Supporting Information

Distributed Drug Discovery, Part 2: Rehearsal of Alkylating Agents for the Synthesis of Resin-Bound Unnatural Amino Acids and Virtual D^3 Library Construction

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Tutorial for Using the Distributed Drug Discovery (D^3) Database on the Collaborative Drug Discovery (CDD) Website

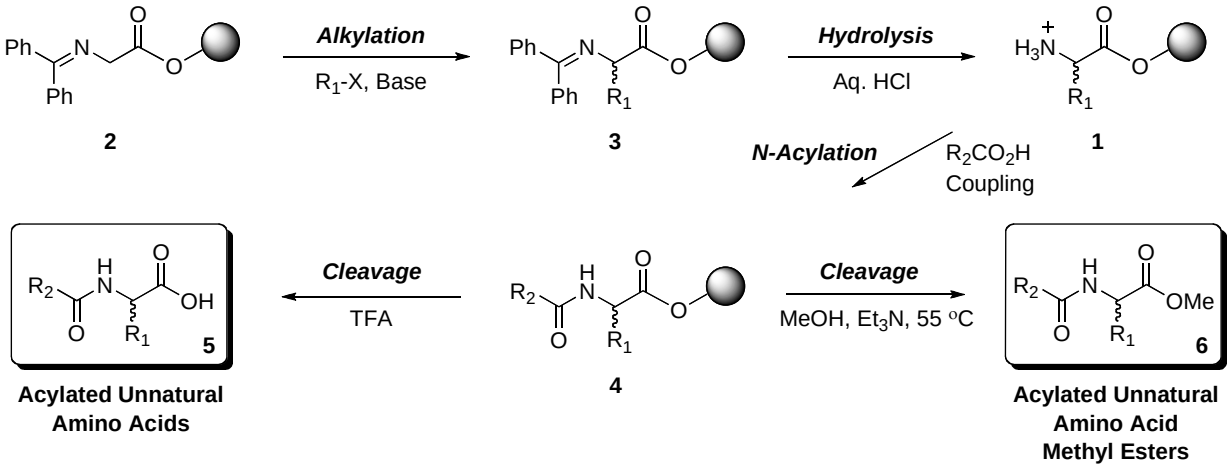
The Distributed Drug Discovery (D^3) database is a virtual catalog of 48,608 unique acylated unnatural amino acid derivatives obtained from a combinatorial enumeration. For access to this database, register for a free read-download account with Collaborative Drug Discovery (CDD) at http://www.collaborativedrug.com/register/iupui-d3 (accessed November 2, 2008).

The following discussion is divided into three parts:

1) Synthesis 2) Enumeration 3) Tutorial

Compound identifiers are those described in the accompanying *Journal of Combinatorial Chemistry* papers [Scott, W. L.; O'Donnell, M. J. et al. *J. Comb. Chem.* DOI: 10.1021/cc800184v (http://dx.doi.org/10.1021/cc800184v) and DOI: 10.1021/cc800185z (http://dx.doi.org/10.1021/cc800185z) and DOI: 10.1021/cc800183m (http://dx.doi.org/10.1021/cc800183m)]. The user is referred to these papers for an in-depth discussion of the D^3 project.

Synthesis. Scheme 1 describes the chemistry involved in the combinatorial enumeration to prepare a virtual catalog of 48,608 unique acylated unnatural amino acids **5** or their methyl esters **6**. The starting material is the Wang resin-bound benzophenone imine of glycine (**2**). The first diversity element (R_1) is attached to the glycine scaffold by reaction of an alkyl halide or Michael acceptor (both abbreviated as "R_1-X") in the presence of base to give **3** in an alkylation or conjugate addition reaction. The imine activating group is removed by hydrolysis and then the second diversity element is added by N-acylation using a standard coupling reaction. Cleavage from the resin is accomplished with either trifluoroacetic acid to give the acylated unnatural amino acid (**5**) or by transesterification with methanol to yield the acylated unnatural amino acid methyl ester (**6**).



Scheme 1. Synthetic Routes to Acylated Unnatural Amino Acids **5** and Methyl Esters **6**.

A total of 100 commercially available electrophiles (R_1X = alkyl halide or Michael acceptor) and 100 commercially available carboxylic acids (R_2CO_2H) were used in an enumeration creating all the possible combinations of R_1 and R_2 for **5** and **6**.

Enumeration. Enumeration with the 100 electrophiles (alkyl halides and Michael acceptors) and 100 carboxylic acids gave 24,416 acylated amino acids **5** and 24,192 acylated amino acid methyl esters **6**. The reason these numbers exceed 10,000 in each case is discussed below.

Issues of stereochemistry were addressed in this enumeration. Examples illustrating the possibilities for the amino acid products **5** are shown (Table 1). The products are identified in three ways: row/column (e.g. **A1**), number in D^3 database (e.g. DDD-000002150), or number from *J. Comb. Chem.* paper [e.g. **(*R*)-5**{9,119}]. The diversity elements, reactants R_1X and R_2CO_2H, include achiral (**1** and **A**), optically pure (**B**), racemic (**2** and **C**) and prochiral (**3**) examples. Only one of the possible stereoisomers for each product is shown in this table, designed to illustrate three main points.

(1) When achiral or optically pure reactants (R_1X and R_2CO_2H) were used, racemic products (2 stereoisomers) resulted, e.g. **A1** and its enantiomer or **B1** and its diastereomer at the α carbon. The database contains 15,308 unique molecules **5** (7,654 pairs) of this class.

(2) When one of the reactants (R_1X and R_2CO_2H) was racemic or, in the case of Michael acceptors, prochiral, 4 stereoisomers were obtained, e.g. **A2** or **A3** and their stereoisomers. The database contains 8,068 unique molecules **5** (2,017 sets of four stereoisomers) of this class.

(3) When both reactants (R_1X and R_2CO_2H) were racemic or prochiral and racemic, 8 stereoisomers were formed. Examples: **C2** or **C3** and their stereoisomers. The database contains 1,040 such unique molecules **5** (130 sets of eight stereoisomers) of this class.

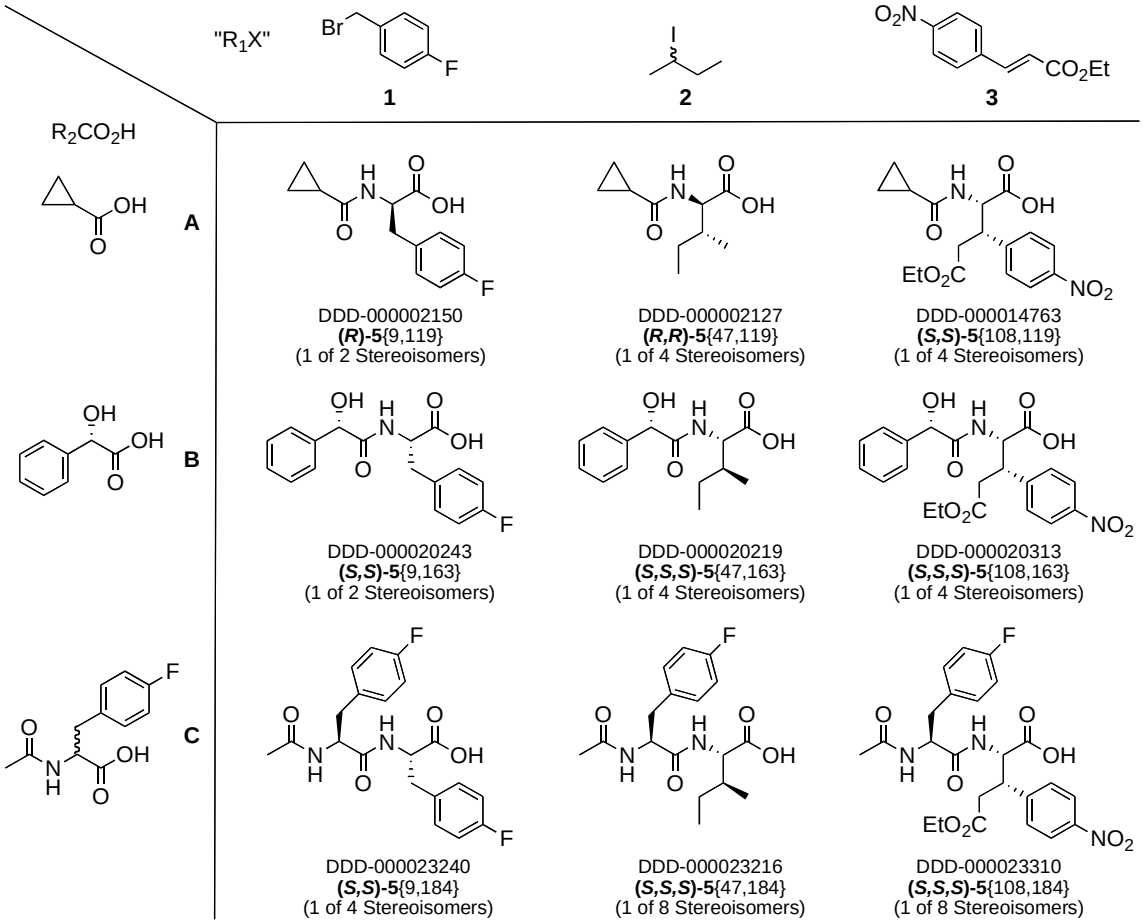
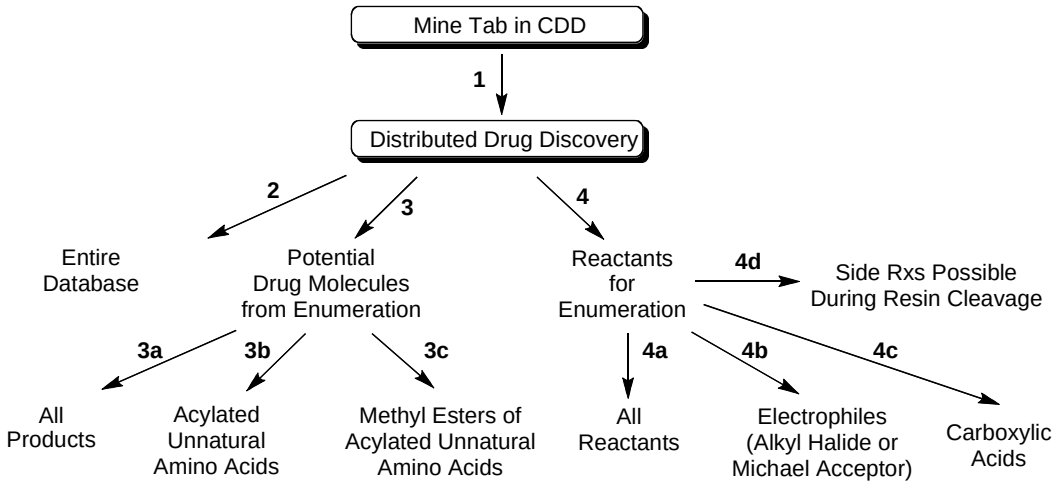


Table 1. Sample 3 x 3 Enumeration Representative of 48,608 Member D^3 Catalog.

Tutorial. This tutorial is a guide to using the IUPUI Distributed Drug Discovery (D^3) database residing on the Collaborative Drug Discovery (CDD) website. The tutorial is accessible from: a) the Supporting Information in Scott, W. L.; O'Donnell, M. J. et al. *J. Comb. Chem.* DOI: 10.1021/cc800184v (http://dx.doi.org/10.1021/cc800184v) and DOI: 10.1021/cc800185z (http://dx.doi.org/10.1021/cc800185z) b) the CDD website; or c) the IUPUI Department of Chemistry and Chemical Biology website [http://chem.iupui.edu/ (accessed November 2, 2008] under faculty & staff directory for O'Donnell or Scott. The tutorial available at (ii) and (iii) will be updated periodically.

1) To Obtain Username and Password for the IUPUI Distributed Drug Discovery (D^3) database.
   For access to the IUPUI - Distributed Drug Discovery (D^3) database, register for a free read-download account with Collaborative Drug Discovery (CDD) at https://www.collaborativedrug.com/register/iupui-d3 (accessed November 2, 2008) by completing the "Sign up for IUPUI – Distributed Drug Discovery (D3)" information.
2) Login to the IUPUI Distributed Drug Discovery (D^3) database.
   URL: http://www.collaborativedrug.com/ (accessed November 2, 2008)
   Username: Your Username
   Password: Your Password
   Select: "Mine" on the Dashboard page (upper right-hand corner)
3) Mining.
   Allows quick searching of the entire D^3 database (or a subset thereof) using "protocols". Searches can be further refined with Structures, Chemical Properties and/or Molecule Keywords. Scheme 2 outlines the D^3 database organization and protocol structure:



1. Select: Distributed Drug Discovery from pull-down "protocol" -> Distributed Drug Discovery Work Site
2. Select: (any Distributed Drug Discovery protocol) -> Entire Distributed Drug Disocovery Database
3. Select: Potential Drug Molecules from Enumeration
  3a. Option: (any readout) -> All Enumerated Products
  3b. Option: Acylated Unnatural Amino Acids -> All Enumerated Acylated Unnatural Amino Acids
  3c. Option: Methyl Esters of Acylated Unnatural Amino Acids -> All Enumerated Methyl Esters
4. Select: Reactants for Enumeration
  4a. Option: (any readout) -> All Reactants
  4b. Option: Electrophiles (Alkyl Halide or Michael Acceptor) -> All Electrophile Reactants
  4c. Option: Carboxylic Acids -> All Carboxylic Acid Reactants
  4d. Option: Side Rxs Possible During Resin Cleavage -> Reactant Functionality Transformed During Cleavage

Scheme 2. D^3 Database Organization and Protocol Structure.

From the Mine tab, “any protocol type”, “any protocol”, and “any readout” pull-down menus can be specified. One or more selections lead to all possible search results within the chosen category. Table 2 lists the results obtained from searches in the indicated categories (numbers in parentheses refer to steps in Scheme 2):

Protocols	Search Results[a]
(any protocol type)	
(any protocol)	Default
Distributed Drug Discovery (1)	
(any Distributed Drug Discovery protocol) (2)	48,818
Potential Drug Molecules from Enumeration (3)	
(any readout) (3a)	48,608
Acylated Unnatural Amino Acids (3b)	24,416
Methyl Esters of Acylated Unnatural Amino Acids (3c)	24,192
Reactants for Enumeration (4)	
(any readout) (4a)	212
Electrophiles (Alkyl Halide or Michael Acceptor) (4b)	112
Carboxylic Acids (4c)	100
Side Rx Possible During Resin Cleavage (4d)	22

[a] “Add a term” to modify a search by: Structures, Chemical Properties and/or Molecule Keywords

Table 2. Results Obtained from Different Protocol Searches.

Example 1: All Products Search

Select: Mine tab
Select: New Query
Select the following from the pull-down protocol menus:
Distributed Drug Discovery
Potential Drug Molecules from Enumeration
(any readout)
Note: “(*any readout*)” means the default has been automatically chosen.
Select: Search Molecules
Result: Displays first 100 of 48,608 acylated unnatural amino acids and methyl esters from enumeration.
Select: Third molecule (DDD-000001000) in list of products. Note that the first two products in the list are both reactant carboxylic acids (DDD-0000000267 and DDD-000000274) and enumeration products (DDD-000001010 and DDD-000013558, respectively).
Result: Left column – information about the product and the reactants used for its preparation in the enumeration; right column – CDD-generated product information (see Appendices 1 and 2 for a listing of product and reactant information).

4) File Downloads

The three files described below are available for download at several locations in the database. The most direct route to these downloads follows:

Select: Archive tab
Select: Protocols

Select: "Potential Drug Molecules from Enumeration"
Select (under Associated Files): Filename

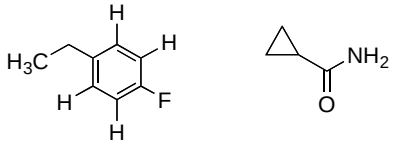
a) "IUPUI D3 Enumerated Products.sdf": The SD File of the 48,608 enumerated products. This file contains the fields described in Appendix 3.
b) "IUPUI D3 Tutorial.pdf": The tutorial will be updated periodically and be available through CDD at this site and also on the IUPUI Department of Chemistry and Chemical Biology website [http://chem.iupui.edu/ (accessed November 2, 2008)] under the faculty & staff directory for O'Donnell or Scott.
c) "IUPUI D3 Refs Rxs Electrophiles.pdf": This file contains selected lead references, cited in Scott, W. L.; O'Donnell, M. J. et al. *J. Comb. Chem.* DOI: 10.1021/cc800184v (http://dx.doi.org/10.1021/cc800184v) for reaction of each electrophile (alkyl halide or Michael acceptor) with Schiff bases of amino acid derivatives under a variety of basic conditions.

5) Substructure or Full Structure Searches

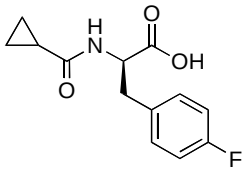
Select: Mine tab
Select: New Query
Select: Structures – by substructure
Select: "Launch the editor" to build a structure for this search (opens MarvinSketch applet)
Note: A dialog box may appear with information about a certificate or digital signature. If this happens, select "Trust" or "Run."

a) Example 2: Substructure Search

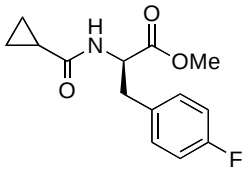
Draw the following search query in MarvinSketch (see Appendix 4 for detailed drawing instructions).



Select: Use This Structure
Result: Structures in Mine Protocols and Molecules structure box.
Note: Sometimes a "?" appears in the resulting structure box, indicating the image did not load but the structure is still stored and one can continue.
Select the following from the pull-down protocol menus:
Distributed Drug Discovery
Potential Drug Molecules from Enumeration
(any readout)
Select: Search Molecules
Result: 4 matching compounds from the 48,606 enumerated products; the two enantiomeric carboxylic acids and their two enantiomeric methyl esters:

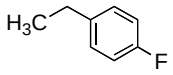


A1
DDD-000002150
***ent*-A1**
DDD-000014693



A1 (Methyl Ester)
DDD-000102150
***ent*-A1 (Methyl Ester)**
DDD-000114693

b) Example 3: Substructure Search
Select: Mine tab
Select: New Query
Select the following from the pull-down protocol menus:
Distributed Drug Discovery
Potential Drug Molecules from Enumeration
Acylated Unnatural Amino Acids
Draw the following search query in MarvinSketch (see Appendix 4 for detailed drawing instructions):

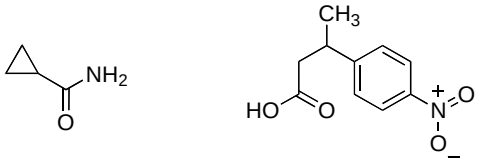


Select: Use This Structure
Select: Search Molecules
Result: 1518 hits from the database of 24,416 amino acid products (Table 3).
The 24 hits from Table 1 are summarized below:

Structure in Table 1	Number of Stereoisomers
A1	2
B1	2
C1	4
C2	8
C3	8

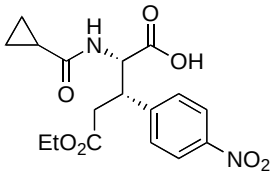
Table 3. Stereochemical Results from Example 3.

c) Example 4: Substructure Search Demonstrating Stereochemistry and Side Reactions
Select: Mine tab
Select: New Query
Select the following from the pull-down protocol menus:
Distributed Drug Discovery
Potential Drug Molecules from Enumeration
(any readout)
Draw the following search query in MarvinSketch (see Appendix 4 for detailed drawing instructions):

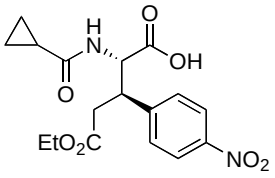


Select: Use This Structure
Select: Search Molecules
Result: 8 matching results from the database of 48,608 amino acid and methyl ester products (Table 4). The 4 stereoisomers of the acylated unnatural amino acids (**5**) are represented in the top row while the 4 stereoisomers of the methyl esters (**6**)

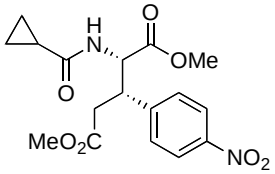
are in the bottom row. For the methyl ester products a possible side reaction during resin cleavage (transesterification of the ethyl ester in the Michael acceptor) has been carried out. Notation of this side reaction plus a lead reference are obtained by searching for the electrophile used in this preparation (Michael acceptor DDD-000000121).



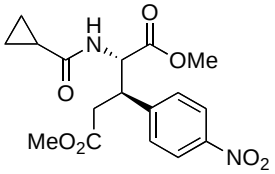
A3
DDD-000014763
***ent*-A3**
DDD-000002219



***diast*-A3**
DDD-000014762
***ent*-(*diast*-A3)**
DDD-000002220



A3 (di-Methyl Ester)
DDD-000114763
***ent*-A3 (di-Methyl Ester)**
DDD-000102219



***diast*-A3 (di-Methyl Ester)**
DDD-000114762
***ent*-(*diast*-A3) (di-Methyl Ester)**
DDD-000102220

Table 4. Results from Example 4.

6) Obtaining Information About a Particular Molecule

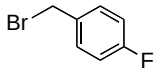
a) Example 5: Product Information Search

- From a Search:
  Under Search Results, select structure or DDD number
- Using a D^3 Number:
  From the original Mine page:
  Select: New Query
  In Molecule Keywords type: DDD-000002150 (shortcut: DDD 2150)
  Select: Search Molecules
  Result: 11 hits. The CDD search strategy returns molecules that begin with "2150": DDD-000002150 and the 10 molecules DDD-000021500 through DDD-000021509. Lower DDD registry numbers appear first in the search results, so DDD-000002150 is the first entry.

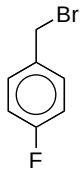
b) Example 6: Reactant Information Search (see Appendix 2 for a listing of reactant information)

Select: Mine tab
Select: New Query
Select the following from the pull-down protocol menus:
Distributed Drug Discovery
Reactants for Enumeration
(any readout)

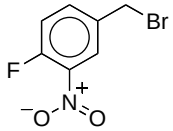
Draw the following search query in MarvinSketch (see Appendix 4 for detailed drawing instructions). To insert the Br: Position the cursor over the H_3C and type Br or select "More", choose Br, Close, Click on H_3C.



Select: Use This Structure
Select: Search Molecules
Result: 2 hits



1-(bromomethyl)-
4-fluorobenzene
DDD-000000048



4-(bromomethyl)-
1-fluoro-2-nitrobenzene
DDD-000000049

Select: Structure or name [1-(bromomethyl)-4-fluorobenzene], to obtain information about this reactant (see Appendix 2 for a listing of reactant information)

7) Selecting Other Public Data Sets

Other public data sets besides the Distributed Drug Discovery (D3) database are available as follows:

Select: Collaborate tab
Select: Data Sets
Select: Select all or make individual selection(s)
Select: Save selections
Select: Mine tab and proceed with search

Appendix 1

Information about Individual Enumeration Products

1) Information about the enumeration product and the reactants used for its generation (left column).
    - Definition (category content):
        - Name (DDD Number)
        - Synonyms
        - Description (Blank)
        - Structure (SMILES or InChI or InChIKey)
        - Molecular Formula
        - Product Type
        - Reactant: Electrophile (Chemical Name)
        - Reactant: Electrophile DDD No.
        - Reactant: Carboxylic Acid (Chemical Name)
        - Reactant: Carboxylic Acid DDD No.

2) CDD-generated information about the enumeration product (right column).
        - Structure
    - Lipinski properties
        - Molecular weight
        - log P
        - H-bond donors
        - H-bond acceptors
        - Lipinski Rule of 5
    - Additional properties
        - Formula
        - pKa
        - Exact mass
        - Atom count
        - Composition
        - Topological polar surface area (PSA)

Appendix 2

Information about Individual Reactants

1) Information about the reactant (left column).
    Definition (category content):
        Name (DDD Number)
        Synonyms (Chemical Name(s))
        Description (Blank)
        Structure (SMILES or InChI or InChIKey)
        Reactant Type
        Molecular Formula
        *Reference No. for Rxs with Schiff Bases of Amino Acid Derivatives
        *Side Rxs Possible During Resin Cleavage
            *These categories are only shown when an entry is present.

2) CDD-generated information about the reactant (right column).
        Structure
    Lipinski properties
        Molecular weight
        log P
        H-bond donors
        H-bond acceptors
        Lipinski Rule of 5
    Additional properties
        Formula
        pKa
        Exact mass
        Atom count
        Composition
        Topological polar surface area (PSA)

Appendix 3

Information Available for Enumeration Products in SD File Download

Structure
SMILES
Name (DDD Number)
Product Type (Acylated Unnatural Amino Acid or Methyl Esters of Unnatural Amino Acids)
Molecular weight
log P
H-bond donors
H-bond acceptors
Lipinski Rule of 5
Formula
pKa
Exact mass
Atom count
Composition
Topological polar surface area (PSA)
Reactant: Electrophile (Chemical Name)
Reactant: Electrophile DDD No.
Reactant: Carboxylic Acid (Chemical Name)
Reactant: Carboxylic Acid DDD No.

Appendix 4

Detailed Instructions for Drawing Structures for Example 2 (page 5)

Repeat Login Procedure

Select the following from the pull-down protocol menus:

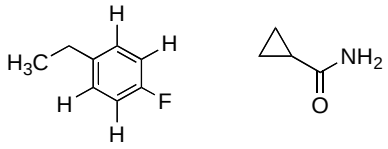
Distributed Drug Discovery

Potential Drug Molecules from Enumeration

(any readout)

Note: "(*any readout*)" means the default has been automatically chosen.

Target Substructures to Draw in Marvin Sketch:



From within the CDD Database:

Select: Mine tab

Select: New Query

Select: Structures – by substructure

Select: "Launch the editor" to build a structure for this search (opens MarvinSketch applet)

Note: A dialog box may appear with information about a certificate or digital signature. If this happens, select "Trust" or "Run."

From within the Structure Editor of MarvinSketch:

(1) Select the benzene ring from the structure palate.

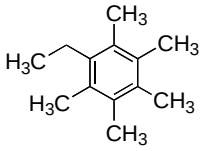
(2) Move the cursor to position the benzene ring on the left side of the drawing surface then click.

(3) Select the bond tool (below "Help").

(4) Position the cursor above one of the carbons so that a blue circle appears then click. Alternatively, you can click/drag/release to position the bond.

(5) Repeat step 4 for all benzene ring carbons.

(6) Position the cursor above one of the CH_3 groups then click.



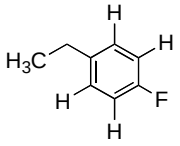
Intermediate
Structure **A**

(7) The hydrogens and fluorine on the benzene ring can be added in one of two ways:

(a) Position the cursor above a CH_3 group so that a blue circle appears then type the atom symbol or

(b) Select the atom ("H" or "F") in the palate then click above each CH_3 to be changed. If the atom symbol is not in the palate, select "More" for a complete list.

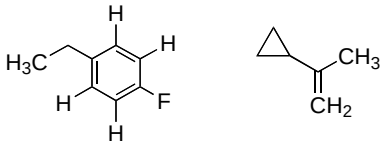
(8) Since not explicitly designated otherwise, the chain H_3C remaining is assumed to be a carbon with 0-3 hydrogens attached.



Intermediate
Structure **B**

(9) Select the bond tool and click in the open space to the right of the previously drawn structure.

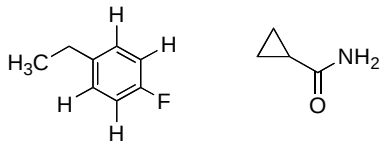
(10) Build the carbon framework of the right-hand structure as before. Click/drag/release to complete the final bond of the cyclopropane ring. To create the second bond of the double bond, position the cursor over the center of the single bond (parentheses will appear) then click.



Intermediate Structures **C**

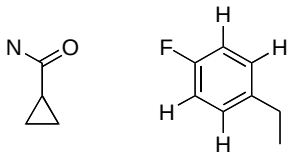
(11) The heteroatoms can be added to the right-hand structure in one of two ways:
   (a) Select the atom ("O" or "N") in the palate then click above the appropriate atom to be changed.
   (b) Position the cursor above the CH_2 or CH_3 group (a circle will appear) then type either an O or an N, respectively.

(12) As before, since not explicitly designated otherwise, the NH_2 is assumed to be a nitrogen with 0-2 hydrogens attached.



Final Search Structures **D**
(in Structure Editor of MarvinSketch)

(13) Select "Use This Structure".
From within the CDD Database:
Result: Structures in Mine Protocols and Molecules structure box.

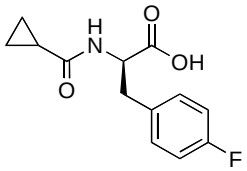


Final Search Structures **E**
(in CDD Search Window)

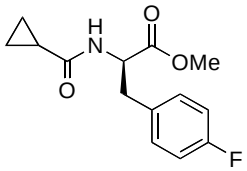
Note: Sometimes a "?" appears in the resulting structure box, indicating the image did not load but the structure is still stored and one can continue.

Select: Search Molecules

Result: 4 matching results from the 48,606 enumerated products; the two enantiomeric carboxylic acids and their two enantiomeric methyl esters:



A1
DDD-000002150
***ent*-A1**
DDD-000014693



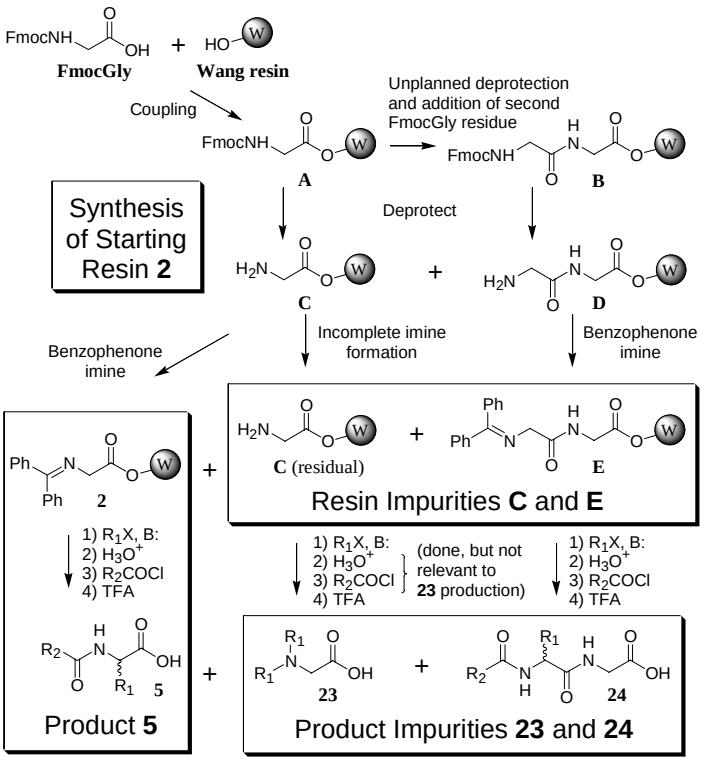
A1 (Methyl Ester)
DDD-000102150
***ent*-A1 (Methyl Ester)**
DDD-000114693

II. Analysis of Resins from Sources I and II, and Interpretation of Results.

The formation of **23** and **24** in A1 products produced from resin source **I** can be explained by assuming the starting material, resin-bound imine **2**, is contaminated with impurities **C** and **E** (Scheme). Resin-bound **C** arises from incomplete transimination with benzophenone imine in the step producing **2** (see text). The presence of **E** in the starting resin has a somewhat more complicated origin. As shown in the scheme, the commercial synthesis of **2** begins with the coupling of FmocGly to a Wang linker attached to a polystyrene polymer. It is well documented in the peptide literature[1] that this coupling process can lead to double coupling product **B** when small amounts of the desired product **A** undergo *in situ* deprotection, and subsequent coupling of a second molecule of FmocGly. When the desired synthesis of imine **2** is completed (by removal of the Fmoc group on **A** to form **C** followed by transimination to **2** with benzophenone imine) the parallel undesired transformation occurs on **B** to give the impurity **E**.

Given the presence of these two impurities, **C** and **E**, in the starting resin **I**, compound **23** is then formed by dialkylation of the primary amine on **C**, and compound **24** (FmocPheGly, R_1 = CH_2Ph) formed when **E** undergoes the same alkylation and acylation chemistry that converts **2** to **5**. Ironically, this FmocPheGly impurity **24** (~11%) also represents successful alkylation, but now on the terminal glycine of a GlyGly residue. Consistent with this interpretation, for almost all the other R_1X alkylations with resin **I** the parallel alkylation impurities **23** and **24** were observed, in addition to desired product **5**. Finally, the third impurity in A1 products from both resins (at 5.3 min, M+1 = 494) is consistent with structure **25**. This would arise from successful alkylation, but subsequent cleavage of product from the resin with the Wang linker still attached.

This byproduct of Wang chemistry, although not often noted in the peptide literature, has been documented.[2]



Scheme. Source of Impurities in Resin **I** Leading to Impurities **23** and **24**.

As can be seen in Figure 2 (see text), there were no significant amounts of either **23** or **24** in products from resin supplier **II**. The only byproduct in A1 samples (at 5.3 min) from resin **II** was **25**. It was present in seven out of eight replicate A1's from teams #18-25. Since this material (with Wang linker attached) also represented successful alkylation, the resin is of high quality and commercial source **II** was used in all the subsequent labs at IUPUI, along with labs conducted in Spain, Russia and Poland.

III. Selected LC/MS and/or NMR analytical data included in Supporting Information.

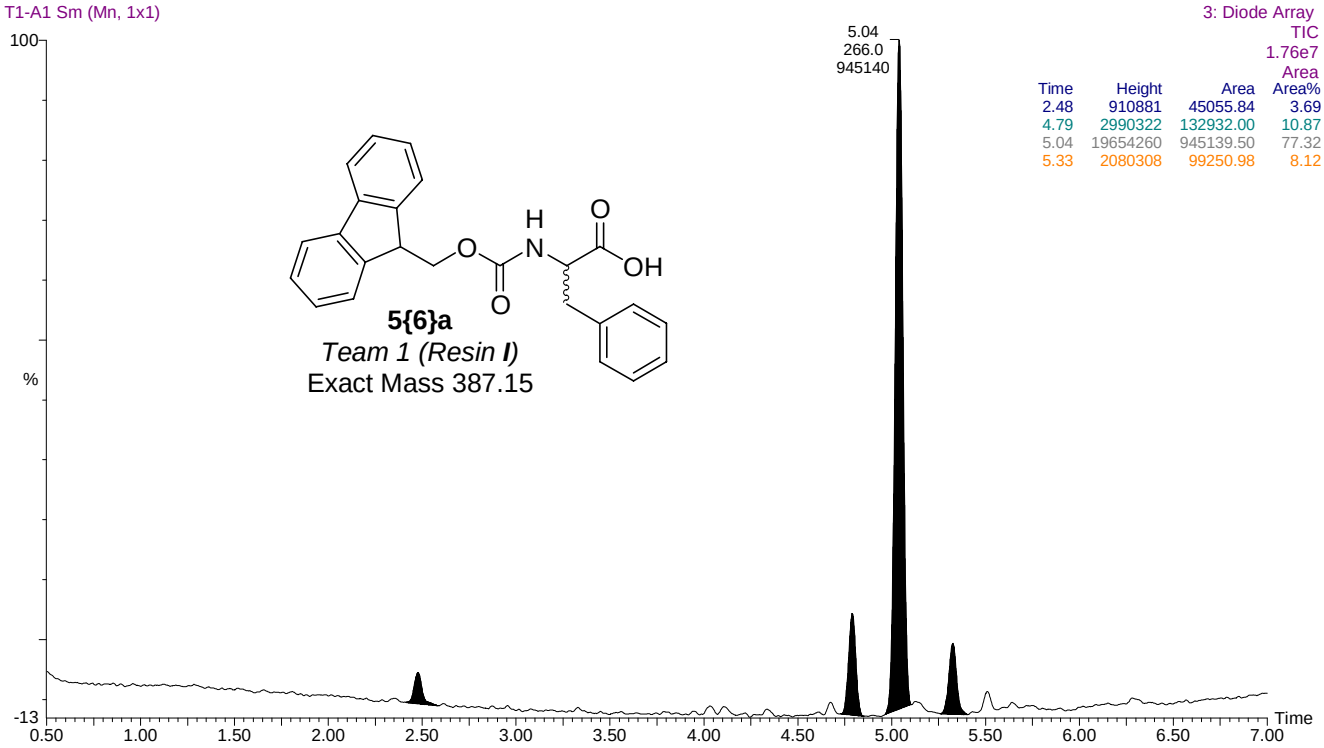
The following Supporting Information provides selected LC/MS and/or NMR data (grouped together by compound) to permit more detailed assessment of:

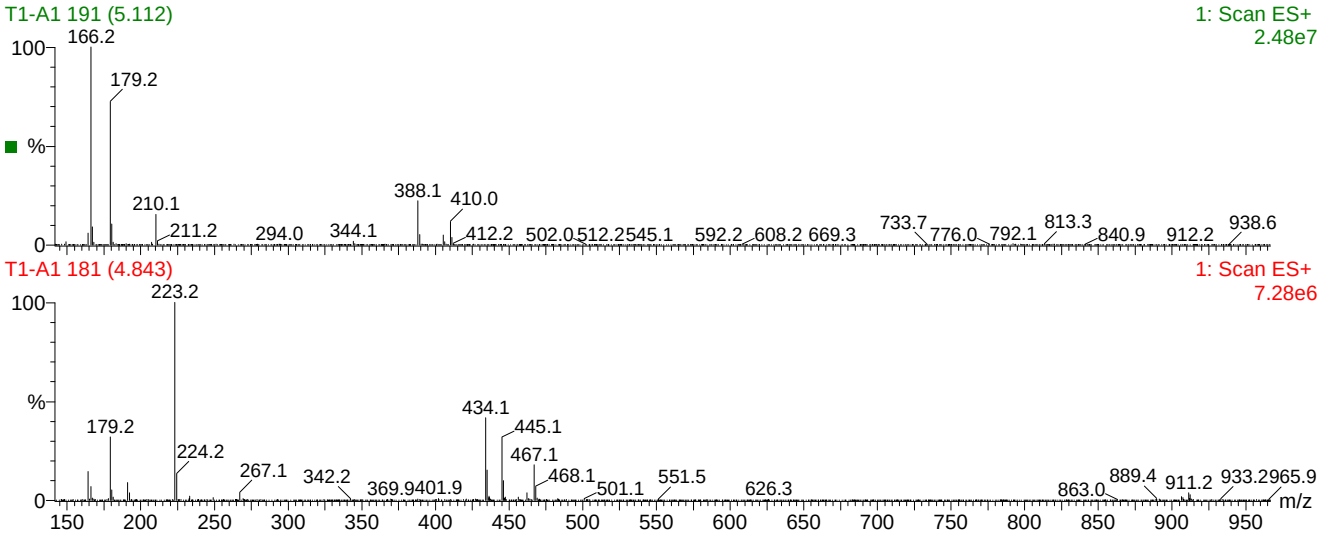
1. The quality and consistency of replicated synthesis, both within a laboratory and globally. For this purpose we provide copies of the LC/MS for all the Fmoc derivatives (the "a" series) of unnatural/natural amino acids prepared at IUPUI, Lublin (Poland) and Moscow (Russia).

2. The identity, as assessed by NMR, of all the final, purified derivatives prepared in the "a" series.

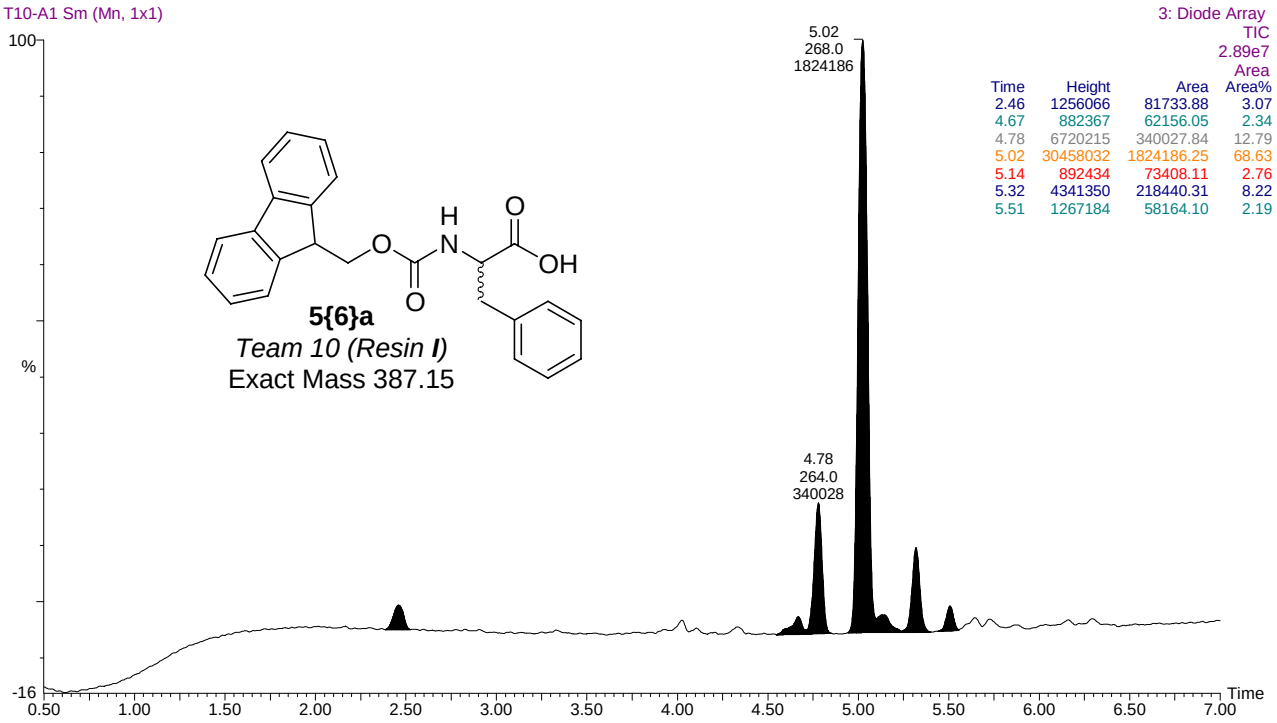
3. The divergent quality, as assessed by LC/MS, of the various preparations of compounds **5{15}b** and **5{17}b** (see pages 104-107 and 108-111, respectively). The syntheses of these compounds represented the rare example where one of the teams (in this case team 28) obtained radically different results from the other replicated samples. As discussed in the text, team 28 obtained none of the expected products **5{15}b** or **5{17}b**, whereas three other teams (teams 12,13, 29 and 11,12, 27 respectively) were successful and had similar results (63% ± 3% and 80% ± 8%, respectively) for each of these compounds in the appropriate Bill-Board positions.[FN - After FN22]

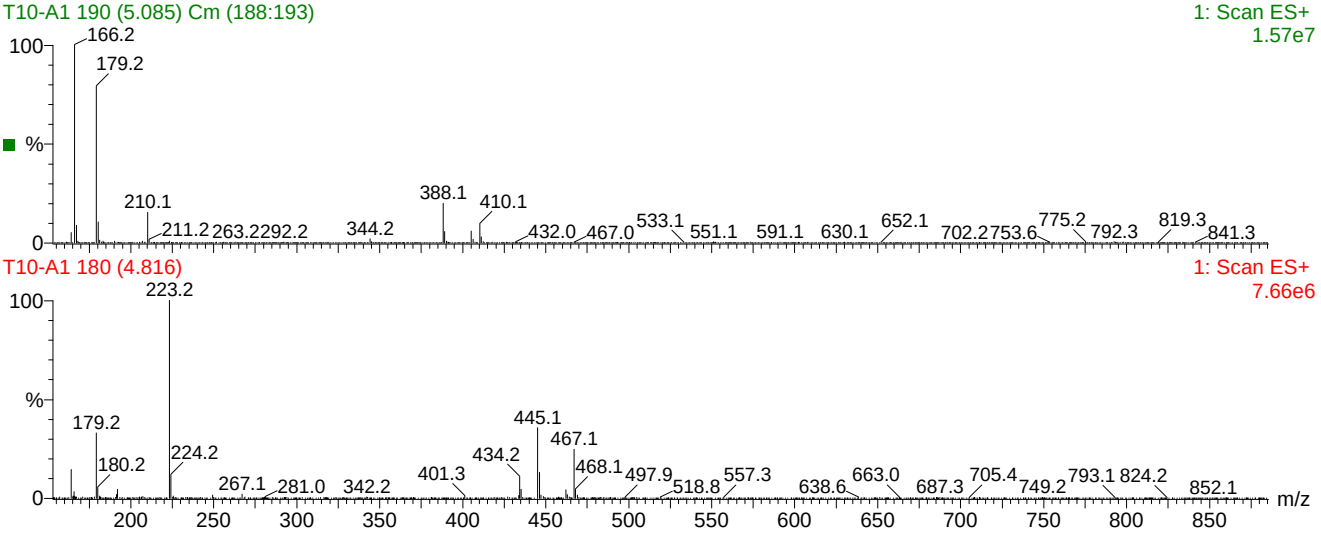
5{6}a


T1-A1 Sm (Mn, 1x1)
3: Diode Array
TIC
1.76e7
Area
Time Height Area Area%
2.48 910881 45055.84 3.69
4.79 2990322 132932.00 10.87
5.04 19654260 945139.50 77.32
5.33 2080308 99250.98 8.12
5.04
266.0
945140
5{6}a
Team 1 (Resin I)
Exact Mass 387.15
%
Time


T1-A1 191 (5.112)
1: Scan ES+
2.48e7
166.2
179.2
210.1
211.2
294.0
344.1
388.1
410.0
412.2
502.0
512.2
545.1
592.2
608.2
669.3
733.7
776.0
792.1
813.3
840.9
912.2
938.6
T1-A1 181 (4.843)
1: Scan ES+
7.28e6
223.2
179.2
224.2
267.1
342.2
369.9
401.9
434.1
445.1
467.1
468.1
501.1
551.5
626.3
863.0
889.4
911.2
933.2
965.9
m/z

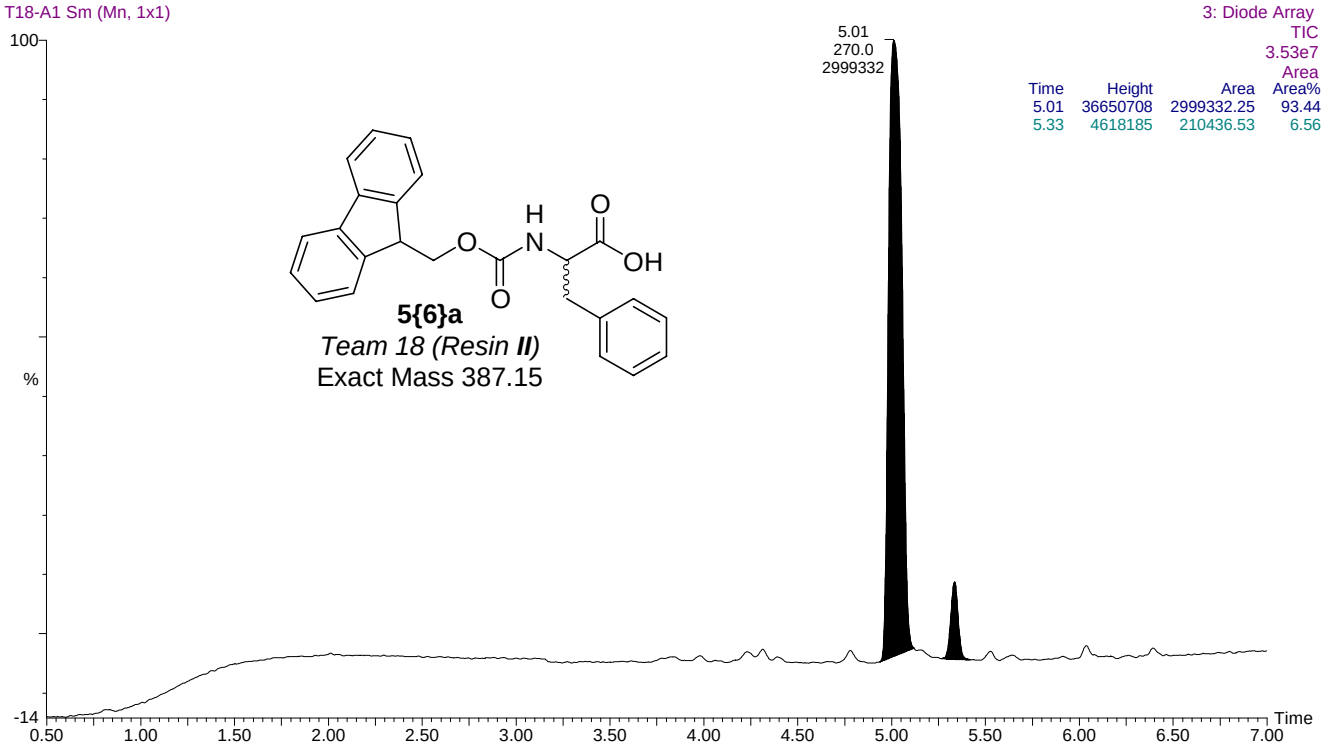
5{6}a

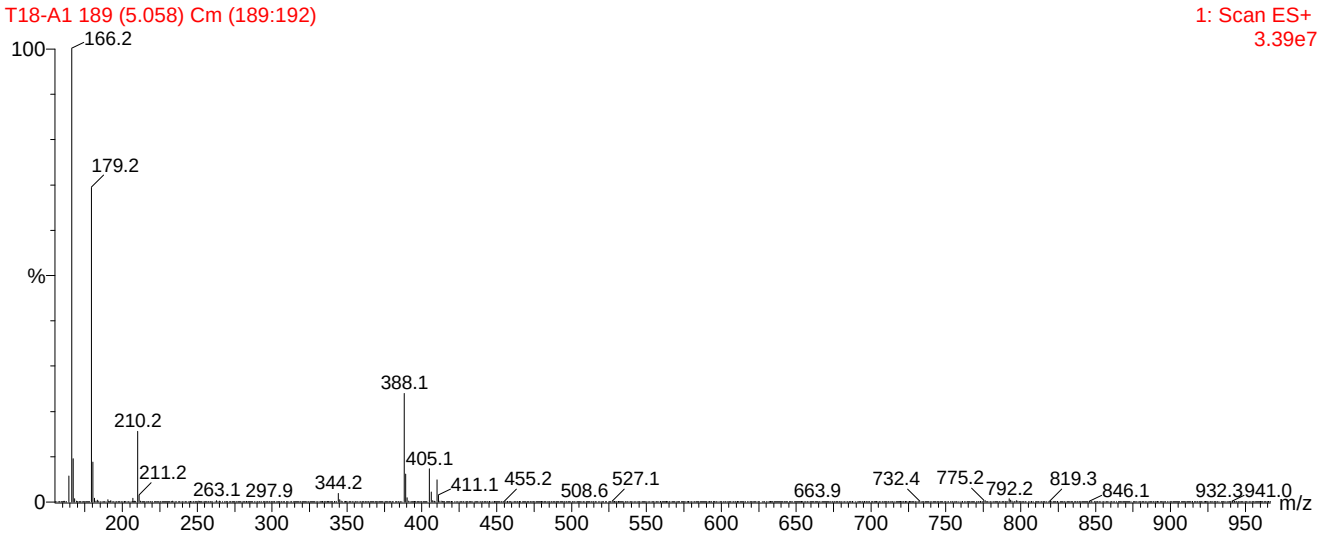

T10-A1 Sm (Mn, 1x1)
3: Diode Array
TIC
2.89e7
Area
Time Height Area Area%
2.46 1256066 81733.88 3.07
4.67 882367 62156.05 2.34
4.78 6720215 340027.84 12.79
5.02 30458032 1824186.25 68.63
5.14 892434 73408.11 2.76
5.32 4341350 218440.31 8.22
5.51 1267184 58164.10 2.19
5.02
268.0
1824186
4.78
264.0
340028
5{6}a
Team 10 (Resin I)
Exact Mass 387.15
100
%
-16
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time


T10-A1 190 (5.085) Cm (188:193)
1: Scan ES+
1.57e7
100
%
0
166.2
179.2
210.1
211.2 263.2 292.2
344.2
388.1
410.1
432.0 467.0 533.1 551.1 591.1 630.1 652.1 702.2 753.6 775.2 792.3 819.3 841.3

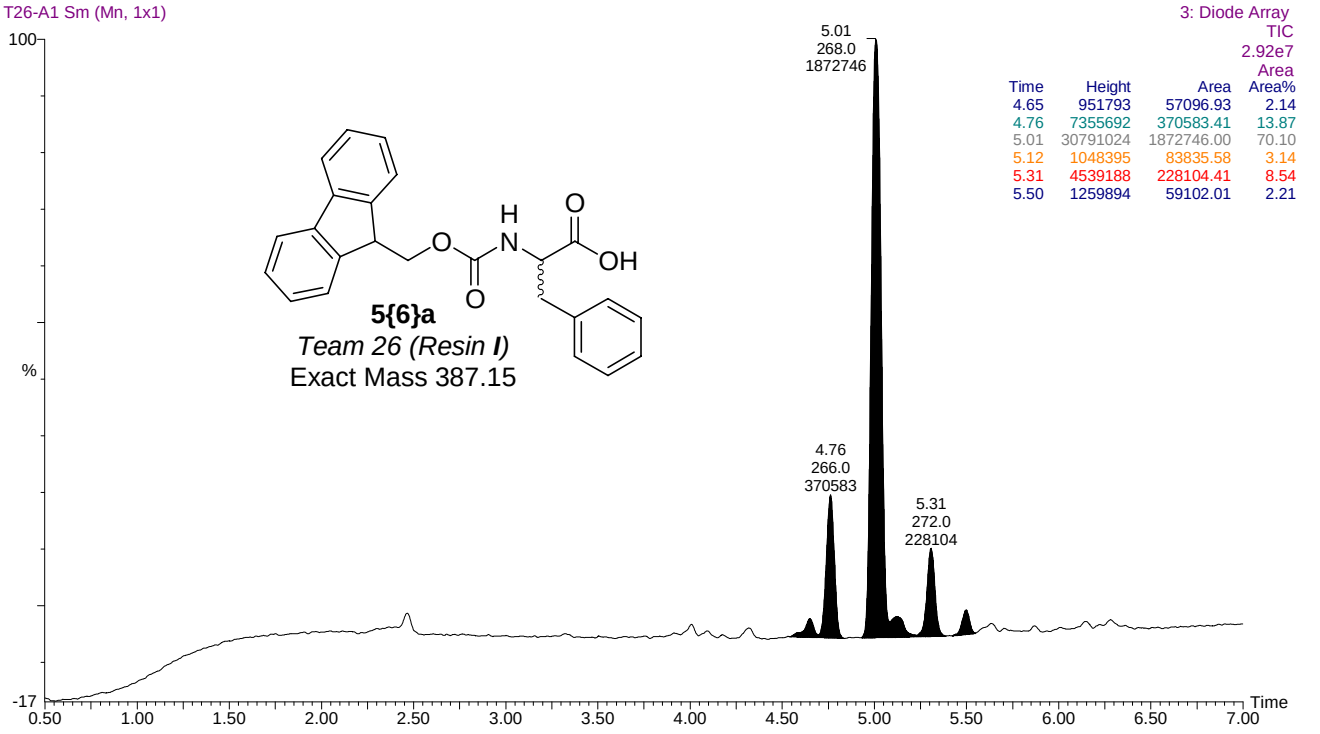
T10-A1 180 (4.816)
1: Scan ES+
7.66e6
100
%
0
223.2
179.2
180.2
224.2
267.1 281.0 342.2 401.3 434.2 445.1 467.1 468.1 497.9 518.8 557.3 638.6 663.0 687.3 705.4 749.2 793.1 824.2 852.1
200 250 300 350 400 450 500 550 600 650 700 750 800 850
m/z

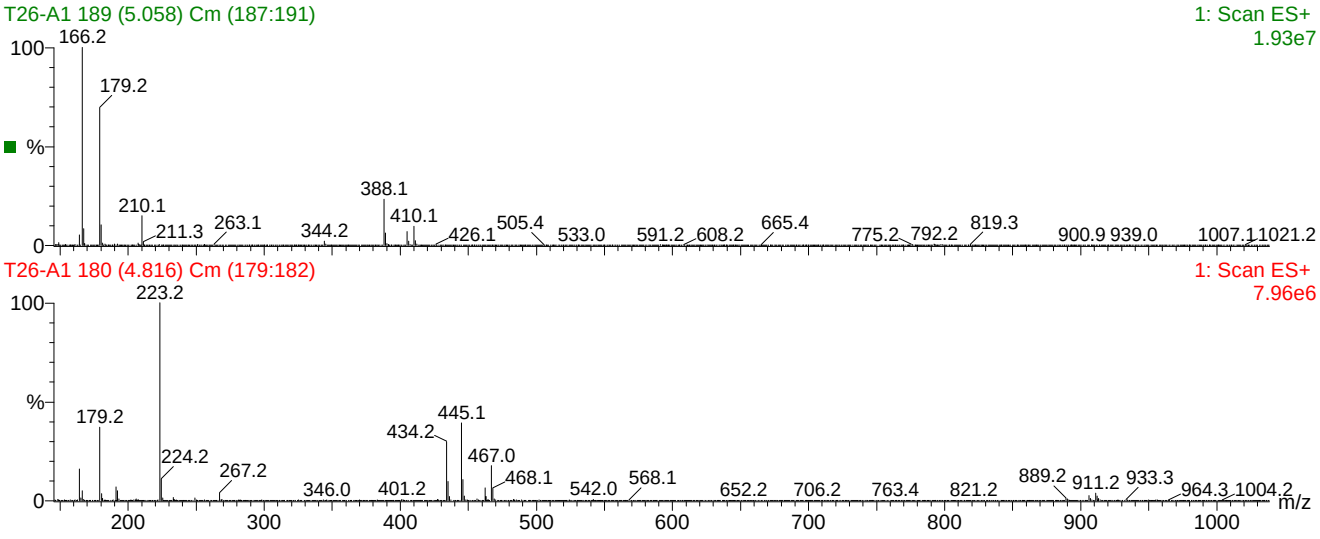
5{6}a


T18-A1 Sm (Mn, 1x1)
3: Diode Array
TIC
3.53e7
Area
Time Height Area Area%
5.01 36650708 2999332.25 93.44
5.33 4618185 210436.53 6.56
5.01
270.0
2999332
100
%
-14
H
N
O
O
OH
O
5{6}a
Team 18 (Resin II)
Exact Mass 387.15
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time


T18-A1 189 (5.058) Cm (189:192)
1: Scan ES+
3.39e7
100
%
0
166.2
179.2
210.2
211.2
263.1
297.9
344.2
388.1
405.1
411.1
455.2
508.6
527.1
663.9
732.4
775.2
792.2
819.3
846.1
932.3
941.0
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950
m/z

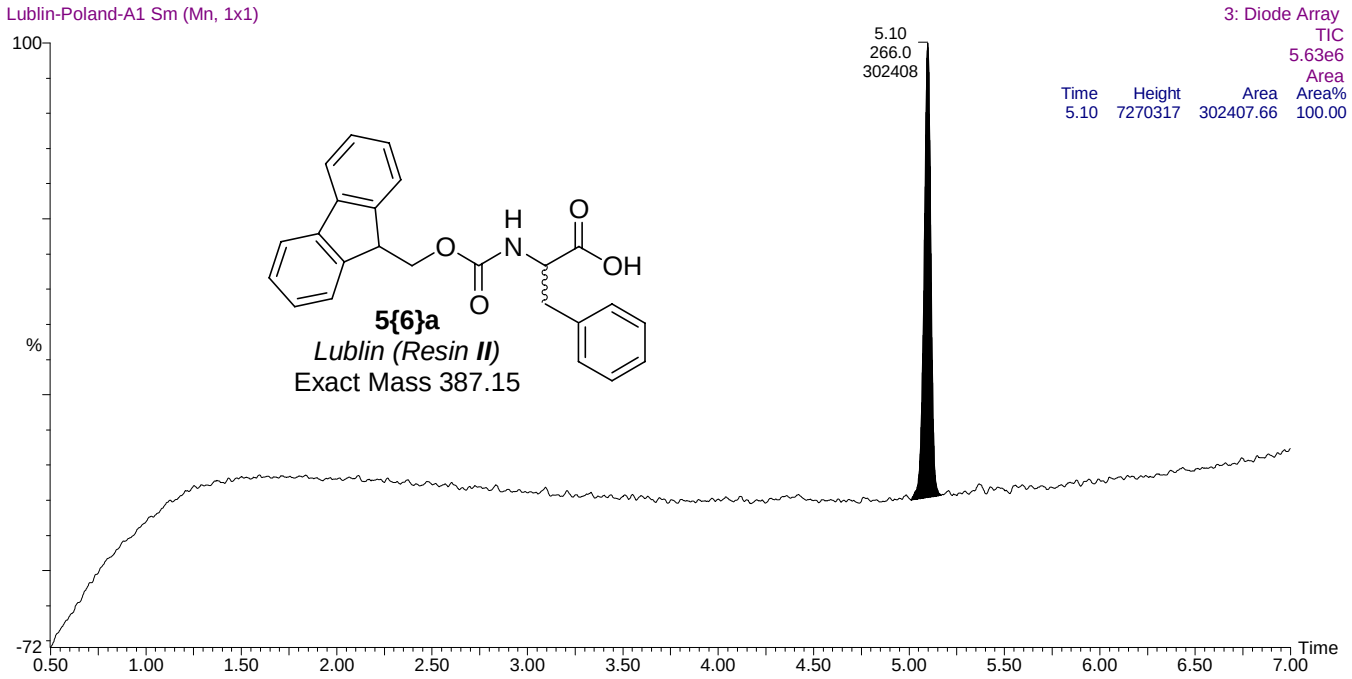
5{6}a

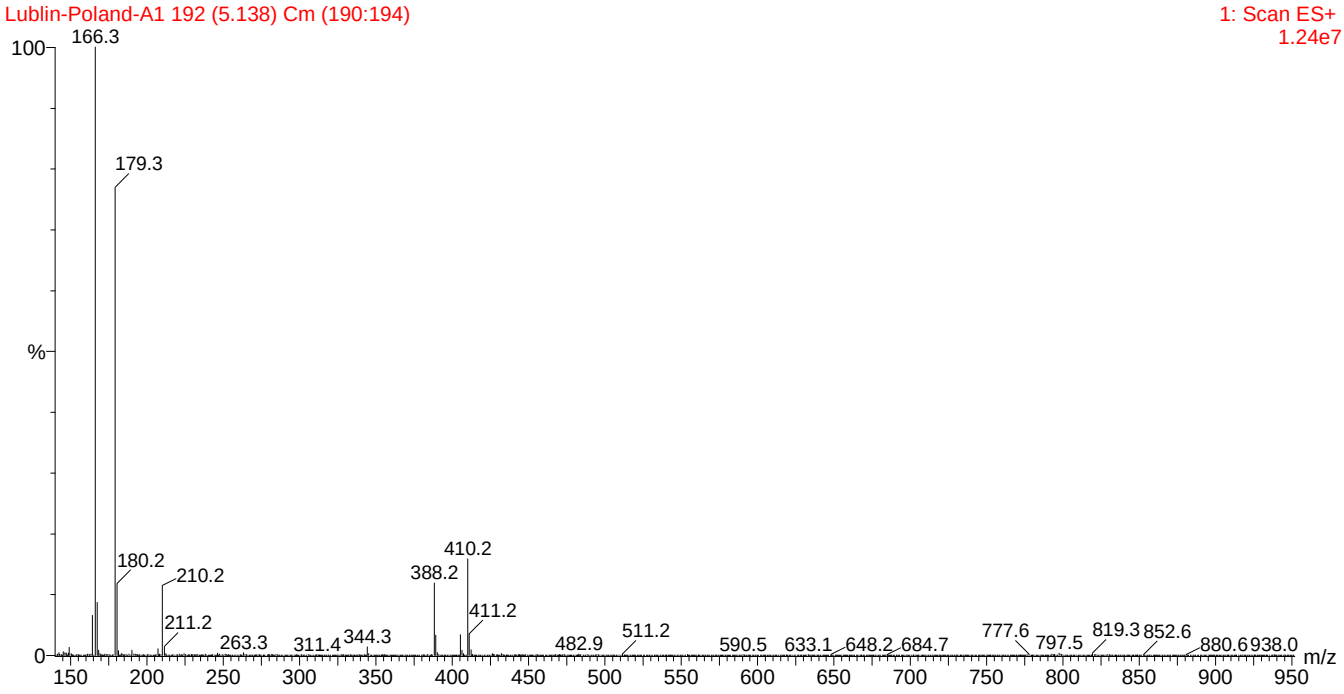

T26-A1 Sm (Mn, 1x1)
3: Diode Array
TIC
2.92e7
Area
Time Height Area Area%
4.65 951793 57096.93 2.14
4.76 7355692 370583.41 13.87
5.01 30791024 1872746.00 70.10
5.12 1048395 83835.58 3.14
5.31 4539188 228104.41 8.54
5.50 1259894 59102.01 2.21
5.01
268.0
1872746
4.76
266.0
370583
5.31
272.0
228104
5{6}a
Team 26 (Resin I)
Exact Mass 387.15
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

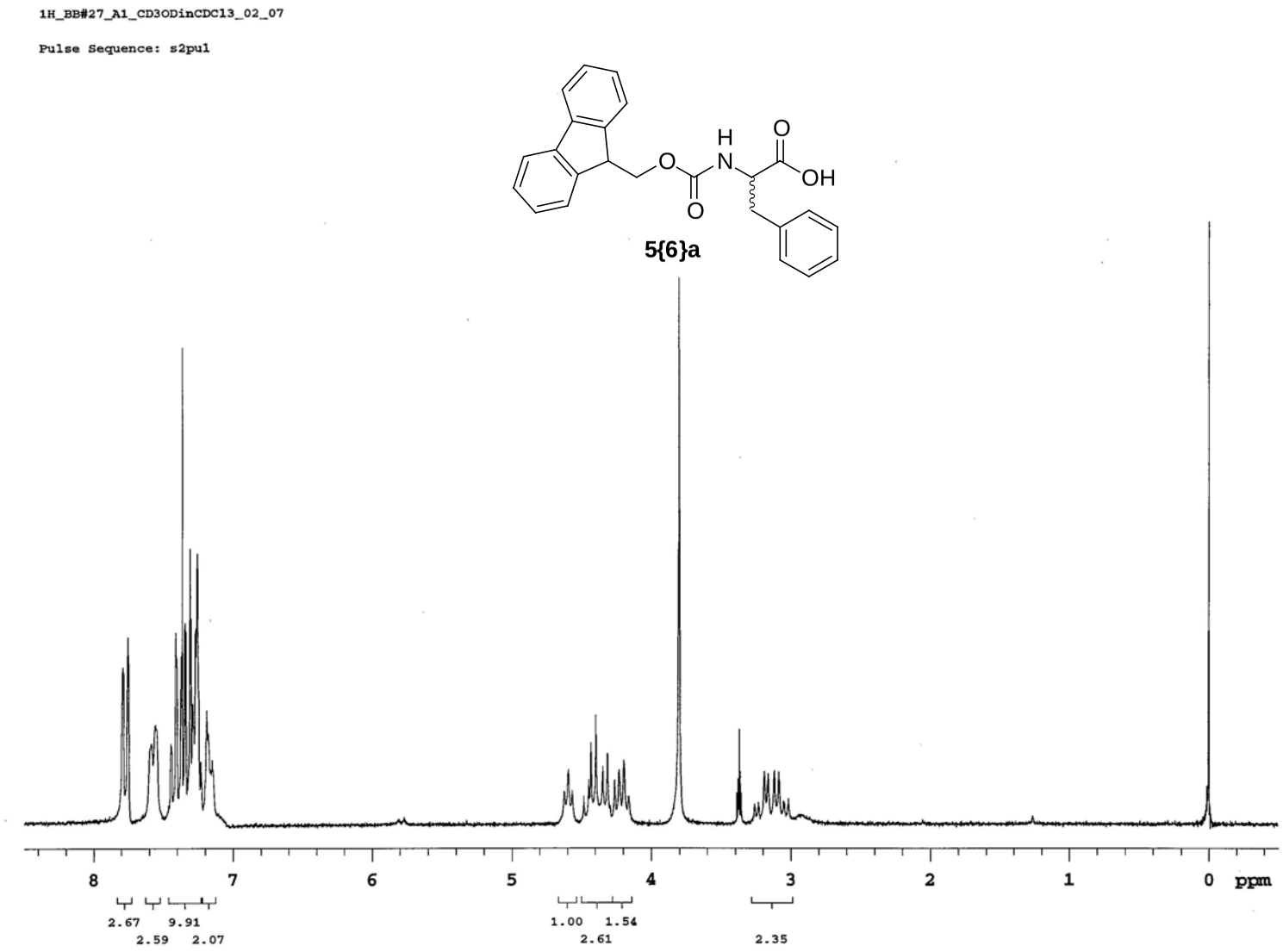

T26-A1 189 (5.058) Cm (187:191)
1: Scan ES+
1.93e7
100
%
0
166.2
179.2
210.1
211.3
263.1
344.2
388.1
410.1
426.1
505.4
533.0
591.2
608.2
665.4
775.2
792.2
819.3
900.9
939.0
1007.1
1021.2

T26-A1 180 (4.816) Cm (179:182)
1: Scan ES+
7.96e6
100
%
0
223.2
179.2
224.2
267.2
346.0
401.2
434.2
445.1
467.0
468.1
542.0
568.1
652.2
706.2
763.4
821.2
889.2
911.2
933.3
964.3
1004.2
200 300 400 500 600 700 800 900 1000
m/z

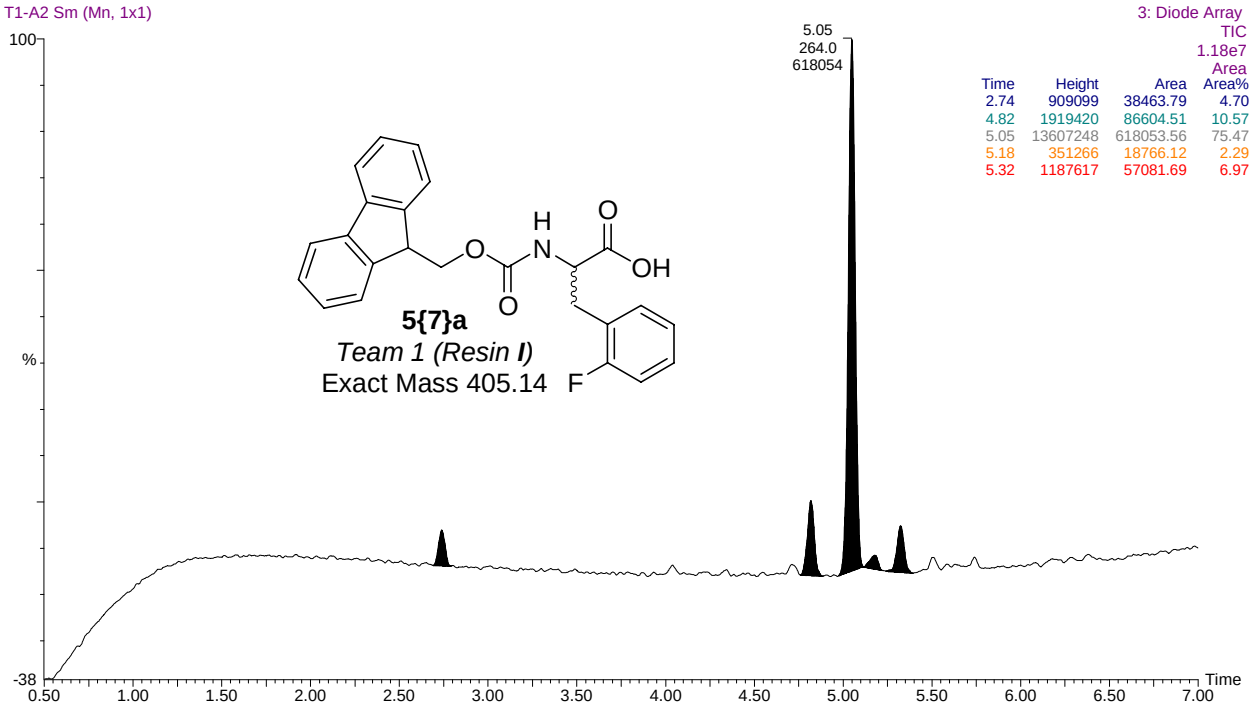
5{6}a

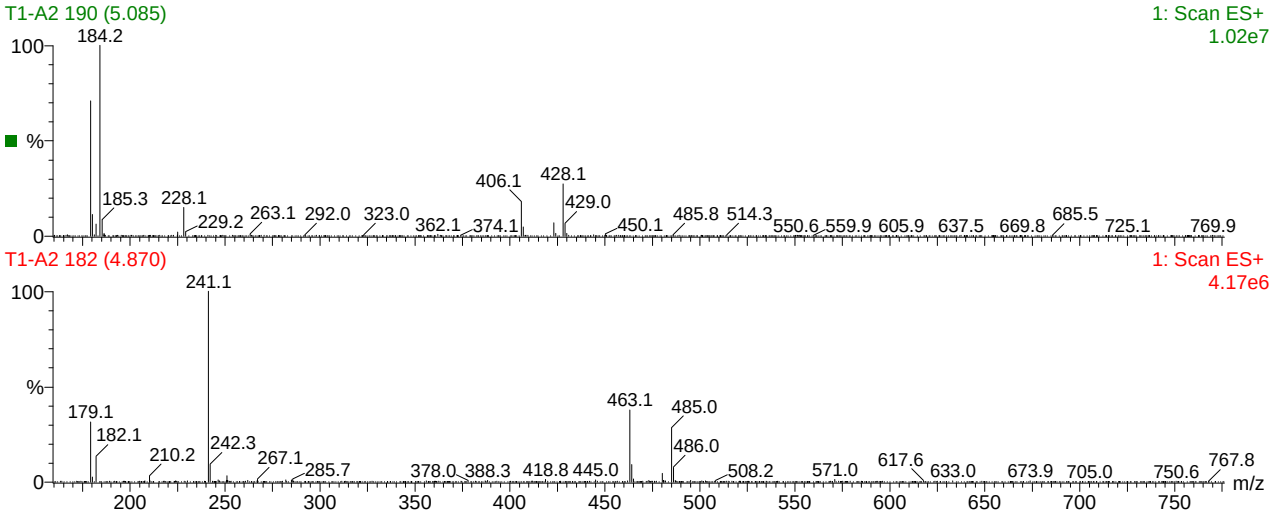

Lublin-Poland-A1 Sm (Mn, 1x1)
3: Diode Array
TIC
5.63e6
Area
Time Height Area Area%
5.10 7270317 302407.66 100.00
5.10
266.0
302408
100
%
-72
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
OH
O
5{6}a
Lublin (Resin II)
Exact Mass 387.15


Lublin-Poland-A1 192 (5.138) Cm (190:194)
1: Scan ES+
1.24e7
100
%
0
166.3
179.3
180.2
210.2
211.2
263.3
311.4
344.3
388.2
410.2
411.2
482.9
511.2
590.5
633.1
648.2
684.7
777.6
797.5
819.3
852.6
880.6
938.0
m/z
150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

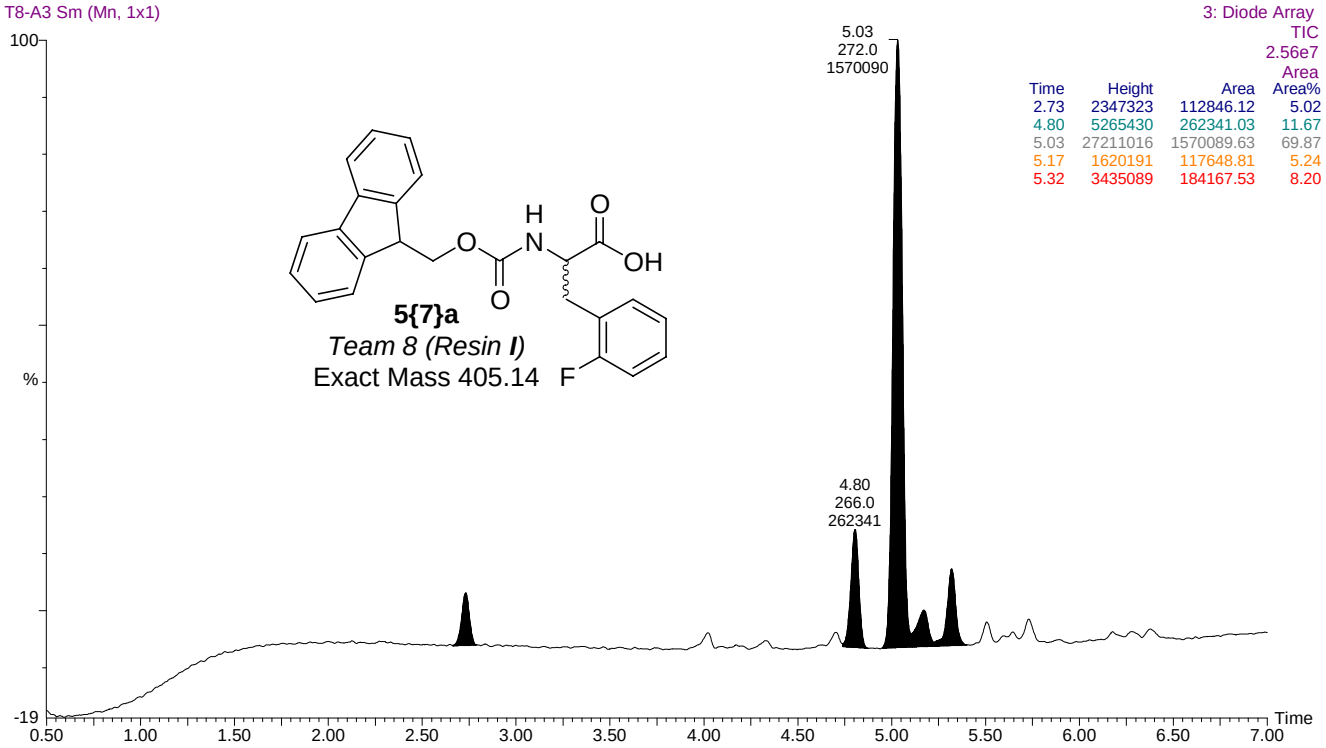

1H_BB#27_A1_CD3ODinCDCl3_02_07
Pulse Sequence: s2pul
H
N
O
O
O
OH
5{6}a
8
7
6
5
4
3
2
1
0
ppm
2.67
2.59
9.91
2.07
1.00
2.61
1.54
2.35

