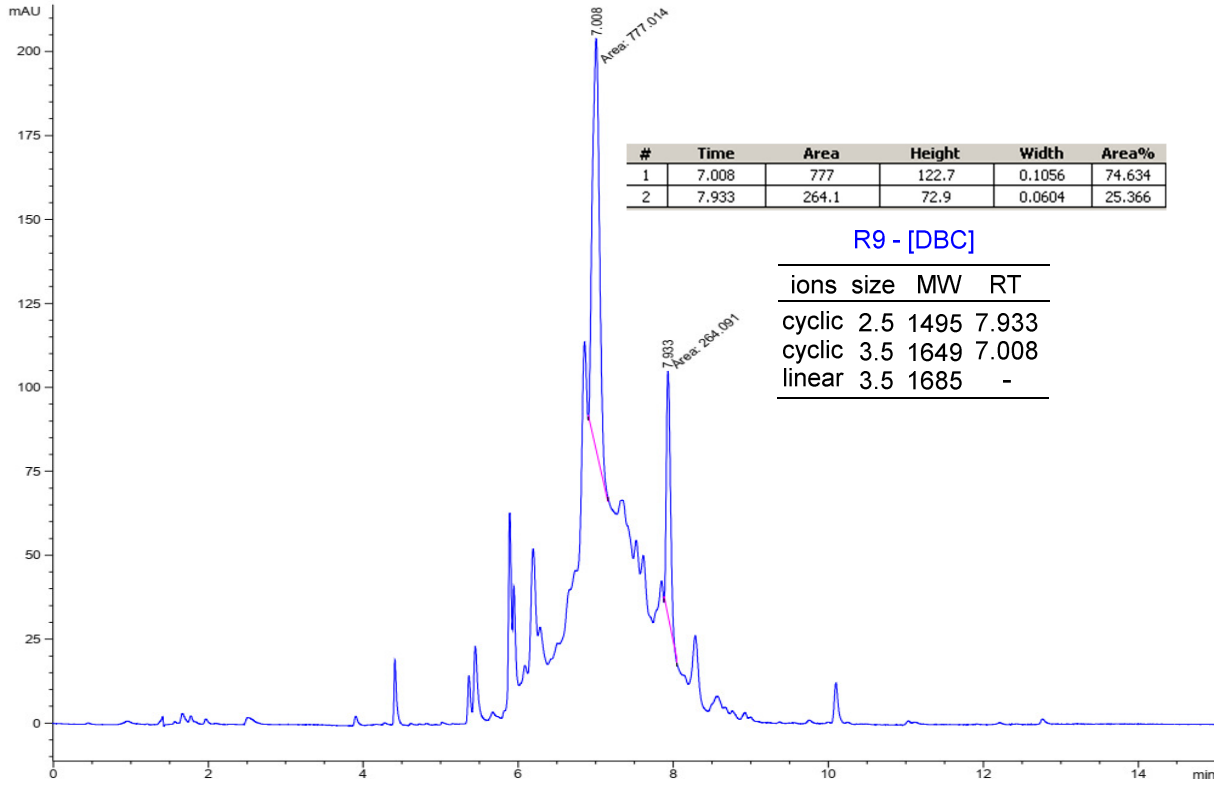

mAU
8.292
Area: 550.918
Time Area Height Width Area%
1 8.292 550.9 120.5 0.0762 100.000
R7 - [DAC]
ions size MW RT
cyclic 3.5 1700 8.292
linear 3.5 1736 -
min


[M+2H+]
Max: 17488
[M+H+]
Exact Mass: 1700.67
cyclic - 3.5 mer
m/

R8-[DBC]: Cyclization was complete on both 10um & 160um.



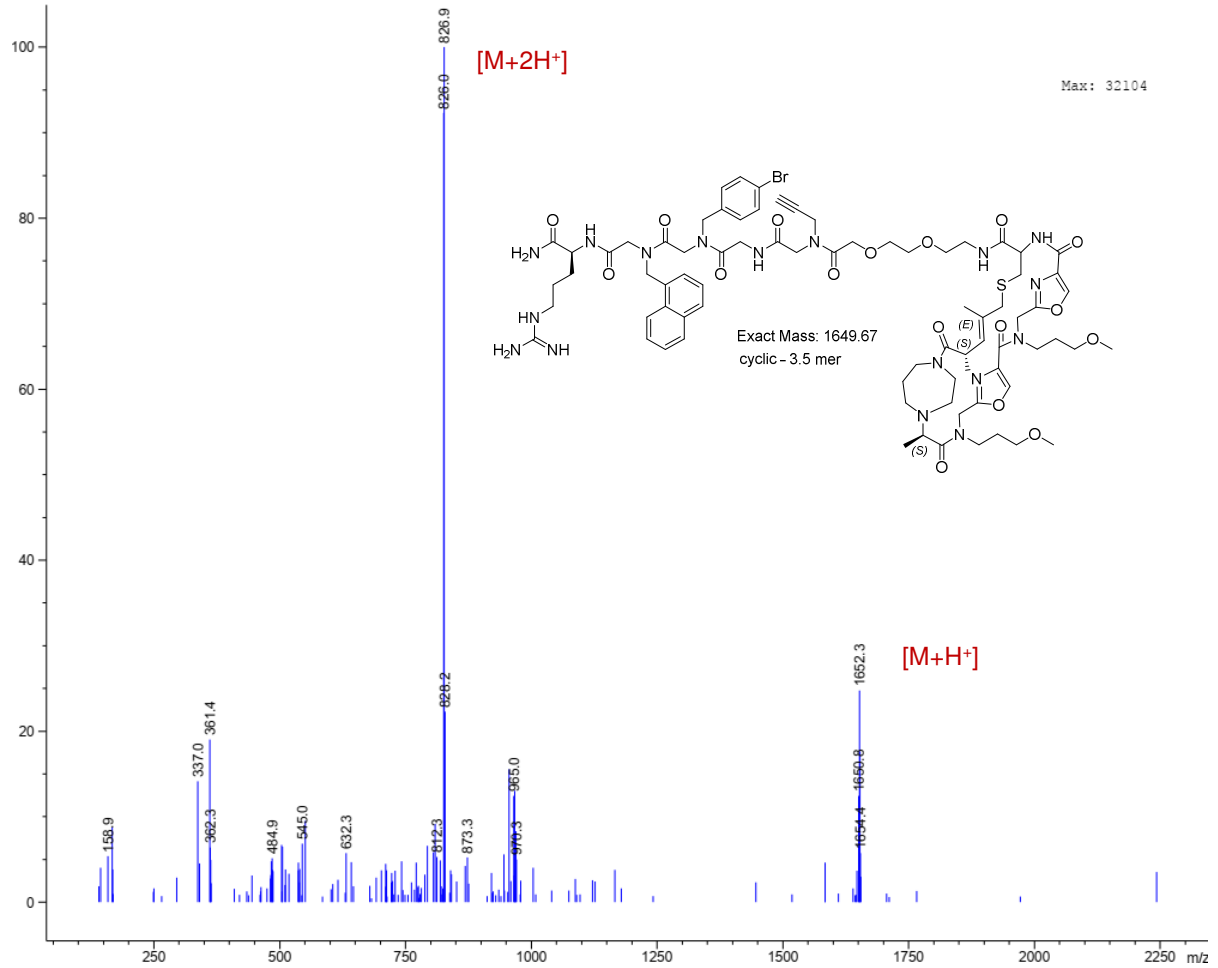


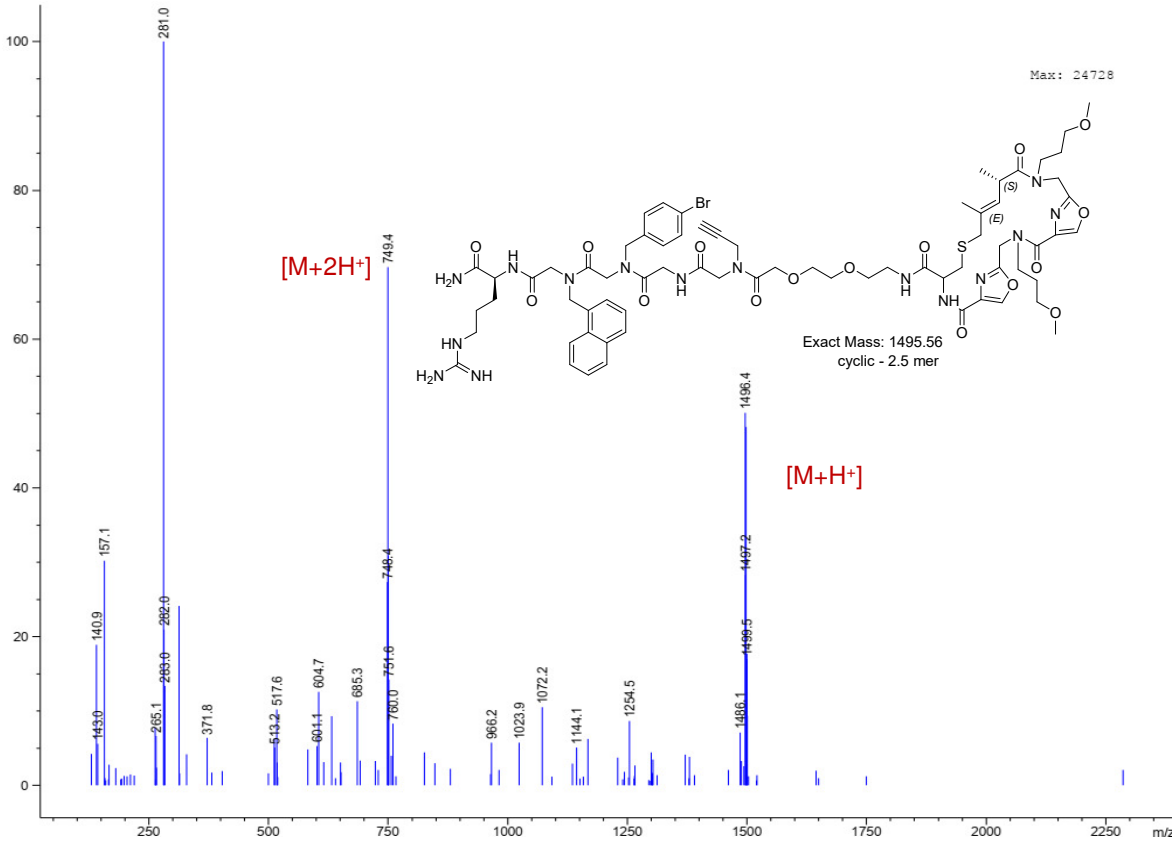


#	Time	Area	Height	Width	Area%
1	7.008	777	122.7	0.1056	74.634
2	7.933	264.1	72.9	0.0604	25.366

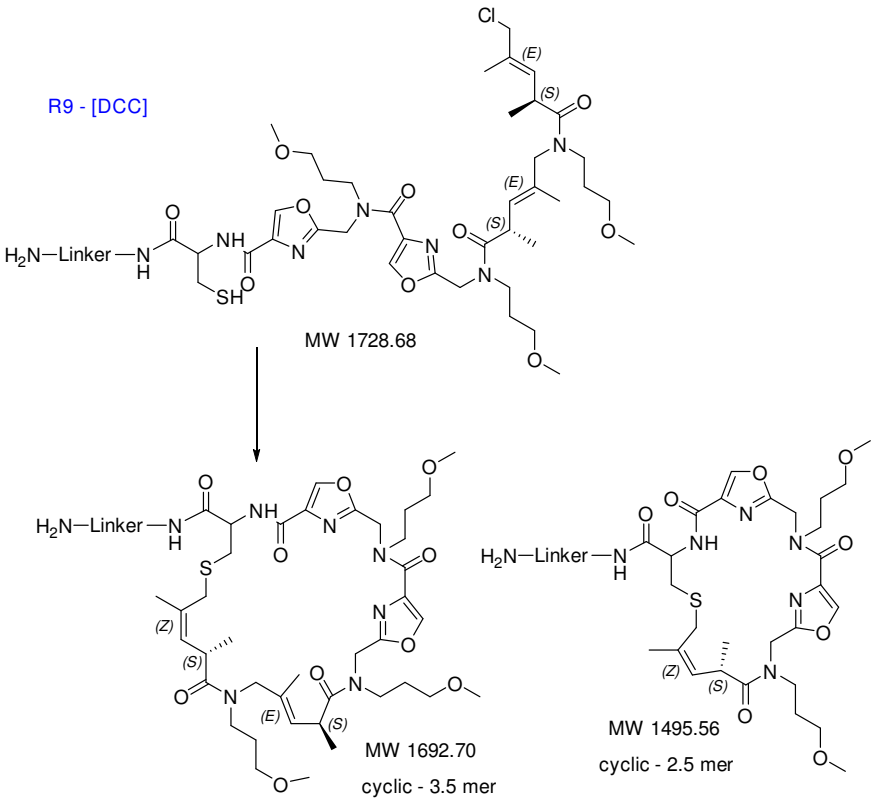
R9 - [DBC]

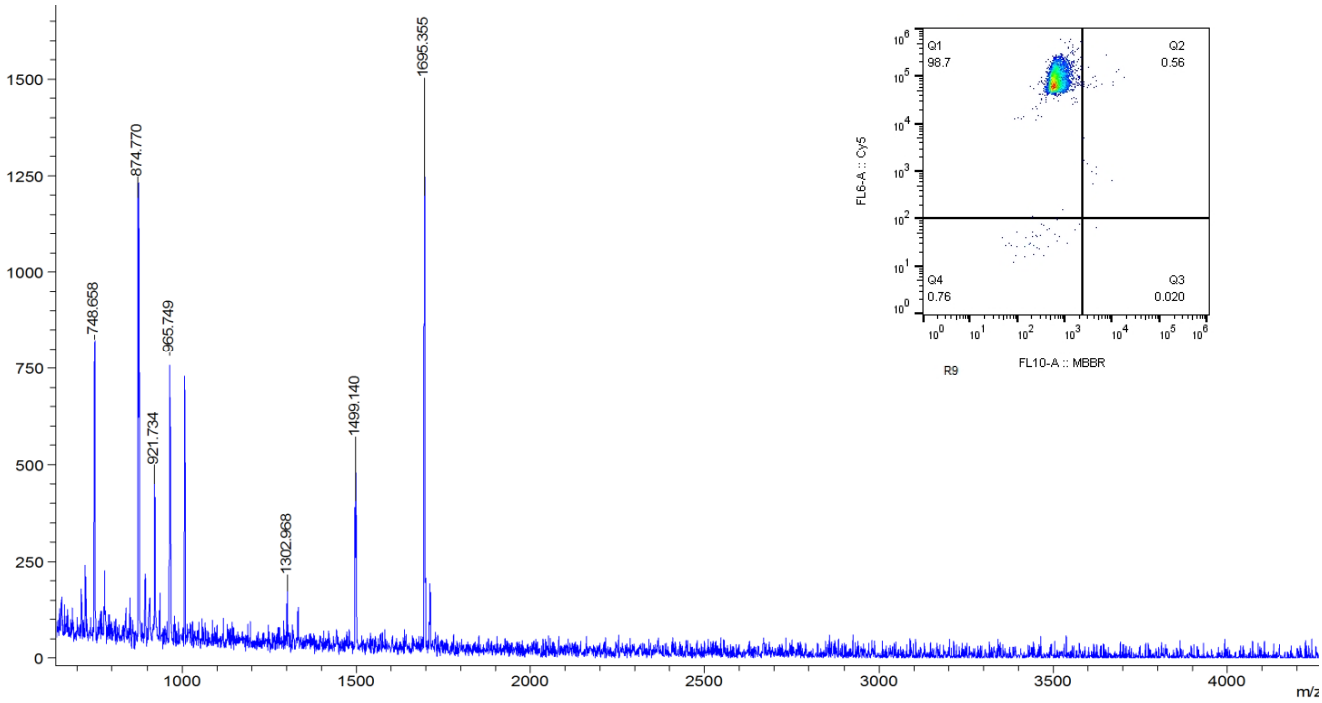
ions	size	MW	RT
cyclic	2.5	1495	7.933
cyclic	3.5	1649	7.008
linear	3.5	1685	-

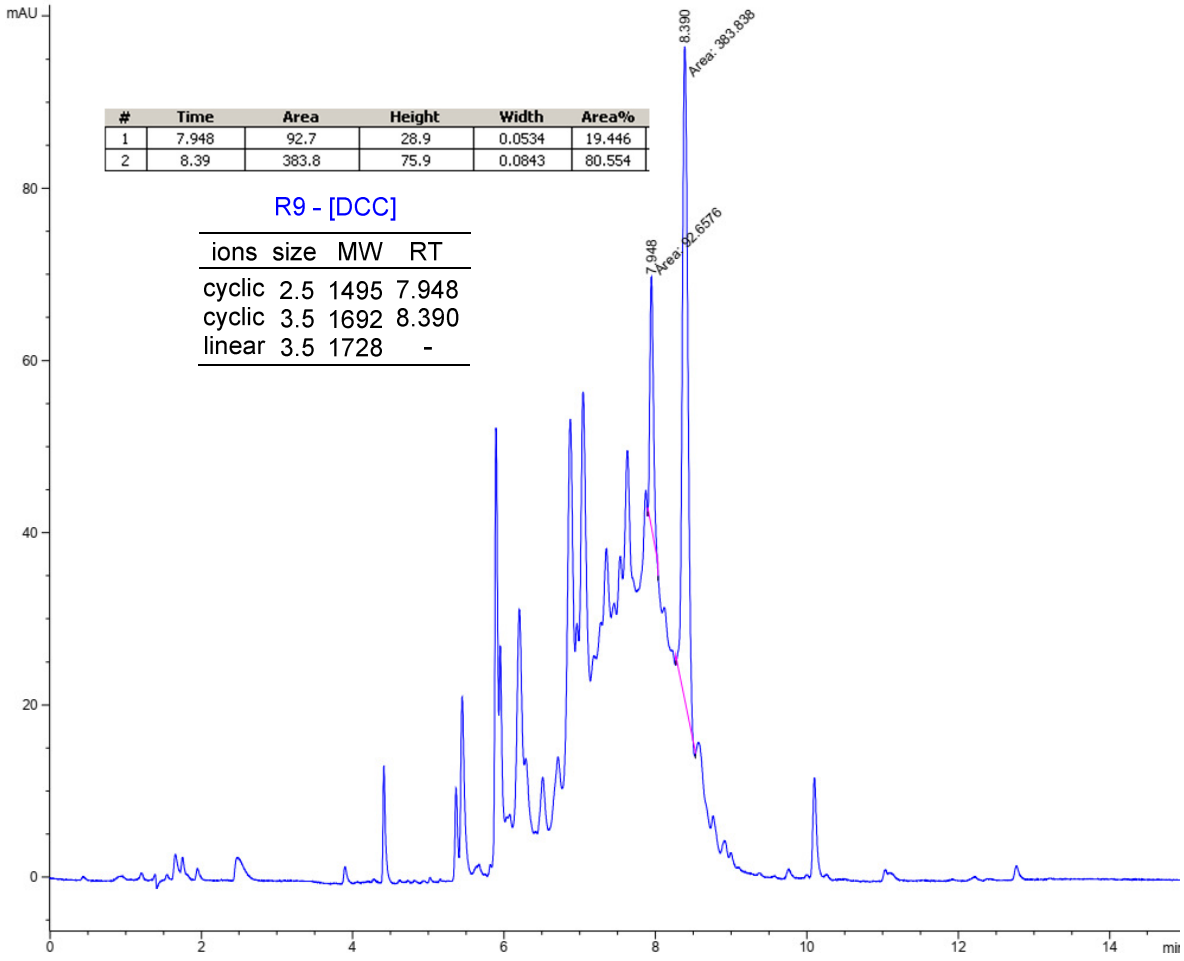




R9-[DCC]: Cyclization was complete on both 10um & 160um.



