

Supporting Information

Development and Clinical Potential of ^{18}F -PSiMA for Prostate Cancer PET Imaging

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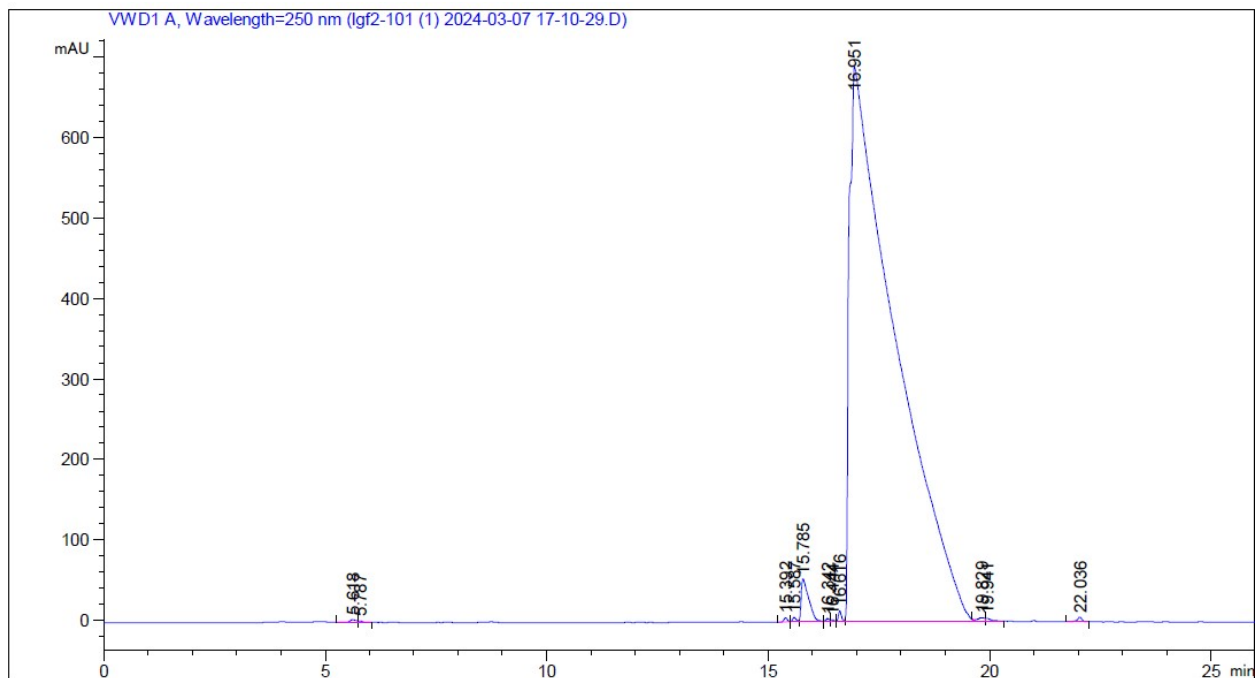
Table of Contents

HPLC Chromatograms	S3-S15
Compound HPLC Traces	S3

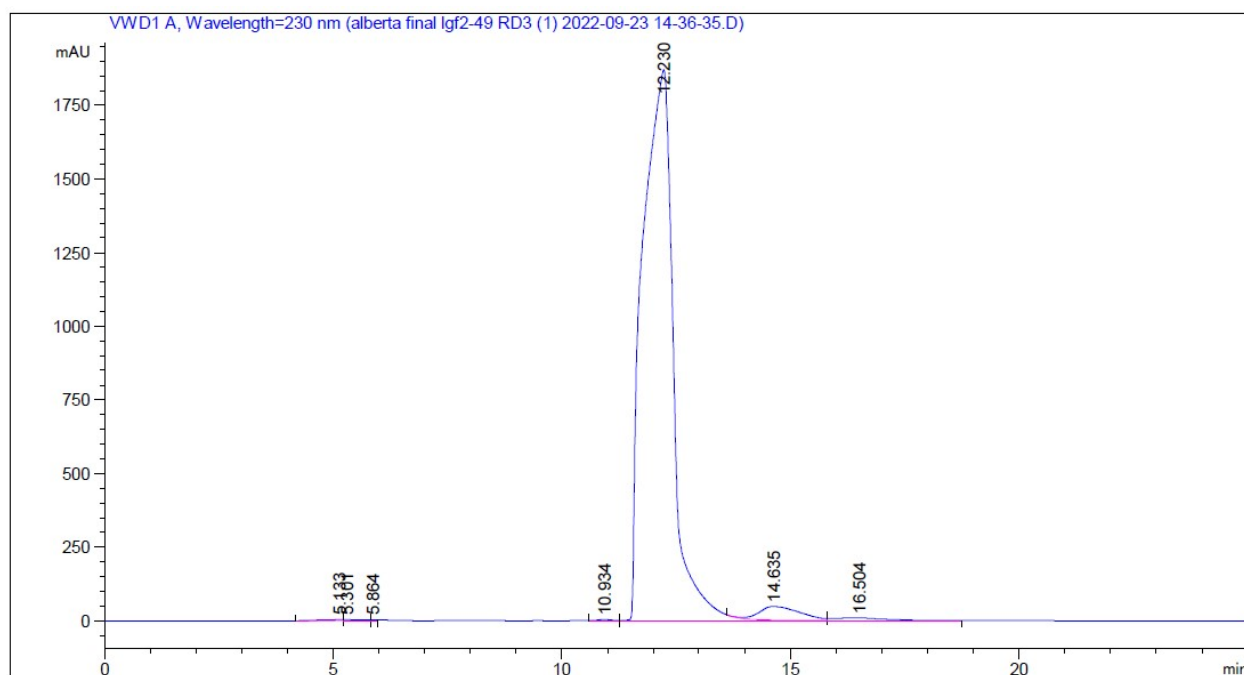
Radiosynthesis and QC Traces	S4-S5
HPLC Calibration Curve Data	S6-S9
Blood pool clearance.....	S10
Figure S1	S10
In vivo metabolism data	S10-S13
Gamma Spectroscopy Data of Cell Compartment Distribution	S14-S15
Select NMR Spectra	S16-S28

Select Compound HPLC Traces.

HPLC trace of Compound 12.

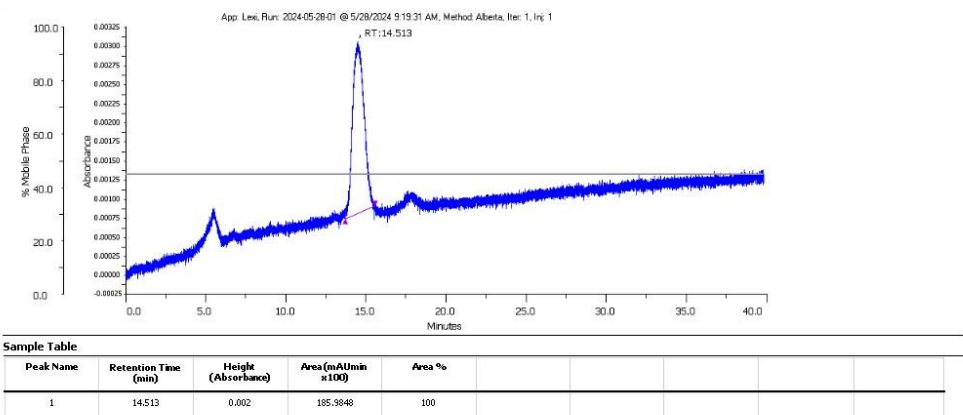


HPLC trace of Compound 14.

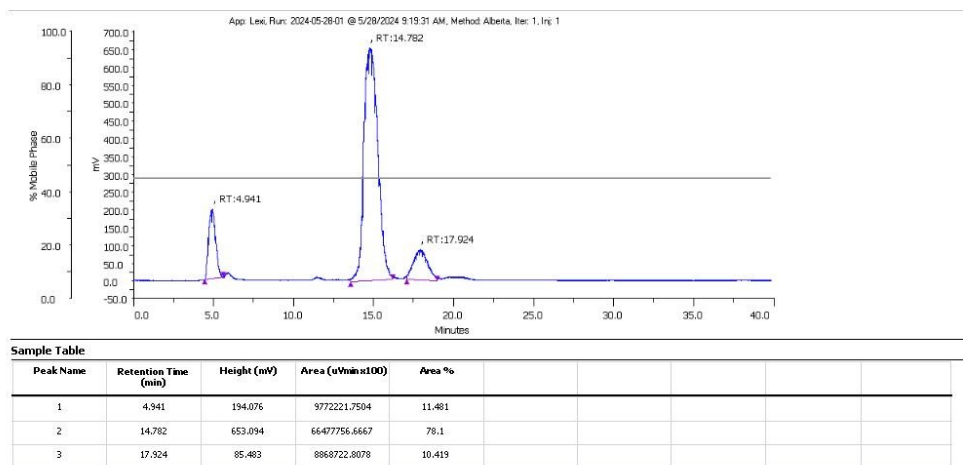


Radiosynthesis and QC Traces.