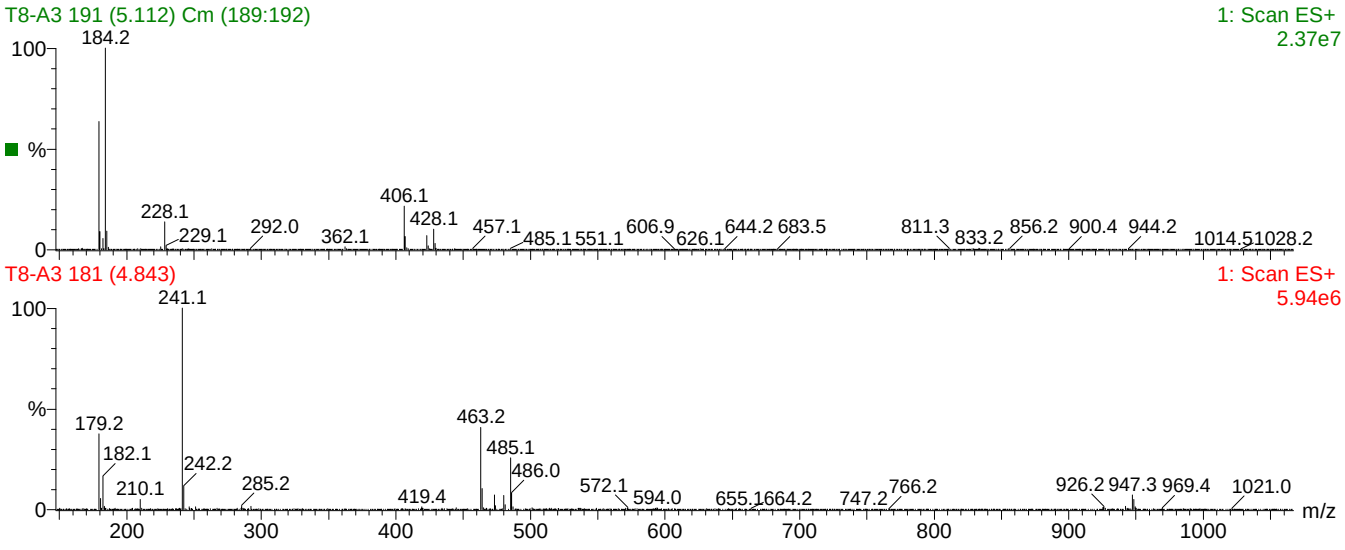
5{7}a


T1-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
1.18e7
Area
5.05
264.0
618054
Time Height Area Area%
2.74 909099 38463.79 4.70
4.82 1919420 86604.51 10.57
5.05 13607248 618053.56 75.47
5.18 351266 18766.12 2.29
5.32 1187617 57081.69 6.97
100
%
-38
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time
5{7}a
Team 1 (Resin I)
Exact Mass 405.14

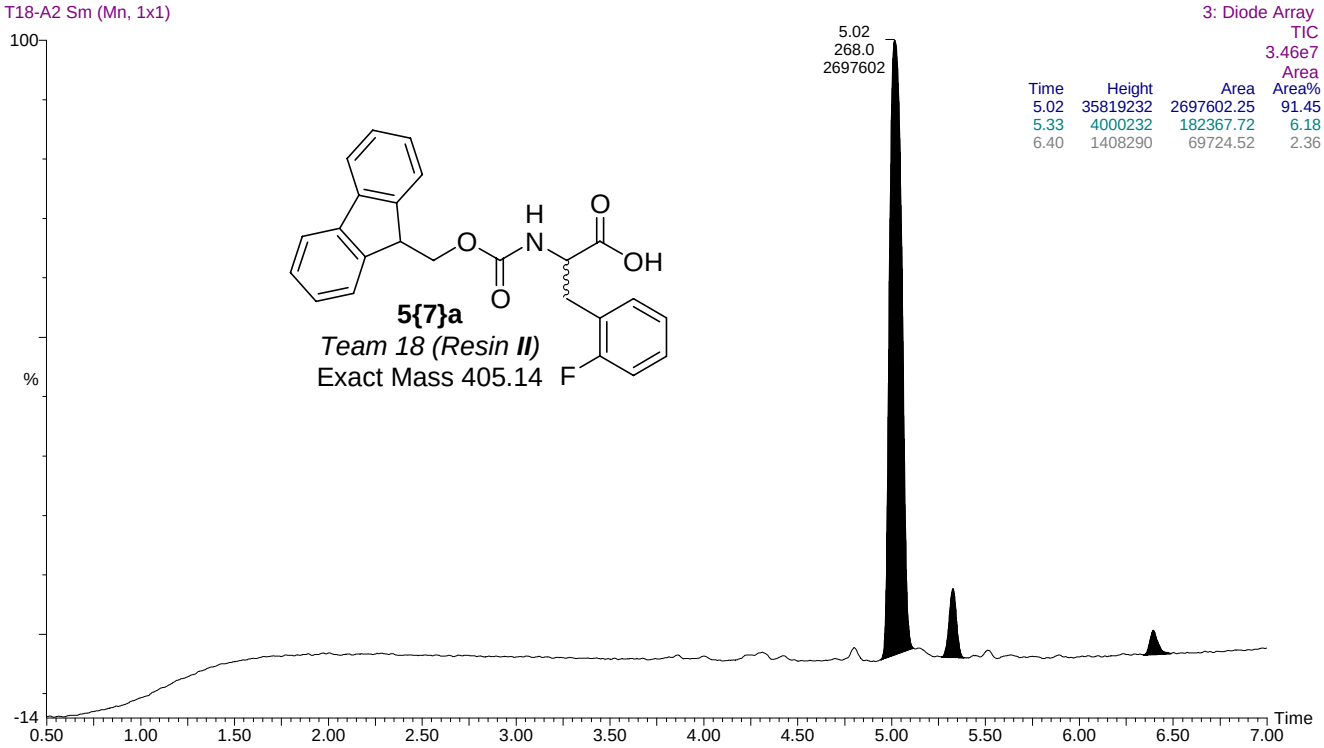

T1-A2 190 (5.085)
1: Scan ES+
1.02e7
100
%
0
184.2
185.3 228.1 229.2 263.1 292.0 323.0 362.1 374.1 406.1 428.1 429.0 450.1 485.8 514.3 550.6 559.9 605.9 637.5 669.8 685.5 725.1 769.9
T1-A2 182 (4.870)
1: Scan ES+
4.17e6
100
%
0
241.1
179.1 182.1 210.2 242.3 267.1 285.7 378.0 388.3 418.8 445.0 463.1 485.0 486.0 508.2 571.0 617.6 633.0 673.9 705.0 750.6 767.8
200 250 300 350 400 450 500 550 600 650 700 750
m/z

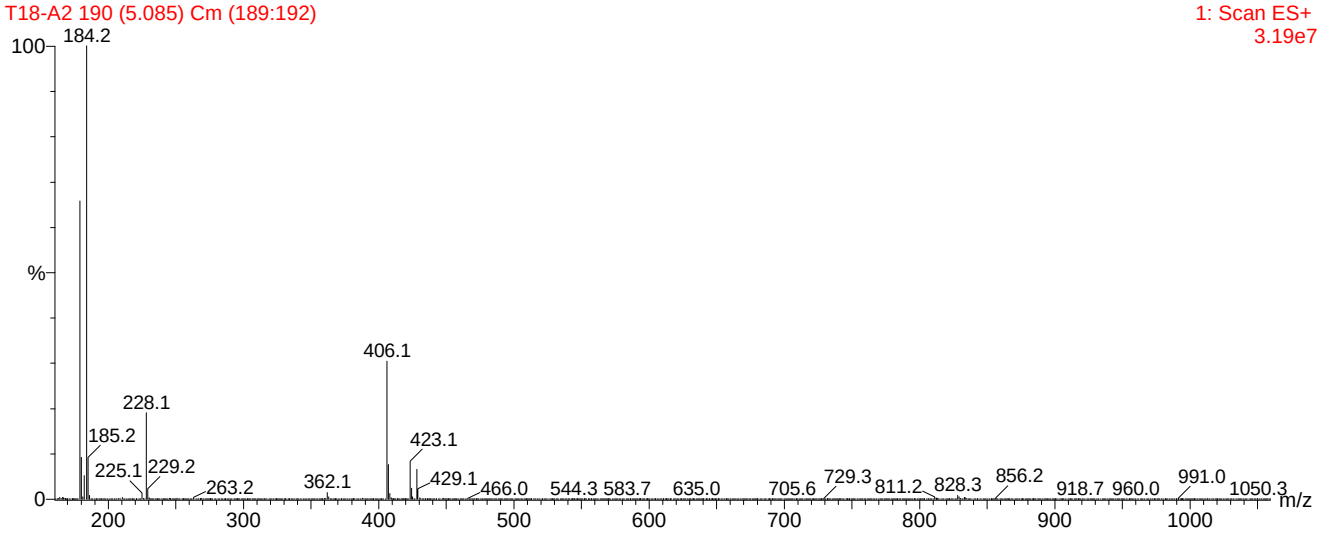
5{7}a


T8-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.56e7
Area
Time Height Area Area%
2.73 2347323 112846.12 5.02
4.80 5265430 262341.03 11.67
5.03 27211016 1570089.63 69.87
5.17 1620191 117648.81 5.24
5.32 3435089 184167.53 8.20
5.03
272.0
1570090
4.80
266.0
262341
5{7}a
Team 8 (Resin I)
Exact Mass 405.14
100
%
-19
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

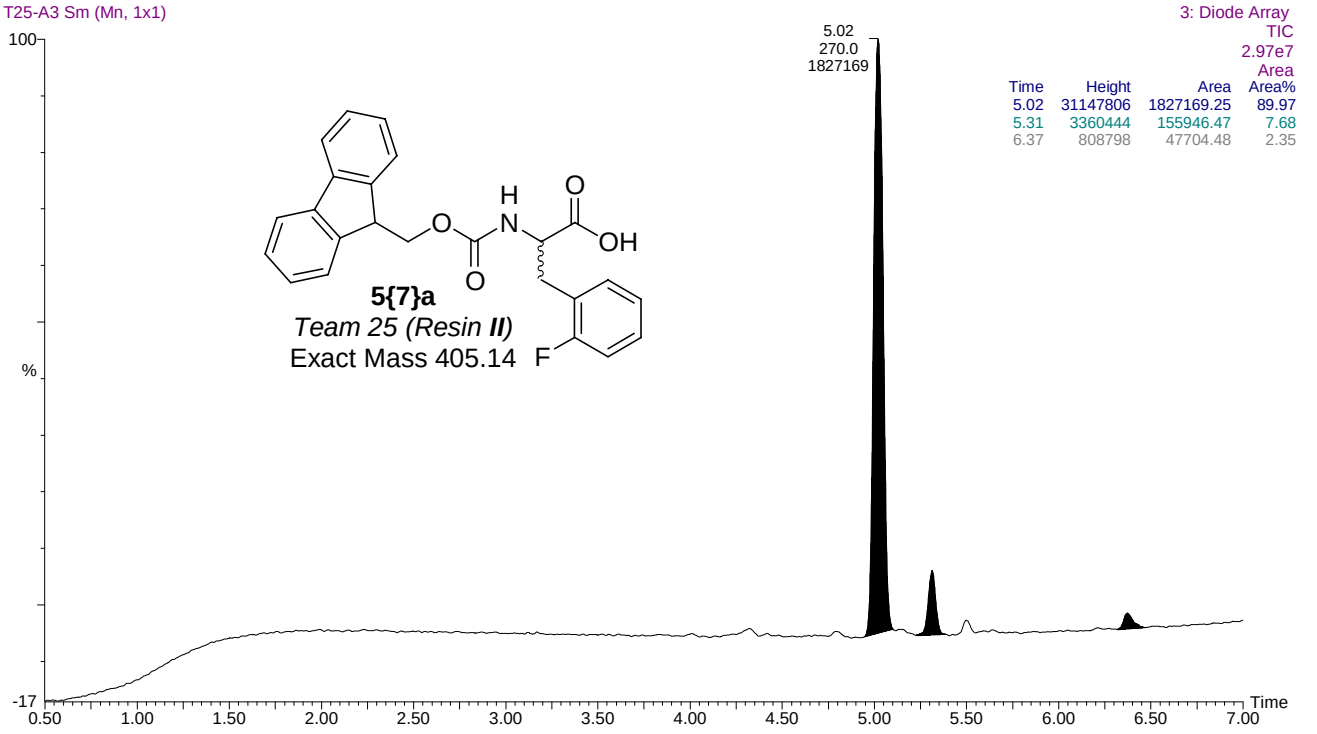

T8-A3 191 (5.112) Cm (189:192)
1: Scan ES+
2.37e7
184.2
228.1
229.1
292.0
362.1
406.1
428.1
457.1
485.1 551.1
606.9
626.1
644.2 683.5
811.3
833.2
856.2
900.4
944.2
1014.5 1028.2
T8-A3 181 (4.843)
1: Scan ES+
5.94e6
241.1
179.2
182.1
210.1
242.2
285.2
419.4
463.2
485.1
486.0
572.1
594.0
655.1 664.2
747.2
766.2
926.2 947.3 969.4
1021.0
100
%
0
200 300 400 500 600 700 800 900 1000
m/z

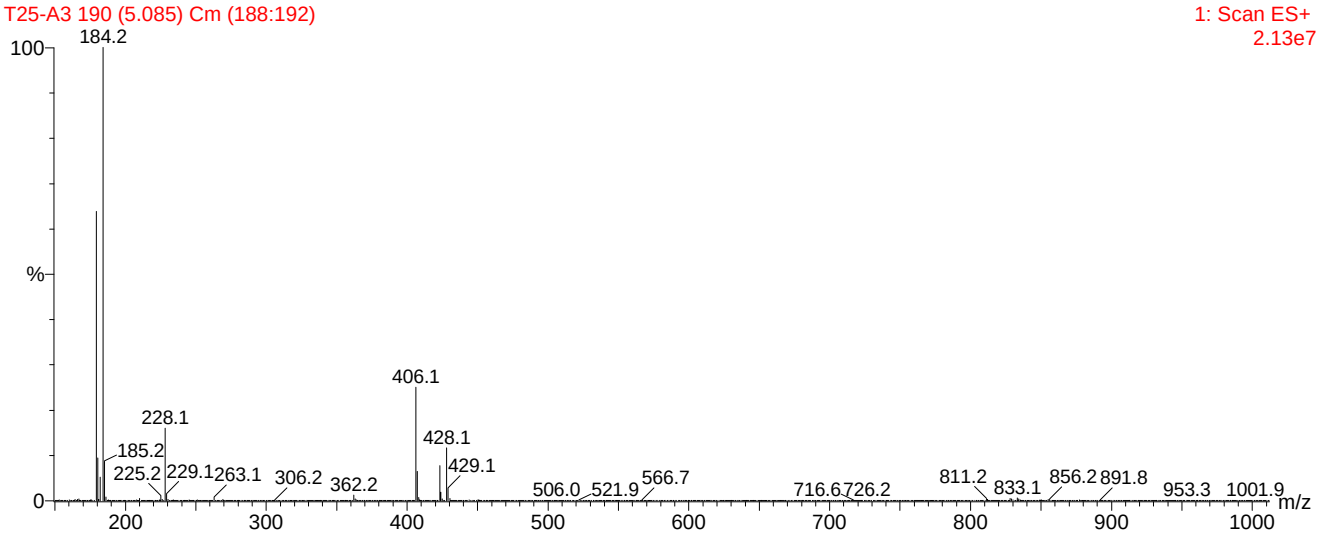
5{7}a


T18-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.46e7
Area
Time Height Area Area%
5.02 35819232 2697602.25 91.45
5.33 4000232 182367.72 6.18
6.40 1408290 69724.52 2.36
5.02
268.0
2697602
5{7}a
Team 18 (Resin II)
Exact Mass 405.14
100
%
-14
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time


T18-A2 190 (5.085) Cm (189:192)
1: Scan ES+
3.19e7
100
%
0
184.2
406.1
228.1
185.2
423.1
225.1
229.2
263.2
362.1
429.1
466.0
544.3 583.7
635.0
705.6
729.3
811.2
828.3
856.2
918.7 960.0
991.0
1050.3
200 300 400 500 600 700 800 900 1000
m/z

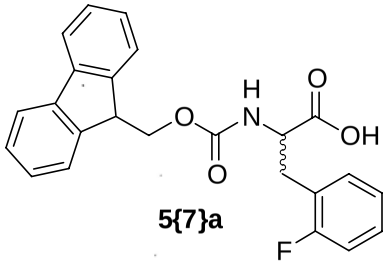
5{7}a


T25-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.97e7
Area
Time Height Area Area%
5.02 31147806 1827169.25 89.97
5.31 3360444 155946.47 7.68
6.37 808798 47704.48 2.35
5.02
270.0
1827169
5{7}a
Team 25 (Resin II)
Exact Mass 405.14
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

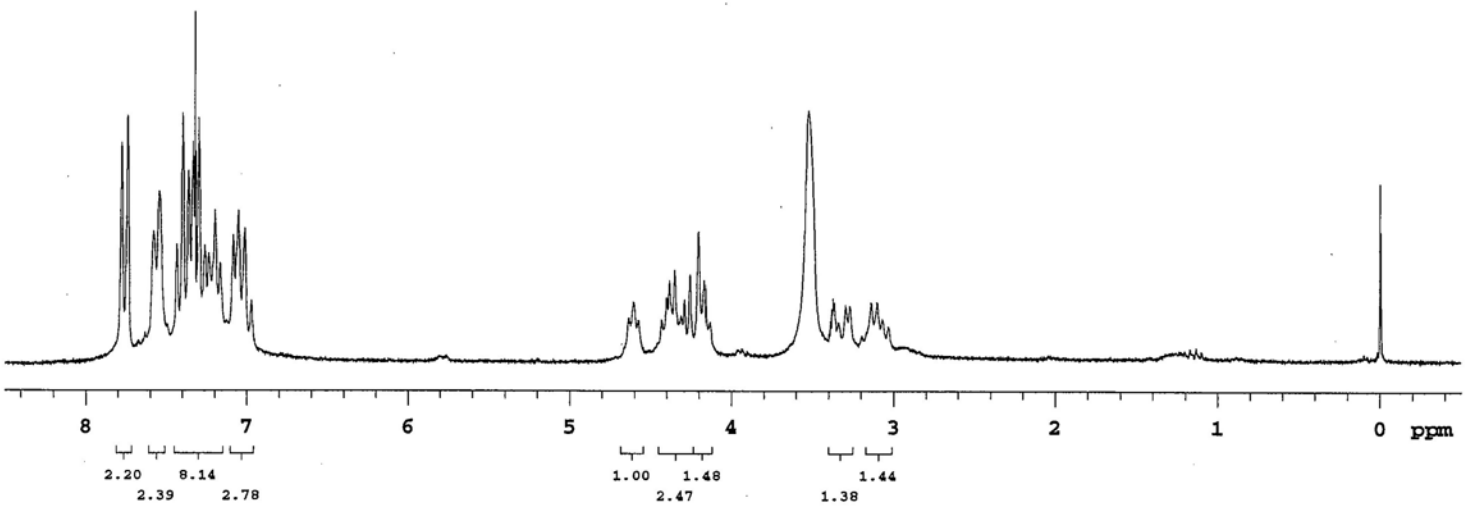

T25-A3 190 (5.085) Cm (188:192)
1: Scan ES+
2.13e7
100
%
0
184.2
228.1
185.2
225.2
229.1
263.1
306.2
362.2
406.1
428.1
429.1
506.0
521.9
566.7
716.6
726.2
811.2
833.1
856.2
891.8
953.3
1001.9
200 300 400 500 600 700 800 900 1000
m/z

1H_RR#27_A2_CD3ODinCDCl3_02_18_07

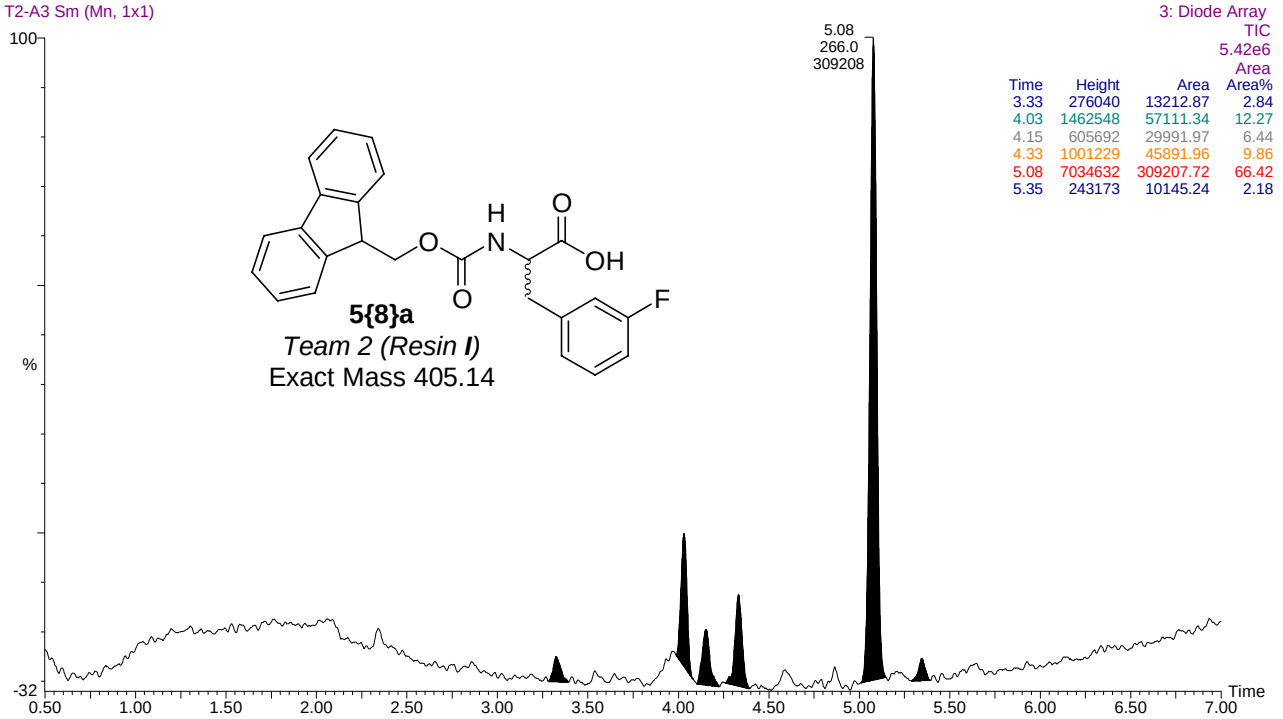
Pulse Sequence: s2pul

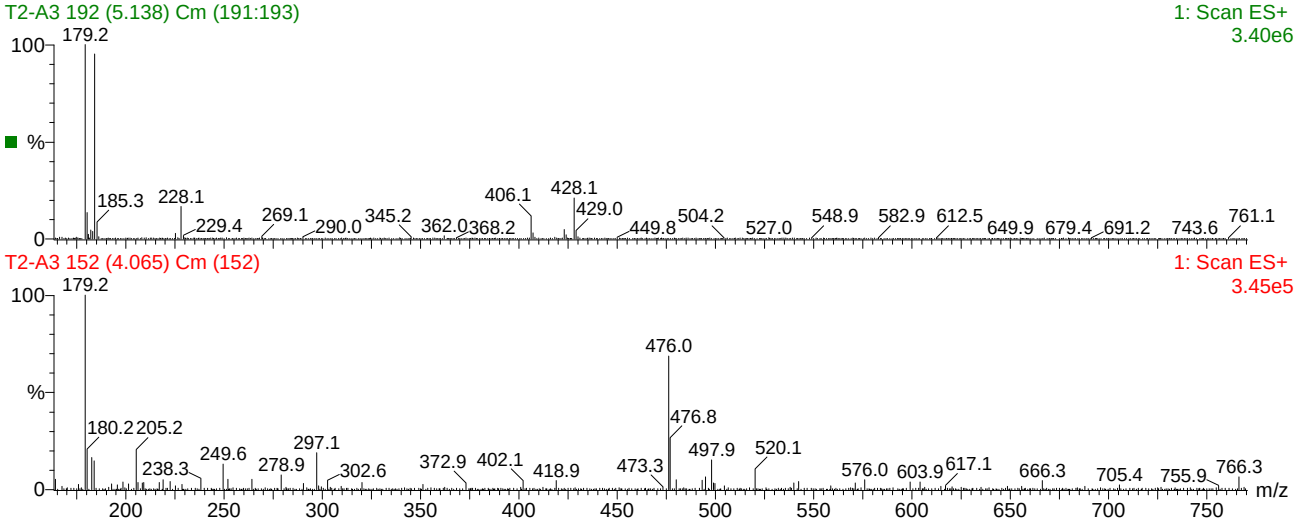


5{7}a

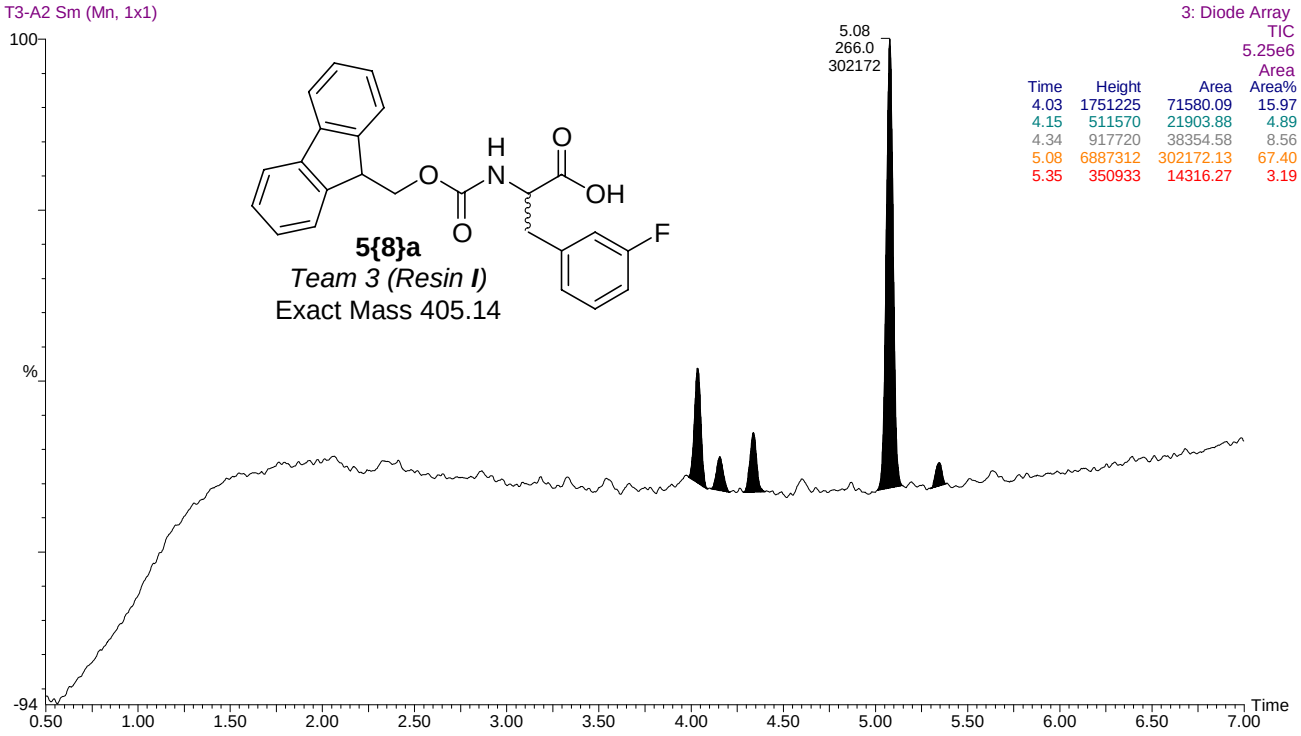


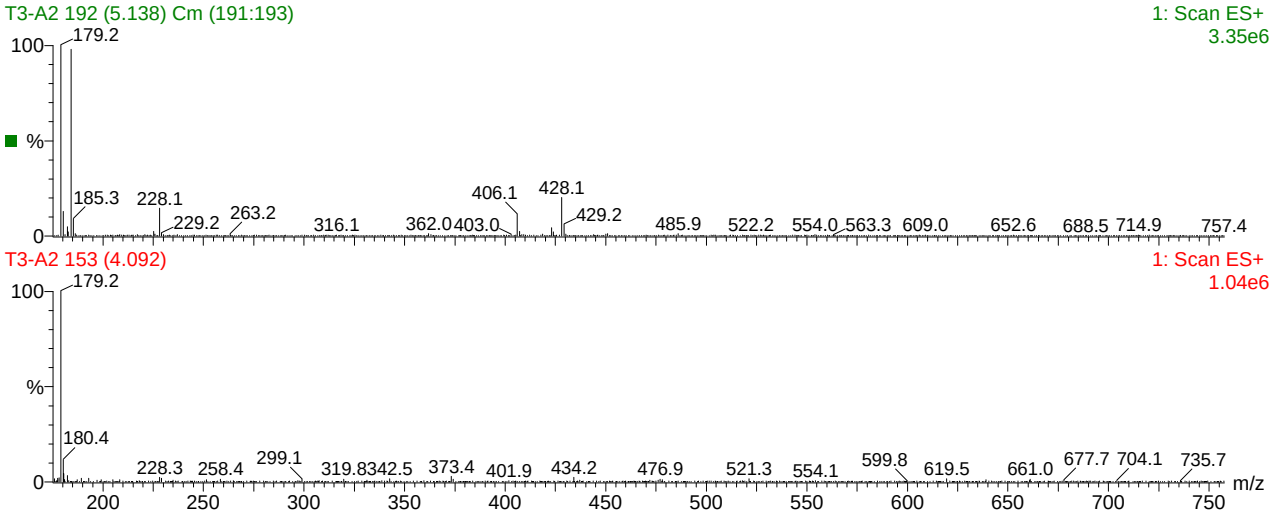
5{8}a


T2-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
5.42e6
Area
Time Height Area Area%
3.33 276040 13212.87 2.84
4.03 1462548 57111.34 12.27
4.15 605692 29991.97 6.44
4.33 1001229 45891.96 9.86
5.08 7034632 309207.72 66.42
5.35 243173 10145.24 2.18
5.08
266.0
309208
100
%
-32
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
O
OH
F
5{8}a
Team 2 (Resin I)
Exact Mass 405.14

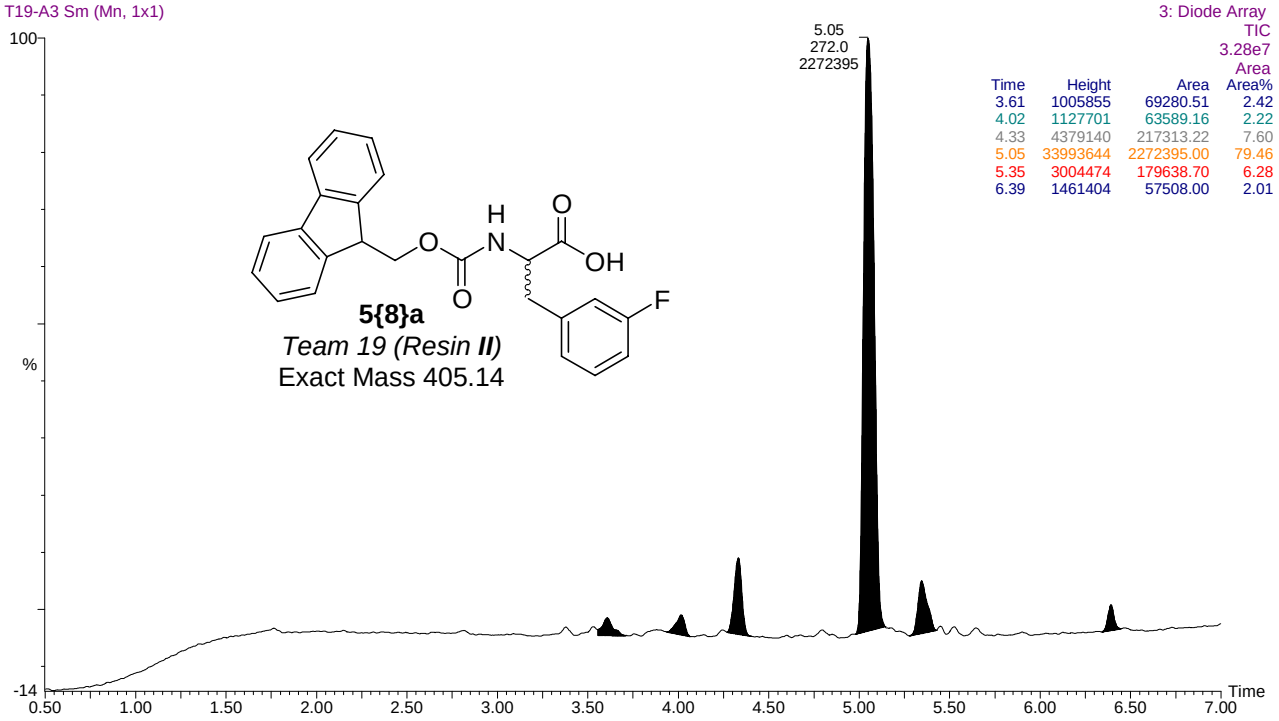

T2-A3 192 (5.138) Cm (191:193)
1: Scan ES+
3.40e6
100
%
0
179.2
185.3
228.1
229.4
269.1
290.0
345.2
362.0
368.2
406.1
428.1
429.0
449.8
504.2
527.0
548.9
582.9
612.5
649.9
679.4
691.2
743.6
761.1
T2-A3 152 (4.065) Cm (152)
1: Scan ES+
3.45e5
100
%
0
179.2
180.2
205.2
238.3
249.6
278.9
297.1
302.6
372.9
402.1
418.9
473.3
476.0
476.8
497.9
520.1
576.0
603.9
617.1
666.3
705.4
755.9
766.3
200 250 300 350 400 450 500 550 600 650 700 750
m/z

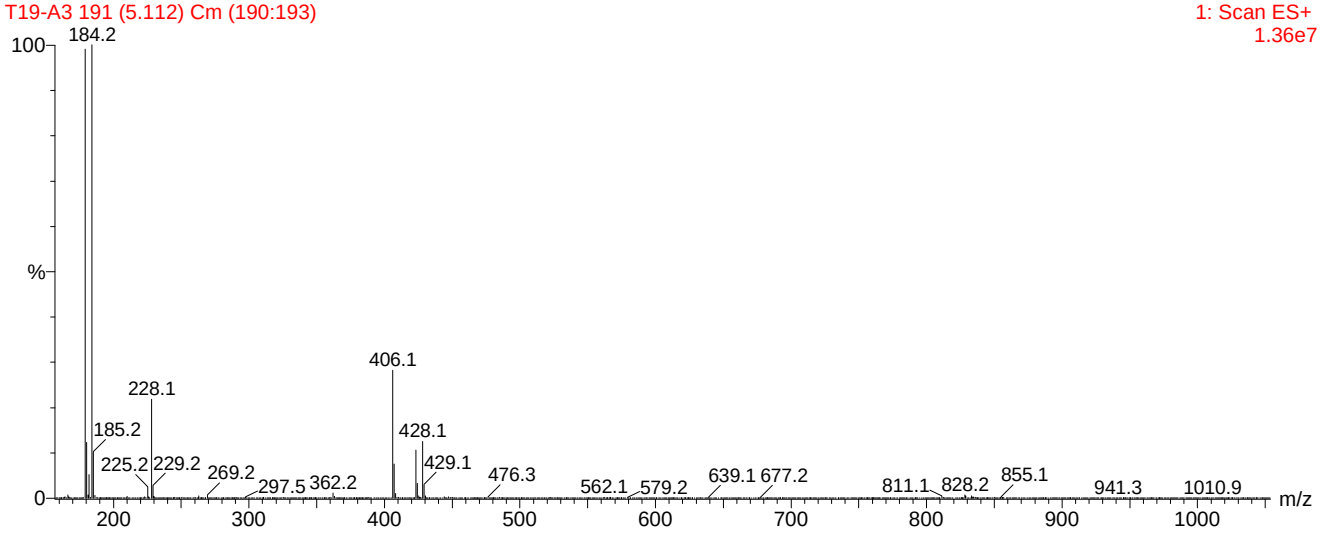
5{8}a


T3-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
5.25e6
Area
Time Height Area Area%
4.03 1751225 71580.09 15.97
4.15 511570 21903.88 4.89
4.34 917720 38354.58 8.56
5.08 6887312 302172.13 67.40
5.35 350933 14316.27 3.19
5.08
266.0
302172
5{8}a
Team 3 (Resin I)
Exact Mass 405.14
100
%
-94
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time

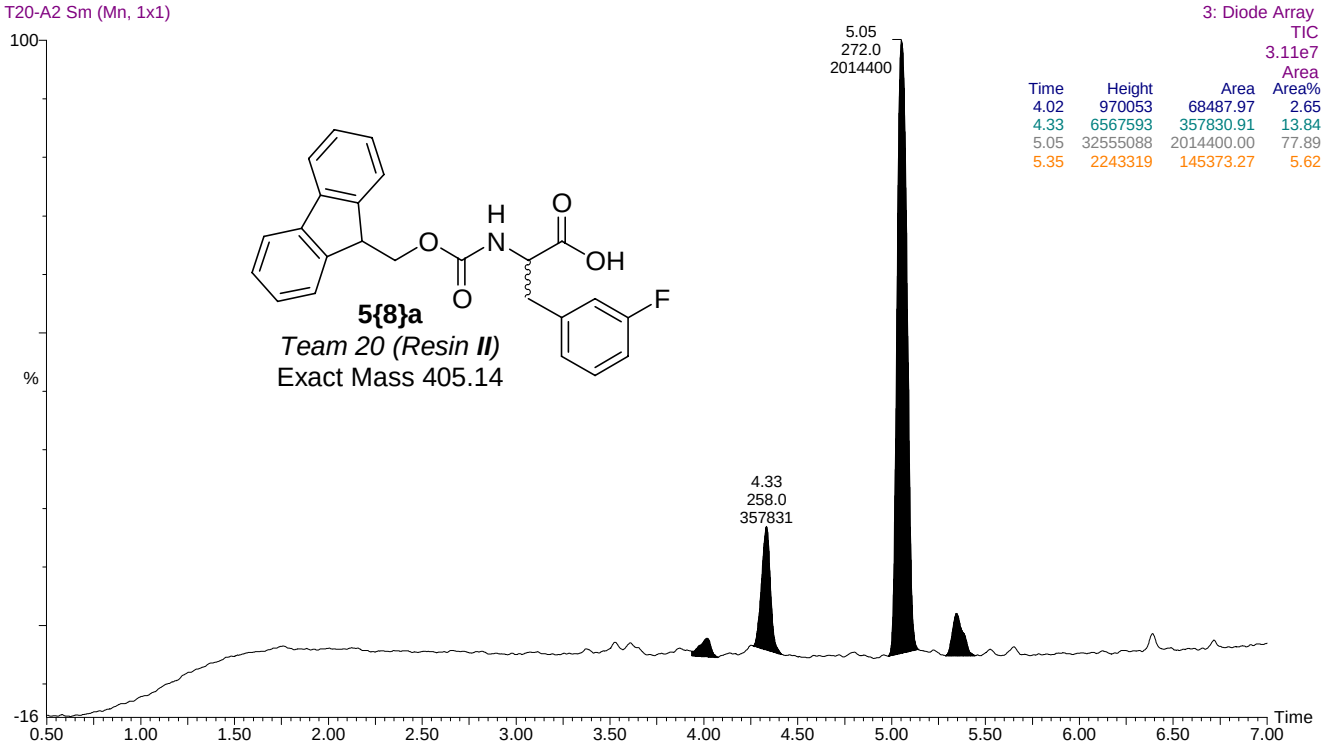

T3-A2 192 (5.138) Cm (191:193)
1: Scan ES+
3.35e6
100
%
0
179.2
185.3 228.1 229.2 263.2 316.1 362.0 403.0 406.1 428.1 429.2 485.9 522.2 554.0 563.3 609.0 652.6 688.5 714.9 757.4
T3-A2 153 (4.092)
1: Scan ES+
1.04e6
100
%
0
179.2
180.4
228.3 258.4 299.1 319.8 342.5 373.4 401.9 434.2 476.9 521.3 554.1 599.8 619.5 661.0 677.7 704.1 735.7
200 250 300 350 400 450 500 550 600 650 700 750
m/z

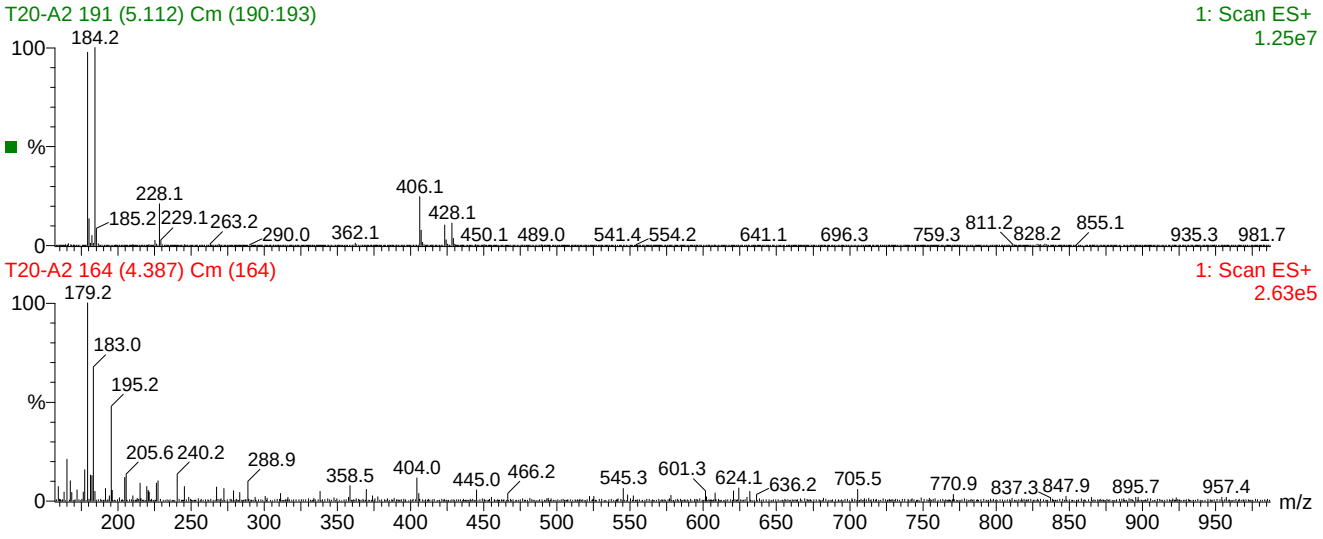
5{8}a


T19-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.28e7
Area
Time Height Area Area%
3.61 1005855 69280.51 2.42
4.02 1127701 63589.16 2.22
4.33 4379140 217313.22 7.60
5.05 33993644 2272395.00 79.46
5.35 3004474 179638.70 6.28
6.39 1461404 57508.00 2.01
5.05
272.0
2272395
100
%
-14
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
O
OH
F
5{8}a
Team 19 (Resin II)
Exact Mass 405.14


T19-A3 191 (5.112) Cm (190:193)
1: Scan ES+
1.36e7
100
%
0
184.2
228.1
185.2
225.2
229.2
269.2
297.5
362.2
406.1
428.1
429.1
476.3
562.1
579.2
639.1
677.2
811.1
828.2
855.1
941.3
1010.9
200 300 400 500 600 700 800 900 1000
m/z

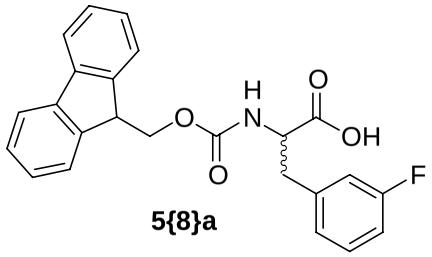
5{8}a


T20-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.11e7
Area
Time Height Area Area%
4.02 970053 68487.97 2.65
4.33 6567593 357830.91 13.84
5.05 32555088 2014400.00 77.89
5.35 2243319 145373.27 5.62
5.05
272.0
2014400
4.33
258.0
357831
5{8}a
Team 20 (Resin II)
Exact Mass 405.14
100
%
-16
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

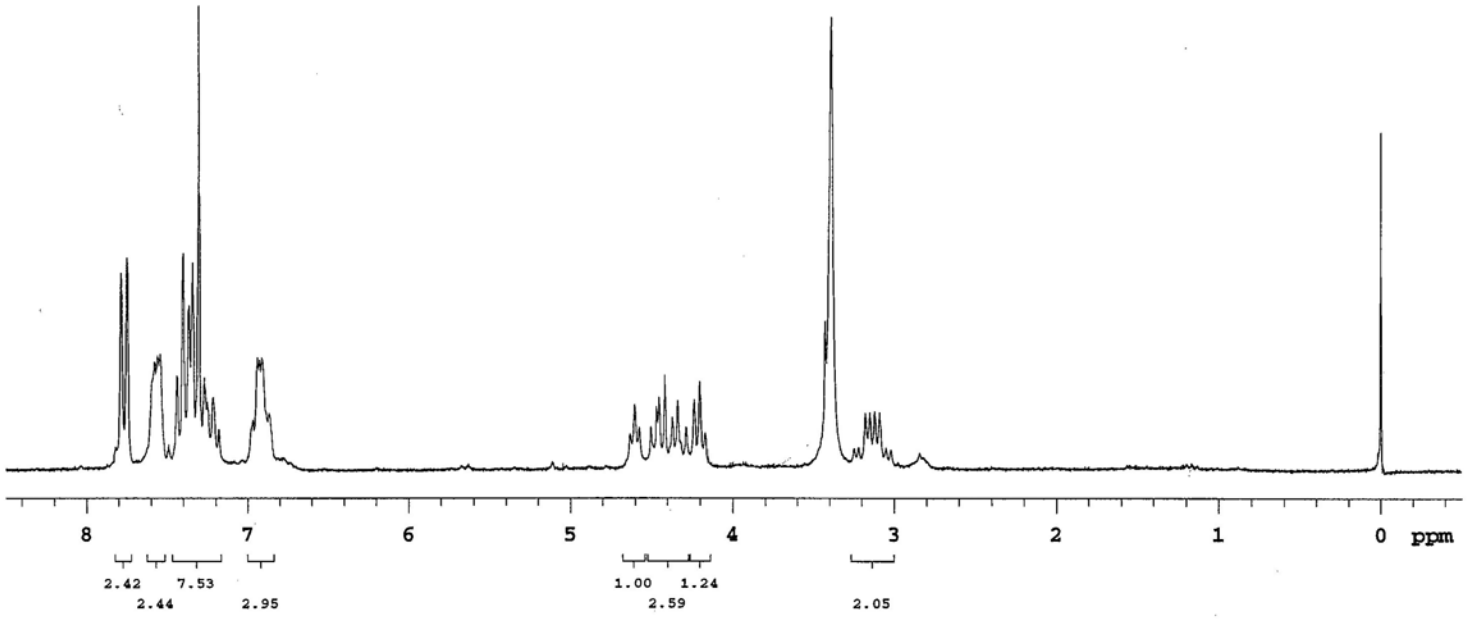

T20-A2 191 (5.112) Cm (190:193)
1: Scan ES+
1.25e7
100
%
0
184.2
228.1
185.2
229.1
263.2
290.0
362.1
406.1
428.1
450.1
489.0
541.4
554.2
641.1
696.3
759.3
811.2
828.2
855.1
935.3
981.7
T20-A2 164 (4.387) Cm (164)
1: Scan ES+
2.63e5
100
%
0
179.2
183.0
195.2
205.6
240.2
288.9
358.5
404.0
445.0
466.2
545.3
601.3
624.1
636.2
705.5
770.9
837.3
847.9
895.7
957.4
m/z
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

1H_RR#40_A1_CD3ODinCDCl3_03_07

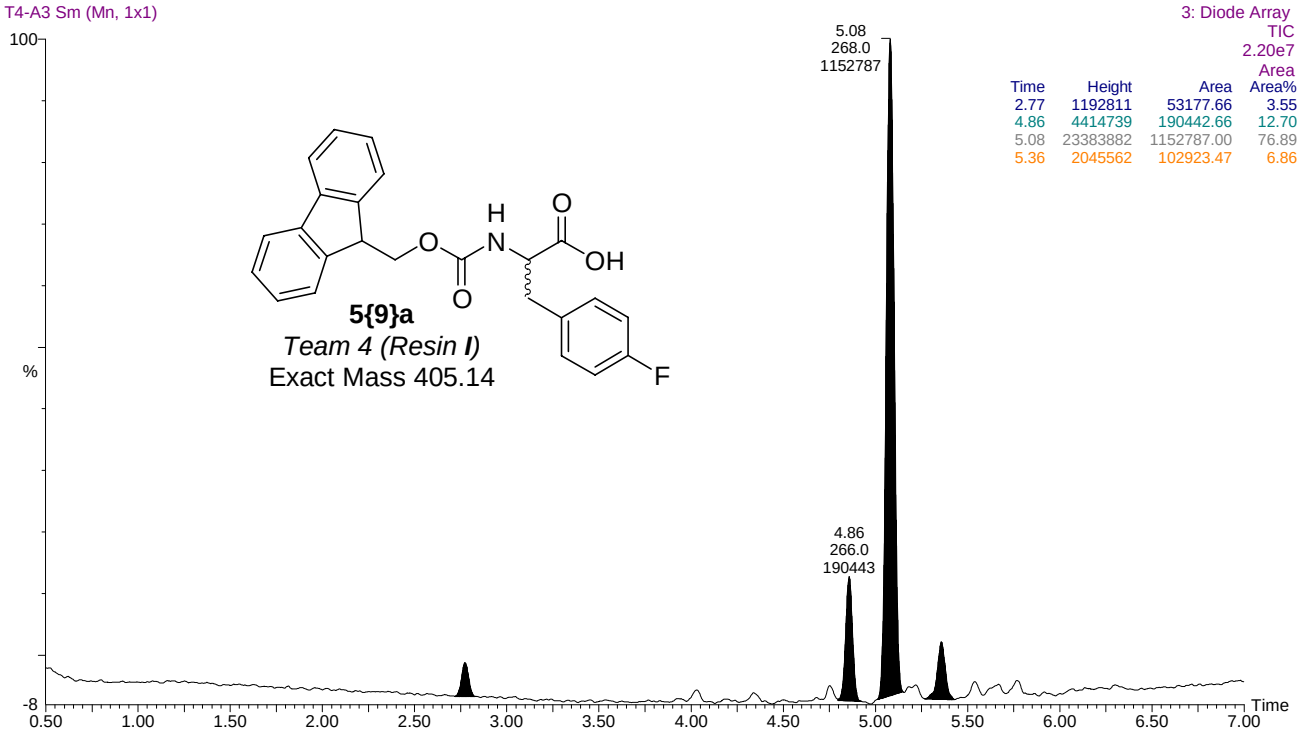
Pulse Sequence: s2pul

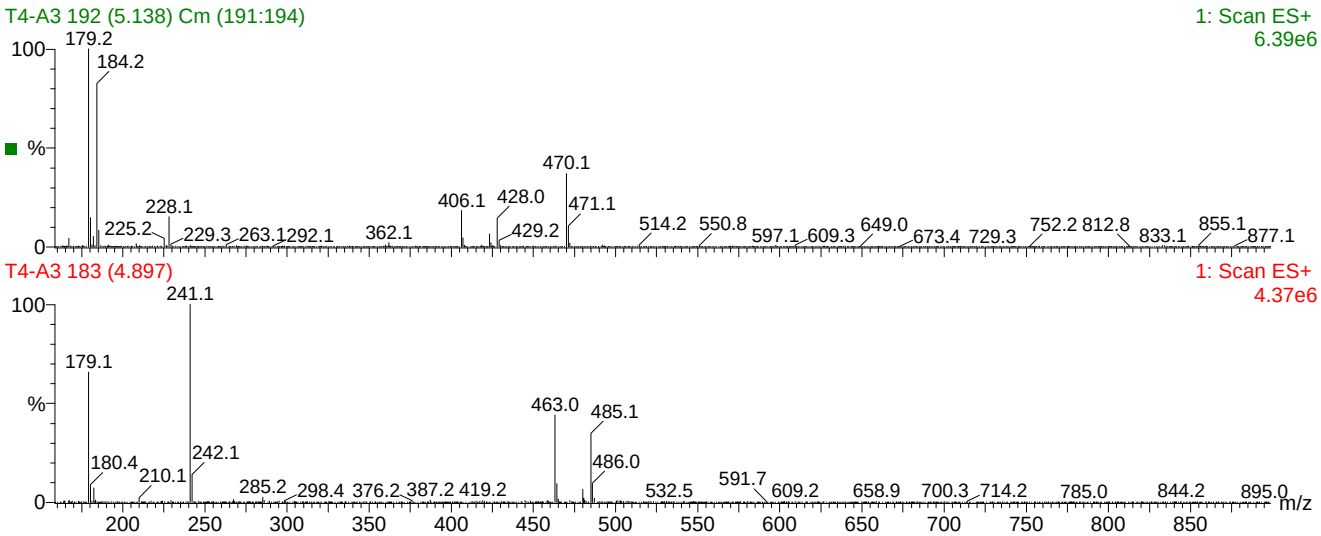


5{8}a

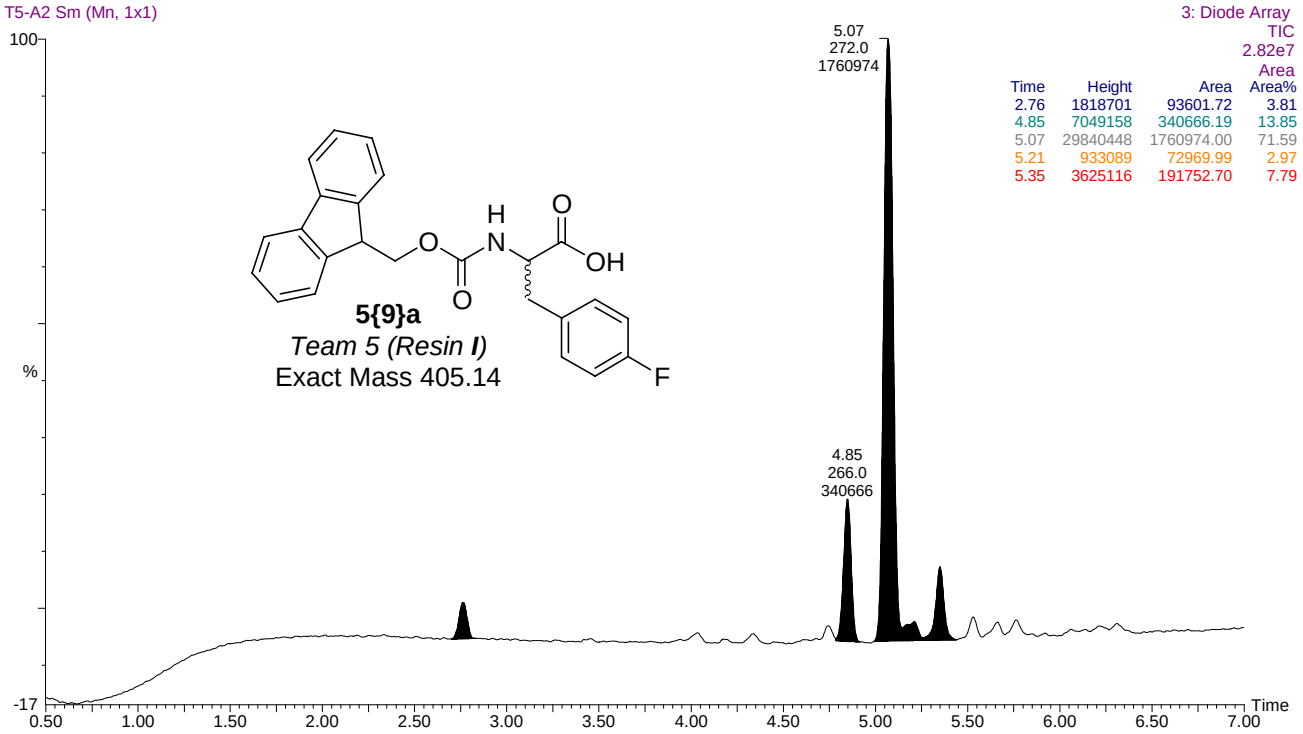


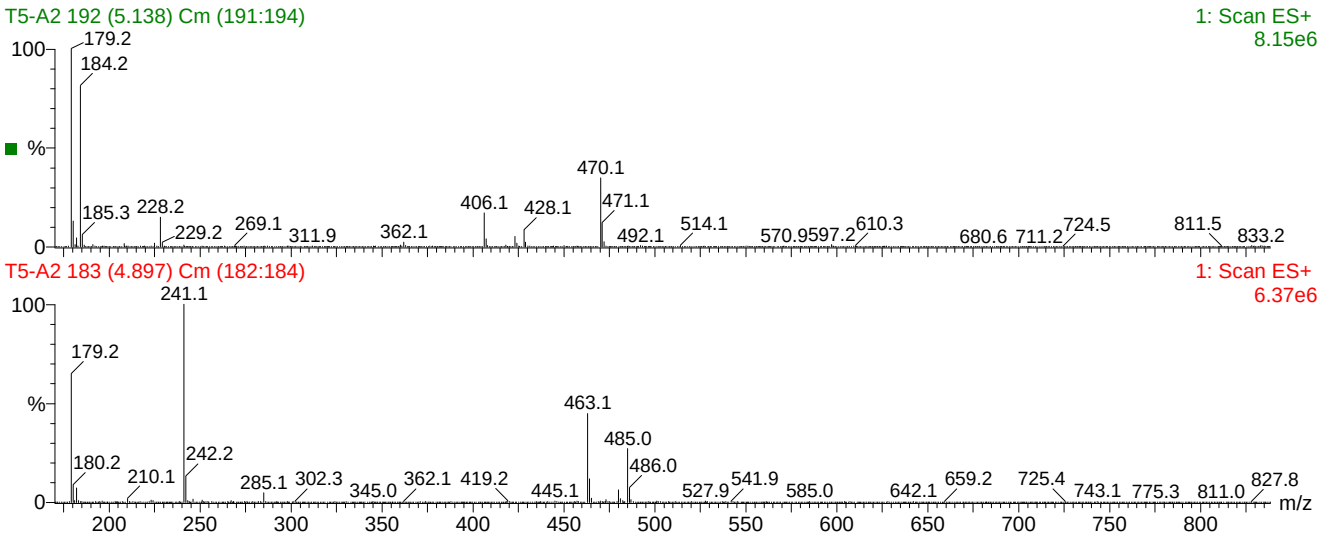
5{9}a


T4-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.20e7
Area
Time Height Area Area%
2.77 1192811 53177.66 3.55
4.86 4414739 190442.66 12.70
5.08 23383882 1152787.00 76.89
5.36 2045562 102923.47 6.86
5.08
268.0
1152787
4.86
266.0
190443
5{9}a
Team 4 (Resin I)
Exact Mass 405.14
Time

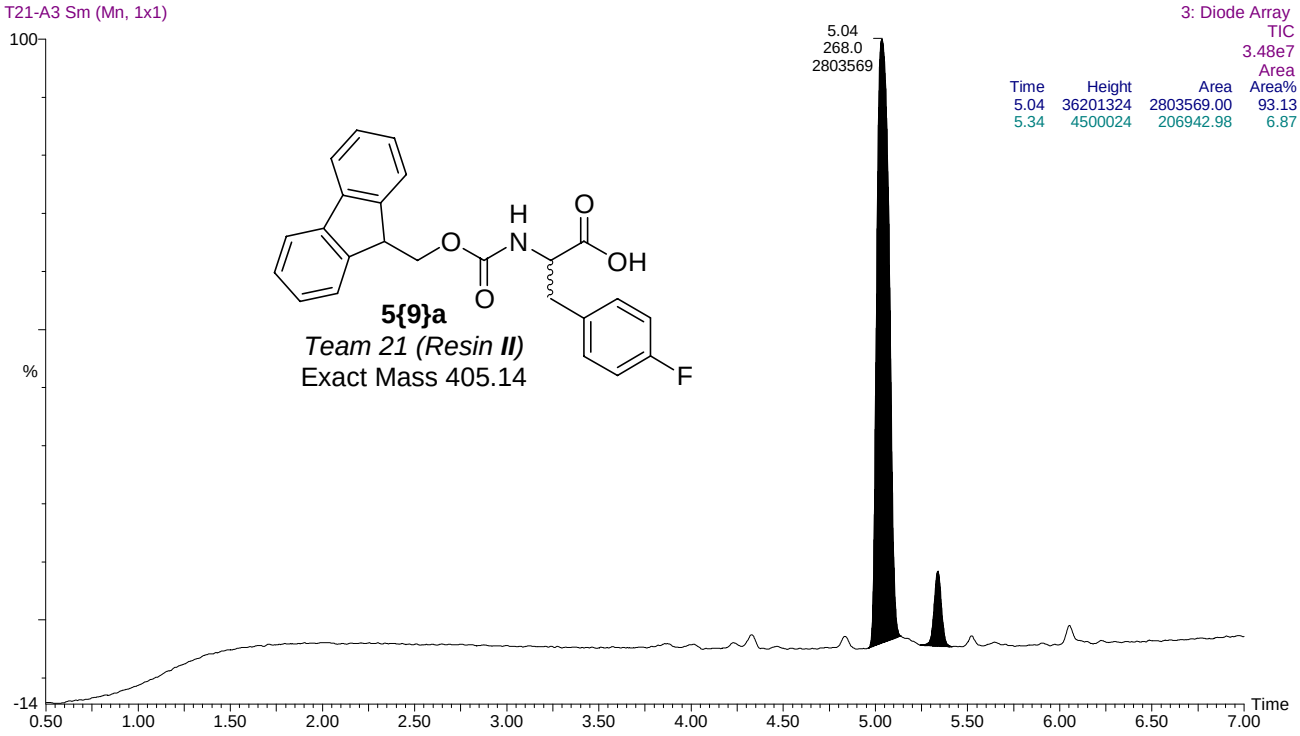

T4-A3 192 (5.138) Cm (191:194)
1: Scan ES+
6.39e6
T4-A3 183 (4.897)
1: Scan ES+
4.37e6
m/z

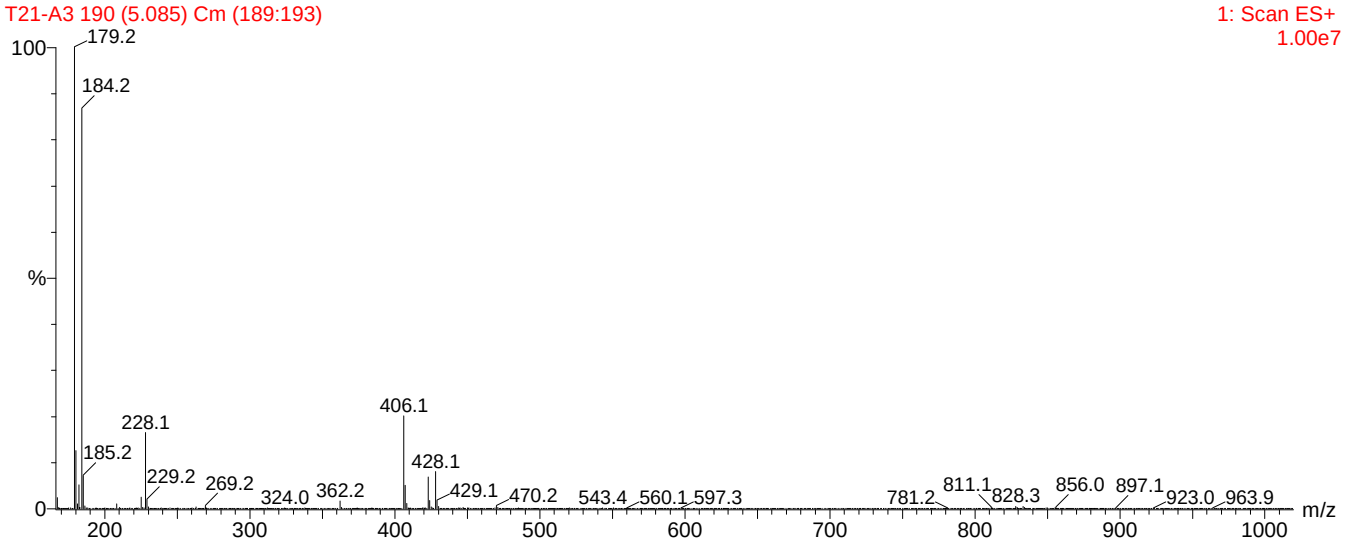
5{9}a


T5-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.82e7
Area
Time Height Area Area%
2.76 1818701 93601.72 3.81
4.85 7049158 340666.19 13.85
5.07 29840448 1760974.00 71.59
5.21 933089 72969.99 2.97
5.35 3625116 191752.70 7.79
5.07
272.0
1760974
4.85
266.0
340666
5{9}a
Team 5 (Resin I)
Exact Mass 405.14
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

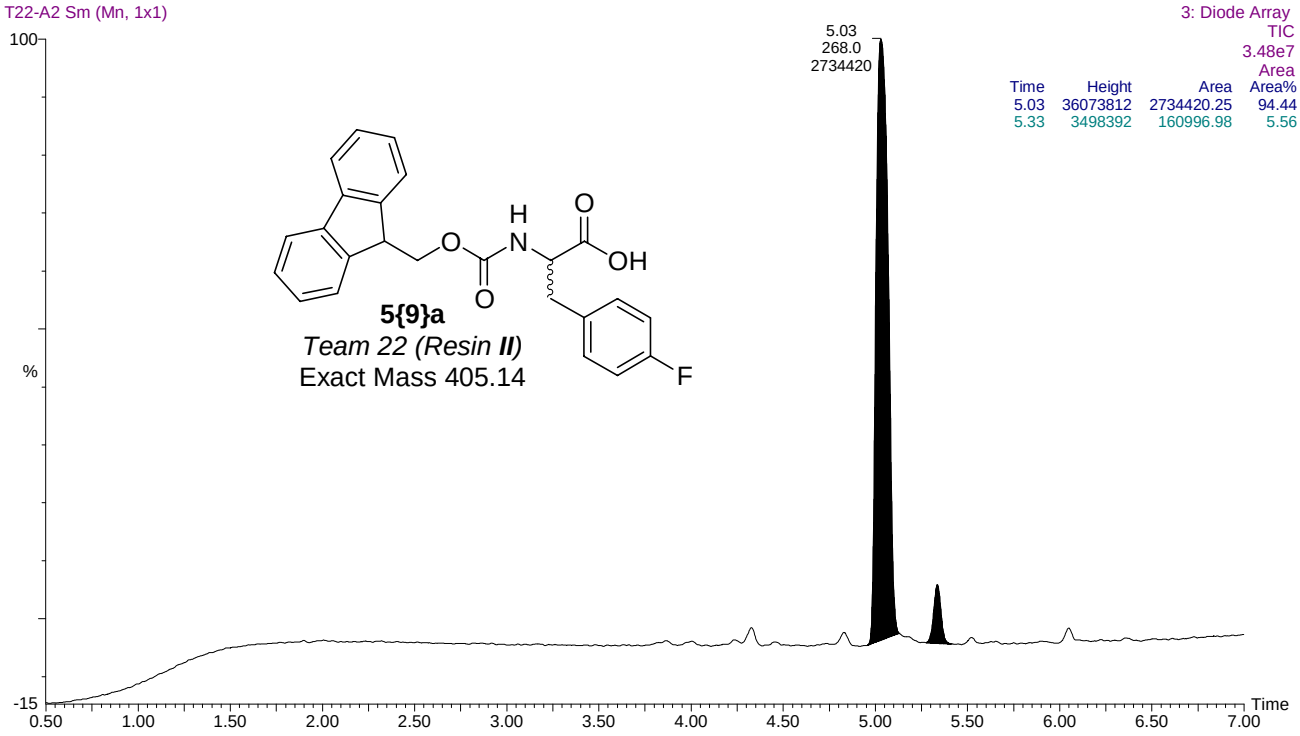

T5-A2 192 (5.138) Cm (191:194)
1: Scan ES+
8.15e6
100
%
0
179.2
184.2
185.3
228.2
229.2
269.1
311.9
362.1
406.1
428.1
470.1
471.1
492.1
514.1
570.9597.2
610.3
680.6
711.2
724.5
811.5
833.2
T5-A2 183 (4.897) Cm (182:184)
1: Scan ES+
6.37e6
100
%
0
241.1
179.2
180.2
210.1
242.2
285.1
302.3
345.0
362.1
419.2
445.1
463.1
485.0
486.0
527.9
541.9
585.0
642.1
659.2
725.4
743.1
775.3
811.0
827.8
200 250 300 350 400 450 500 550 600 650 700 750 800
m/z

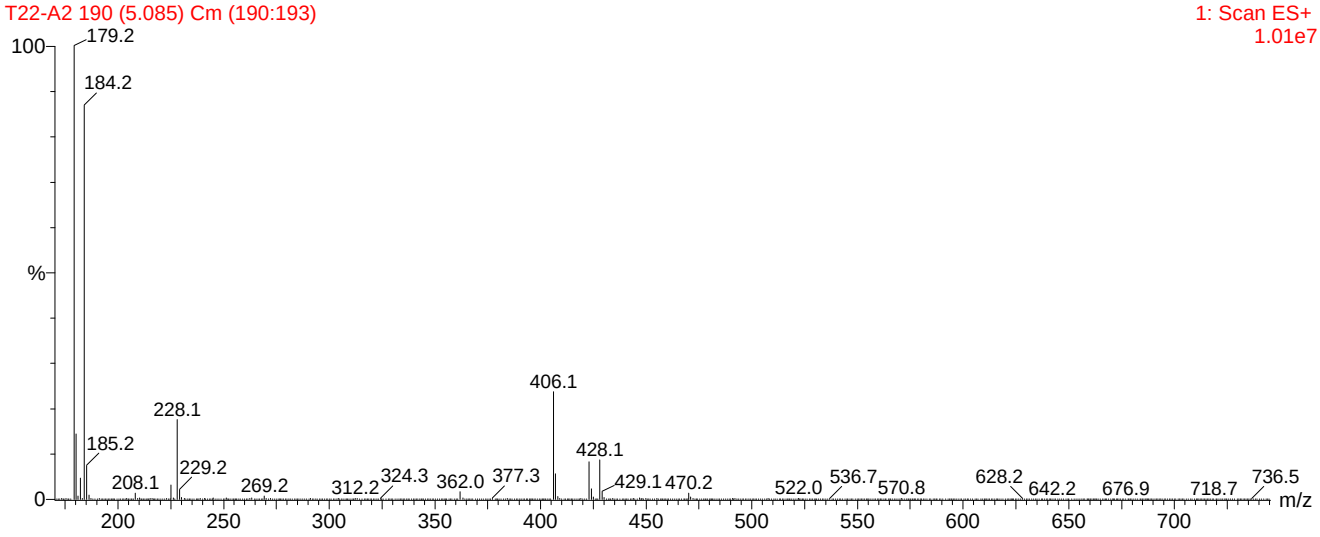
5{9}a

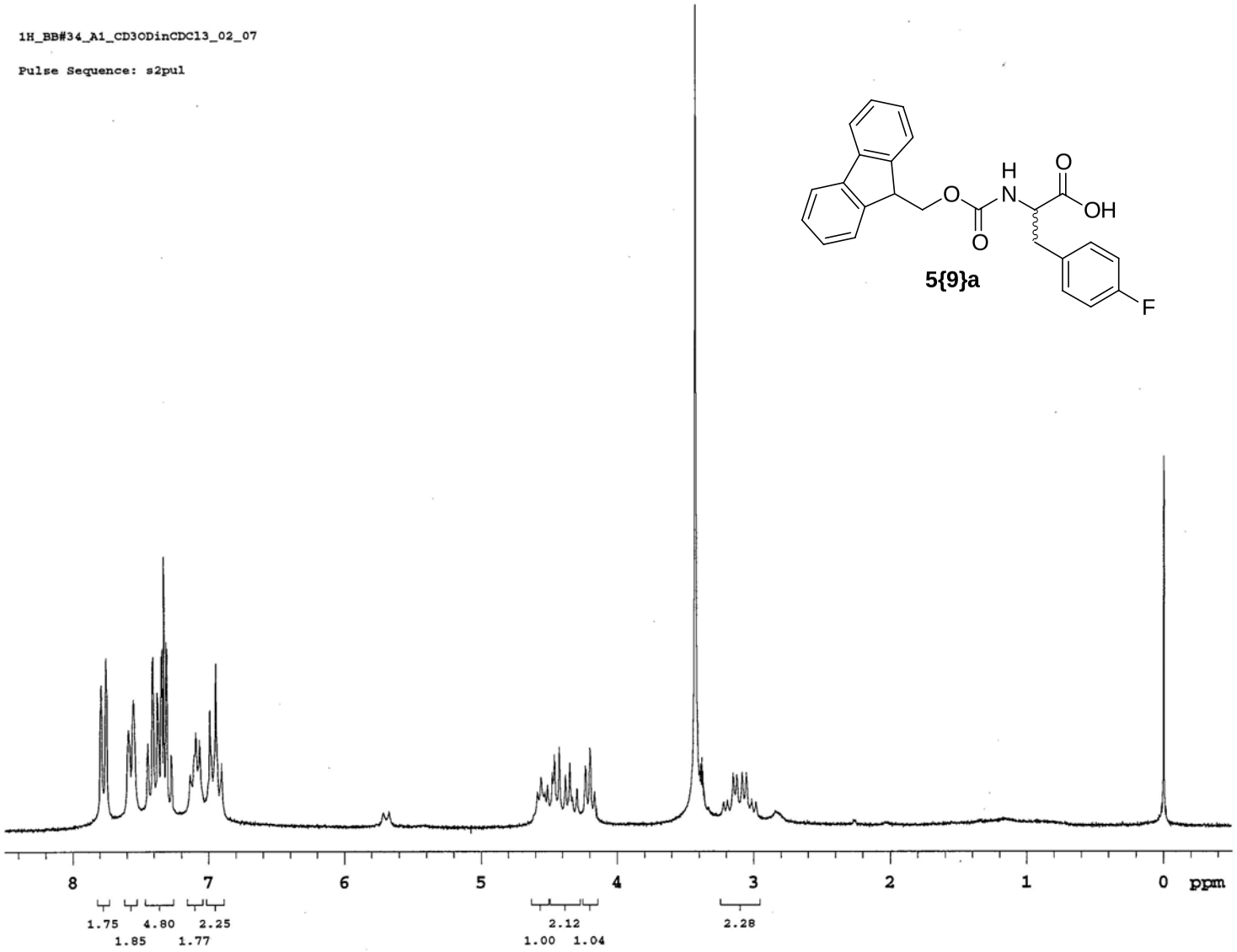

T21-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.48e7
Area
Time Height Area Area%
5.04 36201324 2803569.00 93.13
5.34 4500024 206942.98 6.87
5.04
268.0
2803569
100
%
-14
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
5{9}a
Team 21 (Resin II)
Exact Mass 405.14


T21-A3 190 (5.085) Cm (189:193)
1: Scan ES+
1.00e7
100
%
0
m/z
179.2
184.2
185.2
228.1
229.2
269.2
324.0
362.2
406.1
428.1
429.1
470.2
543.4
560.1
597.3
781.2
811.1
828.3
856.0
897.1
923.0
963.9
200 300 400 500 600 700 800 900 1000

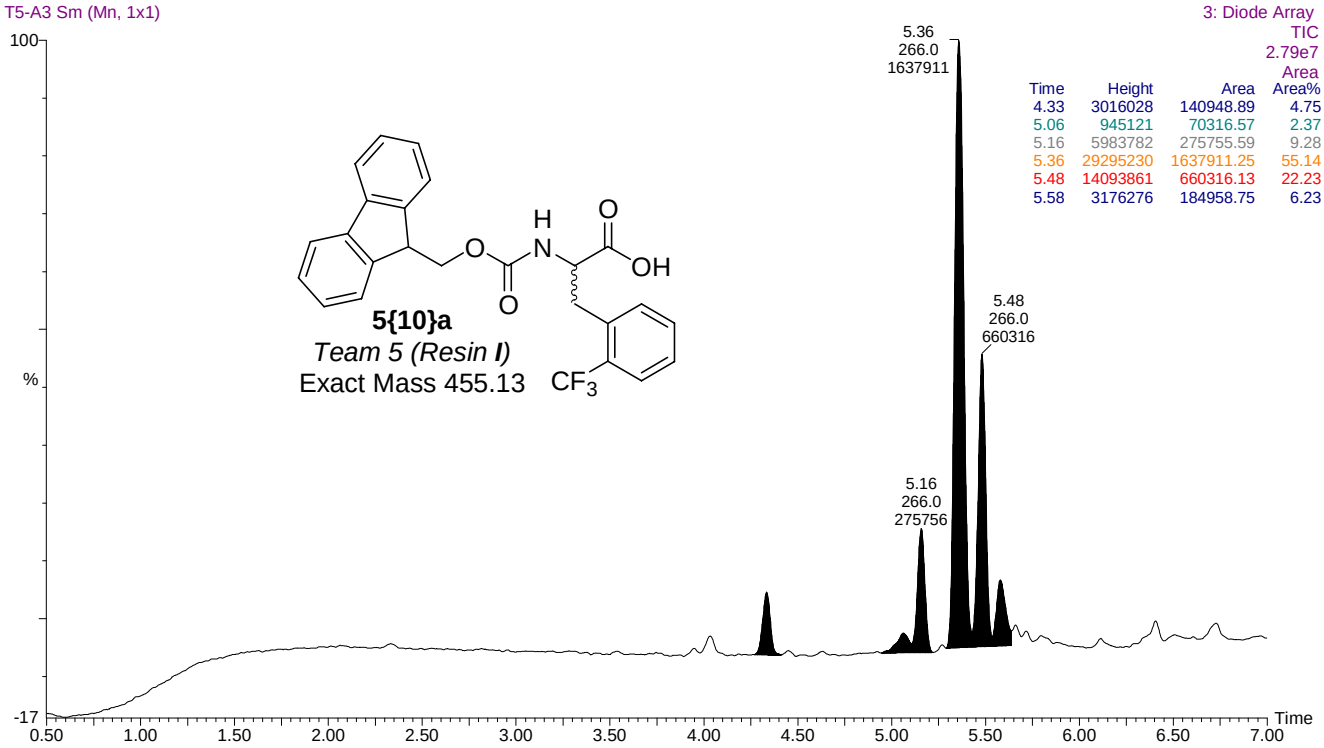
5{9}a

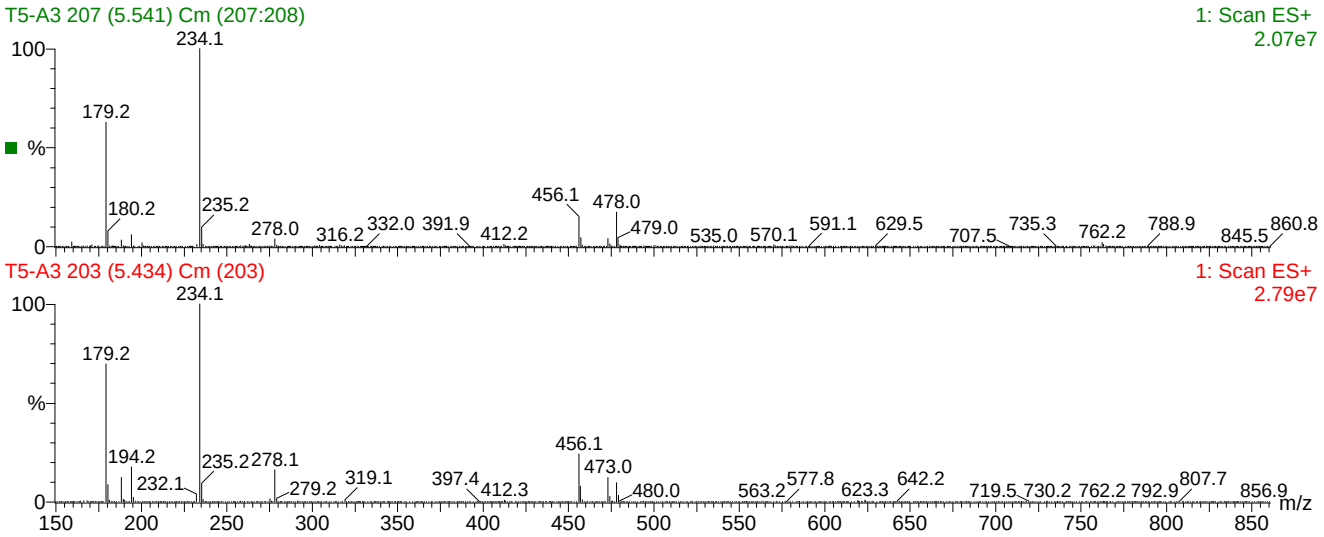

T22-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.48e7
Area
Time Height Area Area%
5.03 36073812 2734420.25 94.44
5.33 3498392 160996.98 5.56
5.03
268.0
2734420
100
%
-15
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
5{9}a
Team 22 (Resin II)
Exact Mass 405.14