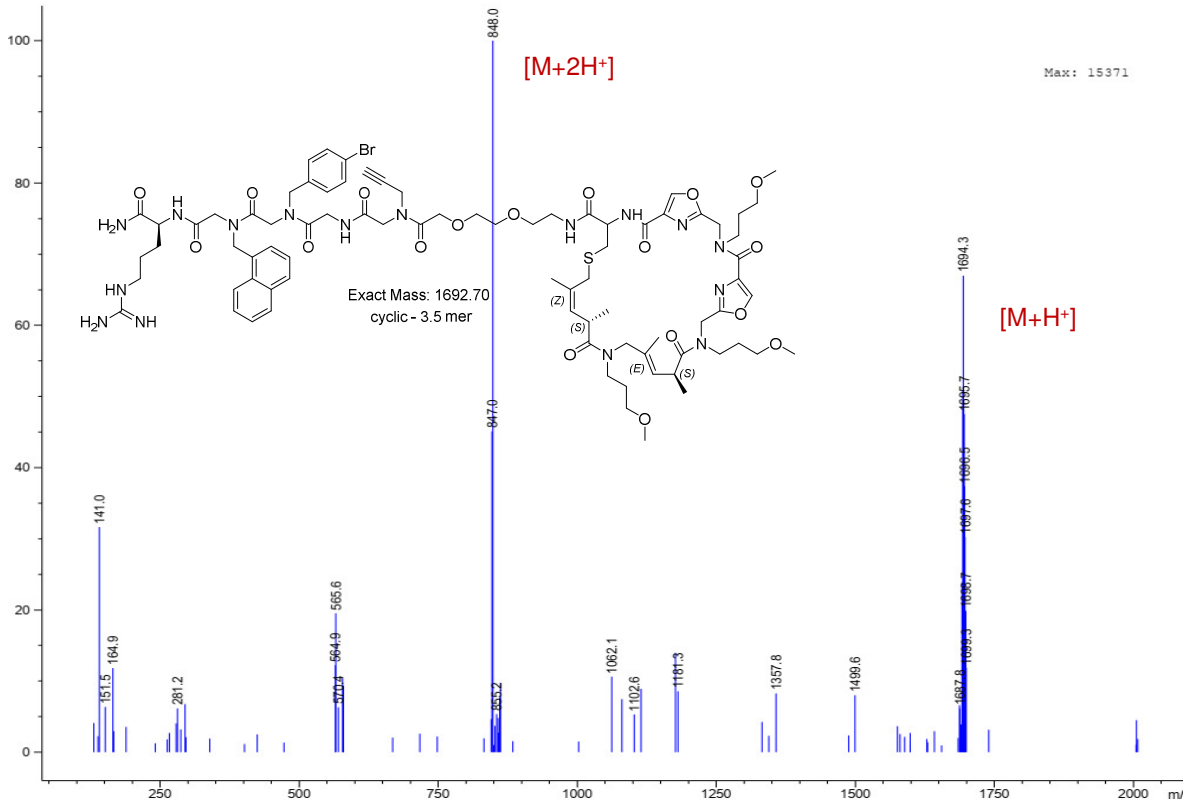


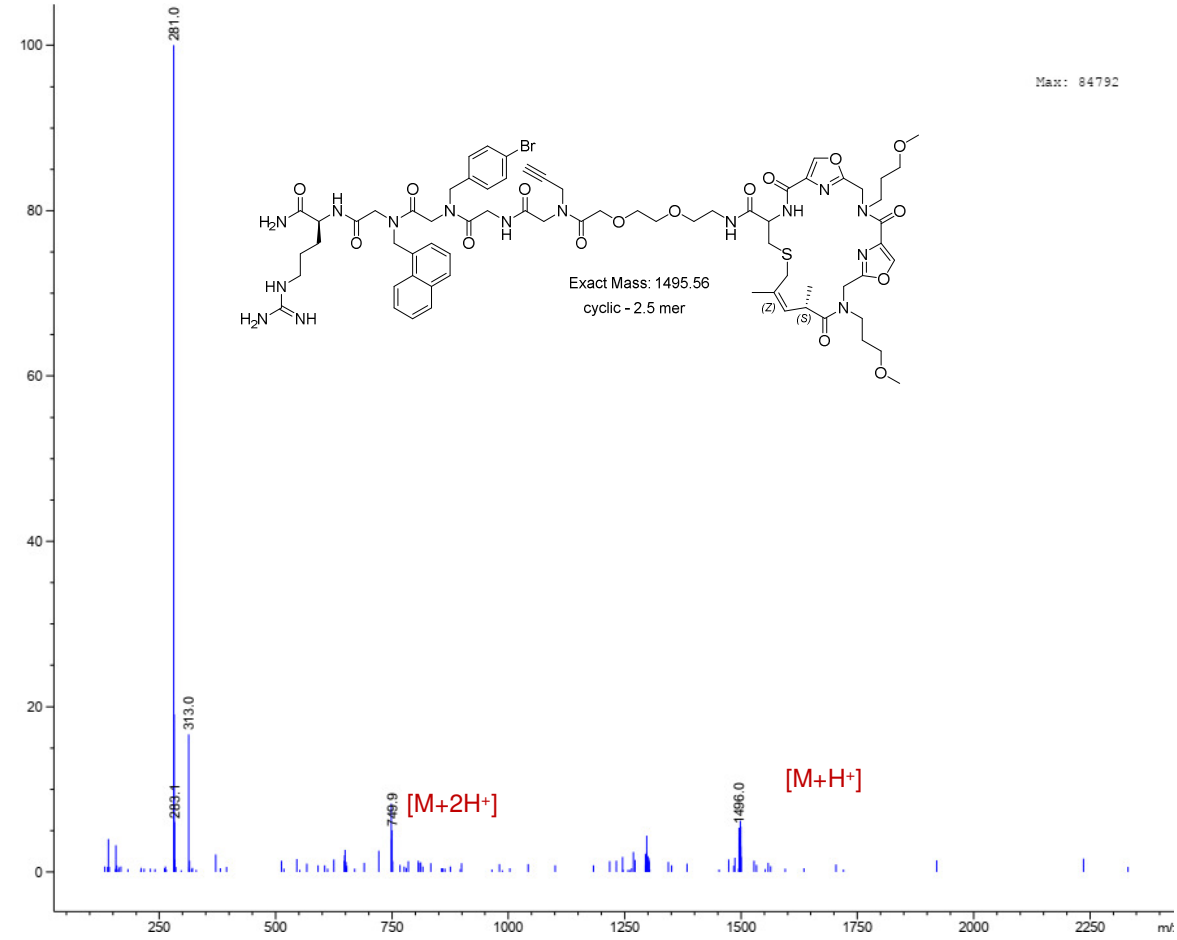


#	Time	Area	Height	Width	Area%
1	7.948	92.7	28.9	0.0534	19.446
2	8.39	383.8	75.9	0.0843	80.554

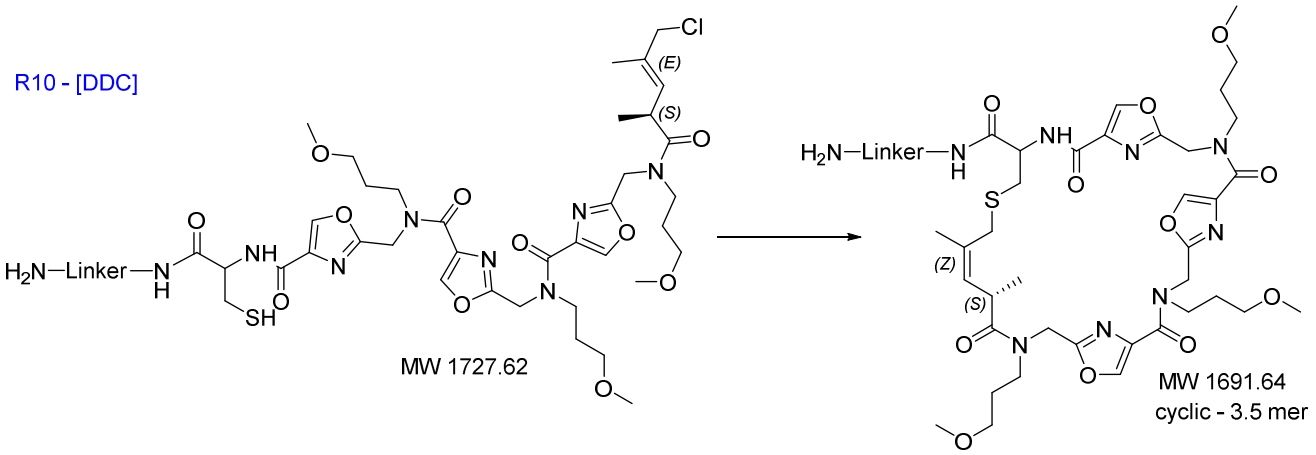
R9 - [DCC]

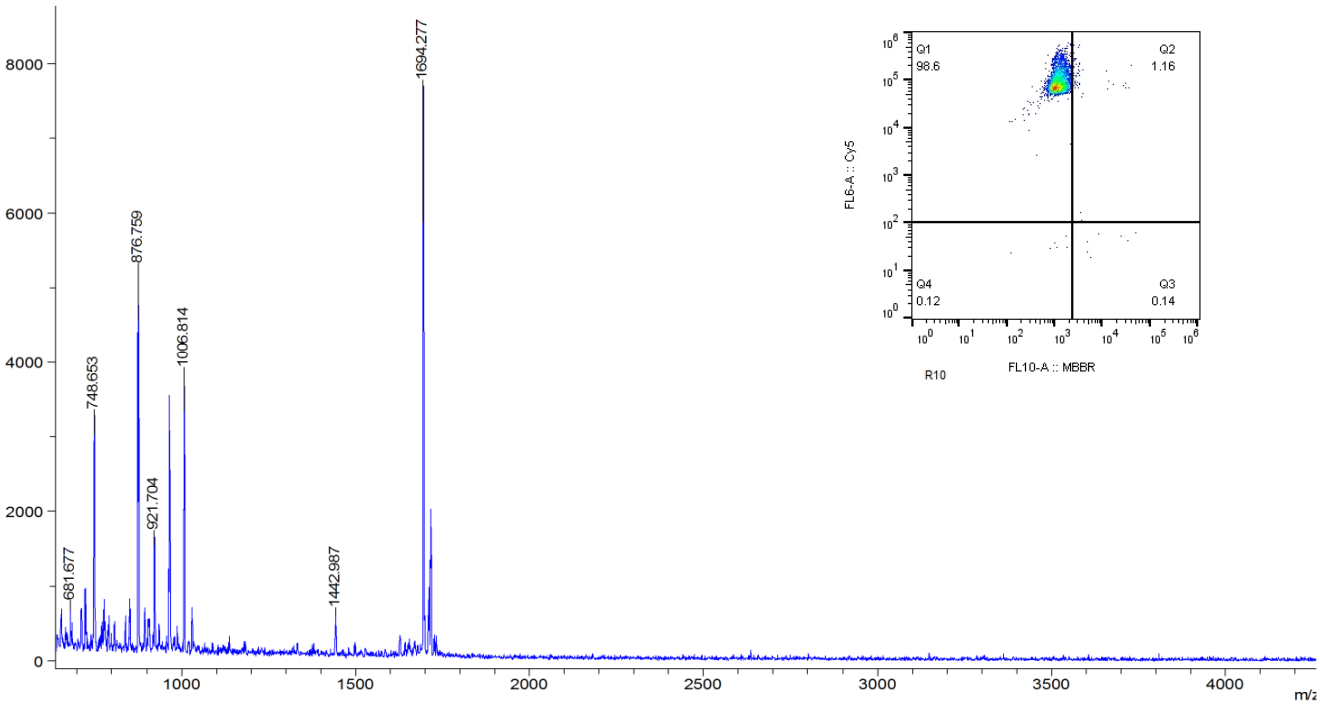
ions	size	MW	RT
cyclic	2.5	1495	7.948
cyclic	3.5	1692	8.390
linear	3.5	1728	-

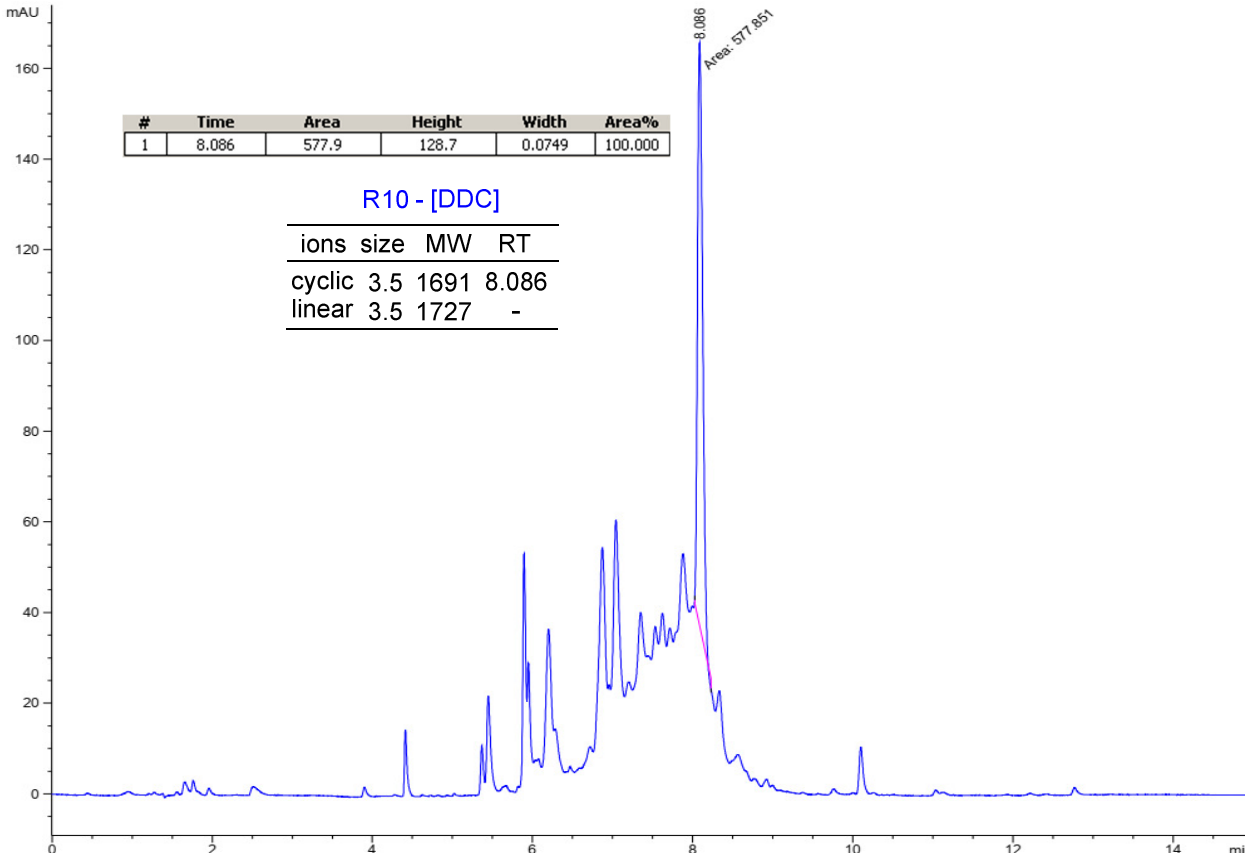

[M+2H+]
Max: 15371
Exact Mass: 1692.70
cyclic - 3.5 mer
[M+H+]
848.0
847.0
1694.3
141.0
565.6
1062.1
1357.8
1499.6
281.2

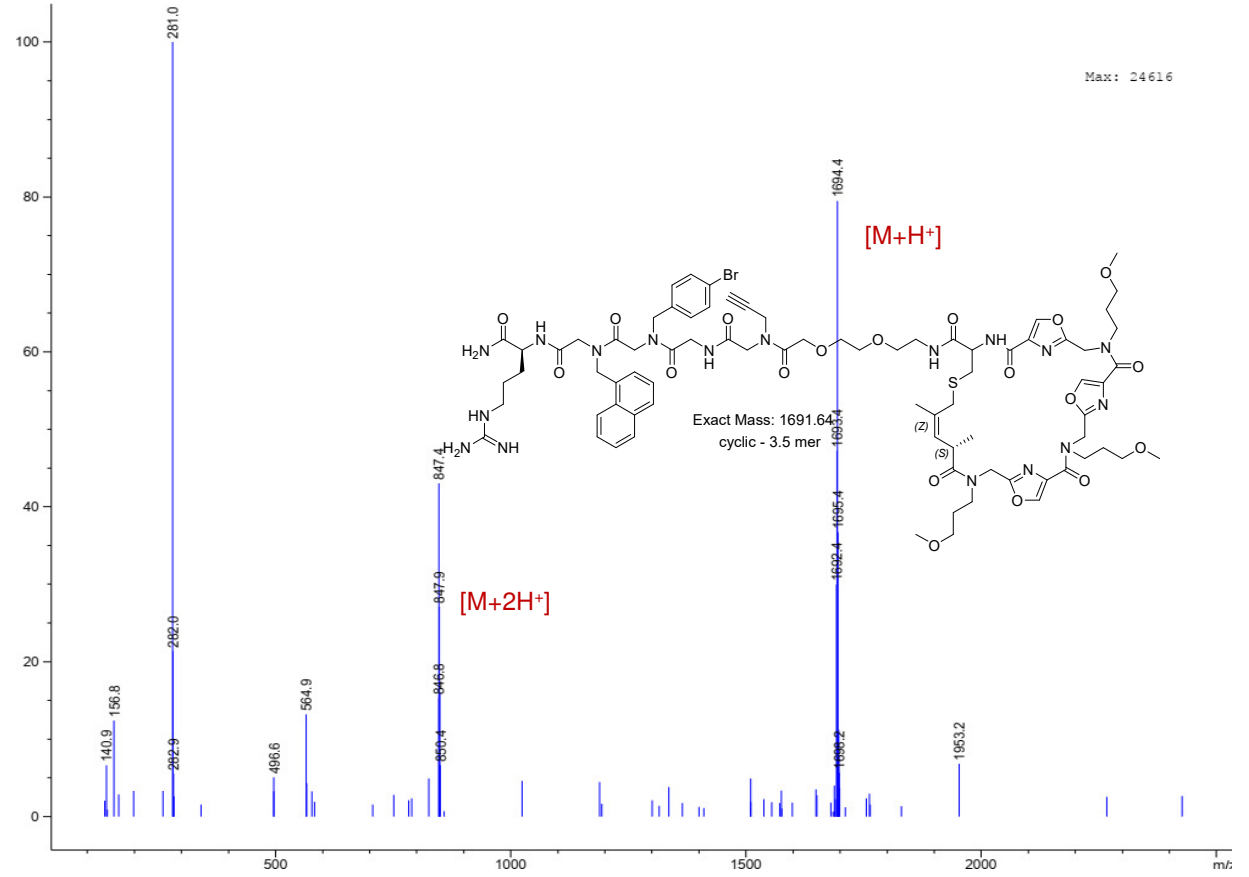

Max: 84792
Exact Mass: 1495.56
cyclic - 2.5 mer
281.0
313.0
283.1
749.9
[M+2H+]
1496.0
[M+H+]

R10-[DDC]: Cyclization was complete on both 10um & 160um.






mAU
8.086
Area: 577.851
Time Area Height Width Area%
1 8.086 577.9 128.7 0.0749 100.000
R10 - [DDC]
ions size MW RT
cyclic 3.5 1691 8.086
linear 3.5 1727 -