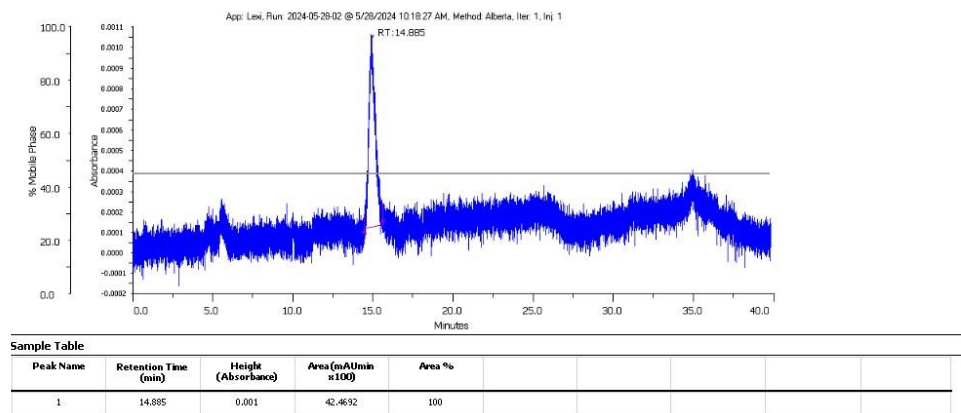
Example of HPLC of [^{18}F]PSiMA – UV.



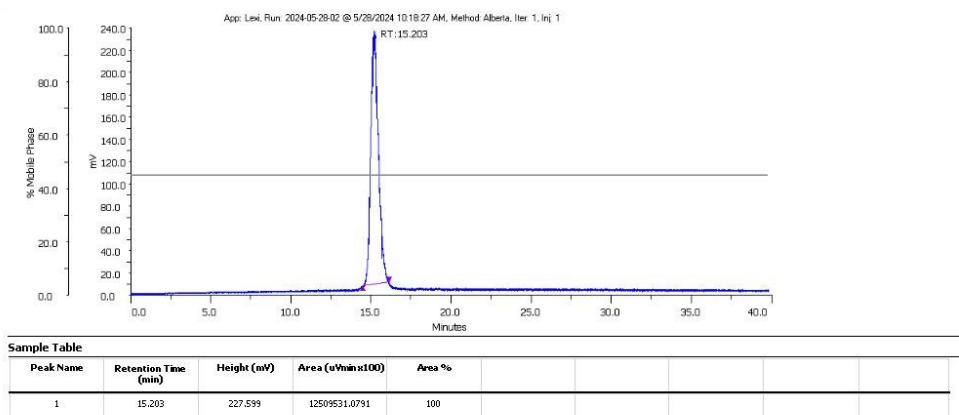
Example of HPLC of [^{18}F]PSiMA – Radiodetector.



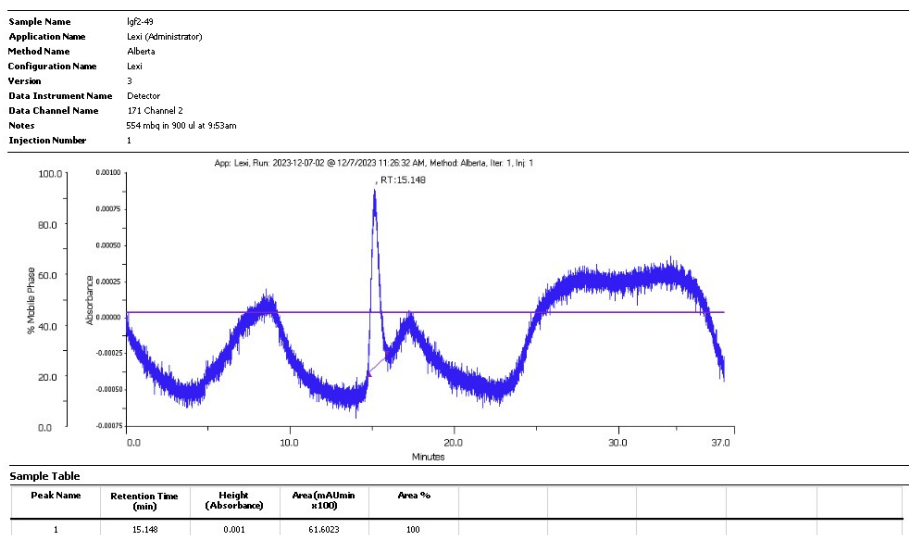
Example of QC HPLC – UV.



Example of QC HPLC- Radiodetector.



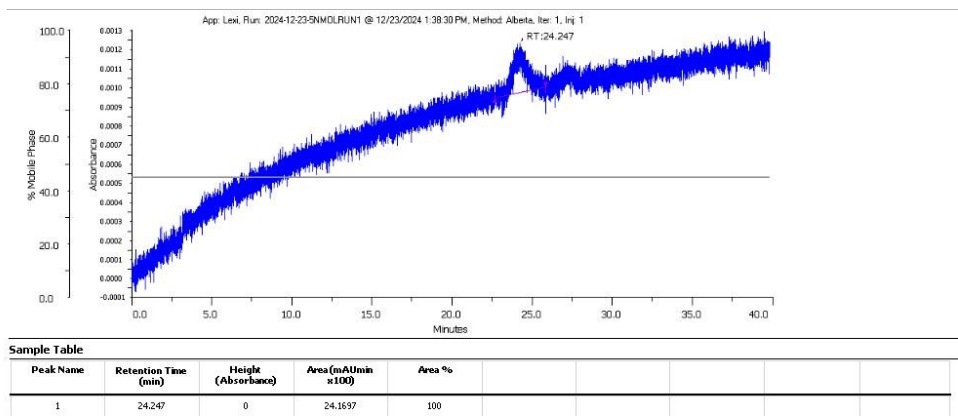
Example of QC with 5 nmol ^{19}F -PSiMA spike – UV.



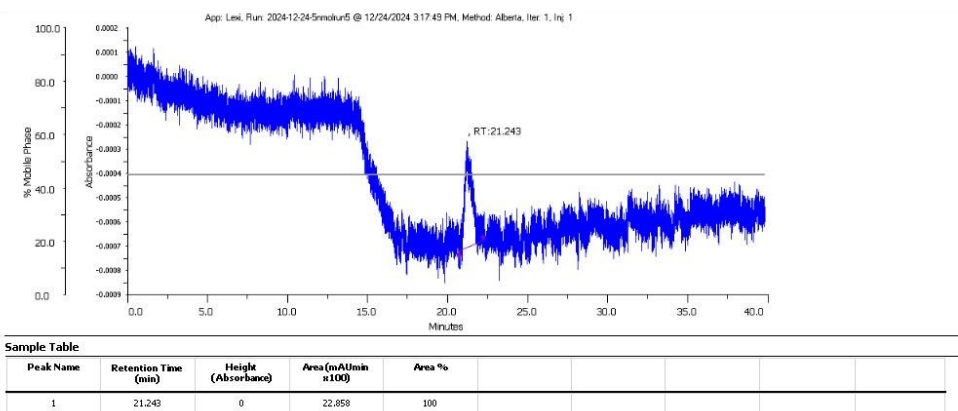
Calibration Curve HPLCs for calculation of A_m .

(*column was altered giving a slight change in retention time)

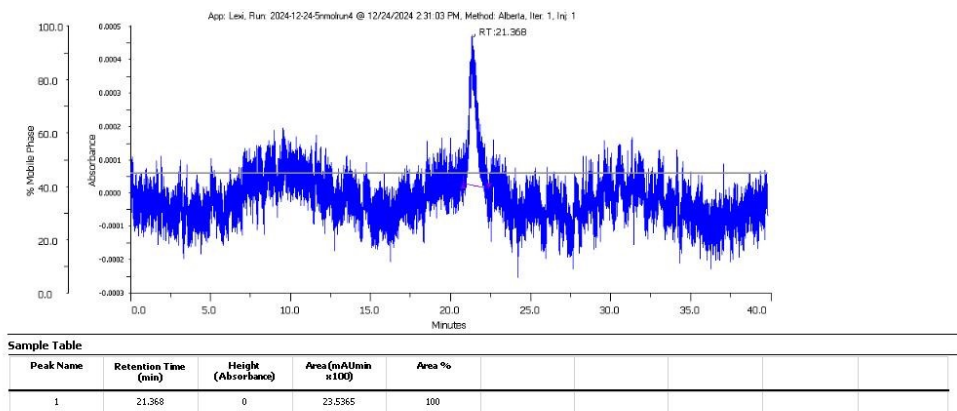
5 nmol A:



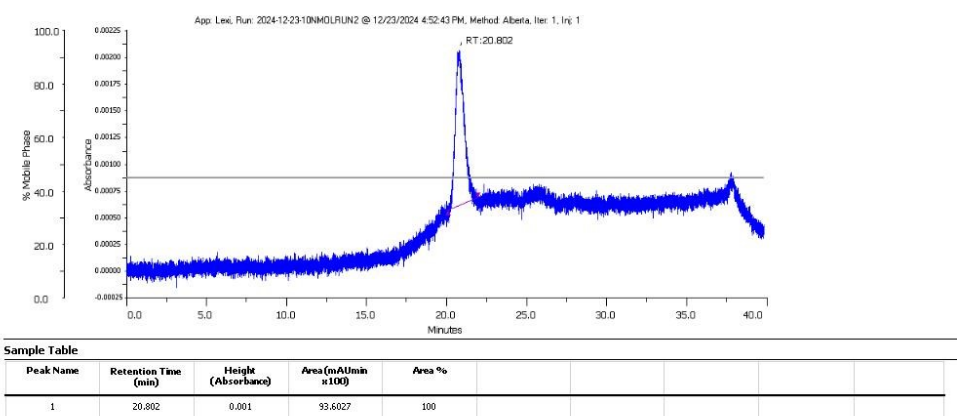
5 nmol B:



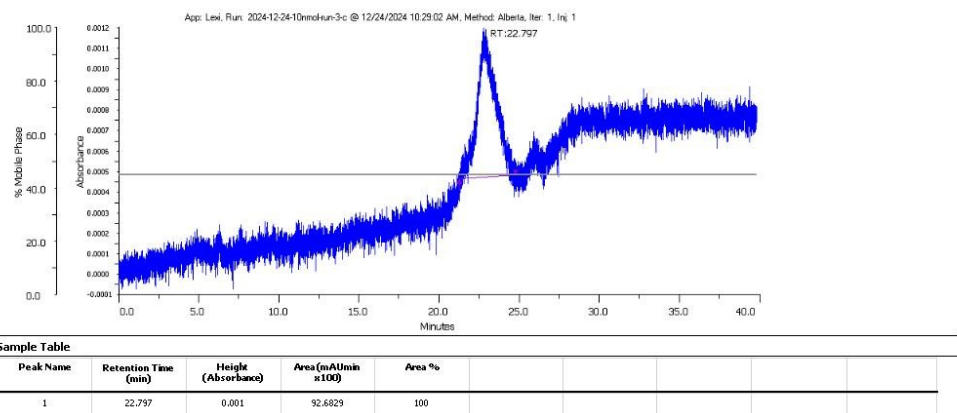
5 nmol C:



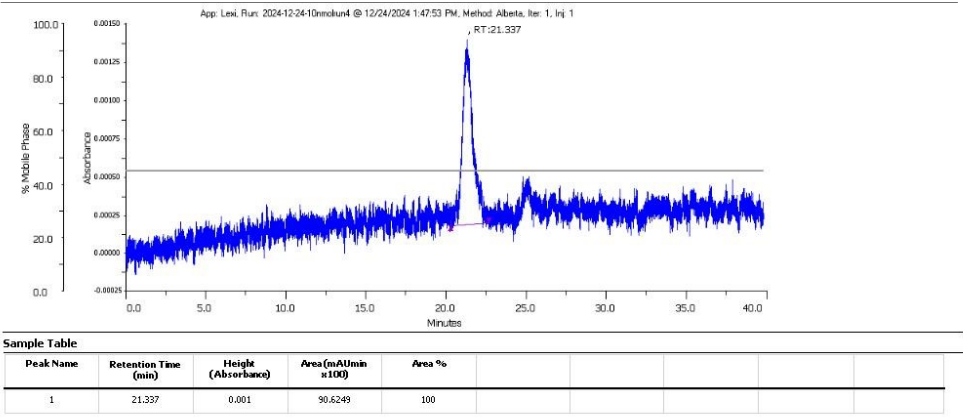
10 nmol A:



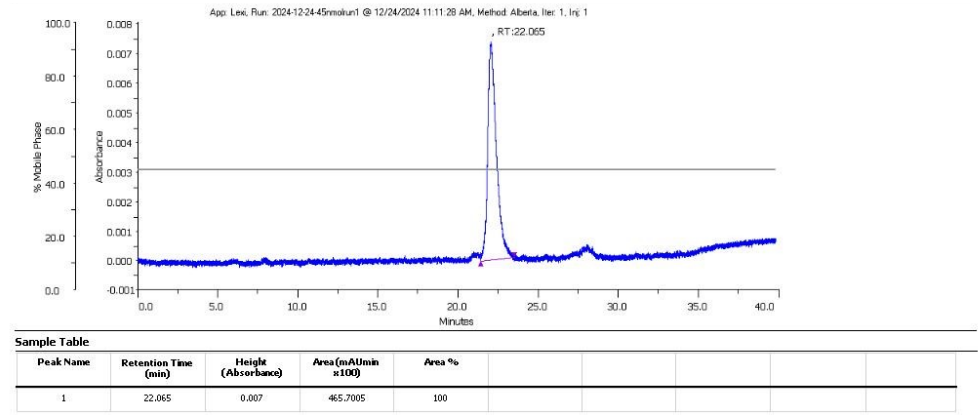
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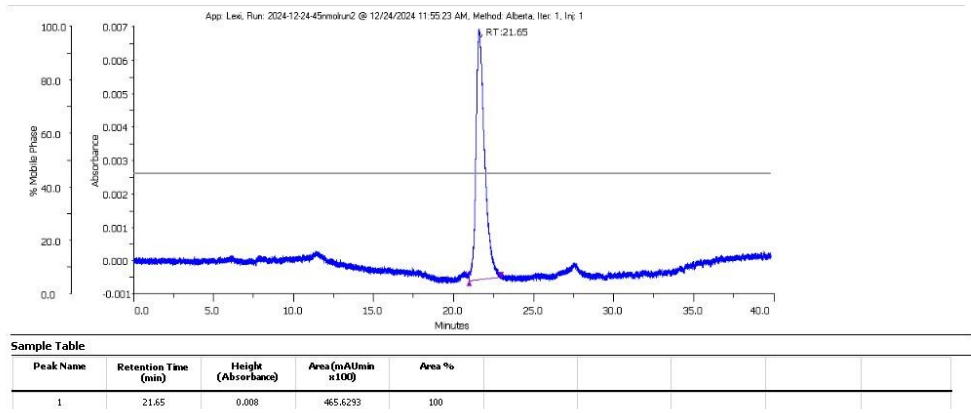
10 nmol C:



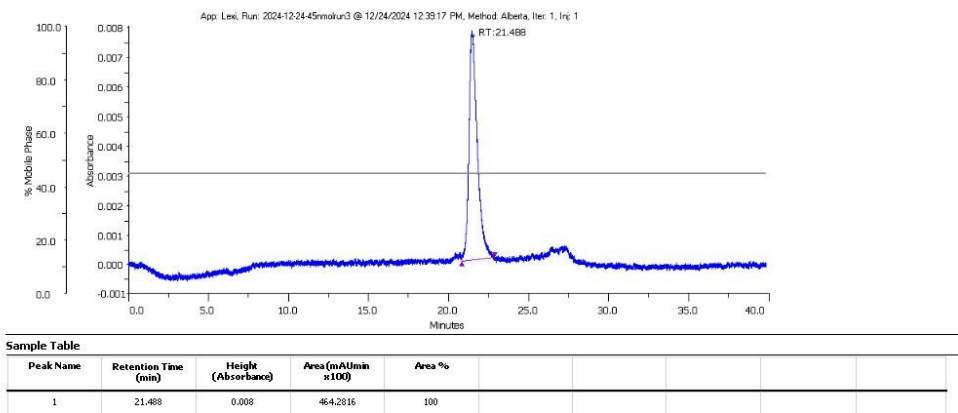
45 nmol A:



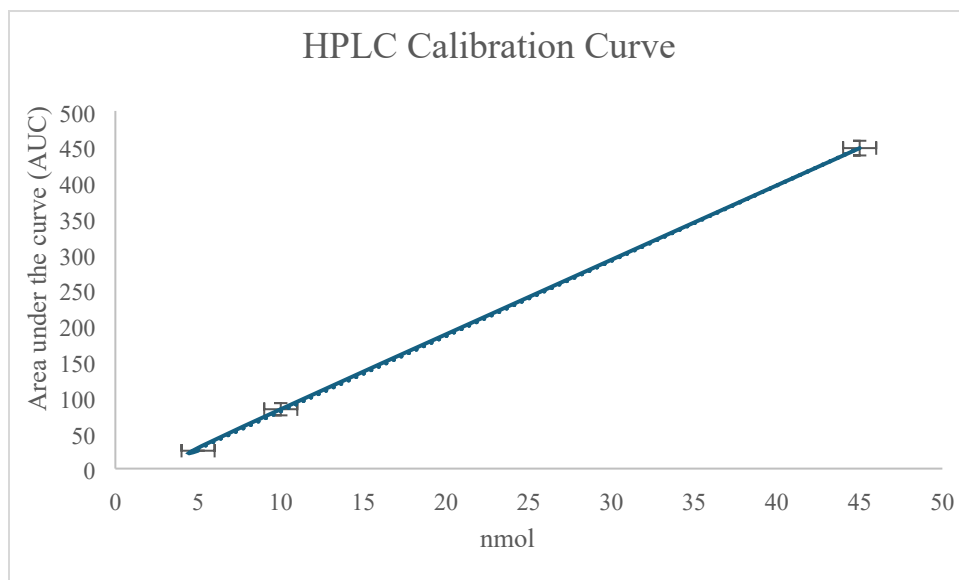
45 nmol B:



45 nmol C:



HPLC Calibration Curve Graph:



Blood pool clearance.