T22-A2 190 (5.085) Cm (190:193)
1: Scan ES+
1.01e7
100
%
0
179.2
184.2
185.2
208.1
228.1
229.2
269.2
312.2
324.3
362.0
377.3
406.1
428.1
429.1
470.2
522.0
536.7
570.8
628.2
642.2
676.9
718.7
736.5
200 250 300 350 400 450 500 550 600 650 700
m/z

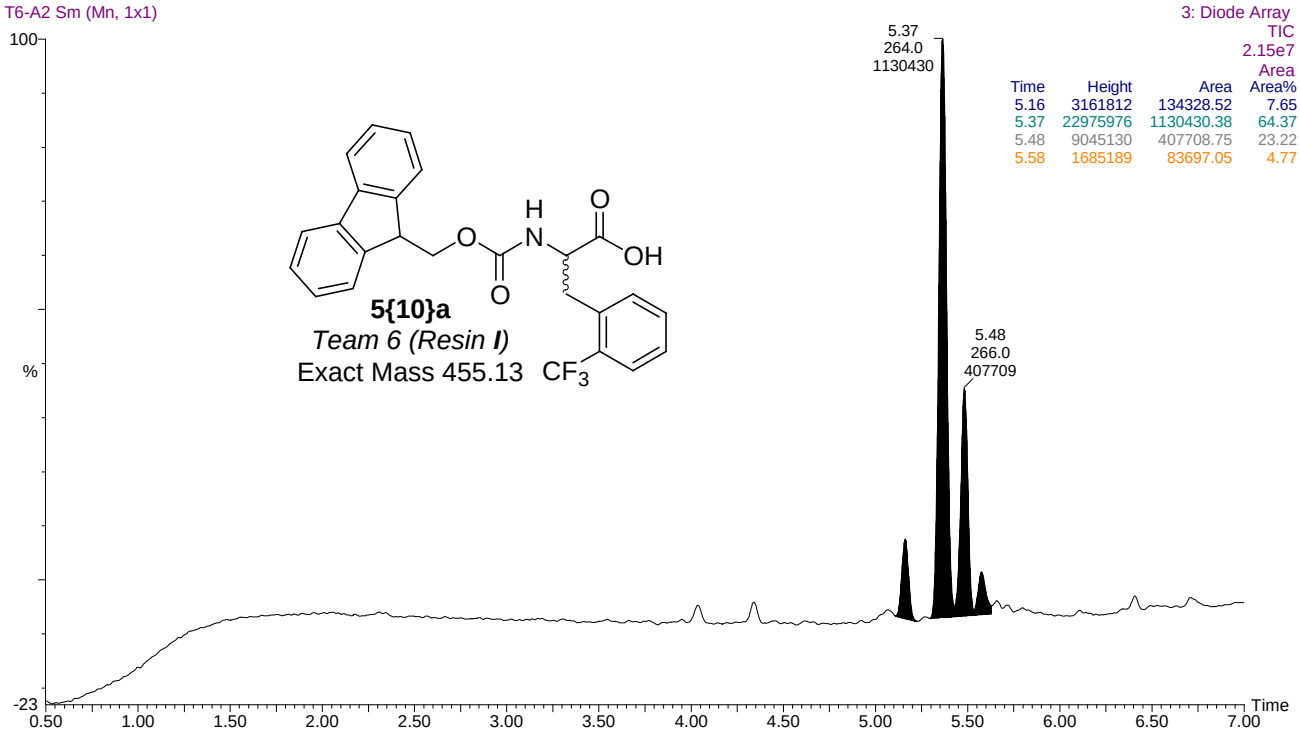

1H_BB#34_A1_CD3ODinCDCl3_02_07
Pulse Sequence: s2pul
H
N
O
O
O
OH
F
5{9}a
8
7
6
5
4
3
2
1
0
ppm
1.75
4.80
2.25
1.85
1.77
2.12
1.00
1.04
2.28

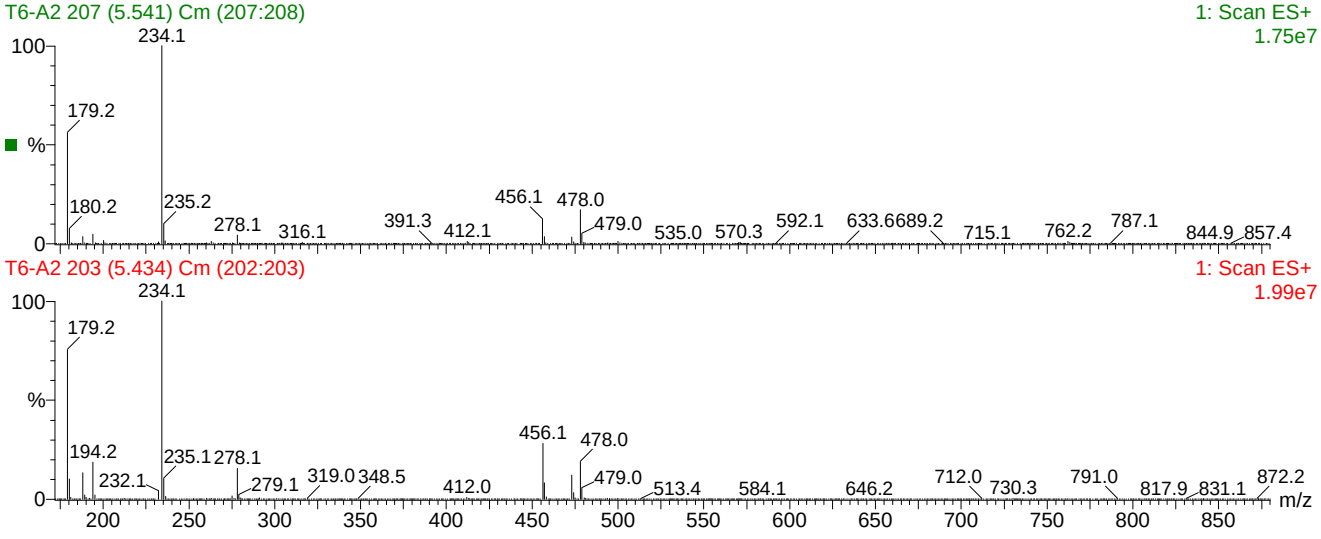
5{10}a


T5-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.79e7
Area
Time Height Area Area%
4.33 3016028 140948.89 4.75
5.06 945121 70316.57 2.37
5.16 5983782 275755.59 9.28
5.36 29295230 1637911.25 55.14
5.48 14093861 660316.13 22.23
5.58 3176276 184958.75 6.23
5.36
266.0
1637911
5.48
266.0
660316
5.16
266.0
275756
5{10}a
Team 5 (Resin I)
Exact Mass 455.13
CF3
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

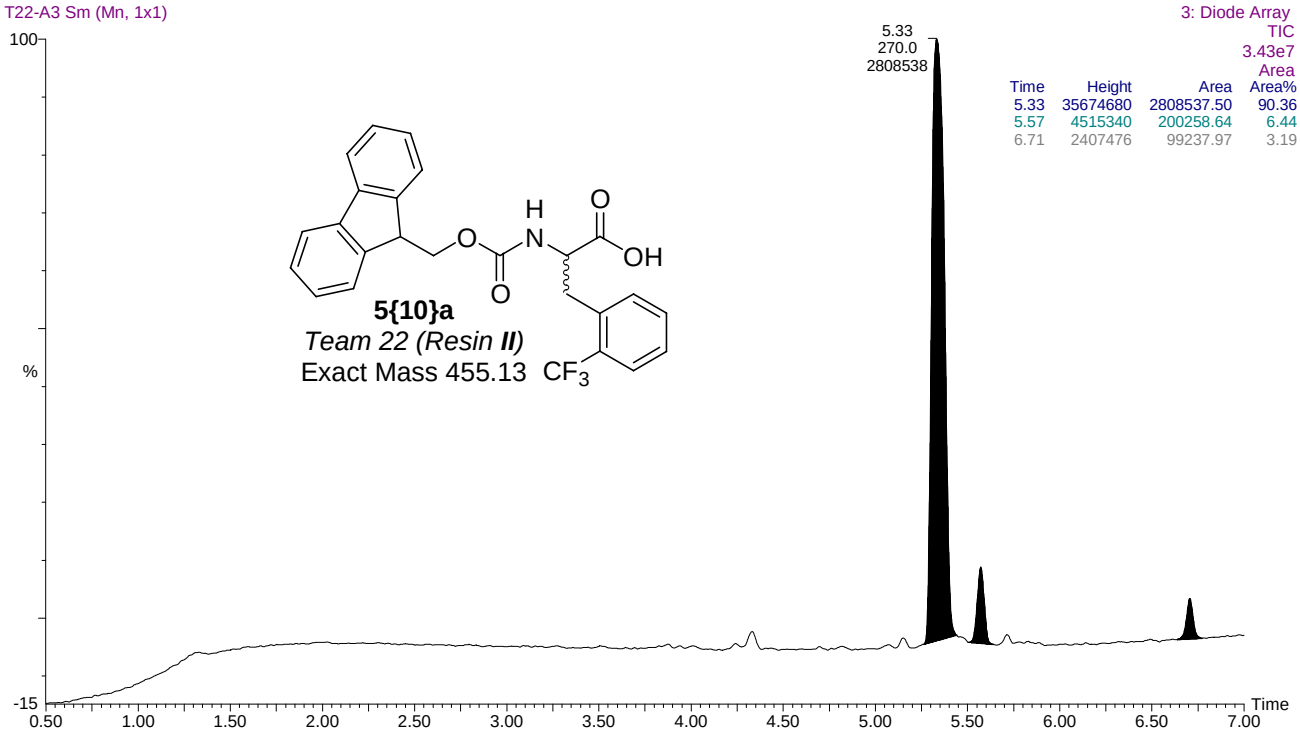

T5-A3 207 (5.541) Cm (207:208)
1: Scan ES+
2.07e7
100
%
0
234.1
179.2
180.2
235.2
278.0
316.2
332.0
391.9
412.2
456.1
478.0
479.0
535.0
570.1
591.1
629.5
707.5
735.3
762.2
788.9
845.5
860.8
T5-A3 203 (5.434) Cm (203)
1: Scan ES+
2.79e7
100
%
0
234.1
179.2
194.2
232.1
235.2
278.1
279.2
319.1
397.4
412.3
456.1
473.0
480.0
563.2
577.8
623.3
642.2
719.5
730.2
762.2
792.9
807.7
856.9
m/z
150 200 250 300 350 400 450 500 550 600 650 700 750 800 850

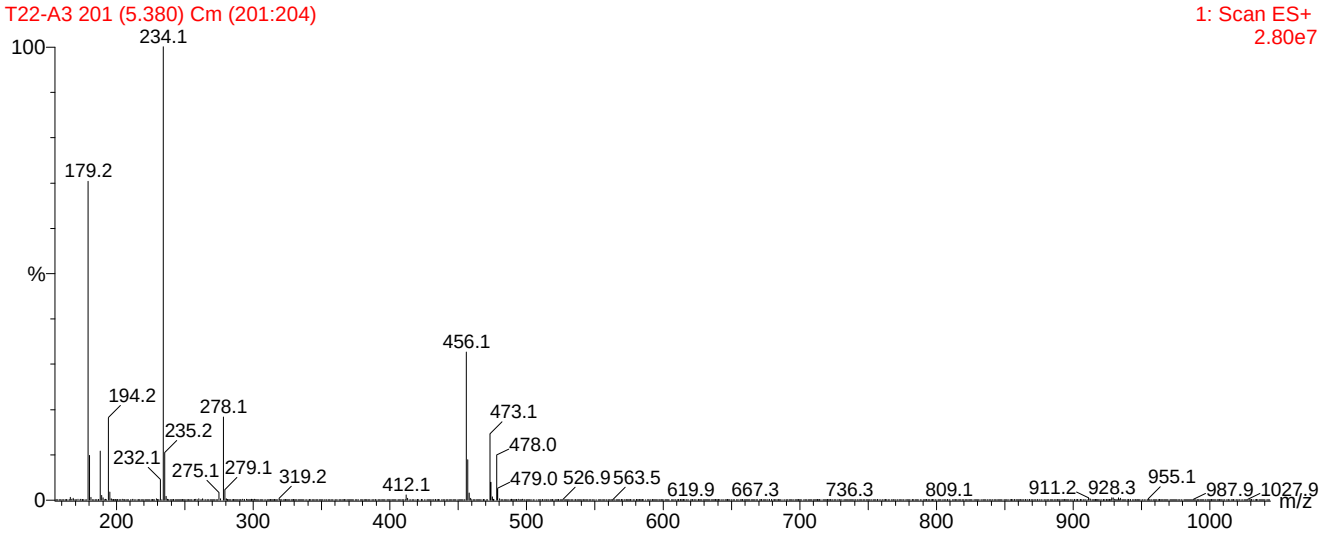
5{10}a


T6-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.15e7
Area
Time Height Area Area%
5.16 3161812 134328.52 7.65
5.37 22975976 1130430.38 64.37
5.48 9045130 407708.75 23.22
5.58 1685189 83697.05 4.77
5.37
264.0
1130430
5.48
266.0
407709
5{10}a
Team 6 (Resin I)
Exact Mass 455.13
CF3
%
Time

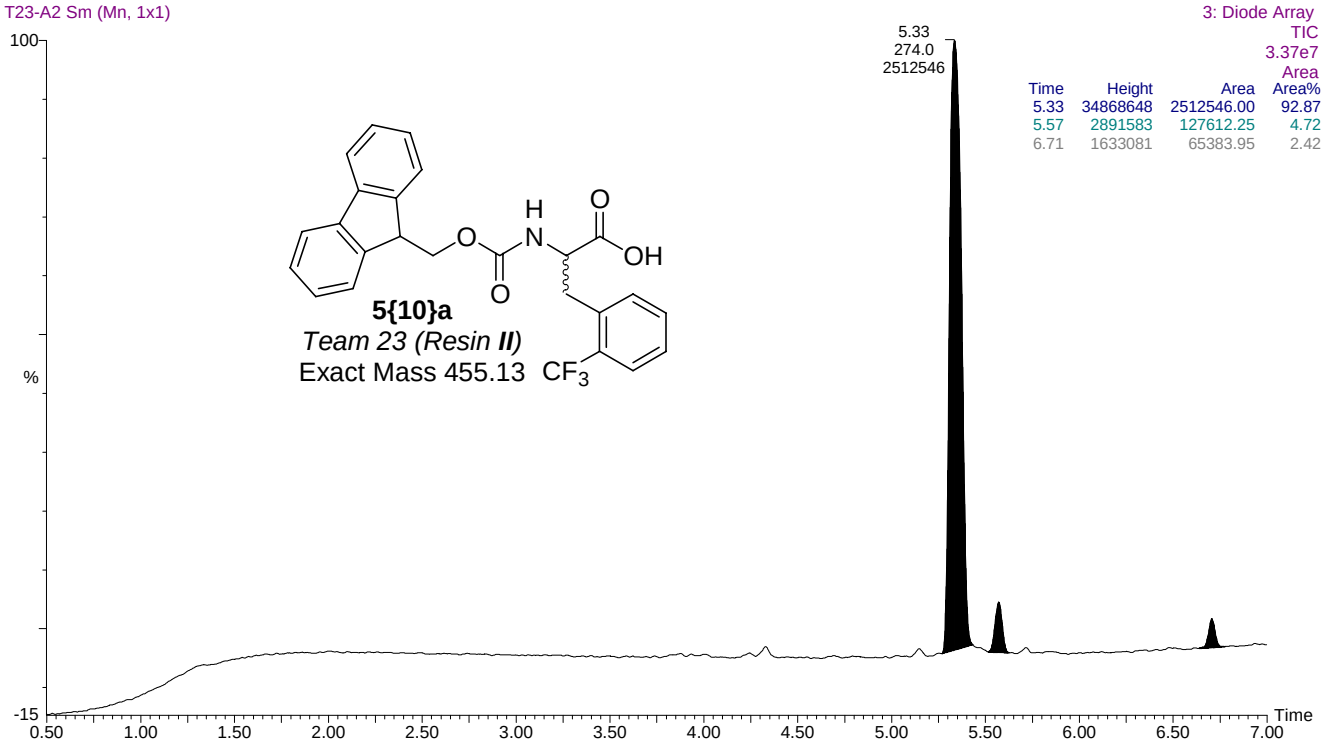

T6-A2 207 (5.541) Cm (207:208)
1: Scan ES+
1.75e7
T6-A2 203 (5.434) Cm (202:203)
1: Scan ES+
1.99e7
%
m/z

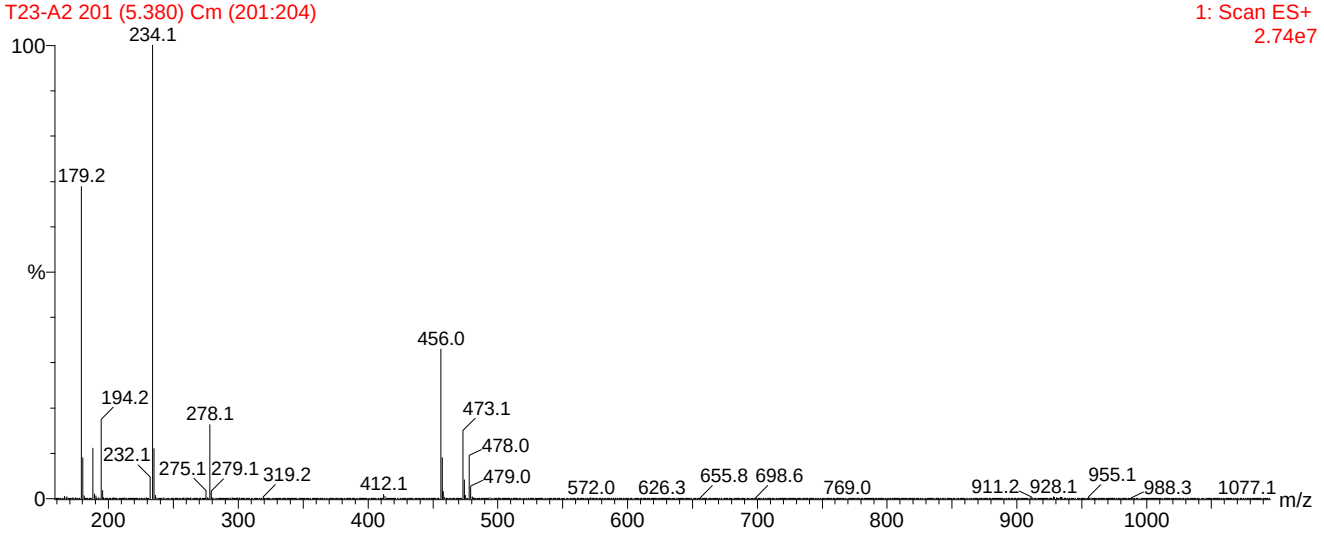
5{10}a


T22-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.43e7
Area
Time Height Area Area%
5.33 35674680 2808537.50 90.36
5.57 4515340 200258.64 6.44
6.71 2407476 99237.97 3.19
5.33
270.0
2808538
5{10}a
Team 22 (Resin II)
Exact Mass 455.13
%
Time


T22-A3 201 (5.380) Cm (201:204)
1: Scan ES+
2.80e7
234.1
179.2
456.1
194.2
278.1
473.1
235.2
478.0
232.1
275.1
279.1
319.2
412.1
479.0
526.9
563.5
619.9
667.3
736.3
809.1
911.2
928.3
955.1
987.9
1027.9
%
m/z

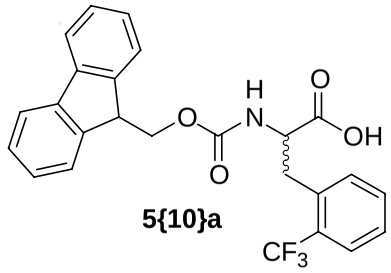
5{10}a


T23-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.37e7
Area
Time Height Area Area%
5.33 34868648 2512546.00 92.87
5.57 2891583 127612.25 4.72
6.71 1633081 65383.95 2.42
5.33
274.0
2512546
100
%
-15
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
OH
O
CF3
5{10}a
Team 23 (Resin II)
Exact Mass 455.13

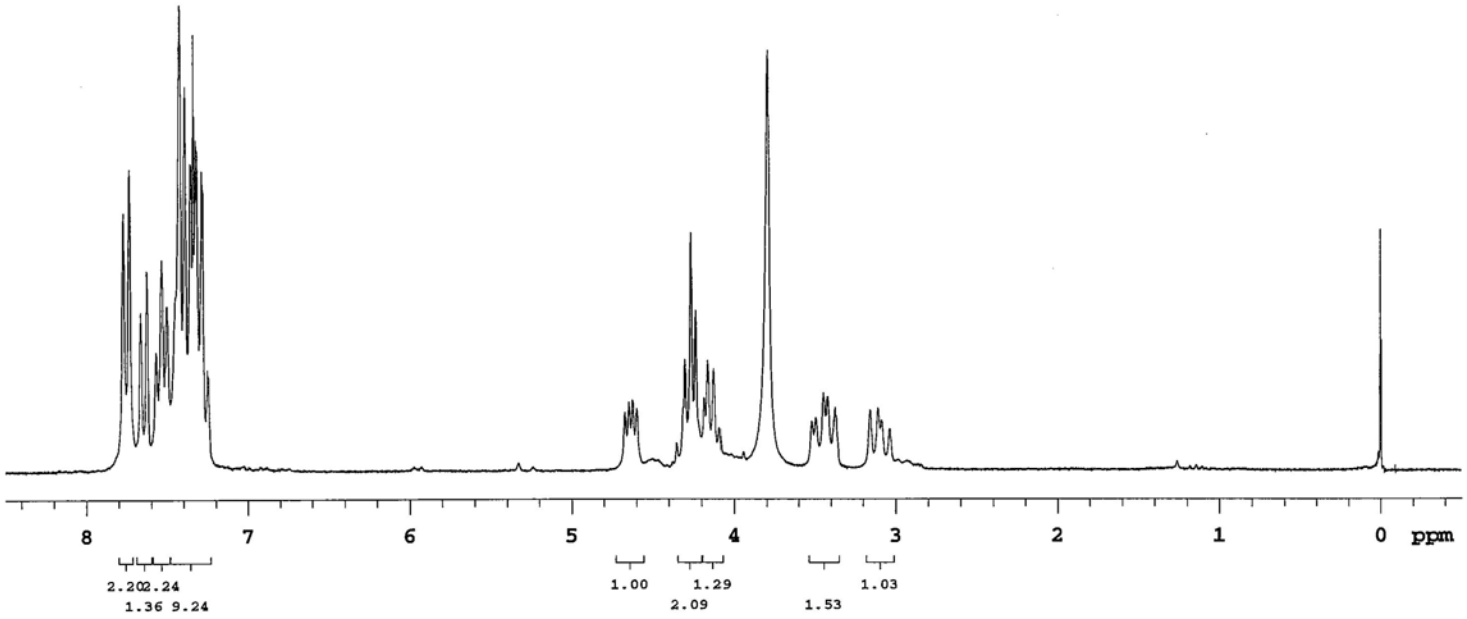

T23-A2 201 (5.380) Cm (201:204)
1: Scan ES+
2.74e7
100
%
0
234.1
179.2
194.2
278.1
232.1
275.1
279.1
319.2
412.1
456.0
473.1
478.0
479.0
572.0
626.3
655.8
698.6
769.0
911.2
928.1
955.1
988.3
1077.1
200 300 400 500 600 700 800 900 1000
m/z

1H_RR#27_B3_1eastCD3ODinCDCl3_02_17_02_17_07

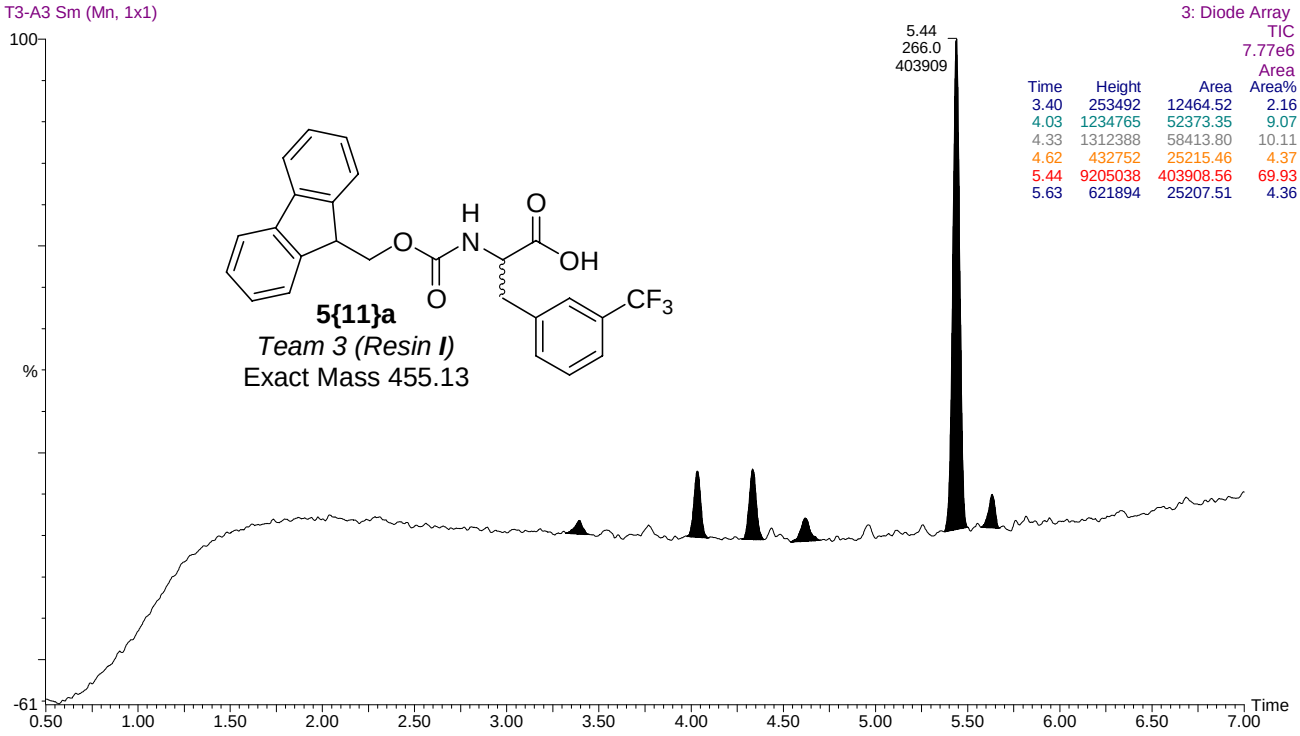
Pulse Sequence: s2pul

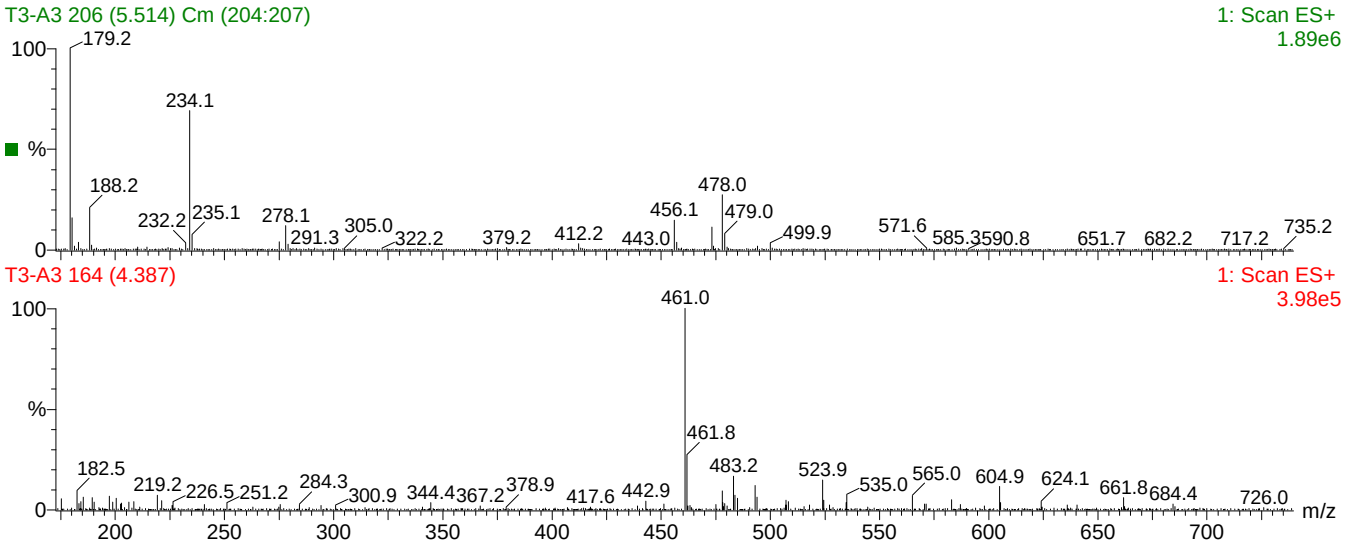


5{10}a

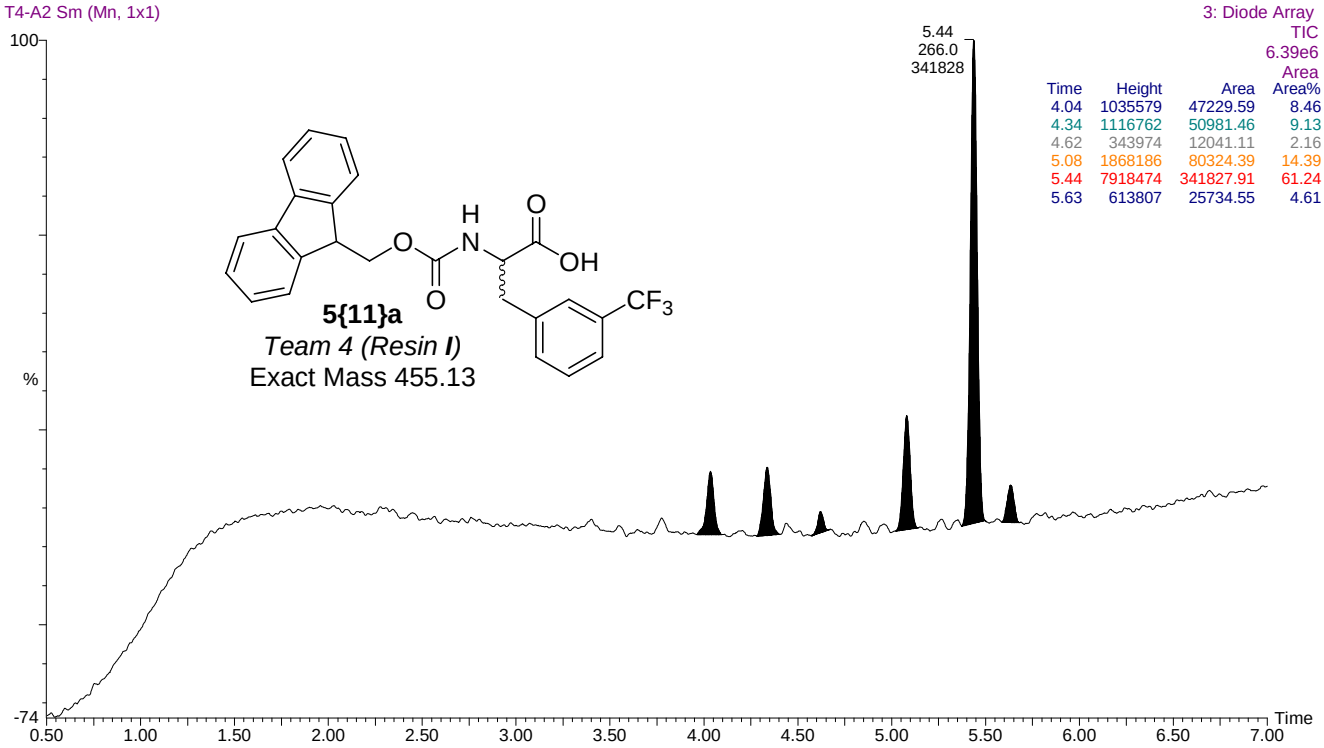


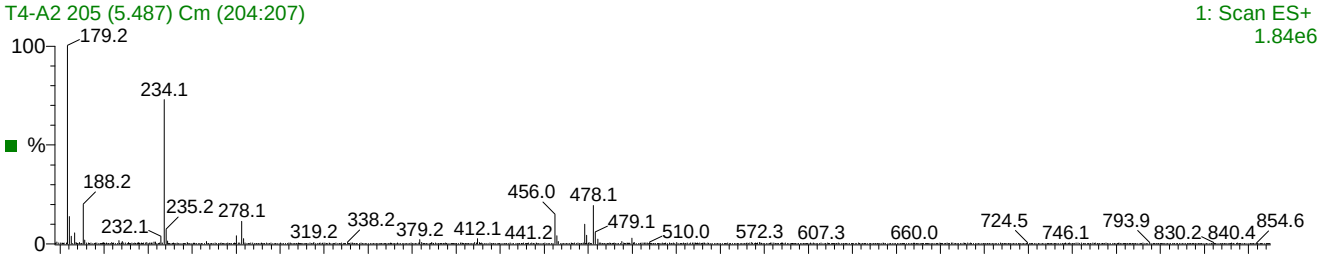
5{11}a

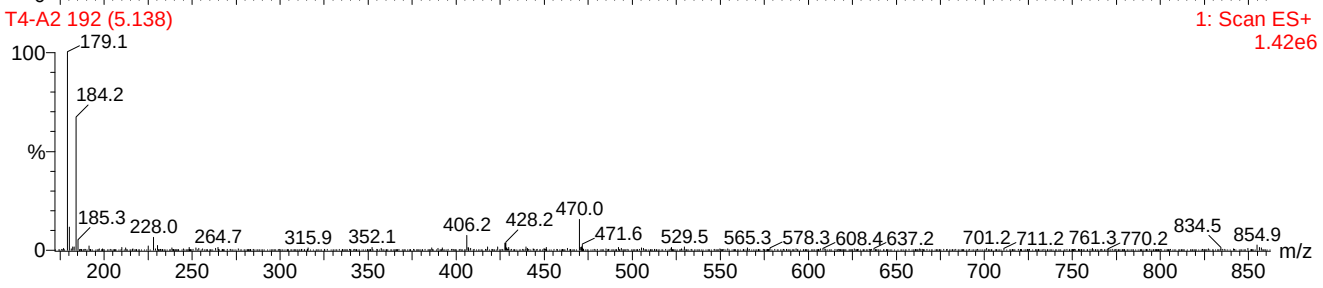

T3-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
7.77e6
Area
Time Height Area Area%
3.40 253492 12464.52 2.16
4.03 1234765 52373.35 9.07
4.33 1312388 58413.80 10.11
4.62 432752 25215.46 4.37
5.44 9205038 403908.56 69.93
5.63 621894 25207.51 4.36
5.44
266.0
403909
5{11}a
Team 3 (Resin I)
Exact Mass 455.13
Time


T3-A3 206 (5.514) Cm (204:207)
1: Scan ES+
1.89e6
T3-A3 164 (4.387)
1: Scan ES+
3.98e5
m/z

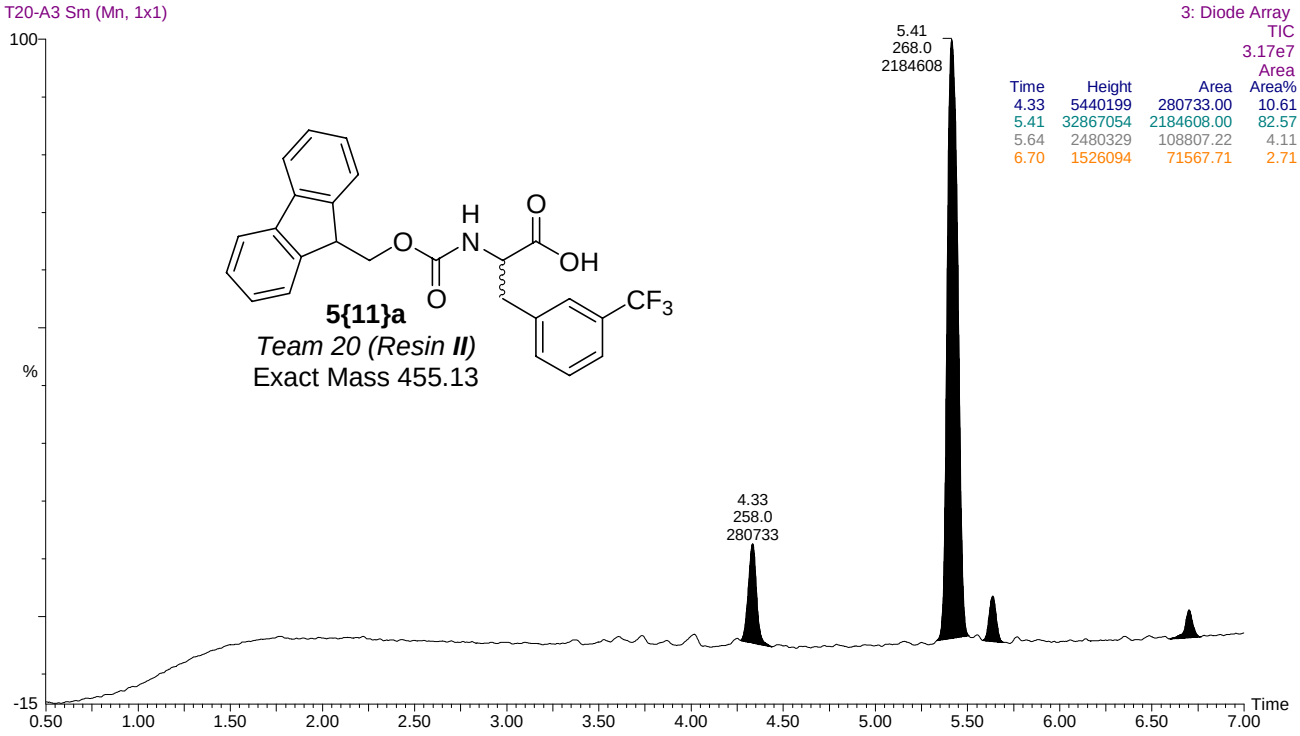
5{11}a

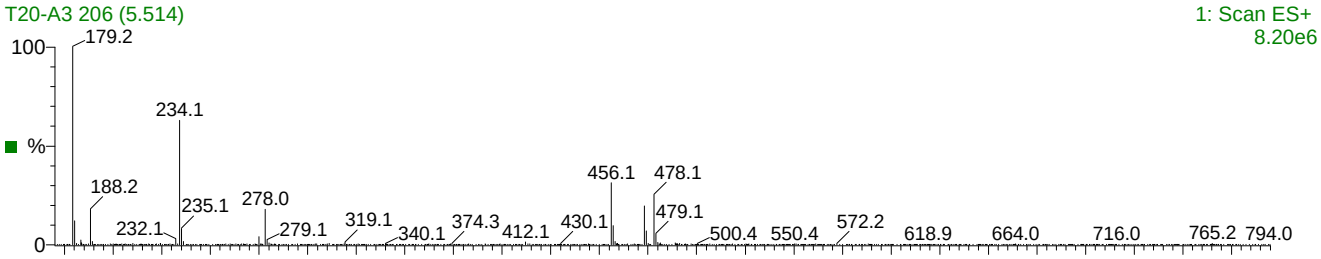

T4-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
6.39e6
Area
Time Height Area Area%
4.04 1035579 47229.59 8.46
4.34 1116762 50981.46 9.13
4.62 343974 12041.11 2.16
5.08 1868186 80324.39 14.39
5.44 7918474 341827.91 61.24
5.63 613807 25734.55 4.61
5.44
266.0
341828
5{11}a
Team 4 (Resin I)
Exact Mass 455.13
Time

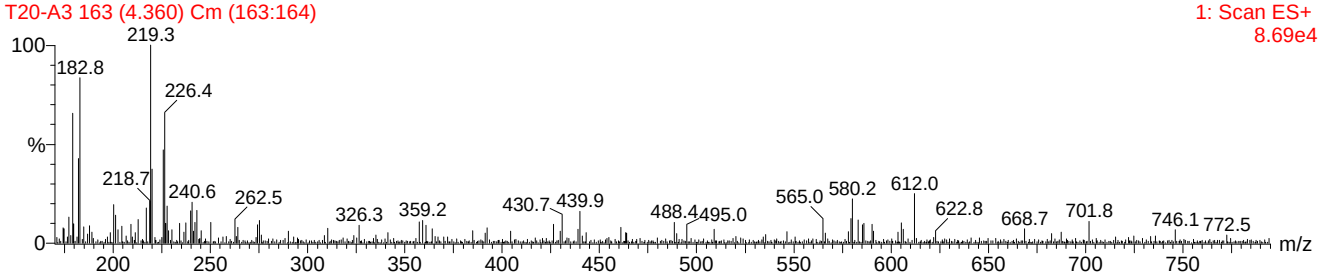

T4-A2 205 (5.487) Cm (204:207)
1: Scan ES+
1.84e6


T4-A2 192 (5.138)
1: Scan ES+
1.42e6
m/z

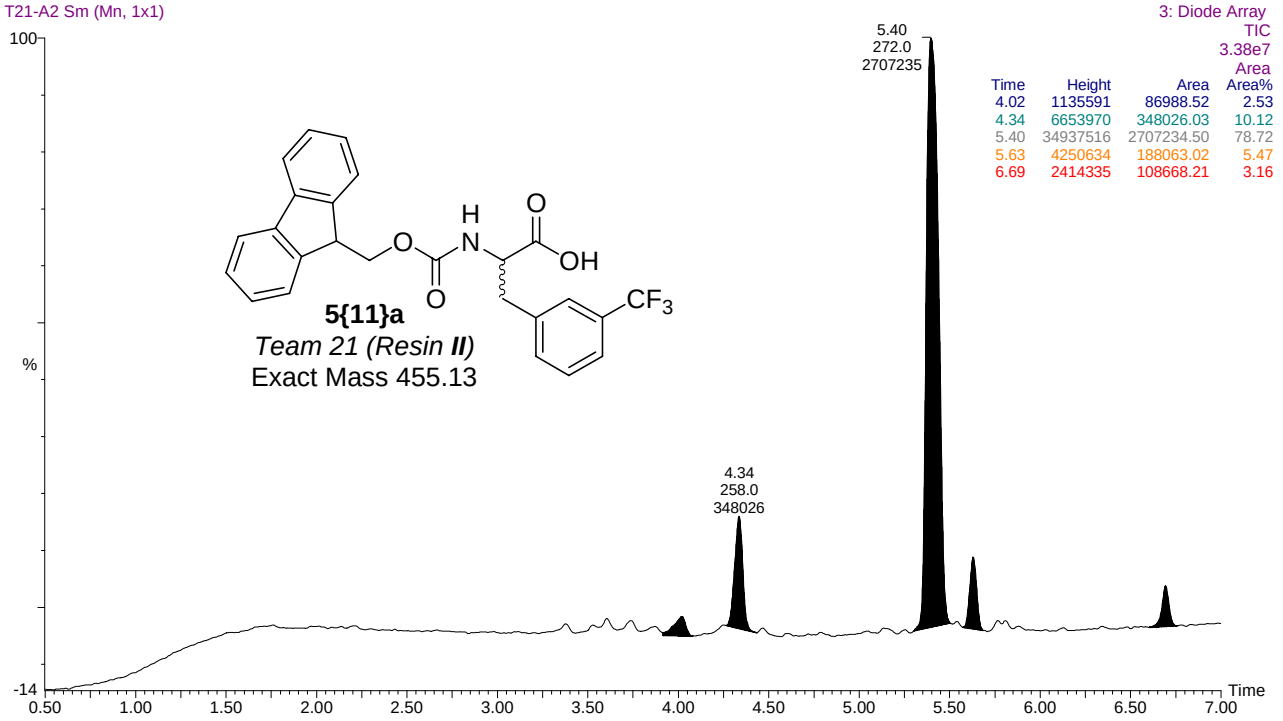
5{11}a

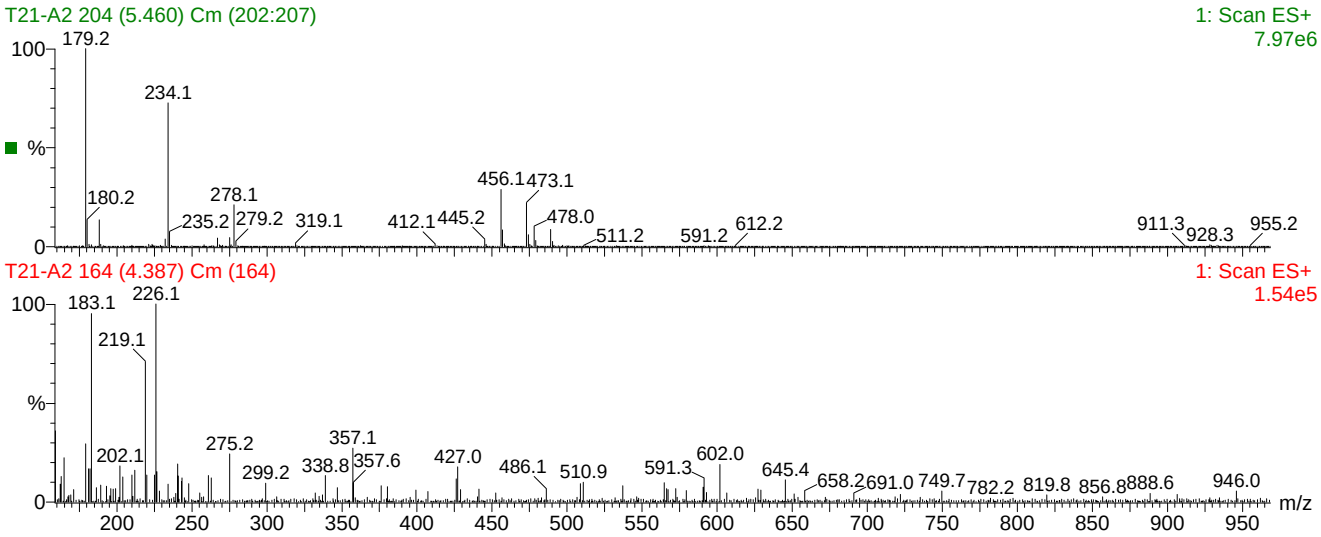

T20-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.17e7
Area
Time Height Area Area%
4.33 5440199 280733.00 10.61
5.41 32867054 2184608.00 82.57
5.64 2480329 108807.22 4.11
6.70 1526094 71567.71 2.71
5.41
268.0
2184608
4.33
258.0
280733
5{11}a
Team 20 (Resin II)
Exact Mass 455.13
%
Time


T20-A3 206 (5.514)
1: Scan ES+
8.20e6
179.2
234.1
188.2
235.1
278.0
232.1
279.1
319.1
340.1
374.3
412.1
430.1
456.1
478.1
479.1
500.4
550.4
572.2
618.9
664.0
716.0
765.2
794.0


T20-A3 163 (4.360) Cm (163:164)
1: Scan ES+
8.69e4
219.3
182.8
226.4
218.7
240.6
262.5
326.3
359.2
430.7
439.9
488.4
495.0
565.0
580.2
612.0
622.8
668.7
701.8
746.1
772.5
m/z

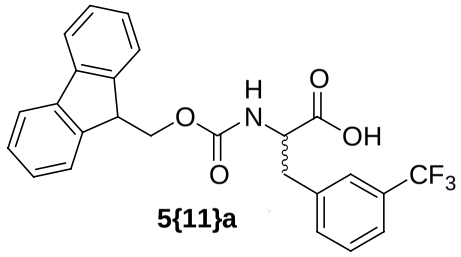
5{11}a


T21-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.38e7
Area
Time Height Area Area%
4.02 1135591 86988.52 2.53
4.34 6653970 348026.03 10.12
5.40 34937516 2707234.50 78.72
5.63 4250634 188063.02 5.47
6.69 2414335 108668.21 3.16
5.40
272.0
2707235
4.34
258.0
348026
5{11}a
Team 21 (Resin II)
Exact Mass 455.13
100
%
-14
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

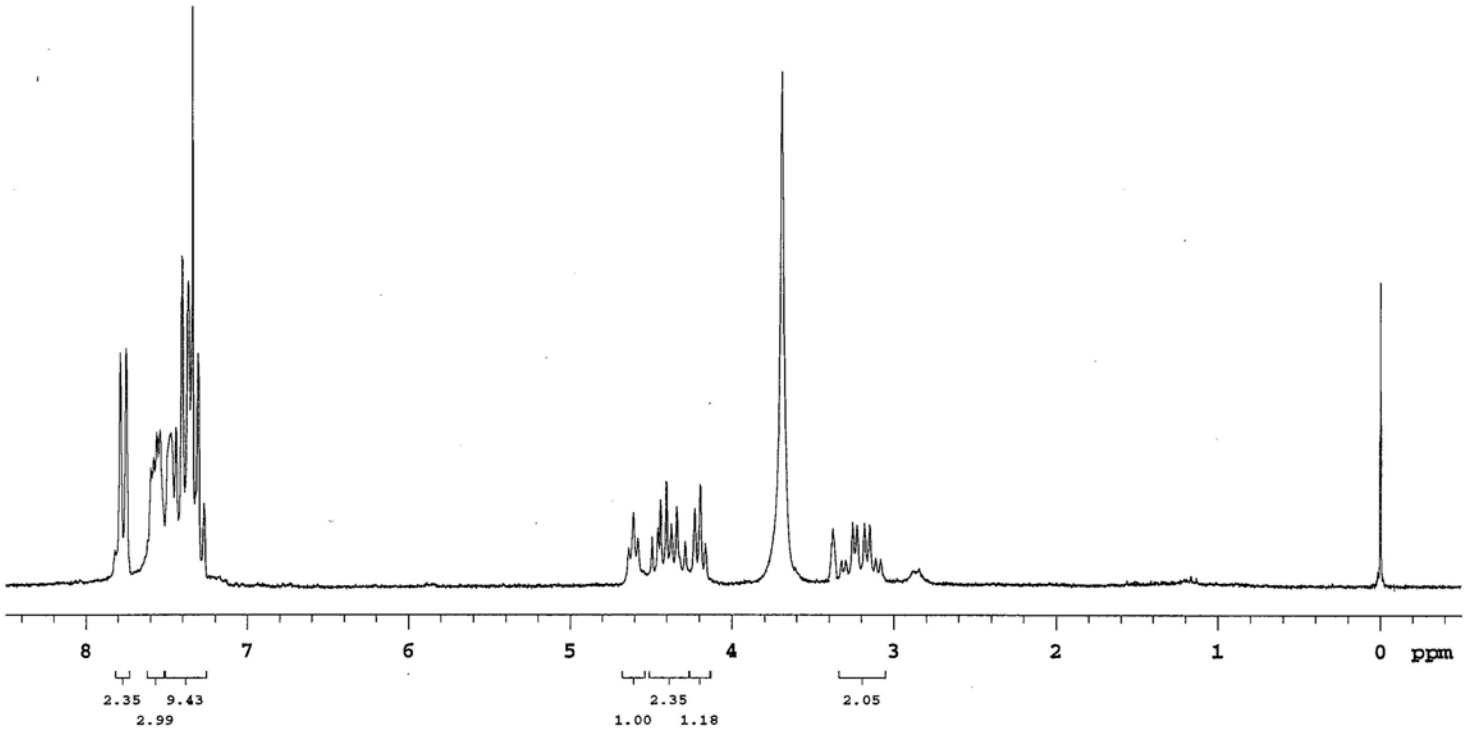

T21-A2 204 (5.460) Cm (202:207)
1: Scan ES+
7.97e6
100
%
0
179.2
234.1
180.2
278.1
235.2
279.2
319.1
412.1
445.2
456.1
473.1
478.0
511.2
591.2
612.2
911.3
928.3
955.2
T21-A2 164 (4.387) Cm (164)
1: Scan ES+
1.54e5
100
%
0
183.1
226.1
219.1
202.1
275.2
299.2
338.8
357.1
357.6
427.0
486.1
510.9
591.3
602.0
645.4
658.2
691.0
749.7
782.2
819.8
856.8
888.6
946.0
m/z
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

1H_RR#40_A2_CD3ODinCDCl3_03_07

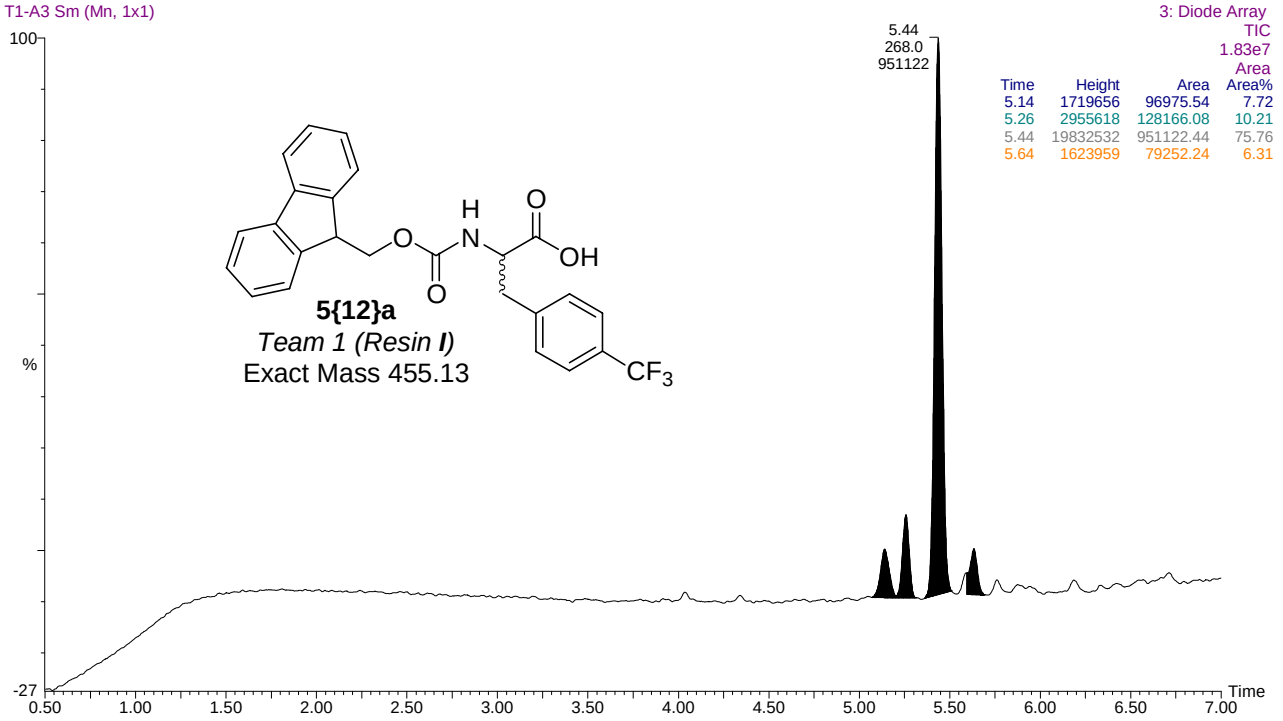
Pulse Sequence: s2pul

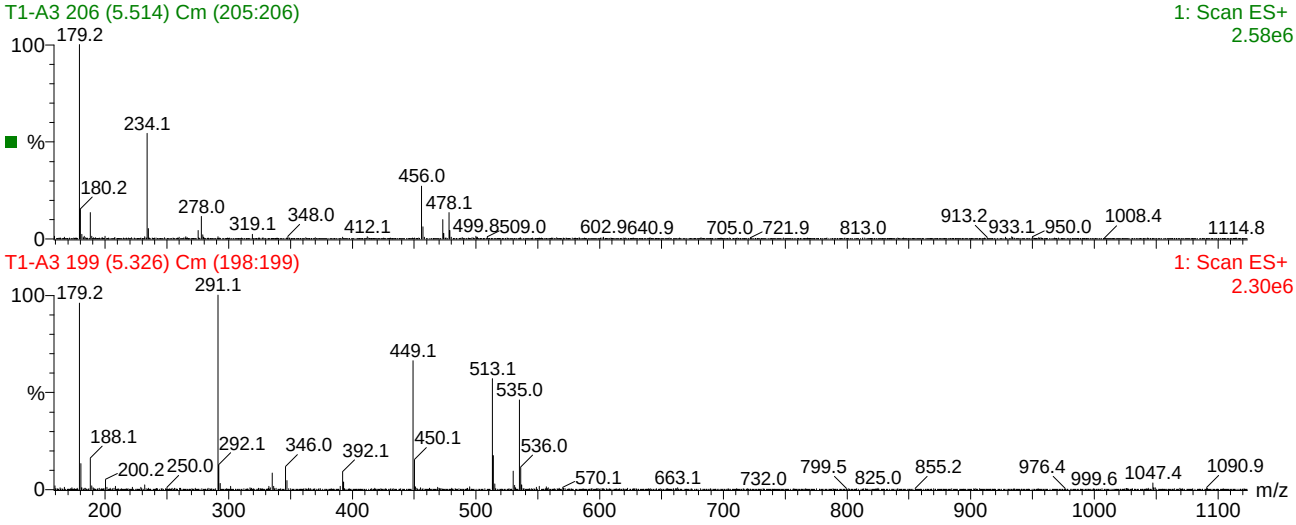


5{11}a

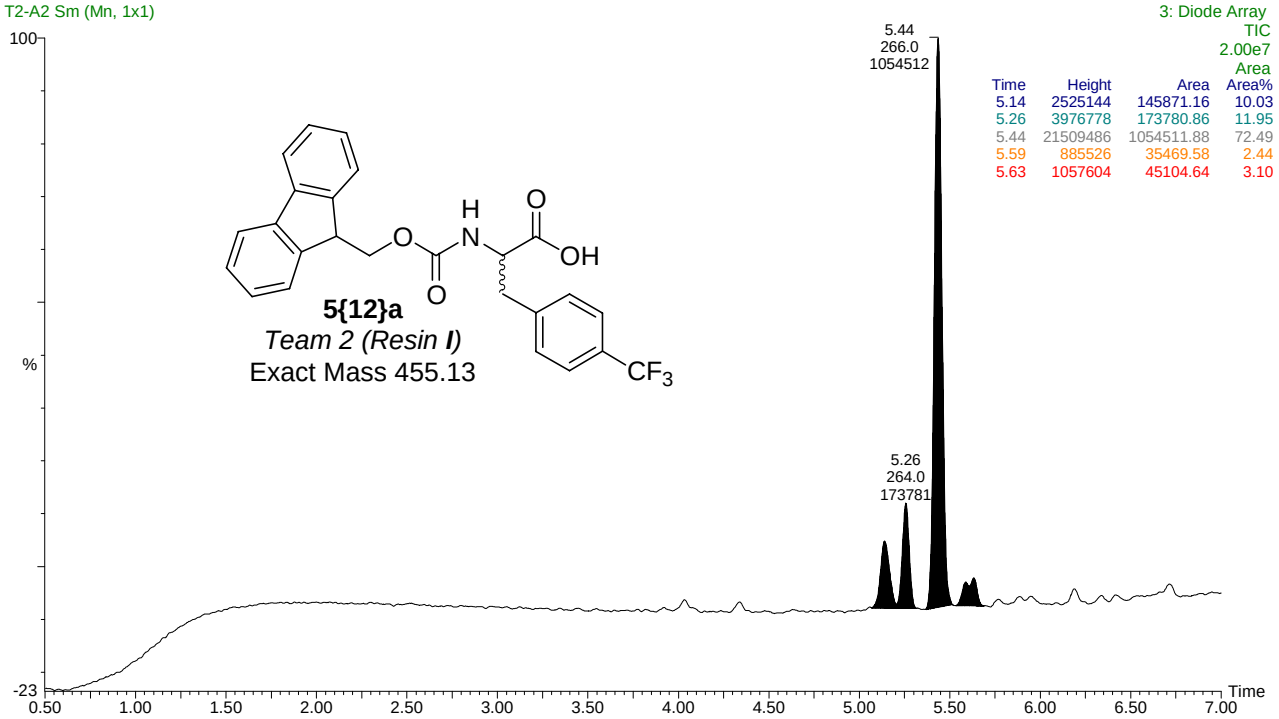


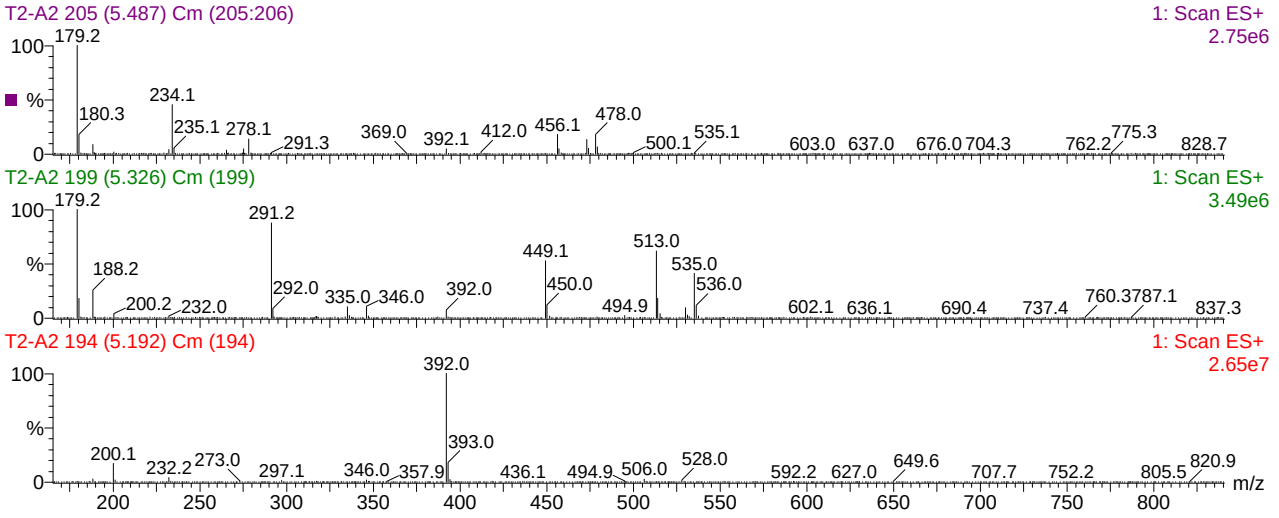
5{12}a


T1-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
1.83e7
Area
5.44
268.0
951122
Time Height Area Area%
5.14 1719656 96975.54 7.72
5.26 2955618 128166.08 10.21
5.44 19832532 951122.44 75.76
5.64 1623959 79252.24 6.31
5{12}a
Team 1 (Resin I)
Exact Mass 455.13
Time

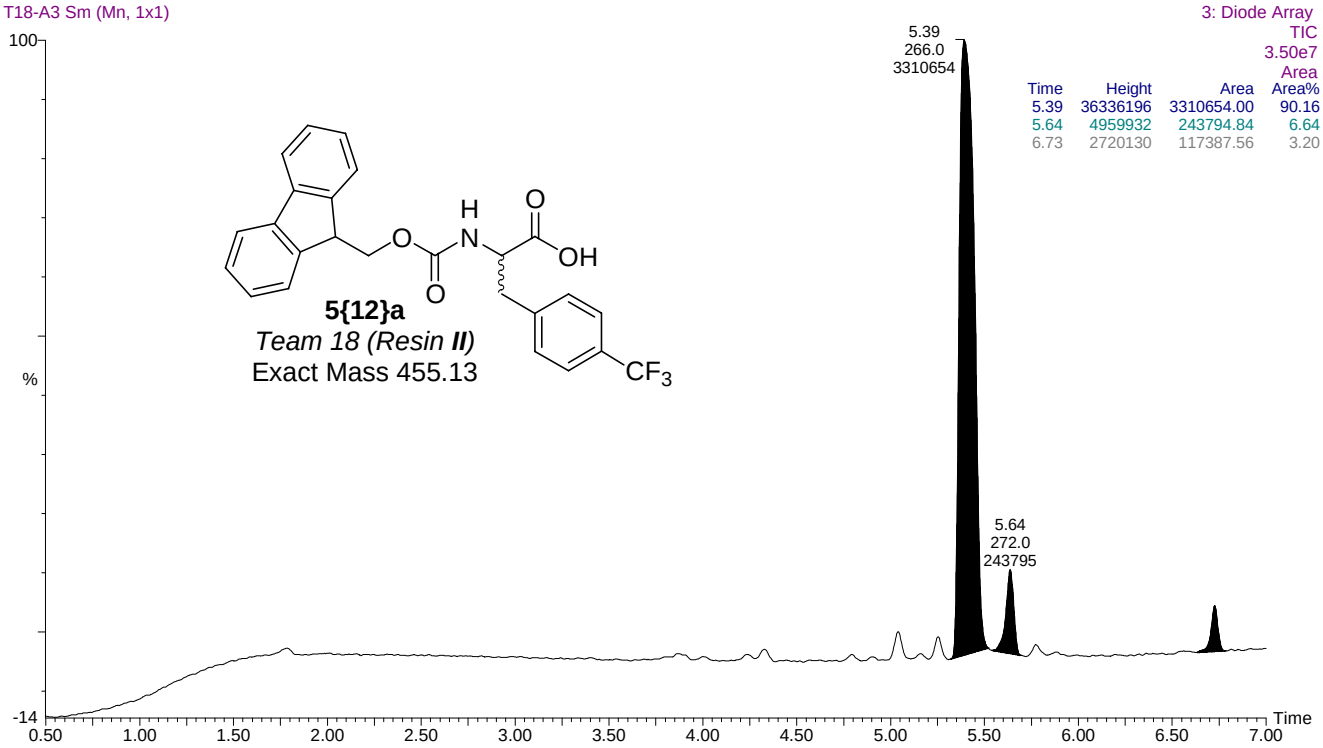

T1-A3 206 (5.514) Cm (205:206)
1: Scan ES+
2.58e6
179.2
234.1
180.2
456.0
478.1
T1-A3 199 (5.326) Cm (198:199)
1: Scan ES+
2.30e6
179.2
291.1
449.1
513.1
535.0
188.1
292.1
346.0
392.1
450.1
536.0
m/z

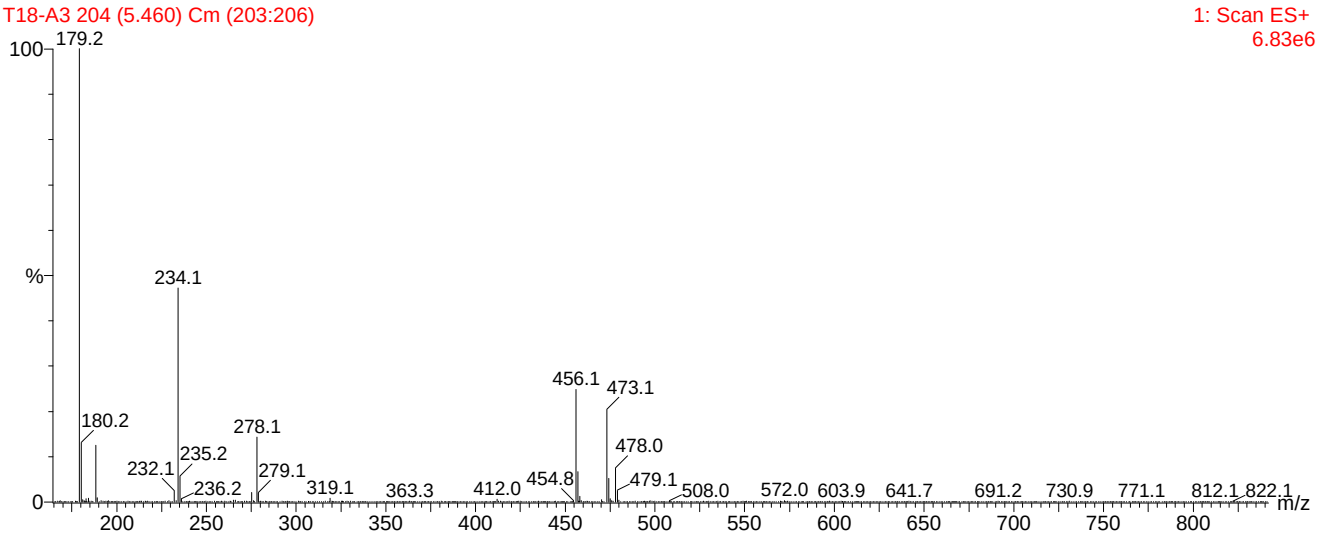
5{12}a


T2-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.00e7
Area
Time Height Area Area%
5.14 2525144 145871.16 10.03
5.26 3976778 173780.86 11.95
5.44 21509486 1054511.88 72.49
5.59 885526 35469.58 2.44
5.63 1057604 45104.64 3.10
5.44
266.0
1054512
5.26
264.0
173781
5{12}a
Team 2 (Resin I)
Exact Mass 455.13
%
Time

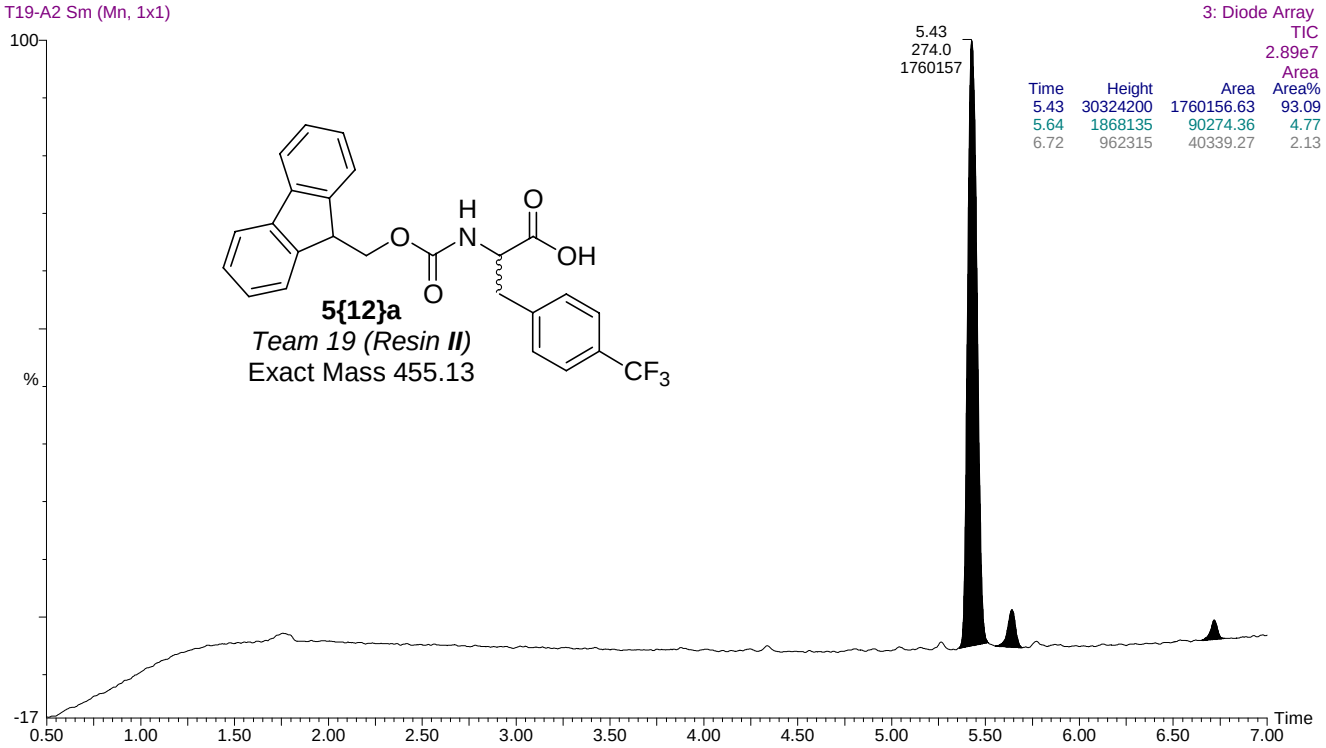

T2-A2 205 (5.487) Cm (205:206)
1: Scan ES+
2.75e6
T2-A2 199 (5.326) Cm (199)
1: Scan ES+
3.49e6
T2-A2 194 (5.192) Cm (194)
1: Scan ES+
2.65e7
m/z

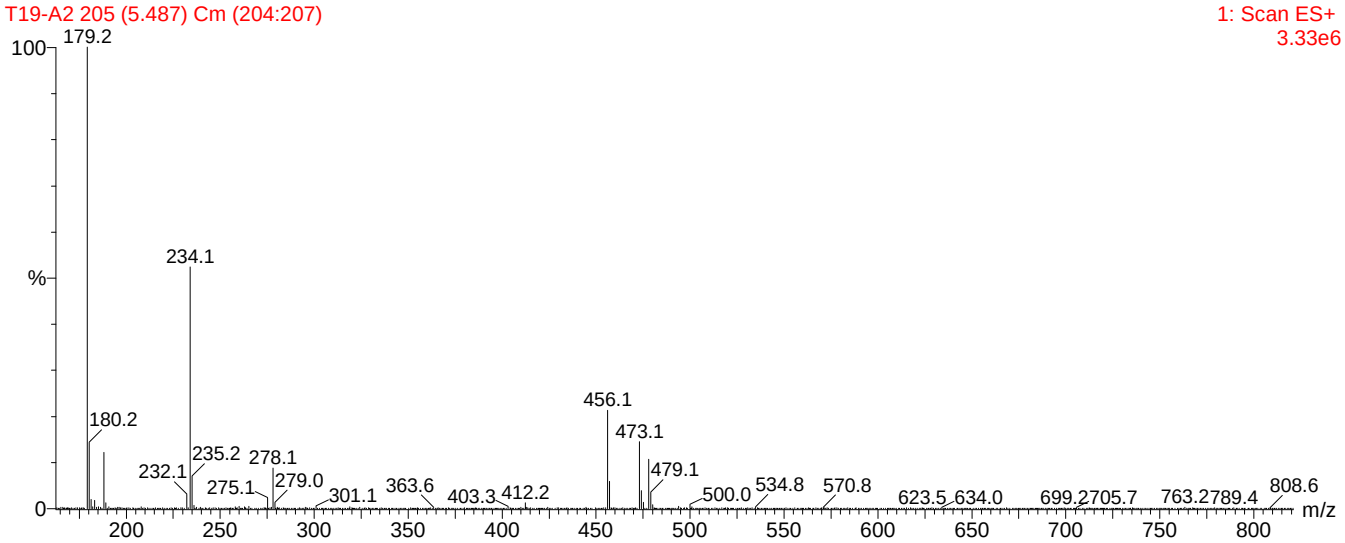
5{12}a


T18-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.50e7
Area
Time Height Area Area%
5.39 36336196 3310654.00 90.16
5.64 4959932 243794.84 6.64
6.73 2720130 117387.56 3.20
5.39
266.0
3310654
5.64
272.0
243795
5{12}a
Team 18 (Resin II)
Exact Mass 455.13
100
%
-14
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

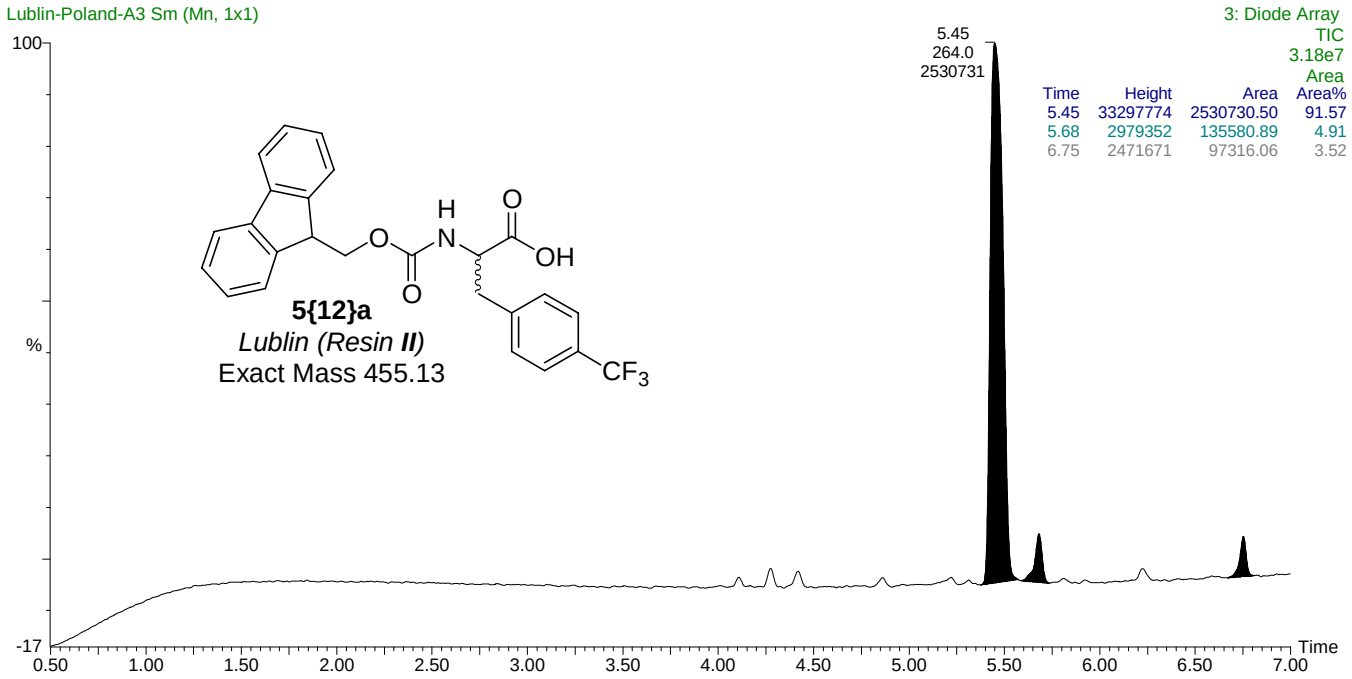

T18-A3 204 (5.460) Cm (203:206)
1: Scan ES+
6.83e6
100
%
0
179.2
234.1
180.2
278.1
235.2
232.1
279.1
236.2
319.1
363.3
412.0
454.8
456.1
473.1
478.0
479.1
508.0
572.0
603.9
641.7
691.2
730.9
771.1
812.1
822.1
m/z
200 250 300 350 400 450 500 550 600 650 700 750 800