Max: 24616
[M+H+]
[M+2H+]
Exact Mass: 1691.64
cyclic - 3.5 mer

Section-9: Sequencing result of beads separated by flow cytometer due to incomplete cyclization (upto 3 copies)

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
1	13012405150126061102804	18		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(Cl)=NN1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
2	13032405150126081704280 3	18		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
3	13012405150228031702804	17		NCC1=CC=C(C)C=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
4	13042407150126031702803	12		NCC1=CC=C(C)C=C1		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
5	13092403150126061702804	12		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
6	13012407150226041703280 3	11		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
7	13032403150926041702804	11		NCCCOC		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(Cl)C(=O)[C@@H](C)C(=O)O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
9	13022407150126071703280 3	10		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
10	13032407150926031703280 3	10		NCC1=CC=C(C)C=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(Cl)C(=O)[C@@H](C)C(=O)O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
11	13092402150326081702804	10		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
8	13022403150126041709280 3	10		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
12	13032410150326071703280 3	9		C1CNCCN1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
15	13022407150326041704280 3	8		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
16	13032405150226031702803	8		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
17	13032405150428041703280 3	8		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CO)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
19	13092403150126031702803	8		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
20	13092403150226041702804	8		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
13	13022403150126021704280 9	8		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
14	13022403150226031702803	8		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
18	13042403150126071703280 3	8		NCCCOC		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
22	13012407150326061703280 3	7		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
23	13012407150326091702804	7		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
24	13012407150426021703280 9	7		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
25	13022407150426071704280 9	7		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
21	13012405150426091703280 3	7		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
27	13092403150226041702803	7		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
26	13042403150126101703280 1	7		NCCCOC		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		NCC1=CC=C(Cl)C=C1		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
39	13032408150426091702804	6		N1CCNCCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
45	13102403150326071703280 3	6		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
33	13022407150126031703280 3	6		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
34	13022407150126041710280 4	6		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
35	13022407150226071703280 3	6		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
36	13022407150229101704280 3	6		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
37	13022407150326031710280 4	6		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
38	13022407150926041709280 3	6		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
28	13012405150126061702803	6		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
32	13022405150126081704280 4	6		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
42	13092403150226071703280 4	6		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
43	13092403150326081709280 4	6		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
44	13092403150926011703280 3	6		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
41	13042409150226031709280 3	6		NCCCN1C=CN=C1		ClC(Cl)C(=O)[C@@H](C)C(C)(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
29	13022403150226041709280 4	6		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O

Entry	MoleculeID	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
30	13022403150226101702804	6		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
31	13022403150326021702804	6		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
40	13024403150226101702809	6		NCCCOC		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1COCCO1		OC(=O)[C@@H](C)Cl
60	13022410150926021702801	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC(=O)[C@@H](C)Cl
61	13022410151026011702804	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
74	13102403150226021702803	5		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC(=O)[C@H](C)Cl
48	13012407150126061703203	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
49	13012407150126091703203	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCO1		OC(=O)[C@H](C)Cl
50	13012407150326041702804	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
51	13012407151026041702804	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
57	13022407150226071702803	5		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CN(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
58	13022407150426031703203	5		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
59	13022407151026031703204	5		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CO1		OC(=O)[C@H](C)Cl
65	13032407150126021704204	5		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC(=O)[C@H](C)Br
66	13032407151026041704203	5		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Br
70	13042407150126041703209	5		NCC1=CC=C(C)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COCCO1		OC(=O)[C@H](C)Cl
46	13012405150926041703205	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC(=O)[C@H](C)Cl
47	13012405151026041703201	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CNC2=CC=CC=C21		OC(=O)[C@H](C)Cl
63	13032405150126021702803	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
64	13032405150226061703203	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC(=O)[C@H](C)Cl
71	13092403150926041701203	5		NCCC1COCOC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
72	13092403150926041703210	5		NCCC1COCOC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(=O)[C@H](C)Cl
73	13092404150426041703206	5		NCCC1COCOC1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1		OC(=O)[C@H](C)Cl
52	13022403150126041703206	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1		OC(=O)[C@H](C)Cl
53	13022403150126081703203	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
54	13022403150126101702803	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Br
55	13022403150126101702804	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
56	13022403150326101703203	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
62	13032403150226081703203	5		NCCCOC		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC(=O)[C@H](C)Cl
67	13042403150126031703209	5		NCCCOC		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCO1		OC(=O)[C@H](C)Cl
68	13042403150226041702805	5		NCCCOC		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC(=O)[C@H](C)Br
69	13042403150226061703206	5		NCCCOC		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1		OC(=O)[C@H](C)Cl
66	13022410150126061703203	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
114	13042410150426081703203	4		C1CNCCN1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
115	13042410150926041703203	4		C1CNCCN1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
85	13012408150326031701203	4		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
107	13032408150226031703204	4		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC(=O)[C@H](C)Cl
79	13012407150126031703204	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC(=O)[C@H](C)Cl
80	13012407150126081703205	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC(=O)[C@H](C)Cl
81	13012407150226061703203	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
82	13012407150326021702803	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		OC(=O)[C@H](C)Cl
83	13012407150426081703205	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC(=O)[C@H](C)Cl

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
84	13012407151029031701 2803	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CO)=N1)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)Cl(C)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
91	13022407150228041703 2805	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C[C@H](C)Cl)=O [S]
92	13022407150328041702 2804	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(=CC(=C1)F)F		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
93	13022407150328101704 2803	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Br)=O [R]
94	13022407150428041704 2803	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Br)=O [R]
95	13022407150926021704 2809	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1COCCC1		OC(C[C@H](C)Br)=O [R]
104	13032407150126031703 2803	4		NCC1=CC=C(C)C=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
105	13032407150126071703 2803	4		NCC1=CC=C(C)C=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
106	13032407150326101703 2803	4		NCC1=CC=C(C)C=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
78	13012405152229091703 2803	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CO)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
100	13032405152126091703 2803	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
101	13032405152229031703 2805	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C[C@H](C)Cl)=O [S]
102	13032405152229041703 2804	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CO)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC(C[C@H](C)Cl)=O [S]
103	13032405152428041703 2802	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CO)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC(C[C@H](C)Cl)=O [S]
112	13042405152229071704 2810	4		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C\C(=O)[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		BrC1=CC=C(C(O)=O)C=C1
113	13042405152326071703 2803	4		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C\C(=O)[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
75	13012401152326031703 2803	4		NCC1=CC=C(Br)C=C1		OC(C1=COC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
77	13012404152226081703 2803	4		NCC=C		OC(C1=COC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
116	13092402152022681703 2804	4		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC(C[C@H](C)Cl)=O [S]
117	13092402152228081709 2803	4		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC(C[C@H](C)Cl)=O [S]
118	13092403152326081703 2802	4		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC(C[C@H](C)Cl)=O [S]
119	13092403152326081703 2809	4		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC(C[C@H](C)Cl)=O [S]
120	13092403152426031703 2810	4		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(C[C@H](C)Cl)=O [S]
121	13092403152926011703 2810	4		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(C[C@H](C)Cl)=O [S]
122	13092403152926031709 2804	4		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
123	13092403151029031703 2804	4		NCCC1CCOCC1		OC(C1=CSC(CO)=N1)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CO1		OC(C[C@H](C)Cl)=O [S]
76	13012403151022907 1703 2810	4		NCCCOC		OC(C1=COC(CO)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(C[C@H](C)Cl)=O [S]
86	13022403151026091702 2809	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		ClCC1=CC(C(O)=O)=CC=C1
87	13022403151026101710 2804	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
88	13022403151022610703 2803	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
89	13022403151032607170 3804	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC(C[C@H](C)Cl)=O [S]
90	13022403151032609170 3803	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
97	13032403151029061703 2809	4		NCCCOC		OC(C1=CSC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC(C[C@H](C)Cl)=O [S]
98	13032403151032609171 0203 4	4		NCCCOC		OC(C1=CSC(CO)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
99	13032403151042608170 2209	4		NCCCOC		OC(C1=CSC(CO)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		ClCC1=CC(C(O)=O)=CC=C1
108	13042403151032602170 9204	4		NCCCOC		ClC/C(C)=C\C(=O)[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
109	13042403151092604170 9203	4		NCCCOC		ClC/C(C)=C\C(=O)[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC(C[C@H](C)Cl)=O [S]
110	13042403151026041703 2807	4		NCCCOC		ClC/C(C)=C\C(=O)[C@@H](C)C(O)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC(C[C@H](C)Cl)=O [S]
111	13042403151026041709 2803	4		NCCCOC		ClC/C(C)=C\C(=O)[C@@H](C)C(O)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC(C[C@H](C)Cl)=O [S]
157	13012410150126031703 2803	3		C1CNCCN1		OC(C1=COC(CO)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C[C@H](C)Cl)=O [S]
191	13022410150326041710 2803	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		OC(C[C@H](C)Cl)=O [S]
192	13022410150428031701 2803	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O

Entry	MoleculeID	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
193	13022410150426091709280 4	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
194	13022410150926021703280 7	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O [S]
195	13022410151026021709280 3	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC(C(=O)[C@@H](C)C(O)=O)=O		N[C@@H](C)C1=CC=CC=C1 [R]		OC([C@H](C)Cl)=O [S]
238	13042410150426091703280 9	3		C1CNCCN1		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O [S]
190	13022408150426071703280 3	3		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=O/N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
253	13102403150326081703280 3	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
254	13102403150426091703280 3	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
135	13012407150126021703280 7	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O [S]
136	13012407150126031703280 9	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O [S]
137	13012407150126081710280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
138	13012407150226011710280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
139	13012407150226021710280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		OC([C@H](C)Cl)=O [S]
140	13012407150226031710280 9	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COCCC1		OC(C1=CSC(CCl)=N1)=O
141	13012407150228041704280 7	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Br)=O [R]
142	13012407150226061709280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
143	13012407150226091703280 7	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O [S]
144	13012407150228101703281 0	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O [S]
145	13012407150326041710280 2	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		ClCC1=CC(C(O)=O)=CC=C1
146	13012407150326091703280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O [S]
147	13012407150426041703280 9	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O [S]
148	13012407150426051710280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		OC([C@H](C)Cl)=O [S]
149	13012407150426081703280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O [S]
150	13012407150426091703280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
151	13012407150426091703280 6	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O [S]
152	13012407150926011709280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC([C@H](C)Cl)=O [S]
153	13012407150926031710280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
154	13012407151026091710280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC(C(=O)[C@@H](C)C(O)=O)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
155	13012407151026031702280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
171	13022407150126041709280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC([C@H](C)Cl)=O [S]
172	13022407150126071709280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=O/N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
173	13022407150126071703280 2	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=O/N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O [S]
174	13022407150126081704280 9	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Br)=O [R]
175	13022407150226041703280 7	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O [S]
176	13022407150226051703280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
177	13022407150326051703280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
178	13022407150426031710280 4	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
179	13022407150426051703280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
180	13022407150426071712803 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=O/N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
181	13022407150426081703280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
182	13022407150926021703280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O [S]
183	13022407150926031702280 9	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCC1COCCC1		ClCC1=CC(C(O)=O)=CC=C1
184	13022407150926031703280 9	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O)=O		NCC1COCCC1		OC([C@H](C)Cl)=O [S]

Entry	MoleculeID	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
185	13022407150926031703 2810	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
186	13022407150926041703 2802	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
187	13022407150926041102 2804	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
188	13022407151026021710 2804	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
189	13022407151026031704 2807	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Br)=O.[R]
207	13032407150126021704 2803	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
208	13032407150126021710 2804	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
209	13032407150126031703 2808	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
210	13032407150126041703 2803	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
211	13032407150326081703 2809	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O.[S]
212	13032407150326101709 2803	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
213	13032407150426041704 2801	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Br)=O.[R]
214	13032407151026031703 2808	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
232	13042407150126081703 2803	3		NCC1=CC=C(C)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
233	13042407150426081710 2804	3		NCC1=CC=C(C)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
234	13042407150926031701 2803	3		NCC1=CC=C(C)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
235	13042407150926041709 2804	3		NCC1=CC=C(C)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
128	13012405150126061704 2804	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
129	13012405150126061704 2808	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Br)=O.[R]
130	13012405150326091703 2803	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
131	13012405150426041702 2809	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCC1COCCC1		ClCC1=CC(C(O)=O)=CC=C1
132	13012405150926021703 2807	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
133	13012405150926031702 2806	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=C1
134	13012405151026041702 2806	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=C1
168	13022405150126081709 2803	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
168	13022405150326071703 2804	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CN(N)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
170	13022405150426091704 2804	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
197	13032405150126061703 2805	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=D(Cl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
198	13032405150126091703 2809	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O.[S]
199	13032405150226071703 2804	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
200	13032405150226101703 2803	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
201	13032405150326031703 2803	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
202	13032405150326071703 2810	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
203	13032405150426091702 2809	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		ClCC1=CC(C(O)=O)=CC=C1
204	13032405150926021703 2801	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
205	13032405150926021704 2803	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
206	13032405151026041703 2805	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
228	13042405150226071703 2801	3		NCC1=CC=C(OCO2)C2=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CN(N)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
229	13042405150226071703 2803	3		NCC1=CC=C(OCO2)C2=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC=CN(N)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
230	13042405150426081710 2801	3		NCC1=CC=C(OCO2)C2=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC(C1=CSC(CCl)=N1)=O
231	13042405150426091703 2805	3		NCC1=CC=C(OCO2)C2=C1		ClC(C)C(=O)[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
124	13012401150226091703 2809	3		NCC1=CC=CC(Br)=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O.[S]

Entry	MoleculeID	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
239	13092402150428091703280 3	3		NCCC1CCOCC1		ClCC1=CC(=CO)N=CC=C1		NCC1=CC(F)=CC(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)C(=O)=O [S]
240	13092403150126061704280 4	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CC)C=C1)=O		NCC1=CC=CO1		OC[C@H](C)Br)=O [R]
241	13092403150126081704280 3	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CC)=N1)=O		NCCCN1C=NN=C1		OC(C1=CSC(CC)=N1)=O
242	13092403150226031703280 4	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CC)=N1)=O		NCC1=CC=CO1		OC[C@H](C)Cl)=O [S]
243	13092403150226031703280 8	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CC)=N1)=O		BrC1=CC=C(CN)C=C1		OC[C@H](C)Cl)=O [S]
244	13092403150226061701280 3	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CC)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CC)=N1)=O
245	13092403150226061704280 8	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CC)C=C1)=O		BrC1=CC=C(CN)C=C1		OC[C@H](C)Br)=O [R]
246	13092403150226081701280 9	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CC)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CC)=N1)=O
247	13092403150228101701280 3	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC(C(=O)[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CC)=N1)=O
248	13092403150426081703280 6	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CC)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC[C@H](C)Cl)=O [S]
249	13092403150926011701280 9	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CC)=N1)=O
250	13092403150926011702280 5	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1
251	13092403150926041702280 4	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
252	13092403151026041702280 9	3		NCCC1CCOCC1		OC(C1=CSC(CC)=N1)=O		CC(C)CCN		ClC(C(=O)[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
156	13012409150126091703280 4	3		NCCCN1C=CN=C1		OC(C1=COC(CC)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		NCC1=CC=CO1		OC[C@H](C)Cl)=O [S]
236	13042409150426071703280 5	3		NCCCN1C=CN=C1		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CC)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC[C@H](C)Cl)=O [S]
237	13042409150926031702280 3	3		NCCCN1C=CN=C1		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(C)=C[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
125	13012403150226071703280 6	3		NCCCOC		OC(C1=COC(CC)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CC)=N1)=O		N[C@H](C)C1=CC=CC=C1		OC[C@H](C)Cl)=O [S]
126	13012403150226091701280 9	3		NCCCOC		OC(C1=COC(CC)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		NCC1COCCC1		OC(C1=CSC(CC)=N1)=O
127	13012403151026041703280 4	3		NCCCOC		OC(C1=COC(CC)=N1)=O		CC(C)CCN		ClC(C(=O)[C@@H](C)C(O)=O		NCC1=CC=CO1		OC[C@H](C)Cl)=O [S]
158	13022403150226061703280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CC)C=C1)=O		NCC1=CC=CO1		OC[C@H](C)Cl)=O [S]
159	13022403150226071703280 9	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CC)=N1)=O		NCC1COCCC1		OC[C@H](C)Cl)=O [S]
160	13022403150226101703280 5	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC[C@H](C)Cl)=O [S]
161	13022403150326031703280 3	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CC)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O [S]
162	13022403150326061703280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CC)C=C1)=O		NCC1=CC=CO1		OC[C@H](C)Cl)=O [S]
163	13022403150426061703280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [R]		O=C(O)C1=C(C)OC=C1
164	13022403150826021702280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(C)=C[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
165	13022403150826041702280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(C)=C[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
166	13022403150826041702280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(C)=C[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(C)OC=C1
167	13022403151026011702280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC(C(C)=C[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
196	13032403150226051704280 3	3		NCCCOC		OC(C1=CSC(CC)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CC)C=C1)=O		NCCCN1C=CN=C1		OC[C@H](C)Br)=O [R]
215	13042403150126091703280 2	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		NCCO		OC[C@H](C)Cl)=O [S]
216	13042403150126091703280 6	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		N[C@H](C)C1=CC=CC=C1		OC[C@H](C)Cl)=O [S]
217	13042403150226021703280 2	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(=O)C)=O)C=C1		OC(C1=COC(CC)=N1)=O		NCCO		OC[C@H](C)Cl)=O [S]
218	13042403150326081703280 3	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CC)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O [S]
219	13042403150326081703280 5	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CC)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC[C@H](C)Cl)=O [S]
220	13042403150326091703280 3	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O [S]
221	13042403150326091702280 3	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CC)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		OC[C@H](C)Cl)=O [S]
222	13042403150426031702280 3	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CC)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CC)=N1)=O
223	13042403150426081703280 9	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CC)=N1)=O		NCC1COCCC1		OC[C@H](C)Cl)=O [S]
224	13042403150826021702280 3	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(C)=C[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
225	13042403150826021703280 3	3		NCCCOC		ClC(C(C)=C[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C(C)=C[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC[C@H](C)Cl)=O [S]