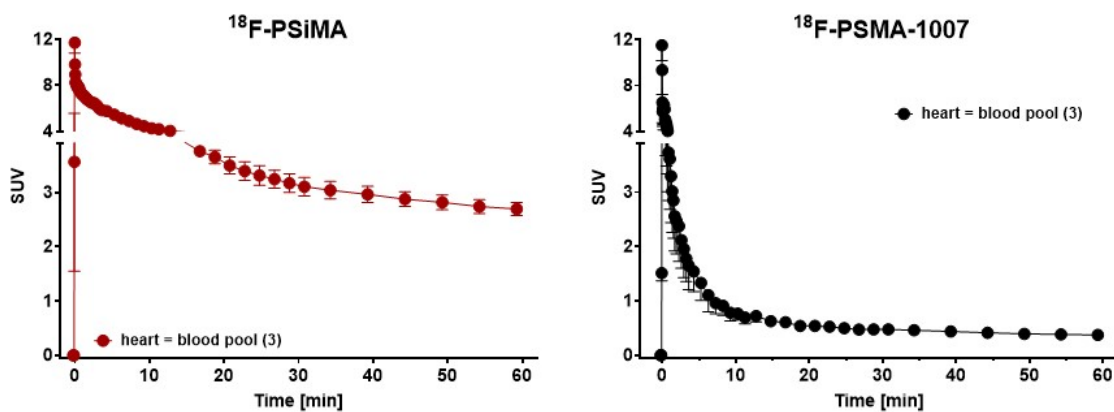


Figure S1: Blood pool clearance data (n=3).

In vivo metabolism HPLC data.

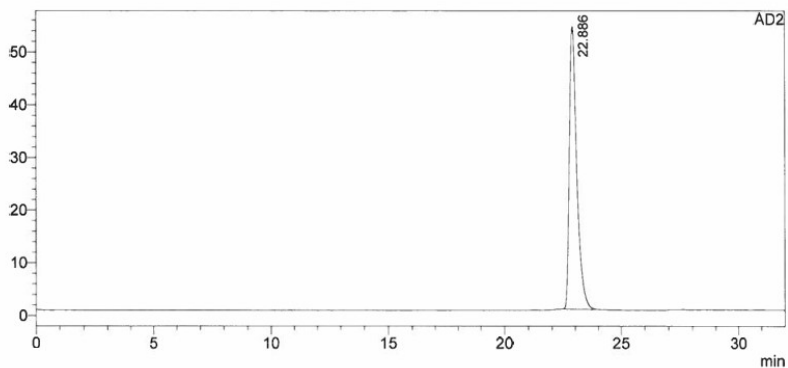
QC:

<Sample Information>

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Sample ID	: 18F-Alberta		
Data Filename	: 20240528_18F-Alberta_QC.lcd	Acquired by	: System Administrator
Method Filename	: SiFA.lcm	Processed by	: System Administrator
Batch Filename	:		
Vial #	: 1-1		
Injection Volume	: 10 uL		
Date Acquired	: 28/05/2024 10:05:47 AM		
Date Processed	: 28/05/2024 10:37:56 AM		
0.366MBq in 1uL+39uL saline, Luna C18 'metab.stab.'			
100000cps=1V			

<Chromatogram>

mV



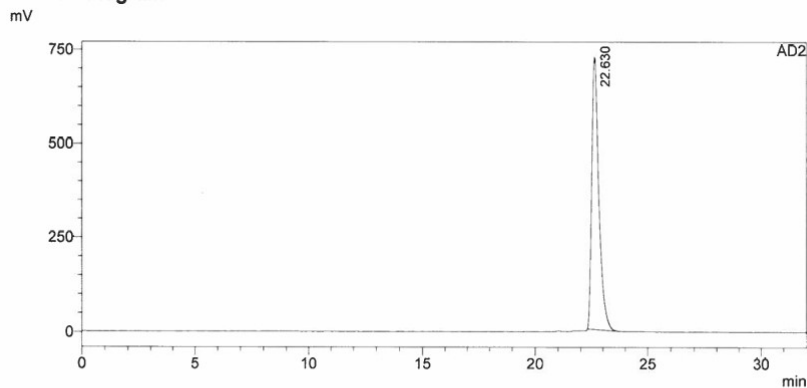
5 min time point:

<Sample Information>

Sample Name : 20240528_18F-Alberta_5min
Sample ID : 18F-Alberta
Data Filename : 20240528_18F-Alberta_5min.lcd
Method Filename : SiFA.lcm
Batch Filename :
Vial # : 1-1
Injection Volume : 20 uL
Date Acquired : 28/05/2024 11:07:40 AM
Date Processed : 28/05/2024 11:39:48 AM
280kBq in ~200uL, Luna C18 'metab.stab.'
10000cps=1V

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>



<Peak Table>

AD2

Peak#	Ret. Time	Height	Area	Area%	Name
1	22.630	721144	15973087	100.000	
Total		721144	15973087	100.000	

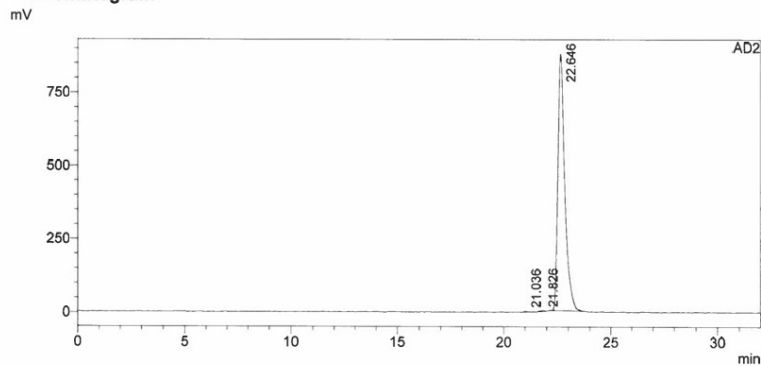
15 min time point:

<Sample Information>

Sample Name : 20240528_18F-Alberta_15min
Sample ID : 18F-Alberta
Data Filename : 20240528_18F-Alberta_15min.lcd
Method Filename : SiFA.lcm
Batch Filename :
Vial # : 1-1
Injection Volume : 20 uL
Date Acquired : 28/05/2024 11:48:44 AM
Date Processed : 28/05/2024 12:20:52 PM
22kBq in ~200uL, Luna C18 'metab.stab.'
1000cps=1V

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>



<Peak Table>

AD2

Peak#	Ret. Time	Height	Area	Area%	Name
1	21.036	2441	21497	0.112	
2	21.826	2649	39644	0.207	
3	22.646	872746	19120293	99.681	
Total		877836	19181434	100.000	

30 minute time point:

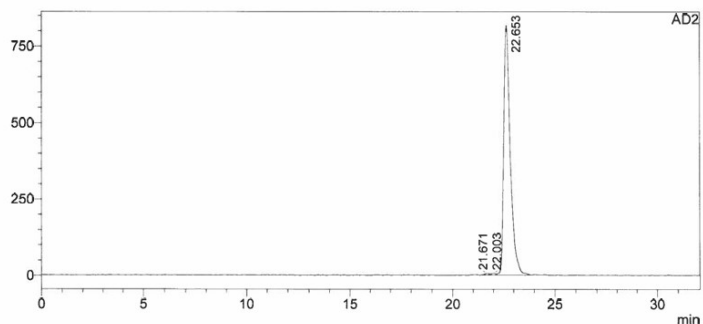
<Sample Information>

Sample Name : 20240528_18F-Alberta_30min
Sample ID : 18F-Alberta
Data Filename : 20240528_18F-Alberta_30min.lcd
Method Filename : SiFA.lcm
Batch Filename :
Vial # : 1-1
Injection Volume : 20 uL
Date Acquired : 28/05/2024 12:30:44 PM
Date Processed : 28/05/2024 1:02:52 PM
27kBq in ~200uL, Luna C18 'metab.stab.'
1000cps=1V