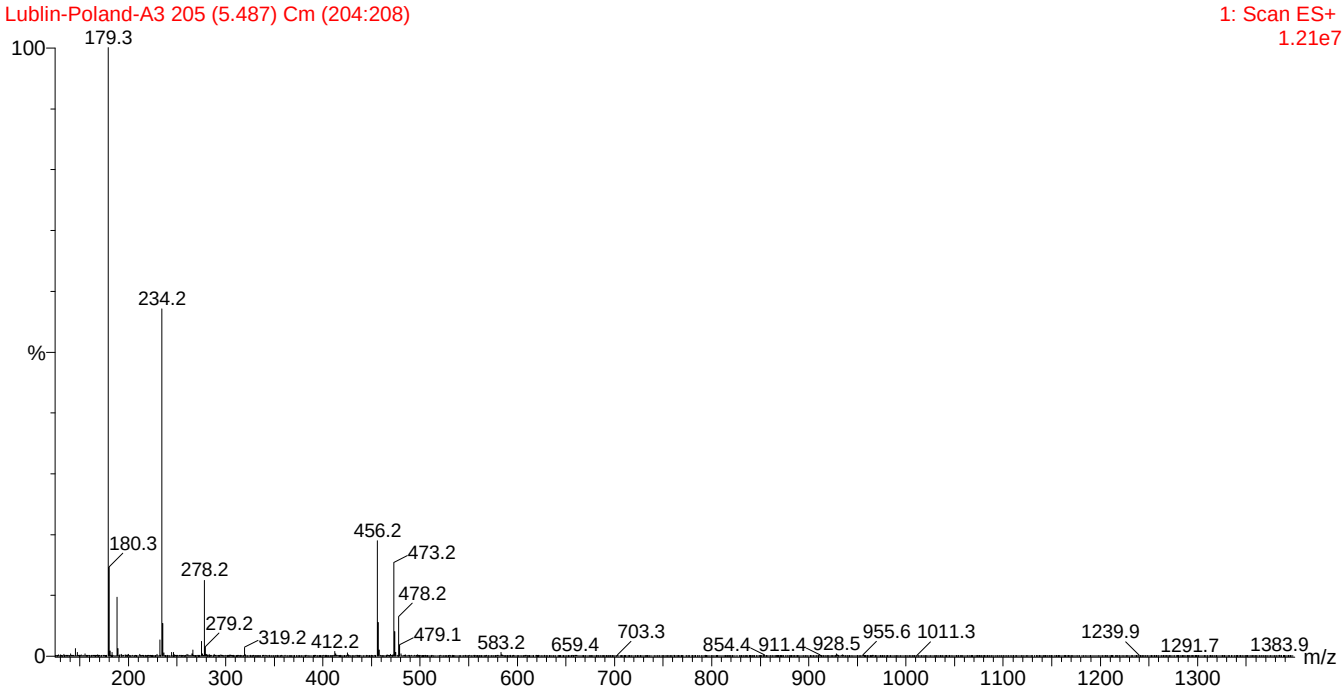
5{12}a


T19-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.89e7
Area
Time Height Area Area%
5.43 30324200 1760156.63 93.09
5.64 1868135 90274.36 4.77
6.72 962315 40339.27 2.13
5.43
274.0
1760157
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
O
OH
CF3
5{12}a
Team 19 (Resin II)
Exact Mass 455.13

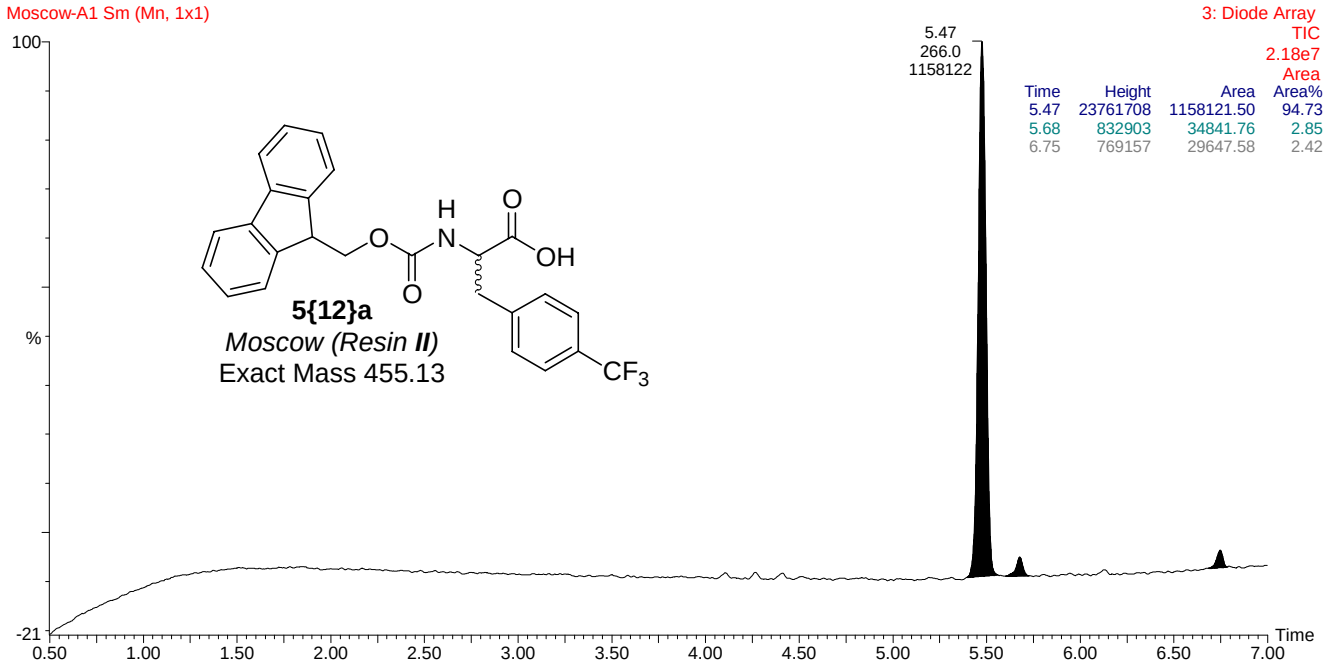

T19-A2 205 (5.487) Cm (204:207)
1: Scan ES+
3.33e6
100
%
0
m/z
179.2
234.1
180.2
235.2
232.1
278.1
275.1
279.0
301.1
363.6
403.3
412.2
456.1
473.1
479.1
500.0
534.8
570.8
623.5
634.0
699.2
705.7
763.2
789.4
808.6
200 250 300 350 400 450 500 550 600 650 700 750 800

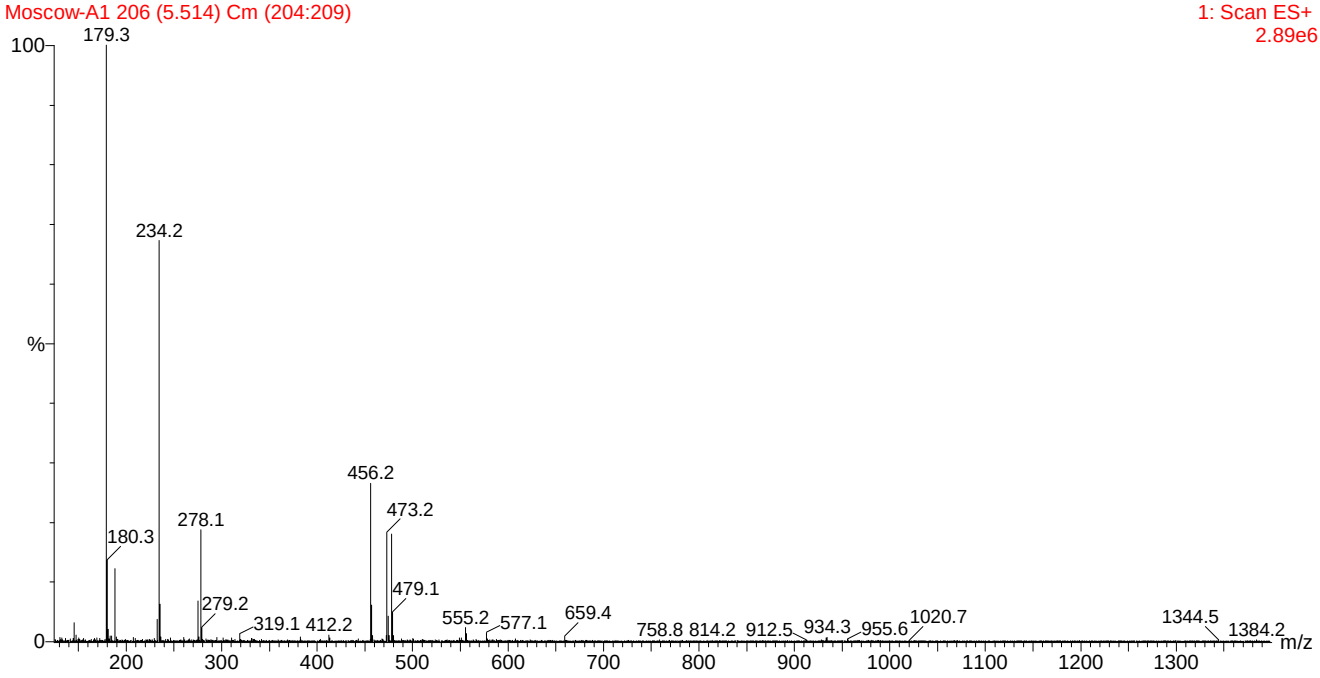
5{12}a


Lublin-Poland-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.18e7
Area
Time Height Area Area%
5.45 33297774 2530730.50 91.57
5.68 2979352 135580.89 4.91
6.75 2471671 97316.06 3.52
5.45
264.0
2530731
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
5{12}a
Lublin (Resin II)
Exact Mass 455.13
H
N
O
O
O
OH
CF3


Lublin-Poland-A3 205 (5.487) Cm (204:208)
1: Scan ES+
1.21e7
100
%
0
m/z
179.3
234.2
180.3
278.2
279.2
319.2
412.2
456.2
473.2
478.2
479.1
583.2
659.4
703.3
854.4
911.4
928.5
955.6
1011.3
1239.9
1291.7
1383.9
200 300 400 500 600 700 800 900 1000 1100 1200 1300

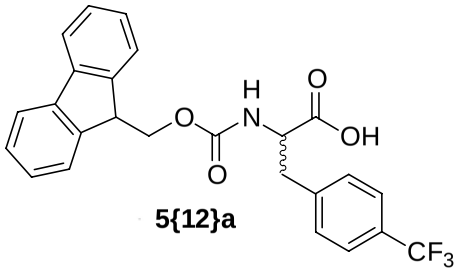
5{12}a


Moscow-A1 Sm (Mn, 1x1)
3: Diode Array
TIC
2.18e7
Area
Time Height Area Area%
5.47 23761708 1158121.50 94.73
5.68 832903 34841.76 2.85
6.75 769157 29647.58 2.42
5.47
266.0
1158122
100
%
-21
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
5{12}a
Moscow (Resin II)
Exact Mass 455.13

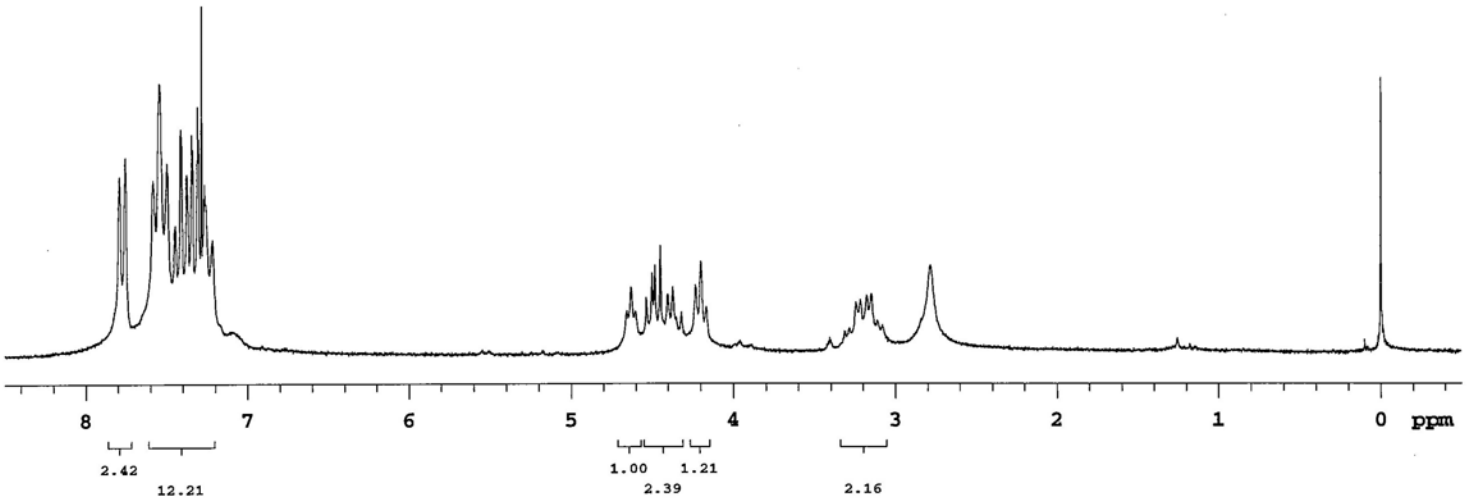

Moscow-A1 206 (5.514) Cm (204:209)
1: Scan ES+
2.89e6
100
%
0
m/z
179.3
234.2
180.3
278.1
279.2
319.1 412.2
456.2
473.2
479.1
555.2
577.1
659.4
758.8 814.2
912.5
934.3
955.6
1020.7
1344.5
1384.2
200 300 400 500 600 700 800 900 1000 1100 1200 1300

1H_BB#27_A3_P_CDCl3withCD3OD_02_01_07

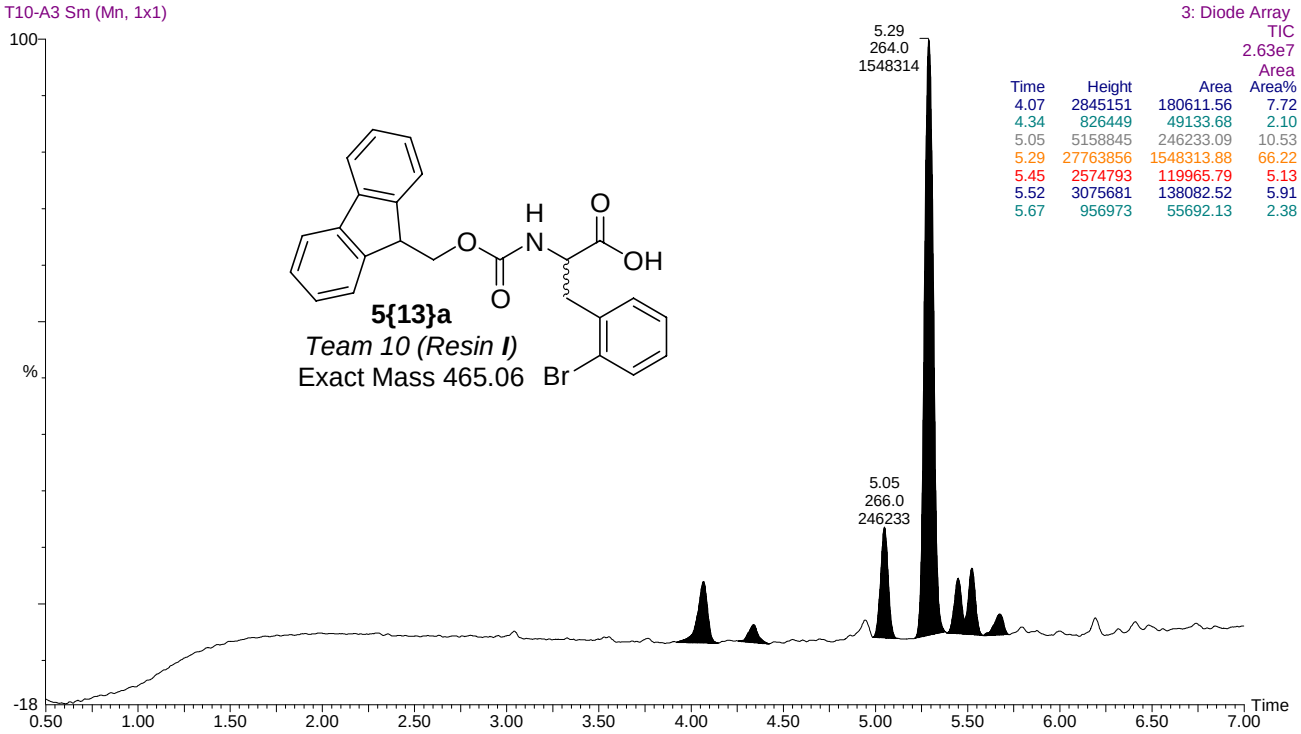
Pulse Sequence: s2pul

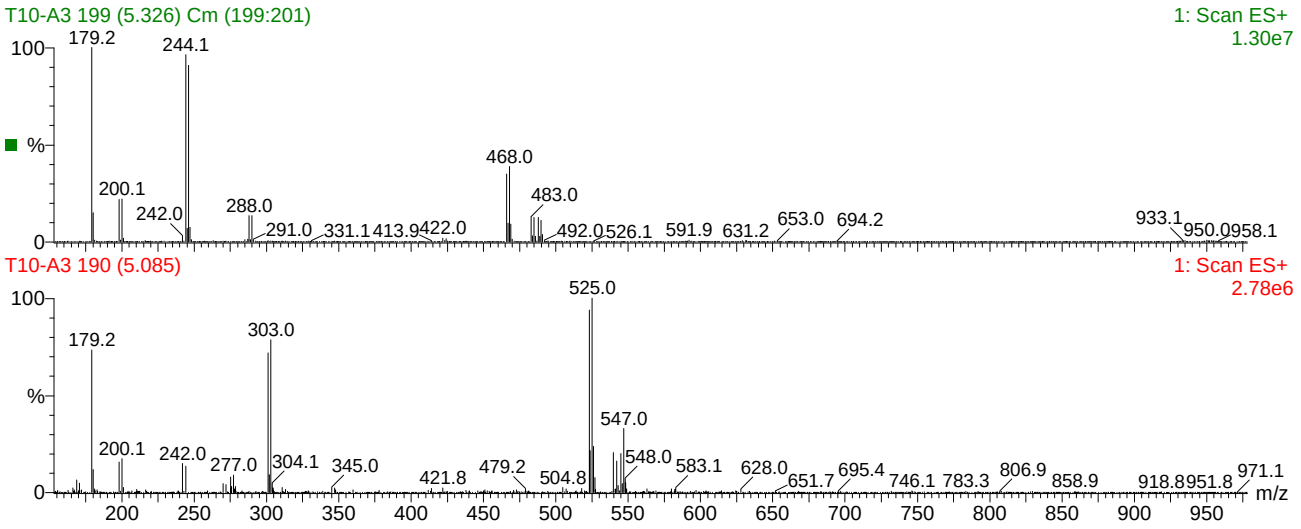


5{12}a

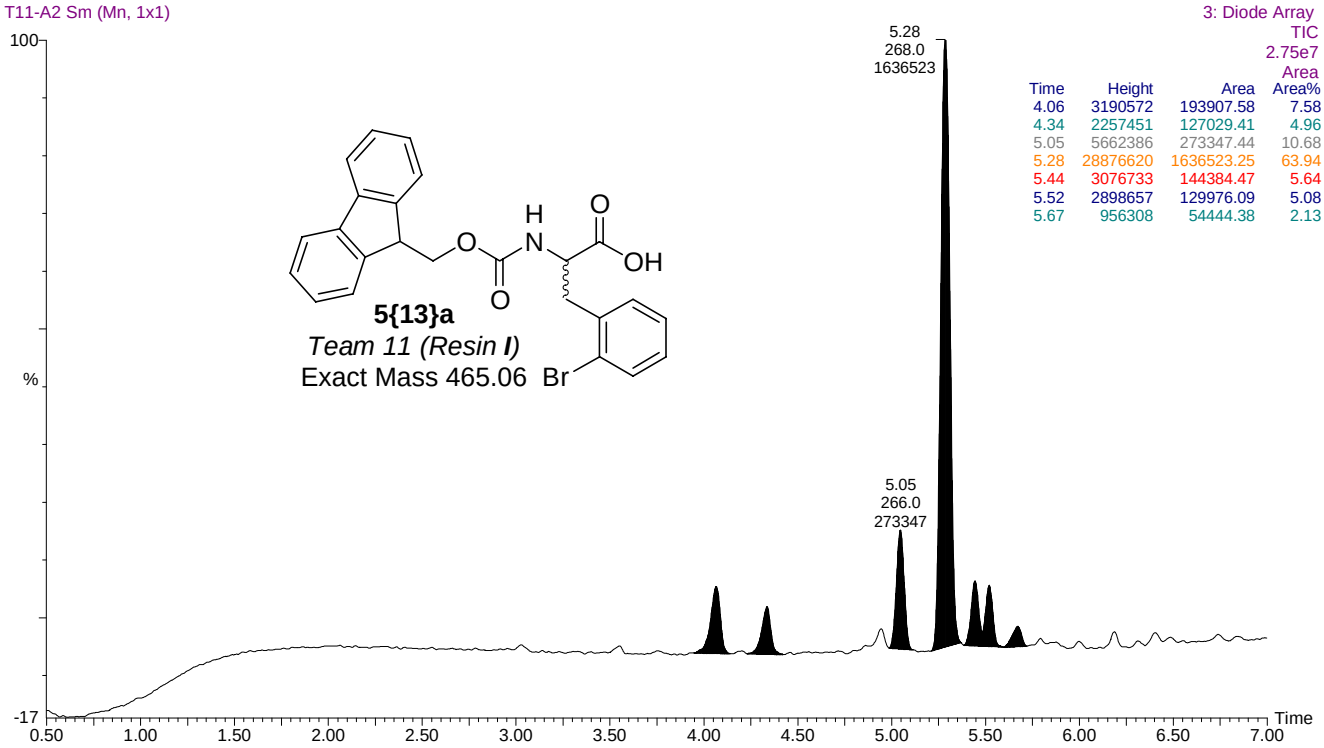


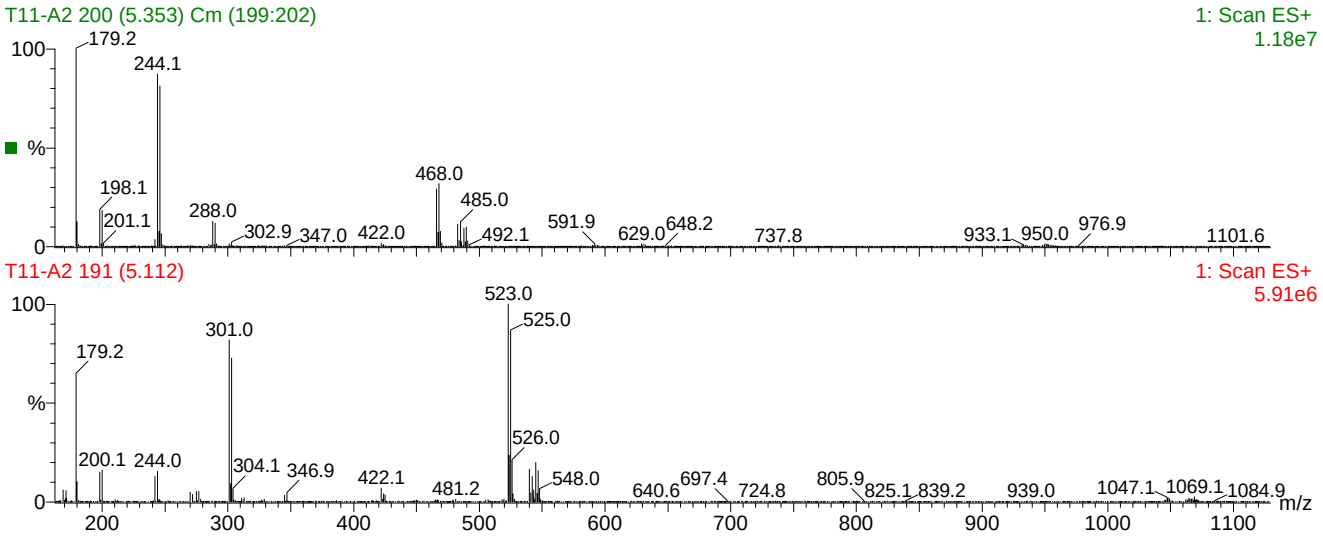
5{13}a


T10-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.63e7
Area
Time Height Area Area%
4.07 2845151 180611.56 7.72
4.34 826449 49133.68 2.10
5.05 5158845 246233.09 10.53
5.29 27763856 1548313.88 66.22
5.45 2574793 119965.79 5.13
5.52 3075681 138082.52 5.91
5.67 956973 55692.13 2.38
5.29
264.0
1548314
5.05
266.0
246233
5{13}a
Team 10 (Resin I)
Exact Mass 465.06
Br
OH
100
%
-18
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

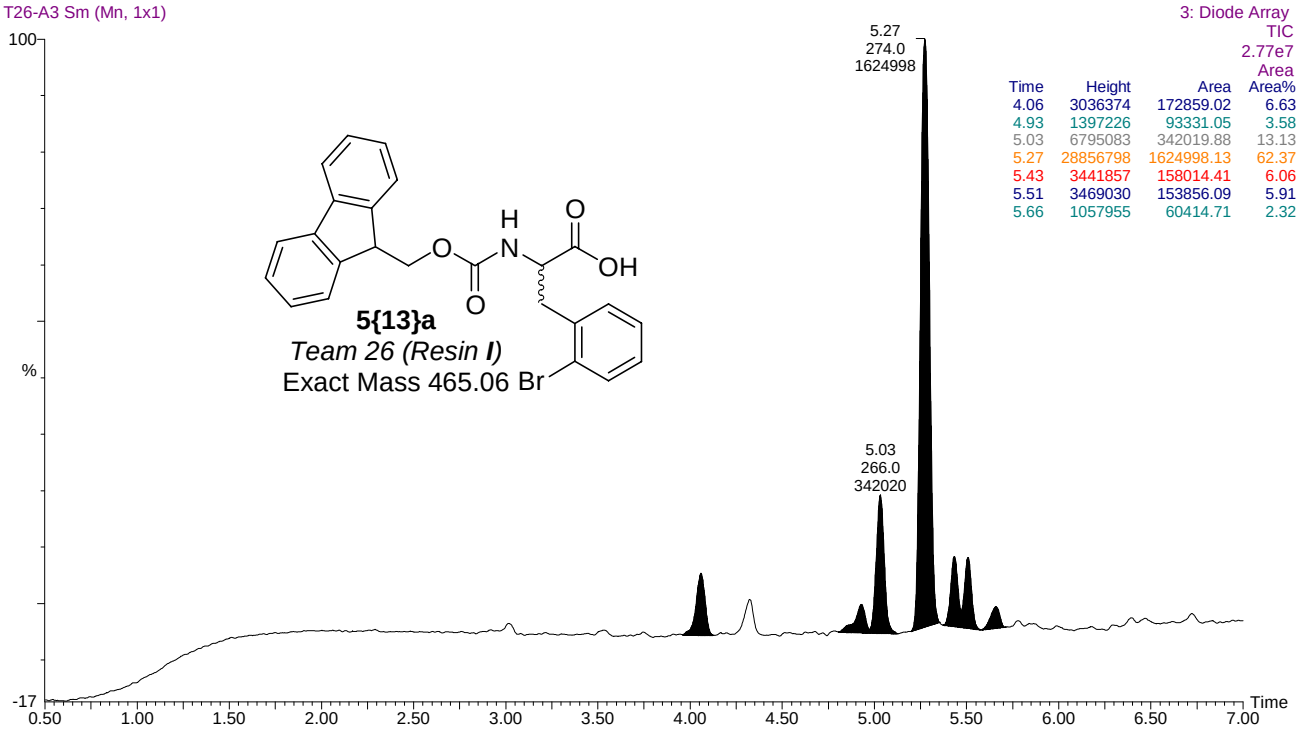

T10-A3 199 (5.326) Cm (199:201)
1: Scan ES+
1.30e7
179.2
244.1
200.1
242.0
288.0
291.0
331.1
413.9
422.0
468.0
483.0
492.0
526.1
591.9
631.2
653.0
694.2
933.1
950.0
958.1
T10-A3 190 (5.085)
1: Scan ES+
2.78e6
525.0
303.0
179.2
547.0
548.0
200.1
242.0
277.0
304.1
345.0
421.8
479.2
504.8
583.1
628.0
651.7
695.4
746.1
783.3
806.9
858.9
918.8
951.8
971.1
m/z
100
%
0
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

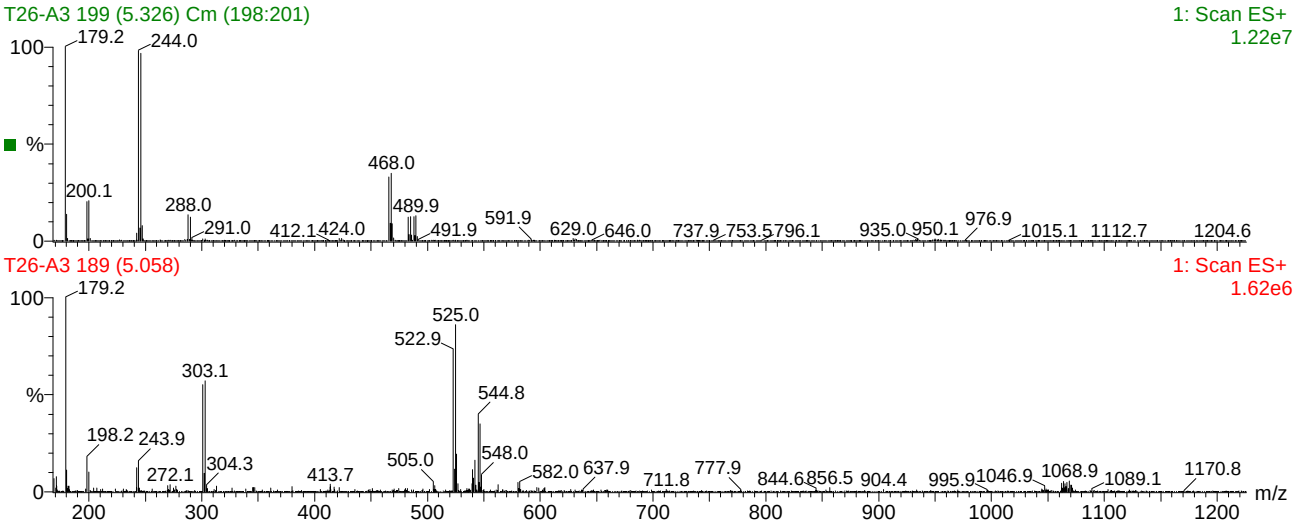
5{13}a


T11-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.75e7
Area
Time Height Area Area%
4.06 3190572 193907.58 7.58
4.34 2257451 127029.41 4.96
5.05 5662386 273347.44 10.68
5.28 28876620 1636523.25 63.94
5.44 3076733 144384.47 5.64
5.52 2898657 129976.09 5.08
5.67 956308 54444.38 2.13
5.28
268.0
1636523
5.05
266.0
273347
5{13}a
Team 11 (Resin I)
Exact Mass 465.06 Br
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

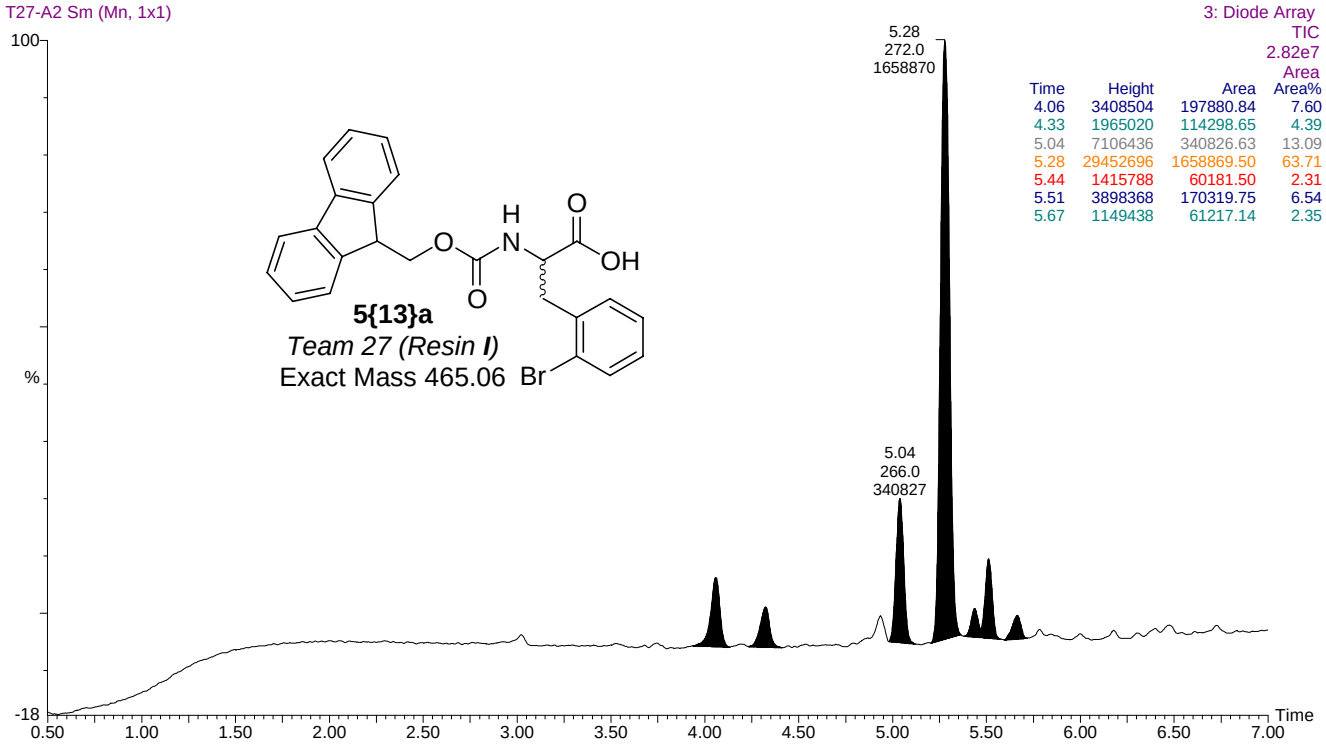

T11-A2 200 (5.353) Cm (199:202)
1: Scan ES+
1.18e7
100
%
0
179.2
244.1
198.1
201.1
288.0
302.9
347.0
422.0
468.0
485.0
492.1
591.9
629.0
648.2
737.8
933.1
950.0
976.9
1101.6
T11-A2 191 (5.112)
1: Scan ES+
5.91e6
100
%
0
523.0
525.0
301.0
179.2
526.0
200.1
244.0
304.1
346.9
422.1
481.2
548.0
640.6
697.4
724.8
805.9
825.1
839.2
939.0
1047.1
1069.1
1084.9
200 300 400 500 600 700 800 900 1000 1100
m/z

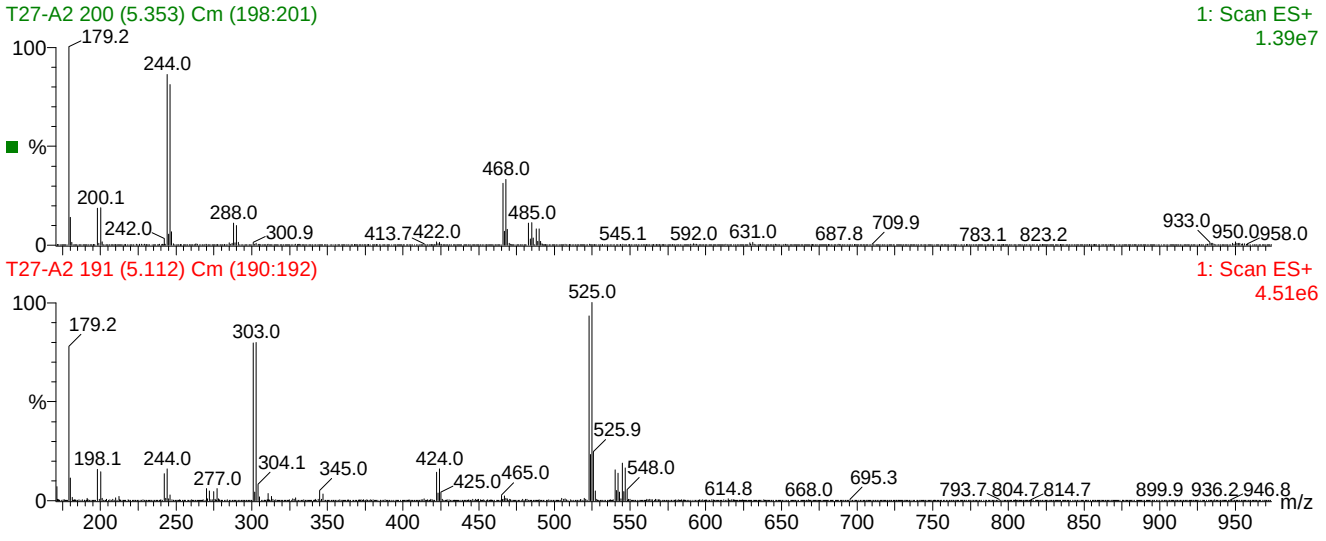
5{13}a


T26-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.77e7
Area
Time Height Area Area%
4.06 3036374 172859.02 6.63
4.93 1397226 93331.05 3.58
5.03 6795083 342019.88 13.13
5.27 28856798 1624998.13 62.37
5.43 3441857 158014.41 6.06
5.51 3469030 153856.09 5.91
5.66 1057955 60414.71 2.32
5.27
274.0
1624998
5.03
266.0
342020
5{13}a
Team 26 (Resin I)
Exact Mass 465.06 Br
100
%
-17
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time


T26-A3 199 (5.326) Cm (198:201)
1: Scan ES+
1.22e7
100
%
0
179.2 244.0 200.1 288.0 291.0 412.1 424.0 468.0 489.9 491.9 591.9 629.0 646.0 737.9 753.5 796.1 935.0 950.1 976.9 1015.1 1112.7 1204.6
T26-A3 189 (5.058)
1: Scan ES+
1.62e6
100
%
0
179.2 198.2 243.9 272.1 303.1 304.3 413.7 505.0 522.9 525.0 544.8 548.0 582.0 637.9 711.8 777.9 844.6 856.5 904.4 995.9 1046.9 1068.9 1089.1 1170.8
200 300 400 500 600 700 800 900 1000 1100 1200
m/z

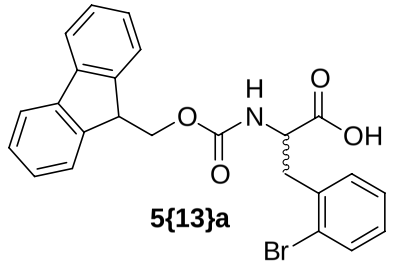
5{13}a


T27-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.82e7
Area
Time Height Area Area%
4.06 3408504 197880.84 7.60
4.33 1965020 114298.65 4.39
5.04 7106436 340826.63 13.09
5.28 29452696 1658869.50 63.71
5.44 1415788 60181.50 2.31
5.51 3898368 170319.75 6.54
5.67 1149438 61217.14 2.35
5.28
272.0
1658870
5.04
266.0
340827
5{13}a
Team 27 (Resin I)
Exact Mass 465.06
Br
OH
100
%
-18
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

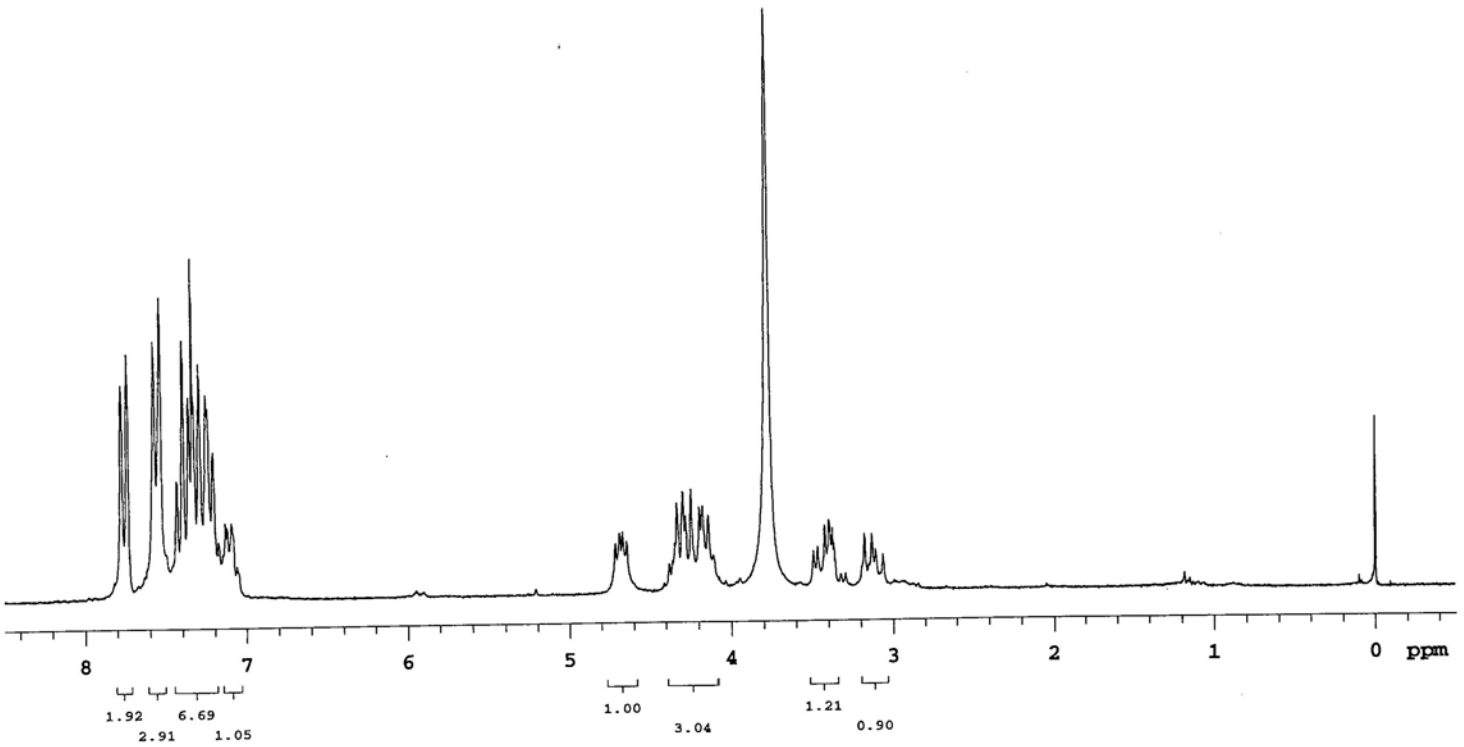

T27-A2 200 (5.353) Cm (198:201)
1: Scan ES+
1.39e7
100
%
0
179.2
244.0
200.1
242.0
288.0
300.9
413.7422.0
468.0
485.0
545.1
592.0
631.0
687.8
709.9
783.1
823.2
933.0
950.0958.0
T27-A2 191 (5.112) Cm (190:192)
1: Scan ES+
4.51e6
100
%
0
179.2
303.0
525.0
525.9
198.1
244.0
277.0
304.1
345.0
424.0
425.0
465.0
548.0
614.8
668.0
695.3
793.7804.7814.7
899.9
936.2946.8
m/z
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

1H_RR#40_A3_CD3ODinCDCl3_02_22_07

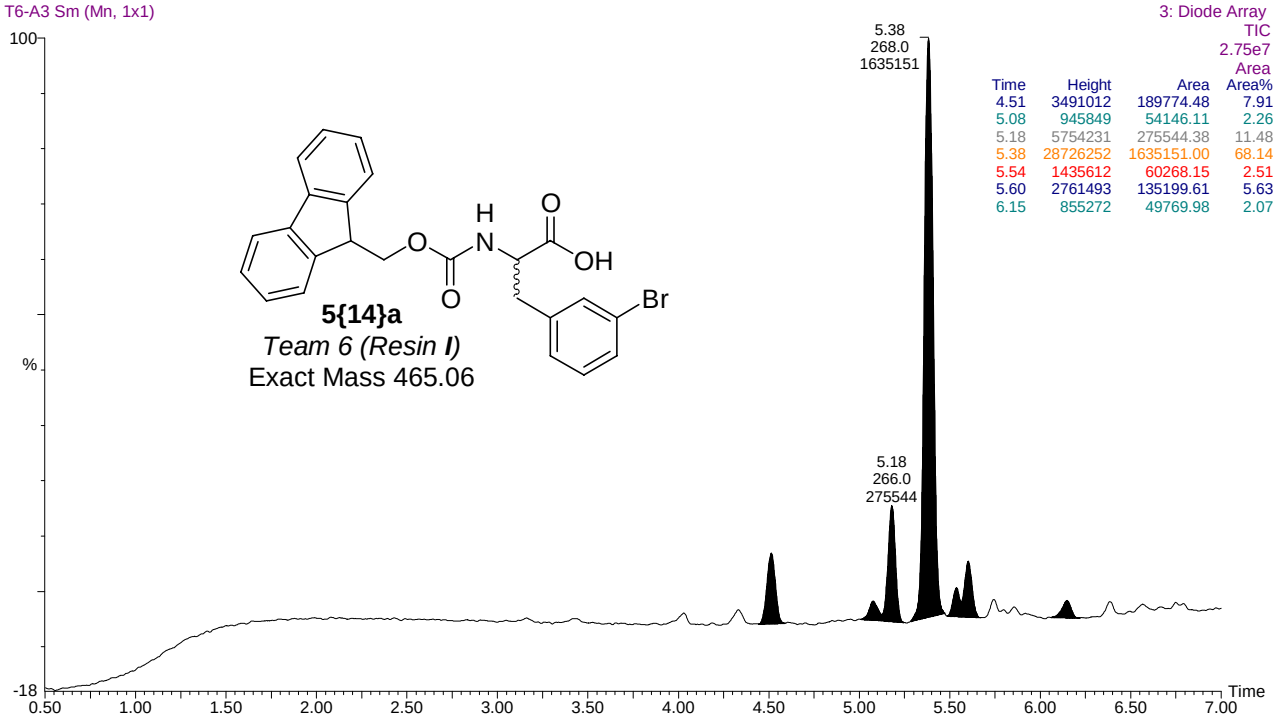
Pulse Sequence: s2pul

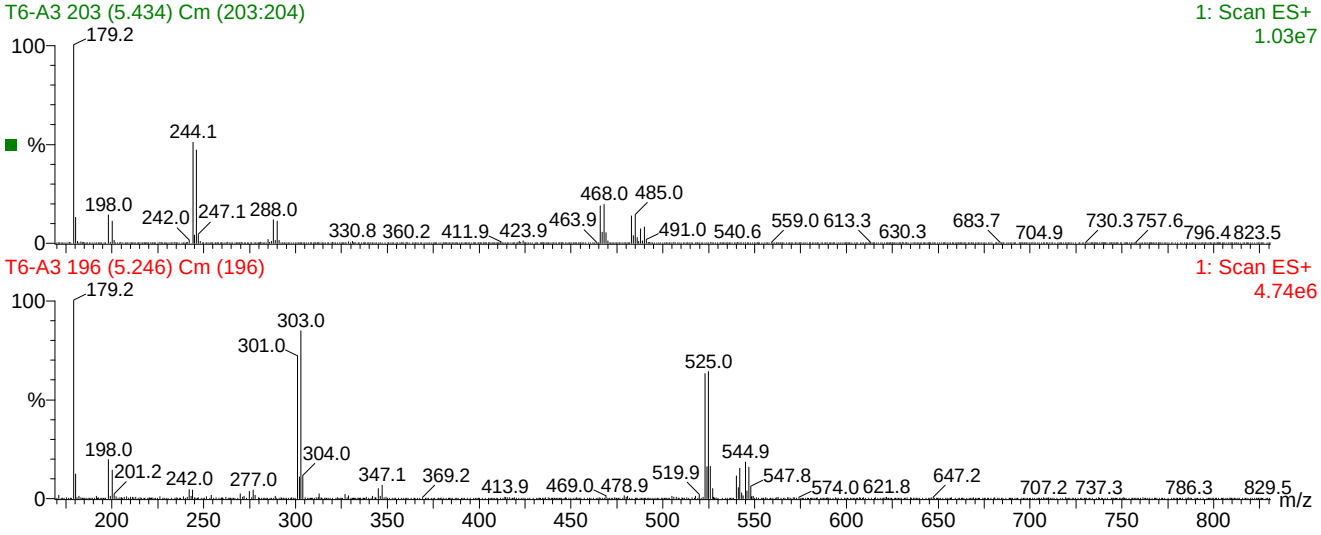


5{13}a

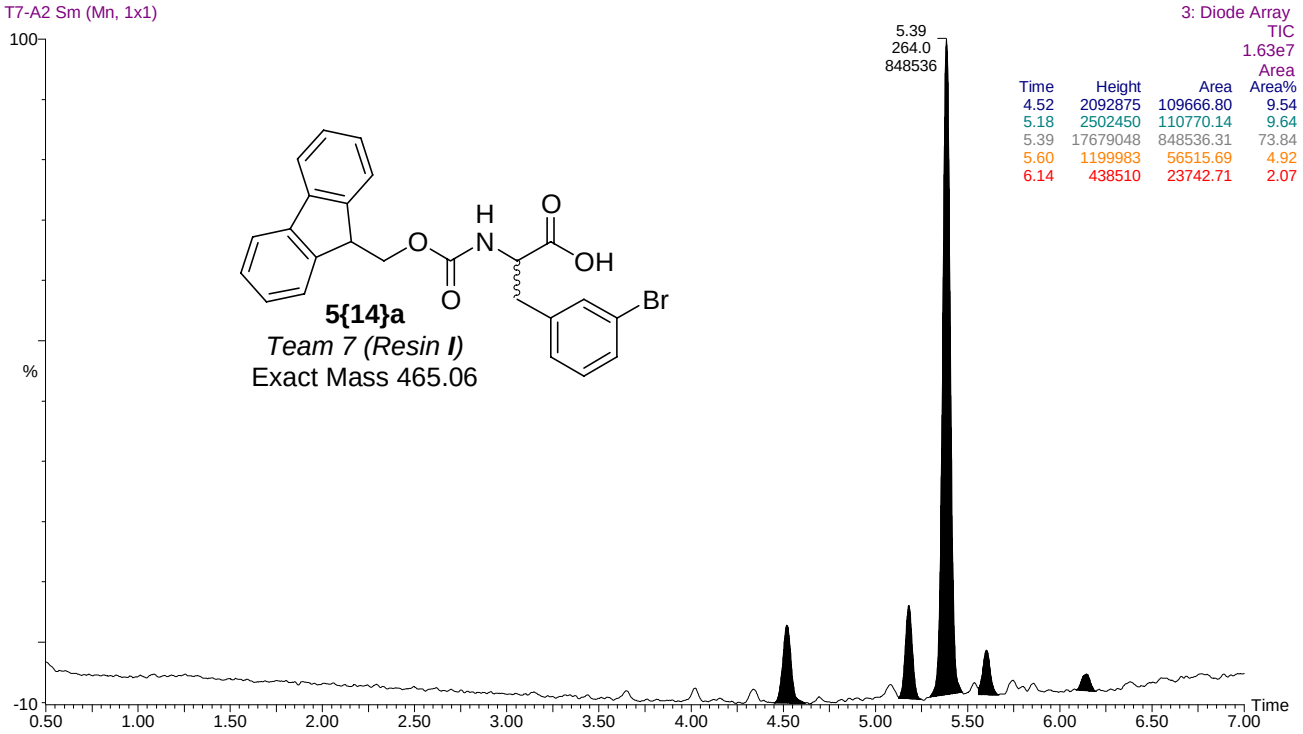


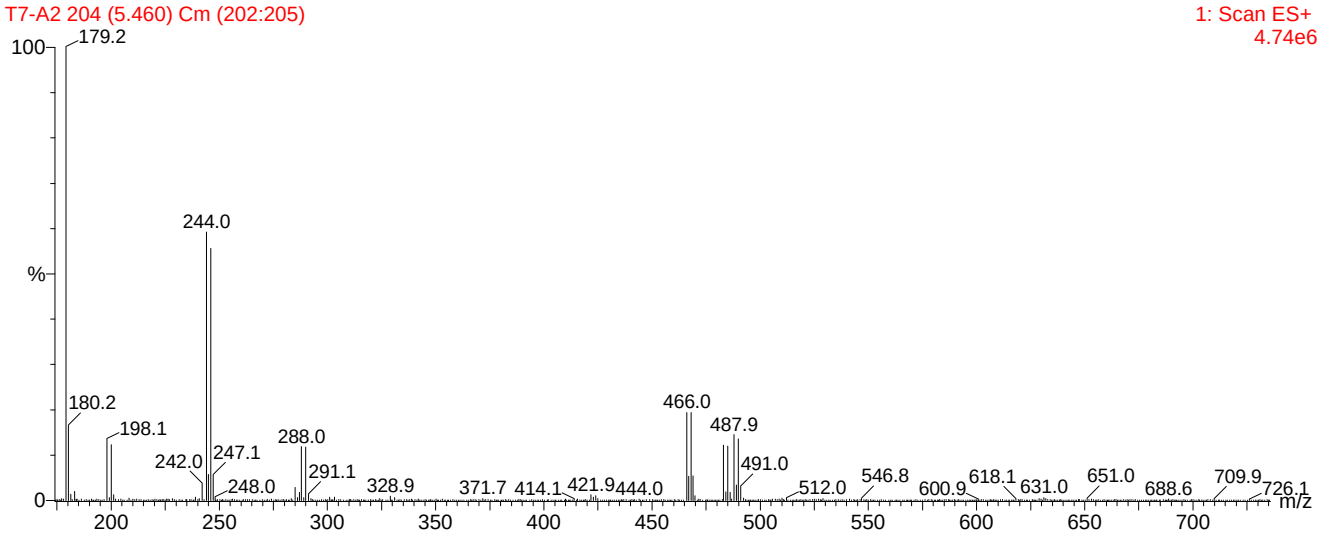
5{14}a


T6-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.75e7
Area
Time Height Area Area%
4.51 3491012 189774.48 7.91
5.08 945849 54146.11 2.26
5.18 5754231 275544.38 11.48
5.38 28726252 1635151.00 68.14
5.54 1435612 60268.15 2.51
5.60 2761493 135199.61 5.63
6.15 855272 49769.98 2.07
5.38
268.0
1635151
5.18
266.0
275544
5{14}a
Team 6 (Resin I)
Exact Mass 465.06
Time

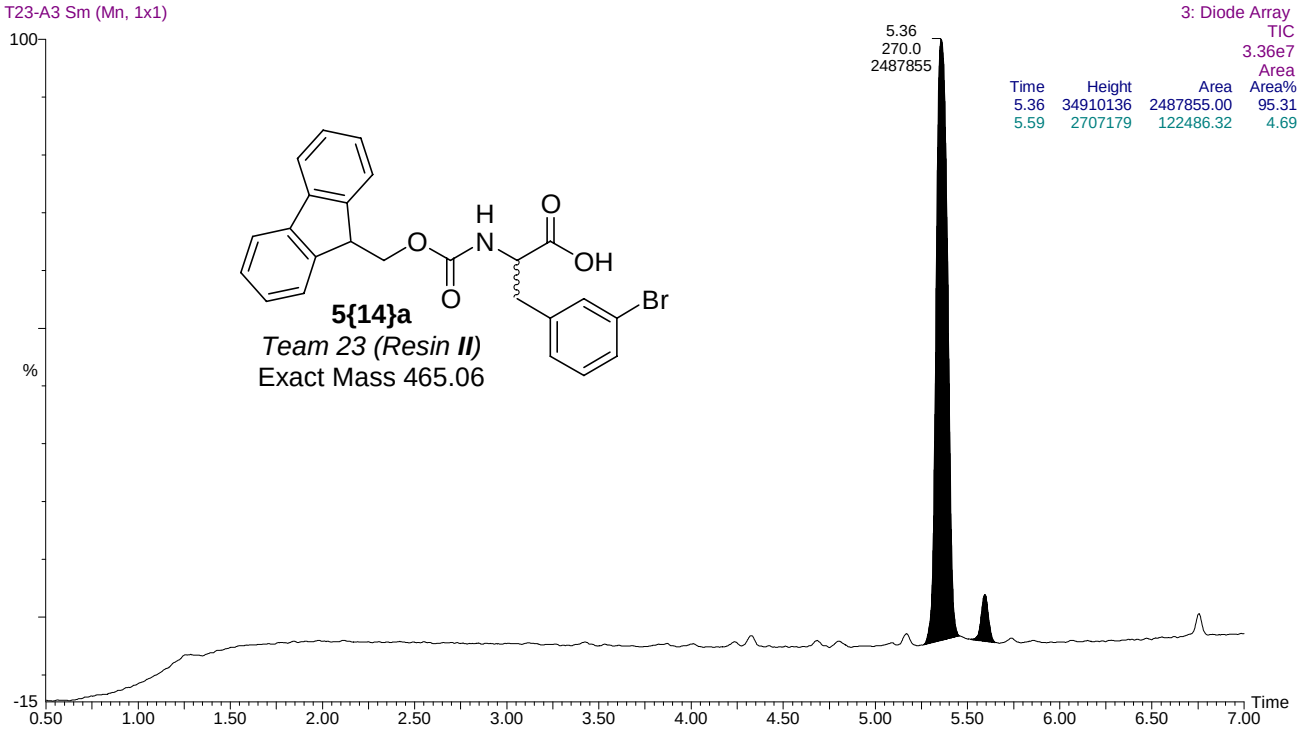

T6-A3 203 (5.434) Cm (203:204)
1: Scan ES+
1.03e7
T6-A3 196 (5.246) Cm (196)
1: Scan ES+
4.74e6
m/z

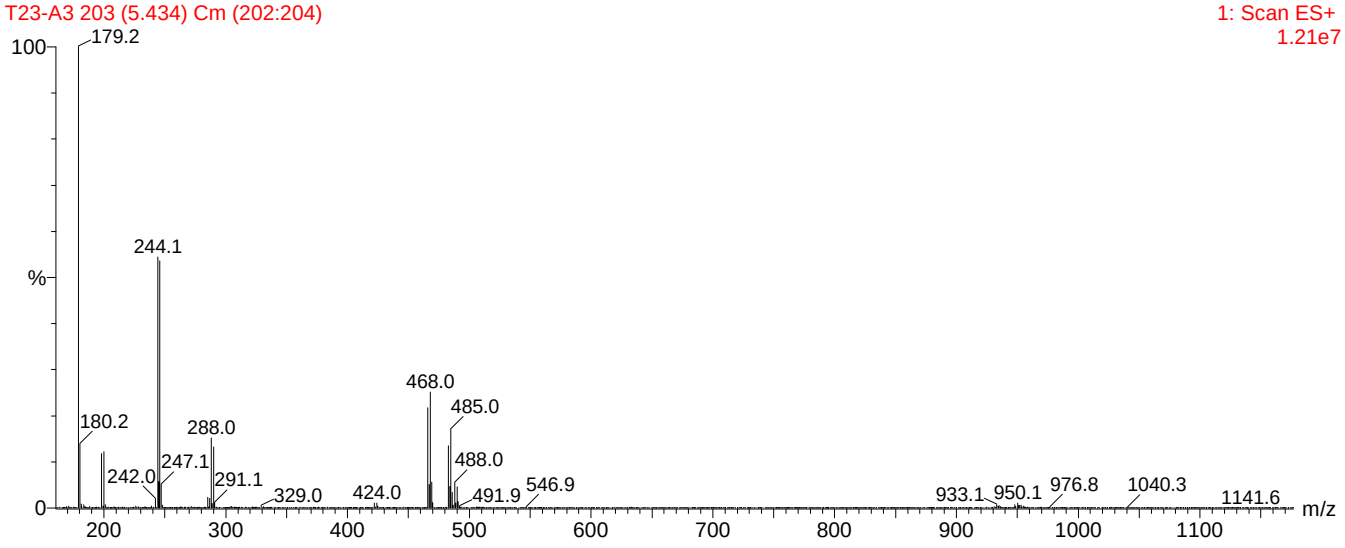
5{14}a


T7-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
1.63e7
Area
Time Height Area Area%
4.52 2092875 109666.80 9.54
5.18 2502450 110770.14 9.64
5.39 17679048 848536.31 73.84
5.60 1199983 56515.69 4.92
6.14 438510 23742.71 2.07
5.39
264.0
848536
100
%
-10
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time
H
N
O
O
O
OH
Br
5{14}a
Team 7 (Resin I)
Exact Mass 465.06

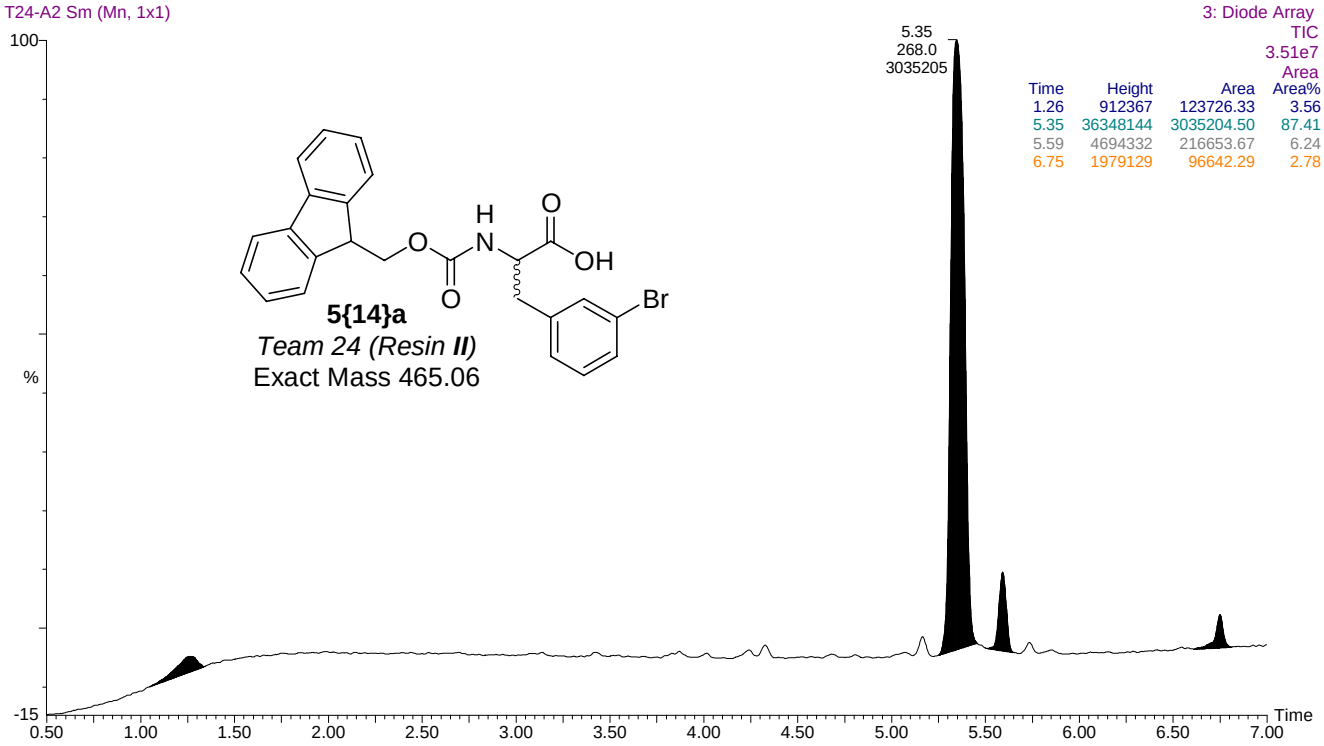

T7-A2 204 (5.460) Cm (202:205)
1: Scan ES+
4.74e6
100
%
0
179.2
244.0
180.2
198.1
242.0
247.1
248.0
288.0
291.1
328.9
371.7
414.1
421.9
444.0
466.0
487.9
491.0
512.0
546.8
600.9
618.1
631.0
651.0
688.6
709.9
726.1
200 250 300 350 400 450 500 550 600 650 700
m/z

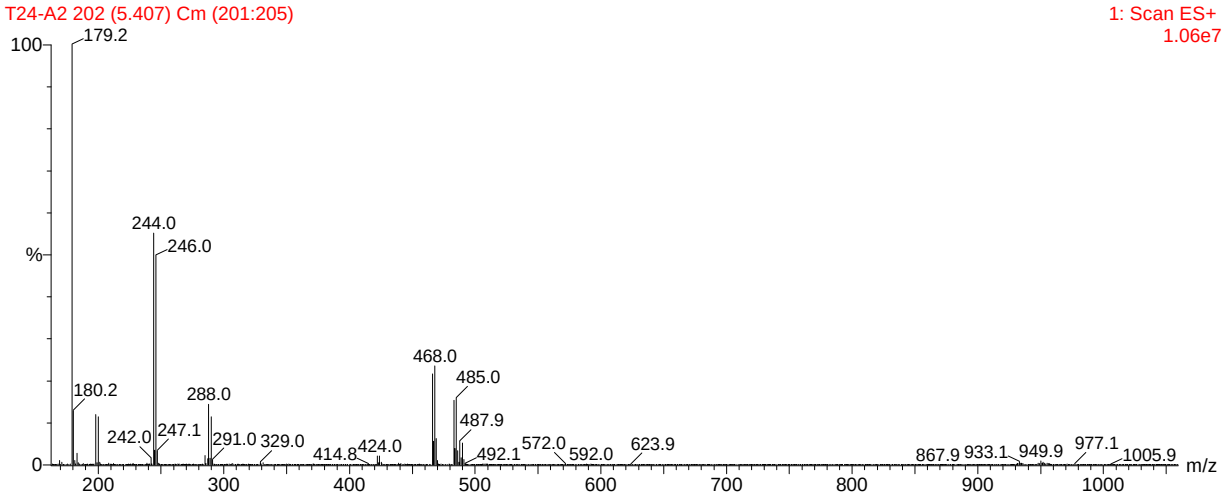
5{14}a


T23-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.36e7
Area
Time Height Area Area%
5.36 34910136 2487855.00 95.31
5.59 2707179 122486.32 4.69
5.36
270.0
2487855
100
%
-15
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
OH
O
O
Br
5{14}a
Team 23 (Resin II)
Exact Mass 465.06

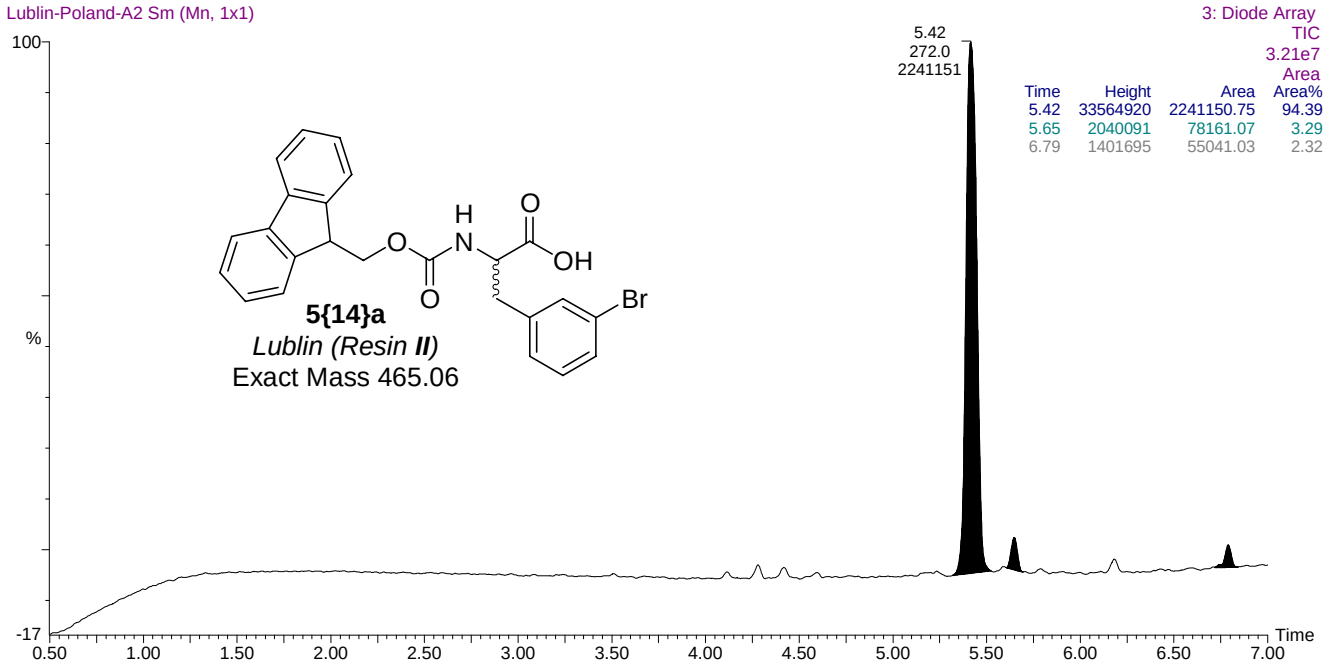

T23-A3 203 (5.434) Cm (202:204)
1: Scan ES+
1.21e7
100
%
0
m/z
179.2
244.1
180.2
288.0
247.1
242.0
291.1
329.0
424.0
468.0
485.0
488.0
491.9
546.9
933.1
950.1
976.8
1040.3
1141.6
200 300 400 500 600 700 800 900 1000 1100

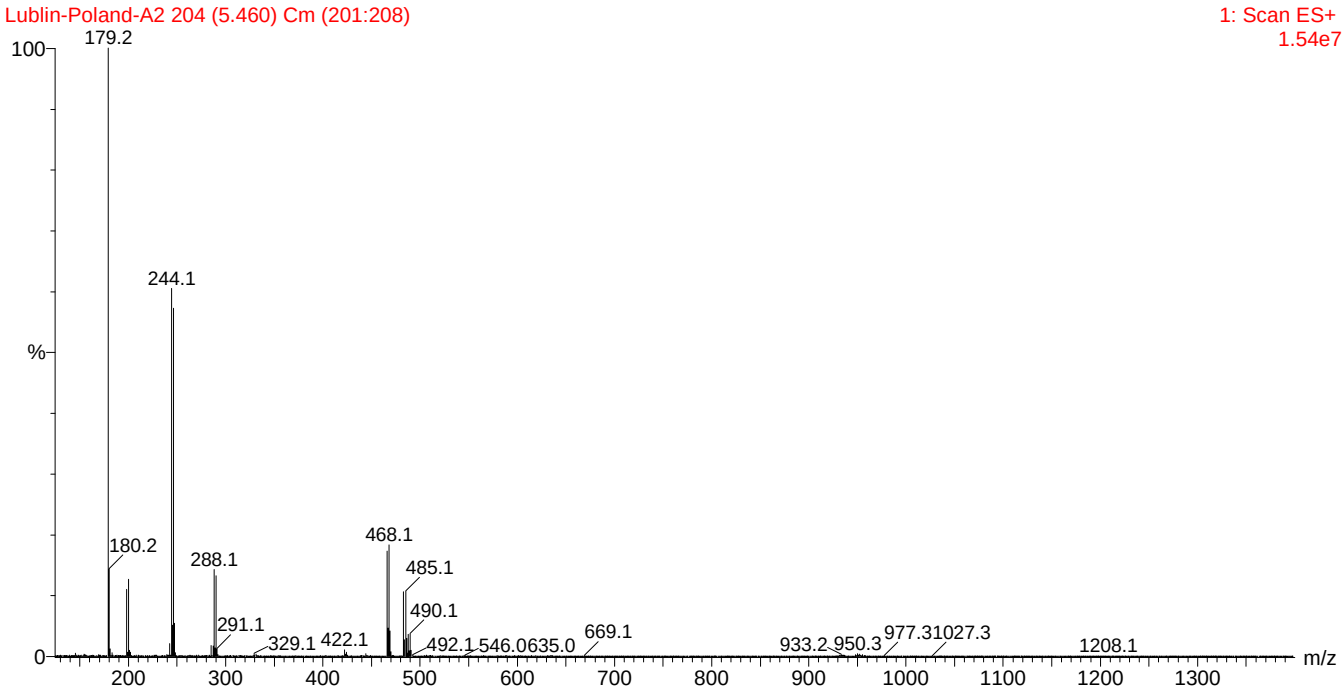
5{14}a


T24-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.51e7
Area
Time Height Area Area%
1.26 912367 123726.33 3.56
5.35 36348144 3035204.50 87.41
5.59 4694332 216653.67 6.24
6.75 1979129 96642.29 2.78
5.35
268.0
3035205
100
%
-15
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
OH
O
Br
5{14}a
Team 24 (Resin II)
Exact Mass 465.06

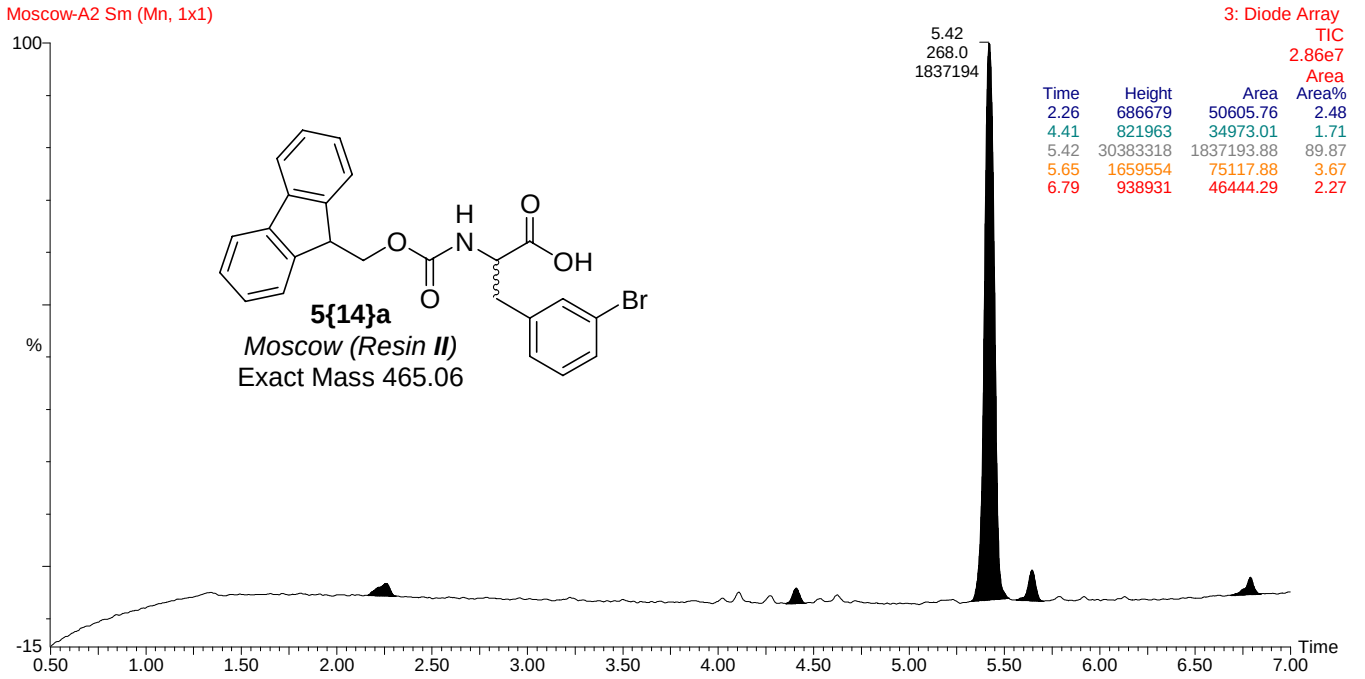

T24-A2 202 (5.407) Cm (201:205)
1: Scan ES+
1.06e7
100
%
0
179.2
244.0
246.0
180.2
288.0
242.0
247.1
291.0
329.0
414.8
424.0
468.0
485.0
487.9
492.1
572.0
592.0
623.9
867.9
933.1
949.9
977.1
1005.9
200 300 400 500 600 700 800 900 1000
m/z

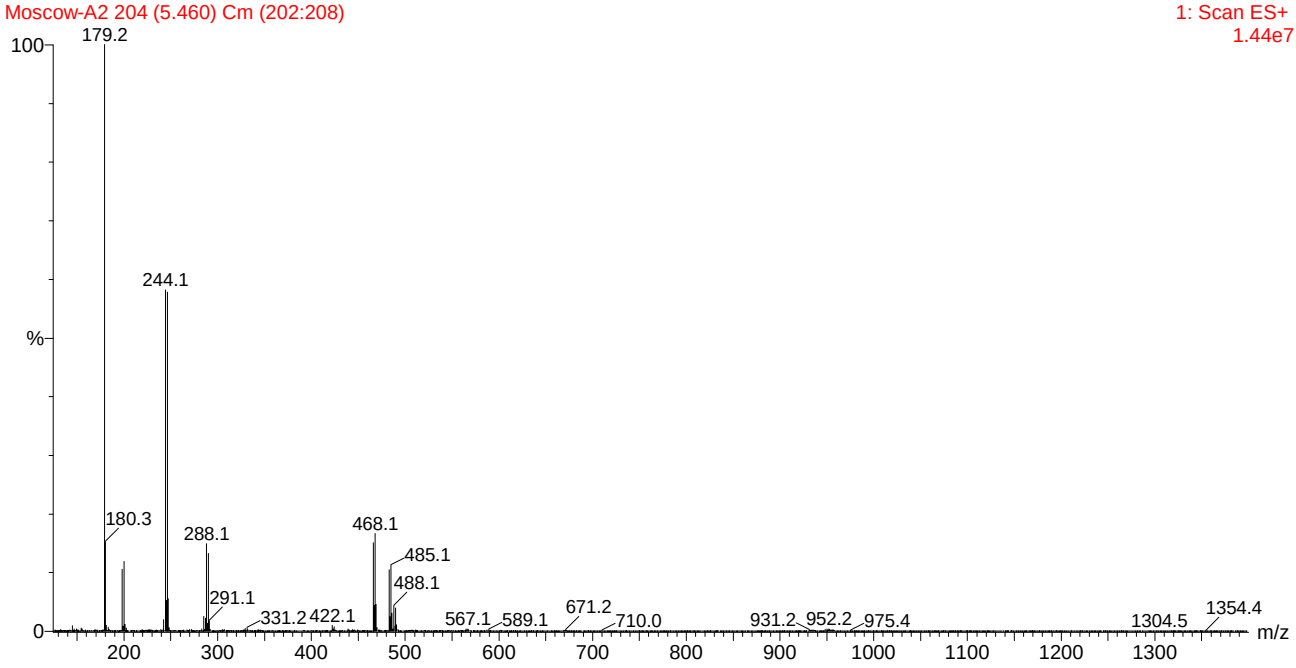
5{14}a


Lublin-Poland-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.21e7
Area
5.42
272.0
2241151
Time Height Area Area%
5.42 33564920 2241150.75 94.39
5.65 2040091 78161.07 3.29
6.79 1401695 55041.03 2.32
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
OH
O
Br
5{14}a
Lublin (Resin II)
Exact Mass 465.06


Lublin-Poland-A2 204 (5.460) Cm (201:208)
1: Scan ES+
1.54e7
100
%
0
m/z
179.2
244.1
180.2
288.1
291.1
329.1
422.1
468.1
485.1
490.1
492.1
546.0
635.0
669.1
933.2
950.3
977.3
1027.3
1208.1
200 300 400 500 600 700 800 900 1000 1100 1200 1300

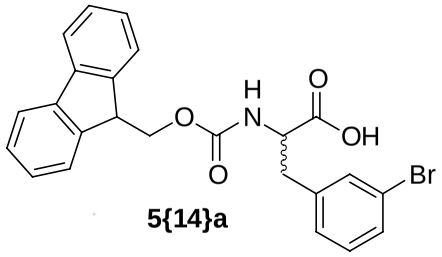
5{14}a


Moscow-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.86e7
Area
5.42
268.0
1837194
Time Height Area Area%
2.26 686679 50605.76 2.48
4.41 821963 34973.01 1.71
5.42 30383318 1837193.88 89.87
5.65 1659554 75117.88 3.67
6.79 938931 46444.29 2.27
100
%
-15
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
OH
O
O
Br
5{14}a
Moscow (Resin II)
Exact Mass 465.06