Entry	MoleculariD	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
226	13024031509260417032802	3		NCCOCC		ClC(C(C)=O)C[C@@H](C)C(C)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)C[C@@H](C)C(C)=O		NCCO		OC(=O)[C@H](C)Cl
227	13024031511026031032802	3		NCCCOC		ClC(C)C(=O)C[C@@H](C)C(C)=O		CC(C)CCN		ClC(C)C(=O)C[C@@H](C)C(C)=O		NCCO		OC(=O)[C@H](C)Cl
332	13024101501260717032803	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
333	13012410150426091703280 3	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Cl
427	13022410150126021702280 6	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=C1
428	13022410150126101702280 9	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)C[C@@H](C)C(C)=O		NCC1COCCC1		ClCC1=CC(C(O)=O)=CC=C1
429	13022410150126101703280 8	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC(C)C(=O)C[C@@H](C)C(C)=O		BrC1=CC=C(CN)C=C1		OC(=O)[C@H](C)Cl
430	13022410150226051703280 2	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCCO		OC(=O)[C@H](C)Cl
431	13022410150226061702280 3	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
432	13022410150226081703280 3	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl
433	13022410150226081703280 8	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC[C@H](C)Cl
434	13022410150326081703280 2	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC[C@H](C)Cl
435	13022410150426051709280 4	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
436	13022410150428081704261 0	2		C1CNCCN1		ClC(C1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		BrC1=CC=C(C(O)=O)C=C1
517	13032410150226061703280 4	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCC1=CC=CO1		OC[C@H](C)Cl
556	13042410150126061710280 4	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(Cl)OC=C1
557	13042410150126091703280 9	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC[C@H](C)Cl
558	13042410150126091709280 3	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC[C@H](C)Cl
559	13042410150226031709280 3	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC[C@H](C)Cl
560	13042410150326071703280 7	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC[C@H](C)Cl
561	13042410150326091701280 3	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
562	13042410150426081709280 4	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1 [R]		CCC(O)=O
563	13042410150926041703280 7	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)C[C@@H](C)C(C)=O		NCC1=CC(OC)=CC(OC)=C1		OC[C@H](C)Cl
564	13042410151026041702804	2		C1CNCCN1		ClC(C(C)=C[C@@H](C)C(C)=O		CC(C)CCN		ClC(C)C(=O)C[C@@H](C)C(C)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
327	13012408150126091710280 3	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		OC[C@H](C)Cl
328	13012408150126091710280 4	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		O=C(O)C1=C(Cl)OC=C1
330	13012408150426071703280 4	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC[C@H](C)Cl
331	13012408150426081703280 3	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl
420	13022408150126071703280 1	2		N1CCNCCC1		ClC(C1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl
421	13022408150426071710280 3	2		N1CCNCCC1		ClC(C1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1 [S]		OC[C@H](C)Cl
511	13032408150326061703280 3	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl
512	13032408150426041704260 8	2		N1CCNCCC1		OC(C1=CSC(CO)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C(Cl)=C1)=O		BrC1=CC=C(CN)C=C1		OC(=O)[C@H](C)Br)=O.[R]
513	13032408150426061704280 4	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		NCC1=CC=CO1		OC(=O)[C@H](C)Br)=O.[R]
514	13032408150426071703280 2	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCO		OC(=O)[C@H](C)Cl
547	13042408150926021704280 3	2		N1CCNCCC1		ClC(C(C)=C[C@@H](C)C(C)=O		NCC1=CC=C(C(F)(F)F)=C1		ClC(C)C(=O)C[C@@H](C)C(C)=O		NCCCN1C=CN=C1		OC(=O)[C@H](C)Br)=O.[R]
618	13102403150226061709280 3	2		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C(Cl)=C1)=O		N[C@H](C)C1=CC=CC=C1 [R]		OC[C@H](C)Cl
619	13102403150426071703280 4	2		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC[C@H](C)Cl
620	13102403150426081702280 3	2		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
621	13102403150926041701280 3	2		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC(C)C(=O)C[C@@H](C)C(C)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
283	13012407150126031702280 6	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1OOC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1
284	13012407150126031703280 6	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1		OC(C)[C@H](C)Cl

Entry	MoleculariD	Copies	Amines (X1)	Amines (X1) smiles	Acids (X1)	Acids (X1) smiles	Amines (X2)	Amines (X2) smiles	Acids (X2)	Acids (X2) smiles	Amines (X3)	Amines (X3) smiles	Acids (X3)	Acids (X3) smiles
285	13012407150128061703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
286	13012407150128071703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
287	13012407150128091717032803	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC[C@H](C)Cl)=O.[S]
288	13012407150128081703280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
289	13012407150128081709280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
290	13012407150126091703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
291	13012407150126091704280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC[C@H](C)Br)=O.[R]
292	13012407150126101703280 8	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		Cl[C@H](C)C(=O)O		BrC1=CC=C(CN)C=C1		OC[C@H](C)Cl)=O.[S]
293	13012407150228021703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
294	13012407150228021703280 6	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1		OC[C@H](C)Cl)=O.[S]
295	13012407150228031703281 0	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC[C@H](C)Cl)=O.[S]
296	13012407150226041703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
297	13012407150226041704280 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC[C@H](C)Br)=O.[R]
298	13012407150228051709280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC[C@H](C)Cl)=O.[S]
299	13012407150229071703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=O)N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC[C@H](C)Cl)=O.[S]
300	13012407150226081704280 9	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC[C@H](C)Br)=O.[R]
301	13012407150226091702280 9	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		ClCC1=CC(C(O)=O)=CC=C1
302	13012407150226101702280 5	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		Cl[C@H](C)C(=O)O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1
303	13012407150328031703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
304	13012407150328031703280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
305	13012407150328041704280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC[C@H](C)Br)=O.[R]
306	13012407150328081703280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC[C@H](C)Cl)=O.[S]
307	13012407150326091703280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
308	13012407150326091704280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Br)=O.[R]
309	13012407150326091709280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
310	13012407150426031703280 5	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
311	13012407150426031703280 6	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1		OC[C@H](C)Cl)=O.[S]
312	13012407150426041702280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
314	13012407150426041703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
315	13012407150426041703280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
316	13012407150426041703280 8	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC[C@H](C)Cl)=O.[S]
317	13012407150426041704280 9	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COCCC1		OC[C@H](C)Br)=O.[R]
318	13012407150426061703280 5	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC[C@H](C)Cl)=O.[S]
319	13012407150426091701280 8	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
320	13012407150926011701280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		Cl[C@H](C)C(=O)O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
321	13012407150926021703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		Cl[C@H](C)C(=O)O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
322	13012407150926021703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		Cl[C@H](C)C(=O)O		NCCO		OC[C@H](C)Cl)=O.[S]
323	13012407150926031701280 9	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		Cl[C@H](C)C(=O)O		NCC1COCCC1		OC(C1=CSC(CCl)=N1)=O
324	13012407150926031704280 9	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		Cl[C@H](C)C(=O)O		NCC1COCCC1		OC[C@H](C)Br)=O.[R]
325	13012407150926041709280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		Cl[C@H](C)C(=O)O		N[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
326	13012407151028041702280 5	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		Cl[C@H](C)C(=O)O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1

Section-11: Analysis of Naive bead population: These beads are deep sequenced after DEL synthesis

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
1	13042408150126011703280	47		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC[C@H](C)Cl)=O.[S]
2	13012407150126071702281 0	44		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
4	13022410150326031710280 4	37		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
3	13022403150426051703280 2	37		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
5	13032404150426041709280 4	33		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
6	13042407150226091703280 5	31		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC[C@H](C)Cl)=O.[S]
7	13042406150226051703280 2	25		NCC1=CC=CO1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC[C@H](C)Cl)=O.[S]
8	13102402150226101702280 9	23		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
9	13022409150926031703280 3	19		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
11	13092403150926021710280 4	18		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
10	13012404150926031702280 4	18		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
12	13012407150126041710280 4	17		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
13	13022403150326041709280 4	16		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
14	13102402150126041710280 4	16		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
15	13012406150926011710280 4	15		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
16	13012407161026041703280 3	15		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
17	13012410151026031709280 4	14		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
18	13022410151026031703280 3	14		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
19	13022402150126041704280 6	13		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC[C@H](C)Br)=O.[R]
23	13022403151026041709280 4	12		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
22	13012408150426041710280 4	12		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
26	13042403151026031703280 3	12		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
21	13012406150226101704260 3	12		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC[C@H](C)Br)=O.[R]
20	13012405150226041704280 3	12		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC[C@H](C)Br)=O.[R]
24	13032410150126041702280 3	12		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
25	13042401150326051703280 2	12		NCC1=CC=CC(Br)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
29	13042403150926031709280 4	11		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
28	13042403150426081702280 3	11		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
27	13012403150426041703280 3	11		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
30	13102402150126021701280 8	11		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
32	13012405150926031703280 7	10		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
33	13012407150226041709280 3	10		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
34	13032403150926021710280 4	10		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
36	13032410150226021702280 3	10		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
35	13032405150326011702280	10		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
37	13042405150426091702280	10		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
31	13012405150226041702280	10		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
38	13012403150226101709280	9		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
45	13092403150426041709280	9		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
40	13022410150926011702280	9		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
41	13032410151026031702280	9		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
42	13042403150926021703280	9		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
43	13042408150326071703280	9		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
44	13092403150126091703280	9		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
39	13012409150126101703280	9		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
46	13012403150326041709280	8		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
49	13012405150326061709280	8		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
59	13042408150926031702280	8		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
48	13012405150126101702280	8		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
63	13032407160126061702280	8		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
55	13042403150426061703280	8		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
58	13042407150226021702280	8		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
60	13042409150426061702280	8		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
57	13042405150226041703280	8		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
52	13022404150426071702280	8		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
50	13012405150926031702280	8		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
61	13042410150126061703280	8		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
56	13042403150426091702280	8		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
47	13012403150426081703280	8		NCCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
54	13042403150426051703280	8		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
51	13022403150226081702280	8		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=C1
66	13042407150226031703280	7		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
70	13092404150126041709280	7		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
63	13012407150226001709280	7		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
71	13102402150326041702280	7		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
65	13042403150126101702280	7		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
67	13042407150926041703280	7		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
68	13042409150226031703280	7		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
62	13012403150226021703280 3	7		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
63	13092403150126071704280 3	7		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
64	13032405150426061703280 3	7		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
84	13042403150326051709280 4	6		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
85	13042405150926021709280 4	6		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
75	13012407150226031709280 4	6		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
81	13032406150326041709280 4	6		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
77	13022404150126051710280 4	6		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
79	13022408150326041710280 4	6		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
76	13012407150426021710280 4	6		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
82	13032408150926021710280 4	6		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
88	13092403150226101710280 4	6		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
83	13042403150226021703280 3	6		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
78	13022408150226071703280 3	6		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
87	13092402150126031703280 3	6		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
73	13012404160126101703280 3	6		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
72	13012403150226101703280 3	6		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
74	13012405151026031703280 3	6		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
80	13032404150226041704280 3	6		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC[C@H](C)Br)=O.[R]
89	13092403150326101703280 3	6		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]
90	13102401150426061704280 3	6		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC[C@H](C)Br)=O.[R]
86	13042410150926021702280 4	6		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
91	13102403150426051703280 3	6		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC[C@H](C)Cl)=O.[S]
125	13042403150226041702280 5	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1
122	13032410150226041703280 1	5		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC[C@H](C)Cl)=O.[S]
113	13022410150226101709280 4	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
126	13042403150426041710280 3	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC[C@H](C)Cl)=O.[S]
128	13042405150426101710280 4	5		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
110	13022408151026031710280 4	5		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
111	13022409150426001710280 4	5		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
134	13102402150126101710280 4	5		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
135	13102402150226061710280 4	5		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
99	13012407150426041710280 4	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
131	13042410150426031703280 3	5		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC[C@H](C)Cl)=O.[S]

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
130	13042409150226081703280 3	5		NCCCN1C=CN=C1		ClC(C(C)=O)[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
112	13022410150126081703280 3	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
114	13022410150926031703280 3	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
108	13022403150226071703280 3	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
109	13022403150226071703280 3	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
132	13092402150926041702280 3	5		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
106	13012410150226041704280 3	5		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
107	13012410150326041702280 3	5		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
95	13012407150126041703280 3	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
96	13012407150126061703280 3	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
98	13012407150126101704280 3	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
101	13012407150926041702280 3	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
103	13012409150126061702280 3	5		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
104	13012409150126071703280 3	5		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
92	13012405150326101704280 3	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
93	13012406160926011703280 3	6		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
94	13012405150926041703280 3	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
123	13032401150326041702280 3	5		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
115	13032403150326041702280 3	5		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
120	13032407150326101702280 3	5		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
121	13032409151026031703280 3	5		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
117	13032405150226101704280 3	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
118	13032405150426001702280 3	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
119	13032405150926041702280 3	5		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
124	13042403150226031703280 9	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
127	13042403150426061703280 9	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
102	13012408150226041702280 9	5		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
100	13012407150926011702280 9	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
105	13012409150426021702280 9	5		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
133	13092403150126021703280 9	5		NCCC1CCOCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
97	13012407150126081703280 4	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
116	13032404150926031702280 4	5		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
129	13042409150226021703280 2	5		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
131	13022410150126041702281 0	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
138	13012403150926011703281O	4		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
161	13012408150226101701281O	4		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(C1=CSC(CCl)=N1)=O
204	13032410150926021704281O	4		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		BrC1=CC=C(C(O)=O)C=C1
223	13102403150126041703281O	4		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
227	13102403150426081703281O	4		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
207	13042404150226051703280S	4		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
206	13042403150426061703280S	4		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
211	13042405150926021703280S	4		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
187	13022410150426081703280S	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
188	13022410150926011703280I	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
170	13022407150126021703280I	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
142	13012405150126041703280I	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
221	13042410150226101702280I	4		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
209	13042405150126051709280I	4		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
182	13022410150126071709280I	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
183	13022410160226041709280I	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=C1
177	13022409150426041709280I	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
222	13102402150226041709280I	4		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
164	13012409150326061709280I	4		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
200	13032408150926011709280I	4		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
208	13042404150326071710280I	4		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
216	13042409150426051710280I	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
184	13022410150226051710280I	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
185	13022410150326051710280I	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
186	13022410150326101710280I	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
176	13022408151026041710280I	4		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
174	13022407150926041710280I	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
169	13022405150126041710280I	4		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC(C1=CSC(CCl)=N1)=O
162	13012408150926011710280I	4		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
130	13012402150926031710280I	4		NCC1=CC=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
159	13012407150926041710280I	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
145	13012405150226051710280I	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
202	13032410150226041710280I	4		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
191	13032403150126041710280I	4		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
224	13102403150326031703280 6	4		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
195	13032405150126041703280 6	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
219	13042410150226021703280 3	4		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
214	13042409150126031703280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
215	13042409150126041703280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
217	13042409150426101702280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
218	13042409150926021702280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
189	13022410151026041702280 3	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
190	13022410151026041703280 3	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
167	13022403150426061703280 3	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
175	13022408150426031703280 3	4		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
171	13022407150126061704280 3	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
172	13022407150226031704280 3	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
178	13022409150426081701280 3	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
180	13022409151026031702280 3	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
168	13022406160126021702280 3	4		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
139	13012404150226041703280 3	4		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
141	13012404151026021703280 3	4		NCC=C		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
160	13012408150226021701280 3	4		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
152	13012407150126081704280 3	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
154	13012407150226031703280 3	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
155	13012407150326031703280 3	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
156	13012407150326071702280 3	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
157	13012407150426091702280 3	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
158	13012407150426091704280 3	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
144	13012405150226041703280 3	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
148	13012405150426031704280 3	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
151	13012405150926021702280 3	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
194	13032404150226021703280 3	4		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
203	13032410150426101703280 3	4		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
192	13032403150126071703280 3	4		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
193	13032403150926041703280 3	4		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
199	13032408150226061702280 3	4		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
201	13032409150426021703280 3	4		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
226	13102403150326041704280 3	4		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
196	13032405150926011703280 3	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
205	13042403150226061701280 3	4		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
212	13042407150126061702280 3	4		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
166	13022403150226071701280 3	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
173	13022407150326031703280 3	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
146	13012405150226081704280 3	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
197	13032405151026041703280 3	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
220	13042401150226081702280 4	4		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
165	13022403150126041703280 4	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
179	13022409150926031703280 4	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
153	13012407150126101703280 4	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
163	13012409150226061703280 4	4		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
143	13012405150126081703280 4	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
150	13012405150426081703280 4	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
226	13102403160326041703280 4	4		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
213	13042407150926021703280 4	4		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
210	13042405150426051703280 2	4		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
140	13012404150426051703280 2	4		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
137	13012403150426051703280 2	4		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
147	13012405150326081702280 2	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=C1
149	13012405150426051703280 2	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
196	13032407150426051703280 2	4		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
408	13042409150926041702281 0	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
318	13022410150126061702281 0	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
296	13022403150926041703281 0	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
305	13022405150426041703281 0	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
231	13012403150226031703281 0	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
325	13032403150226081702281 0	3		NCCCOC		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
329	13032403150426081702281 0	3		NCCCOC		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
417	13042401150426061703280 5	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
398	13042408151026041702280 5	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1
407	13042409150926031703280 5	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
292	13022403150126061702280 5	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
311	13022407150126017032805	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
316	13022409150226071703280	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
286	13012410150426101701280	3		C1CNCCN1		OC(C1=COC(Cl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(Cl)=N1)=O
267	13012408150126051703280	3		N1CCNCCC1		OC(C1=COC(Cl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
243	13012405150126091702280	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(Cl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(Cl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=C1
365	13032410150426061703280	3		C1CNCCN1		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
397	13042408150426041703280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
323	13022410151026031703280	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
233	13012403150326081703280	3		NCCCOC		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
254	13012407150126061703280	3		NCC1=CC=C(C)C=C1		OC(C1=COC(Cl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
349	13032407150926041703280	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
302	13022405150326041703280	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
382	13042404150326041709280	3		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
372	13042403150126041709280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
373	13042403150126101709280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
377	13042403160326101709280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
395	13042408150326041709280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
435	13092404151026011709280	3		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
403	13042409150226051709280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
447	13102404150326041709280	3		NCC1=CC(F)=C(F)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
390	13042405150926011709280	3		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
297	13022404150426041709280	3		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
296	13022404150926021709280	3		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
324	13022410151026031709280	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
308	13022406150326081709280	3		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
310	13022407150126051709280	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
423	13092402150426071709280	3		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
425	13092402150926041709280	3		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
240	13012404150426041709280	3		NCC=C		OC(C1=COC(Cl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
230	13012403150126041709280	3		NCCCOC		OC(C1=COC(Cl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
270	13012408150326051709280	3		N1CCNCCC1		OC(C1=COC(Cl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
258	13012407150126091709280	3		NCC1=CC=C(C)C=C1		OC(C1=COC(Cl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
260	13012407150226101709280	3		NCC1=CC=C(C)C=C1		OC(C1=COC(Cl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
228	13012401150226091709280	3		NCC1=CC=CC(Br)=C1		OC(C1=COC(Cl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=C1