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>

mV



<Peak Table>

AD2	Peak#	Ret. Time	Height	Area	Area%	Name
	1	21.671	5404	68025	0.372	
	2	22.003	4809	90392	0.494	
	3	22.653	813947	18141771	99.134	
	Total		824159	18300189	100.000	

60 minute time point:

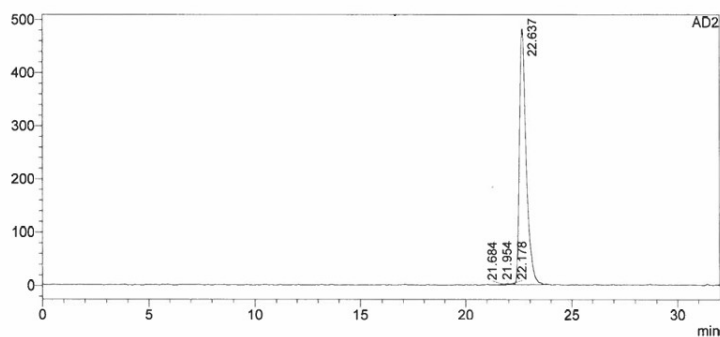
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Sample Name : 20240528_18F-Alberta_60min
Sample ID : 18F-Alberta
Data Filename : 20240528_18F-Alberta_60min.lcd
Method Filename : SiFA.lcm
Batch Filename :
Vial # : 1-1
Injection Volume : 20 uL
Date Acquired : 28/05/2024 1:11:22 PM
Date Processed : 28/05/2024 1:43:30 PM
11kBq in ~200uL, Luna C18 'metab.stab.'
1000cps=1V

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>

mV



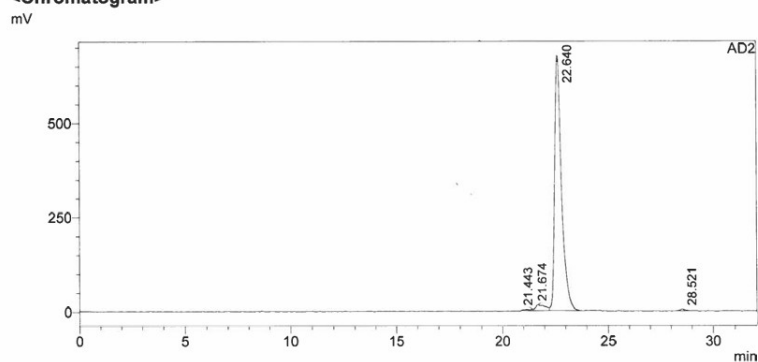
<Peak Table>

AD2	Peak#	Ret. Time	Height	Area	Area%	Name
	1	21.684	1591	11614	0.111	
	2	21.954	2374	24481	0.234	
	3	22.178	2630	25174	0.240	
	4	22.637	479984	10420702	99.415	
	Total		486579	10481971	100.000	

Urine sample:

Sample Name : 20240528_18F-Alberta_urine
 Sample ID : 18F-Alberta
 Data Filename : 20240528_18F-Alberta_urine.lcd
 Method Filename : SIFA.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 28/05/2024 1:51:49 PM
 Date Processed : 28/05/2024 2:23:56 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator
 30kBq in ~200uL (diuted in saline), Luna C18 'metab.stab.'
 1000cps=1V

<Chromatogram>



<Peak Table>

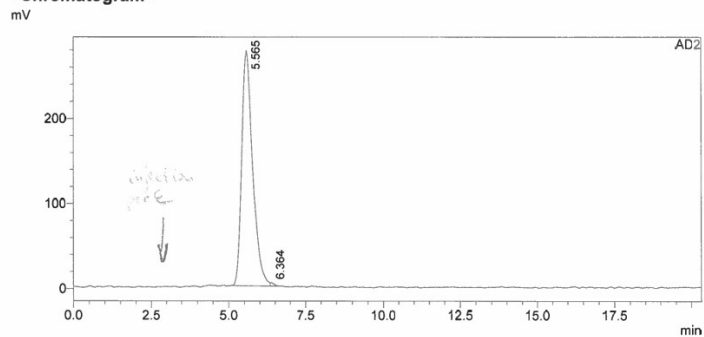
Peak#	Ret. Time	Height	Area	Area%	Name
1	21.443	3824	79530	0.501	
2	21.674	15337	501484	3.160	
3	22.640	674505	15201808	95.795	
4	28.521	4913	86358	0.544	
Total		698580	15869180	100.000	

60 minute time point isocratic run:

<Sample Information>

Sample Name : 20240528_18F-Alberta_60min_iso
 Sample ID : 18F-Alberta
 Data Filename : 20240528_18F-Alberta_60min_iso.lcd
 Method Filename : SIFA_45_iso.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 28/05/2024 2:32:24 PM
 Date Processed : 28/05/2024 2:52:49 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator
 3kBq in ~180uL, Luna C18 'metab.stab.'
 1000cps=1V

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Height	Area	Area%	Name
1	5.565	275487	6765089	99.480	
2	6.364	4152	35375	0.520	
Total		279639	6800465	100.000	

Blood cell compartment distribution data.

5 minute post injection (p.i.):

Hidex Automatic Gamma Counter

18F Counts

Run
Template 18F Counts
Run status Finished
Run startec #####
Run type Count only, multiple racks
Software v.1.8.0.0
AMG serial 2210234
Firmware v 0: 50, 1: 50, F: 100
Counting ti 60
Result norr #####
Comment

5 min p.i.

Counting windows

Window st Window er Additional Isotope Counting e Half-life
400 600 [950-1100] ¹⁸F 0.409 1.82951 h

Racks

Rack	Time	Barcode	Slot count	Latest QC c	QC status
1	#####	001	6	#####	QC pass

Results

Rack	Vial	Time	Counted ti	Dead time	¹⁸ F (counts)	¹⁸ F (CPM)	Normalized	Normalized
1	1	#####	60	1.285	1,269,090	1,630,865	1,644,490	67,013
1	2	#####	60	1.057	311,978	329,717	335,690	13,679
1	3	#####	60	2.368	2,967,051	7,025,266	7,222,191	294,303
1	4	#####	60	1.000	48	48	50	2

↓

blood cells
protein
plasma
background

15 minute post injection:

Hidex Automatic Gamma Counter

18F Counts

Run
Template 18F Counts
Run status Finished
Run startec #####
Run type Count only, multiple racks
Software v.1.8.0.0
AMG serial 2210234
Firmware v 0: 50, 1: 50, F: 100
Counting ti 60
Result norr #####
Comment

15 min p.i.

Counting windows

Window st Window er Additional Isotope Counting e Half-life
400 600 [950-1100] ¹⁸F 0.409 1.82951 h

Racks

Rack	Time	Barcode	Slot count	Latest QC c	QC status
1	#####	001	6	#####	QC pass

Results

Rack	Vial	Time	Counted ti	Dead time	¹⁸ F (counts)	¹⁸ F (CPM)	Normalized	Normalized
1	1	#####	60	1.041	229,332	238,613	240,541	9,802
1	2	#####	60	1.010	57,931	58,522	59,563	2,427
1	3	#####	60	1.170	833,085	974,885	1,001,788	40,823
1	4	#####	60	1.000	56	56	58	2

↓

blood cells
protein
plasma
background

30 minute post injection:

18F Counts

30 min p.i.

Run
Template 18F Counts
Run status Finished
Run startec #####
Run type Count only, multiple racks
Software v 1.8.0.0
AMG serial 2210234
Firmware v 0: 50, 1: 50, F: 100
Counting ti 60
Result norr #####
Comment

Counting windows

Window st	Window er	Additional	Isotope	Counting e	Half-life
400	600	[950-1100]	¹⁸ F	0.409	1.82951 h

Racks

Rack	Time	Barcode	Slot count	Latest QC c	QC status
1	#####	001	6	#####	QC pass

Results

Rack	Vial	Time	Counted ti	Dead time	¹⁸ F (counts)	¹⁸ F (CPM)	Normalized	Normalized
1	1	#####	60	1.061	334,298	354,591	357,462	14,566
1	2	#####	60	1.015	87,852	89,179	90,768	3,699
1	3	#####	60	1.215	979,482	1,189,570	1,222,482	49,816
1	4	#####	60	1.000	53	53	55	2

blood cells
protein
plasma
background

60 minute post injection:

Hidex Automatic Gamma Counter

18F Counts

60 min p.i.