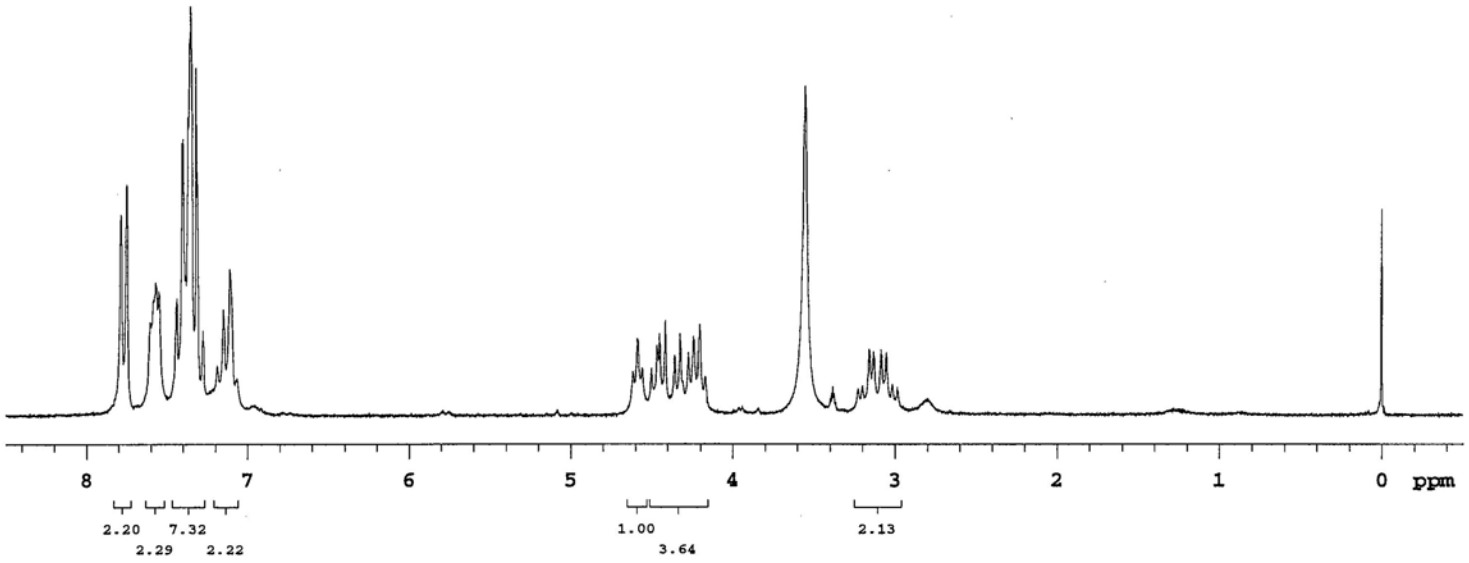

Moscow-A2 204 (5.460) Cm (202:208)
1: Scan ES+
1.44e7
100
%
0
179.2
244.1
180.3
288.1
291.1
331.2
422.1
468.1
485.1
488.1
567.1
589.1
671.2
710.0
931.2
952.2
975.4
1304.5
1354.4
m/z
200 300 400 500 600 700 800 900 1000 1100 1200 1300

1H_BB#40_B1_CD3ODinCDCl3_02_07

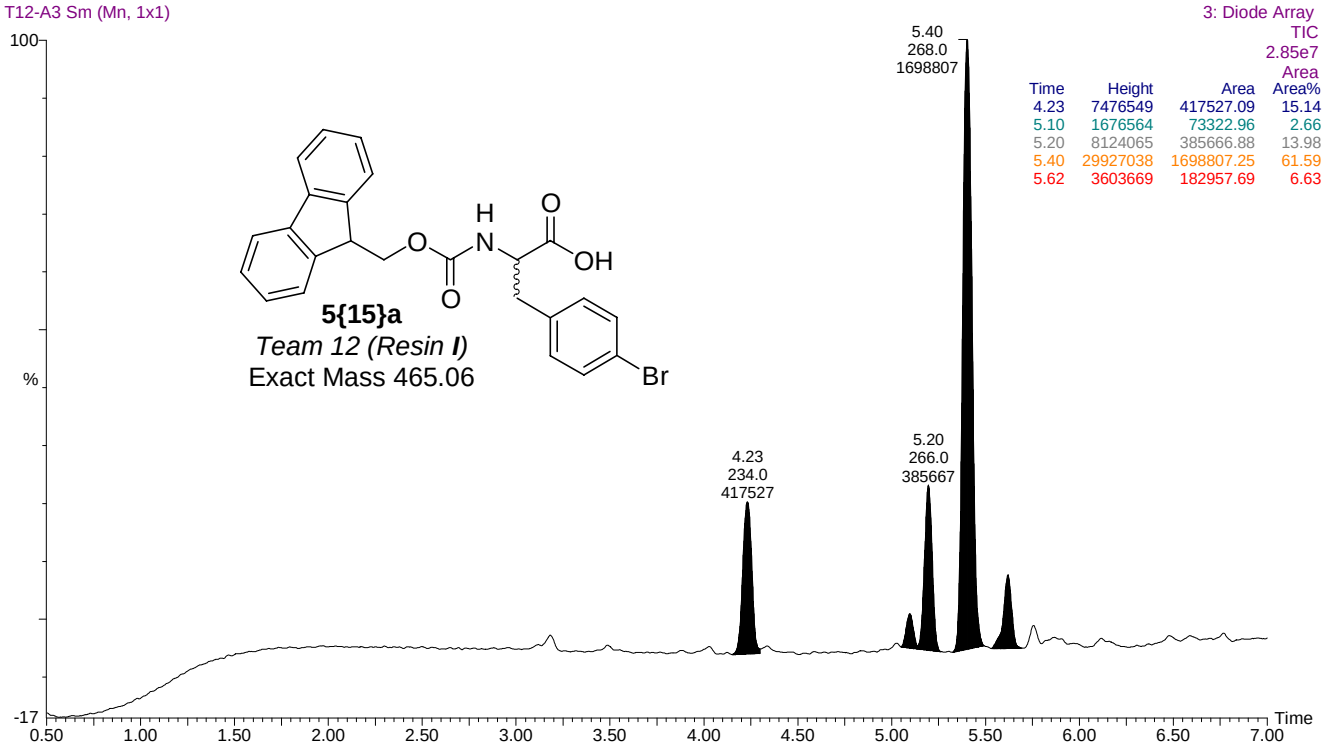
Pulse Sequence: s2pul

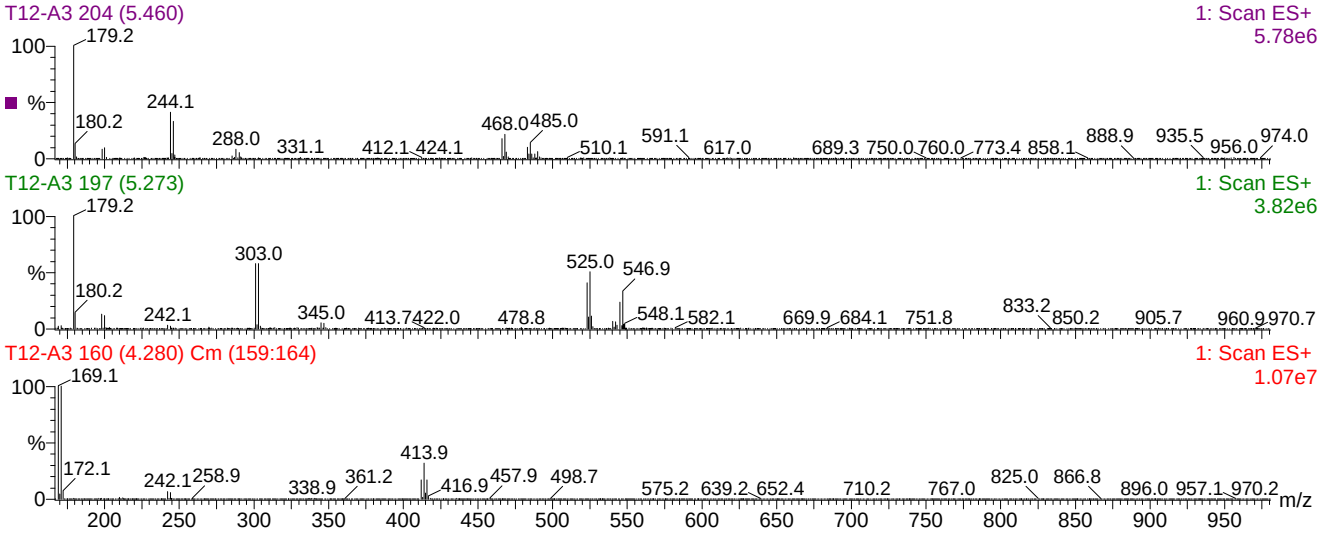


5{14}a

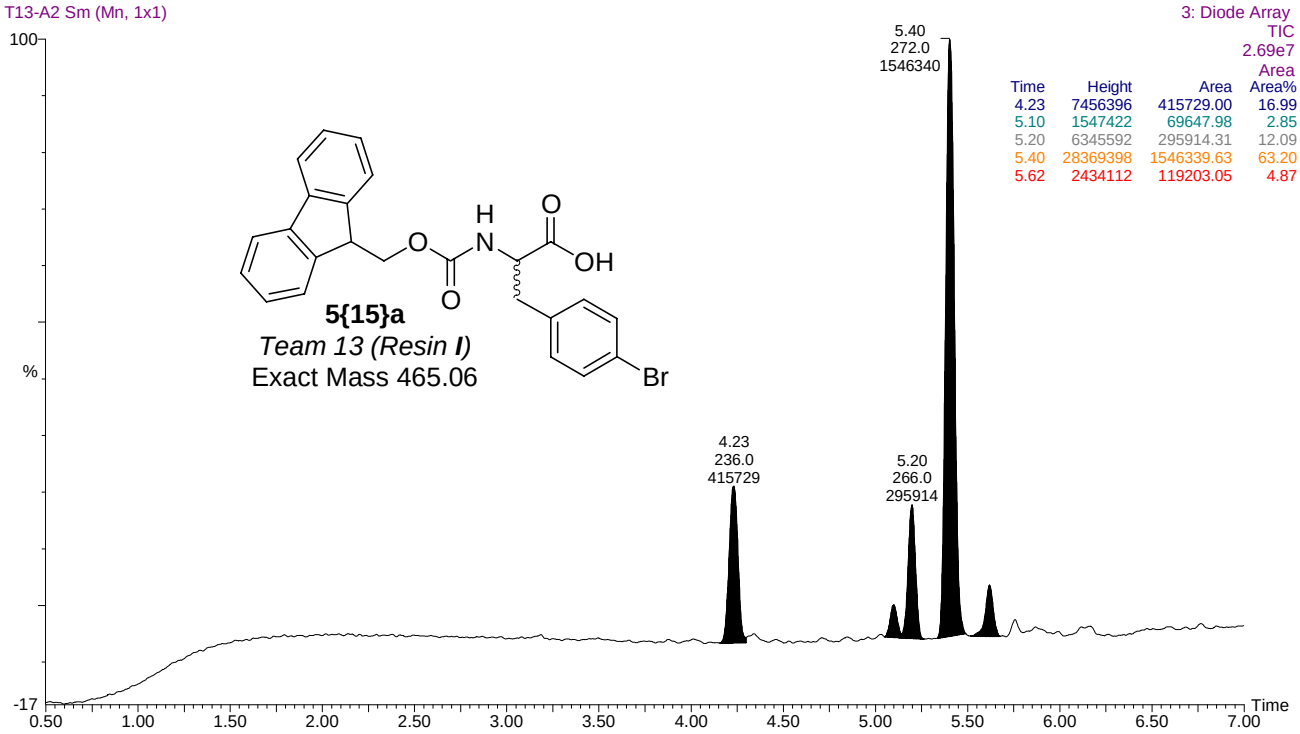


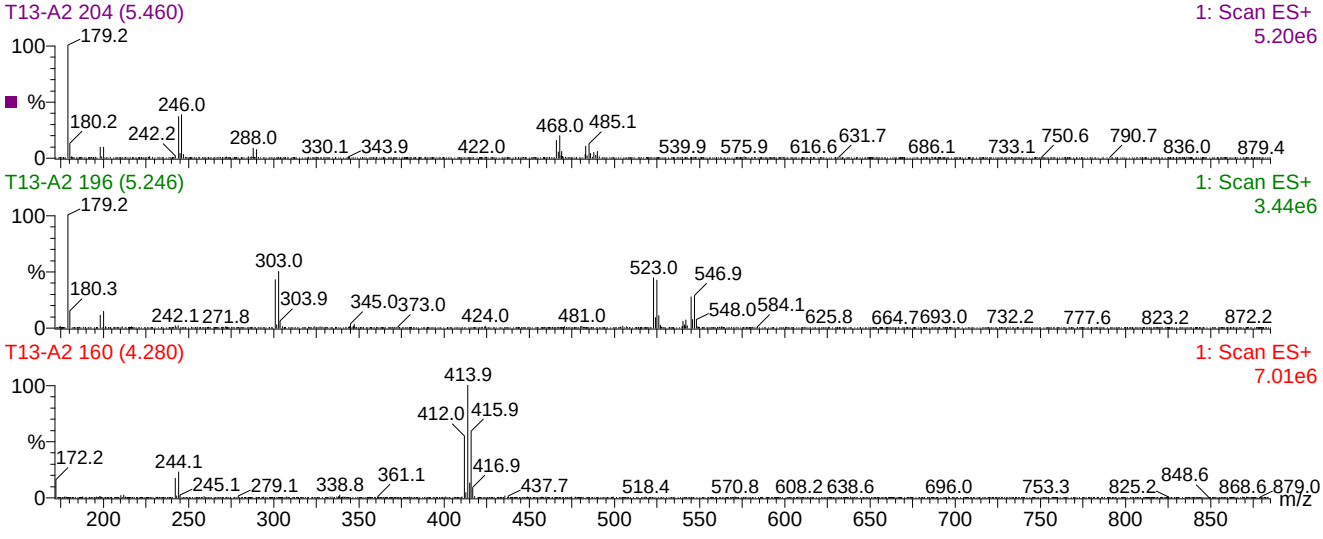
5{15}a


T12-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.85e7
Area
Time Height Area Area%
4.23 7476549 417527.09 15.14
5.10 1676564 73322.96 2.66
5.20 8124065 385666.88 13.98
5.40 29927038 1698807.25 61.59
5.62 3603669 182957.69 6.63
5.40
268.0
1698807
5.20
266.0
385667
4.23
234.0
417527
5{15}a
Team 12 (Resin I)
Exact Mass 465.06
Br
OH
Time

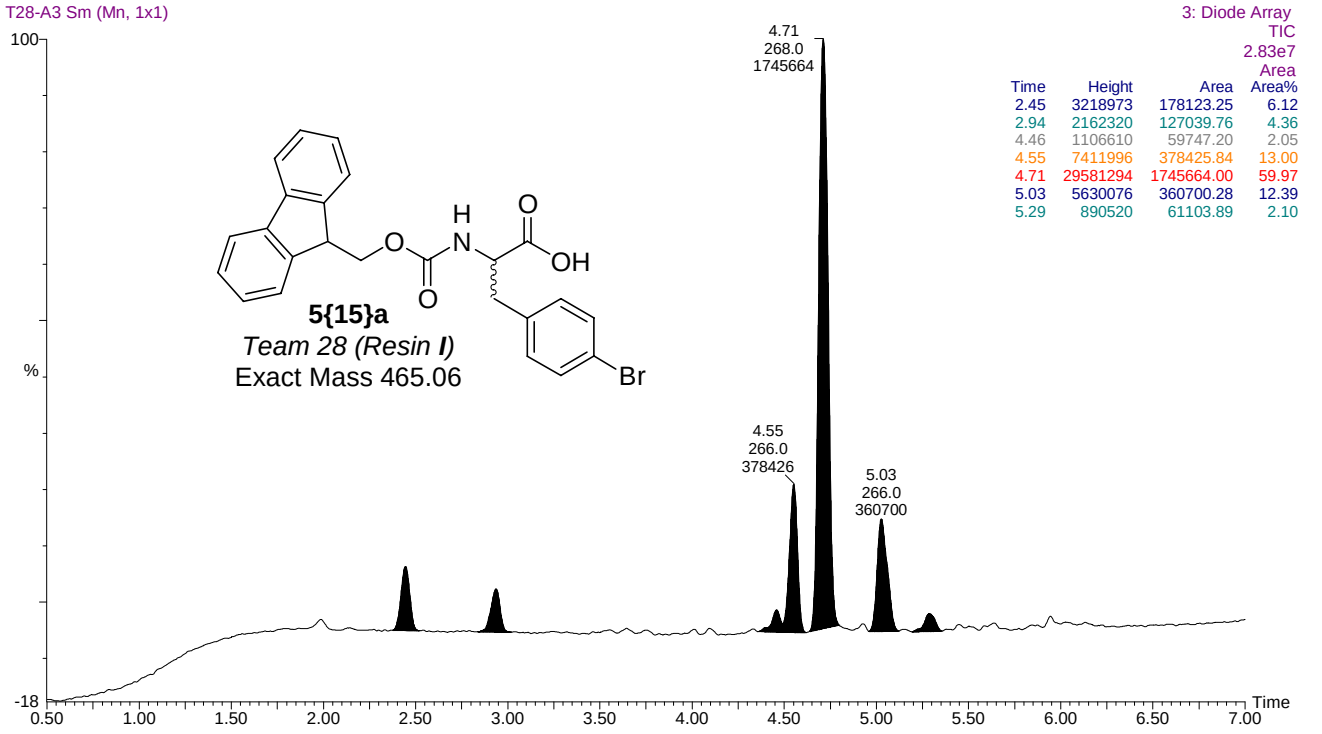

T12-A3 204 (5.460)
1: Scan ES+
5.78e6
T12-A3 197 (5.273)
1: Scan ES+
3.82e6
T12-A3 160 (4.280) Cm (159:164)
1: Scan ES+
1.07e7
m/z

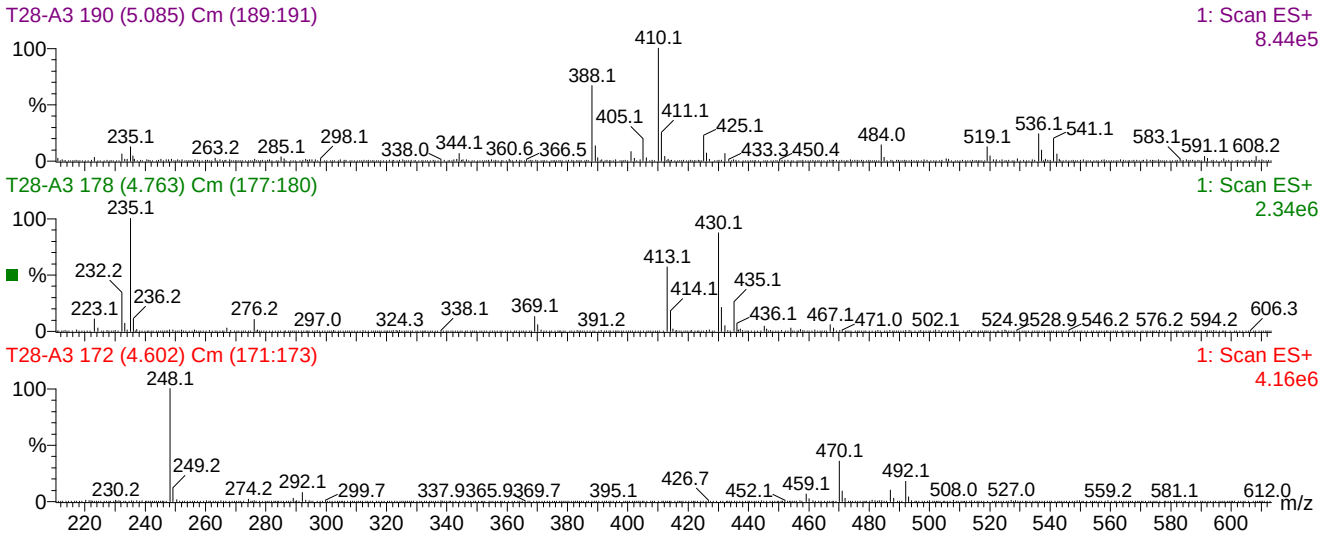
5{15}a


T13-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.69e7
Area
Time Height Area Area%
4.23 7456396 415729.00 16.99
5.10 1547422 69647.98 2.85
5.20 6345592 295914.31 12.09
5.40 28369398 1546339.63 63.20
5.62 2434112 119203.05 4.87
5.40
272.0
1546340
4.23
236.0
415729
5.20
266.0
295914
5.10
5.20
5.40
5.62
5{15}a
Team 13 (Resin I)
Exact Mass 465.06
Br
OH
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

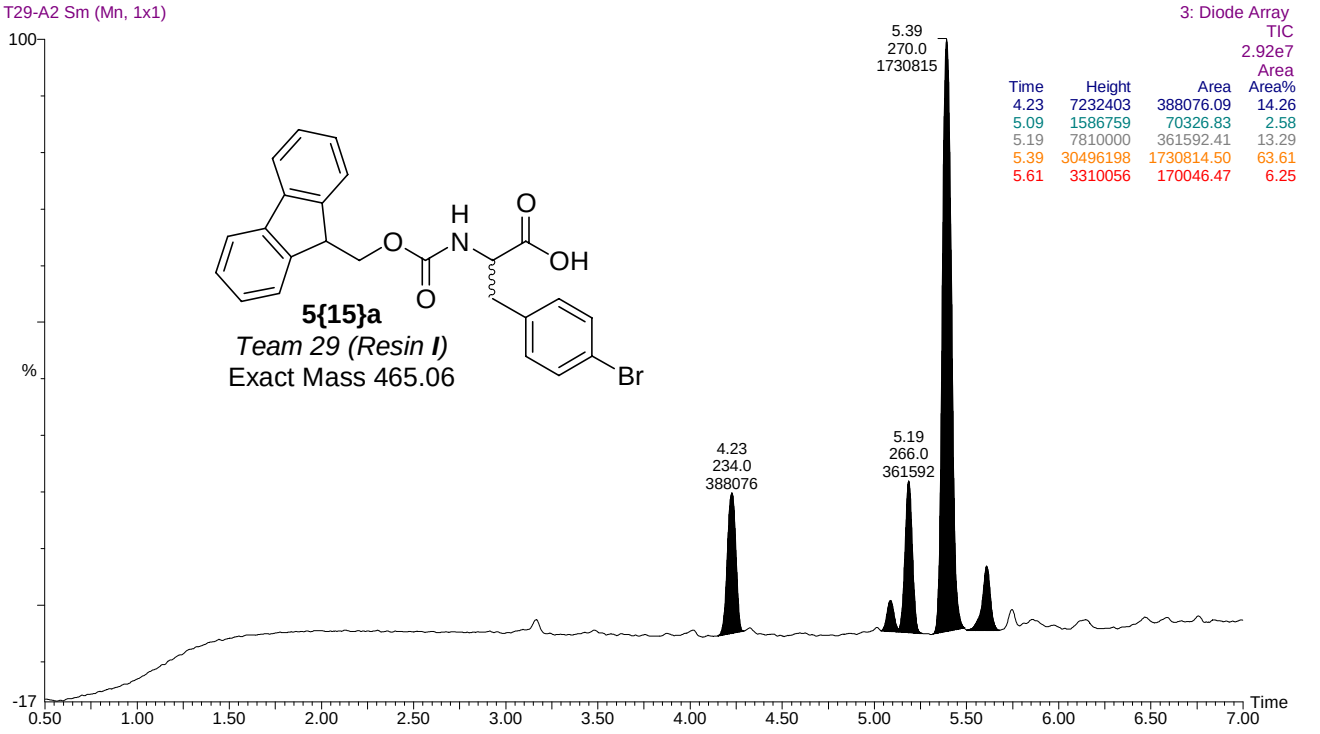

T13-A2 204 (5.460)
1: Scan ES+
5.20e6
100
%
0
179.2
180.2
242.2
246.0
288.0
330.1
343.9
422.0
468.0
485.1
539.9
575.9
616.6
631.7
686.1
733.1
750.6
790.7
836.0
879.4
T13-A2 196 (5.246)
1: Scan ES+
3.44e6
179.2
180.3
242.1
271.8
303.0
303.9
345.0
373.0
424.0
481.0
523.0
546.9
548.0
584.1
625.8
664.7
693.0
732.2
777.6
823.2
872.2
T13-A2 160 (4.280)
1: Scan ES+
7.01e6
413.9
412.0
415.9
416.9
172.2
244.1
245.1
279.1
338.8
361.1
437.7
518.4
570.8
608.2
638.6
696.0
753.3
825.2
848.6
868.6
879.0
200 250 300 350 400 450 500 550 600 650 700 750 800 850
m/z

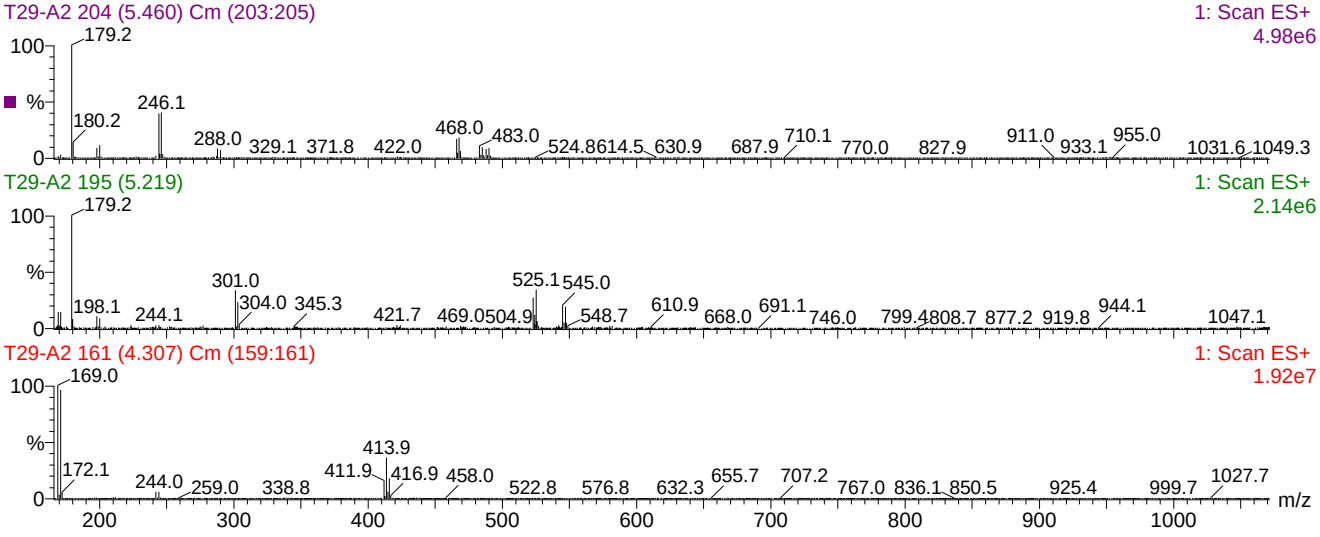
5{15}a

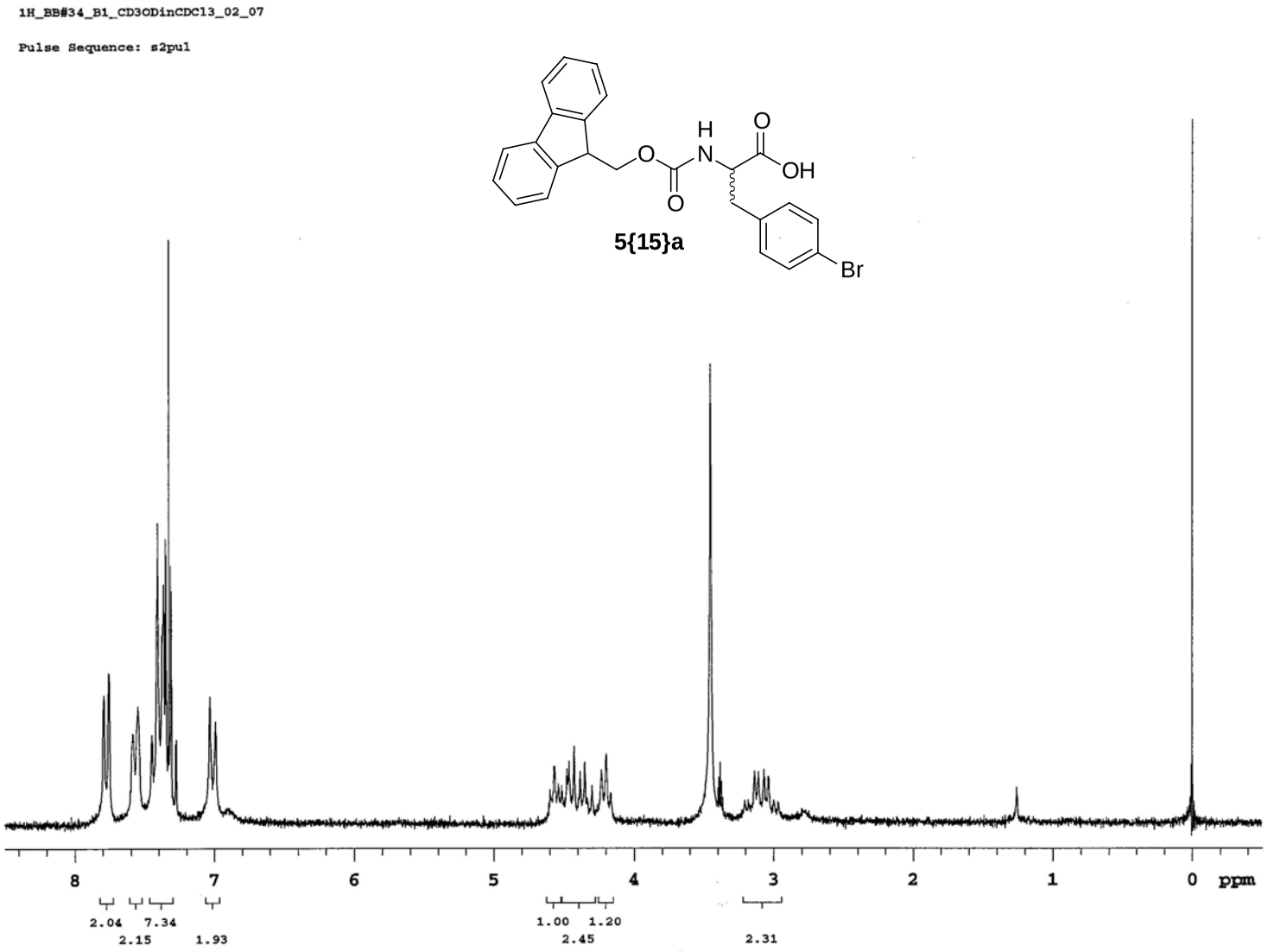

T28-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.83e7
Area
Time Height Area Area%
2.45 3218973 178123.25 6.12
2.94 2162320 127039.76 4.36
4.46 1106610 59747.20 2.05
4.55 7411996 378425.84 13.00
4.71 29581294 1745664.00 59.97
5.03 5630076 360700.28 12.39
5.29 890520 61103.89 2.10
4.71
268.0
1745664
4.55
266.0
378426
5.03
266.0
360700
5{15}a
Team 28 (Resin I)
Exact Mass 465.06
Br
%
Time


T28-A3 190 (5.085) Cm (189:191)
1: Scan ES+
8.44e5
T28-A3 178 (4.763) Cm (177:180)
1: Scan ES+
2.34e6
T28-A3 172 (4.602) Cm (171:173)
1: Scan ES+
4.16e6
m/z

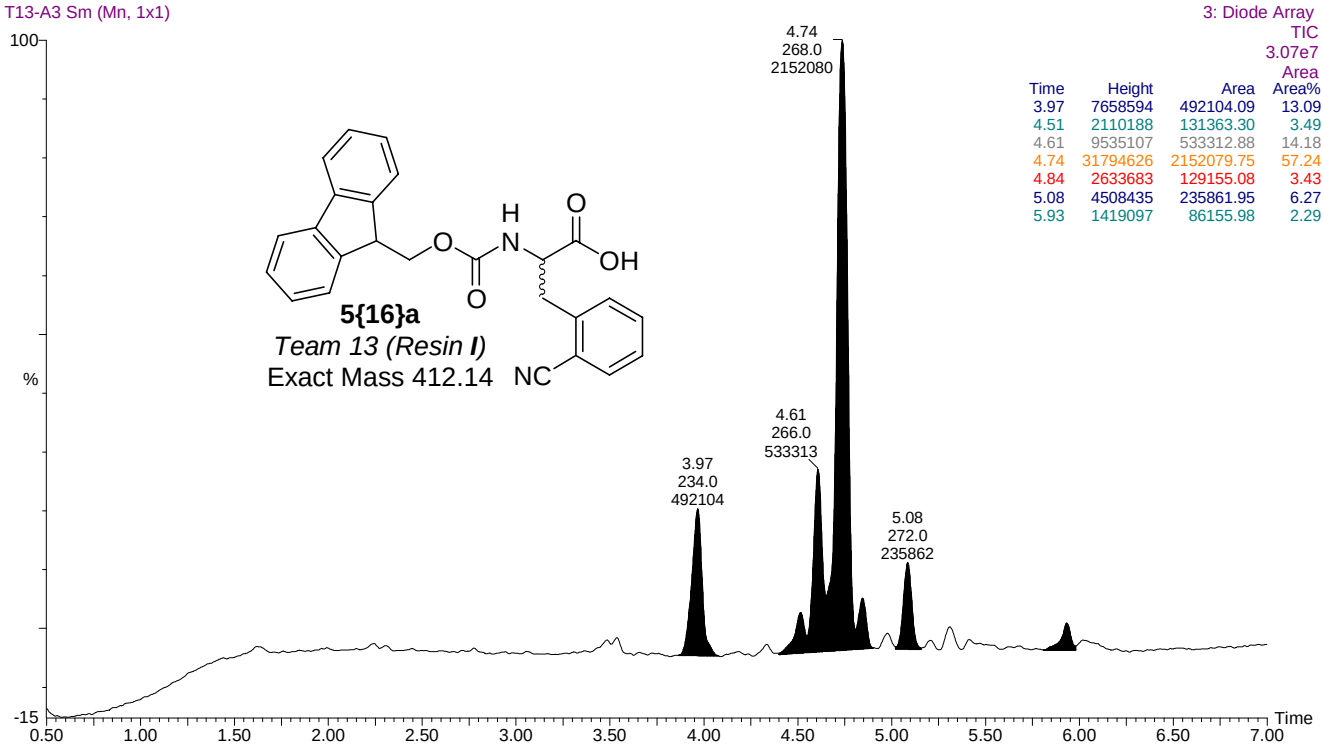
5{15}a

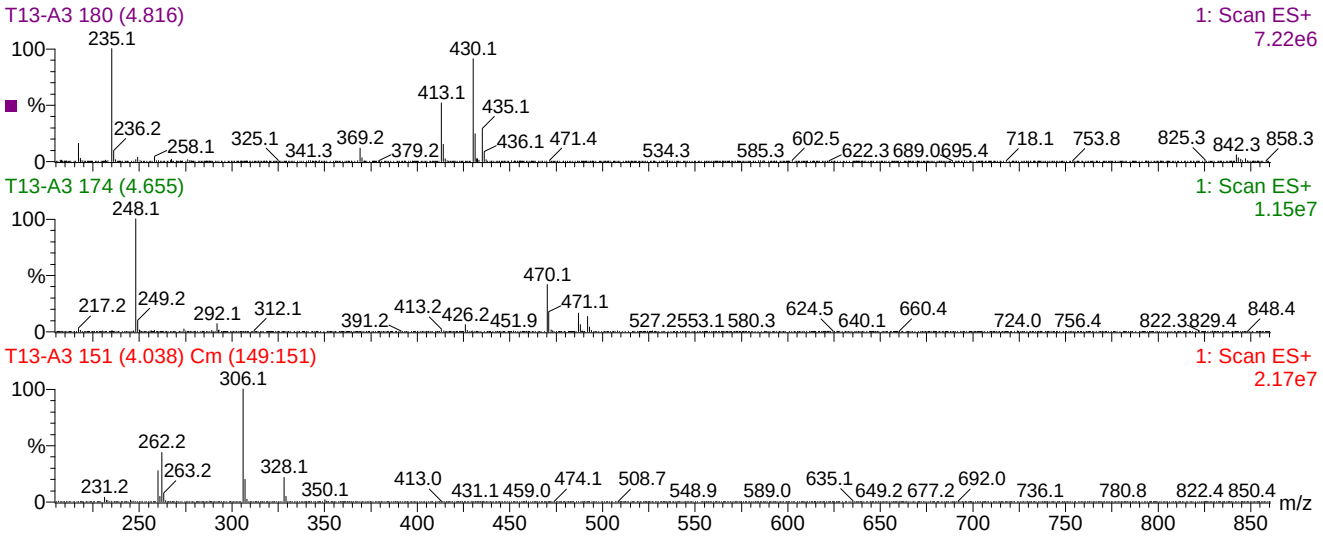

T29-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.92e7
Area
Time Height Area Area%
4.23 7232403 388076.09 14.26
5.09 1586759 70326.83 2.58
5.19 7810000 361592.41 13.29
5.39 30496198 1730814.50 63.61
5.61 3310056 170046.47 6.25
5.39
270.0
1730815
4.23
234.0
388076
5.19
266.0
361592
5{15}a
Team 29 (Resin I)
Exact Mass 465.06
Br
OH
Time


T29-A2 204 (5.460) Cm (203:205)
1: Scan ES+
4.98e6
T29-A2 195 (5.219)
1: Scan ES+
2.14e6
T29-A2 161 (4.307) Cm (159:161)
1: Scan ES+
1.92e7
m/z

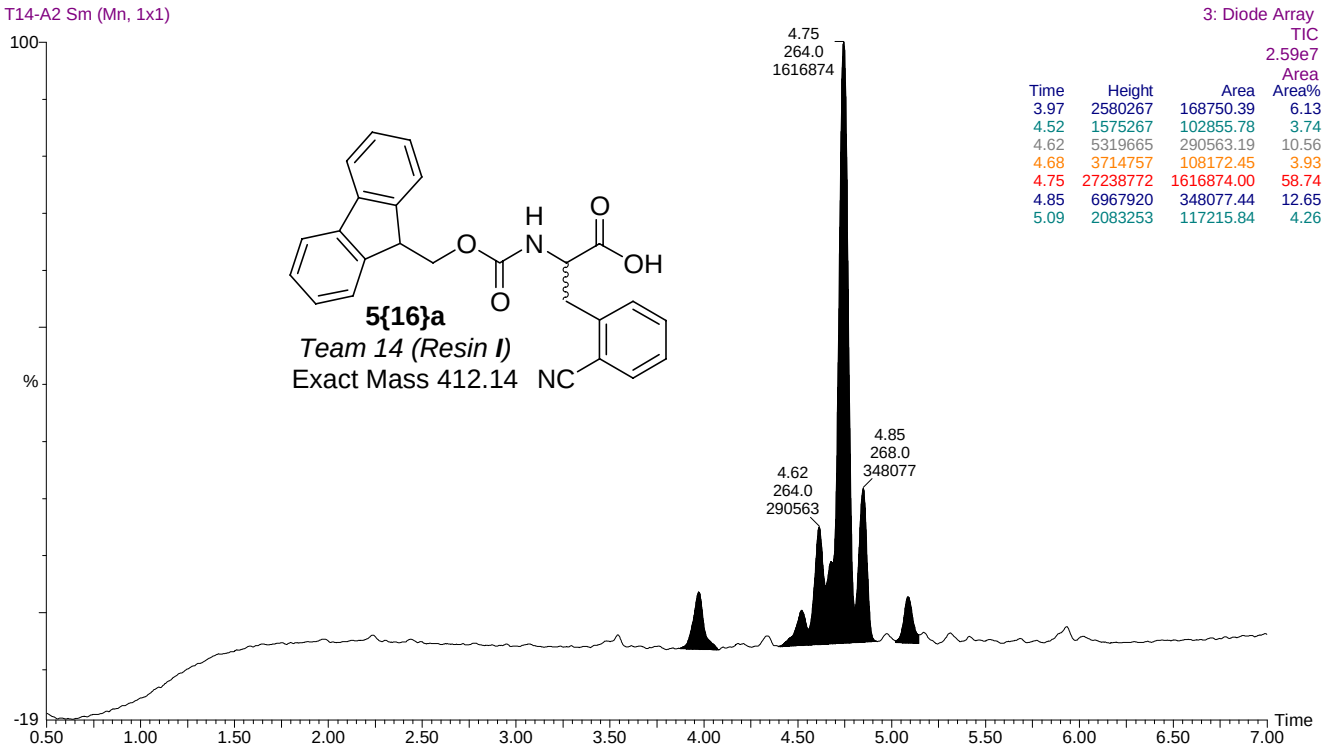

1H_BB#34_B1_CD3ODinCDCl3_02_07
Pulse Sequence: s2pul
H
N
O
O
O
OH
Br
5{15}a
8
7
6
5
4
3
2
1
0
ppm
2.04
2.15
7.34
1.93
1.00
2.45
1.20
2.31

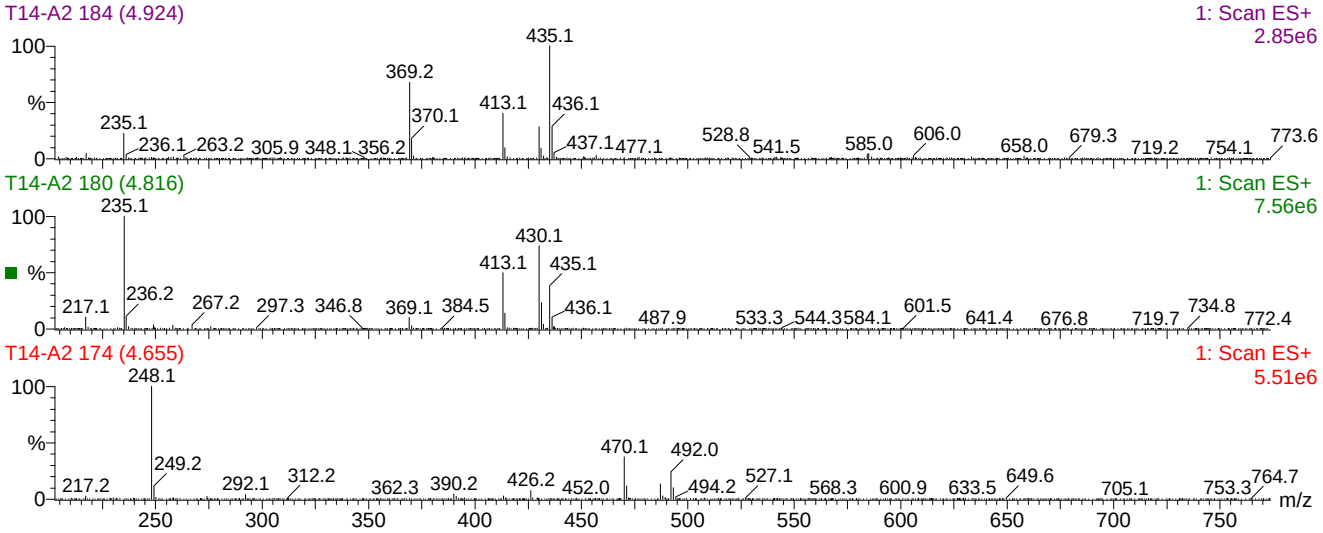
5{16}a


T13-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.07e7
Area
Time Height Area Area%
3.97 7658594 492104.09 13.09
4.51 2110188 131363.30 3.49
4.61 9535107 533312.88 14.18
4.74 31794626 2152079.75 57.24
4.84 2633683 129155.08 3.43
5.08 4508435 235861.95 6.27
5.93 1419097 86155.98 2.29
4.74
268.0
2152080
4.61
266.0
533313
3.97
234.0
492104
5.08
272.0
235862
5{16}a
Team 13 (Resin I)
Exact Mass 412.14
NC
OH
H
N
O
O
O
100
%
-15
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

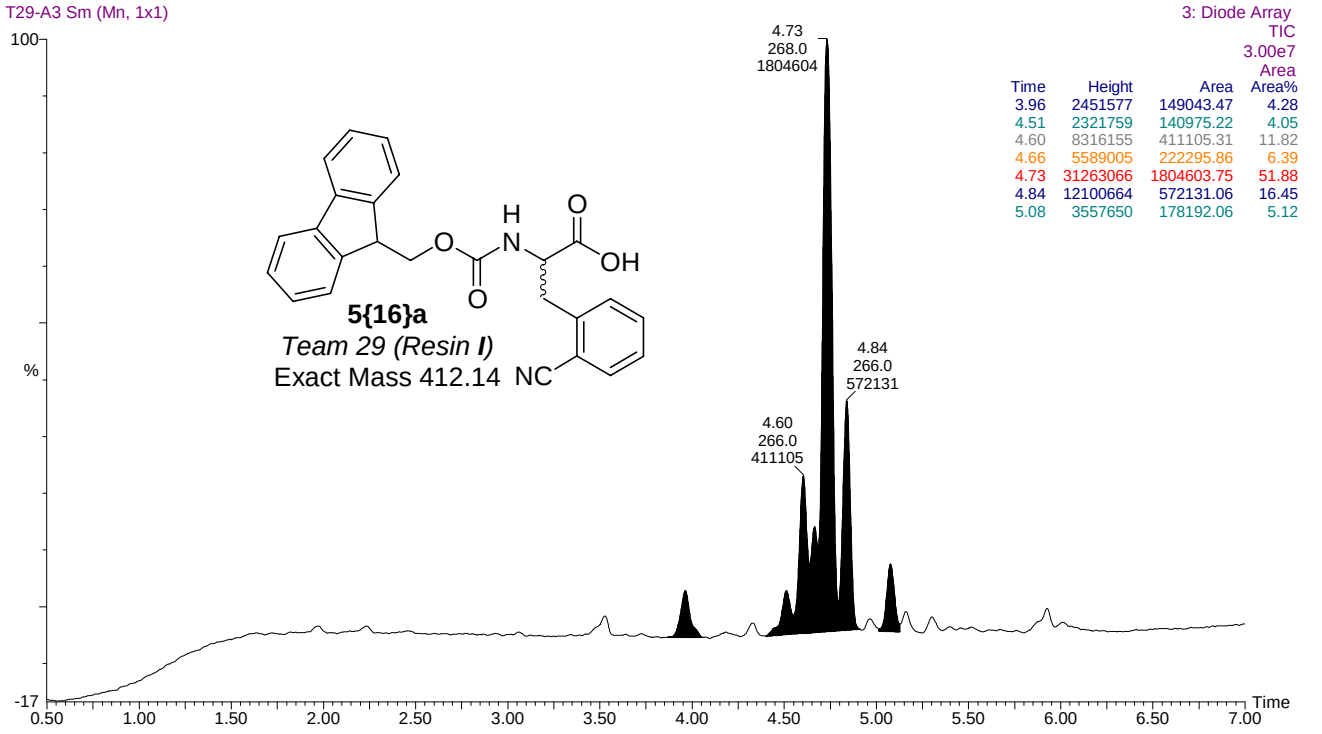

T13-A3 180 (4.816)
1: Scan ES+
7.22e6
235.1
430.1
413.1
435.1
236.2
258.1
325.1
341.3
369.2
379.2
436.1
471.4
534.3
585.3
602.5
622.3
689.0
695.4
718.1
753.8
825.3
842.3
858.3
T13-A3 174 (4.655)
1: Scan ES+
1.15e7
248.1
470.1
471.1
217.2
249.2
292.1
312.1
391.2
413.2
426.2
451.9
527.2
553.1
580.3
624.5
640.1
660.4
724.0
756.4
822.3
829.4
848.4
T13-A3 151 (4.038) Cm (149:151)
1: Scan ES+
2.17e7
306.1
262.2
263.2
328.1
231.2
350.1
413.0
431.1
459.0
474.1
508.7
548.9
589.0
635.1
649.2
677.2
692.0
736.1
780.8
822.4
850.4
100
%
0
250 300 350 400 450 500 550 600 650 700 750 800 850
m/z

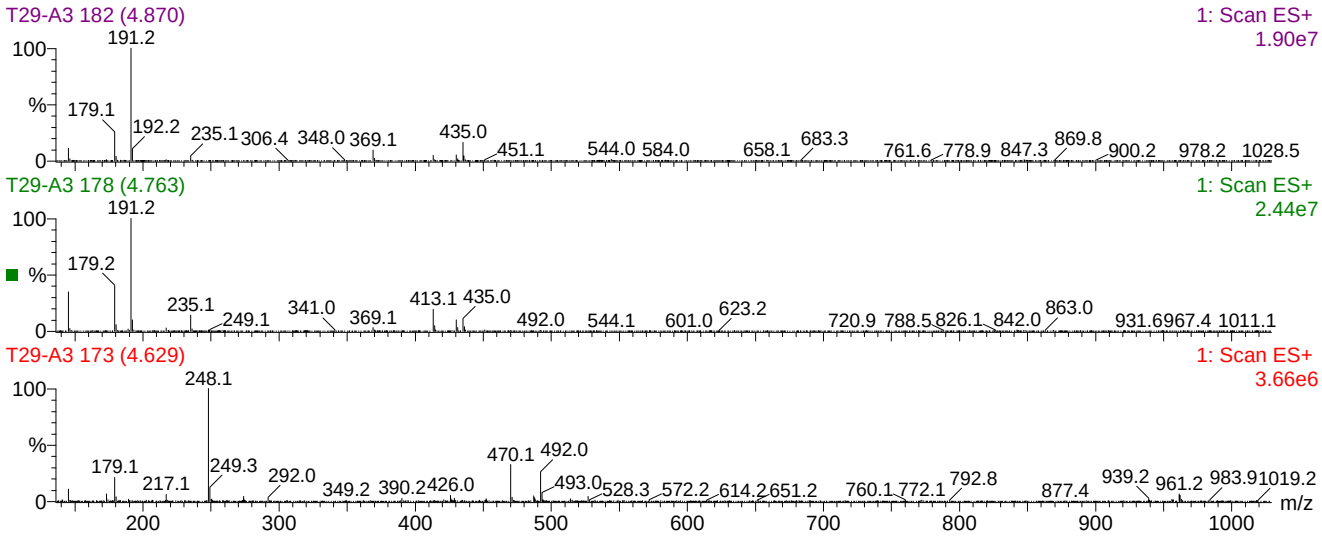
5{16}a


T14-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.59e7
Area
Time Height Area Area%
3.97 2580267 168750.39 6.13
4.52 1575267 102855.78 3.74
4.62 5319665 290563.19 10.56
4.68 3714757 108172.45 3.93
4.75 27238772 1616874.00 58.74
4.85 6967920 348077.44 12.65
5.09 2083253 117215.84 4.26
4.75
264.0
1616874
4.85
268.0
348077
4.62
264.0
290563
5{16}a
Team 14 (Resin I)
Exact Mass 412.14
NC
OH
100
%
-19
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

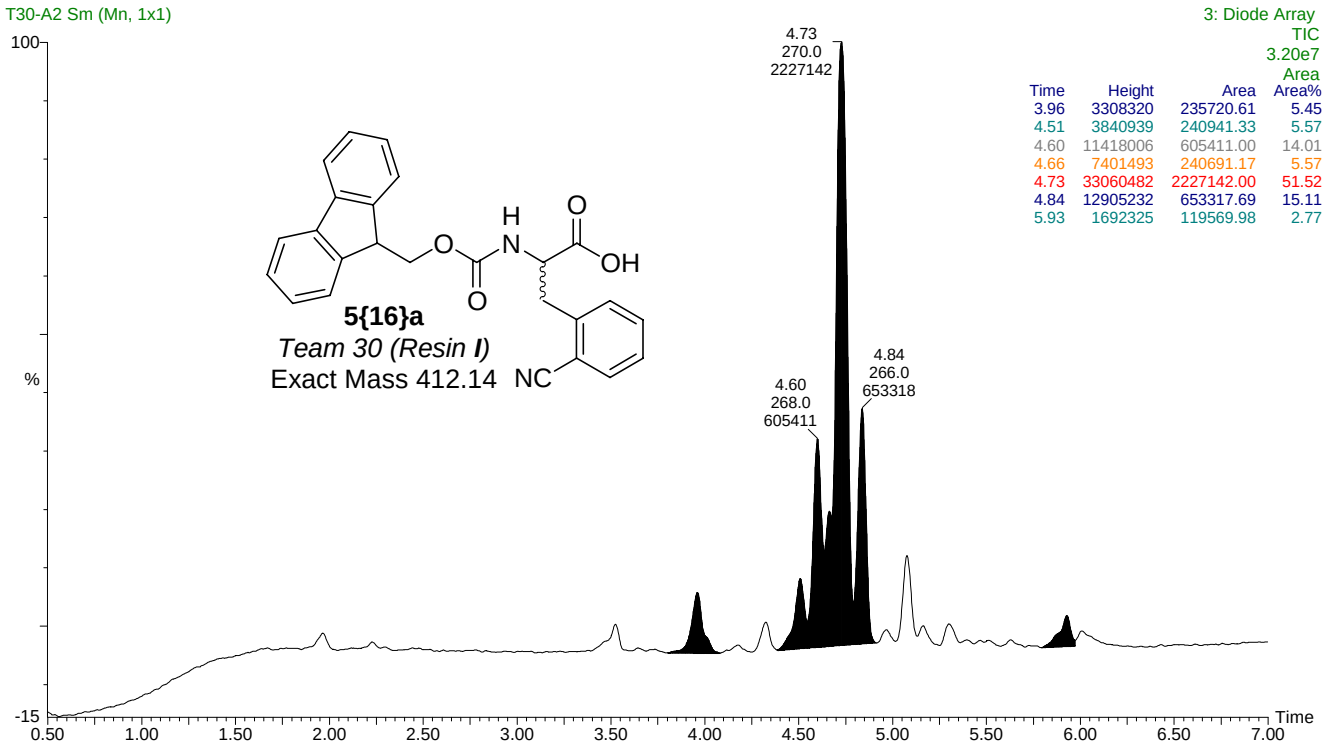

T14-A2 184 (4.924)
1: Scan ES+
2.85e6
435.1
369.2
413.1
436.1
370.1
235.1
236.1 263.2 305.9 348.1 356.2 437.1 477.1 528.8 541.5 585.0 606.0 658.0 679.3 719.2 754.1 773.6
T14-A2 180 (4.816)
1: Scan ES+
7.56e6
235.1
430.1
413.1
435.1
236.2
217.1 267.2 297.3 346.8 369.1 384.5 436.1 487.9 533.3 544.3 584.1 601.5 641.4 676.8 719.7 734.8 772.4
T14-A2 174 (4.655)
1: Scan ES+
5.51e6
248.1
249.2
470.1
492.0
217.2 292.1 312.2 362.3 390.2 426.2 452.0 494.2 527.1 568.3 600.9 633.5 649.6 705.1 753.3 764.7
100
%
0
250 300 350 400 450 500 550 600 650 700 750
m/z

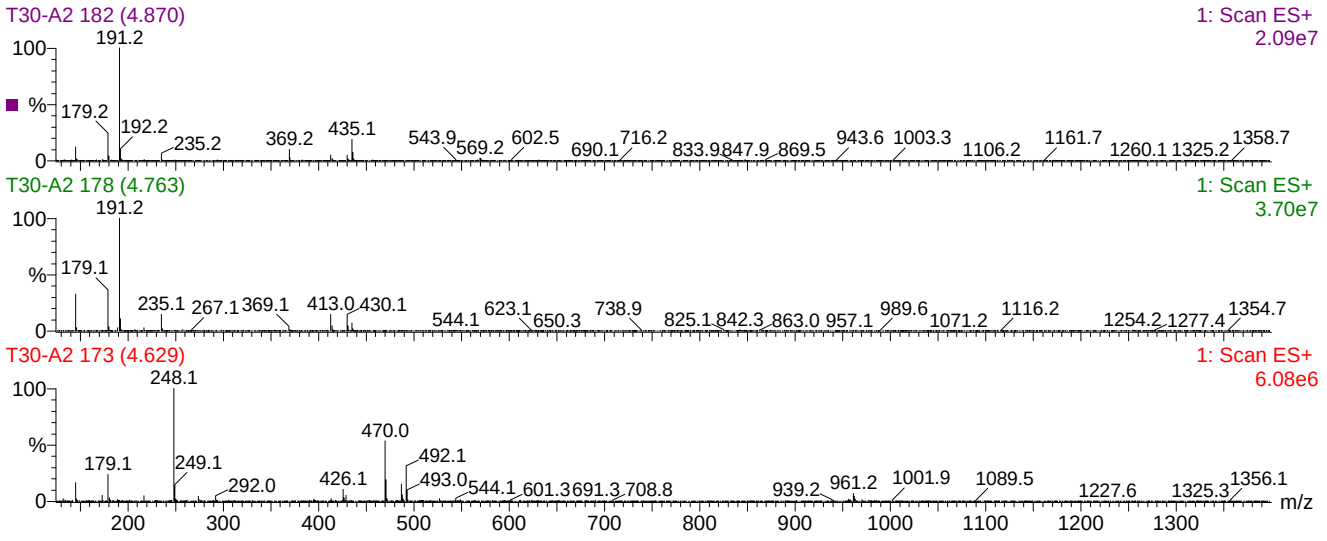
5{16}a


T29-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.00e7
Area
Time Height Area Area%
3.96 2451577 149043.47 4.28
4.51 2321759 140975.22 4.05
4.60 8316155 411105.31 11.82
4.66 5589005 222295.86 6.39
4.73 31263066 1804603.75 51.88
4.84 12100664 572131.06 16.45
5.08 3557650 178192.06 5.12
4.73
268.0
1804604
4.84
266.0
572131
4.60
266.0
411105
5{16}a
Team 29 (Resin I)
Exact Mass 412.14
NC
OH
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00


T29-A3 182 (4.870)
1: Scan ES+
1.90e7
191.2
179.1
192.2
235.1
306.4
348.0
369.1
435.0
451.1
544.0
584.0
658.1
683.3
761.6
778.9
847.3
869.8
900.2
978.2
1028.5
T29-A3 178 (4.763)
1: Scan ES+
2.44e7
191.2
179.2
235.1
249.1
341.0
369.1
413.1
435.0
492.0
544.1
601.0
623.2
720.9
788.5
826.1
842.0
863.0
931.6
967.4
1011.1
T29-A3 173 (4.629)
1: Scan ES+
3.66e6
248.1
179.1
217.1
249.3
292.0
349.2
390.2
426.0
470.1
492.0
493.0
528.3
572.2
614.2
651.2
760.1
772.1
792.8
877.4
939.2
961.2
983.9
1019.2
m/z
200 300 400 500 600 700 800 900 1000

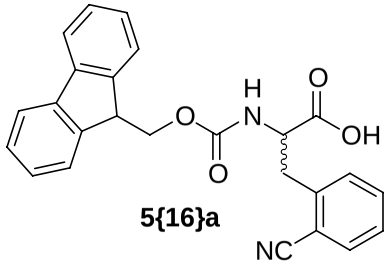
5{16}a


T30-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.20e7
Area
Time Height Area Area%
3.96 3308320 235720.61 5.45
4.51 3840939 240941.33 5.57
4.60 11418006 605411.00 14.01
4.66 7401493 240691.17 5.57
4.73 33060482 2227142.00 51.52
4.84 12905232 653317.69 15.11
5.93 1692325 119569.98 2.77
4.73
270.0
2227142
4.84
266.0
653318
4.60
268.0
605411
5{16}a
Team 30 (Resin I)
Exact Mass 412.14
NC
%
Time

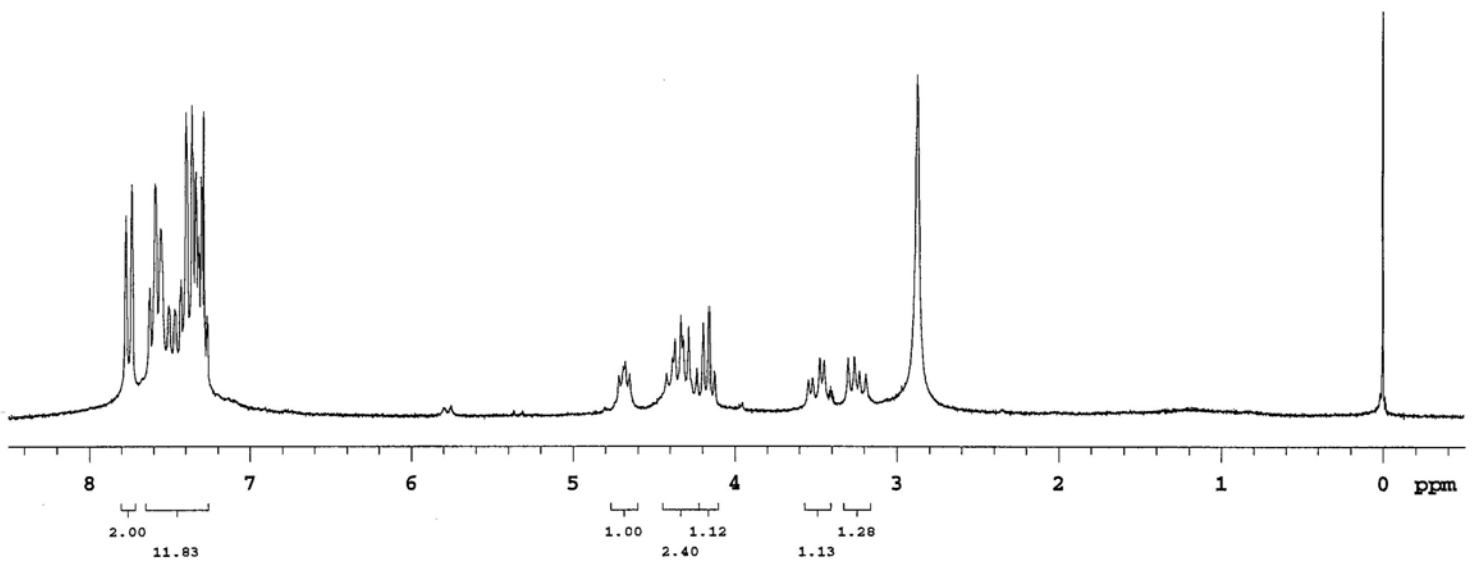

T30-A2 182 (4.870)
1: Scan ES+
2.09e7
191.2
179.2
192.2
235.2
369.2
435.1
543.9
569.2
602.5
690.1
716.2
833.9
847.9
869.5
943.6
1003.3
1106.2
1161.7
1260.1
1325.2
1358.7
T30-A2 178 (4.763)
1: Scan ES+
3.70e7
191.2
179.1
235.1
267.1
369.1
413.0
430.1
544.1
623.1
650.3
738.9
825.1
842.3
863.0
957.1
989.6
1071.2
1116.2
1254.2
1277.4
1354.7
T30-A2 173 (4.629)
1: Scan ES+
6.08e6
248.1
470.0
179.1
249.1
292.0
426.1
492.1
493.0
544.1
601.3
691.3
708.8
939.2
961.2
1001.9
1089.5
1227.6
1325.3
1356.1
m/z

1H_BB#34_A2_CD3ODinCDCl3_02_07

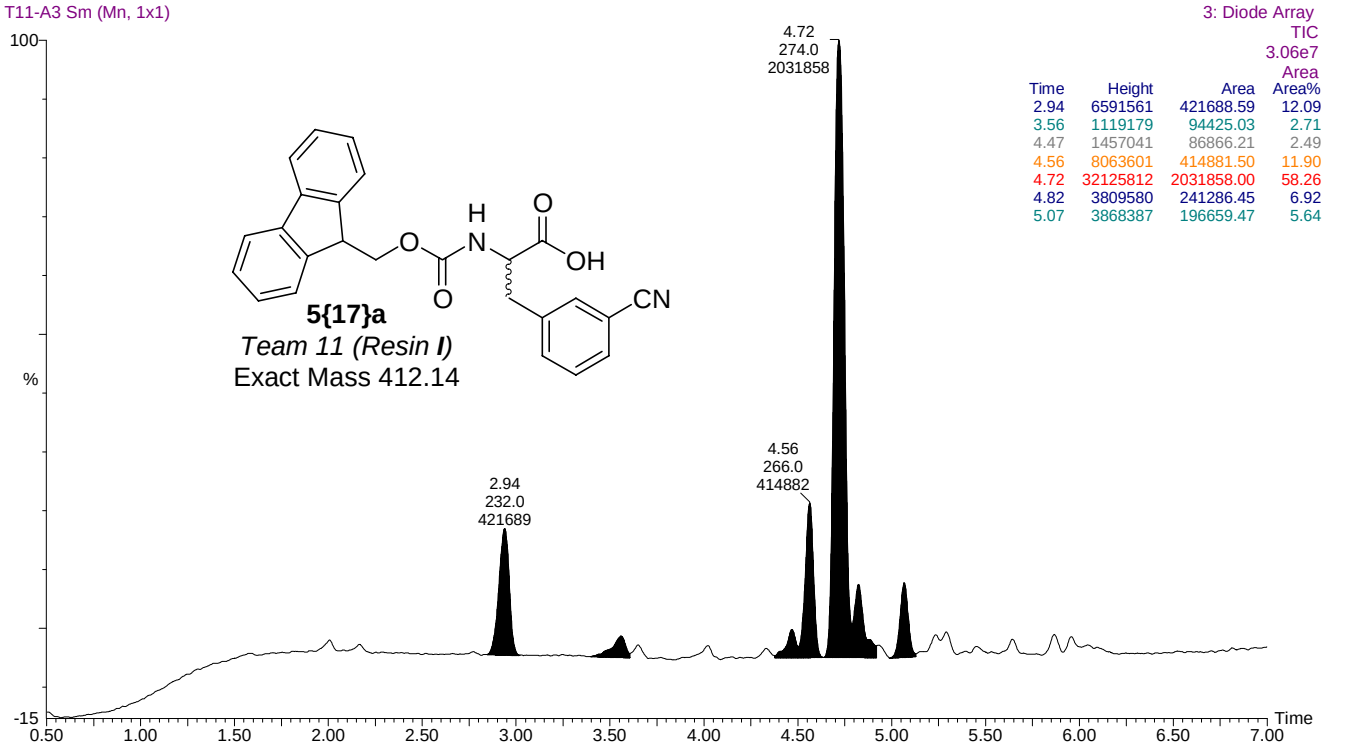
Pulse Sequence: s2pul

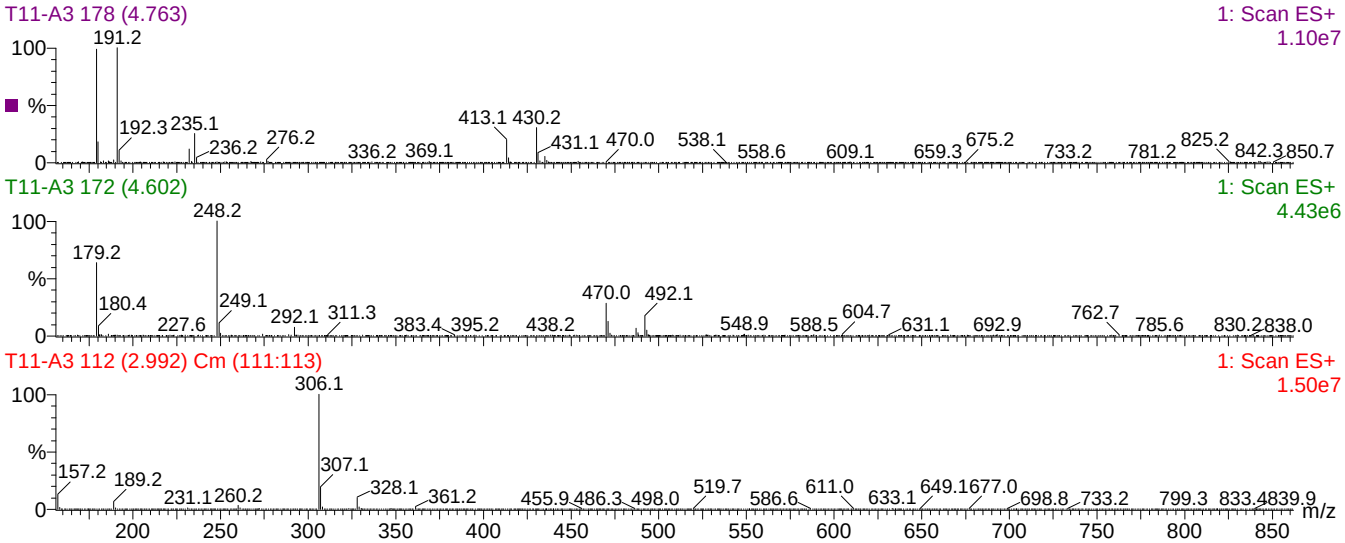


5{16}a

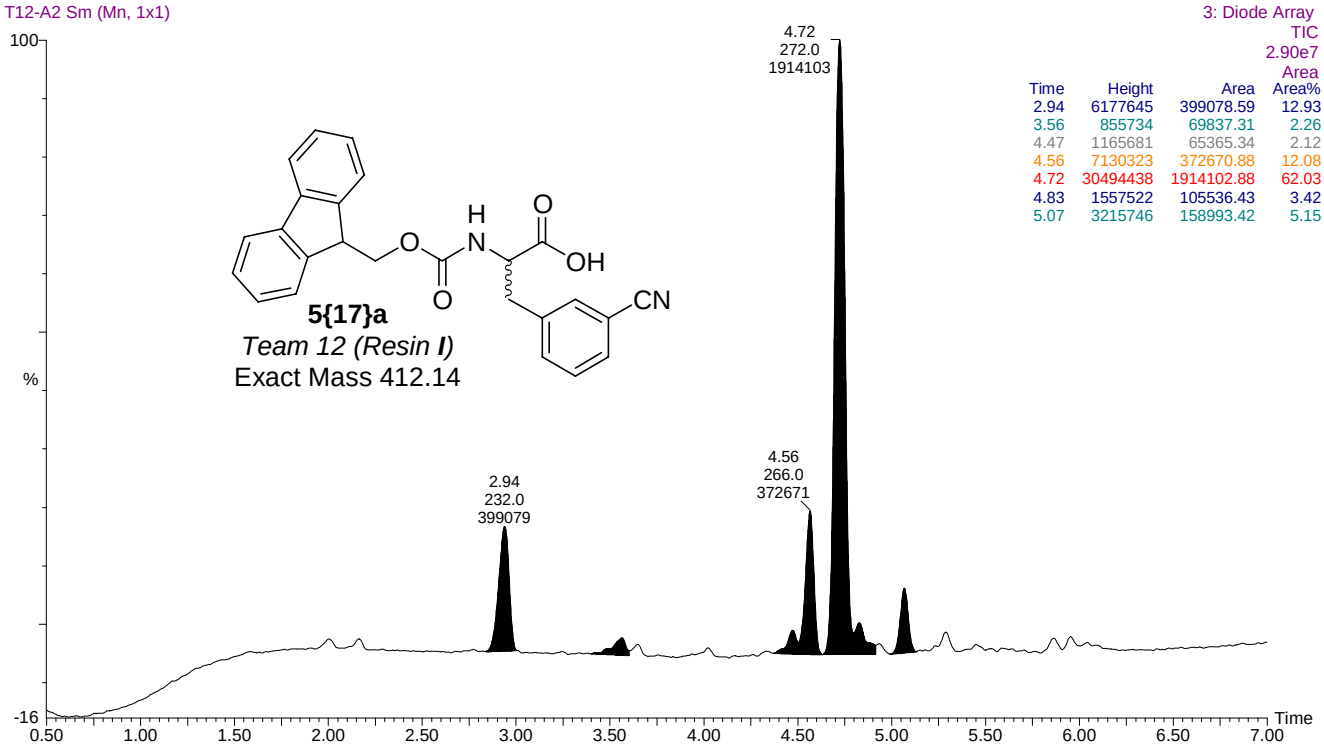


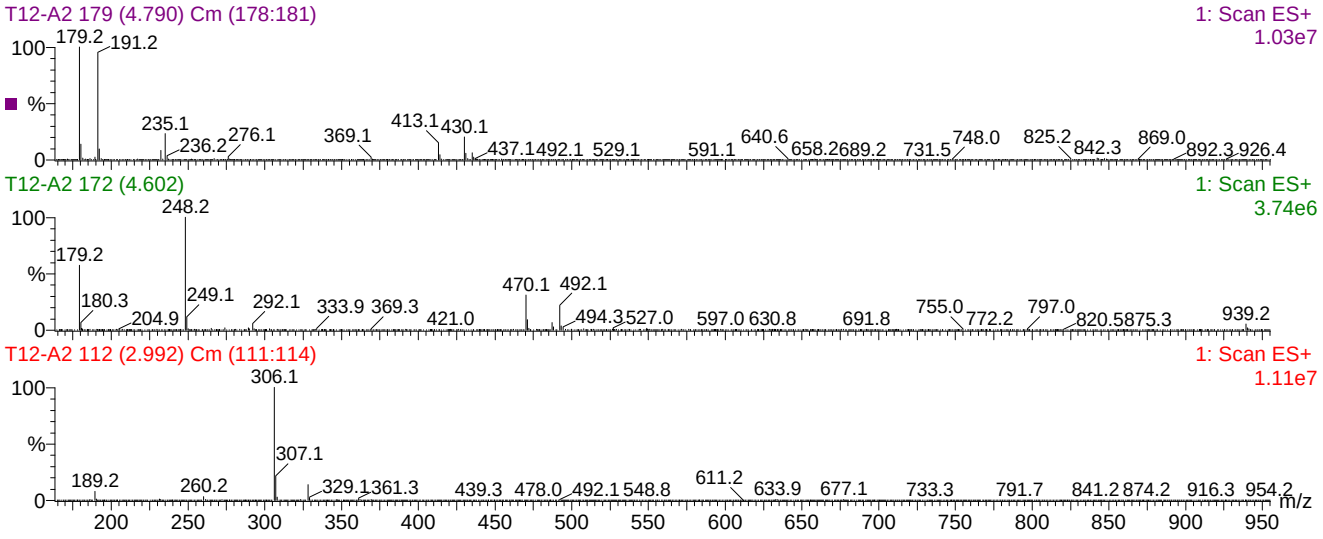
5{17}a


T11-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.06e7
Area
Time Height Area Area%
2.94 6591561 421688.59 12.09
3.56 1119179 94425.03 2.71
4.47 1457041 86866.21 2.49
4.56 8063601 414881.50 11.90
4.72 32125812 2031858.00 58.26
4.82 3809580 241286.45 6.92
5.07 3868387 196659.47 5.64
4.72
274.0
2031858
4.56
266.0
414882
2.94
232.0
421689
5{17}a
Team 11 (Resin I)
Exact Mass 412.14
Time

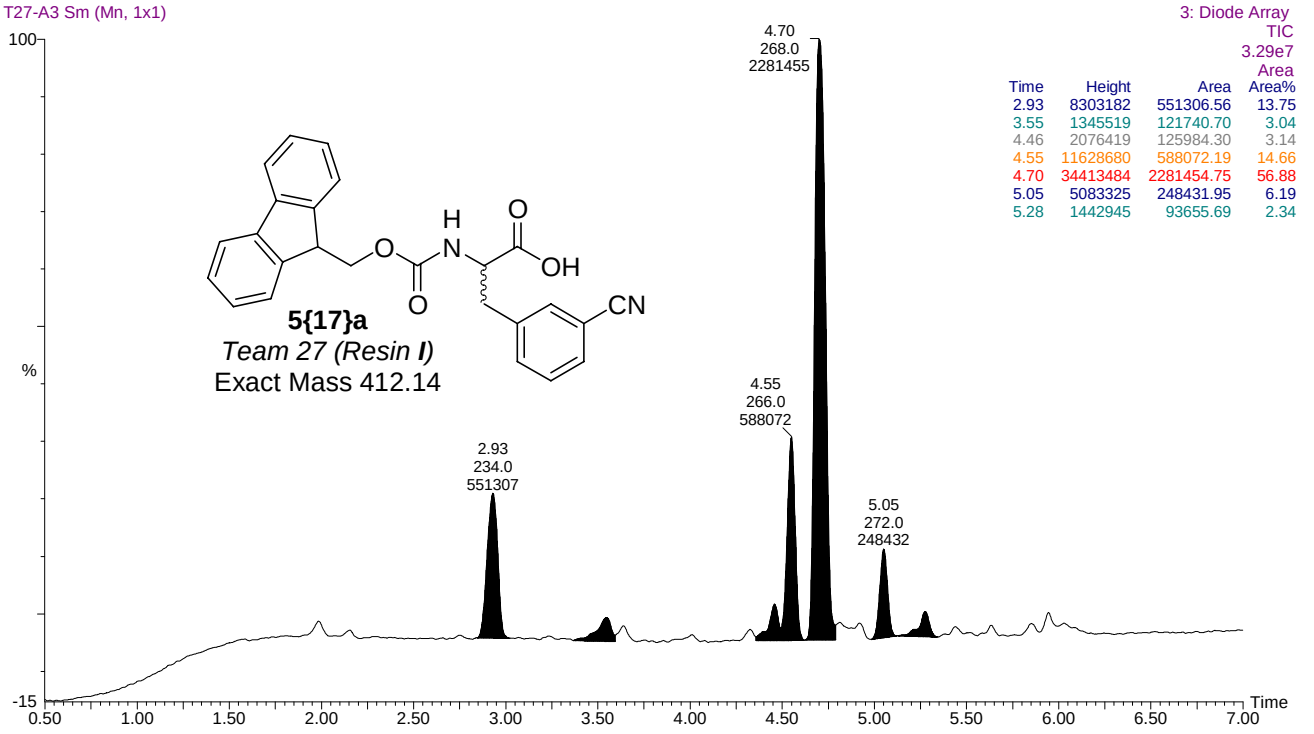

T11-A3 178 (4.763)
1: Scan ES+
1.10e7
T11-A3 172 (4.602)
1: Scan ES+
4.43e6
T11-A3 112 (2.992) Cm (111:113)
1: Scan ES+
1.50e7
m/z

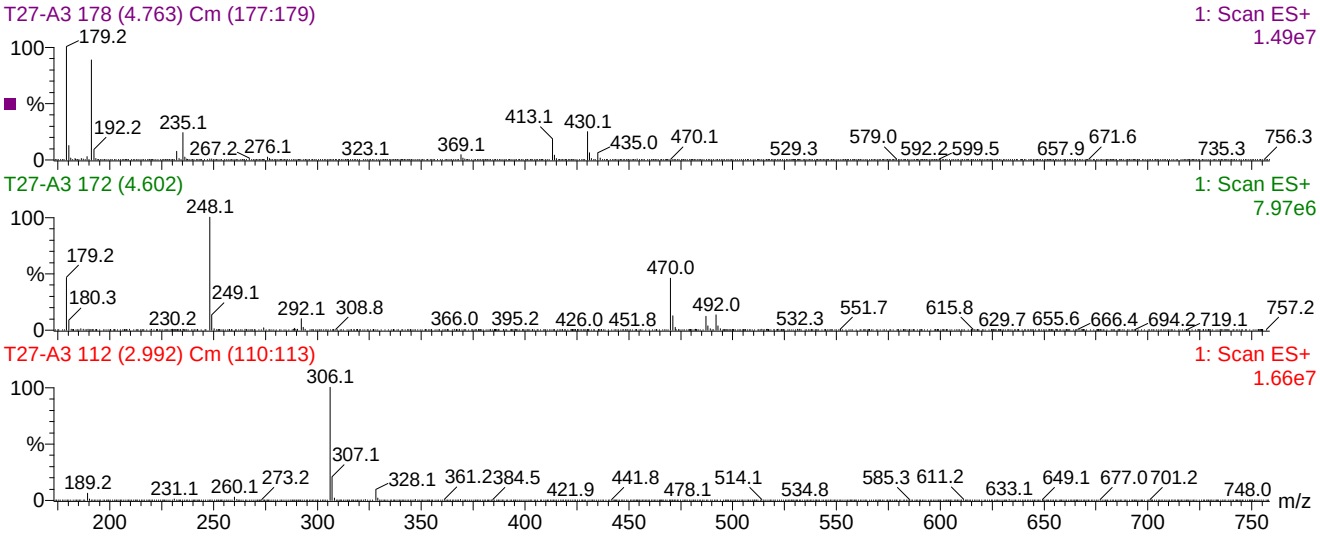
5{17}a


T12-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.90e7
Area
Time Height Area Area%
2.94 6177645 399078.59 12.93
3.56 855734 69837.31 2.26
4.47 1165681 65365.34 2.12
4.56 7130323 372670.88 12.08
4.72 30494438 1914102.88 62.03
4.83 1557522 105536.43 3.42
5.07 3215746 158993.42 5.15
4.72
272.0
1914103
4.56
266.0
372671
2.94
232.0
399079
5{17}a
Team 12 (Resin I)
Exact Mass 412.14
Time