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
272	13012409150126051709280 2	3		NCCCN1C=CN=C1		OC(C1=COC(Cl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=C1
276	13012409150226071709280 4	3		NCCCN1C=CN=C1		OC(C1=COC(Cl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
361	13032410150226051709280 4	3		C1CNCCN1		OC(C1=CSC(Cl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
347	13032407150326031709280 4	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
350	13032407150926041709280 4	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
356	13032409150226031709280 4	3		NCCCN1C=CN=C1		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
338	13032405150426061709280 4	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
342	13032405151026041709280 4	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(Cl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
383	13042404150426031710280 4	3		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
384	13042404150426071710280 4	3		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
371	13042403150126011710280 4	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCOC		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
378	13042403150426091710280 4	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
381	13042403151026031710280 2	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		ClCC1=CC(C(O)=O)=CC=C1
392	13042406150226031710280 4	3		NCC1=CC=CO1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
399	13042409150126041710280 4	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
400	13042409160126091710280 3	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
385	13042405150126061710280 4	3		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
389	13042405150326101710280 3	3		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
293	13022403150326081710280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
420	13092402150226071710280 4	3		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
424	13092402150426081710280 4	3		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
317	13022409150326031710280 4	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
436	13102402150126031710280 4	3		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
306	13022405150926031710280 4	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
307	13022405151026021710280 4	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
238	13012404150226041710280 3	3		NCC=C		OC(C1=COC(Cl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
241	13012404151026031710280 3	3		NCC=C		OC(C1=COC(Cl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
284	13012410150326071710280 4	3		C1CNCCN1		OC(C1=COC(Cl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
251	13012406151026031710280 4	3		NCC1=CC=CO1		OC(C1=COC(Cl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
252	13012407150126011710280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(Cl)=N1)=O		NCCOC		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
264	13012407150926011710280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(Cl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
437	13102401151026031710280 4	3		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(Cl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
360	13032401150226021710280 4	3		C1CNCCN1		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
327	13032403150326051710280 4	3		NCCCOC		OC(C1=CSC(Cl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
352	13032408150326017102804	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
353	13032408150426041710280 4	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
355	13032408151026041710280 2	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		ClCC1=CC(C(O)=O)=CC=C1
343	13032406150926021710280 4	3		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
429	13092403150326081710280 4	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
430	13092403150426031710280 4	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
433	13092403151026031710280 2	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		ClCC1=CC(C(O)=O)=CC=C1
446	13102403151026041710280 3	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
332	13032405150126041710280 4	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
333	13032405150226061710280 1	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC(C1=CSC(CCl)=N1)=O
336	13032405150326081710280 4	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
414	13042410150226041701280 6	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
380	13042403150926021703280 6	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
387	13042405150226071701280 6	3		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
312	13022407150326041701280 6	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
247	13012406160326041703280 6	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
363	13032410150426061702280 6	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=C1
415	13042410150326061701280 3	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
374	13042403150326021703280 3	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
379	13042403150926011704280 3	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
368	13042402150126061703280 3	3		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
370	13042402150426071703280 3	3		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
393	13042407150126051701260 3	3		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
434	13092404150326031703280 3	3		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
401	13042409150226021703280 3	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
402	13042409150226031702280 3	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
448	13102404150426081703280 3	3		NCC1=CC(F)=C(F)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
386	13042405150226061702280 3	3		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
388	13042405150326021703280 3	3		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
299	13022404150926041703280 3	3		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
320	13022410150226071703280 3	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
294	13022403150426081703280 3	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
295	13022403150426101703280 3	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
309	13022407150126021703280 3	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
289	13022401150326071703280 3	3		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
422	13092402150326041703280 3	3		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
313	13022409150126041703280 3	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
314	13022409150126051703280 3	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
439	13102402150326041703280 3	3		NCC1=CC(F)=C(F)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
300	13022405150126051703280 3	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
301	13022405150126091704280 3	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
237	13012404150126101704280 3	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
283	13012410150326071703280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
285	13012410150326081703280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
286	13012410150326081704280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
287	13012410150426061703280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
232	13012403150226071703280 3	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
234	13012403150326091703280 3	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
265	13012408150126021702280 3	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
271	13012408160926031704280 3	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
229	13012402150226031703280 3	3		NCC1=CC=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
253	13012407150126041702280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
256	13012407150126081703280 3	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
273	13012409150126061704280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
275	13012409150226041704280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
278	13012409150326051703280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
279	13012409150426051702280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
280	13012409150426091704280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
281	13012409150926021703280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
436	13102401150426071704280 3	3		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
244	13012405150226031702280 3	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
362	13032410150326061702280 3	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
366	13032410150926041704280 3	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
354	13032406150926041703280 3	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
345	13032407150126081701280 3	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
348	13032407150326081704280 3	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
428	13092403150126081704280 3	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
432	13092403150426081702280 3	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1

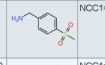
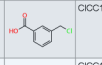
Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
359	13032409150326017022803	3		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1
442	13102403150326017012803	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
444	13102403150926021701 2803	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
335	13032405150326017032803	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
340	13032405150926021701 2803	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
416	13042401150426061702 2808	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=C1
396	13042408150326091703 2808	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
259	13012407150226101702 2808	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=C1
246	13012405150326041702 2808	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
358	13032409150326071702 2808	3		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
412	13042410150126101703 2809	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
413	13042410150226021704 2809	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
369	13042402150226081702 2809	3		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
394	13042407150126051703 2809	3		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
391	13042405150926031702 2809	3		NCC1=CC=C(OCO2)C2=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
321	13022410160326021703 2809	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
322	13022410150326071704 2809	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
291	13022403150126041702 2809	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
290	13022401150426081703 2809	3		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
315	13022409150226021701 2809	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
304	13022405150426031702 2809	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
236	13012404150126101702 2809	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
235	13012403150926021701 2809	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(C(F)(F)F)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
268	13012408150226101702 2809	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
269	13012408150326051702 2809	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
255	13012407150126071702 2809	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
257	13012407150126081702 2809	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
274	13012409150226031702 2809	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
277	13012409150226091702 2809	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
248	13012405150326101702 2809	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
249	13012405150426081703 2809	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
250	13012405150426091702 2809	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
331	13032404150326061702 2809	3		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1
334	13032405150326071703 2809	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
411	13042410150126081703280 4	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(=O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
405	13042409150426041703280 4	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(=O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
421	13092402150226101704280 4	3		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
239	13012404150426041703280 4	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
263	13012407150426061702280 4	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
282	13012409150926031702280 4	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
245	13012405150226041701280 4	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
367	13032401151026031704280 4	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
351	13032407151026031703280 4	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
427	13092403150126071702280 4	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
443	13102403150426091702280 4	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1
339	13032405150926011703280 4	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
418	13042410150426081703280 2	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
375	13042403150326061702280 2	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=C1
376	13042403150326071703280 2	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
404	13042409160226081703280 2	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
406	13042409150426051703280 2	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
409	13042409151026031703280 2	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
410	13042409151026041703280 2	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
319	13022410150126061703280 2	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
419	13092402150226071703280 2	3		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
303	13022405150326081703280 2	3		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
266	13012406150126021703280 2	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
261	13012407150326061703280 2	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
262	13012407150426051703280 2	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
242	13012405150126031703280 2	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
330	13032404150226021703280 2	3		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
364	13032410150426061703280 2	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
326	13032403150226081703280 2	3		NCCCOC		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
328	13032403150426051703280 2	3		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
344	13032407150126041703280 2	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
346	13032407150226031703280 2	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
426	13092403150126071702280 2	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=C1
431	13092403150426051703280 2	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
357	13032409150326041703280 2	3		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
440	13102403150126061703280 2	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
441	13102403150326071703280 2	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
445	13102403150926031703280 2	3		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
337	13032405150426051703280 2	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
341	13032405150926021703280 2	3		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
904	13042403150226021703281 0 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
950	13042407150226051702281 0 2	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
960	13042407150426081702281 0 2	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
984	13042409150226041703281 0 2	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
985	13042409150226051703281 0 2	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
662	13022404151026041703281 0 2	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
744	13022410150226091703281 0 2	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
638	13022403150126101702281 0 2	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
643	13022403150426041702281 0 2	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
710	13022408160926031703281 0 2	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
688	13022407150126031702281 0 2	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
624	13022401150226061703281 0 2	2		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
681	13022405150426101703281 0 2	2		NCC1=CC=C(OCO2)C2=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
483	13012404150326061704281 0 2	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		BrC1=CC=C(C(O)=O)C=C1
468	13012403150426041702281 0 2	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
517	13012407150126031701281 0 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(C1=CSC(CCl)=N1)=O
564	13012409150126061702281 0 2	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=C1
591	13012409150226071703281 0 2	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
594	13012409150426041703281 0 2	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
489	13012405150126091703281 0 2	2		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
510	13012405151026041704281 0 2	2		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		BrC1=CC=C(C(O)=O)C=C1
794	13032404150326091704281 0 2	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		BrC1=CC=C(C(O)=O)C=C1
823	13032407150126071703281 0 2	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
1111	13102403150126031704281 0 2	2		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		BrC1=CC=C(C(O)=O)C=C1
1120	13102403150226041703281 0 2	2		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
807	13032405150126081703281 0 2	2		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
923	13042404150126031701280 5 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
922	13042403151026041704280 5 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]

Section-10: Analysis of Naive bead population: These beads are deep sequenced after DEL synthesis (upto 2 copies)