Run
Template 18F Counts
Run status Finished
Run startec #####
Run type Count only, multiple racks
Software v 1.8.0.0
AMG serial 2210234
Firmware v 0: 50, 1: 50, F: 100
Counting ti 60
Result norr #####
Comment

Counting windows

Window st	Window er	Additional	Isotope	Counting e	Half-life
400	600	[950-1100]	¹⁸ F	0.409	1.82951 h

Racks

Rack	Time	Barcode	Slot count	Latest QC c	QC status
1	#####	001	6	#####	QC pass

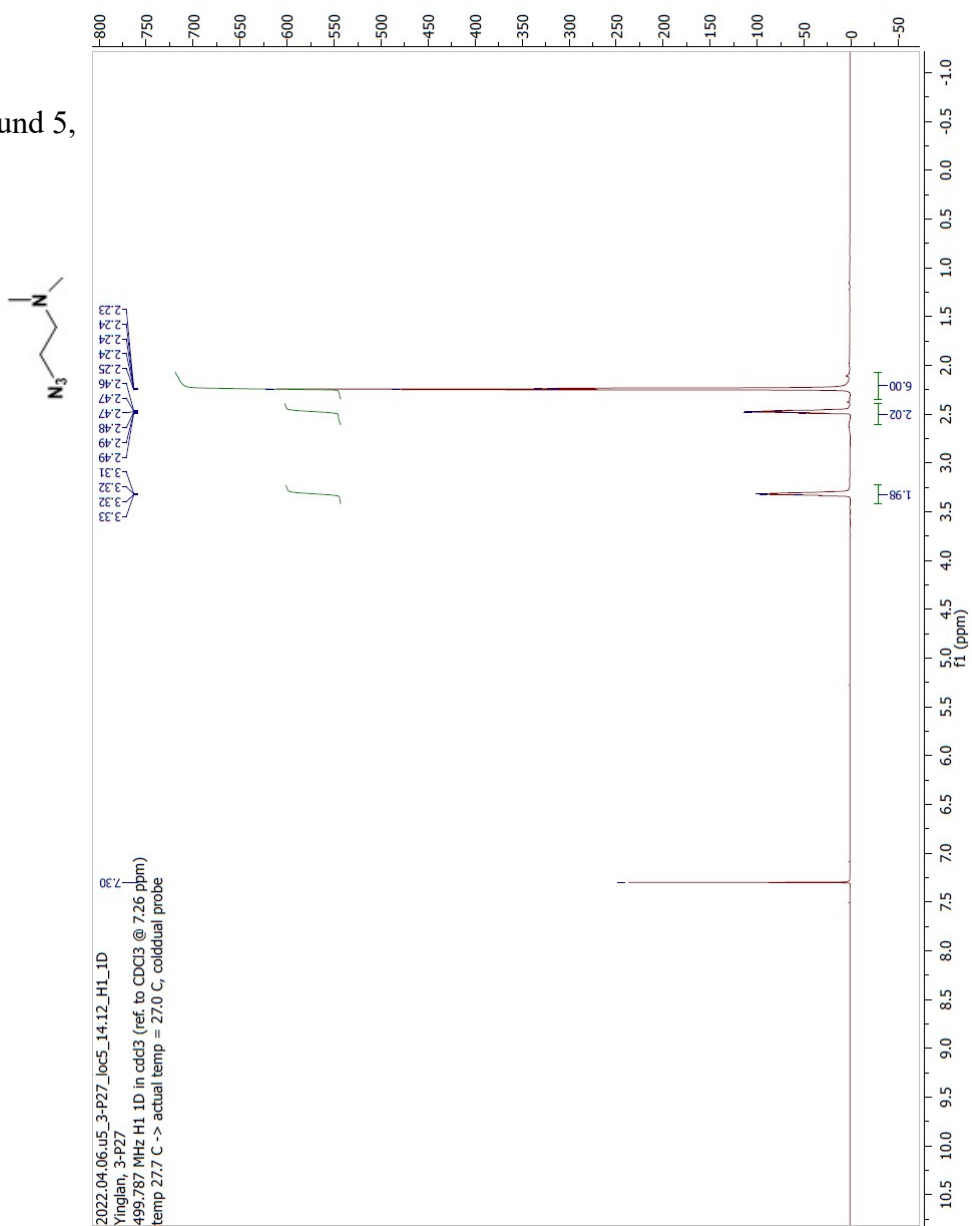
Results

Rack	Vial	Time	Counted ti	Dead time	¹⁸ F (counts)	¹⁸ F (CPM)	Normalized	Normalized
1	1	#####	60	1.028	158,011	162,388	163,697	6,671
1	2	#####	60	1.009	55,666	56,186	57,249	2,333
1	3	#####	60	1.128	655,894	739,795	761,137	31,016
1	4	#####	60	1.000	49	49	51	2

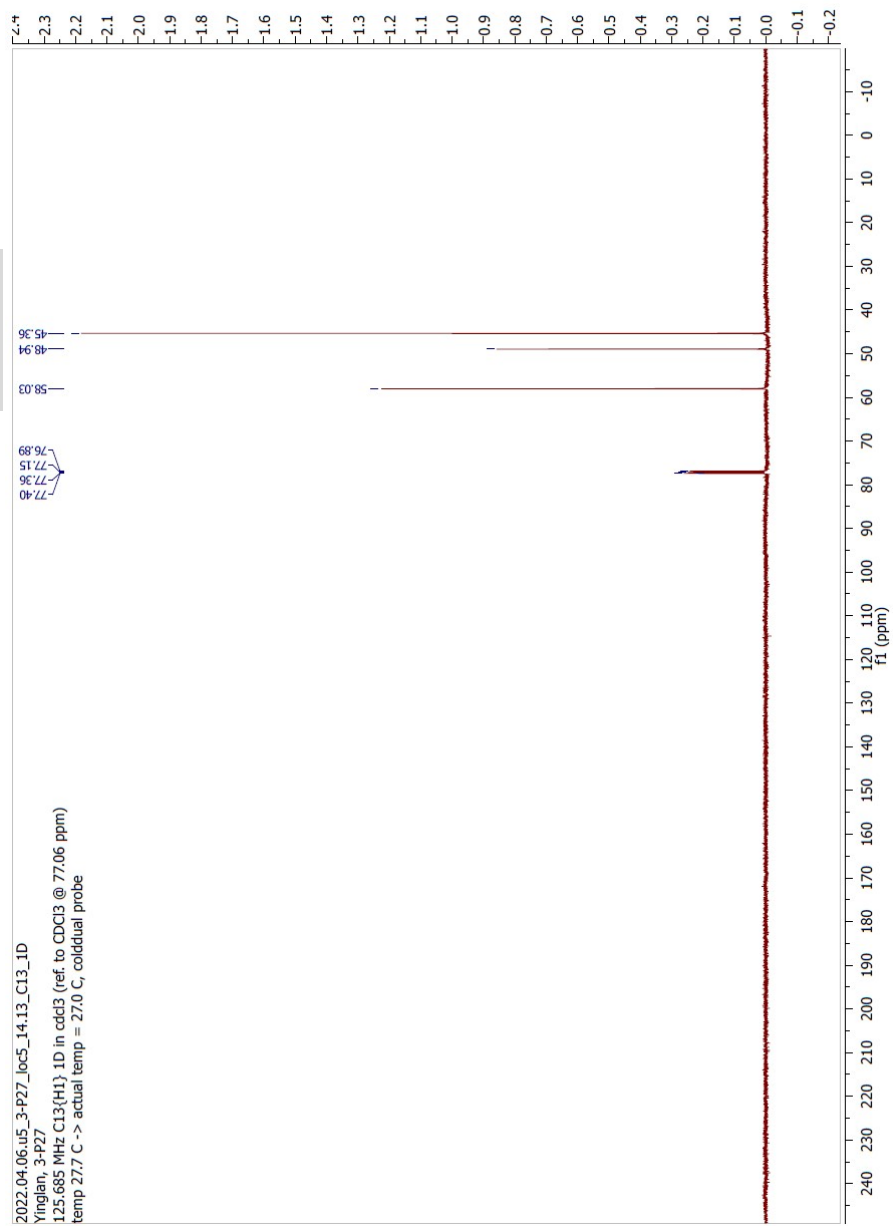
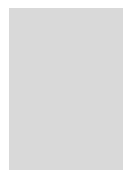
blood cells
protein
plasma
background

Select NMR Spectra.