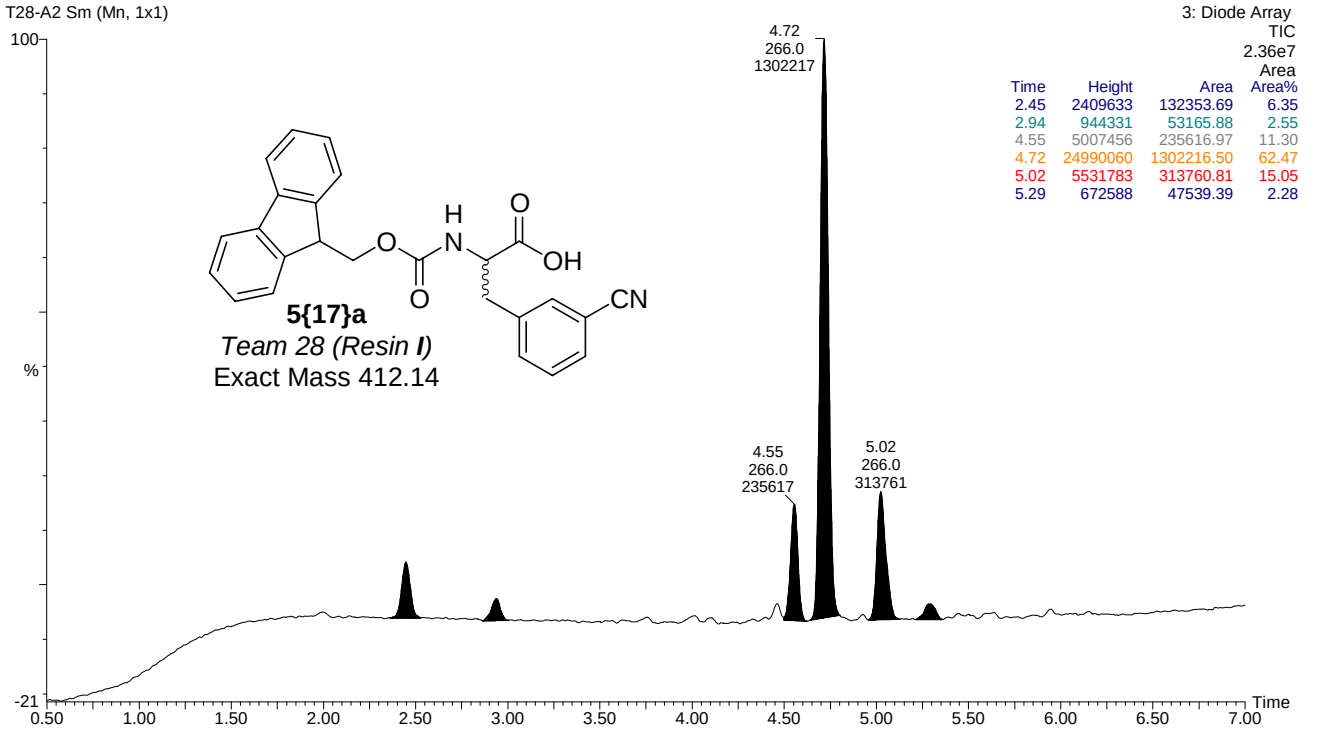

T12-A2 179 (4.790) Cm (178:181)
1: Scan ES+
1.03e7
T12-A2 172 (4.602)
1: Scan ES+
3.74e6
T12-A2 112 (2.992) Cm (111:114)
1: Scan ES+
1.11e7
m/z

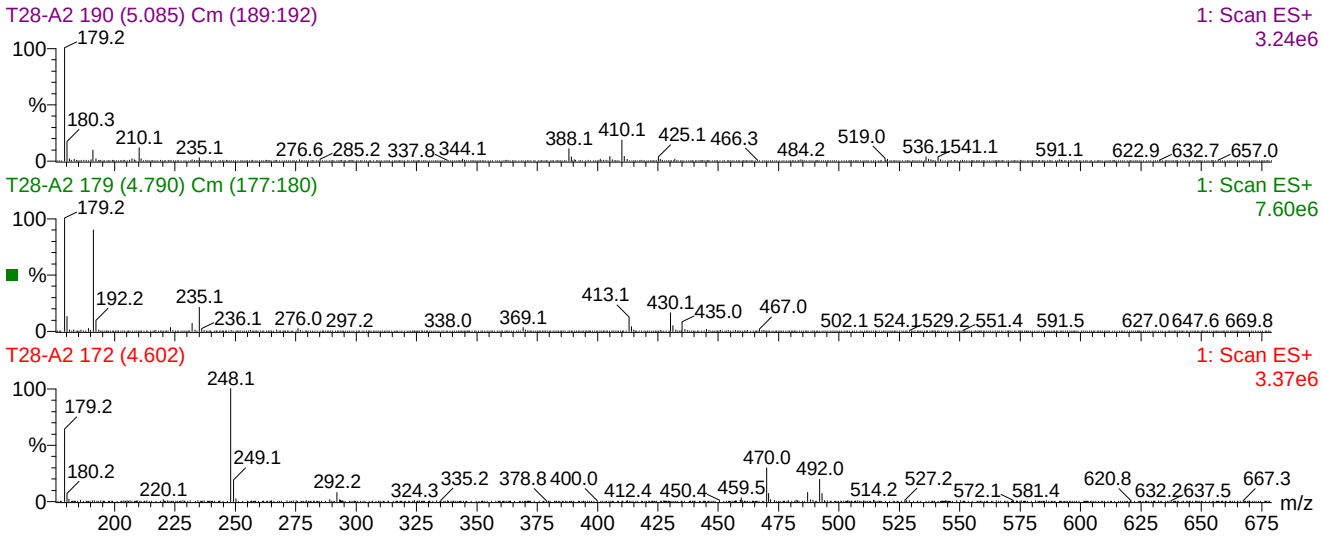
5{17}a


T27-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.29e7
Area
Time Height Area Area%
2.93 8303182 551306.56 13.75
3.55 1345519 121740.70 3.04
4.46 2076419 125984.30 3.14
4.55 11628680 588072.19 14.66
4.70 34413484 2281454.75 56.88
5.05 5083325 248431.95 6.19
5.28 1442945 93655.69 2.34
4.70
268.0
2281455
4.55
266.0
588072
2.93
234.0
551307
5.05
272.0
248432
5{17}a
Team 27 (Resin I)
Exact Mass 412.14
%
Time


T27-A3 178 (4.763) Cm (177:179)
1: Scan ES+
1.49e7
T27-A3 172 (4.602)
1: Scan ES+
7.97e6
T27-A3 112 (2.992) Cm (110:113)
1: Scan ES+
1.66e7
m/z

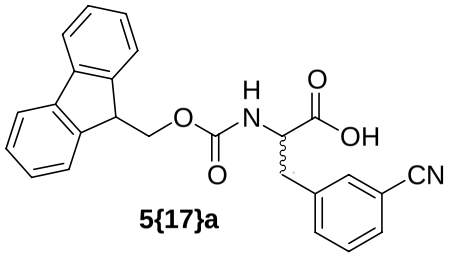
5{17}a


T28-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.36e7
Area
Time Height Area Area%
2.45 2409633 132353.69 6.35
2.94 944331 53165.88 2.55
4.55 5007456 235616.97 11.30
4.72 24990060 1302216.50 62.47
5.02 5531783 313760.81 15.05
5.29 672588 47539.39 2.28
4.72
266.0
1302217
4.55
266.0
235617
5.02
266.0
313761
5{17}a
Team 28 (Resin I)
Exact Mass 412.14
%
Time

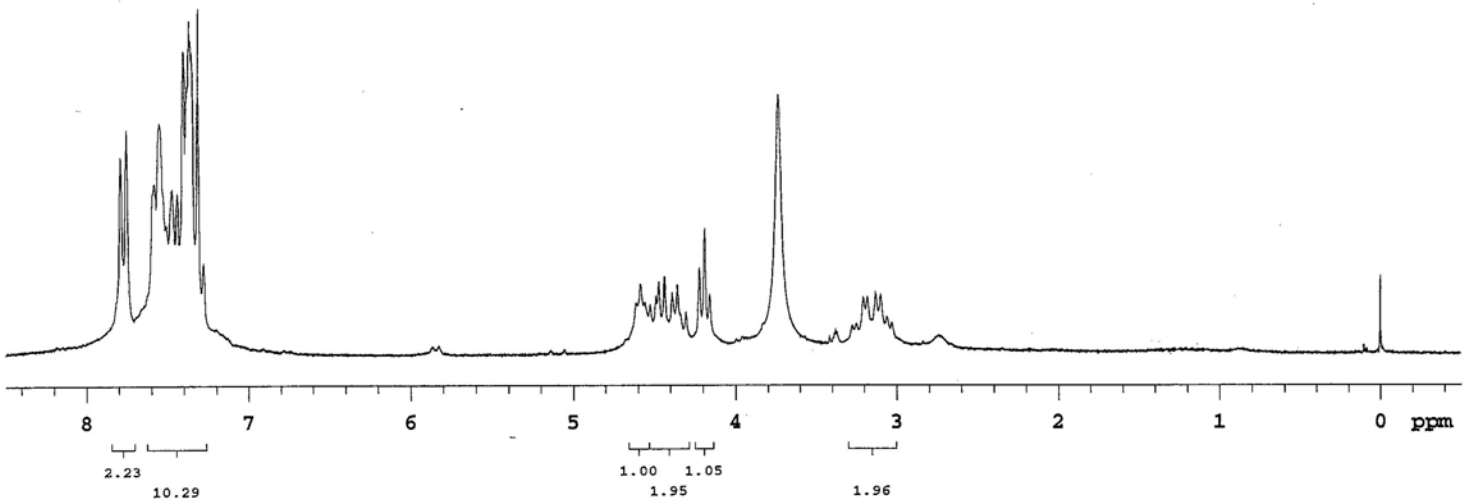

T28-A2 190 (5.085) Cm (189:192)
1: Scan ES+
3.24e6
T28-A2 179 (4.790) Cm (177:180)
1: Scan ES+
7.60e6
T28-A2 172 (4.602)
1: Scan ES+
3.37e6
m/z

1H_BB#27_B1_CD3ODinCDCl3_02_20_07

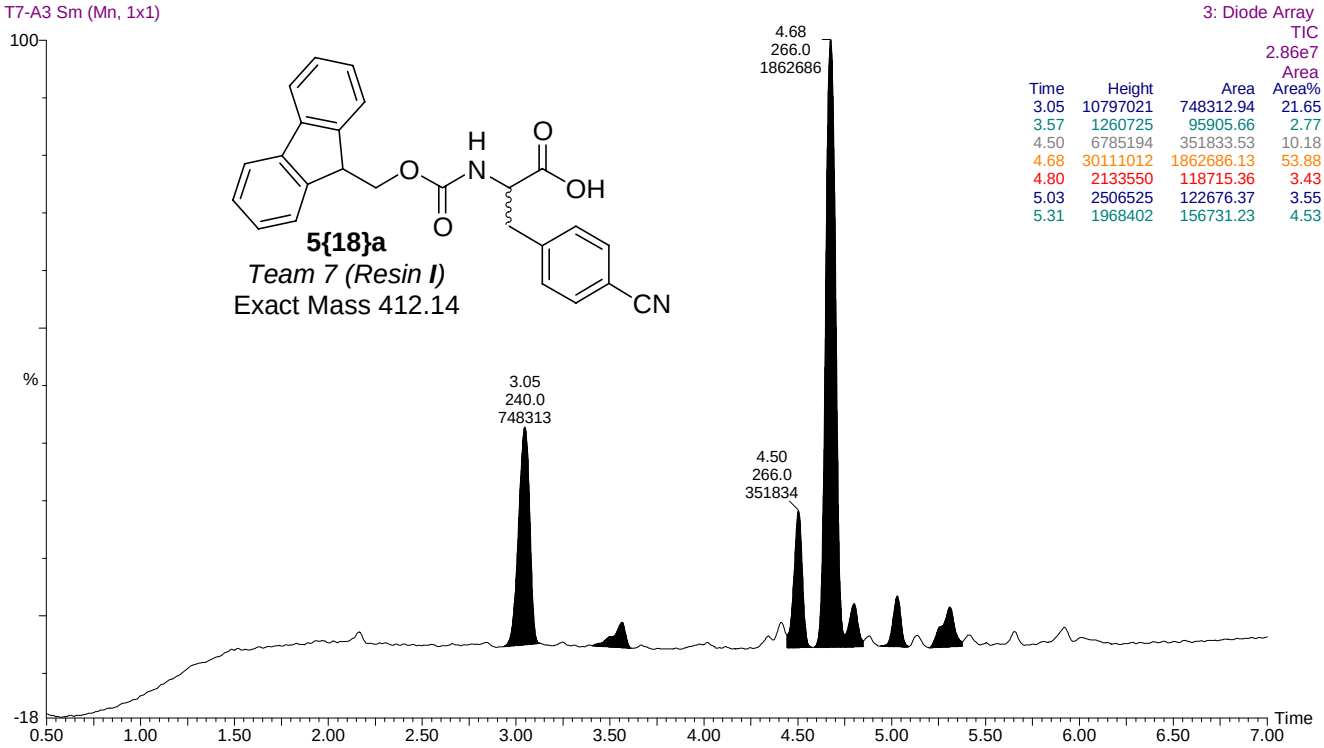
Pulse Sequence: s2pul

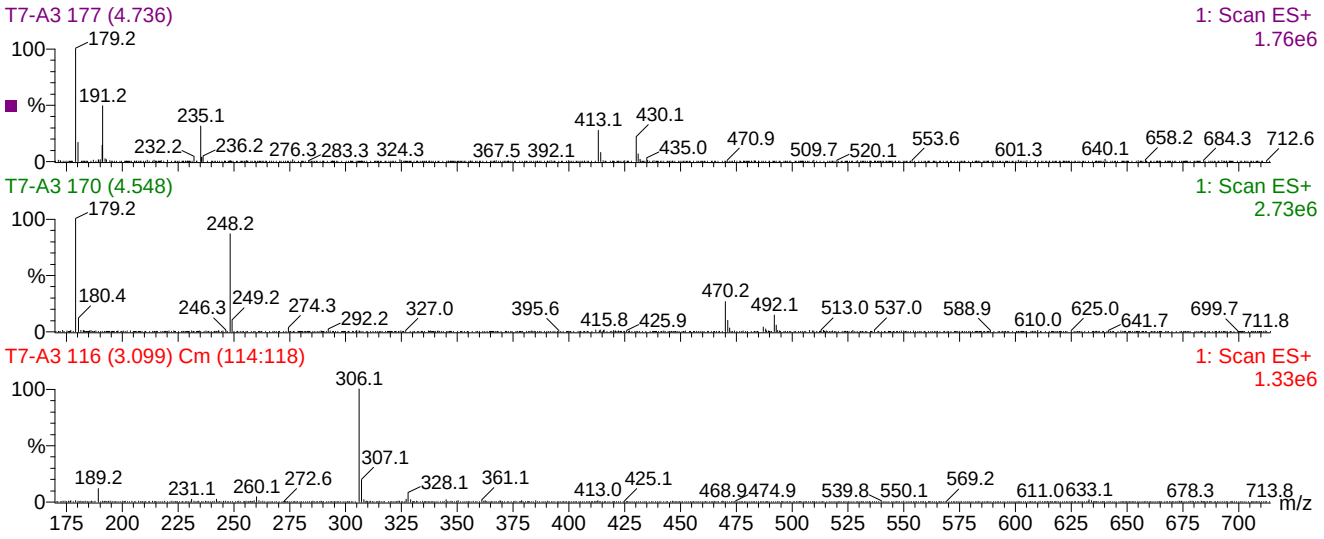


5{17}a

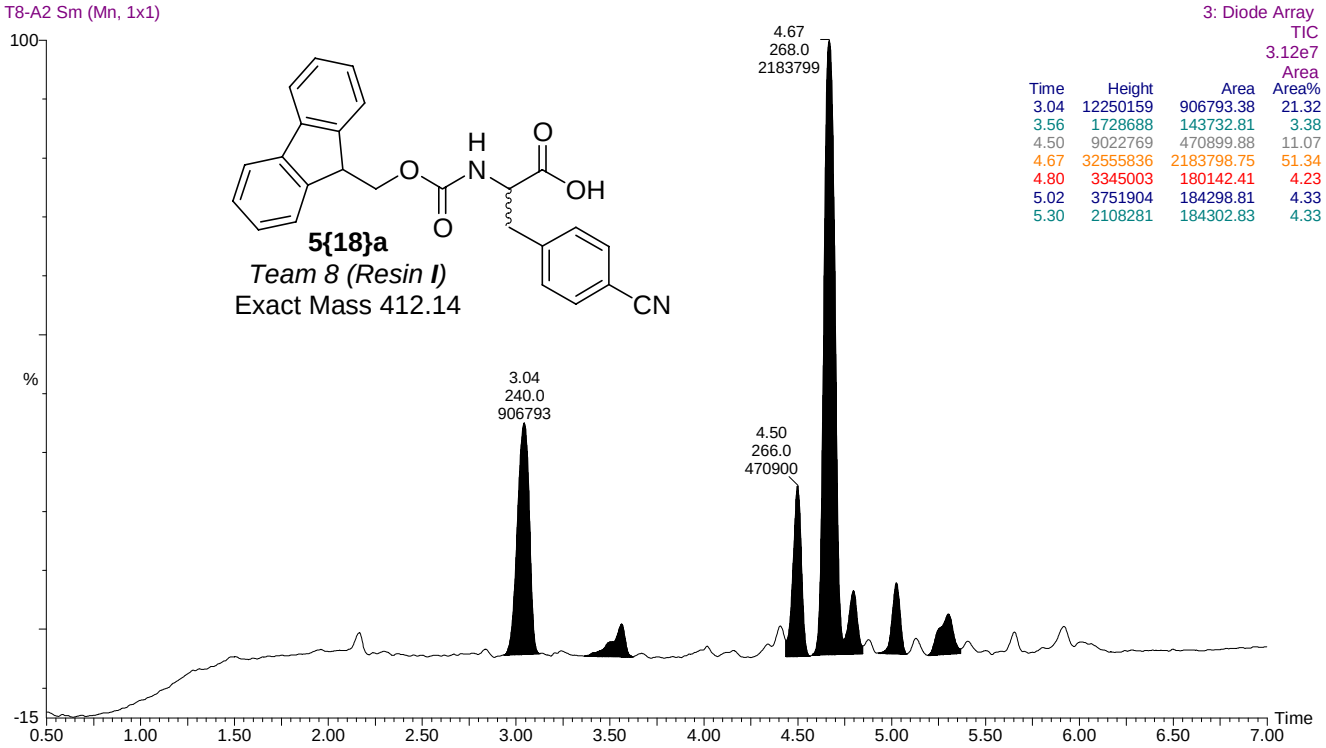


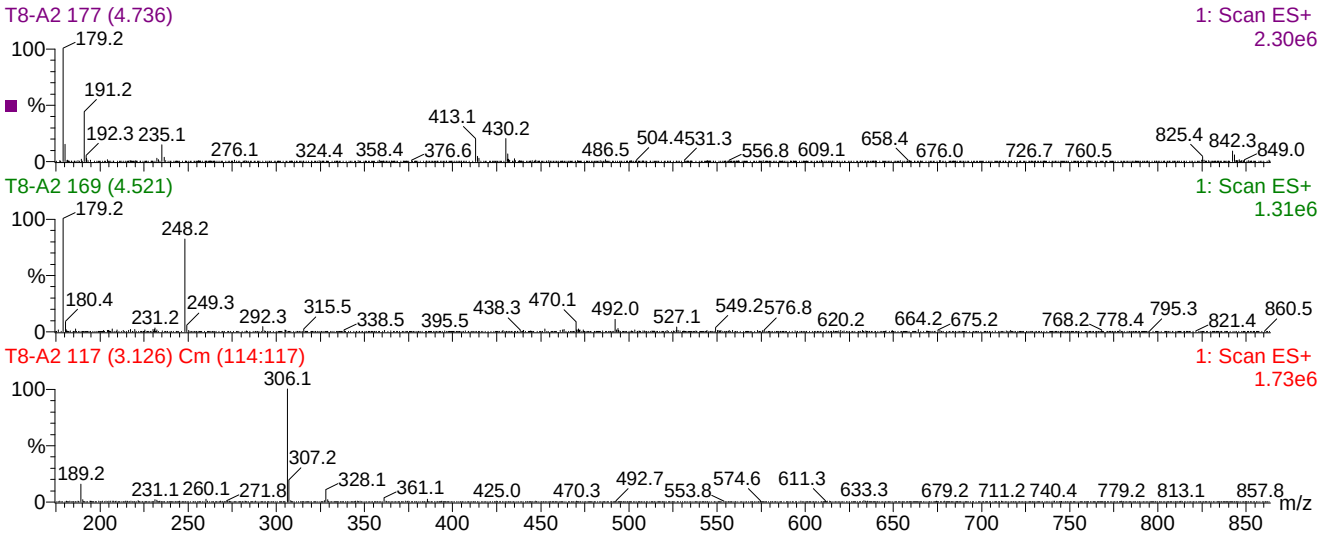
5{18}a


T7-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.86e7
Area
Time Height Area Area%
3.05 10797021 748312.94 21.65
3.57 1260725 95905.66 2.77
4.50 6785194 351833.53 10.18
4.68 30111012 1862686.13 53.88
4.80 2133550 118715.36 3.43
5.03 2506525 122676.37 3.55
5.31 1968402 156731.23 4.53
4.68
266.0
1862686
3.05
240.0
748313
4.50
266.0
351834
5{18}a
Team 7 (Resin I)
Exact Mass 412.14
Time

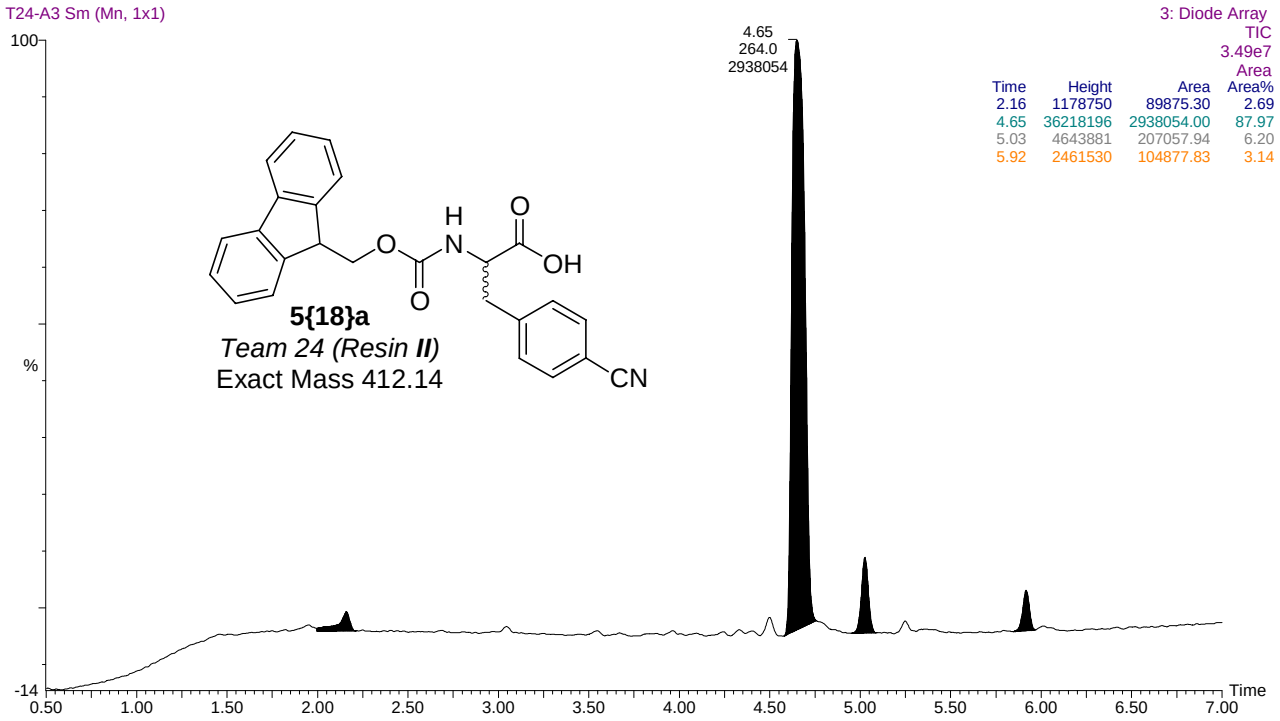

T7-A3 177 (4.736)
1: Scan ES+
1.76e6
T7-A3 170 (4.548)
1: Scan ES+
2.73e6
T7-A3 116 (3.099) Cm (114:118)
1: Scan ES+
1.33e6
m/z

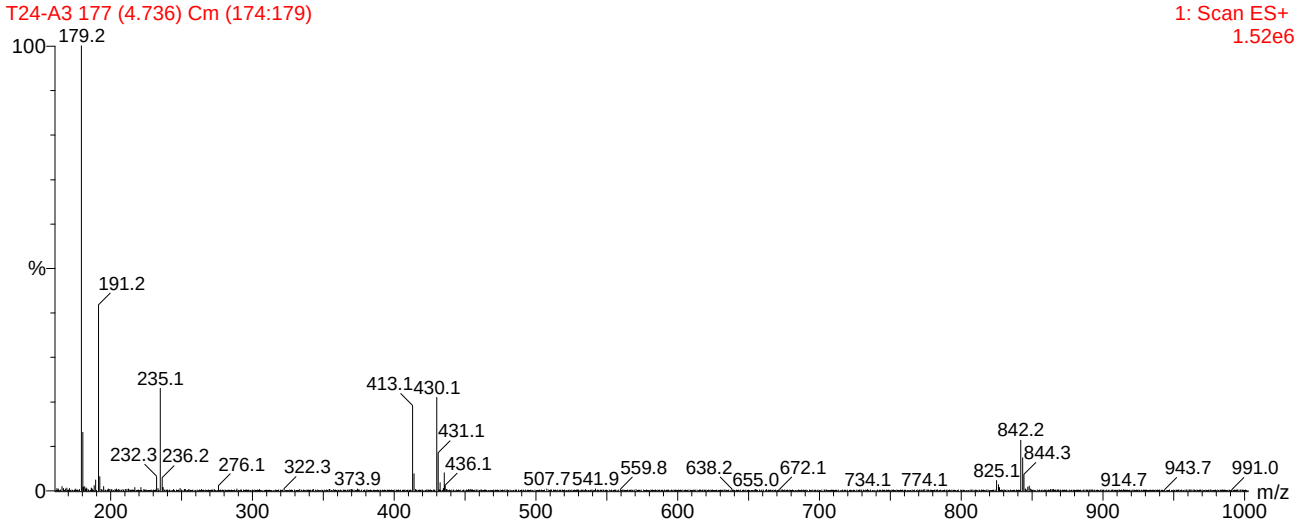
5{18}a


T8-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.12e7
Area
Time Height Area Area%
3.04 12250159 906793.38 21.32
3.56 1728688 143732.81 3.38
4.50 9022769 470899.88 11.07
4.67 32555836 2183798.75 51.34
4.80 3345003 180142.41 4.23
5.02 3751904 184298.81 4.33
5.30 2108281 184302.83 4.33
4.67
268.0
2183799
3.04
240.0
906793
4.50
266.0
470900
5{18}a
Team 8 (Resin I)
Exact Mass 412.14
%
Time

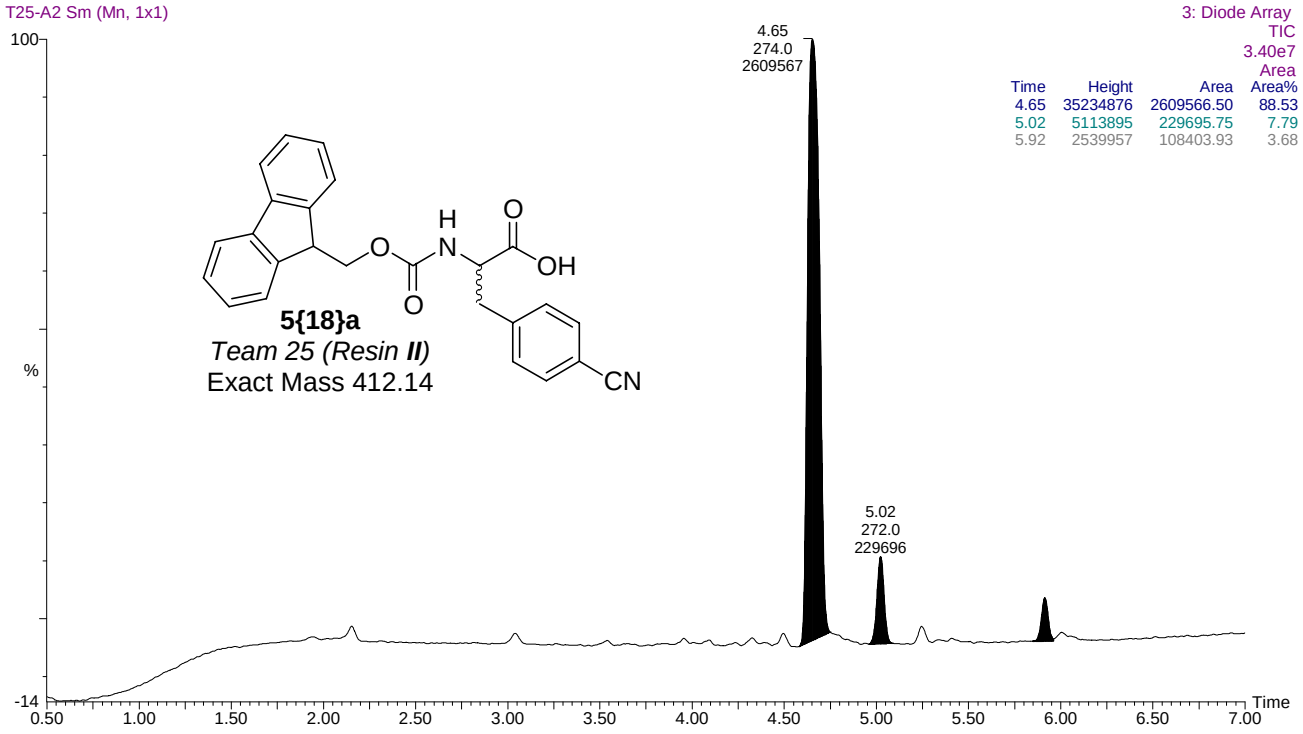

T8-A2 177 (4.736)
1: Scan ES+
2.30e6
T8-A2 169 (4.521)
1: Scan ES+
1.31e6
T8-A2 117 (3.126) Cm (114:117)
1: Scan ES+
1.73e6
m/z

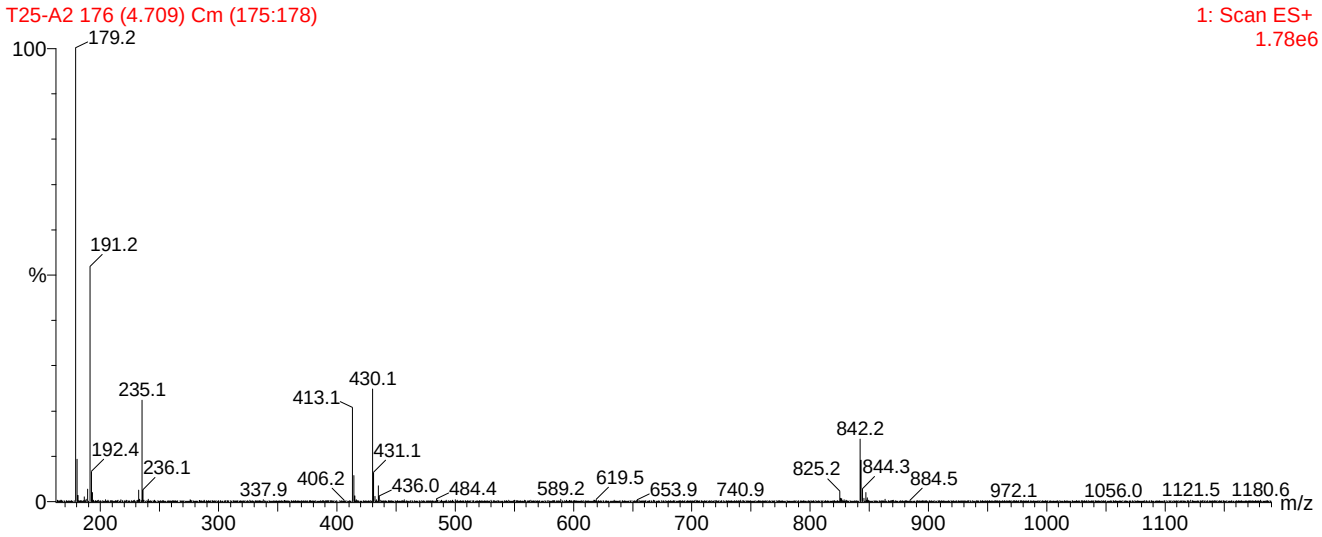
5{18}a


T24-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.49e7
Area
Time Height Area Area%
2.16 1178750 89875.30 2.69
4.65 36218196 2938054.00 87.97
5.03 4643881 207057.94 6.20
5.92 2461530 104877.83 3.14
4.65
264.0
2938054
100
%
-14
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
H
N
O
O
OH
O
O
CN
5{18}a
Team 24 (Resin II)
Exact Mass 412.14


T24-A3 177 (4.736) Cm (174:179)
1: Scan ES+
1.52e6
100
%
0
179.2
191.2
235.1
232.3
236.2
276.1
322.3
373.9
413.1
430.1
431.1
436.1
507.7
541.9
559.8
638.2
655.0
672.1
734.1
774.1
825.1
842.2
844.3
914.7
943.7
991.0
200 300 400 500 600 700 800 900 1000
m/z

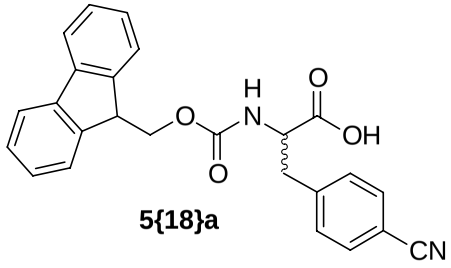
5{18}a


T25-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.40e7
Area
Time Height Area Area%
4.65 35234876 2609566.50 88.53
5.02 5113895 229695.75 7.79
5.92 2539957 108403.93 3.68
4.65
274.0
2609567
5.02
272.0
229696
5{18}a
Team 25 (Resin II)
Exact Mass 412.14
100
%
-14
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

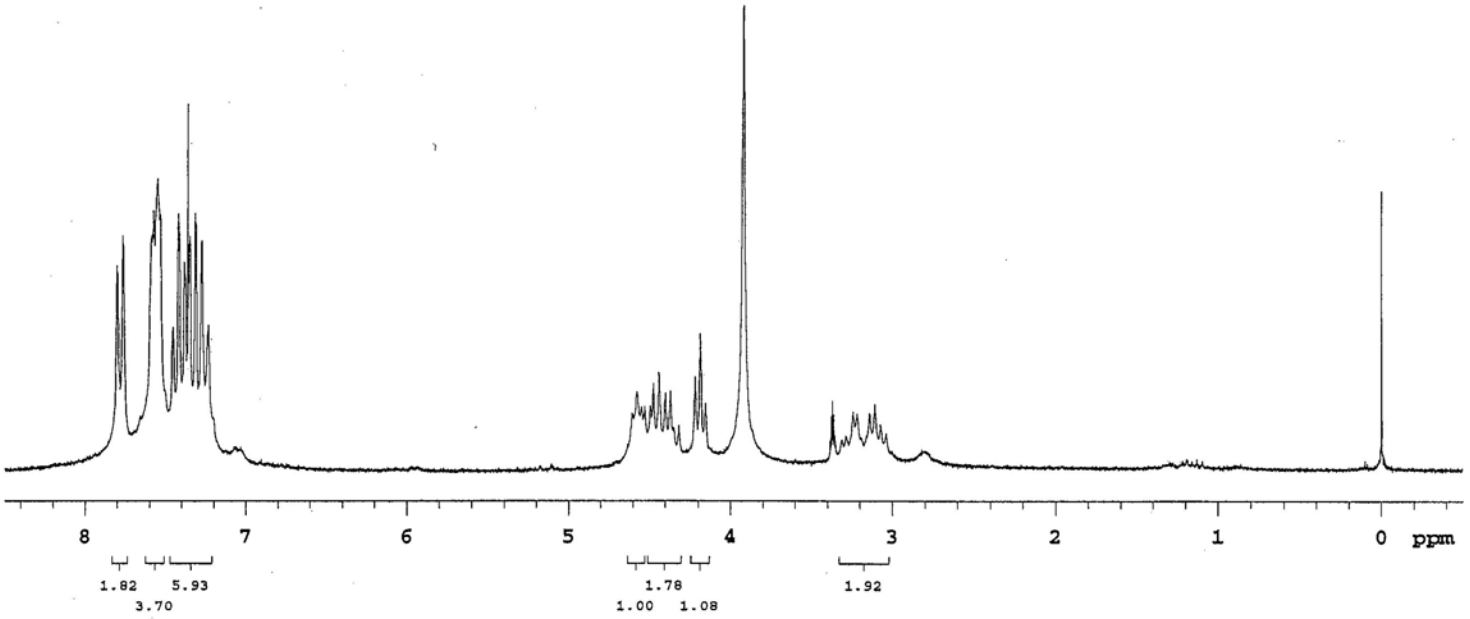

T25-A2 176 (4.709) Cm (175:178)
1: Scan ES+
1.78e6
100
%
0
179.2
191.2
235.1
192.4
236.1
337.9
406.2
413.1
430.1
431.1
436.0
484.4
589.2
619.5
653.9
740.9
825.2
842.2
844.3
884.5
972.1
1056.0
1121.5
1180.6
m/z
200 300 400 500 600 700 800 900 1000 1100

1H_BB#34_A3_CD3ODinCDCl3_02_07

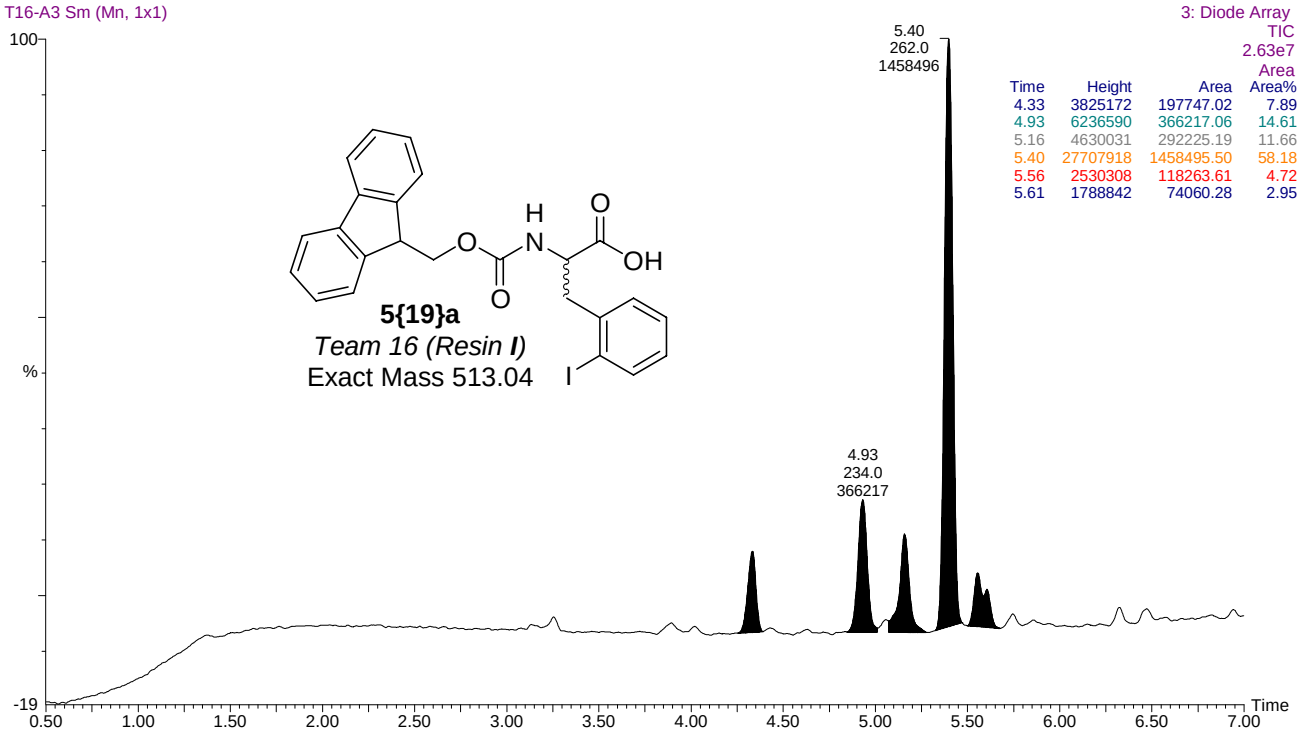
Pulse Sequence: s2pul

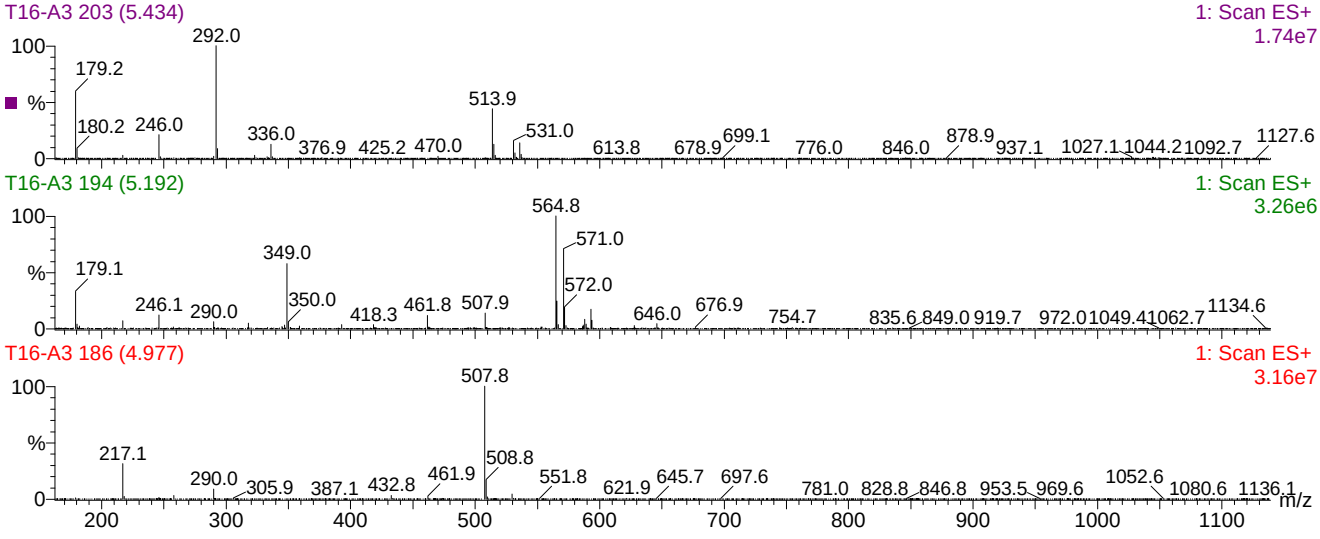


5{18}a

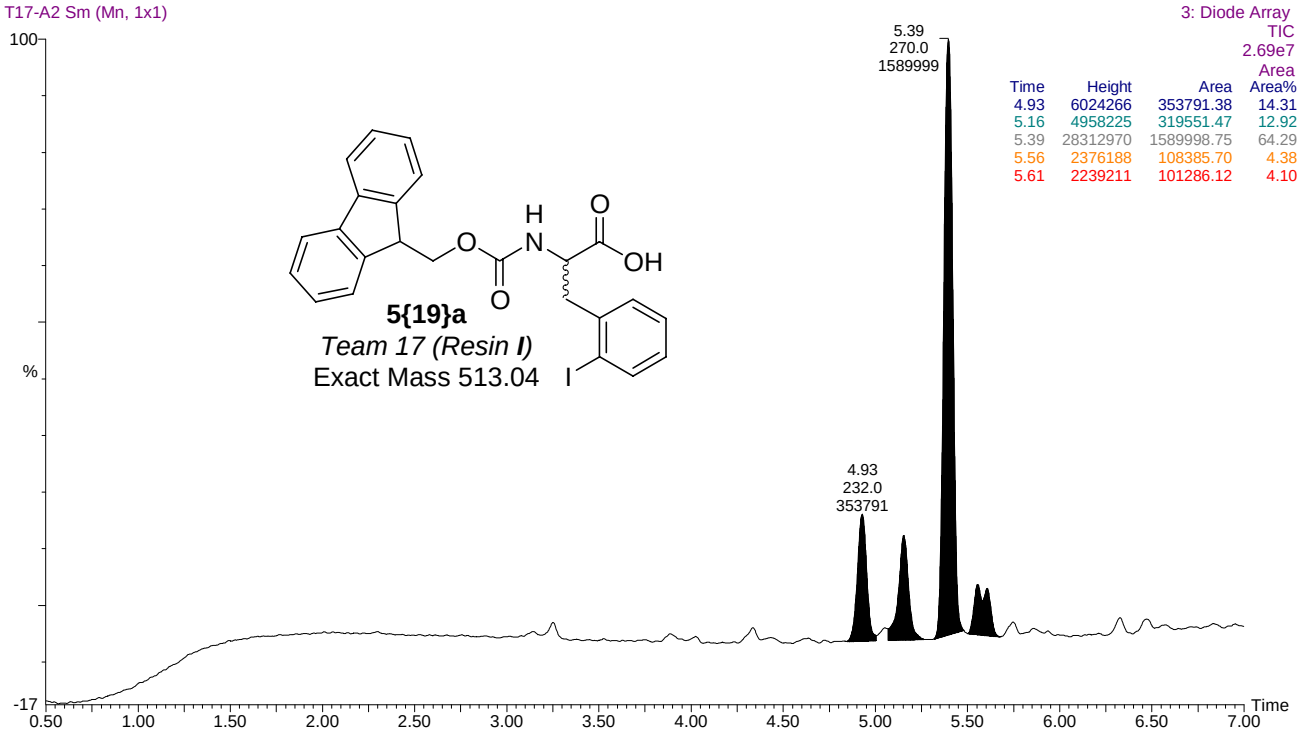


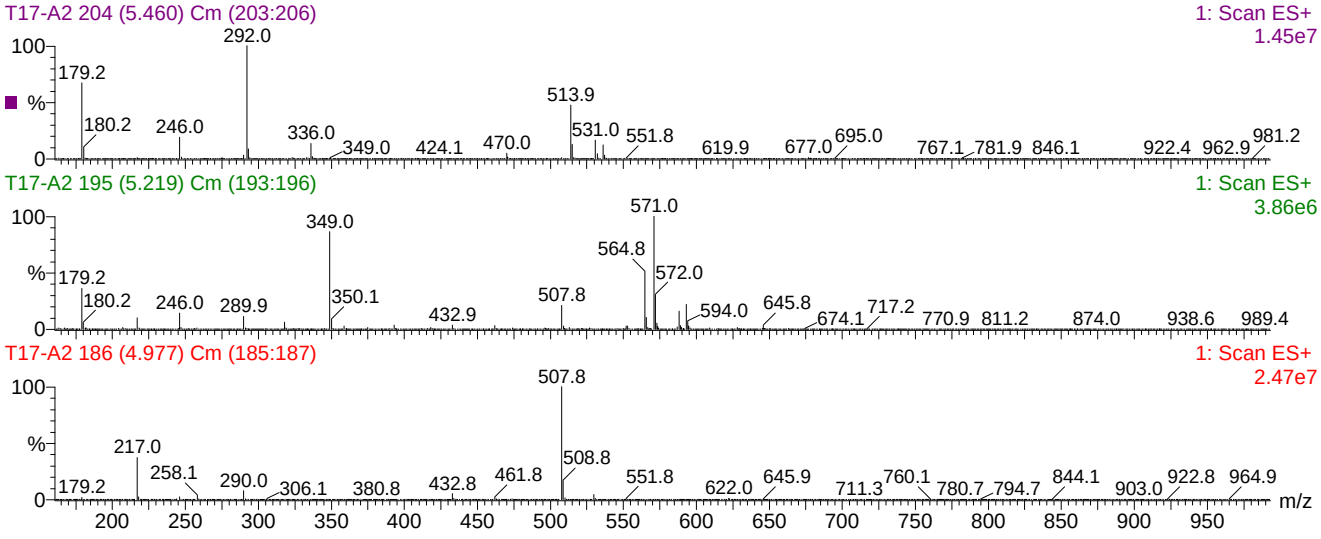
5{19}a


T16-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.63e7
Area
Time Height Area Area%
4.33 3825172 197747.02 7.89
4.93 6236590 366217.06 14.61
5.16 4630031 292225.19 11.66
5.40 27707918 1458495.50 58.18
5.56 2530308 118263.61 4.72
5.61 1788842 74060.28 2.95
5.40
262.0
1458496
4.93
234.0
366217
5{19}a
Team 16 (Resin I)
Exact Mass 513.04
%
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

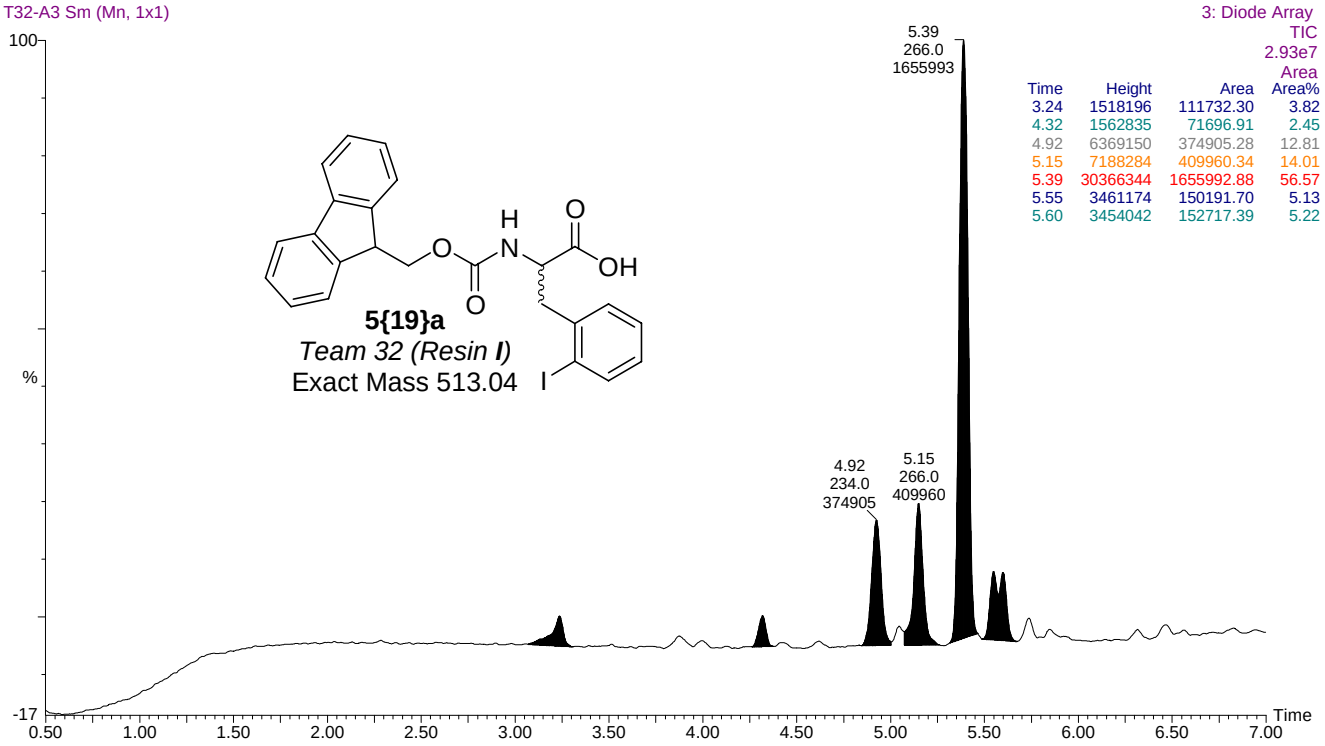

T16-A3 203 (5.434)
1: Scan ES+
1.74e7
T16-A3 194 (5.192)
1: Scan ES+
3.26e6
T16-A3 186 (4.977)
1: Scan ES+
3.16e7
m/z

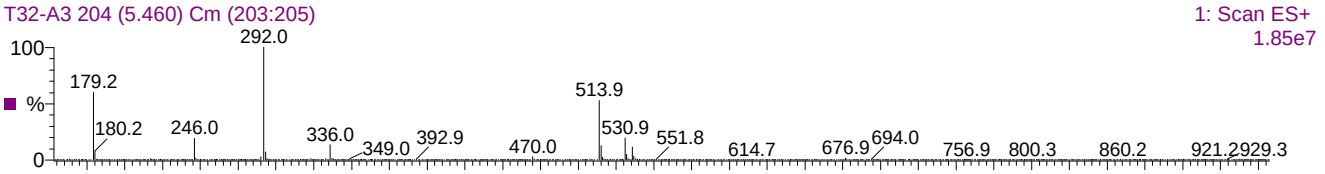
5{19}a

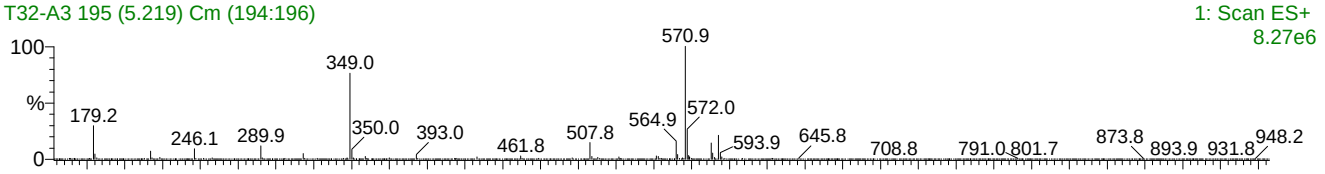

T17-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.69e7
Area
Time Height Area Area%
4.93 6024266 353791.38 14.31
5.16 4958225 319551.47 12.92
5.39 28312970 1589998.75 64.29
5.56 2376188 108385.70 4.38
5.61 2239211 101286.12 4.10
5.39
270.0
1589999
4.93
232.0
353791
5{19}a
Team 17 (Resin I)
Exact Mass 513.04
%
Time

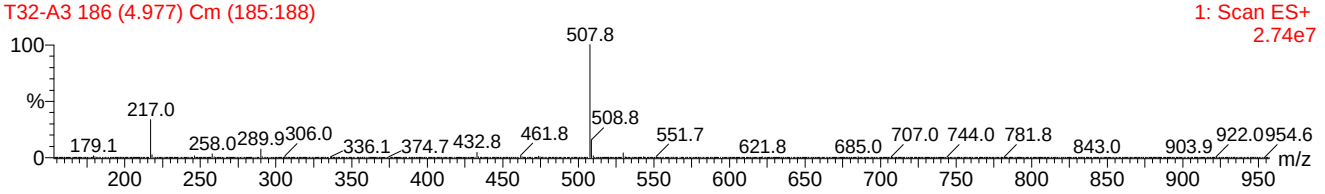

T17-A2 204 (5.460) Cm (203:206)
1: Scan ES+
1.45e7
T17-A2 195 (5.219) Cm (193:196)
1: Scan ES+
3.86e6
T17-A2 186 (4.977) Cm (185:187)
1: Scan ES+
2.47e7
m/z

5{19}a

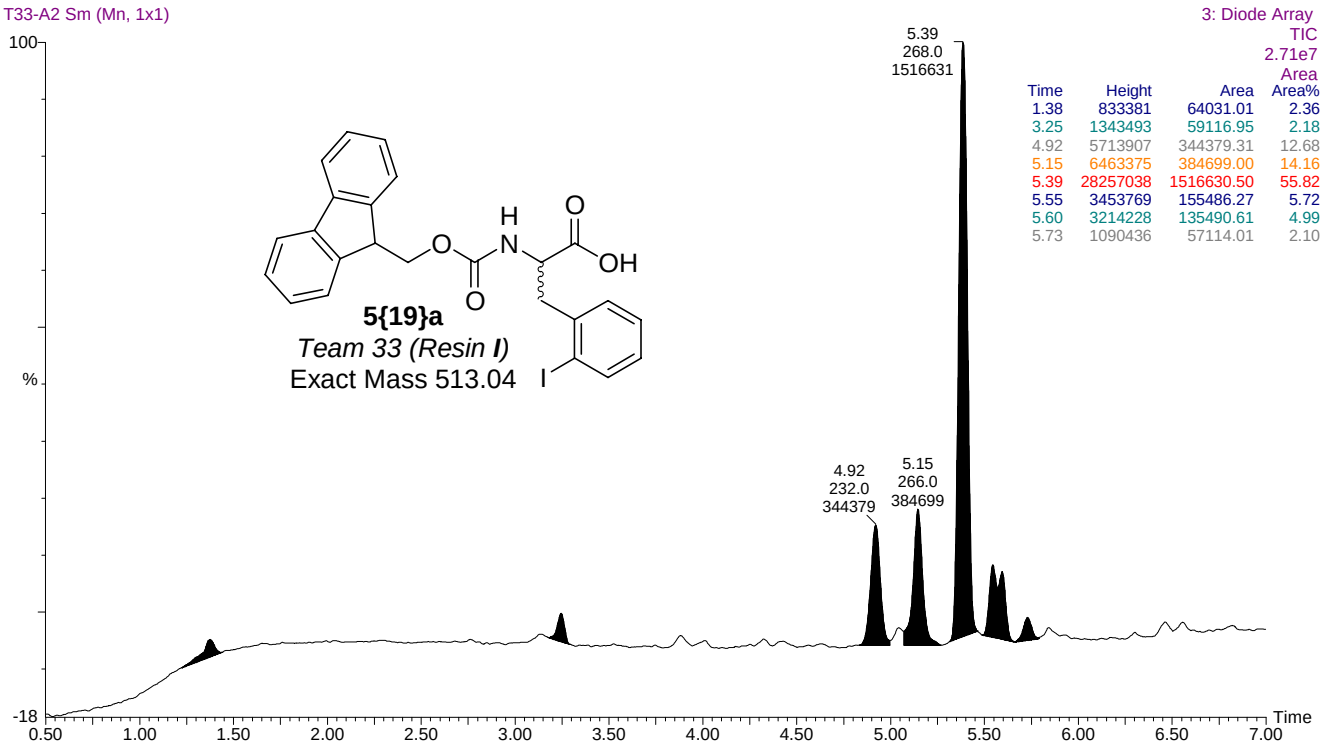

T32-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.93e7
Area
Time Height Area Area%
3.24 1518196 111732.30 3.82
4.32 1562835 71696.91 2.45
4.92 6369150 374905.28 12.81
5.15 7188284 409960.34 14.01
5.39 30366344 1655992.88 56.57
5.55 3461174 150191.70 5.13
5.60 3454042 152717.39 5.22
5.39
266.0
1655993
4.92
234.0
374905
5.15
266.0
409960
5{19}a
Team 32 (Resin I)
Exact Mass 513.04
%
Time

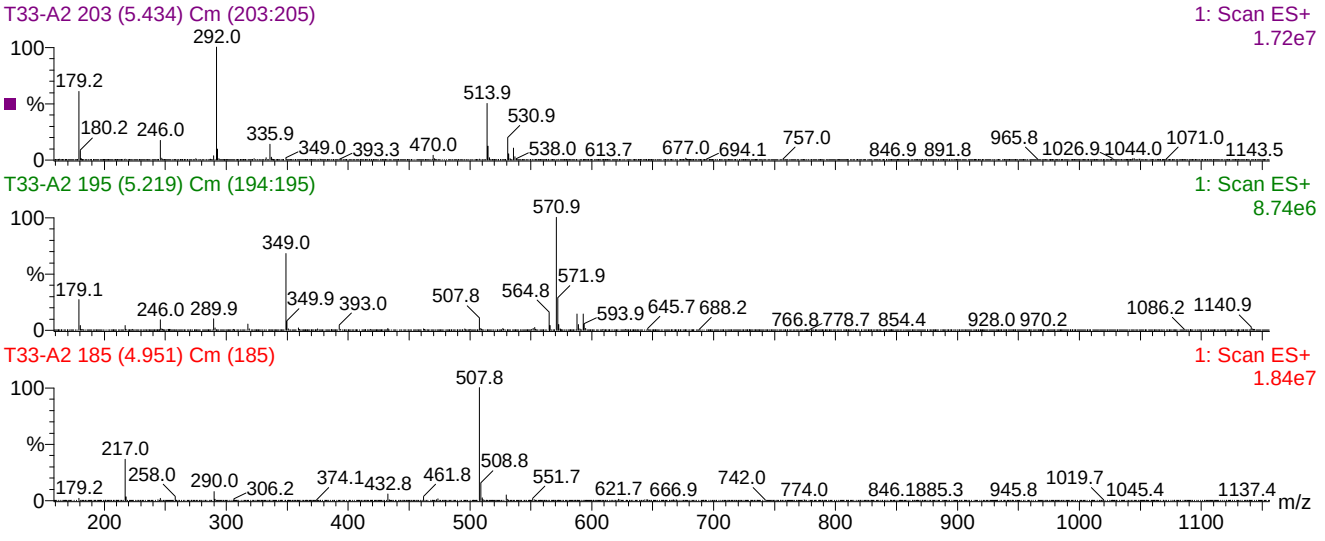

T32-A3 204 (5.460) Cm (203:205)
1: Scan ES+
1.85e7
292.0
179.2
513.9
180.2
246.0
336.0
349.0
392.9
470.0
530.9
551.8
614.7
676.9
694.0
756.9
800.3
860.2
921.2929.3


T32-A3 195 (5.219) Cm (194:196)
1: Scan ES+
8.27e6
570.9
349.0
179.2
572.0
246.1
289.9
350.0
393.0
461.8
507.8
564.9
593.9
645.8
708.8
791.0801.7
873.8
893.9
931.8
948.2


T32-A3 186 (4.977) Cm (185:188)
1: Scan ES+
2.74e7
507.8
217.0
508.8
179.1
258.0289.9306.0
336.1
374.7
432.8
461.8
551.7
621.8
685.0
707.0
744.0
781.8
843.0
903.9
922.0954.6
m/z

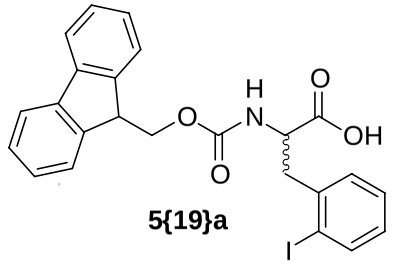
5{19}a


T33-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.71e7
Area
Time Height Area Area%
1.38 833381 64031.01 2.36
3.25 1343493 59116.95 2.18
4.92 5713907 344379.31 12.68
5.15 6463375 384699.00 14.16
5.39 28257038 1516630.50 55.82
5.55 3453769 155486.27 5.72
5.60 3214228 135490.61 4.99
5.73 1090436 57114.01 2.10
5.39
268.0
1516631
4.92
232.0
344379
5.15
266.0
384699
5{19}a
Team 33 (Resin I)
Exact Mass 513.04
%
Time

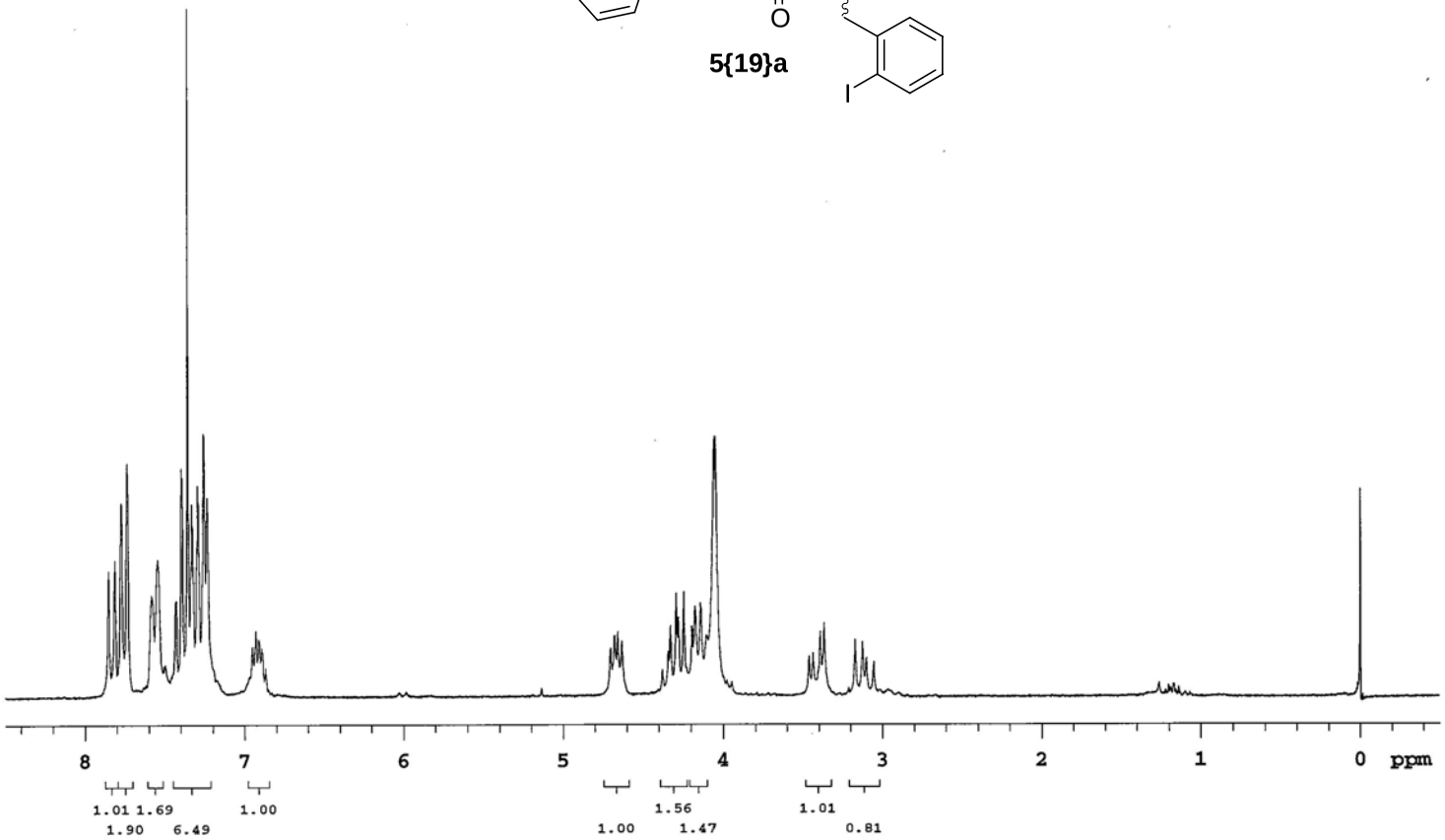

T33-A2 203 (5.434) Cm (203:205)
1: Scan ES+
1.72e7
T33-A2 195 (5.219) Cm (194:195)
1: Scan ES+
8.74e6
T33-A2 185 (4.951) Cm (185)
1: Scan ES+
1.84e7
m/z

BB#34_B3_02_07_07

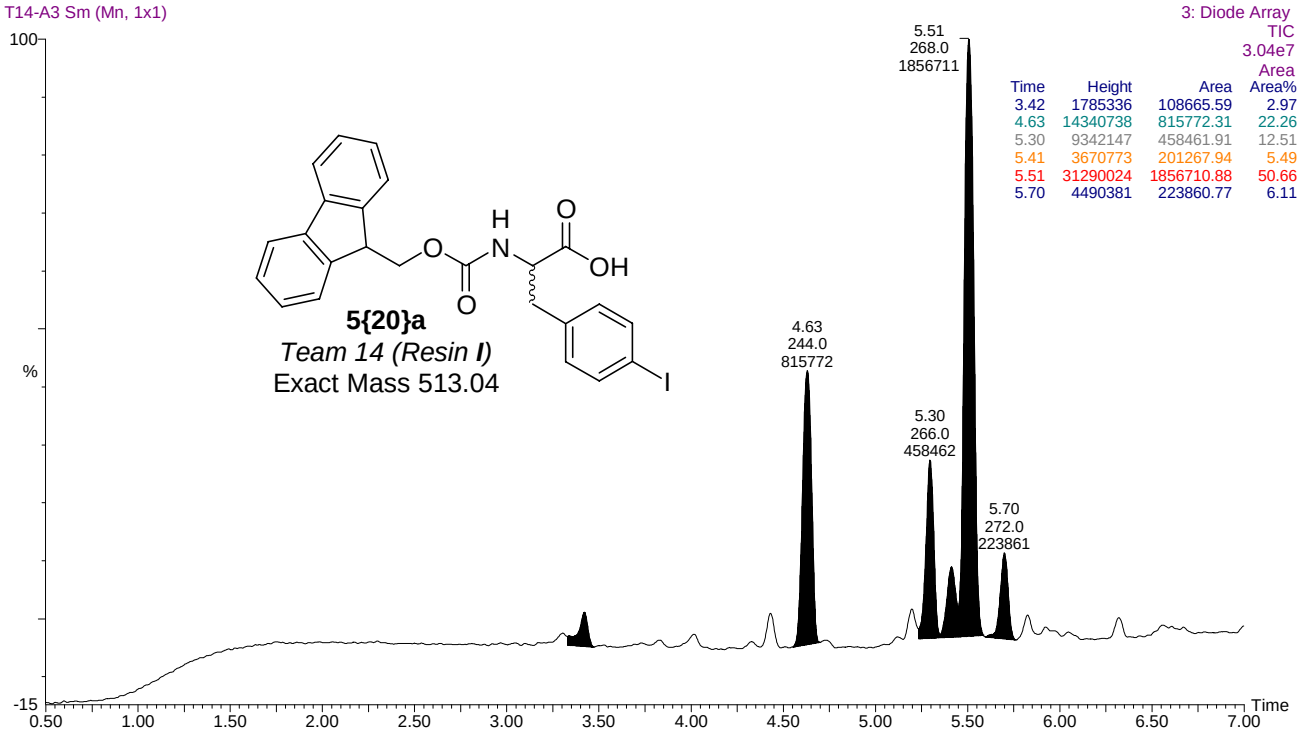
Pulse Sequence: s2pul

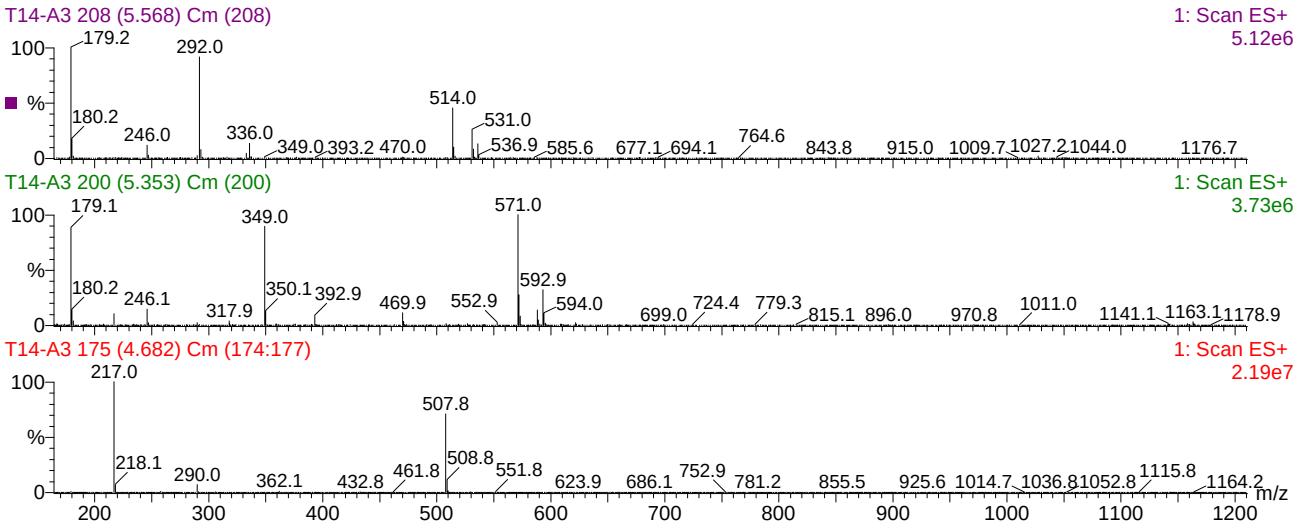


5{19}a

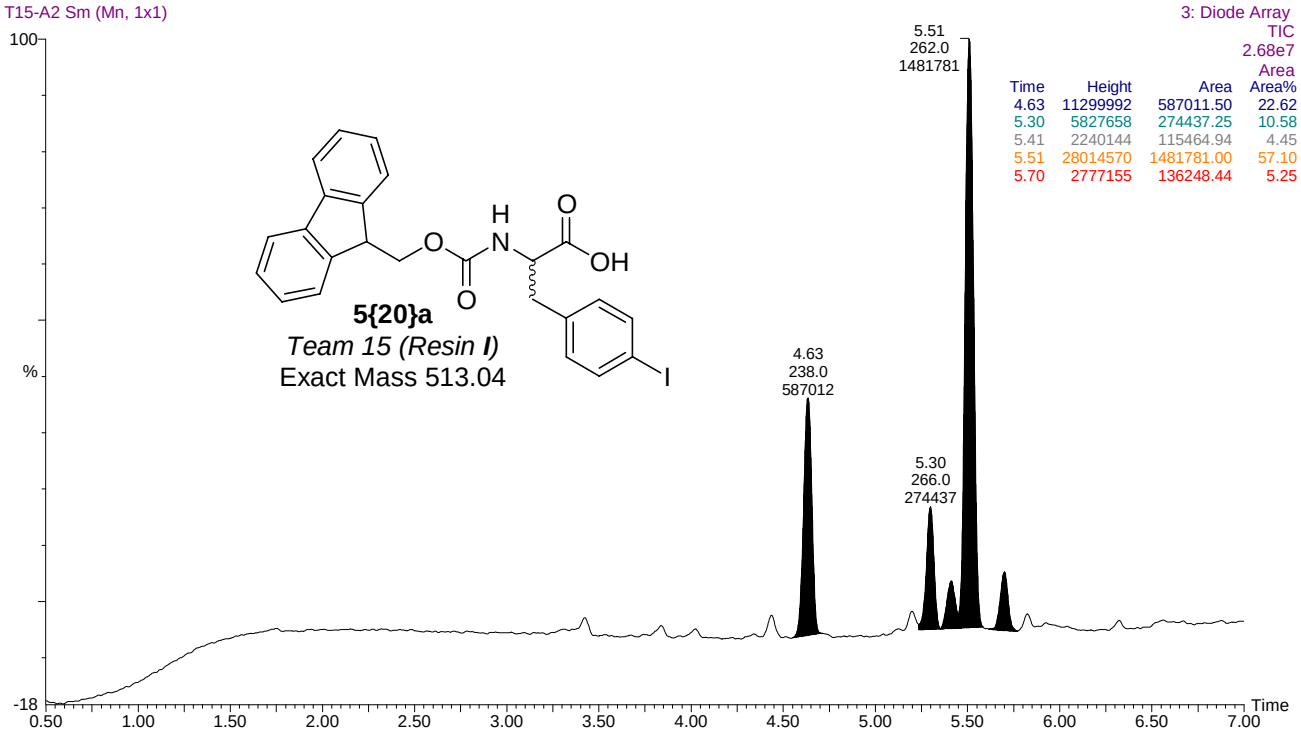


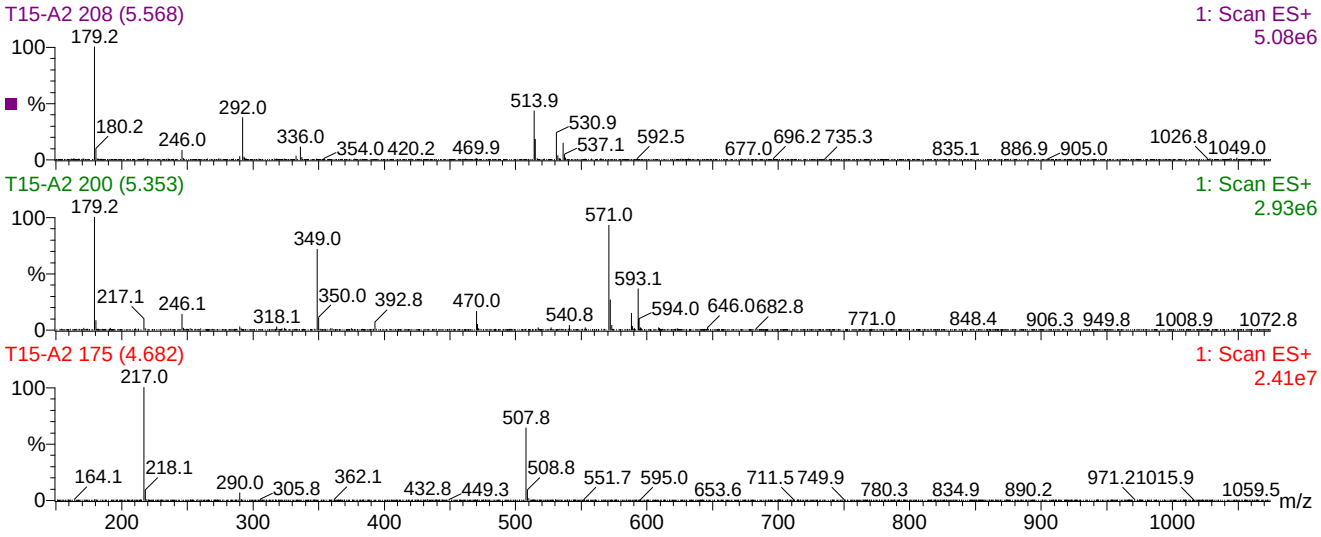
5{20}a


T14-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.04e7
Area
Time Height Area Area%
3.42 1785336 108665.59 2.97
4.63 14340738 815772.31 22.26
5.30 9342147 458461.91 12.51
5.41 3670773 201267.94 5.49
5.51 31290024 1856710.88 50.66
5.70 4490381 223860.77 6.11
5.51
268.0
1856711
4.63
244.0
815772
5.30
266.0
458462
5.70
272.0
223861
5{20}a
Team 14 (Resin I)
Exact Mass 513.04
%
Time