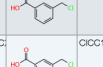
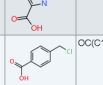
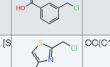
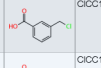
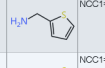
observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
1	13042408150126011703280	47		N1CNCCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
2	13012407150126071702281	44		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
3	13022403150426051703280	37		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
4	13022410150326031710280	37		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
5	13032404150426041709280	33		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
6	13042407150226091703280	31		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
7	13042406150226051703280	25		NCC1=CC=CO1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
8	13102402150226101702280	23		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
9	13022409150926031703280	19		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
10	13012404150926031702280	18		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
11	13092403150926021710280	18		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
12	13012407150126041710280	17		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
13	13022403150326041709280	16		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
14	13102402150126041710280	16		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
15	13012406150926011710280	15		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
16	13012407151026041703280	15		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
17	13012410151026031709280	14		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
18	13022410151026031703280	14		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
19	13022402150126041704280	13		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Br)=O.[R]
20	13012405150226041704280	12		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
21	13012408150226101704280	12		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
22	13012408150426041710280	12		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
23	13022403151026041709280	12		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
24	13032410150126041702280	12		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
25	13042401150326051703280	12		NCC1=CC=CC(Br)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
26	13042403151026031703280	12		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
27	13012403150426041703280	11		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
28	13042403150426081702280	11		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
29	13042403150926031709280	11		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
30	13102402150126021701280	11		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)O)C=C1		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
31	13012405150226041702280	10		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
32	13012405150926031703280	10		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
33	13012407150226041709280	10		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
34	13032403150926021702804	10		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
35	13032405150326021702803	10		NCC1=CC=C(OCO2)C		OC(C1=CSC(CCl)=N1)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
36	13032410150226021702803	10		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
37	13042405150426091702804	10		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
38	13012403150226101702803	9		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
39	13012409150126101703280 2	9		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
40	13022410150926011702804	9		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
41	13032410151026031702804	9		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
42	13042403150926021703803	9		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
43	13042408150326071703803	9		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
44	13092403150126091703280 4	9		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
45	13092403150426041702804	9		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
46	13012403150326041702804	8		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
47	13012403150426081703280 9	8		NCCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
48	13012405150126101702804	8		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
49	13012405150326061702804	8		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
50	13012405150926031702803	8		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
51	13022403150226081702802	8		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
52	13022404150426071702803	8		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
53	13032407150126051702804	8		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
54	13042403150426051703280 2	8		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
55	13042403150426061703280 3	8		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
56	13042403150426091702280 9	8		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
57	13042405150226041703280 3	8		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
58	13042407150226021702803	8		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
59	13042408150926031702804	8		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
60	13042409150426061702803	8		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
61	13042410150126061703280 9	8		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
62	13012403150226021703280 3	7		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
63	13012407150226061702804	7		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
64	13032405150426081703280 3	7		NCC1=CC=C(OCO2)C		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
65	13042403150126101702280 3	7		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
66	13042407150226031703280 5	7		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
67	13042407150926041703280 3	7		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
68	13042409150226031703280 3	7		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
69	13092403150126071704280 3	7		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
70	13092404150126041709280 4	7		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
71	13102402150326041710280 4	7		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
72	13012403150226101703280 3	6		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
73	13012404150126101702280 3	6		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
74	13012405151026031703280 3	6		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
75	13012407150226031709280 4	6		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
76	13012407150426021710280 4	6		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
77	13022404150126051702804 4	6		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
78	13022408150226071703280 3	6		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
79	13022408150326041710280 4	6		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
80	13032404150226041704280 3	6		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
81	13032406150326041709280 4	6		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
82	13032408150926021710280 4	6		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
83	13042403150226021703280 3	6		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
84	13042403150326051709280 4	6		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
85	13042405150926021709280 4	6		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
86	13042410150926021702280 4	6		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
87	13092402150126031703280 3	6		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
88	13092403150226101702804 4	6		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
89	13092403150326101703280 3	6		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
90	13102401150426061704280 9	6		NCC1=CC(F)=C(F)C=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
91	13102403150426051703280 2	6		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
92	13012405150326101704280 3	5		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
93	13012405150926011701280 3	5		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
94	13012405150926041703280 3	5		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
95	13012407150126041703280 3	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
96	13012407150126061702280 3	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
97	13012407150126081703280 4	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
98	13012407150126101704280 3	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
99	13012407150426041710280 4	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
100	13012407150926011702280	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
101	13012407150926041702280	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
102	13012408150226041702280	5		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
103	13012409150126061702280	5		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
104	13012409150126071703280	5		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
105	13012409150426021702280	5		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
106	13012410150226041704280	5		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
107	13012410150326041702280	5		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
108	13022403150226071201280	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
109	13022403150226071703280	5		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
110	13022408151026031702804	5		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
111	13022409150426061702804	5		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
112	13022410150126061701280	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
113	13022410150226101709280	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
114	13022410150926031703280	5		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
115	13032403150326041702280	5		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
116	13032404150926031702280	5		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
117	13032405150226101704280	5		NCC1=CC=C(OCO2)C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
118	13032405150426081701280	5		NCC1=CC=C(OCO2)C		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
119	13032405150926041704280	5		NCC1=CC=C(OCO2)C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
120	13032407150326101702280	5		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
121	13032409151026031703280	5		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
122	13032410150226041703280	5		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
123	13032410150326041702280	5		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
124	13042403150226031703280	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
125	13042403150226041702280	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
126	13042403150426041702803	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
127	13042403150426061703280	5		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
128	13042405150426101702804	5		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
129	13042409150226021703280	5		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
130	13042409150226081703280	5		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
131	13042410150426031703280	5		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
132	13092402150926041702280	5		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
133	13092403150126021703280	9		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O.[S]
134	13102402150126101710280	5		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
135	13102402150226061710280	5		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
136	13012402150926031710280	4		NCC1=CC=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
137	13012403150426051703280	4		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
138	13012403150926011703281	4		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
139	13012404150226041703280	4		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
140	13012404150426051703280	4		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
141	13012404151026021703280	4		NCC=C		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
142	13012405150126041703280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
143	13012405150126081703280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
144	13012405150226041703280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
145	13012405150226051702804	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
146	13012405150226081704280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCCC1		OC([C@H](C)Br)=O.[R]
147	13012405150326081702280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
148	13012405150426031704280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
149	13012405150426051703280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
150	13012405150426081703280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
151	13012405150926021702280	4		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
152	13012407150126081704280	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
153	13012407150126101703280	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
154	13012407150226031703280	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
155	13012407150326031703280	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
156	13012407150326071703280	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
157	13012407150426091702280	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
158	13012407150426091704280	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
159	13012407150926041702804	4		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
160	13012408150226021701280	4		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
161	13012408150226101701281	4		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(C1=CSC(CCl)=N1)=O
162	13012408150926011702804	4		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
163	13012409150226061703280	4		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
164	13012409150326061709280	4		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
165	13022403150126041703280	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
166	13022403150226017012809	4		NCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
167	13022403150426017032803	4		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
168	13022405150126017022803	4		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
169	13022405150126017102801	4		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC(C1=CSC(CCl)=N1)=O
170	13022407150126017032801	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
171	13022407150126017042803	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
172	13022407150226017042803	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
173	13022407150326017032809	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
174	13022407150926017102803	4		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
175	13022408150426017032803	4		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
176	13022408151026017102804	4		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
177	13022409150426017092804	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
178	13022409150426017012803	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
179	13022409150926017032804	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
180	13022409151026017022803	4		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
181	13022410150126017022810	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
182	13022410150126017092804	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
183	13022410150226041709280 2	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
184	13022410150226051702804	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
185	13022410150326051702804	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
186	13022410150326101702804	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
187	13022410150426081703280 5	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
188	13022410150926017032801	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
189	13022410151026041702280 3	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
190	13022410151026041703280 3	4		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
191	13032403150126041710280 3	4		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
192	13032403150126071703280 3	4		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
193	13032403150926041703280 3	4		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
194	13032404150226017032803	4		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
195	13032405150126041703280 6	4		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
196	13032405150926017032803	4		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
197	13032405151026041703280 9	4		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
198	13032407150426051703280 2	4		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
199	13032408150226061702280 3	4		N1CNCCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCCC1=CC(C(O)=O)=CC=
200	13032408150926011709280 4	4		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
201	13032409150426021703280 3	4		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
202	13032410150226041710280 4	4		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
203	13032410150426101703280 3	4		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
205	13042403150226061701280 4	4		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
206	13042403150426061703280 4	4		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
207	13042404150226051703280 4	4		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
208	13042404150326071702804 4	4		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
209	13042405150126051709280 4	4		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
210	13042405150426051703280 2	4		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
211	13042405150926021703280 5	4		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
212	13042407150126061702280 9	4		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCCC1=CC(C(O)=O)=CC=
213	13042407150926021703280 2	4		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
214	13042409150126031703280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
215	13042409150126041703280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
216	13042409150426051702804 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
217	13042409150426101702280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCCC1=CC(C(O)=O)=CC=
218	13042409150926021702280 3	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCCC1=CC(C(O)=O)=CC=
219	13042410150226021702280 3	4		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCCC1=CC(C(O)=O)=CC=
220	13042410150226081702280 4	4		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCCC1=CC(C(O)=O)=CC=
221	13042410150226101702280 7	4		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		ClCCC1=CC(C(O)=O)=CC=
222	13102402150226041709280 4	4		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
223	13102403150126041703281 0	4		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
224	13102403150326031703280 6	4		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
225	13102403150326041703280 4	4		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
226	13102403150326041704280 3	4		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
227	13102403150426081703281 0	4		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
228	13012401150226091709280 2	3		NCC1=CC=CC(Br)=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCCC1=CC(C(O)=O)=CC=
229	13012402150226031703280 3	3		NCC1=CC=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
230	13012403150126041709280 4	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
231	13012403150226031703281 0	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
232	13012403150226071703280 3	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
233	13012403150326017032801	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
234	13012403150326017032803	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
235	13012403150926017012809	3		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
236	13012404150126101 7022809	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
237	13012404150126101 7042803	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
238	13012404150226017102803	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
239	13012404150426017032804	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
240	13012404150426017092804	3		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
241	13012404151026031 7102803	3		NCC=C		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
242	13012405150126031 7032802	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
243	13012405150126091 7022805	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
244	13012405150226031 7022803	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
245	13012405150226041 7012804	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
246	13012405150326041 7012808	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
247	13012405150326041 7032806	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
248	13012405150326101 7012809	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
249	13012405150426081 7032809	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
250	13012405150426091 7012809	3		NCC1=CC=C(OCO2)C		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
251	13012406151026031 7102804	3		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
252	13012407150126011 7102804	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
253	13012407150126041 7022803	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
254	13012407150126061 7032801	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
255	13012407150126071 7012809	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
256	13012407150126081 7032803	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
257	13012407150126081 7032809	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
258	13012407150126091 7092804	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
259	13012407150226101 7022808	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=
260	13012407150226101 7092804	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
261	13012407150326061 7032802	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
262	13012407150426051 7032802	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
263	13012407150426061 7022804	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
264	13012407150926011 7102803	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
265	13012408150126021 7022803	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
266	13012408150126021703280 2	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
267	13012408150126051703280 5	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
268	13012408150226101701280 9	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
269	13012408150326051702280 9	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
270	13012408150326051709280 4	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O	R	N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
271	13012408150926031704280 3	3		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O	R	NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
272	13012409150126051709280 2	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O	R	N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
273	13012409150126061704280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O	R	NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
274	13012409150226031702280 9	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
275	13012409150226041704280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O	R	NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
276	13012409150226071709280 4	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O	R	N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
277	13012409150226091702280 9	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
278	13012409150326051703280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
279	13012409150426051702280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
280	13012409150426091704280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
281	13012409150926021703280 3	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
282	13012409150926031702280 4	3		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
283	13012410150326071703280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
284	13012410150326071702804 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O	S	N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
285	13012410150326081703280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
286	13012410150326081704280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
287	13012410150426061703280 3	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
288	13012410150426101701280 5	3		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
289	13022401150326071703280 3	3		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
290	13022401150426081703280 9	3		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
291	13022403150126041702280 9	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
292	13022403150126061702280 5	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
293	13022403150326081710280 4	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O	S	N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
294	13022403150426081703280 3	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
295	13022403150426101701280 3	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
296	13022403150926041703281 0	3		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
297	13022404150426041709280 4	3		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O	R	N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
298	13022404150926021709280 4	3		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O	R	N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
299	13022404150926041703280	3		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
300	13022405150126051702280	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
301	13022405150126091704280	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(Cl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
302	13022405150326041703280	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
303	13022405150326081703280	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
304	13022405150426031702280	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
305	13022405150426041703281	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
306	13022405150926031710280	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
307	13022405151026021710280	3		NCC1=CC=C(OCO2)C		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
308	13022406150326081709280	3		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
309	13022407150126021701280	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(Cl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(Cl)=N1)=O
310	13022407150126051709280	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
311	13022407150126101703280	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
312	13022407150326041702806	3		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O
313	13022409150126041703280	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
314	13022409150126051703280	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
315	13022409150226021701280	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(Cl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(Cl)=N1)=O
316	13022409150226071703280	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
317	13022409150326031702804	3		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
318	13022410150126061702281	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
319	13022410150126061703280	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
320	13022410150226071703280	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
321	13022410150326021703280	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(Cl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
322	13022410150326071704280	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(Cl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
323	13022410151026031703281	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
324	13022410151026031709280	3		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
325	13032403150226081702281	3		NCCOC		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
326	13032403150226081703280	3		NCCOC		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
327	13032403150326051710280	3		NCCOC		OC(C1=CSC(Cl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
328	13032403150426051703280	3		NCCOC		OC(C1=CSC(Cl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
329	13032403150426081702281	3		NCCOC		OC(C1=CSC(Cl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(Cl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
330	13032404150226021703280	3		NCC=C		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(Cl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
331	13032404150326061702280	3		NCC=C		OC(C1=CSC(Cl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
332	13032405150126041702804	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
333	13032405150226061702801	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC(C1=CSC(CCl)=N1)=O
334	13032405150326071703280 9	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
335	13032405150326081703280 3	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
336	13032405150326081710280 4	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
337	13032405150426051703280 2	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
338	13032405150426061709280 4	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
339	13032405150926011703280 4	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
340	13032405150926021702803	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
341	13032405150926021703280 2	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
342	13032405151026041709280 4	3		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
343	13032406150926021702804	3		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
344	13032407150126041703280 2	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
345	13032407150126081701280 3	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
346	13032407150226031703280 2	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
347	13032407150326031709280 4	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
348	13032407150326081704280 3	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
349	13032407150926041703280 1	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
350	13032407150926041709280 4	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
351	13032407151026031703280 4	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
352	13032408150326101702804	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
353	13032408150426041702804	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
354	13032408150926041703280 3	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
355	13032408151026041702802	3		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
356	13032409150226031709280 4	3		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
357	13032409150326041703280 2	3		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
358	13032409150326071701280 8	3		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
359	13032409150326081702280 3	3		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
360	13032410150226021702804	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
361	13032410150226051709280 4	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
362	13032410150326061702280 3	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
363	13032410150426061702280 6	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
364	13032410150426061703280 2	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
365	13032410150426061703280	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
366	13032410150926041704280	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
367	13032410151026031704280	3		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
368	13042402150126061703280	3		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
369	13042402150226081702280	3		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
370	13042402150426071703280	3		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
371	13042403150126011702804	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
372	13042403150126041709280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
373	13042403150126101709280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
374	13042403150326021703280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
375	13042403150326061702280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
376	13042403150326071703280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
377	13042403150326101709280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
378	13042403150426091710280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
379	13042403150926011704280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
380	13042403150926021703280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
381	13042403151026031710280	3		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
382	13042404150326041709280	3		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
383	13042404150426031710280	3		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
384	13042404150426071702804	3		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
385	13042405150126061702804	3		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
386	13042405150226061702280	3		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
387	13042405150226071712806	3		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
388	13042405150326021703280	3		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
389	13042405150326101710280	3		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
390	13042405150926011709280	3		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
391	13042405150926031702280	3		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
392	13042406150226031710280	3		NCC1=CC=CO1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
393	13042407150126051712803	3		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
394	13042407150126051703280	3		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
395	13042408150326041709280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
396	13042408150326091703280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
397	13042408150426041703280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
398	13042408151026041702280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
399	13042409150126041702280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
400	13042409150126091702280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
401	13042409150226021703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
402	13042409150226031702280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
403	13042409150226051709280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
404	13042409150226081703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
405	13042409150426041703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
406	13042409150426051703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
407	13042409150926031703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
408	13042409150926041702281	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
409	13042409151026031703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
410	13042409151026041703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
411	13042410150126081703280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
412	13042410150126101703280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
413	13042410150226021704280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
414	13042410150226041701280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
415	13042410150326061701280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
416	13042410150426061702280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=
417	13042410150426061703280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
418	13042410150426081703280	3		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
419	13092402150226071703280	3		NCCC1CCOC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
420	13092402150226071710280	3		NCCC1CCOC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
421	13092402150226101704280	3		NCCC1CCOC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
422	13092402150326041703280	3		NCCC1CCOC1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
423	13092402150426071709280	3		NCCC1CCOC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
424	13092402150426081710280	3		NCCC1CCOC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
425	13092402150926041709280	3		NCCC1CCOC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
426	13092403150126071702280	3		NCCC1CCOC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
427	13092403150126071702280	3		NCCC1CCOC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
428	13092403150126081704280	3		NCCC1CCOC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
429	13092403150326081710280	3		NCCC1CCOC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
430	13092403150426031710280	3		NCCC1CCOC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
431	13092403150426051703280 2	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
432	13092403150426081702280 3	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
433	13092403151026031702280 2	3		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
434	13092404150326031703280 3	3		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
435	13092404151026011709280 4	3		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
436	13102401150426071704280 3	3		NCC1=CC(F)=C(F)C=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
437	13102401151026031710280 4	3		NCC1=CC(F)=C(F)C=C		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
438	13102402150126031710280 4	3		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
439	13102402150326041703280 3	3		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
440	13102403150126061703280 2	3		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
441	13102403150326071703280 2	3		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
442	13102403150326081702803 3	3		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
443	13102403150426091702280 4	3		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
444	13102403150926021702803 3	3		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
445	13102403150926031702802 3	3		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
446	13102403151026041710280 3	3		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
447	13102404150326041709280 4	3		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
448	13102404150426081703280 3	3		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
449	13012401150326051702804 2			NCC1=CC=CC(Br)=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
450	13012401150926031703280 9	2		NCC1=CC=CC(Br)=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
451	13012402150226081702280 4	2		NCC1=CC=CN=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
452	13012402150326021709280 4	2		NCC1=CC=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
453	13012402150326101703280 1	2		NCC1=CC=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
454	13012403150126041704280 9	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
455	13012403150126071703280 1	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
456	13012403150126081702280 5	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
457	13012403150126081703280 2	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
458	13012403150126081703280 3	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
459	13012403150126101704280 3	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
460	13012403150226021703280 2	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
461	13012403150226101701280 5	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
462	13012403150326021703280 2	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
463	13012403150326021710280 4	2		NCCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
464	13012403150326041702280 3	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
465	13012403150326061701280 3	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
466	13012403150326071703280 2	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
467	13012403150326071704280 3	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
468	13012403150426041702281 0	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
469	13012403150426081710280 3	2		NCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
470	13012403150926021703280 8	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
471	13012403150926041701280 4	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
472	13012403150926041702280 5	2		NCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
473	13012404150126051702280 4	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
474	13012404150126061703280 5	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
475	13012404150126081703280 7	2		NCC=C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
476	13012404150126091702280 9	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
477	13012404150226041704280 5	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]
478	13012404150226051702280 3	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
479	13012404150226061703280 2	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
480	13012404150226091703280 2	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
481	13012404150326031703280 2	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
482	13012404150326061703280 1	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
484	13012404150326071703280 6	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
485	13012404150326081709280 4	2		NCC=C		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
486	13012404150326091703280 2	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
487	13012404150426041702280 5	2		NCC=C		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
488	13012405150126071703280 2	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
489	13012405150126091703281 0	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
490	13012405150126101703280 9	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COCC1		OC([C@H](C)Cl)=O.[S]
491	13012405150226021710280 2	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		ClCC1=CC(C(O)=O)=CC=
492	13012405150226031703280 6	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
493	13012405150226031704280 4	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
494	13012405150226051703280 2	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
495	13012405150226061703280 2	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
496	13012405150226071710280 2	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		ClCC1=CC(C(O)=O)=CC=
497	13012405150226101709280 4	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
498	13012405150326031702804	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
499	13012405150326041702809	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
500	13012405150426041702809	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
501	13012405150426081703280 2	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
502	13012405150426091702803	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
503	13012405150926011704280 1	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Br)=O.[R]
504	13012405150926021702280 8	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=
505	13012405150926021703280 2	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
506	13012405150926031701280 1	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC(C1=CSC(CCl)=N1)=O
507	13012405150926041702804	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
508	13012405151026011701280 3	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
509	13012405151026011702804	2		NCC1=CC=C(OCO2)C2		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
511	13012406150226031702280 3	2		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
512	13012406150226061702280 3	2		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
513	13012406150226071702803	2		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
514	13012406150426041709280 4	2		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
515	13012406150926031702280 3	2		NCC1=CC=CO1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
516	13012407150126021703280 5	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
517	13012407150126031701281 0	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC(C1=CSC(CCl)=N1)=O
518	13012407150126031709280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
519	13012407150126041703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
520	13012407150126051710280 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
521	13012407150126071702280 7	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=
522	13012407150126071704280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
523	13012407150126081702280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
524	13012407150126081703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
525	13012407150126101701280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC(C1=CSC(CCl)=N1)=O
526	13012407150126101709280 4	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
527	13012407150226031703280 1	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
528	13012407150226041702280 5	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
529	13012407150226051704280 3	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
530	13012407150226061703280 6	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
531	13012407150226081702280 2	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
532	13012407150226017032805	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
533	13012407150326017032808	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=
534	13012407150326017032802	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
535	13012407150326017092804	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
536	13012407150326017032802	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
537	13012407150326017032804	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
538	13012407150326017012805	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
539	13012407150326017102804	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
540	13012407150426017032802	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
541	13012407150426017032802	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
542	13012407150426017032807	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
543	13012407150926017012803	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
544	13012407150926017012807	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC(C1=CSC(CCl)=N1)=O
545	13012407150926017032807	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
546	13012407150926021732802	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
547	13012407150926017022807	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=
548	13012407150926017032802	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
549	13012407150926017032809	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
550	13012407151026011732801	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
551	13012407151026021732809	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
552	13012407151026031732803	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
553	13012408150126041732803	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
554	13012408150126051732809	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
555	13012408150126061732803	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
556	13012408150226011732804	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
557	13012408150226021732802	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
558	13012408150226041732804	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
559	13012408150226061732806	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
560	13012408150226081732802	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
561	13012408150226091742804	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
562	13012408150326041732805	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
563	13012408150326061732804	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
564	13012408150326071732803	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
565	13012408150326071722803	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
566	13012408150326071722805	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
567	13012408150326081722809	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
568	13012408150426011722801	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
569	13012408150426021722802	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
570	13012408150426021709280 4	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
571	13012408150426041701280 7	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC(C1=CSC(CCl)=N1)=O
572	13012408150426041703280 1	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
573	13012408150426051703280 2	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
574	13012408150426051709280 4	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
575	13012408150426081703280 6	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
576	13012408150926021710280 3	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
577	13012408150926031701280 8	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
578	13012408151026011701280 9	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
579	13012408151026031703280 8	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
580	13012408151026031710280 1	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC(C1=CSC(CCl)=N1)=O
581	13012408151026031710280 3	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
582	13012408151026041701280 5	2		N1CCNCCC1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
583	13012409150126041703280 7	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
584	13012409150126081702281 0	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
585	13012409150126091709280 4	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
586	13012409150226021702280 9	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
587	13012409150226031702280 6	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
588	13012409150226031703280 3	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
589	13012409150226041704280 9	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
590	13012409150226061703280 3	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
591	13012409150226071703281 0	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
592	13012409150226081704280 6	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Br)=O.[R]
593	13012409150326061703280 2	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
594	13012409150426041703281 0	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
595	13012409150426051703280 4	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
596	13012409150426051703280 8	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
597	13012409150926041701280 5	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
598	13012409151026011702280 9	2		NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCCC1=CC(C(O)=O)=CC=
599	13012410150126011703280 1	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
600	13012410150126021703280 2	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
601	13012410150126021703280 4	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
602	13012410150126031710280 4	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
603	13012410150126061703280 1	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
604	13012410150126061704280 7	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Br)=O.[R]
605	13012410150126101703280 9	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
606	13012410150226021702280 5	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		ClCCC1=CC(C(O)=O)=CC=
607	13012410150226021709280 3	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
608	13012410150226061709280 3	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
609	13012410150226081703280 5	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
610	13012410150326041701280 4	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
611	13012410150326071704280 3	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
612	13012410150326091703280 3	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
613	13012410150326091703280 4	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
614	13012410150426031701280 9	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
615	13012410150426051703280 2	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
616	13012410150426061703280 2	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
617	13012410150426091703280 3	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
618	13012410150426101703280 5	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
619	13012410150926031701280 4	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
620	13012410150926041701280 9	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
621	13012410150926041703280 9	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
622	13012410151026031701280 9	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
623	13012410151026031709280 2	2		C1CNCCN1		OC(C1=COC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCCC1=CC(C(O)=O)=CC=
624	13022401150226061703281 0	2		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
625	13022401150226071703280 3	2		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
626	13022401150426081702280 3	2		NCC1=CC=CC(Br)=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
627	13022402150126041709280 3	2		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
628	13022402150126071703280 3	2		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
629	13022402150226041702280 4	2		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
630	13022402150226051709280 4	2		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
631	13022402150326021703280 2	2		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
632	13022402151026011710280 4	2		NCC1=CC=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
633	13022403150126031702280 3	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
634	13022403150126031703280 4	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
635	13022403150126041703280 2	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
636	13022403150126061701280 5	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
637	13022403150126071703280 2	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
638	13022403150126101702281 0	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
639	13022403150226071703280 2	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
640	13022403150326071703280 1	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
641	13022403150326081704280 3	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1	R	OC([C@H](C)Br)=O.[R]
642	13022403150426031703280 2	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
643	13022403150426041702281 0	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
644	13022403150926021710280 1	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC(C1=CSC(CCl)=N1)=O
645	13022403150926031703280 5	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
646	13022403150926041709280 3	2		NCCCOC		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]	R	OC([C@H](C)Cl)=O.[S]
647	13022404150126041701280 9	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
648	13022404150226021703280 2	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
649	13022404150226031703280 4	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
650	13022404150226041702280 3	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
651	13022404150226061701280 9	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
652	13022404150226071703280 5	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
653	13022404150326021710280 3	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
654	13022404150326031710280 4	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
655	13022404150326101703280 3	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
656	13022404150426051703280 2	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
657	13022404150926031702280 7	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=
658	13022404150926041702280 3	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
659	13022404151026021709280 3	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]	R	OC([C@H](C)Cl)=O.[S]
660	13022404151026031702280 9	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
661	13022404151026041703280 4	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
662	13022404151026041703281 0	2		NCC=C		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
663	13022405150126081702280 3	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
664	13022405150126081702280 4	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
665	13022405150226031703280 2	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
666	13022405150226031703280 9	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
667	13022405150226041704280 8	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Br)=O.[R]
668	13022405150226051709280 4	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
669	13022405150226081701280 3	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
670	13022405150326031701280 3	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
671	13022405150326031702280 8	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=
672	13022405150326031710280 4	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
673	13022405150326051709280 3	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
674	13022405150326071703280 2	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
675	13022405150326081702280 1	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		ClCC1=CC(C(O)=O)=CC=
676	13022405150326101709280 4	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
677	13022405150426061710280 4	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
678	13022405150426071703280 5	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
679	13022405150426091703280 3	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
680	13022405150426091704280 3	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
681	13022405150426101703281 0	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
682	13022405150926021701280 3	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
683	13022405150926021703280 2	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
684	13022405151026031703280 8	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
685	13022405151026041702280 9	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
686	13022405151026041703280 5	2		NCC1=CC=C(OCO2)C2		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
687	13022406150426051710280 4	2		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
688	13022407150126031702281 0	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
689	13022407150126031703280 2	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
690	13022407150126091702280 9	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
691	13022407150126101702280 9	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
692	13022407150226021703280 2	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
693	13022407150226021703280 3	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
694	13022407150226041703280 3	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
695	13022407150226071702280 8	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
696	13022407150226081702280 3	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
697	13022407150326041702804	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
698	13022407150326081702280	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
699	13022407150326091702280	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
700	13022407150326101703280	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
701	13022407150426081701280	2		NCC1=CC=C(C)C=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
702	13022408150126041703280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
703	13022408150126081702280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
704	13022408150126081704280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
705	13022408150426041709280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
706	13022408150426051703280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
707	13022408150426081709280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
708	13022408150426091704280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
709	13022408150926021704280	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]
710	13022408150926031703281O	2		N1CCNCCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
711	13022409150126031701280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
712	13022409150126061703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
713	13022409150126071704280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Br)=O.[R]
714	13022409150126101702280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
715	13022409150126101703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
716	13022409150126101709280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
717	13022409150226021701280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
718	13022409150226031704280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
719	13022409150226061703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
720	13022409150226071702280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
721	13022409150226071709280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
722	13022409150226081702280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
723	13022409150326021703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
724	13022409150326041703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
725	13022409150326061703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
726	13022409150326071704280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
727	13022409150326101703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
728	13022409150426071703280	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
729	13022409150926011703280 1	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
730	13022409150926041701 2809	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O
731	13022409150926041702 2802	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
732	13022409150926041702 2809	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
733	13022409151026011709 2804	2		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
734	13022410150126021703 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
735	13022410150126031703 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
736	13022410150126031704 2804	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
737	13022410150126051703 2805	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC(C)(C)O		OC(C1=CC=C(Cl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
738	13022410150126071703 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
739	13022410150226041701 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC(C1=CSC(CCl)=N1)=O
740	13022410150226041703 2804	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
741	13022410150226071701 2803	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
742	13022410150226071703 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
743	13022410150226071703 2804	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
744	13022410150226091703 2810	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
745	13022410150326031703 2805	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
746	13022410150326061702 2803	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
747	13022410150326091702 2809	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
748	13022410150426021702 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
749	13022410150426041703 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
750	13022410150426061710 2804	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
751	13022410150426071703 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
752	13022410150426081704 2805	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]
753	13022410150426091709 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
754	13022410150426091709 2804	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
755	13022410150926011701 2803	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
756	13022410150926011702 2801	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		ClCC1=CC(C(O)=O)=CC=
757	13022410150926021702 2803	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
758	13022410150926041702 2802	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		ClCC1=CC(C(O)=O)=CC=
759	13022410151026031702 2809	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
760	13022410151026041703 2801	2		C1CNCCN1		ClCC1=CC(C(O)=O)=CC=C1		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
761	13032402150126041710 2804	2		NCC1=CC=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(Cl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
762	13032402150126061703 2801	2		NCC1=CC=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(Cl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
763	13032402150226041102804	2		NCC1=CC=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
764	13032402150926021709280 2	2		NCC1=CC=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
765	13032403150126021703280 2	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
766	13032403150126031703280 2	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
767	13032403150126051702280 2	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
768	13032403150226021702280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
769	13032403150226031703280 2	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
770	13032403150226041701280 4	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
771	13032403150226051703280 2	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
772	13032403150226051703280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
773	13032403150226051709280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
774	13032403150226091703280 5	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
775	13032403150326041701280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
776	13032403150326051701280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
777	13032403150326061701280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
778	13032403150426041702280 6	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
779	13032403150426041703280 1	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
780	13032403150426101702280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
781	13032403150426101702280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
782	13032403150926011702280 9	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
783	13032403150926021702280 9	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
784	13032403150926021703280 2	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
785	13032403150926021704280 4	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
786	13032403150926021709280 4	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
787	13032403150926031703280 5	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
788	13032403150926041704280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
789	13032403151026011701280 3	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
790	13032403151026031703280 2	2		NCCCOC		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
791	13032404150126021709280 4	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
792	13032404150326031709280 4	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
793	13032404150326041702280 3	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
795	13032404150426041703280 1	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
796	13032404150426061709280 4	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
797	13032404150426017032802	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
798	13032404150926017022803	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
799	13032404150926017032803	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
800	13032404150926017032803	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
801	13032404150926017032801	2		NCC=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
802	13032405150126017022802	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
803	13032405150126017032802	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
804	13032405150126017012804	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
805	13032405150126017032806	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
806	13032405150126017032802	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
807	13032405150126017032810	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
808	13032405150226017032801	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
809	13032405150226017022809	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
810	13032405150326017012803	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
811	13032405150326017032802	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
812	13032405150326017022809	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
813	13032405150426017032808	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
814	13032405150426081702804	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
815	13032405150426091702803	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
816	13032405150926021709280 4	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
817	13032405150926031703280 6	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
818	13032405150926041702280 7	2		NCC1=CC=C(OCO2)C2		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=
819	13032406150426051703280 2	2		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
820	13032407150126021703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
821	13032407150126041703280 8	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
822	13032407150126061703280 6	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
823	13032407150126071703281 0	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
824	13032407150226031710280 4	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
825	13032407150226051703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
826	13032407150226081710280 4	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
827	13032407150326041703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
828	13032407150326051709280 3	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
829	13032407150326101703280 2	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
830	13032407150426031704280 3	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
831	13032407150426041704280 6	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Br)=O.[R]
832	13032407150426051703280 3	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
833	13032407150426101702280 3	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
834	13032407150926041704280 4	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
835	13032407151026011710280 4	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
836	13032407151026041703280 4	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
837	13032408150126021703280 2	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
838	13032408150126031703280 6	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
839	13032408150126061701280 3	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
840	13032408150226071701280 3	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
841	13032408150326021710280 4	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
842	13032408150326031703280 3	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
843	13032408150326061701280 3	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
844	13032408150326071709280 2	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
845	13032408150326071710280 4	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
846	13032408150326081703280 9	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
847	13032408150426051703280 2	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
848	13032408150426101702280 4	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
849	13032408150926021703280 7	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
850	13032408150926021704280 3	2		N1CCNCCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
851	13032409150126021702280 9	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
852	13032409150126031709280 4	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
853	13032409150126071703280 2	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
854	13032409150126091703280 5	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
855	13032409150226061703280 4	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
856	13032409150226071702280 6	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
857	13032409150326031704280 3	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
858	13032409150326041701280 3	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
859	13032409150326071702280 3	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
860	13032409150326081701280 3	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
861	13032409150326081702280 9	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
862	13032409150426031703280 5	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
863	13032409150926021702804	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
864	13032409150926031702808	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=
865	13032409150926041702806	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
866	13032409151026041702804	2		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
867	13032410150126021702801	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Br)=O.[R]
868	13032410150126031702802	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
869	13032410150126061702805	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
870	13032410150126091702802	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
871	13032410150126101702805	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
872	13032410150126101702805	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
873	13032410150226031702807	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
874	13032410150226031704280 5	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]
875	13032410150226041701280 3	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
876	13032410150226071703280 6	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
877	13032410150226081702280 4	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
878	13032410150226081702280 9	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
879	13032410150226081703280 2	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
880	13032410150326031709280 2	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
881	13032410150326071702280 2	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
882	13032410150426021702280 9	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
883	13032410150426031701280 3	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
884	13032410150426031704280 3	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
885	13032410150426081703280 2	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
886	13032410150926031702280 3	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
887	13032410150926041702280 7	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=
888	13032410151026041703280 4	2		C1CNCCN1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
889	13042401150326031702280 8	2		NCC1=CC=CC(Br)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		ClCC1=CC(C(O)=O)=CC=
890	13042401150326061703280 2	2		NCC1=CC=CC(Br)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
891	13042401150426031702280 3	2		NCC1=CC=CC(Br)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
892	13042401150426031710280 4	2		NCC1=CC=CC(Br)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
893	13042402150226021703280 2	2		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
894	13042402150326081702280 3	2		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
895	13042402150426031703280 3	2		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
896	13042402150926041709280 4	2		NCC1=CC=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
897	13042403150126021703280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
898	13042403150126021703280 3 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
899	13042403150126081703280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
900	13042403150126091709280 4 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
901	13042403150126101703280 9 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
902	13042403150226011710280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		ClCC1=CC(C(O)=O)=CC=
903	13042403150226021703280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
904	13042403150226021703281 0 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
905	13042403150226061703280 6 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
906	13042403150226101710280 3 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
907	13042403150326031703280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
908	13042403150326041709280 4 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
909	13042403150326051703280 3 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
910	13042403150326061704280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Br)=O.[R]
911	13042403150326101704280 6 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Br)=O.[R]
912	13042403150426061701280 3 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
913	13042403150426081703280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
914	13042403150926021702280 2 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
915	13042403150926021702280 3 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
916	13042403150926031701280 3 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
917	13042403150926041701280 3 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
918	13042403150926041701280 4 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
919	13042403150926041701280 6 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
920	13042403151026011710280 4 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
921	13042403151026031701280 6 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
922	13042403151026041704280 5 2	2		NCCCOC		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]
923	13042404150126031701280 5 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
924	13042404150126041702280 7 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=
925	13042404150126051703280 6 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
926	13042404150126051710280 4 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
927	13042404150226061702280 2 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCO		ClCC1=CC(C(O)=O)=CC=
928	13042404150226071702280 3 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
929	13042404150326021703280 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
930	13042404150326041703280 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
931	13042404150926011703280 2	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
932	13042404151026041701280 3	2		NCC=C		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
933	13042405150126021701280 9	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1COCC1		OC(C1=CSC(CCl)=N1)=O
934	13042405150126071702280 3	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
935	13042405150126071702280 9	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCC1		ClCC1=CC(C(O)=O)=CC=
936	13042405150226041703280 6	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
937	13042405150326041704280 3	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
938	13042405150326071703280 2	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
939	13042405150426031703280 3	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
940	13042405150926011703280 1	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
941	13042405151026021703280 5	2		NCC1=CC=C(OCO2)C		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
942	13042406150126021710280 4	2		NCC1=CC=CO1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1	[S	C=C(O)C1=C(C)OC=C1
943	13042406150126071702280 9	2		NCC1=CC=CO1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COCC1		ClCC1=CC(C(O)=O)=CC=
944	13042406150426031703280 3	2		NCC1=CC=CO1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
945	13042407150126021701280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
946	13042407150126031703280 2	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
947	13042407150126071702280 5	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
948	13042407150126091703280 8	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
949	13042407150126101703280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
950	13042407150226051702281 0	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
951	13042407150226071702280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
952	13042407150226081702280 4	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
953	13042407150226101702280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
954	13042407150326041702280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
955	13042407150326041703280 6	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
956	13042407150326061703280 4	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
957	13042407150326081702280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
958	13042407150326091703280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1	[R]	OC([C@H](C)Cl)=O.[S]
959	13042407150426081702280 3	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
960	13042407150426081702281 0	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		ClCC1=CC(C(O)=O)=CC=
961	13042407150426081704280 5	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
962	13042407150926017042803	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
963	13042407150926041704280	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Br)=O.[R]
964	13042407151026031710280	2		NCC1=CC=C(C)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
965	13042408150126021703280	2		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
966	13042408150126031703280	2		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
967	13042408150126041703280	2		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
968	13042408150126071703280	2		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
969	13042408150126071704280	2		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
970	13042408150126091702280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
971	13042408150226071710280	4		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
972	13042408150326031701280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
973	13042408150326031703280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
974	13042408150326101701280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
975	13042408150426061704280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
976	13042408150426061709280	4		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
977	13042408150426101703280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
978	13042408150926041704280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
979	13042408151026031702280	3		N1CCNCCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
980	13042409150126071703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
981	13042409150126091703280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
982	13042409150126101702280	5		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		ClCC1=CC(C(O)=O)=CC=
983	13042409150226031704280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
984	13042409150226041703281	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
985	13042409150226051703281	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
986	13042409150226071703280	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
987	13042409150326011710280	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCOC		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
988	13042409150326021702280	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
989	13042409150326061709280	4		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
990	13042409150326091702280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
991	13042409150326101701280	6		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
992	13042409150326101704280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
993	13042409150426051709280	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
994	13042409150426081704280	3		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
995	13042409150426017012809	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COCC1		OC(C1=CSC(CCl)=N1)=O
996	13042409150926017012805	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCl)=N1)=O
997	13042409151026017012806	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
998	13042409151026041702804	2		NCCCN1C=CN=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
999	13042410150126017032802	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1000	13042410150126017022807	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		ClCC1=CC(C(O)=O)=CC=
1001	13042410150126017032802	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1002	13042410150126017012804	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1003	13042410150126017012809	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COCC1		OC(C1=CSC(CCl)=N1)=O
1004	13042410150126017042803	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
1005	13042410150126017042808	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Br)=O.[R]
1006	13042410150126017032802	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1007	13042410150226017012803	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1008	13042410150226017012804	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
1009	13042410150226017032801	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
1010	13042410150226017022802	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
1011	13042410150226017022803	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
1012	13042410150226081702804	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1013	13042410150226091702806	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
1014	13042410150226101702803	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1015	13042410150326041702807	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
1016	13042410150326051702806	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O
1017	13042410150326091702802	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1018	13042410150326091709280 4	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1019	13042410150326091702804	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1020	13042410150426021703280 3	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1021	13042410150426051703280 2	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1022	13042410150426091702280 3	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
1023	13042410150926011702280 4	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
1024	13042410150926011709280 4	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1025	13042410150926021701280 4	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
1026	13042410150926021701280 8	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
1027	13042410150926031709280 1	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		OC(C1=CSC(CCl)=N1)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
1028	13042410151026021702803	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
1029	13042410151026041702802	2		C1CNCCN1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
1030	13092401150226021702804	2		NCCC1CCOCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1031	13092401150326041703280 4	2		NCCC1CCOCC1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1032	13092401150426051709280 2	2		NCCC1CCOCC1		OC(C1=COC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
1033	13092401150926021709280 2	2		NCCC1CCOCC1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
1034	13092402150126041704280 6	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1		OC([C@H](C)Br)=O.[R]
1035	13092402150126061709280 1	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC(C1=CSC(CCl)=N1)=O
1036	13092402150226081703280 6	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
1037	13092402150326081710280 3	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)Cl)=O.[S]
1038	13092402150326091709280 2	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
1039	13092402150426061703280 9	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1COCCC1		OC([C@H](C)Cl)=O.[S]
1040	13092402150426061710280 4	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1041	13092402150426101710280 4	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1042	13092402150926011710280 4	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1043	13092402150926041702280 6	2		NCCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
1044	13092403150126041704280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
1045	13092403150126051710280 2	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
1046	13092403150126061703280 1	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
1047	13092403150126061704280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Br)=O.[R]
1048	13092403150126071703280 7	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
1049	13092403150126071709280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
1050	13092403150126071709280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1051	13092403150226021701280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC(C1=CSC(CCl)=N1)=O
1052	13092403150226041702280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		ClCC1=CC(C(O)=O)=CC=
1053	13092403150226051703280 2	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1054	13092403150226081701280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1055	13092403150226101701280 8	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
1056	13092403150226101703280 1	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
1057	13092403150226101709280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1058	13092403150326031703280 2	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1059	13092403150326031703280 5	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
1060	13092403150326031710280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
1061	13092403150326061702802	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCCC1=CC(C(O)=O)=CC=
1062	13092403150326081709280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1063	13092403150426031702280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
1064	13092403150426031709280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
1065	13092403150426051703280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1066	13092403150926011701280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1067	13092403150926021701280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1068	13092403150926021703280 4	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1069	13092403151026031701280 3	2		NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1070	13092404150126081710280 4	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1071	13092404150126091703280 3	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1072	13092404150126091703280 8	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
1073	13092404150126101702802	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		ClCC1=CC(C(O)=O)=CC=
1074	13092404150226021709280 4	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1075	13092404150226031703280 9	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
1076	13092404150226081701280 8	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCl)=N1)=O
1077	13092404150326021703280 2	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1078	13092404150326091704280 3	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
1079	13092404150426061703280 1	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
1080	13092404150926021703280 2	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1081	13092404150926021703280 9	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
1082	13092404151026031702280 6	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
1083	13092404151026031709280 3	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
1084	13092404151026041703280 5	2		NCCC1CCOCC1		ClC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
1085	13102401150126041702280 9	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
1086	13102401150126101703280 3	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1087	13102401150226021703280 2	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1088	13102401150226041702280 9	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
1089	13102401150226061701280 3	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1090	13102401150226071704280 5	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Br)=O.[R]
1091	13102401150326071703280 2	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1092	13102401150326071702804	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1093	13102401150426061701280 3	2		NCC1=CC(F)=C(F)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
1094	13102401150426071703280 1	2		NCC1=CC(F)=C(F)C=C		OC(C1=COC(CCl)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
1095	13102402150126041701280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1096	13102402150126061703280 2	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1097	13102402150126071703280 2	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1098	13102402150126101702280 6	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
1099	13102402150126101703280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1100	13102402150226011703280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCCOC		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1101	13102402150226021703280 4	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1102	13102402150226071709280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)Cl)=O.[S]
1103	13102402150226101709280 4	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1104	13102402150326041710280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC([C@H](C)Cl)=O.[S]
1105	13102402150326061702280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
1106	13102402150326091704280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
1107	13102402150926011703280 4	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1108	13102402150926031701280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1109	13102402150926041701280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1110	13102402150926041702280 3	2		NCC1=CC(F)=C(F)C=C		ClCC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
1112	13102403150126031709280 4	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCl)=N1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1113	13102403150126041702280 9	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=
1114	13102403150126041703280 9	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
1115	13102403150126041710280 1	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		OC(C1=CSC(CCl)=N1)=O
1116	13102403150126041710280 4	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S]		O=C(O)C1=C(C)OC=C1
1117	13102403150126081702280 2	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		ClCC1=CC(C(O)=O)=CC=
1118	13102403150126101701280 3	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1119	13102403150126101702280 3	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		ClCC1=CC(C(O)=O)=CC=
1120	13102403150226041703281 0	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CC=C(CC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
1121	13102403150226051709280 4	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1122	13102403150326021701280 3	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1123	13102403150326041703280 1	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
1124	13102403150326061703280 3	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1125	13102403150326061703280 9	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
1126	13102403150326091703280 8	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
1127	13102403150426041702280 9	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1CCOCC1		ClCC1=CC(C(O)=O)=CC=