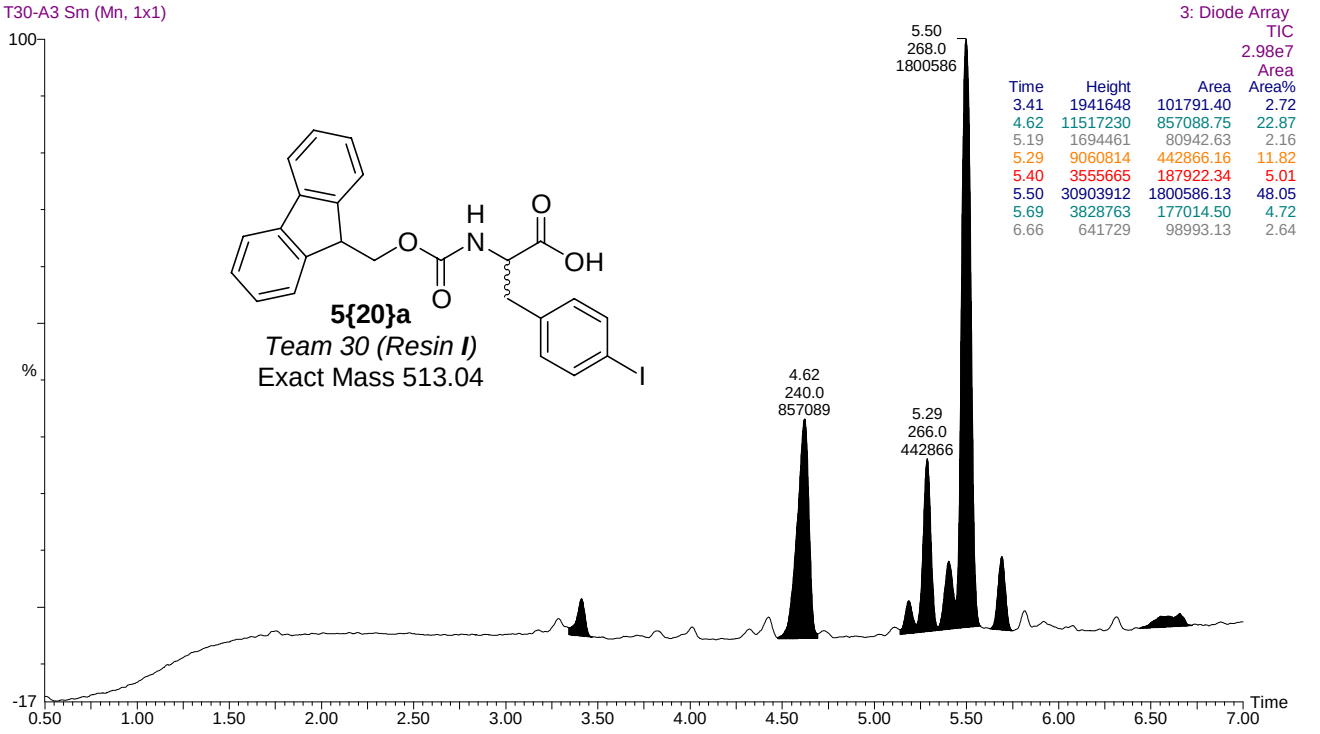

T14-A3 208 (5.568) Cm (208)
1: Scan ES+
5.12e6
T14-A3 200 (5.353) Cm (200)
1: Scan ES+
3.73e6
T14-A3 175 (4.682) Cm (174:177)
1: Scan ES+
2.19e7
m/z

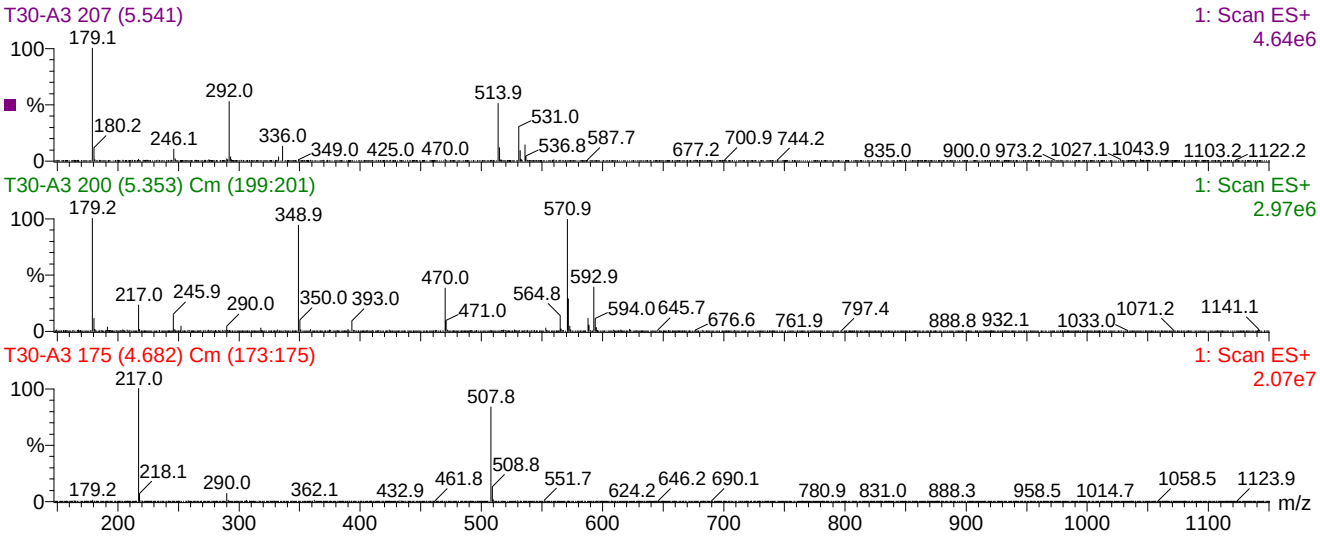
5{20}a


T15-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.68e7
Area
Time Height Area Area%
4.63 11299992 587011.50 22.62
5.30 5827658 274437.25 10.58
5.41 2240144 115464.94 4.45
5.51 28014570 1481781.00 57.10
5.70 2777155 136248.44 5.25
5.51
262.0
1481781
4.63
238.0
587012
5.30
266.0
274437
5{20}a
Team 15 (Resin I)
Exact Mass 513.04
%
Time

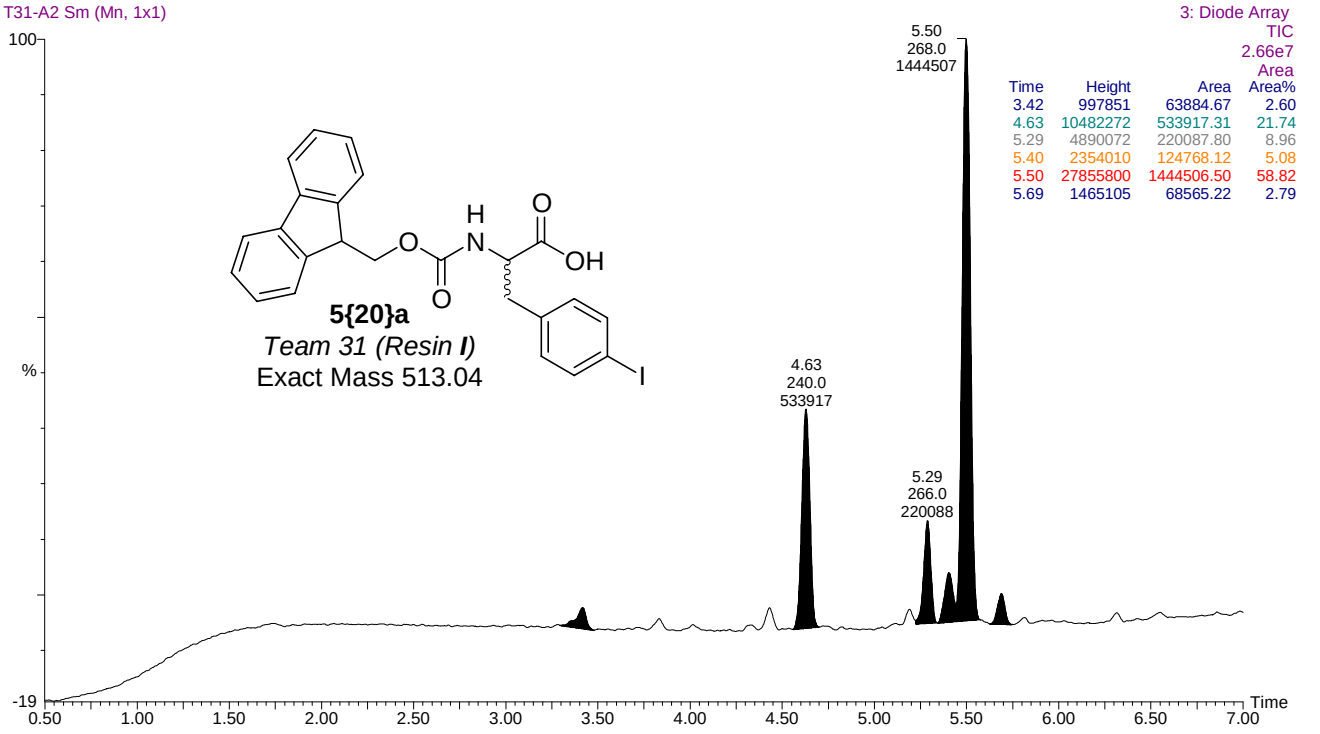

T15-A2 208 (5.568)
1: Scan ES+
5.08e6
T15-A2 200 (5.353)
1: Scan ES+
2.93e6
T15-A2 175 (4.682)
1: Scan ES+
2.41e7
m/z

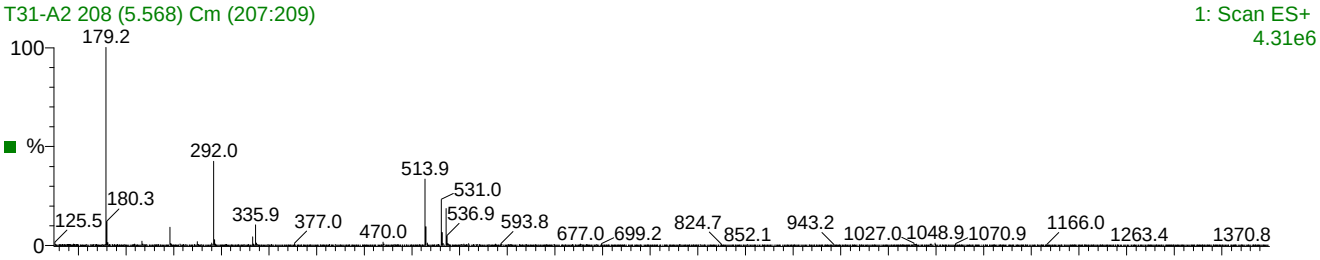
5{20}a

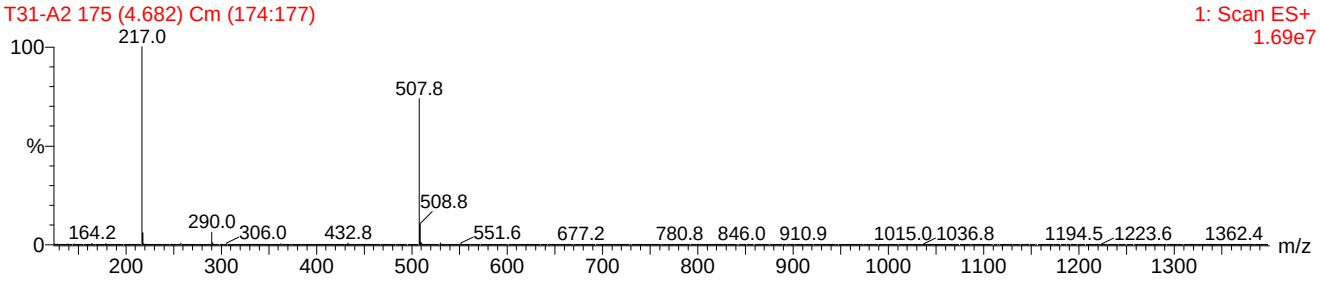

T30-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.98e7
Area
Time Height Area Area%
3.41 1941648 101791.40 2.72
4.62 11517230 857088.75 22.87
5.19 1694461 80942.63 2.16
5.29 9060814 442866.16 11.82
5.40 3555665 187922.34 5.01
5.50 30903912 1800586.13 48.05
5.69 3828763 177014.50 4.72
6.66 641729 98993.13 2.64
5.50
268.0
1800586
4.62
240.0
857089
5.29
266.0
442866
5{20}a
Team 30 (Resin I)
Exact Mass 513.04
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00


T30-A3 207 (5.541)
1: Scan ES+
4.64e6
179.1 292.0 513.9 531.0 180.2 246.1 336.0 349.0 425.0 470.0 536.8 587.7 677.2 700.9 744.2 835.0 900.0 973.2 1027.1 1043.9 1103.2 1122.2
T30-A3 200 (5.353) Cm (199:201)
1: Scan ES+
2.97e6
179.2 348.9 570.9 217.0 245.9 290.0 350.0 393.0 470.0 471.0 564.8 592.9 594.0 645.7 676.6 761.9 797.4 888.8 932.1 1033.0 1071.2 1141.1
T30-A3 175 (4.682) Cm (173:175)
1: Scan ES+
2.07e7
217.0 507.8 179.2 218.1 290.0 362.1 432.9 461.8 508.8 551.7 624.2 646.2 690.1 780.9 831.0 888.3 958.5 1014.7 1058.5 1123.9
100
%
0
200 300 400 500 600 700 800 900 1000 1100
m/z

5{20}a

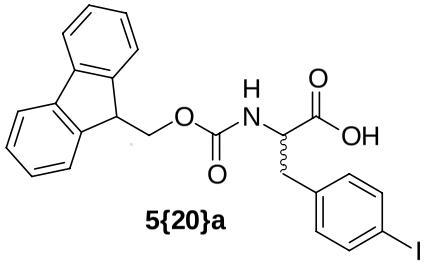

T31-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.66e7
Area
Time Height Area Area%
3.42 997851 63884.67 2.60
4.63 10482272 533917.31 21.74
5.29 4890072 220087.80 8.96
5.40 2354010 124768.12 5.08
5.50 27855800 1444506.50 58.82
5.69 1465105 68565.22 2.79
5.50
268.0
1444507
4.63
240.0
533917
5.29
266.0
220088
5{20}a
Team 31 (Resin I)
Exact Mass 513.04
%
Time


T31-A2 208 (5.568) Cm (207:209)
1: Scan ES+
4.31e6
179.2
292.0
513.9
531.0
180.3
125.5
335.9
377.0
470.0
536.9
593.8
677.0
699.2
824.7
852.1
943.2
1027.0
1048.9
1070.9
1166.0
1263.4
1370.8
%

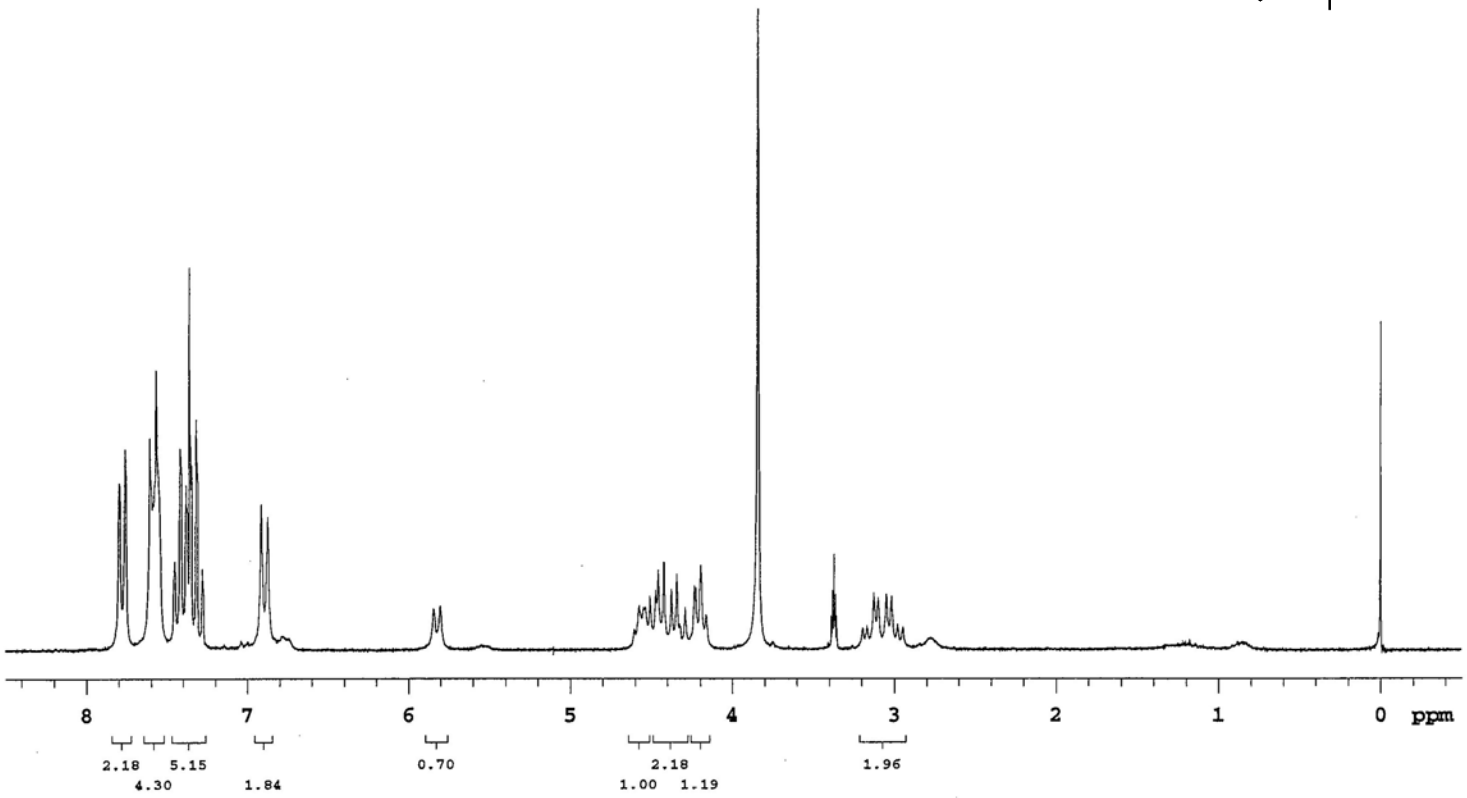

T31-A2 175 (4.682) Cm (174:177)
1: Scan ES+
1.69e7
217.0
507.8
508.8
164.2
290.0
306.0
432.8
551.6
677.2
780.8
846.0
910.9
1015.0
1036.8
1194.5
1223.6
1362.4
%
m/z

1H_BB#34_B2_CD3ODinCDCl3_02_07

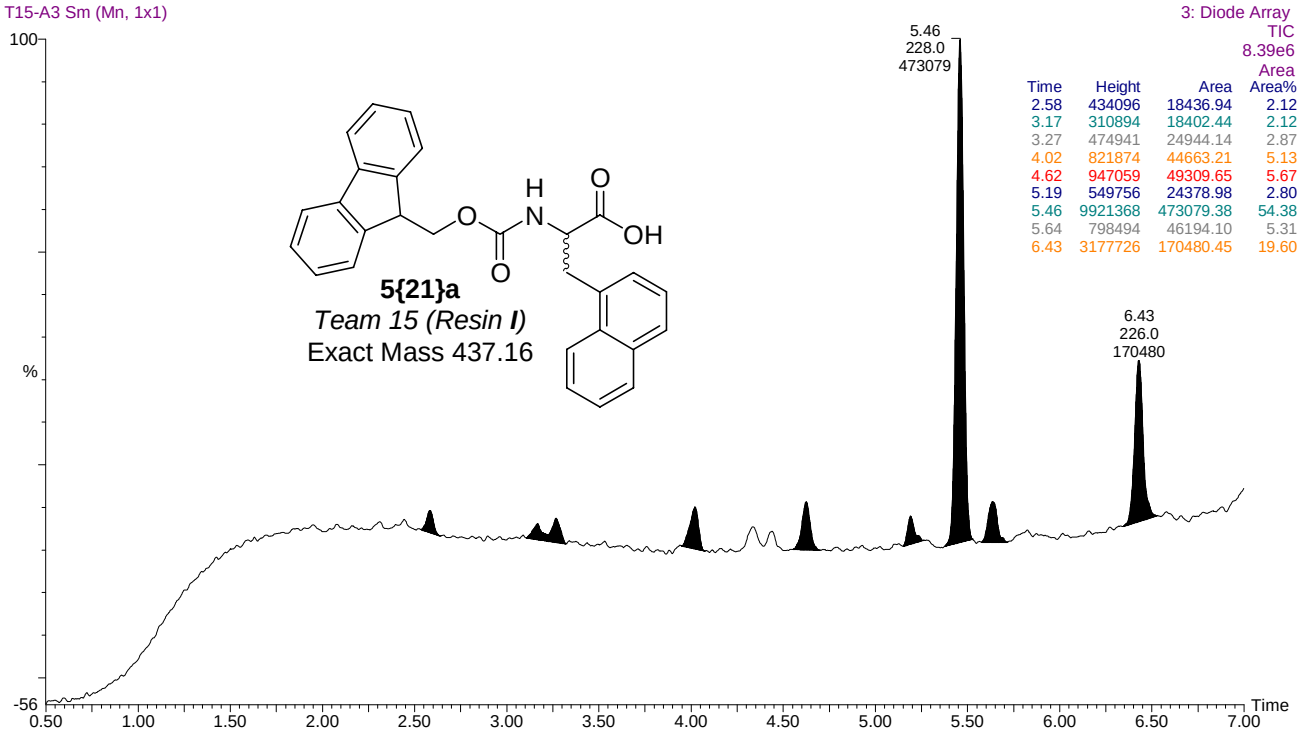
Pulse Sequence: s2pul

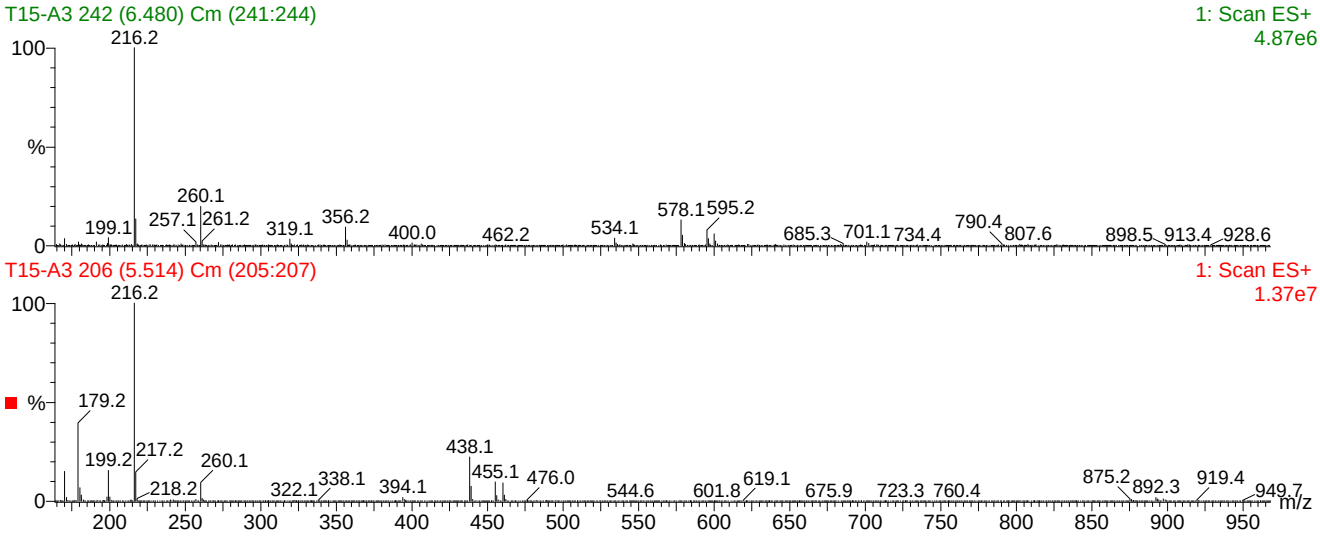


5{20}a

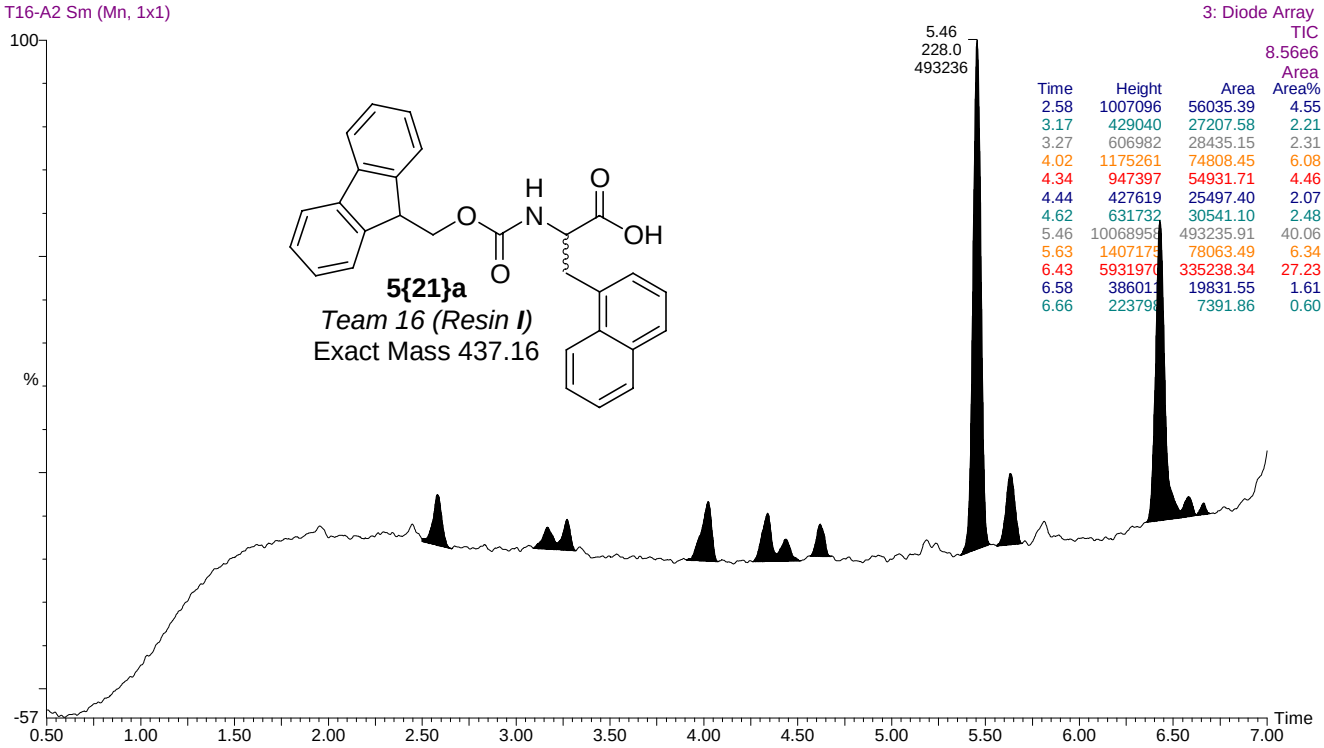


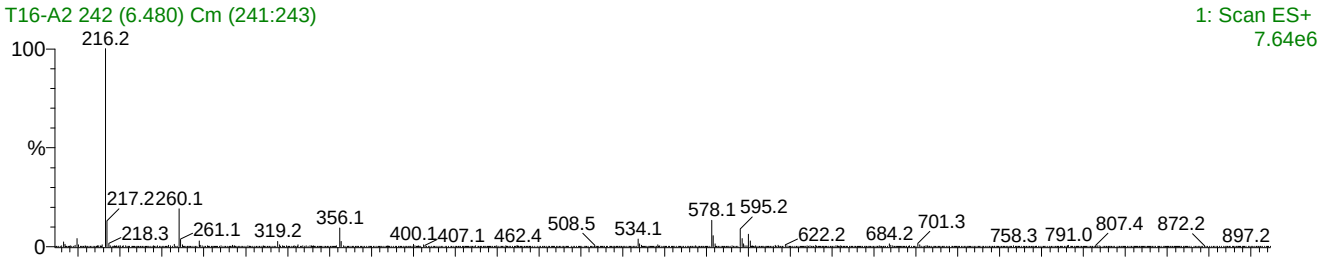
5{21}a

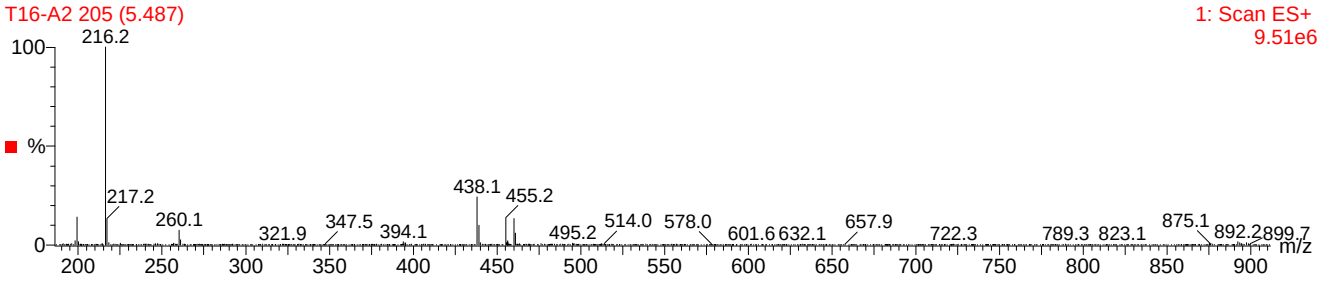

T15-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
8.39e6
Area
Time Height Area Area%
2.58 434096 18436.94 2.12
3.17 310894 18402.44 2.12
3.27 474941 24944.14 2.87
4.02 821874 44663.21 5.13
4.62 947059 49309.65 5.67
5.19 549756 24378.98 2.80
5.46 9921368 473079.38 54.38
5.64 798494 46194.10 5.31
6.43 3177726 170480.45 19.60
5.46
228.0
473079
6.43
226.0
170480
5{21}a
Team 15 (Resin I)
Exact Mass 437.16
100
%
-56
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00


T15-A3 242 (6.480) Cm (241:244)
1: Scan ES+
4.87e6
216.2
260.1
199.1 257.1 261.2 319.1 356.2 400.0 462.2 534.1 578.1 595.2 685.3 701.1 734.4 790.4 807.6 898.5 913.4 928.6
T15-A3 206 (5.514) Cm (205:207)
1: Scan ES+
1.37e7
216.2
179.2
199.2 217.2 218.2 260.1 322.1 338.1 394.1 438.1 455.1 476.0 544.6 601.8 619.1 675.9 723.3 760.4 875.2 892.3 919.4 949.7
m/z
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

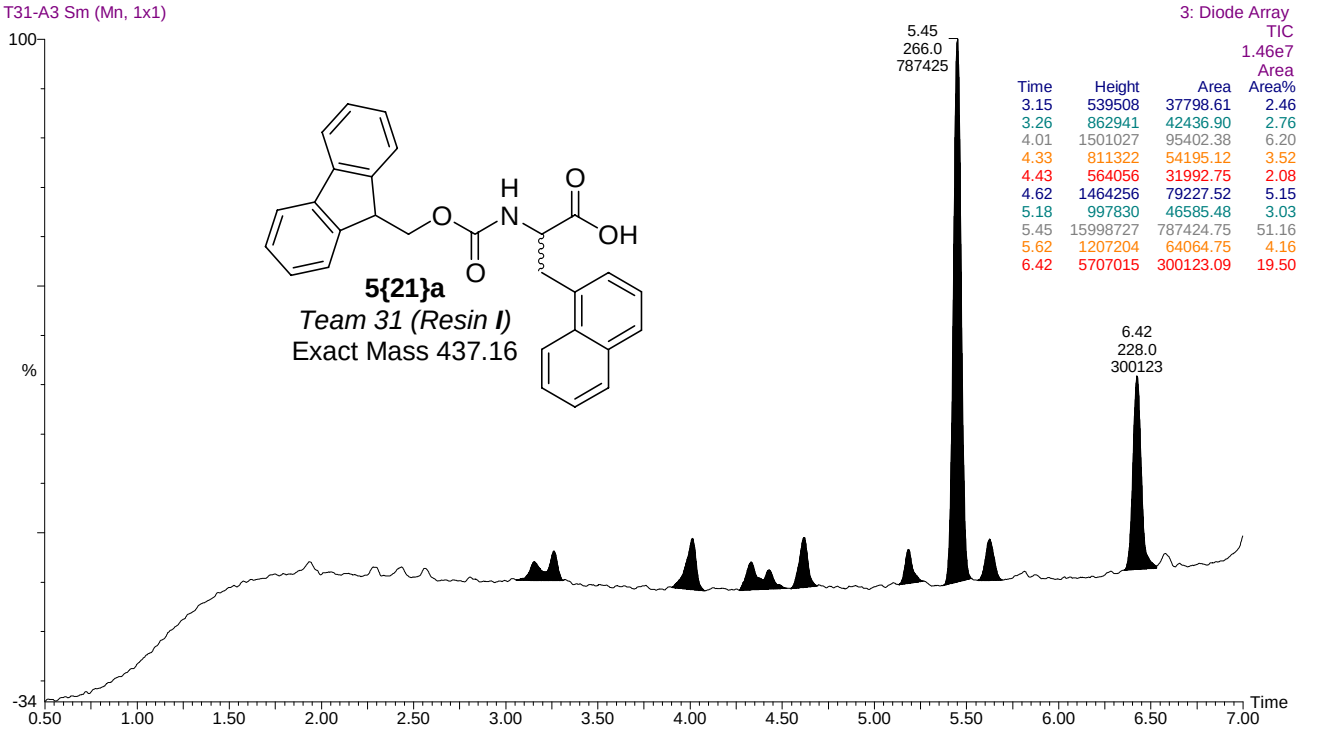
5{21}a

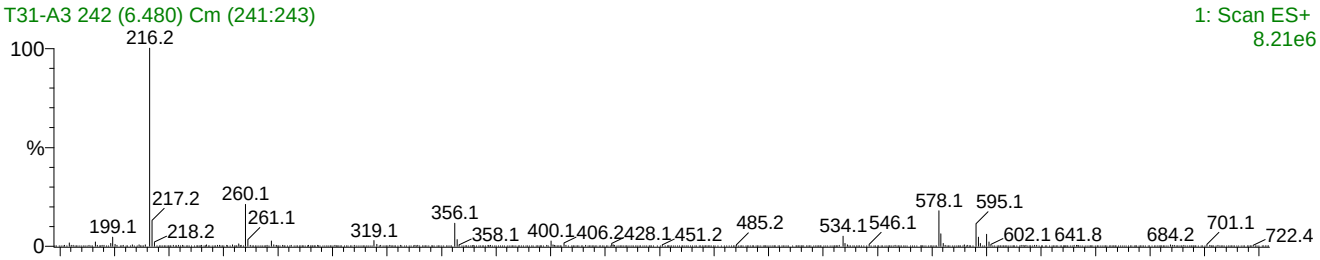

T16-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
8.56e6
Area
5.46
228.0
493236
Time Height Area Area%
2.58 1007096 56035.39 4.55
3.17 429040 27207.58 2.21
3.27 606982 28435.15 2.31
4.02 1175261 74808.45 6.08
4.34 947397 54931.71 4.46
4.44 427619 25497.40 2.07
4.62 631732 30541.10 2.48
5.46 10068958 493235.91 40.06
5.63 1407175 78063.49 6.34
6.43 5931970 335238.34 27.23
6.58 386011 19831.55 1.61
6.66 223798 7391.86 0.60
5{21}a
Team 16 (Resin I)
Exact Mass 437.16
100
%
-57
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time

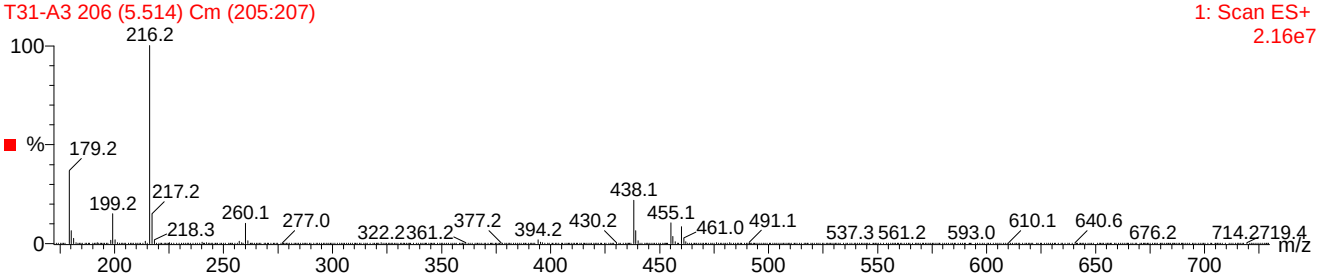

T16-A2 242 (6.480) Cm (241:243)
1: Scan ES+
7.64e6
100
%
0
216.2
217.2 260.1
218.3 261.1 319.2 356.1 400.1 407.1 462.4 508.5 534.1 578.1 595.2 622.2 684.2 701.3 758.3 791.0 807.4 872.2 897.2


T16-A2 205 (5.487)
1: Scan ES+
9.51e6
100
%
0
216.2
217.2 260.1 321.9 347.5 394.1 438.1 455.2 495.2 514.0 578.0 601.6 632.1 657.9 722.3 789.3 823.1 875.1 892.2 899.7
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900
m/z

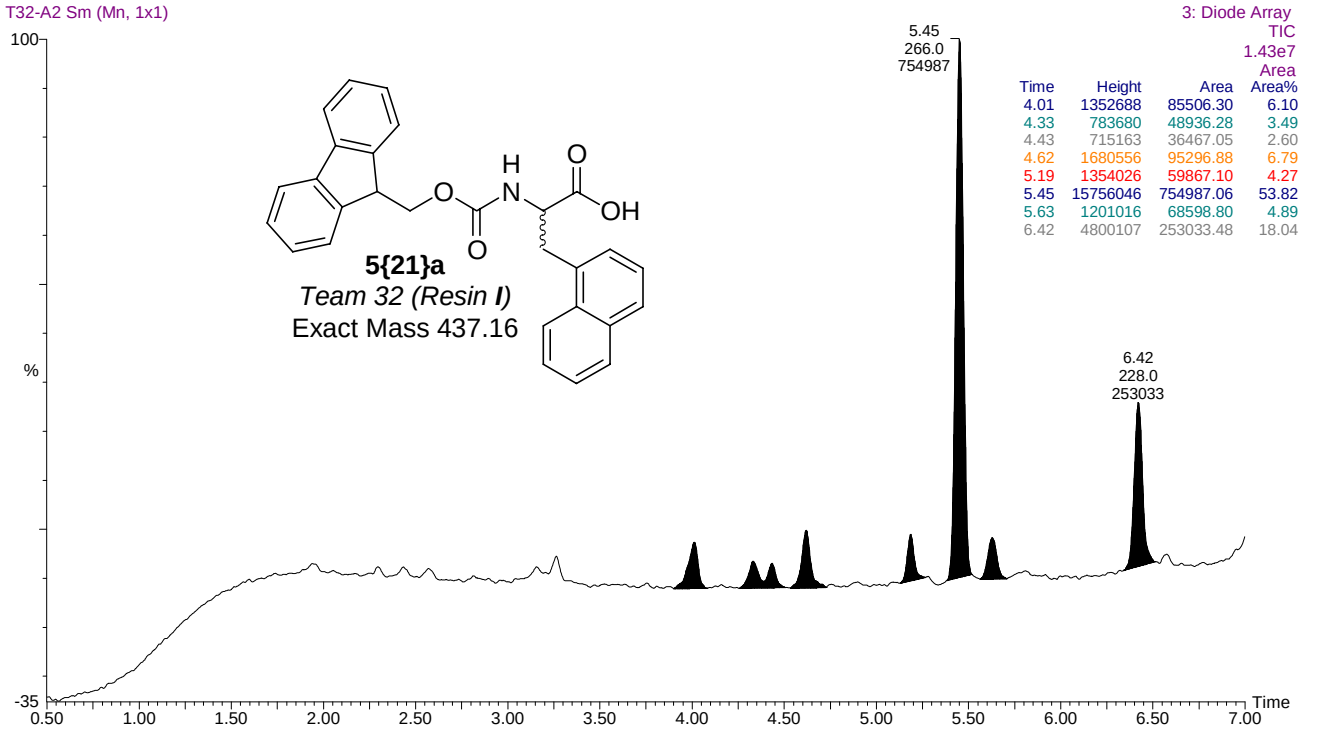
5{21}a

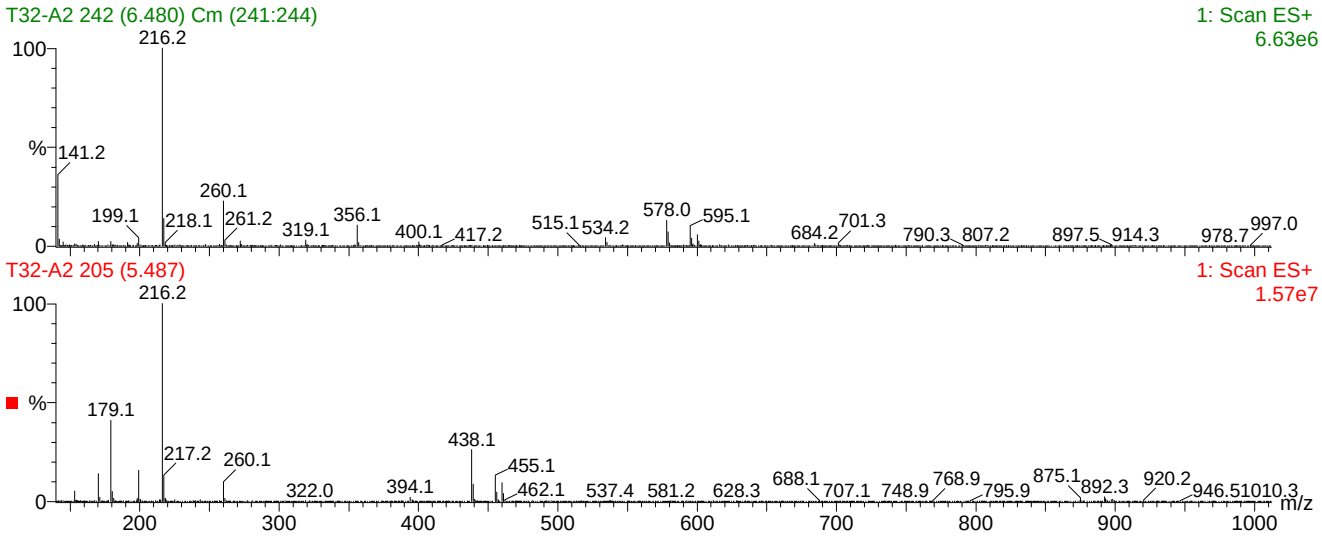

T31-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
1.46e7
Area
Time Height Area Area%
3.15 539508 37798.61 2.46
3.26 862941 42436.90 2.76
4.01 1501027 95402.38 6.20
4.33 811322 54195.12 3.52
4.43 564056 31992.75 2.08
4.62 1464256 79227.52 5.15
5.18 997830 46585.48 3.03
5.45 15998727 787424.75 51.16
5.62 1207204 64064.75 4.16
6.42 5707015 300123.09 19.50
5.45
266.0
787425
6.42
228.0
300123
5{21}a
Team 31 (Resin I)
Exact Mass 437.16
%
Time

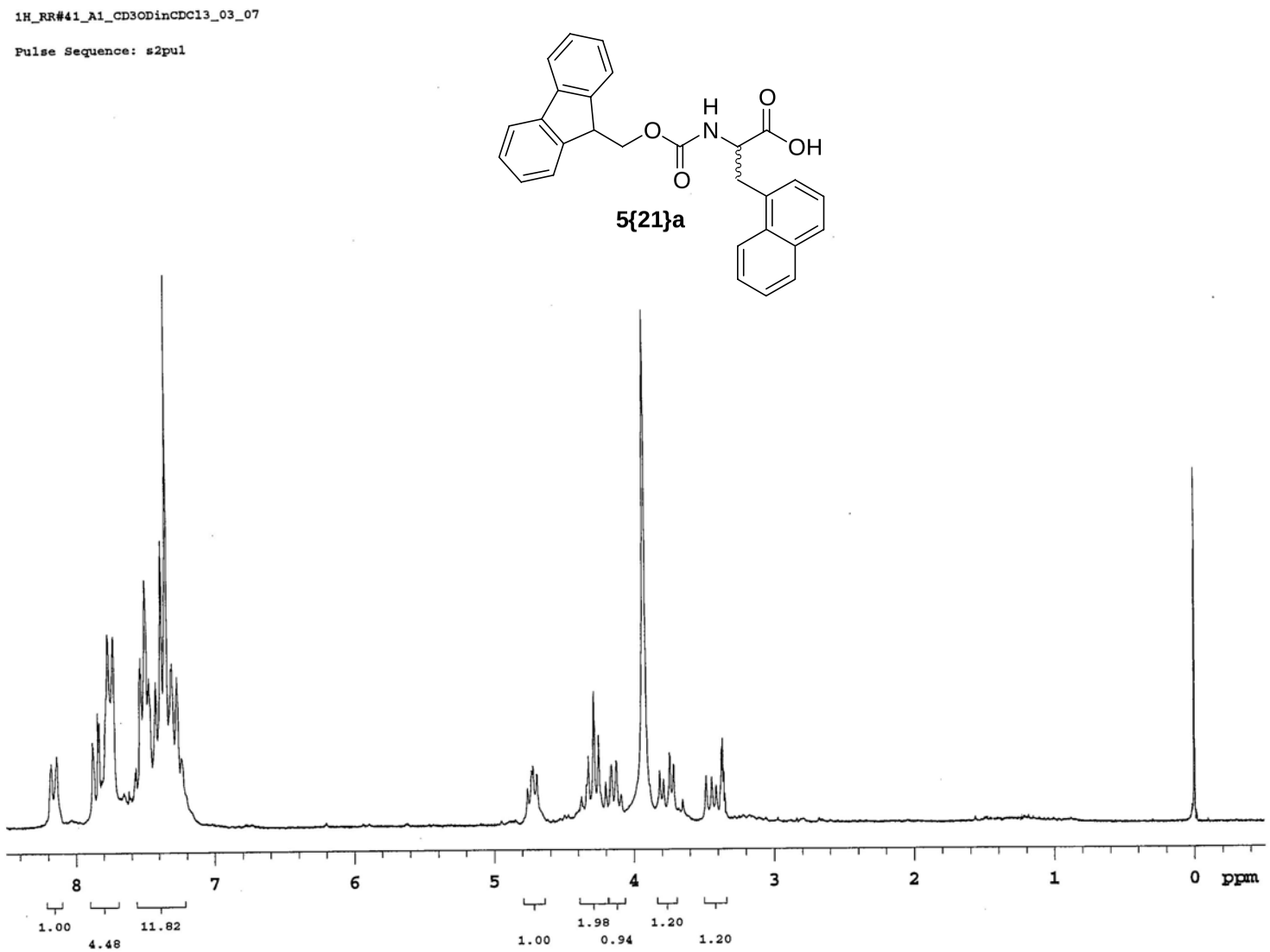

T31-A3 242 (6.480) Cm (241:243)
1: Scan ES+
8.21e6
216.2
217.2
260.1
199.1
218.2
261.1
319.1
356.1
358.1
400.1
406.2
428.1
451.2
485.2
534.1
546.1
578.1
595.1
602.1
641.8
684.2
701.1
722.4


T31-A3 206 (5.514) Cm (205:207)
1: Scan ES+
2.16e7
216.2
179.2
199.2
217.2
218.3
260.1
277.0
322.2
361.2
377.2
394.2
430.2
438.1
455.1
461.0
491.1
537.3
561.2
593.0
610.1
640.6
676.2
714.2
719.4
m/z

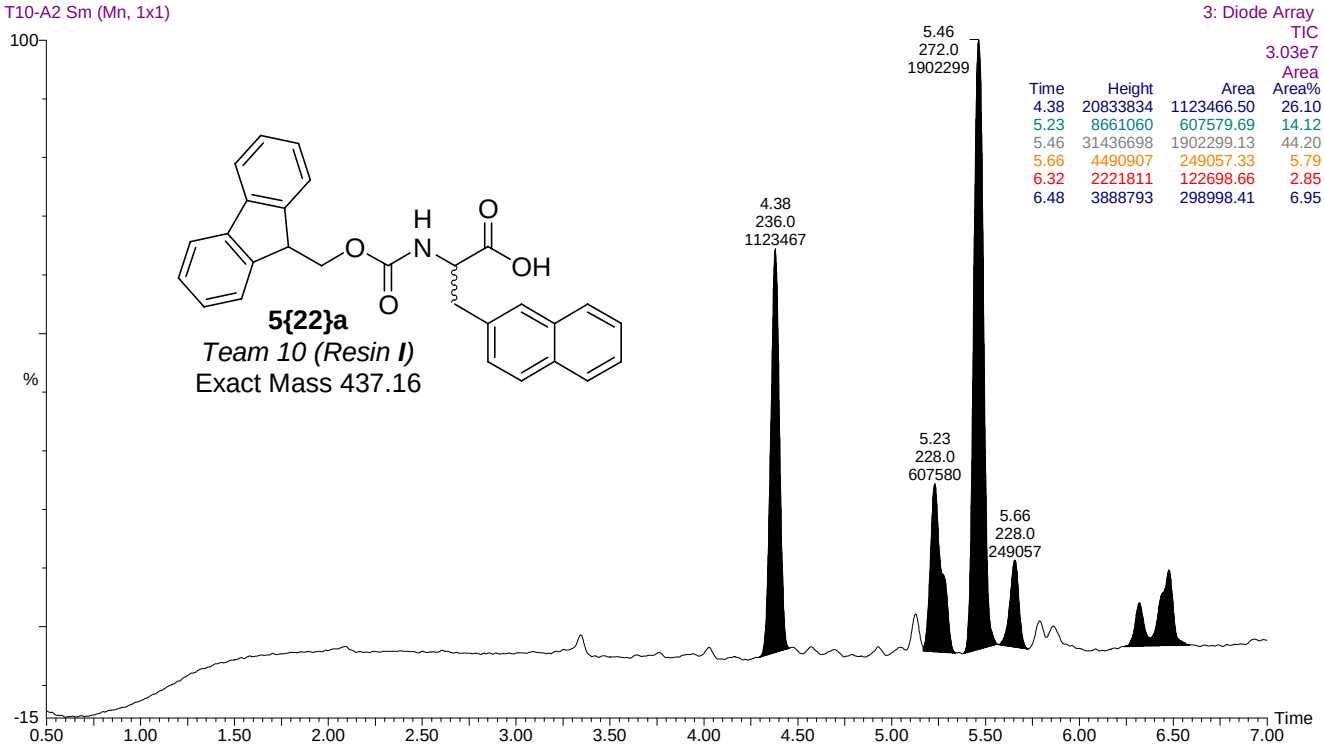
5{21}a

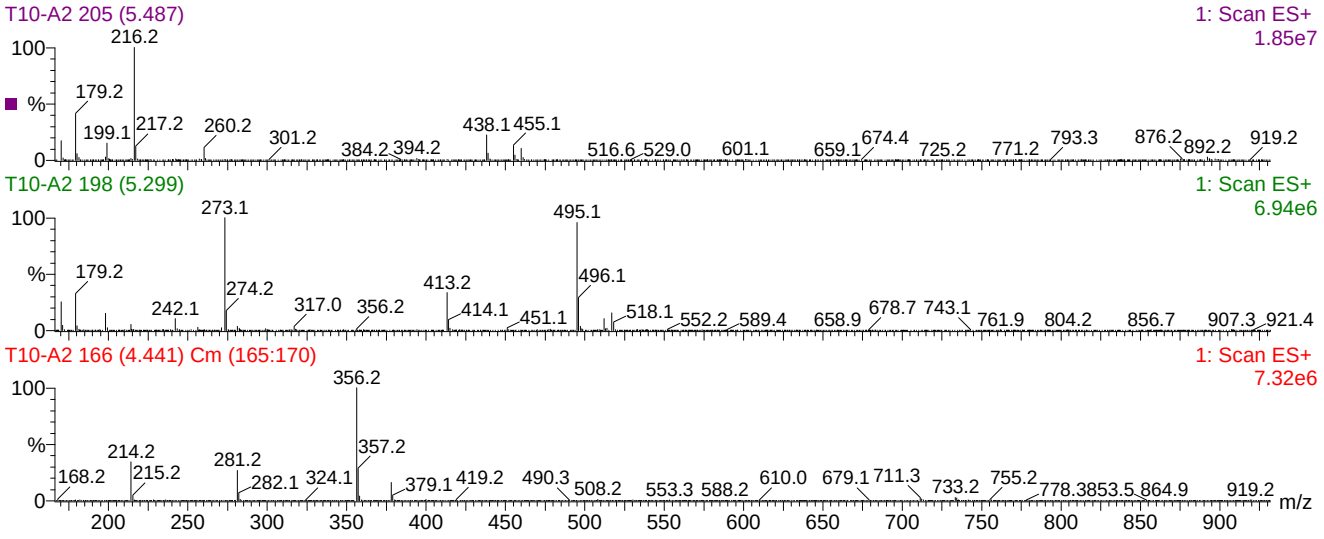

T32-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
1.43e7
Area
Time Height Area Area%
4.01 1352688 85506.30 6.10
4.33 783680 48936.28 3.49
4.43 715163 36467.05 2.60
4.62 1680556 95296.88 6.79
5.19 1354026 59867.10 4.27
5.45 15756046 754987.06 53.82
5.63 1201016 68598.80 4.89
6.42 4800107 253033.48 18.04
5.45
266.0
754987
6.42
228.0
253033
5{21}a
Team 32 (Resin I)
Exact Mass 437.16
%
Time


T32-A2 242 (6.480) Cm (241:244)
1: Scan ES+
6.63e6
T32-A2 205 (5.487)
1: Scan ES+
1.57e7
m/z

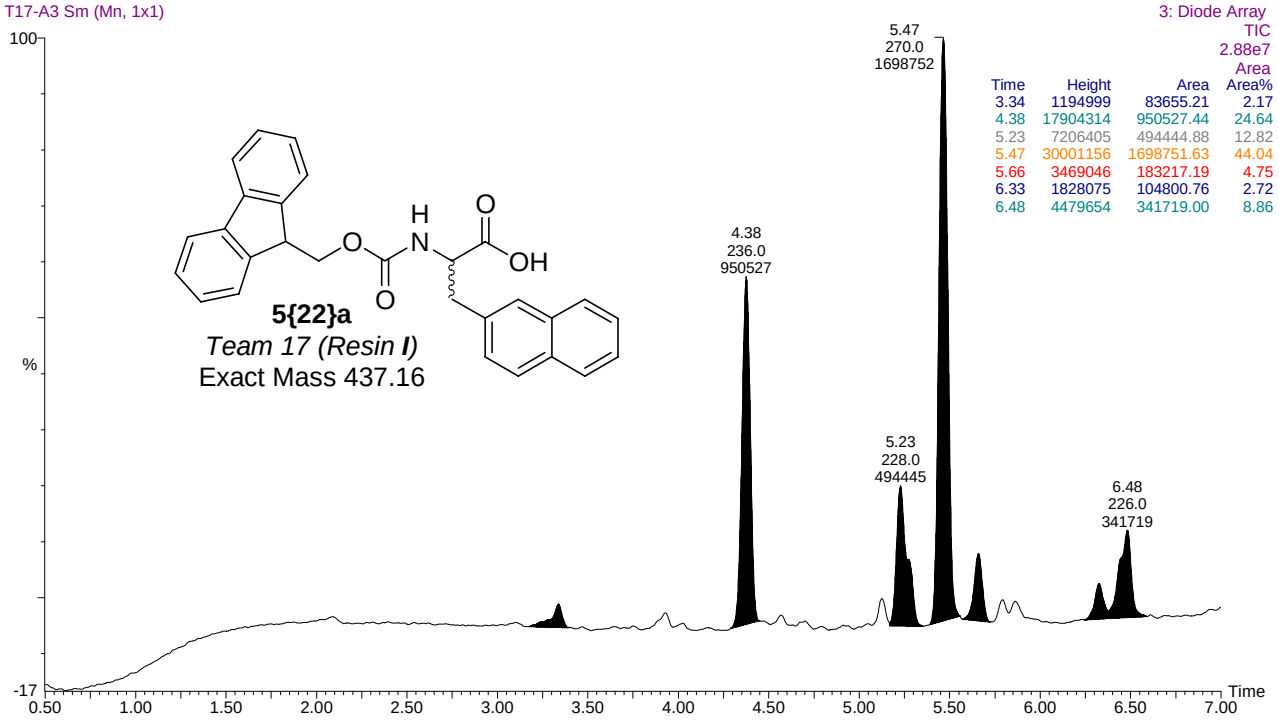

1H_RR#41_A1_CD3ODinCDCl3_03_07
Pulse Sequence: s2pul
H
N
O
O
O
OH
O
5{21}a
8
7
6
5
4
3
2
1
0
ppm
1.00
4.48
11.82
1.00
1.98
0.94
1.20
1.20

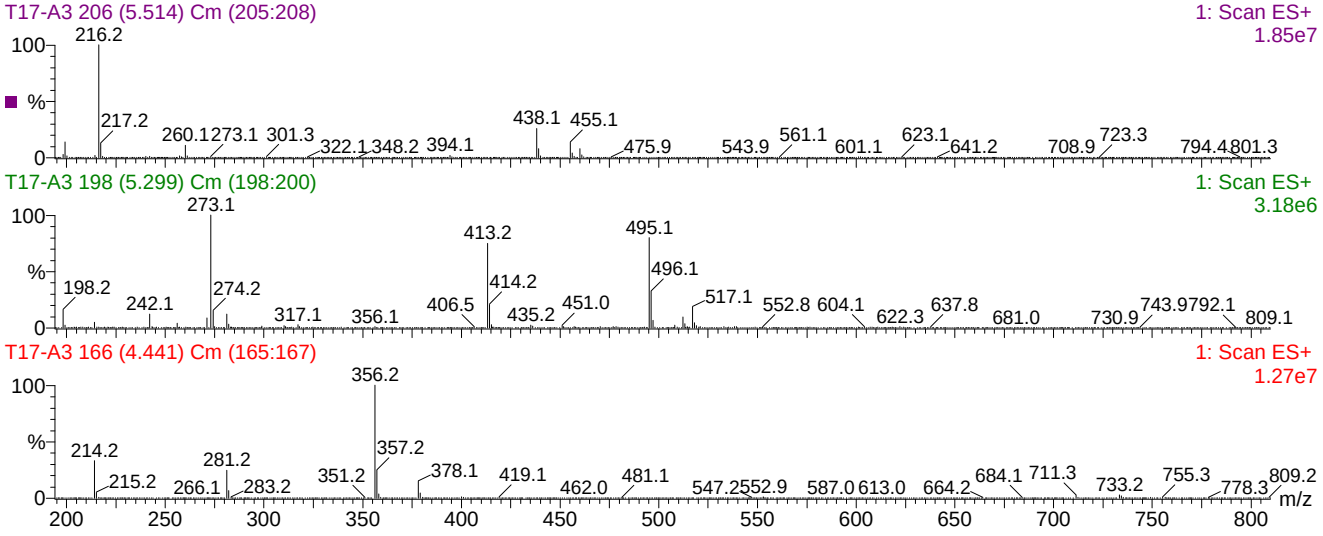
5{22}a


T10-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.03e7
Area
Time Height Area Area%
4.38 20833834 1123466.50 26.10
5.23 8661060 607579.69 14.12
5.46 31436698 1902299.13 44.20
5.66 4490907 249057.33 5.79
6.32 2221811 122698.66 2.85
6.48 3888793 298998.41 6.95
5.46
272.0
1902299
4.38
236.0
1123467
5.23
228.0
607580
5.66
228.0
249057
5{22}a
Team 10 (Resin I)
Exact Mass 437.16
%
Time

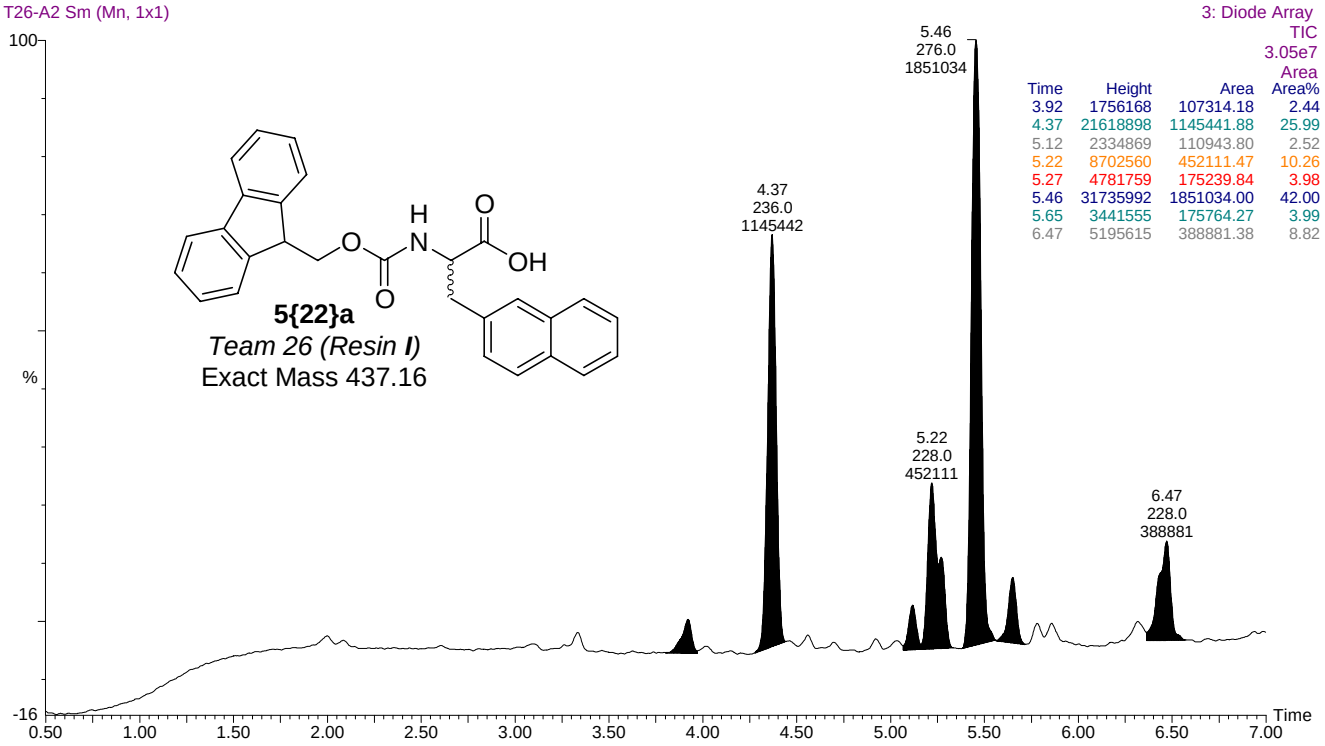

T10-A2 205 (5.487)
1: Scan ES+
1.85e7
T10-A2 198 (5.299)
1: Scan ES+
6.94e6
T10-A2 166 (4.441) Cm (165:170)
1: Scan ES+
7.32e6
m/z

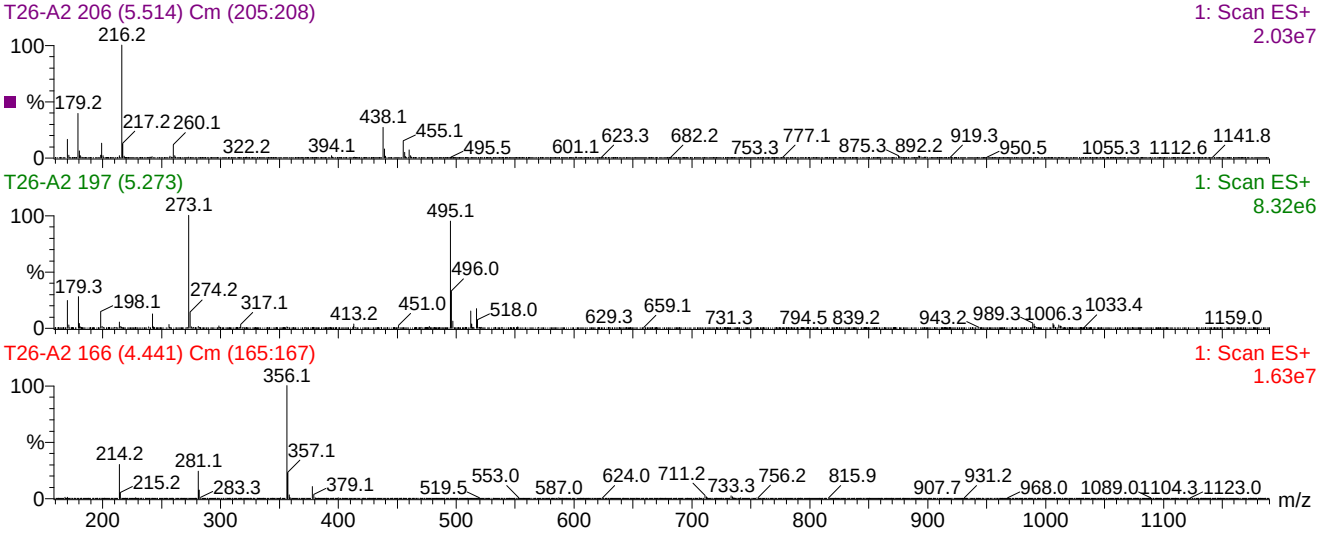
5{22}a


T17-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.88e7
Area
Time Height Area Area%
3.34 1194999 83655.21 2.17
4.38 17904314 950527.44 24.64
5.23 7206405 494444.88 12.82
5.47 30001156 1698751.63 44.04
5.66 3469046 183217.19 4.75
6.33 1828075 104800.76 2.72
6.48 4479654 341719.00 8.86
5.47
270.0
1698752
4.38
236.0
950527
5.23
228.0
494445
6.48
226.0
341719
5{22}a
Team 17 (Resin I)
Exact Mass 437.16
%
Time

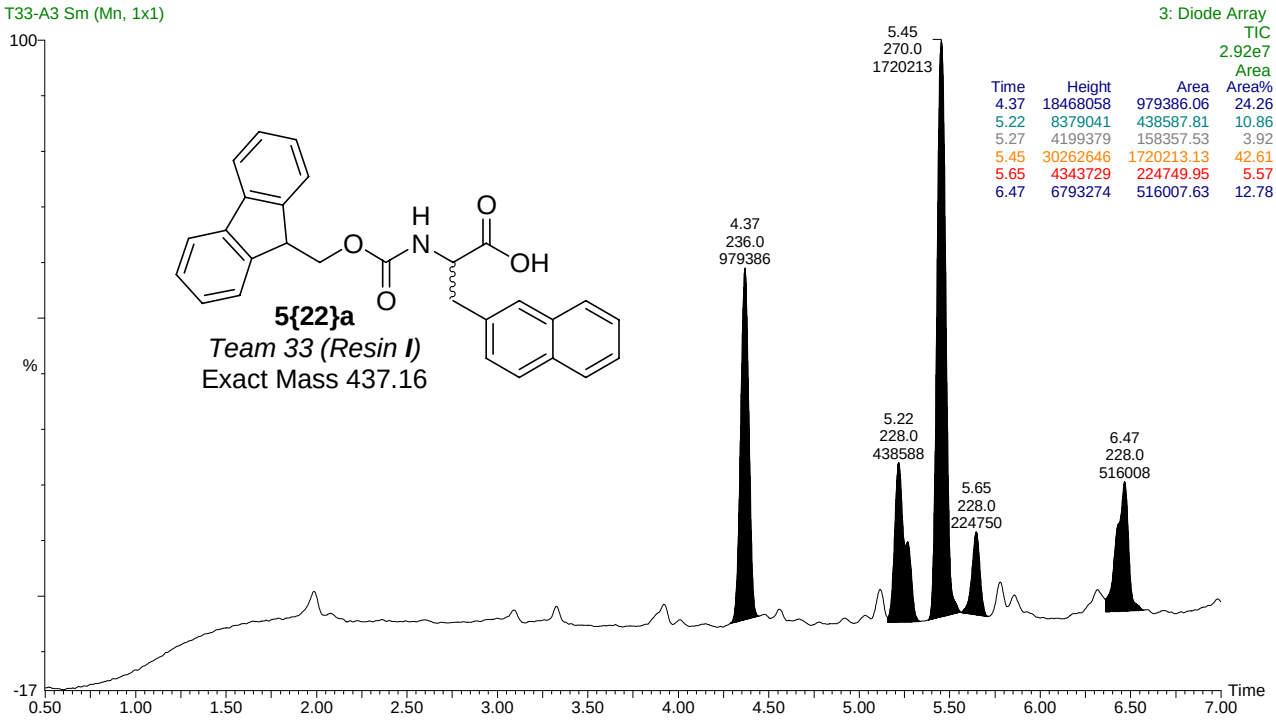

T17-A3 206 (5.514) Cm (205:208)
1: Scan ES+
1.85e7
T17-A3 198 (5.299) Cm (198:200)
1: Scan ES+
3.18e6
T17-A3 166 (4.441) Cm (165:167)
1: Scan ES+
1.27e7
m/z

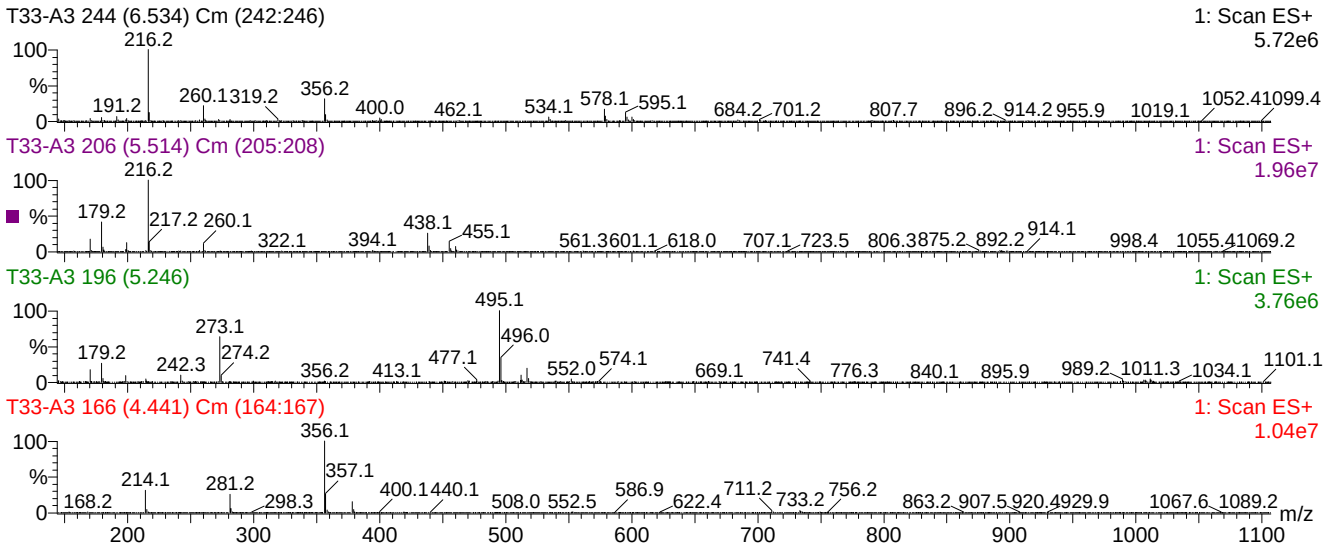
5{22}a


T26-A2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.05e7
Area
Time Height Area Area%
3.92 1756168 107314.18 2.44
4.37 21618898 1145441.88 25.99
5.12 2334869 110943.80 2.52
5.22 8702560 452111.47 10.26
5.27 4781759 175239.84 3.98
5.46 31735992 1851034.00 42.00
5.65 3441555 175764.27 3.99
6.47 5195615 388881.38 8.82
5.46
276.0
1851034
4.37
236.0
1145442
5.22
228.0
452111
6.47
228.0
388881
5{22}a
Team 26 (Resin I)
Exact Mass 437.16
%
Time


T26-A2 206 (5.514) Cm (205:208)
1: Scan ES+
2.03e7
T26-A2 197 (5.273)
1: Scan ES+
8.32e6
T26-A2 166 (4.441) Cm (165:167)
1: Scan ES+
1.63e7
m/z

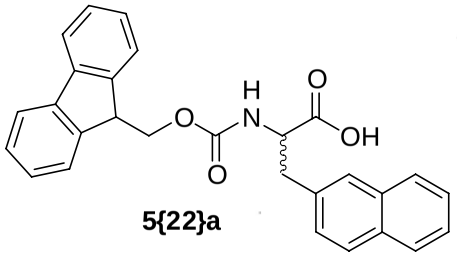
5{22}a


T33-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
2.92e7
Area
Time Height Area Area%
4.37 18468058 979386.06 24.26
5.22 8379041 438587.81 10.86
5.27 4199379 158357.53 3.92
5.45 30262646 1720213.13 42.61
5.65 4343729 224749.95 5.57
6.47 6793274 516007.63 12.78
5.45
270.0
1720213
4.37
236.0
979386
5.22
228.0
438588
5.65
228.0
224750
6.47
228.0
516008
5{22}a
Team 33 (Resin I)
Exact Mass 437.16
Time

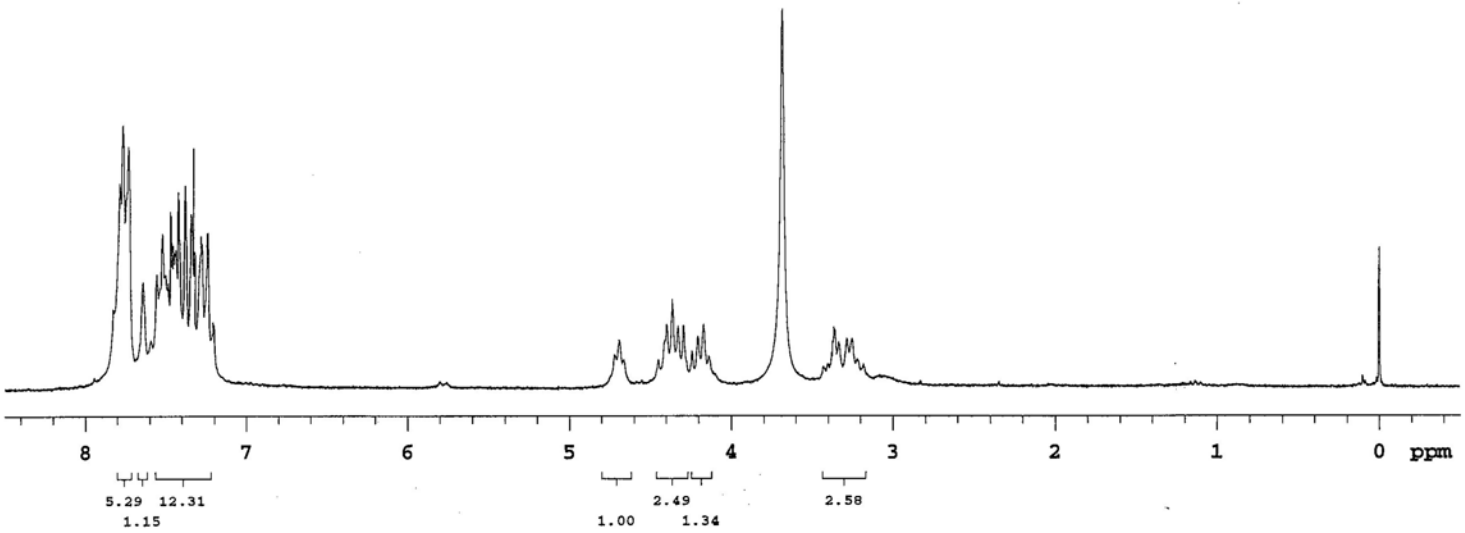

T33-A3 244 (6.534) Cm (242:246)
1: Scan ES+
5.72e6
T33-A3 206 (5.514) Cm (205:208)
1: Scan ES+
1.96e7
T33-A3 196 (5.246)
1: Scan ES+
3.76e6
T33-A3 166 (4.441) Cm (164:167)
1: Scan ES+
1.04e7
m/z

1H_BB#27_B2_CD3ODinCDCl3_02_07

Pulse Sequence: s2pul

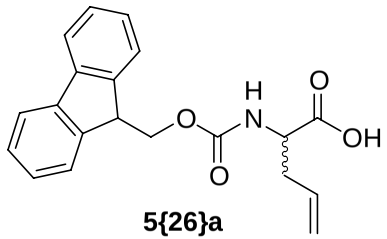


5{22}a

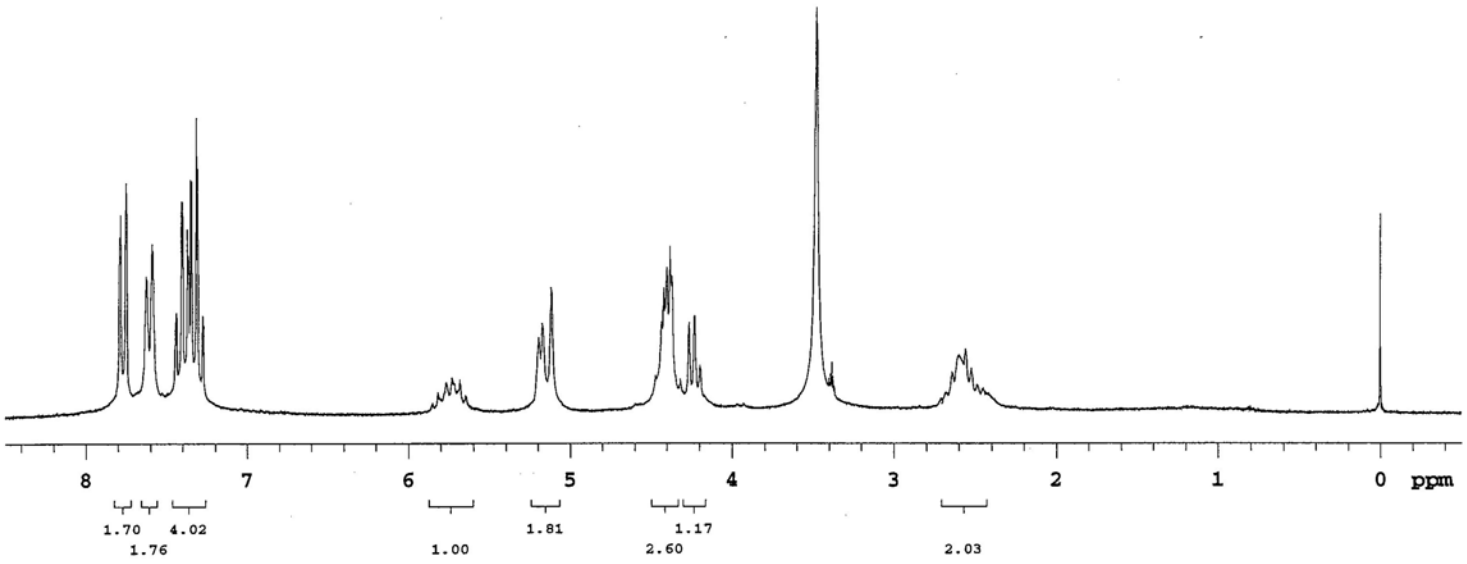


1H_BB#41_A2_CD3ODinCDCl3_03_07

Pulse Sequence: s2pul

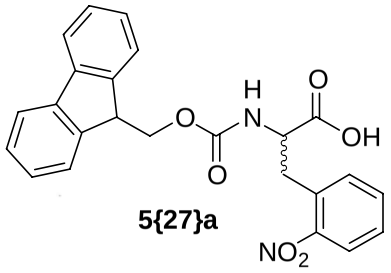


5{26}a

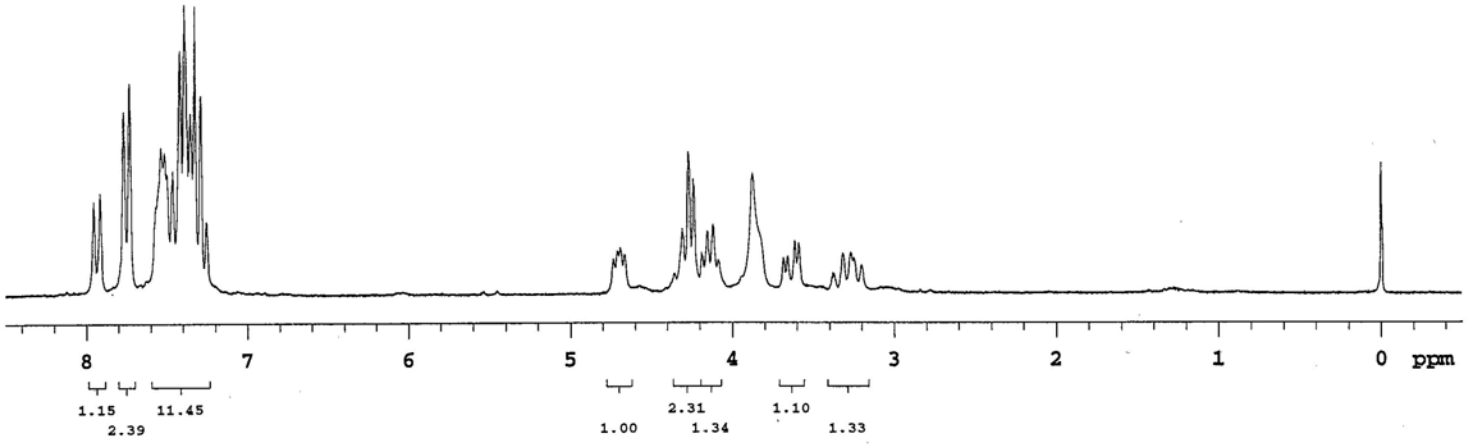


1H_RR#40_B2_CDCl3withCD3OD_03_09_07

Pulse Sequence: s2pul

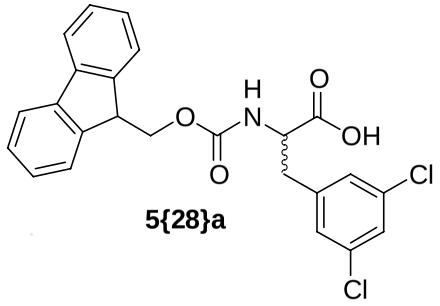


5{27}a

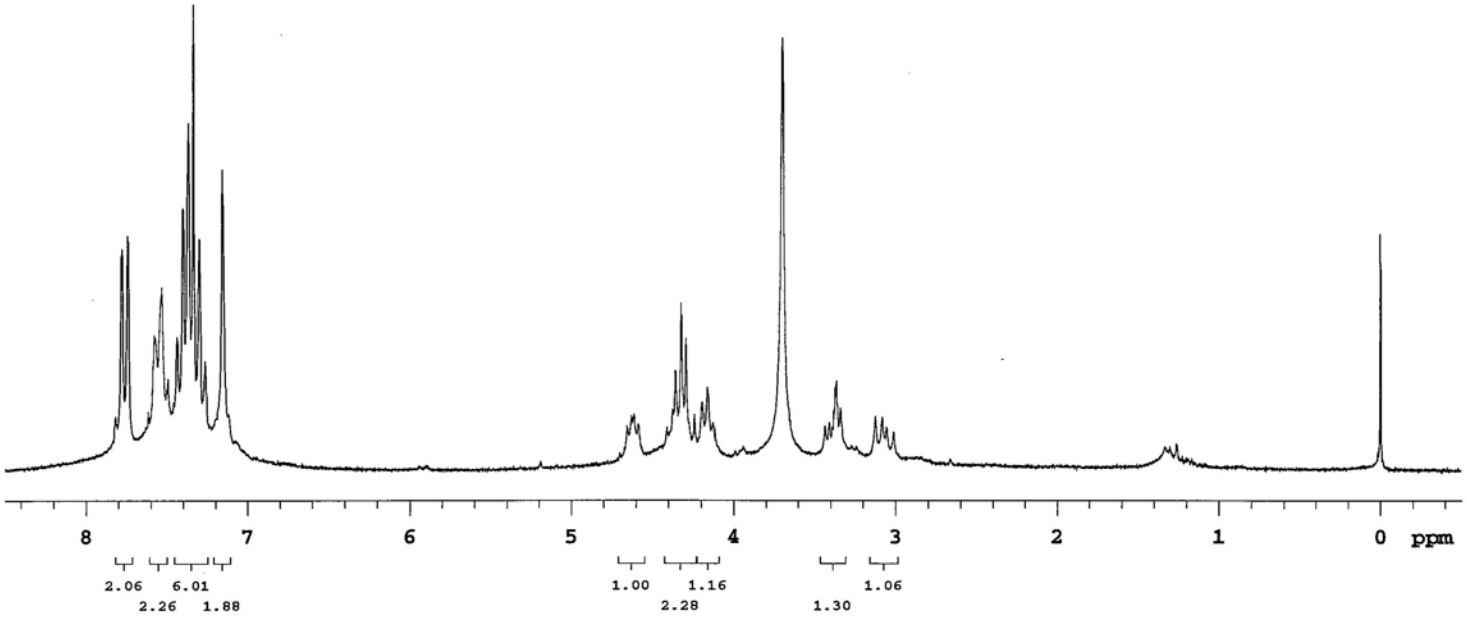


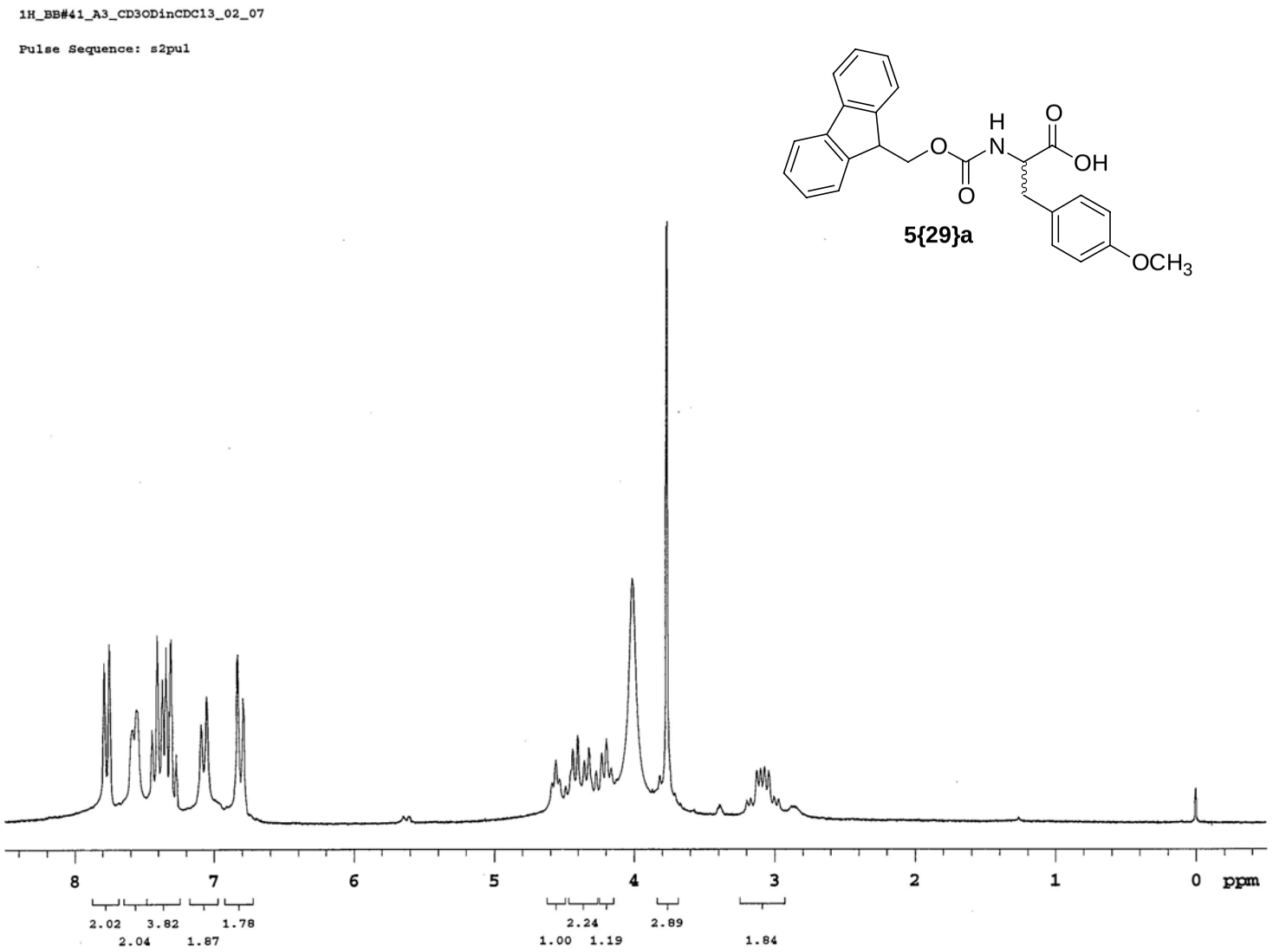
1H_BB#40_B3_CD3ODinCDCl3_02_07

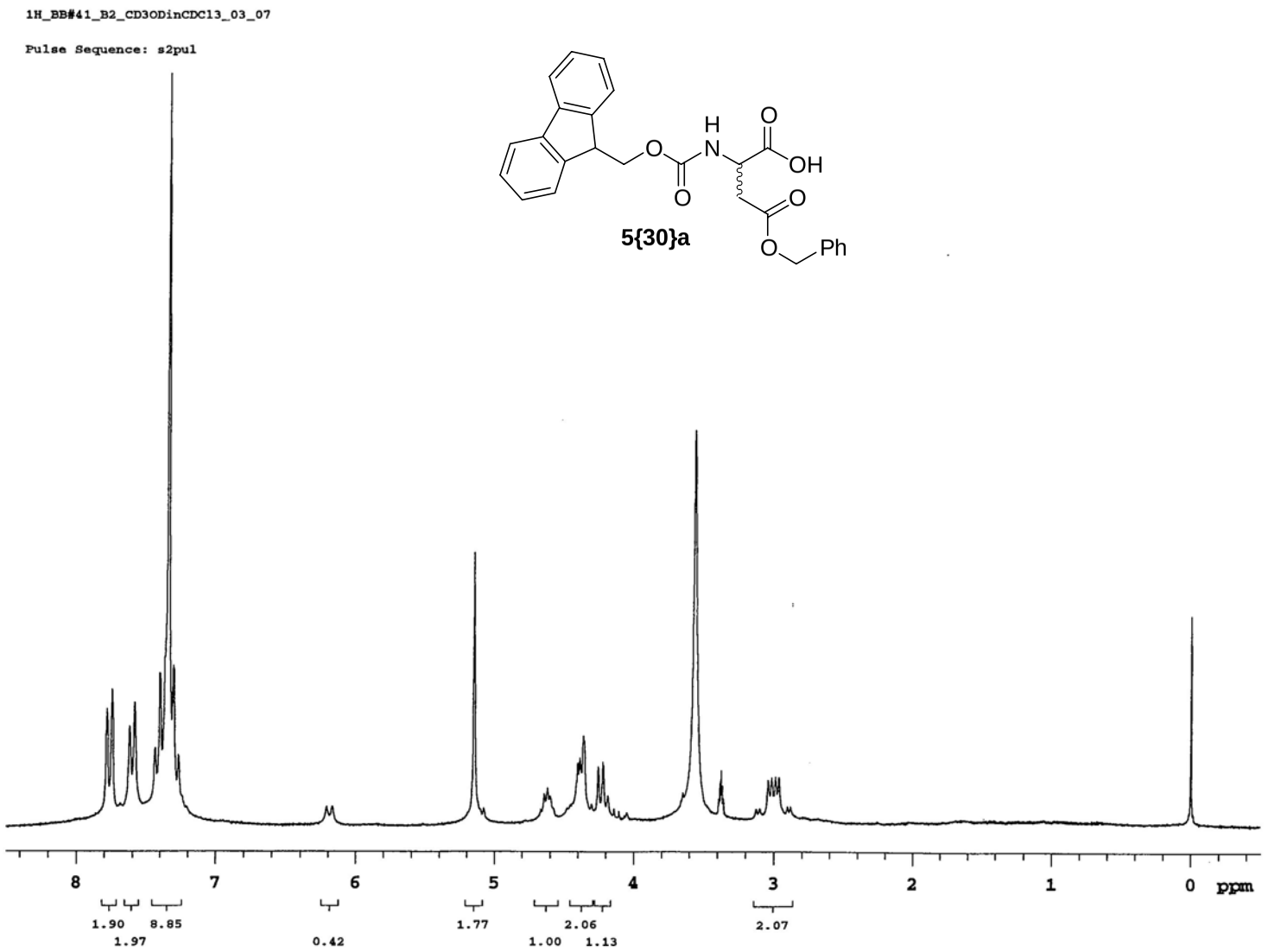
Pulse Sequence: s2pul

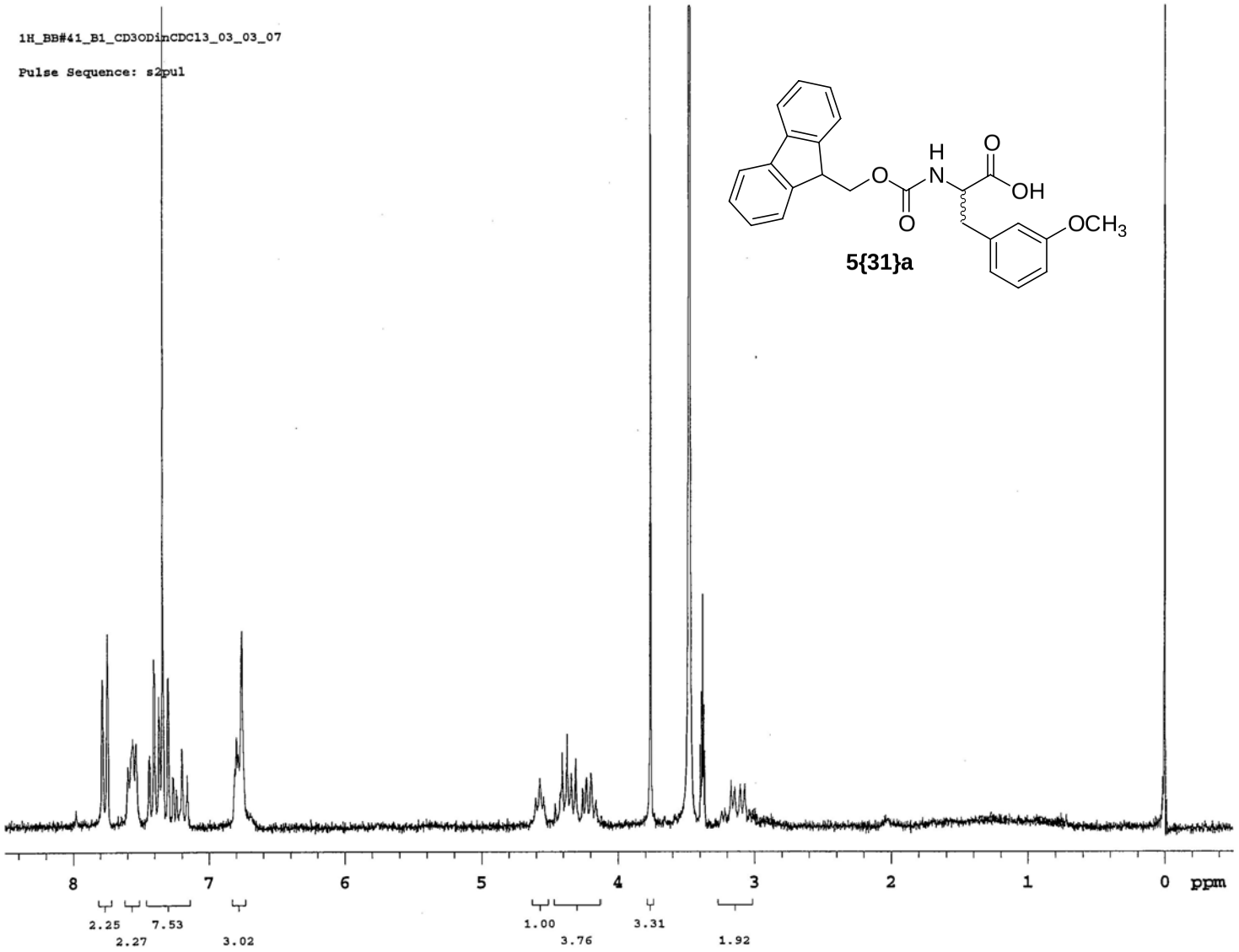


5{28}a

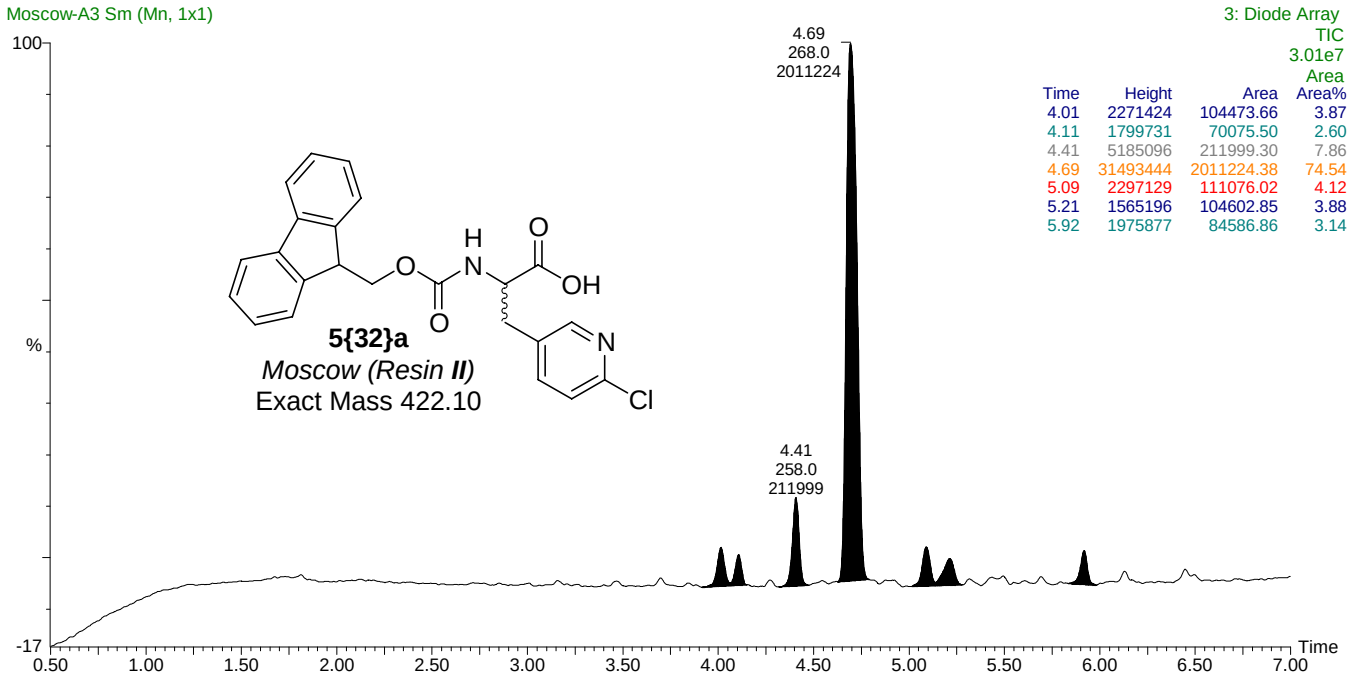


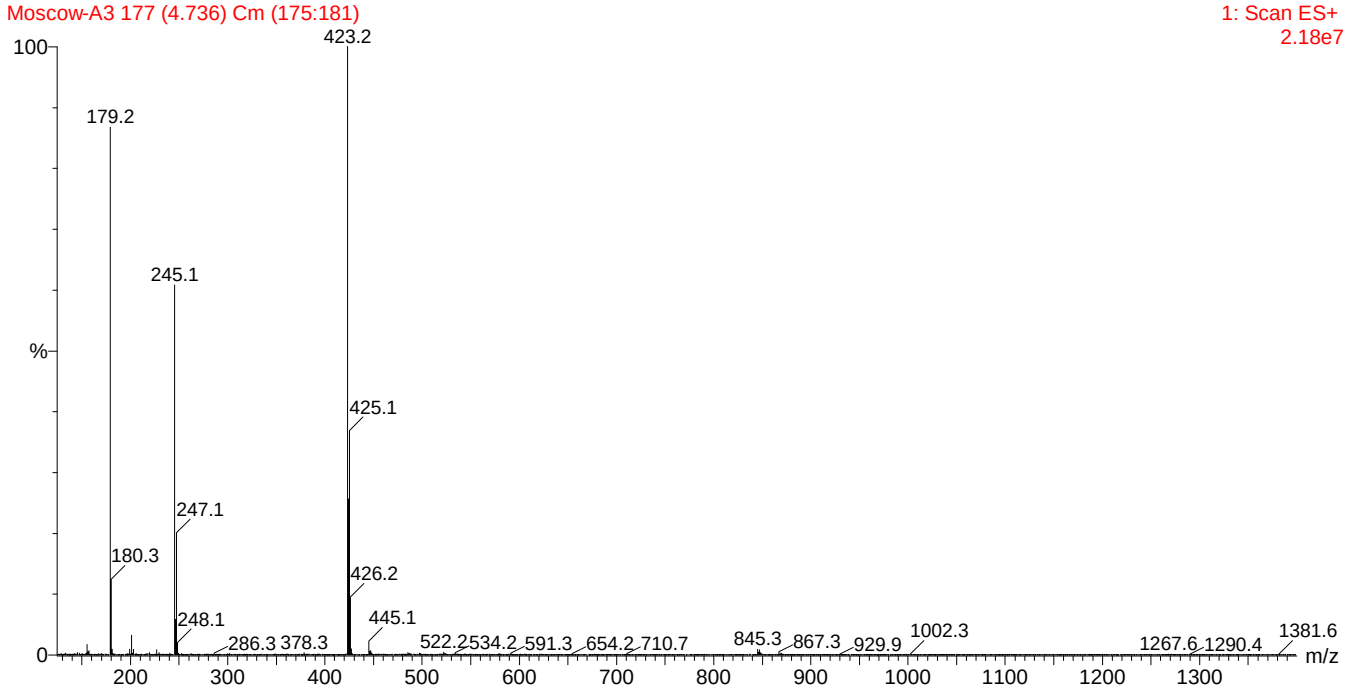

1H_BB#41_A3_CD3ODinCDC13_02_07
Pulse Sequence: s2pul
5{29}a
8
7
6
5
4
3
2
1
0
ppm
2.02
3.82
1.78
2.04
1.87
2.24
2.89
1.00
1.19
1.84


1H_BB#41_B2_CD3ODinCDCl3_03_07
Pulse Sequence: s2pul
5{30}a
8
7
6
5
4
3
2
1
0
ppm
1.90
1.97
8.85
0.42
1.77
1.00
2.06
1.13
2.07


1H_BB#41_B1_CD3ODinCDCl3_03_03_07
Pulse Sequence: s2pul
H
N
O
O
O
OH
O
OCH3
5{31}a
8
7
6
5
4
3
2
1
0
ppm
2.25
2.27
7.53
3.02
1.00
3.76
3.31
1.92

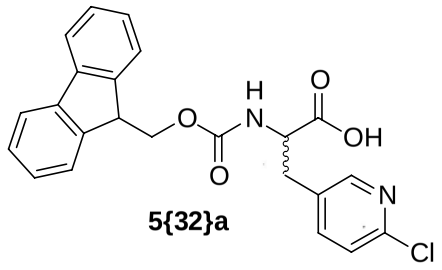
5{32}a


Moscow-A3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.01e7
Area
Time Height Area Area%
4.01 2271424 104473.66 3.87
4.11 1799731 70075.50 2.60
4.41 5185096 211999.30 7.86
4.69 31493444 2011224.38 74.54
5.09 2297129 111076.02 4.12
5.21 1565196 104602.85 3.88
5.92 1975877 84586.86 3.14
4.69
268.0
2011224
4.41
258.0
211999
5{32}a
Moscow (Resin II)
Exact Mass 422.10
100
%
-17
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

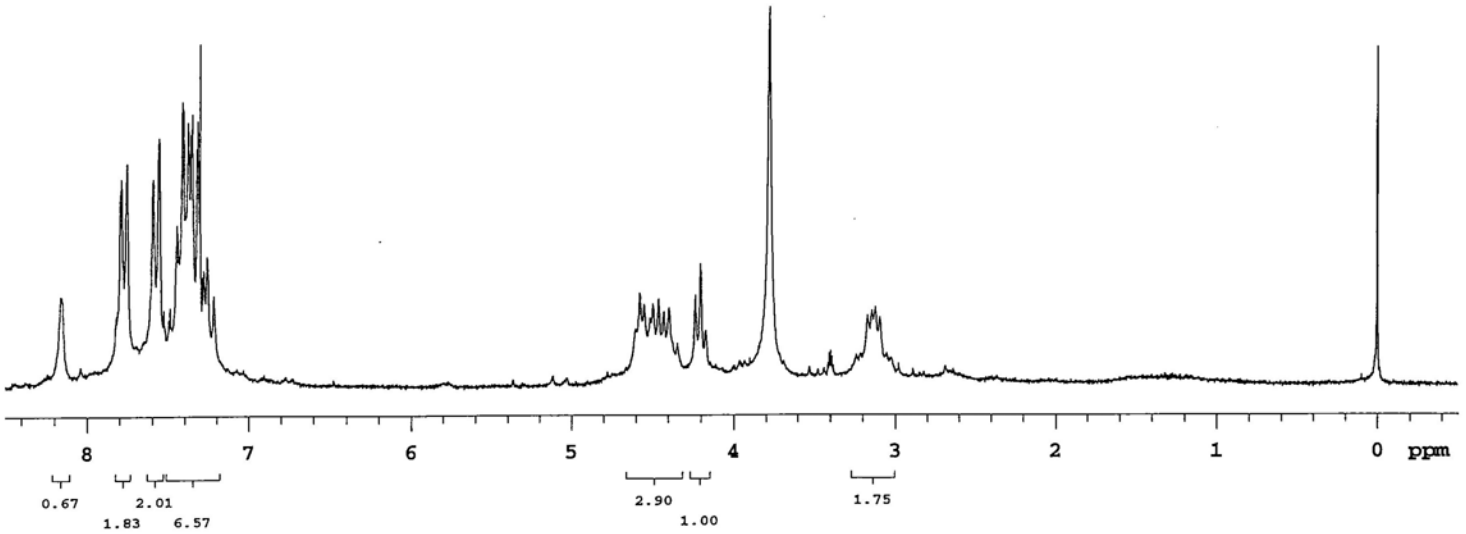

Moscow-A3 177 (4.736) Cm (175:181)
1: Scan ES+
2.18e7
100
%
0
423.2
179.2
245.1
425.1
247.1
180.3
426.2
248.1
445.1
286.3 378.3
522.2 534.2 591.3 654.2 710.7
845.3 867.3 929.9 1002.3
1267.6 1290.4 1381.6
m/z
200 300 400 500 600 700 800 900 1000 1100 1200 1300

1H_ZZN#47_B_CD3ODinCDCl3_04_24_07

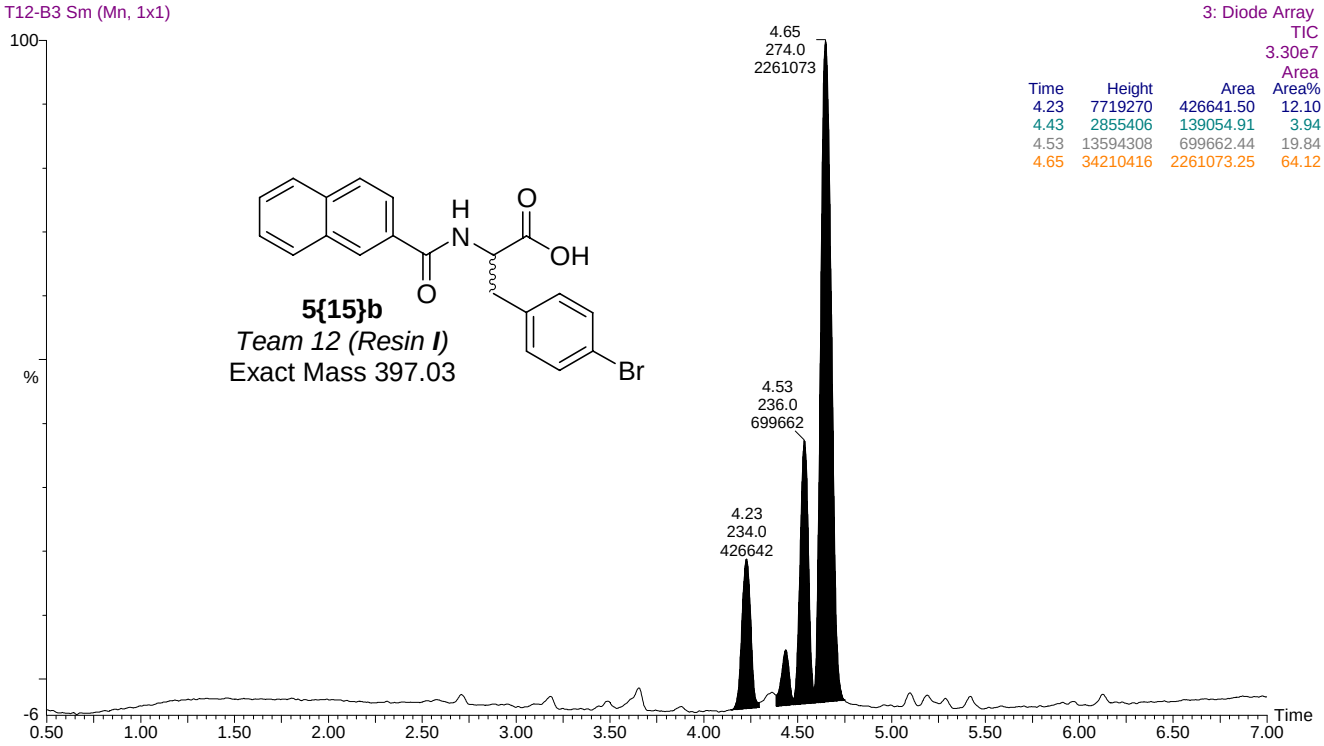
Pulse Sequence: s2pul

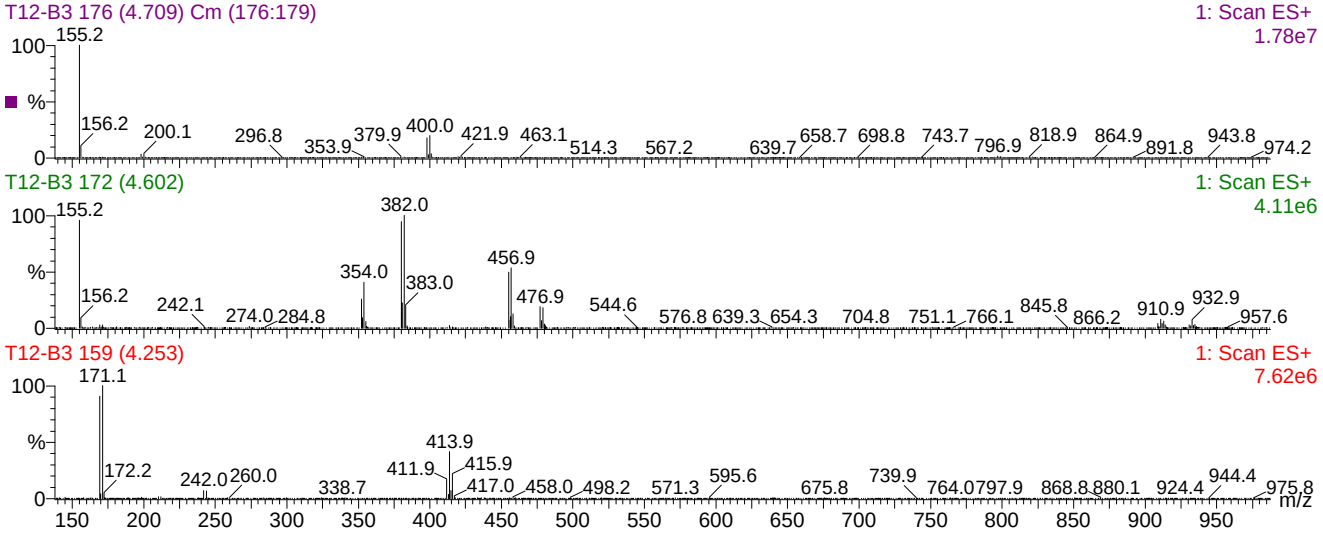


5{32}a

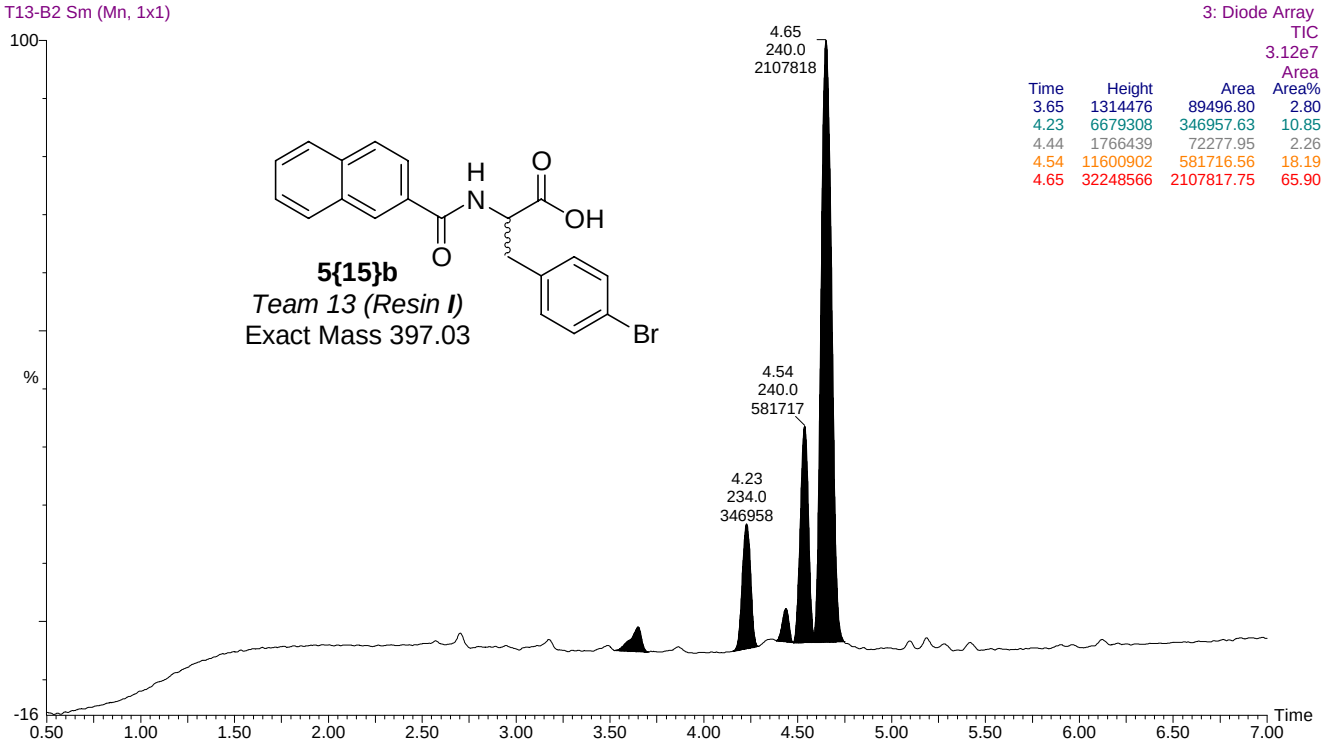


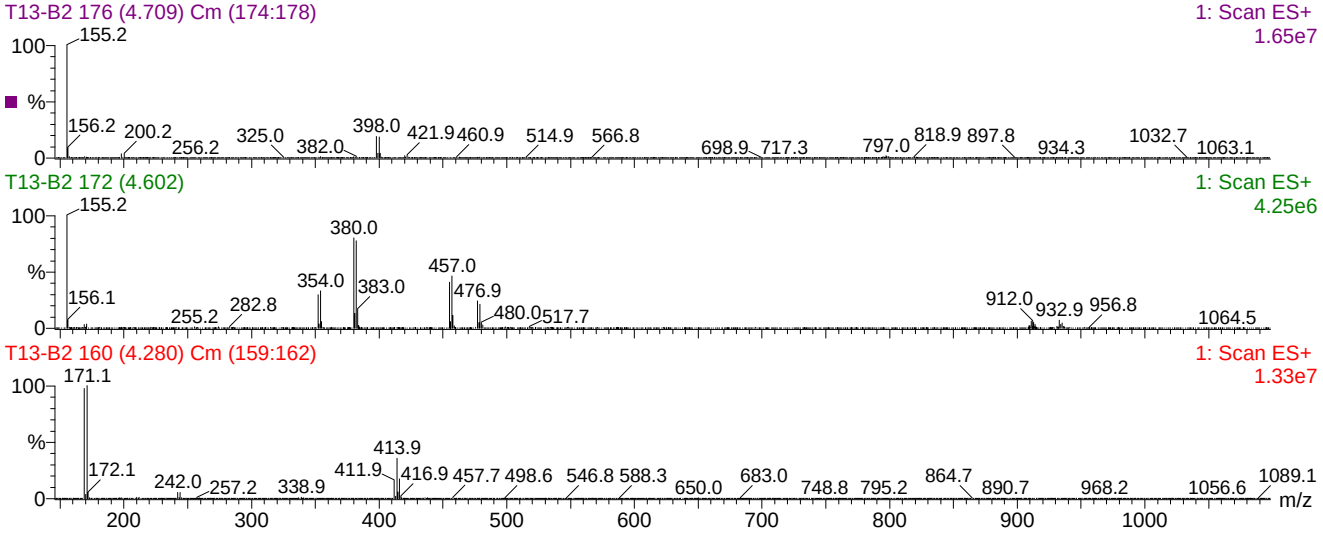
5{15}b


T12-B3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.30e7
Area
Time Height Area Area%
4.23 7719270 426641.50 12.10
4.43 2855406 139054.91 3.94
4.53 13594308 699662.44 19.84
4.65 34210416 2261073.25 64.12
4.65
274.0
2261073
4.53
236.0
699662
4.23
234.0
426642
5{15}b
Team 12 (Resin I)
Exact Mass 397.03
Br
OH
H
N
O
O
100
%
-6
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00
Time

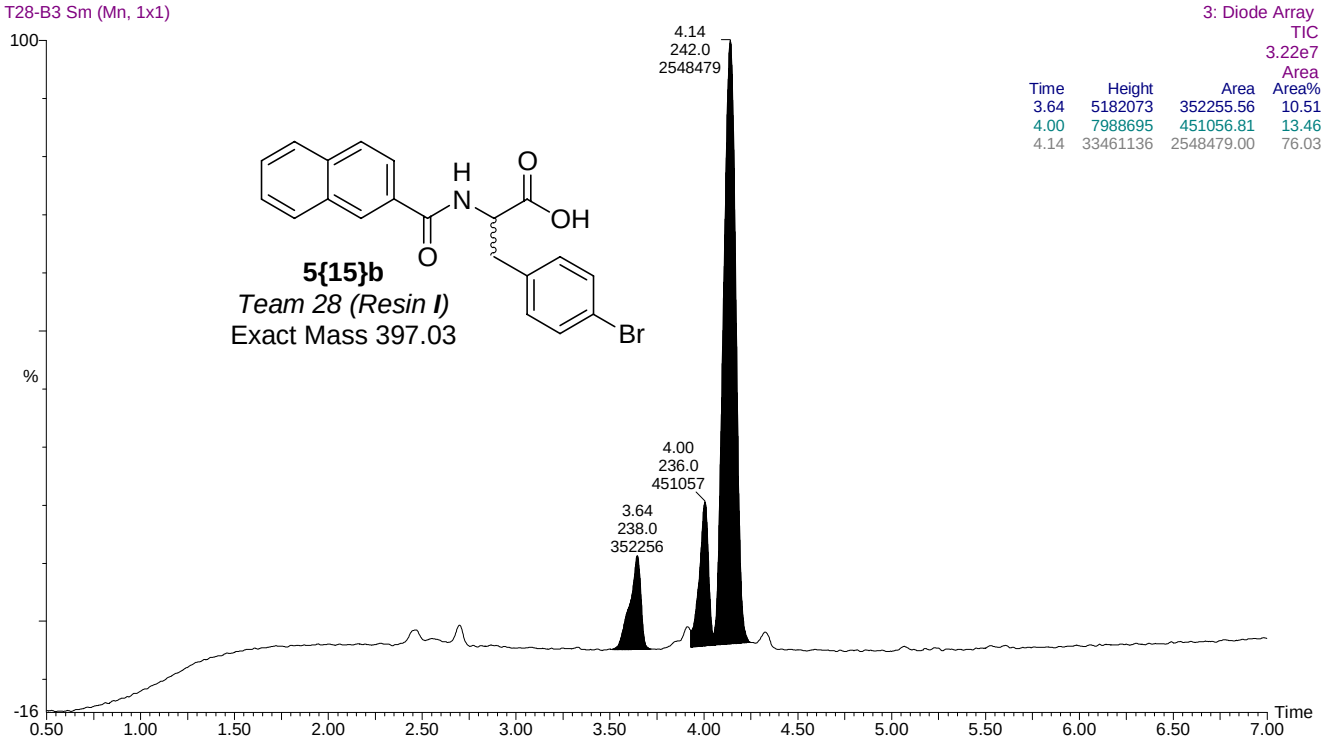

T12-B3 176 (4.709) Cm (176:179)
1: Scan ES+
1.78e7
155.2 156.2 200.1 296.8 353.9 379.9 400.0 421.9 463.1 514.3 567.2 639.7 658.7 698.8 743.7 796.9 818.9 864.9 891.8 943.8 974.2
T12-B3 172 (4.602)
1: Scan ES+
4.11e6
155.2 156.2 242.1 274.0 284.8 354.0 382.0 383.0 456.9 476.9 544.6 576.8 639.3 654.3 704.8 751.1 766.1 845.8 866.2 910.9 932.9 957.6
T12-B3 159 (4.253)
1: Scan ES+
7.62e6
171.1 172.2 242.0 260.0 338.7 411.9 413.9 415.9 417.0 458.0 498.2 571.3 595.6 675.8 739.9 764.0 797.9 868.8 880.1 924.4 944.4 975.8
100
%
0
150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950
m/z

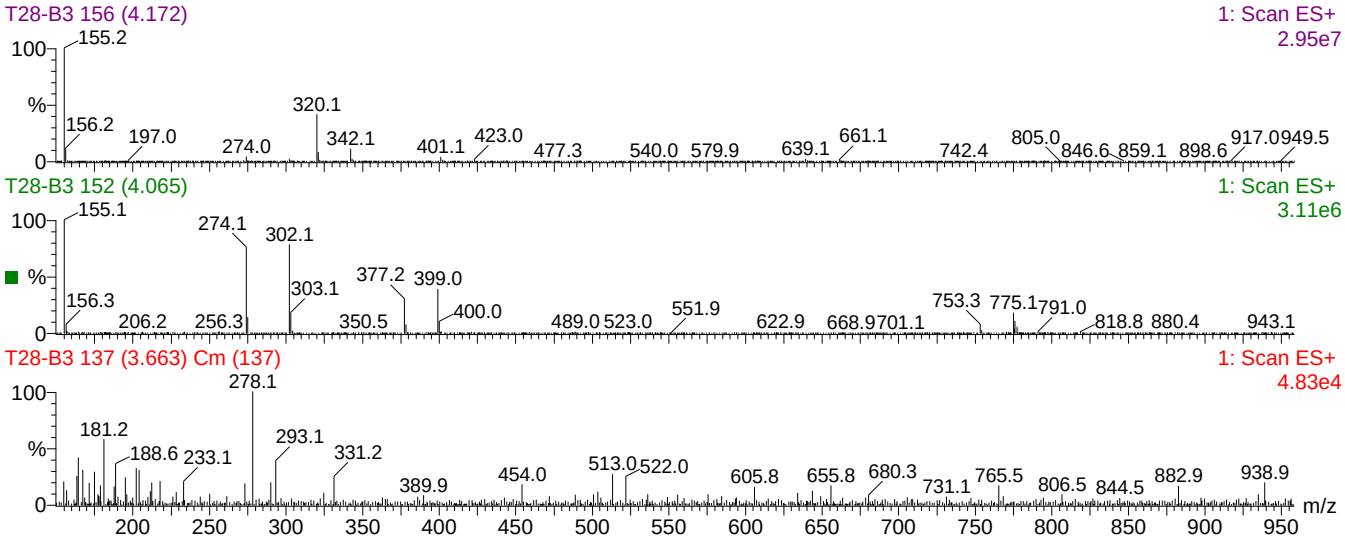
5{15}b


T13-B2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.12e7
Area
Time Height Area Area%
3.65 1314476 89496.80 2.80
4.23 6679308 346957.63 10.85
4.44 1766439 72277.95 2.26
4.54 11600902 581716.56 18.19
4.65 32248566 2107817.75 65.90
4.65
240.0
2107818
4.54
240.0
581717
4.23
234.0
346958
5{15}b
Team 13 (Resin I)
Exact Mass 397.03
Br
OH
H
N
O
O
100
%
-16
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

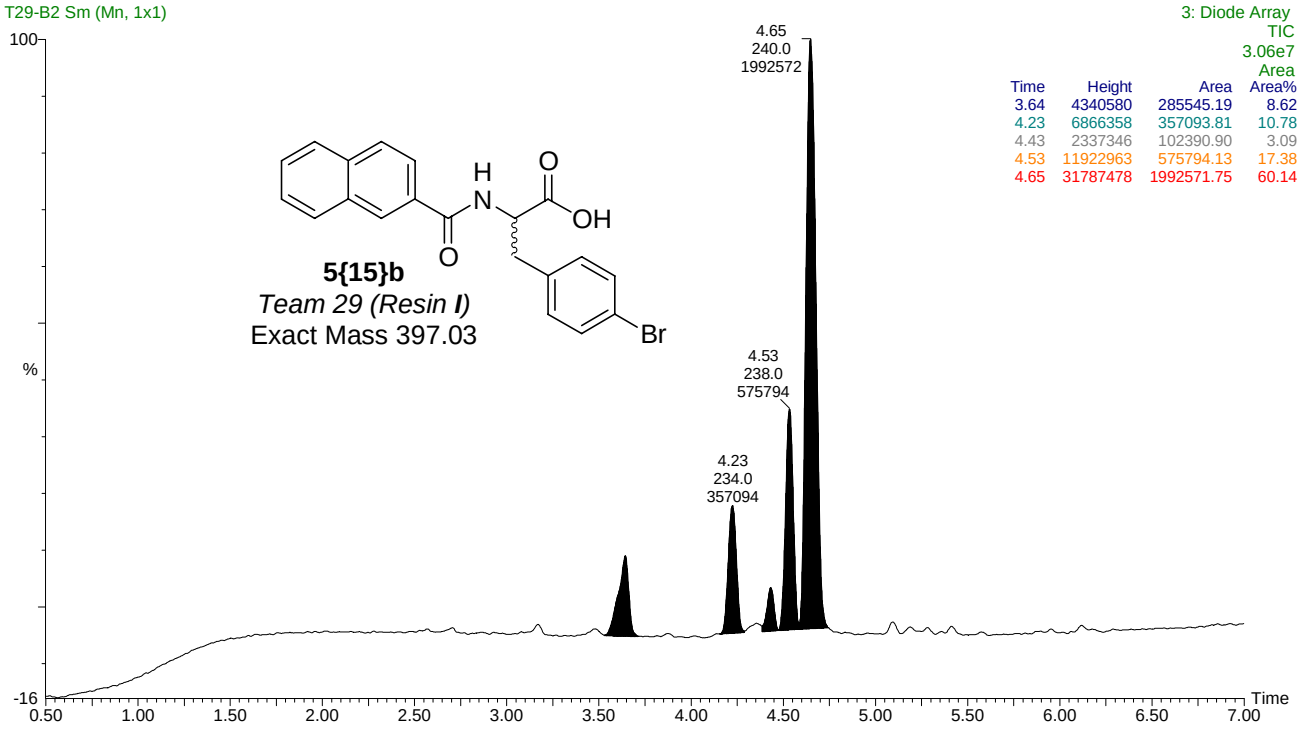

T13-B2 176 (4.709) Cm (174:178)
1: Scan ES+
1.65e7
155.2
156.2 200.2 256.2 325.0 382.0 398.0 421.9 460.9 514.9 566.8 698.9 717.3 797.0 818.9 897.8 934.3 1032.7 1063.1
T13-B2 172 (4.602)
1: Scan ES+
4.25e6
155.2
156.1 255.2 282.8 354.0 380.0 383.0 457.0 476.9 480.0 517.7 912.0 932.9 956.8 1064.5
T13-B2 160 (4.280) Cm (159:162)
1: Scan ES+
1.33e7
171.1
172.1 242.0 257.2 338.9 411.9 413.9 416.9 457.7 498.6 546.8 588.3 650.0 683.0 748.8 795.2 864.7 890.7 968.2 1056.6 1089.1
100
%
0
200 300 400 500 600 700 800 900 1000
m/z

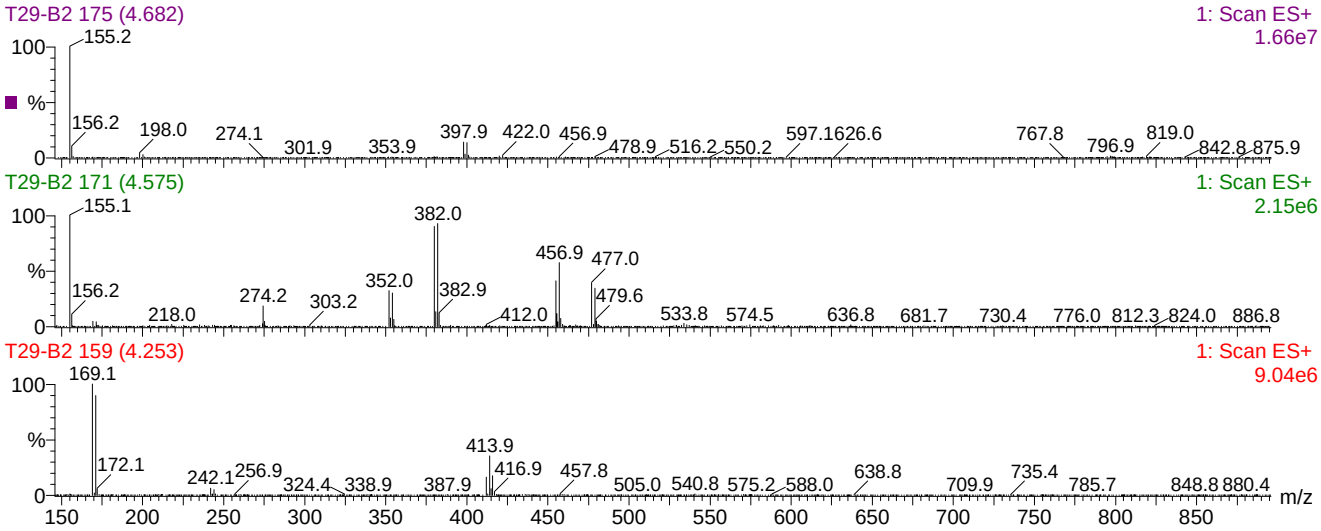
5{15}b


T28-B3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.22e7
Area
Time Height Area Area%
3.64 5182073 352255.56 10.51
4.00 7988695 451056.81 13.46
4.14 33461136 2548479.00 76.03
4.14
242.0
2548479
4.00
236.0
451057
3.64
238.0
352256
5{15}b
Team 28 (Resin I)
Exact Mass 397.03
Br
OH
H
N
O
O
100
%
-16
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

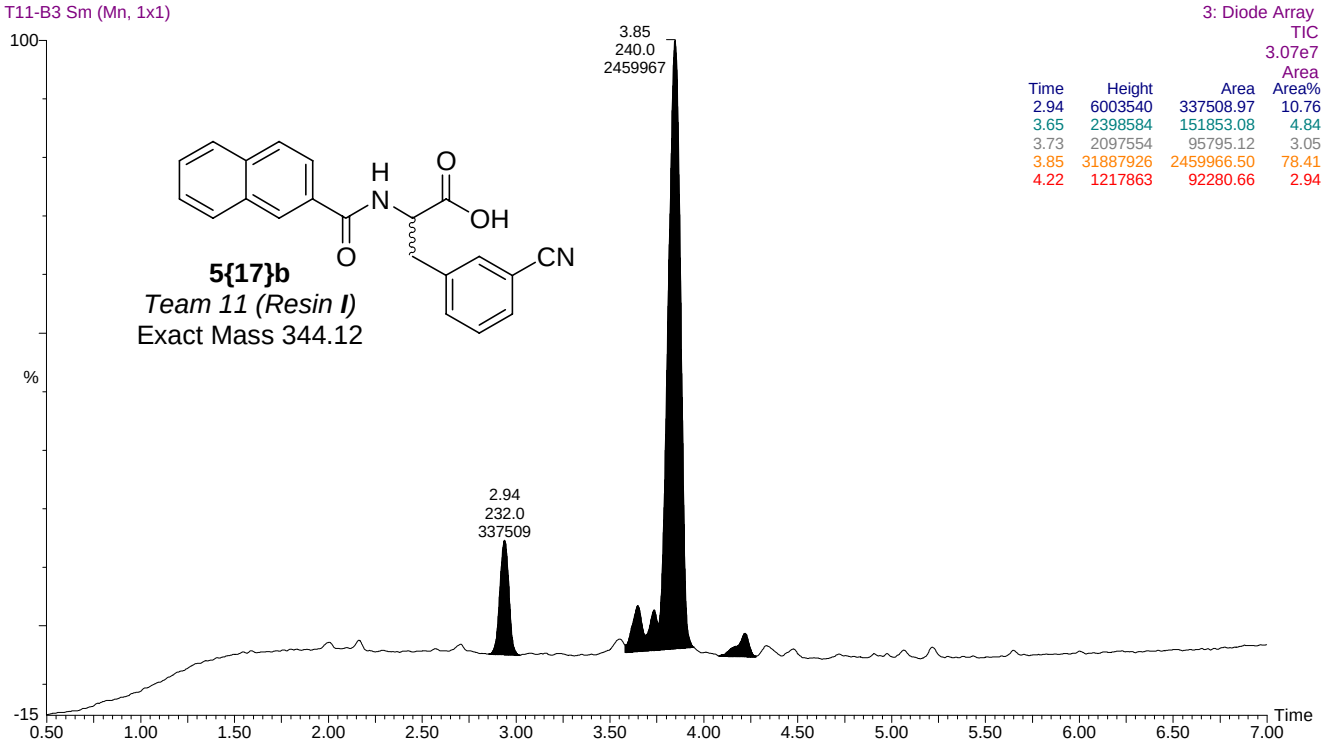

T28-B3 156 (4.172)
1: Scan ES+
2.95e7
155.2
156.2
197.0
274.0
320.1
342.1
401.1
423.0
477.3
540.0
579.9
639.1
661.1
742.4
805.0
846.6
859.1
898.6
917.0
949.5
T28-B3 152 (4.065)
1: Scan ES+
3.11e6
155.1
156.3
206.2
256.3
274.1
302.1
303.1
350.5
377.2
399.0
400.0
489.0
523.0
551.9
622.9
668.9
701.1
753.3
775.1
791.0
818.8
880.4
943.1
T28-B3 137 (3.663) Cm (137)
1: Scan ES+
4.83e4
181.2
188.6
233.1
278.1
293.1
331.2
389.9
454.0
513.0
522.0
605.8
655.8
680.3
731.1
765.5
806.5
844.5
882.9
938.9
100
%
0
m/z
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

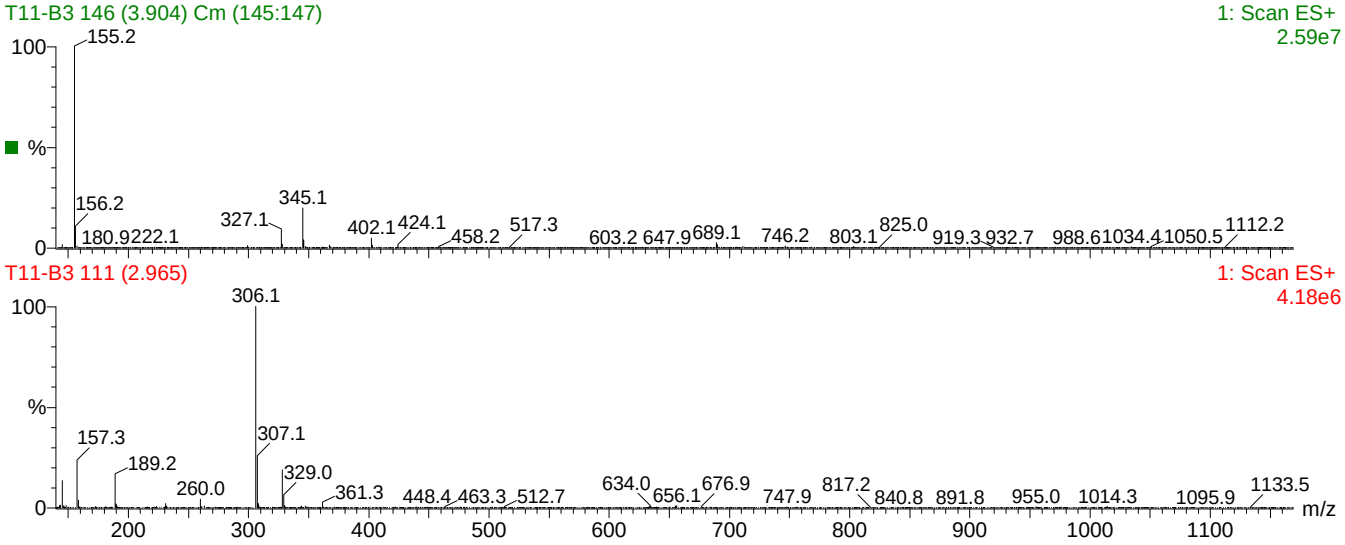
5{15}b


T29-B2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.06e7
Area
Time Height Area Area%
3.64 4340580 285545.19 8.62
4.23 6866358 357093.81 10.78
4.43 2337346 102390.90 3.09
4.53 11922963 575794.13 17.38
4.65 31787478 1992571.75 60.14
4.65
240.0
1992572
4.53
238.0
575794
4.23
234.0
357094
5{15}b
Team 29 (Resin I)
Exact Mass 397.03
Br
OH
H
N
O
O
100
%
-16
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00


T29-B2 175 (4.682)
1: Scan ES+
1.66e7
155.2
156.2
198.0
274.1
301.9
353.9
397.9
422.0
456.9
478.9
516.2
550.2
597.1
626.6
767.8
796.9
819.0
842.8
875.9
T29-B2 171 (4.575)
1: Scan ES+
2.15e6
155.1
156.2
218.0
274.2
303.2
352.0
382.0
382.9
412.0
456.9
477.0
479.6
533.8
574.5
636.8
681.7
730.4
776.0
812.3
824.0
886.8
T29-B2 159 (4.253)
1: Scan ES+
9.04e6
169.1
172.1
242.1
256.9
324.4
338.9
387.9
413.9
416.9
457.8
505.0
540.8
575.2
588.0
638.8
709.9
735.4
785.7
848.8
880.4
100
%
0
150 200 250 300 350 400 450 500 550 600 650 700 750 800 850
m/z

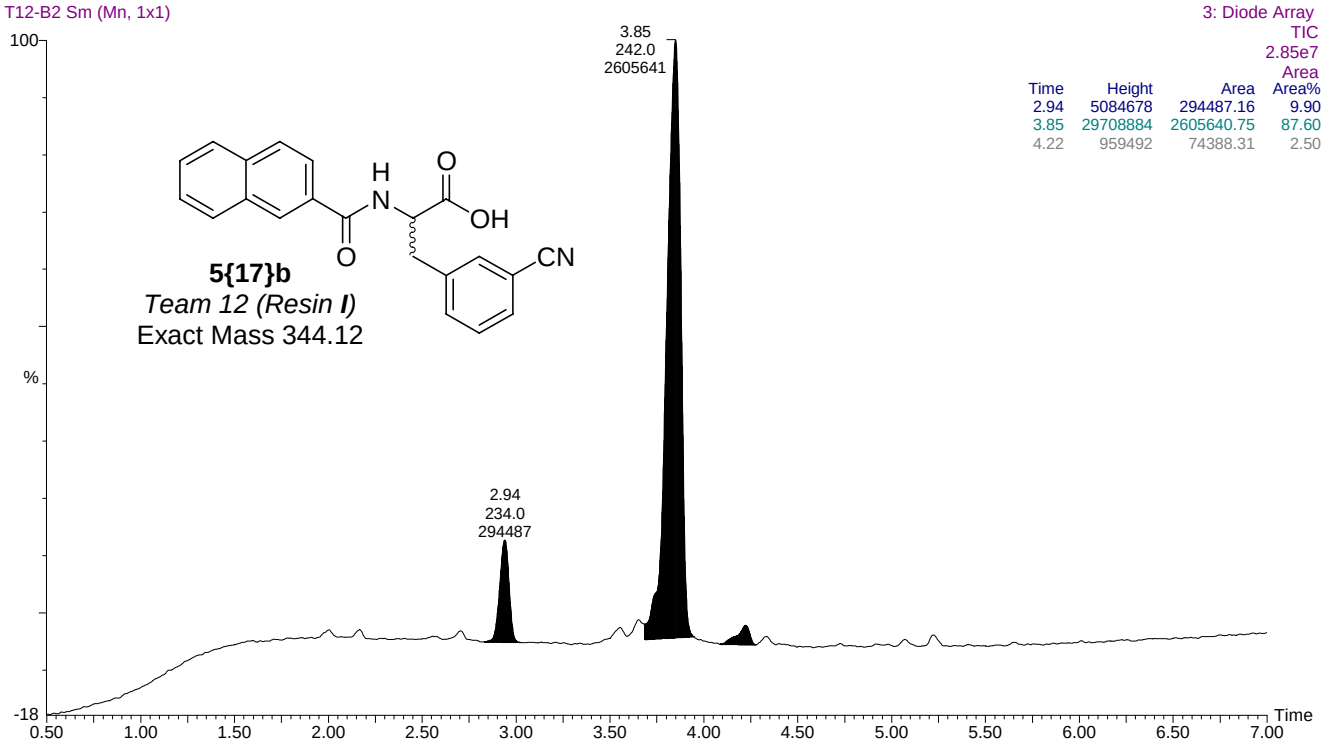
5{17}b

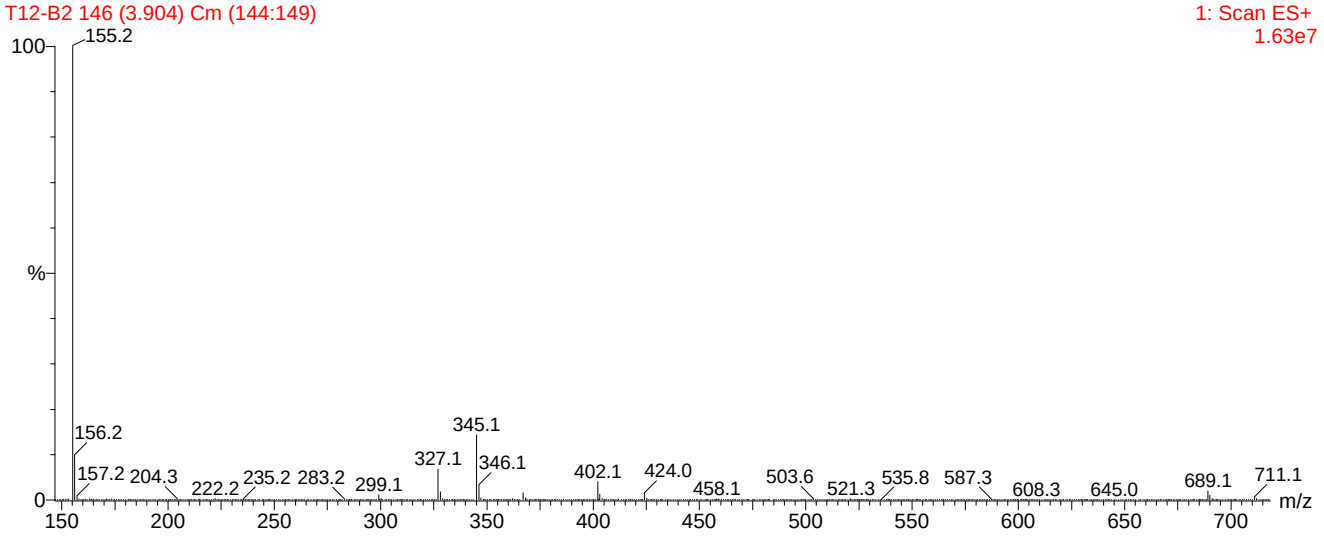

T11-B3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.07e7
Area
Time Height Area Area%
2.94 6003540 337508.97 10.76
3.65 2398584 151853.08 4.84
3.73 2097554 95795.12 3.05
3.85 31887926 2459966.50 78.41
4.22 1217863 92280.66 2.94
3.85
240.0
2459967
2.94
232.0
337509
5{17}b
Team 11 (Resin I)
Exact Mass 344.12
100
%
-15
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00


T11-B3 146 (3.904) Cm (145:147)
1: Scan ES+
2.59e7
100
%
0
155.2
156.2
180.9
222.1
327.1
345.1
402.1
424.1
458.2
517.3
603.2
647.9
689.1
746.2
803.1
825.0
919.3
932.7
988.6
1034.4
1050.5
1112.2

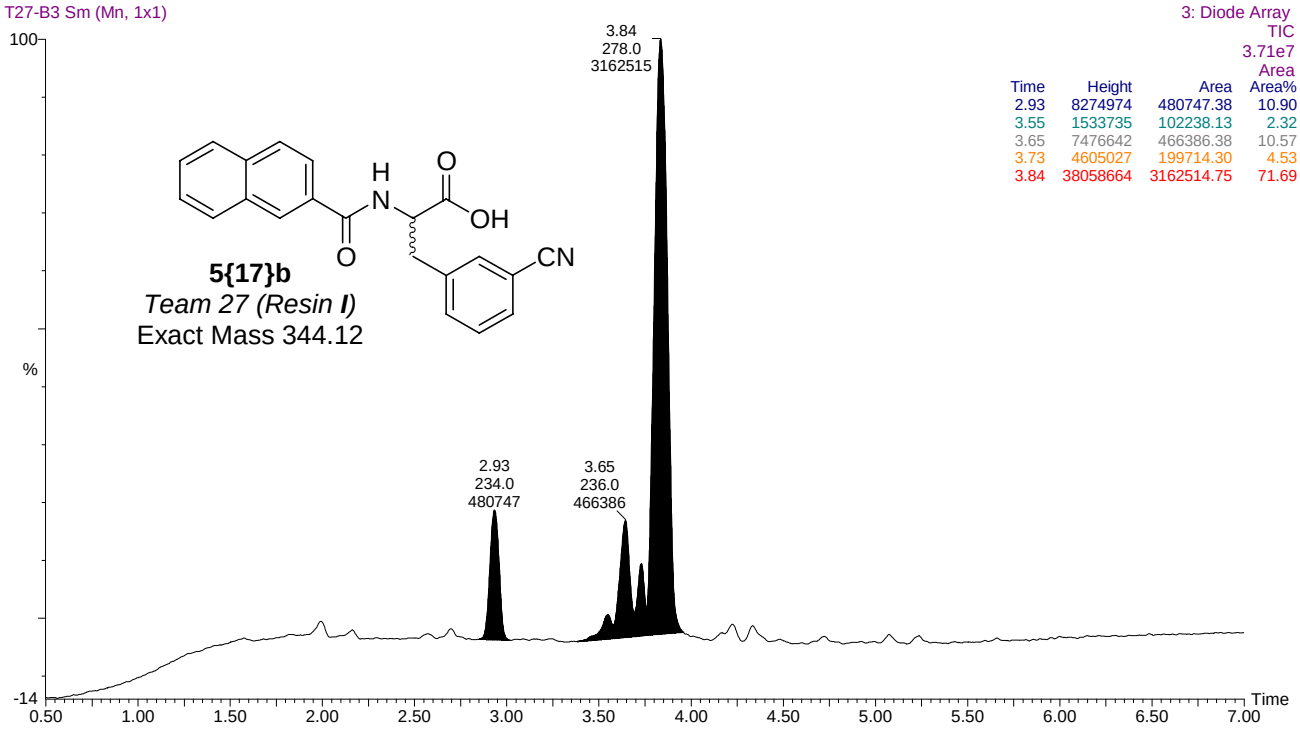
T11-B3 111 (2.965)
1: Scan ES+
4.18e6
100
%
0
306.1
157.3
189.2
260.0
307.1
329.0
361.3
448.4
463.3
512.7
634.0
656.1
676.9
747.9
817.2
840.8
891.8
955.0
1014.3
1095.9
1133.5
200 300 400 500 600 700 800 900 1000 1100
m/z

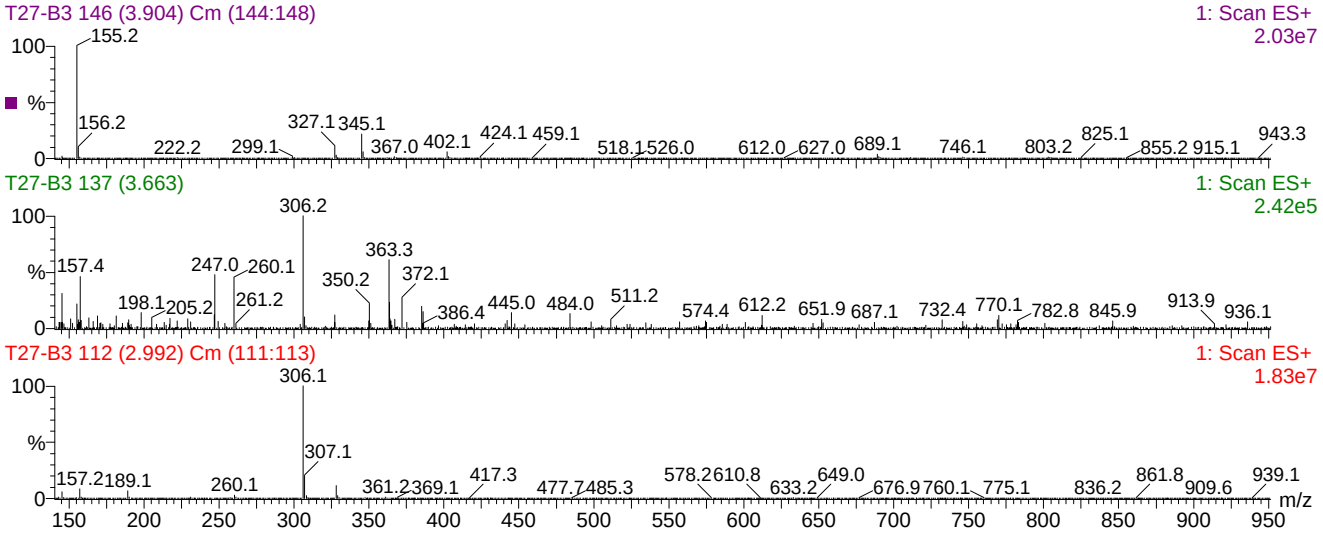
5{17}b


T12-B2 Sm (Mn, 1x1)
3: Diode Array
TIC
2.85e7
Area
Time Height Area Area%
2.94 5084678 294487.16 9.90
3.85 29708884 2605640.75 87.60
4.22 959492 74388.31 2.50
3.85
242.0
2605641
2.94
234.0
294487
5{17}b
Team 12 (Resin I)
Exact Mass 344.12
100
%
-18
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00

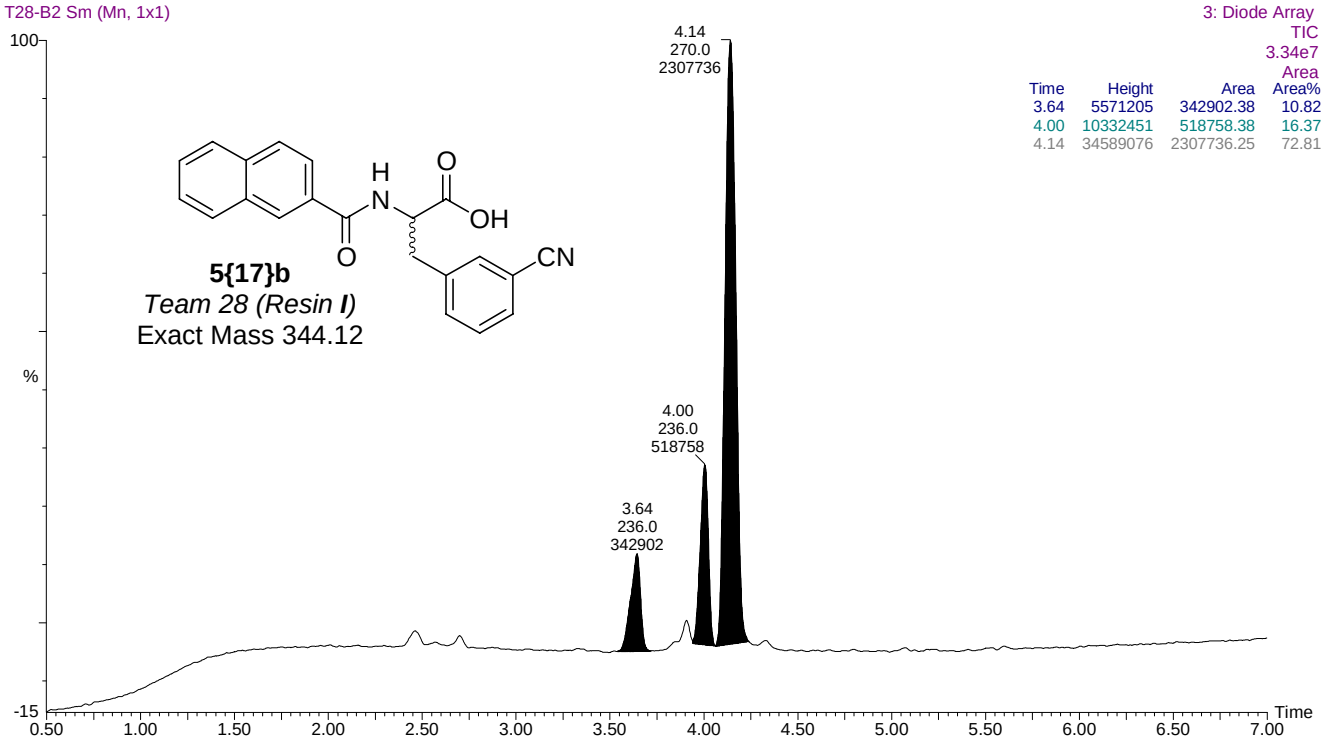

T12-B2 146 (3.904) Cm (144:149)
1: Scan ES+
1.63e7
100
%
0
155.2
156.2
157.2
204.3
222.2
235.2
283.2
299.1
327.1
345.1
346.1
402.1
424.0
458.1
503.6
521.3
535.8
587.3
608.3
645.0
689.1
711.1
m/z
150 200 250 300 350 400 450 500 550 600 650 700

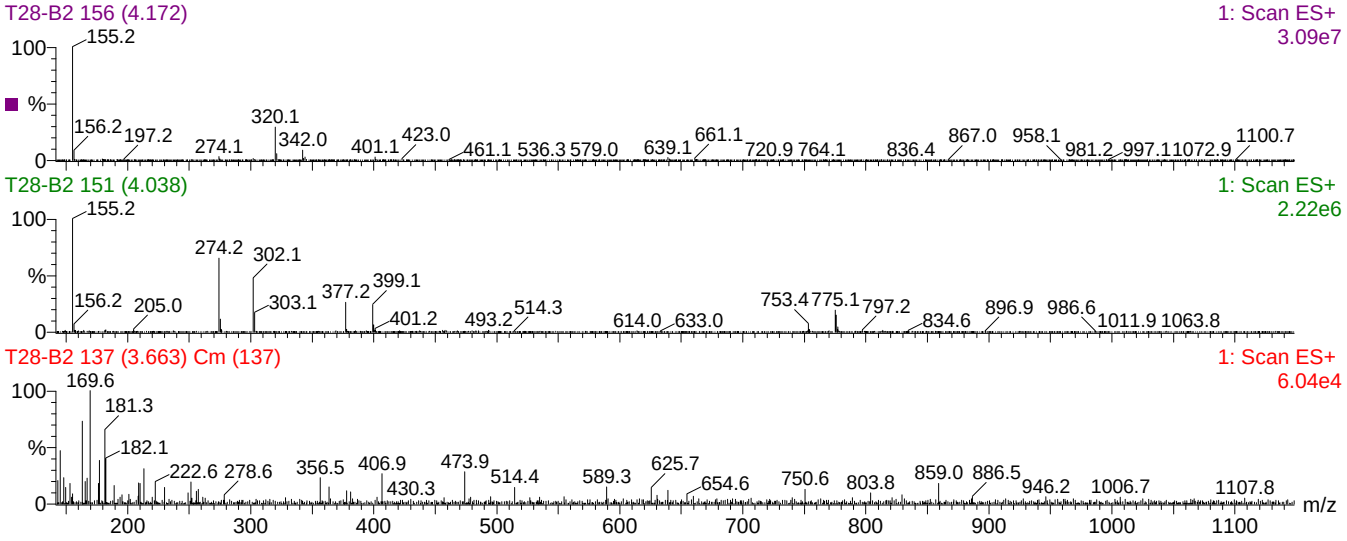
5{17}b


T27-B3 Sm (Mn, 1x1)
3: Diode Array
TIC
3.71e7
Area
Time Height Area Area%
2.93 8274974 480747.38 10.90
3.55 1533735 102238.13 2.32
3.65 7476642 466386.38 10.57
3.73 4605027 199714.30 4.53
3.84 38058664 3162514.75 71.69
3.84
278.0
3162515
2.93
234.0
480747
3.65
236.0
466386
5{17}b
Team 27 (Resin I)
Exact Mass 344.12
Time


T27-B3 146 (3.904) Cm (144:148)
1: Scan ES+
2.03e7
T27-B3 137 (3.663)
1: Scan ES+
2.42e5
T27-B3 112 (2.992) Cm (111:113)
1: Scan ES+
1.83e7
m/z

5{17}b


T28-B2 Sm (Mn, 1x1)
3: Diode Array
TIC
3.34e7
Area
Time Height Area Area%
3.64 5571205 342902.38 10.82
4.00 10332451 518758.38 16.37
4.14 34589076 2307736.25 72.81
4.14
270.0
2307736
4.00
236.0
518758
3.64
236.0
342902
5{17}b
Team 28 (Resin I)
Exact Mass 344.12
%
Time


T28-B2 156 (4.172)
1: Scan ES+
3.09e7
T28-B2 151 (4.038)
1: Scan ES+
2.22e6
T28-B2 137 (3.663) Cm (137)
1: Scan ES+
6.04e4
m/z

References

Numbers in this Supporting Information refer to compounds in the article text; letters refer to compounds not in the article text.

1. (a) Atherton, E.; Gait, M. J.; Sheppard, R. C.; Williams, B. J. *Bioorg. Chem.* **1979**, *8*, 351-370. (b) Grandas, A.; Jorba, X.; Giralt, E.; Pedroso, E. *Int. J. Pept. Protein Res.* **1989**, *33*, 386-390.
2. Stanger, K. J.; Krchnak, V. *J. Comb. Chem.* **2006**, *8*, 652-654.

(Ref for Wang Linker adduct) Stanger, K. J.; Krchnak, V. *J. Comb. Chem.* **2006**, *8*, 652-654.