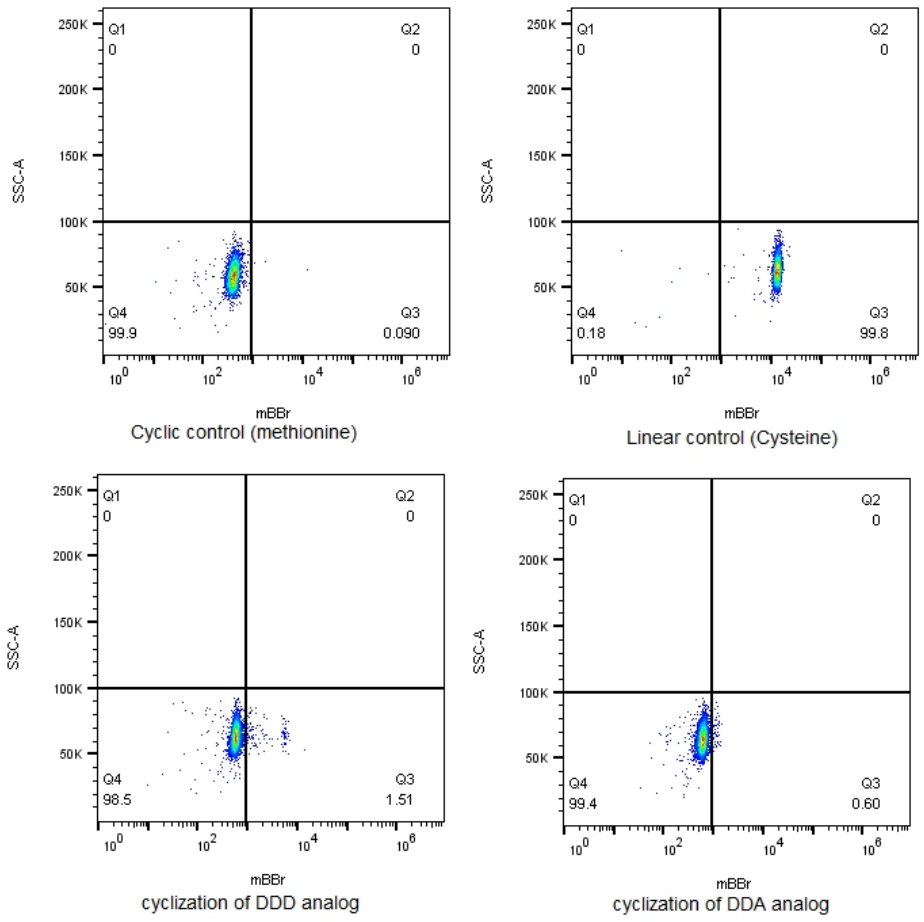
observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair...	Pair3.Acids
1128	13102403150426017102804	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1129	13102403150426017032802	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1130	13102403150426101709280 4	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1131	13102403150926031710280 4	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1132	13102403150926041702280 9	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1COOCC1		ClCC1=CC(C(O)=O)=CC=
1133	13102403151026031701280 3	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1134	13102403151026031703280 3	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1135	13102403151026041703280 4	2		NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1136	13102404150126021703280 5	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
1137	13102404150126041702280 6	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=
1138	13102404150126041703280 6	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)Cl)=O.[S]
1139	13102404150126041703280 7	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
1140	13102404150126061703280 4	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1141	13102404150126081703280 7	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=O.[S]
1142	13102404150126091701280 3	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCl)=N1)=O
1143	13102404150126091703280 9	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCl)=N1)=O		NCC1CCOCC1		OC([C@H](C)Cl)=O.[S]
1144	13102404150226061703280 8	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O		BrC1=CC=C(CN)C=C1		OC([C@H](C)Cl)=O.[S]
1145	13102404150226101709280 2	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(Cl)C=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[R]		ClCC1=CC(C(O)=O)=CC=
1146	13102404150326041703280 1	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=O.[S]
1147	13102404150426041703280 4	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1148	13102404150426041709280 4	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O		N[C@@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
1149	13102404150426071703280 2	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCl)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
1150	13102404150426081703280 5	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCl)=N1)=O		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
1151	13102404150926031703280 3	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1		OC([C@H](C)Cl)=O.[S]
1152	13102404150926031710280 4	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1153	13102404150926041702280 6	2		NCC1=CC(F)=C(F)C=C		ClC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC(C(F)(F)F)=C1		ClC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		ClCC1=CC(C(O)=O)=CC=

Section 11: Analysis of ring-closure via the Michael (thiol-enone) reaction

Linear analogs of DDD and DDA were synthesized with acrylic acid at the X3 position on 10 & 160 μM beads following general SPS method. Compound DDD and DDA have complete cyclization after 8hrs. Thiol protecting STMP group was removed from the linear precursor and it was suspended in 2x PBST buffer at 37°C for 12 hrs. DMSO solution of BnBr was added to beads suspended in PBST buffer (final conc, 1.0M, 150uL) and incubated for an hour at 37°C. Similarly, 10 μM beads were treated with DMSO solution of mBBr dye (final conc, 1mM, 150ul, PBS). After thiol alkylations, they were washed, 160 μM beads were TFA cleaved and analyzed over LCMS. 10 μM beads were suspended in PBST buffer, transferred to BD FACS tube and their fluorescence was measured.

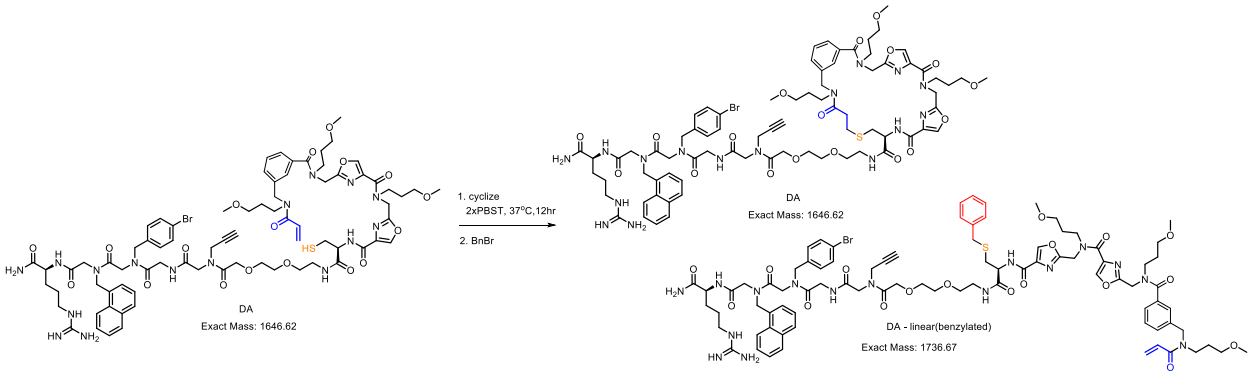
Incomplete cyclization was observed for both DDD and DDA analogs for thiol-ene based ring closure.

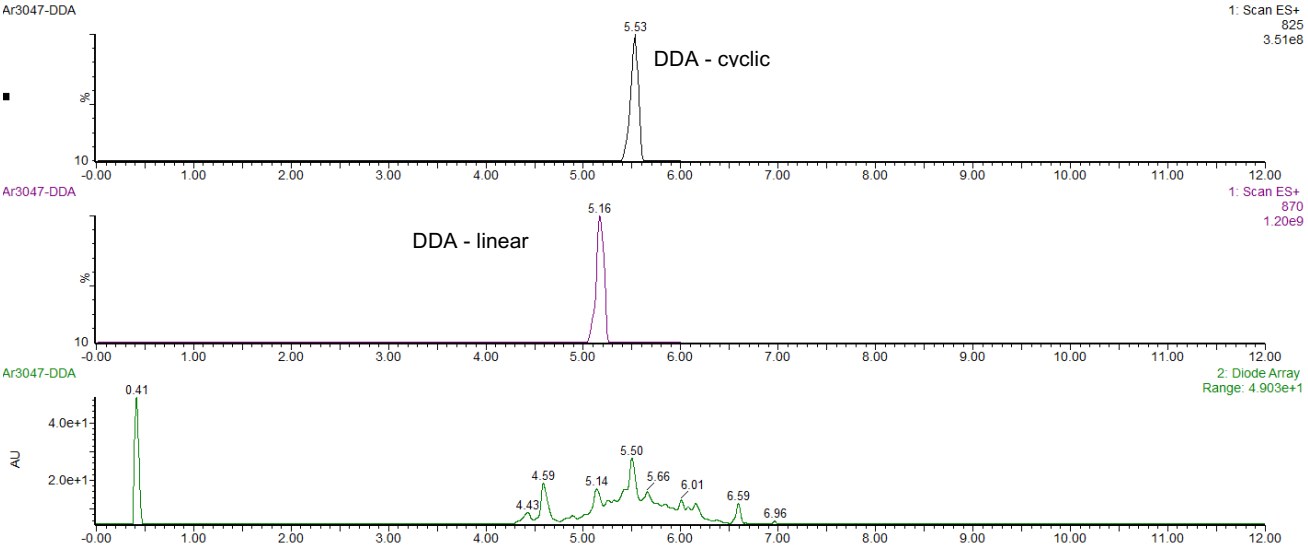
<u>Analysis of ring-closure via flow-cytometry:</u>

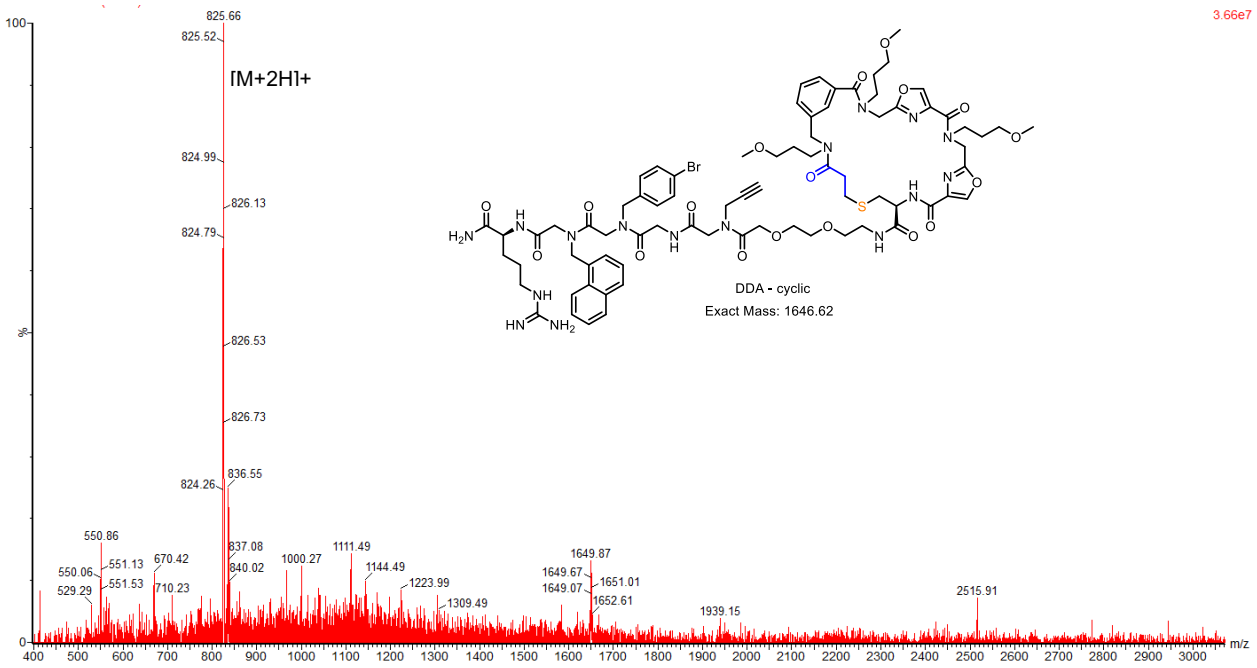


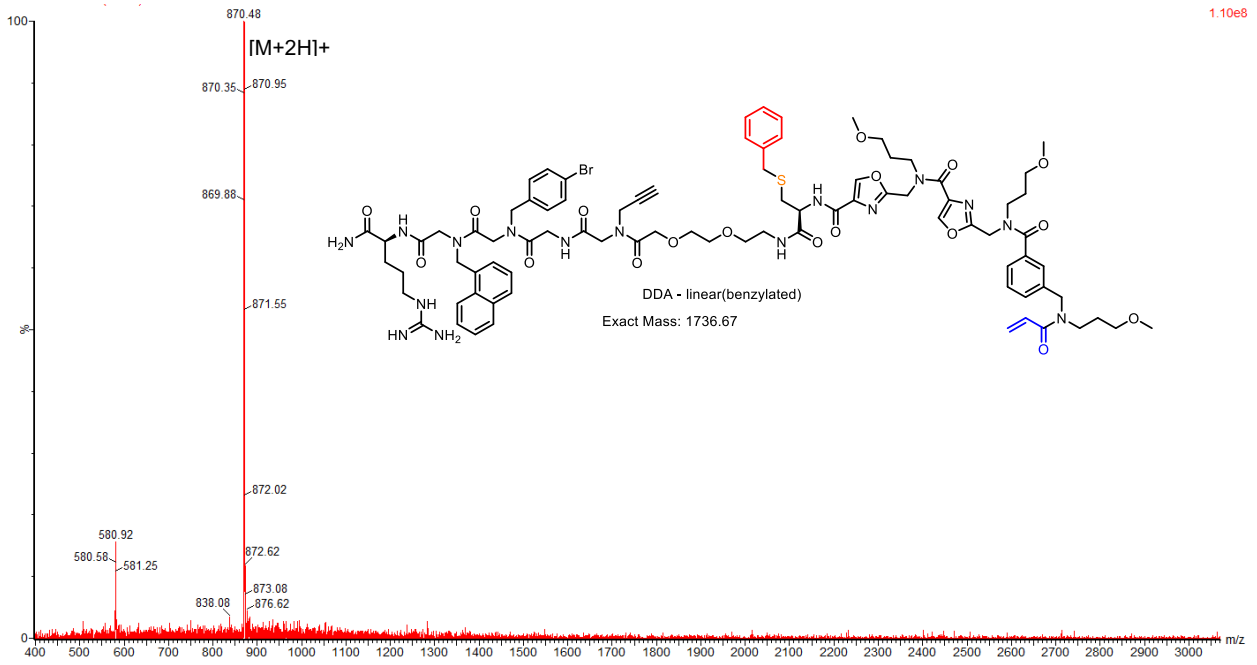
Cyclization of DDA-analog:

Incomplete cyclization was observed on 160 µM beads but 10 µM beads seems to have completed cyclization. Ring closure via thiol-ene reaction appears to be slower compared to halide displacement based reaction.



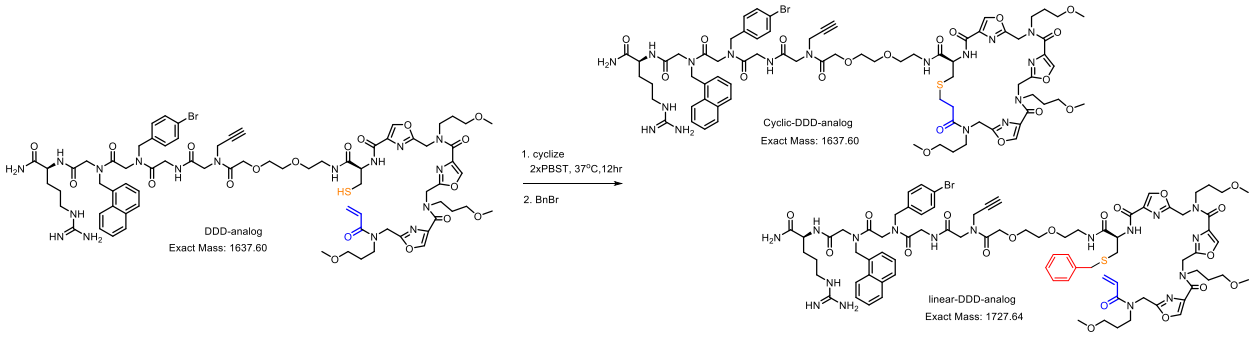


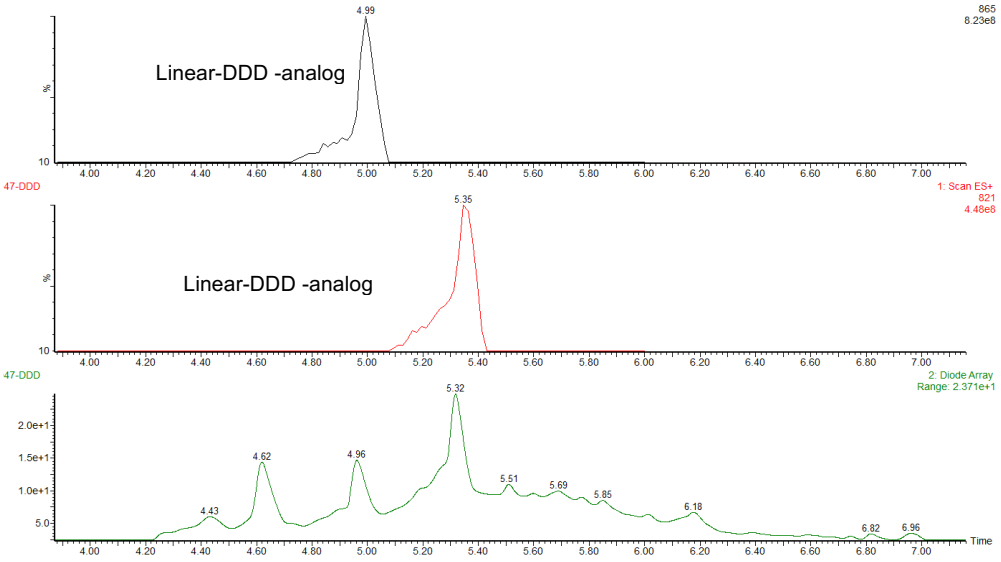

3.66e7
[M+2H]+
825.66
825.52
824.99
826.13
824.79
826.53
826.73
836.55
824.26
837.08
840.02
550.86
551.13
550.06
551.53
529.29
670.42
710.23
1000.27
1111.49
1144.49
1223.99
1309.49
1649.87
1649.67
1649.07
1651.01
1652.61
1939.15
2515.91
DDA - cyclic
Exact Mass: 1646.62
m/z

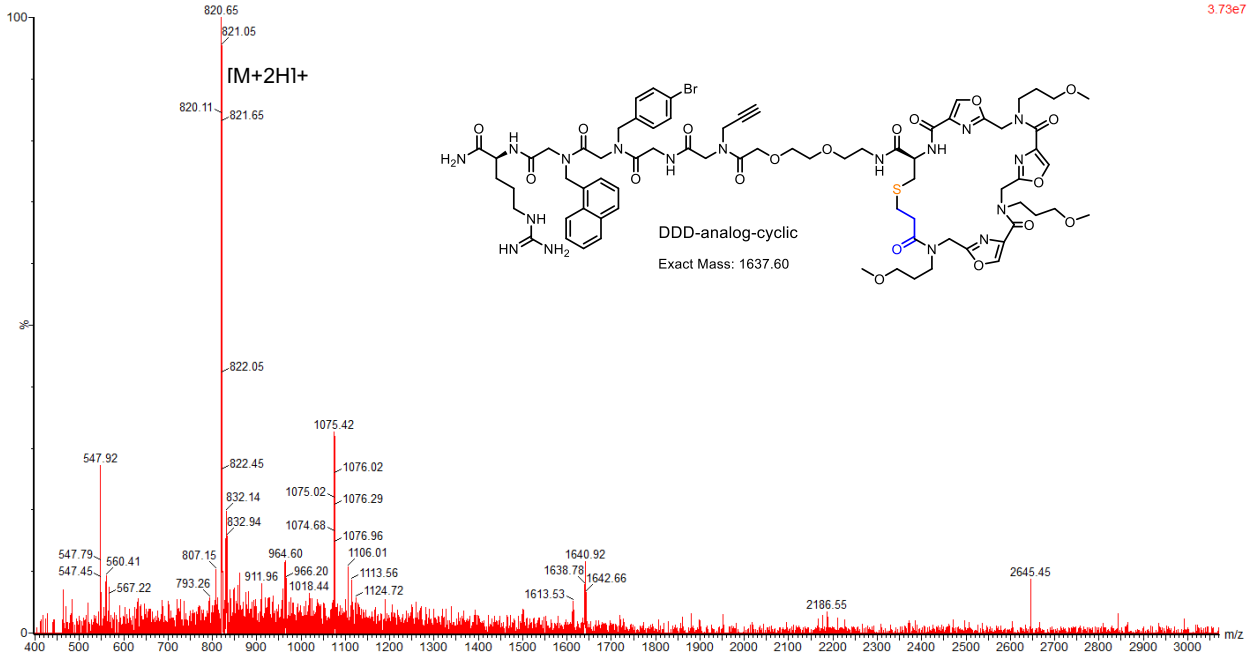

1.10e8
[M+2H]+
870.48
870.35
870.95
869.88
871.55
872.02
872.62
873.08
876.62
838.08
580.92
580.58
581.25
DDA - linear(benzylated)
Exact Mass: 1736.67
m/z

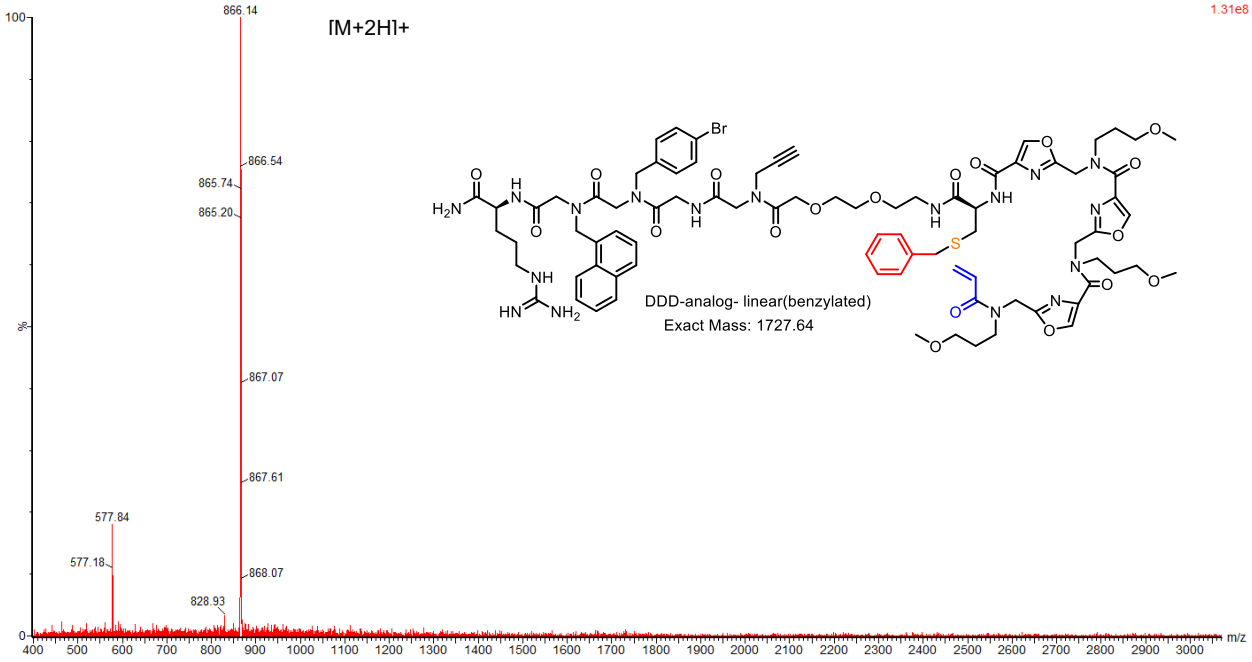
Cyclization of DDD analog:

Incomplete cyclization was observed on 160 µM beads but 10 µM beads seems to have completed cyclization. Ring closure via thiol-ene reaction appears to be slower compared to halide displacement based reaction.






3.73e7
[M+2H]+
820.65
821.05
820.11
821.65
822.05
1075.42
547.92
822.45
1076.02
832.14
1075.02
1076.29
832.94
1074.68
1076.96
547.79
560.41
807.15
964.60
1106.01
547.45
567.22
793.26
911.96
966.20
1018.44
1113.56
1124.72
1640.92
1638.78
1642.66
1613.53
2645.45
2186.55
DDD-analog-cyclic
Exact Mass: 1637.60
%
m/z


1.31e8
[M+2H]+
866.14
866.54
865.74
865.20
867.07
867.61
577.84
577.18
868.07
828.93
DDD-analog- linear(benzylated)
Exact Mass: 1727.64
%
m/z