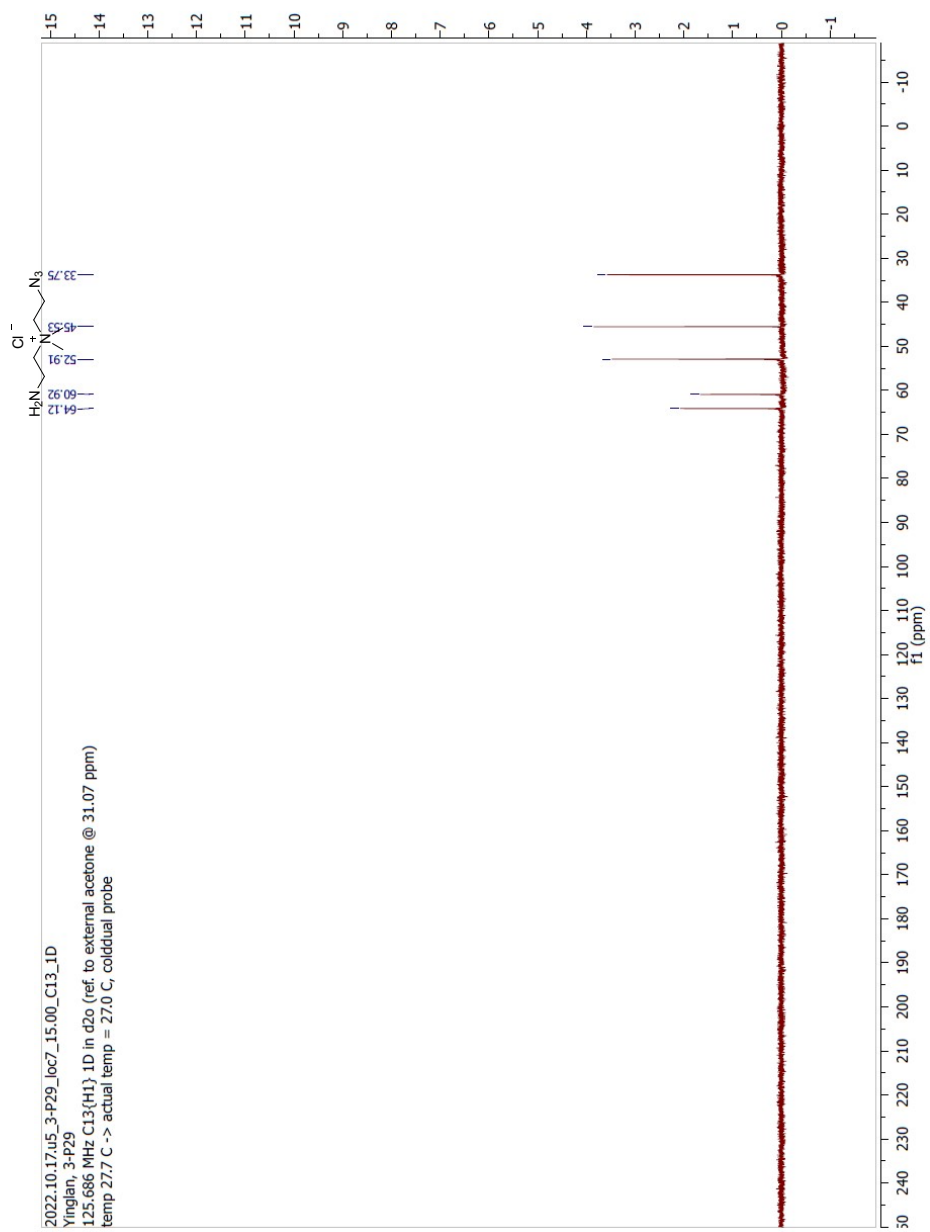
Compound 5,



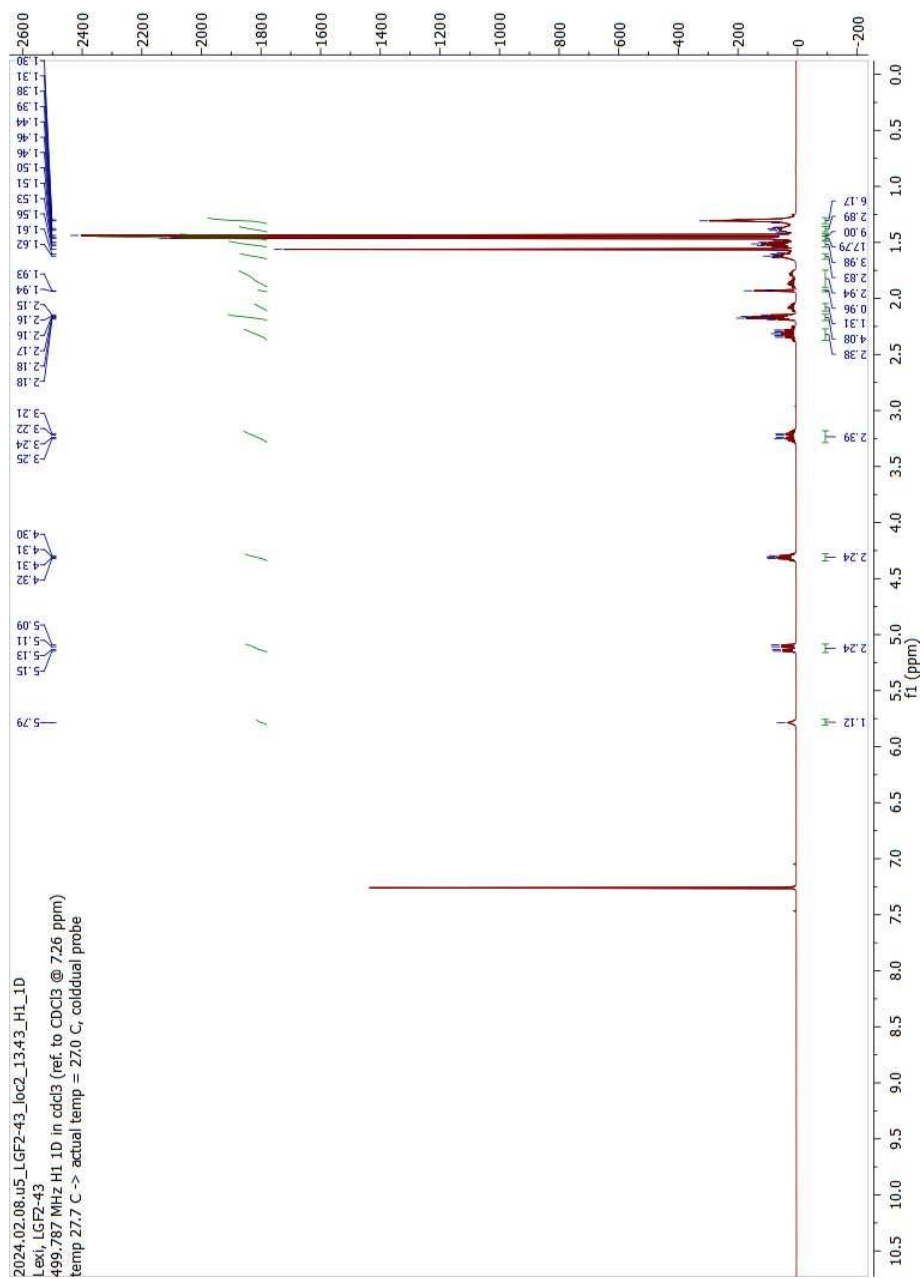
Compound 5, ¹³C NMR

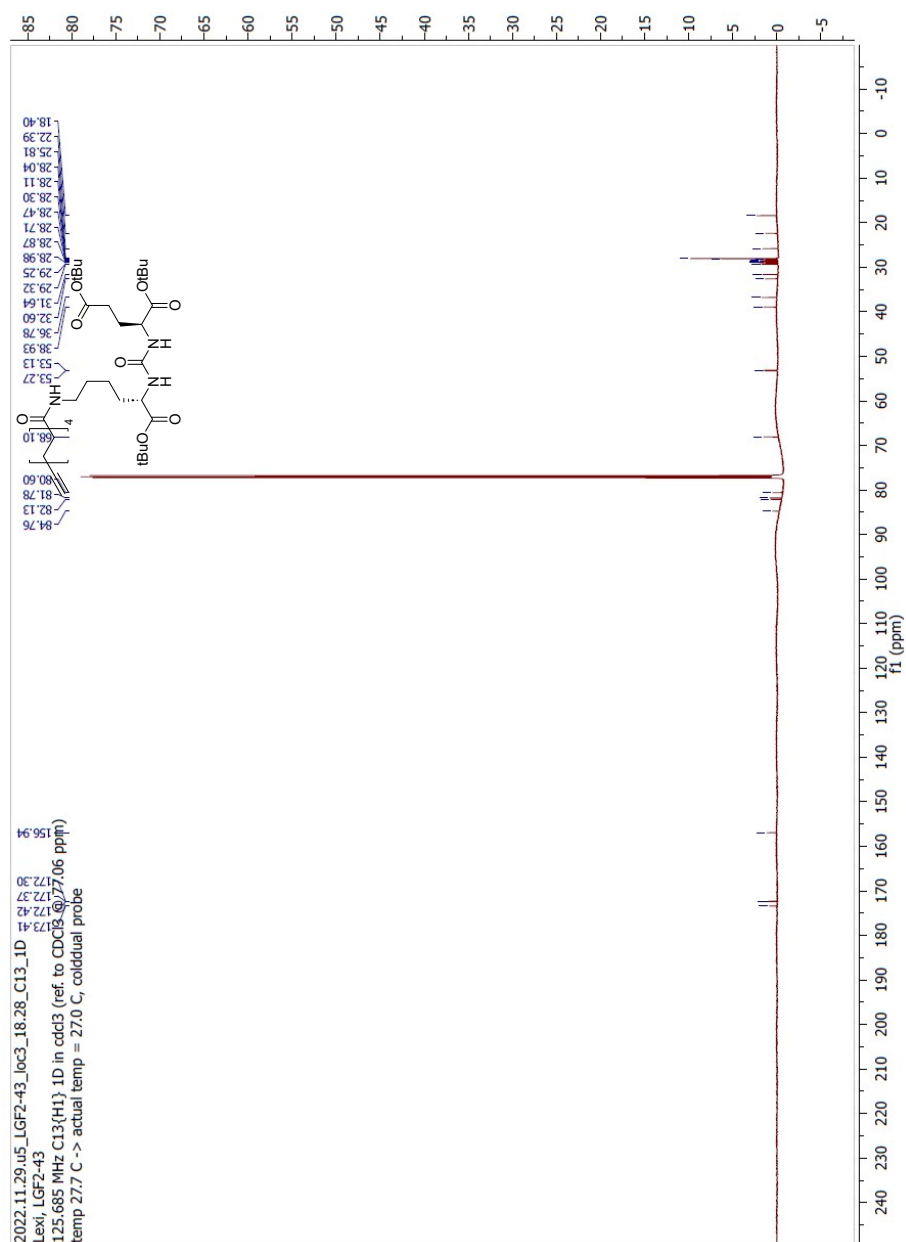


Compound 7, ¹H NMR

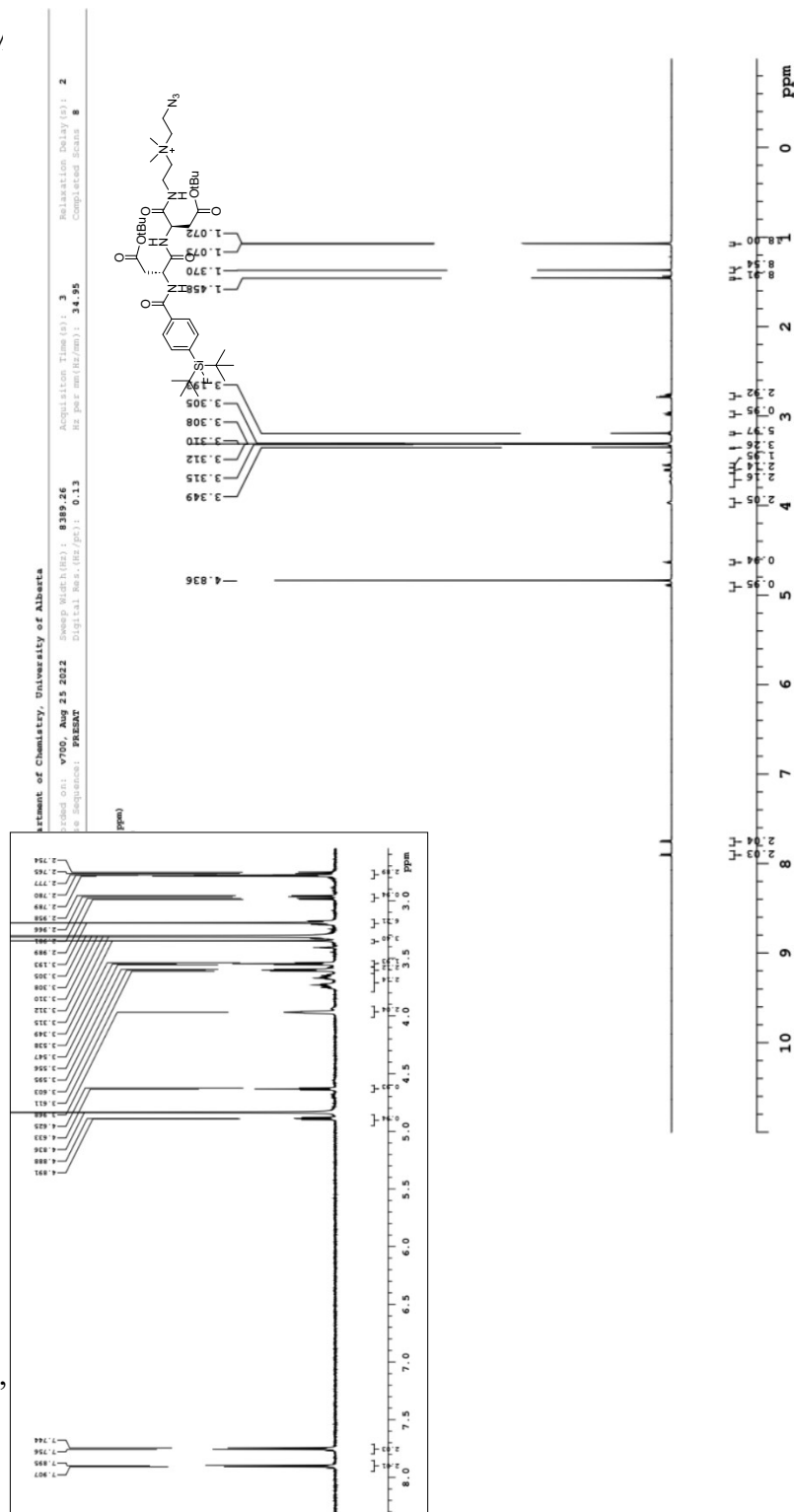


Compound 11, ^1H NMR



[illegible]

Compound 12,

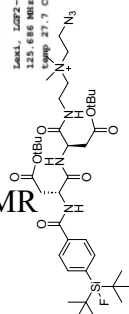


Compound 14, ¹H NMR

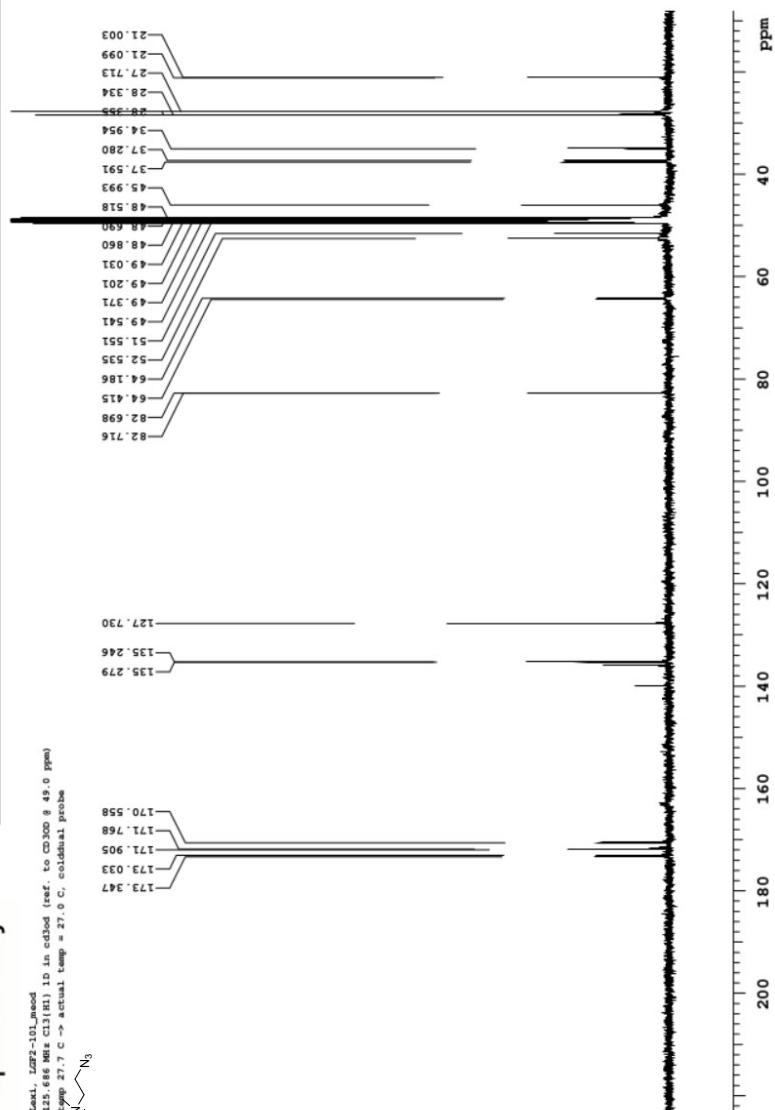
Department of Chemistry, University of Alberta

OpenVnmrJ

1x41, 1272-101_msd
125.686 MHz CHCl₃ 1D in cdh3d (ref. to CDCl₃ @ 49.0 ppm)
Temp: 27.7 C → actual temp = 27.0 C; external probe



Recorded on: 1550, Mar 14 2024 Sweep Width(Hz): 33793.8 Acquisition Time(s): 1 Relaxation Delay(s): 1
Pulse Sequence: szpul Digital Res.(Hz/ppm): 0.26 Hz per ms(Hz/ms): 112.61 Completed Scans: 512

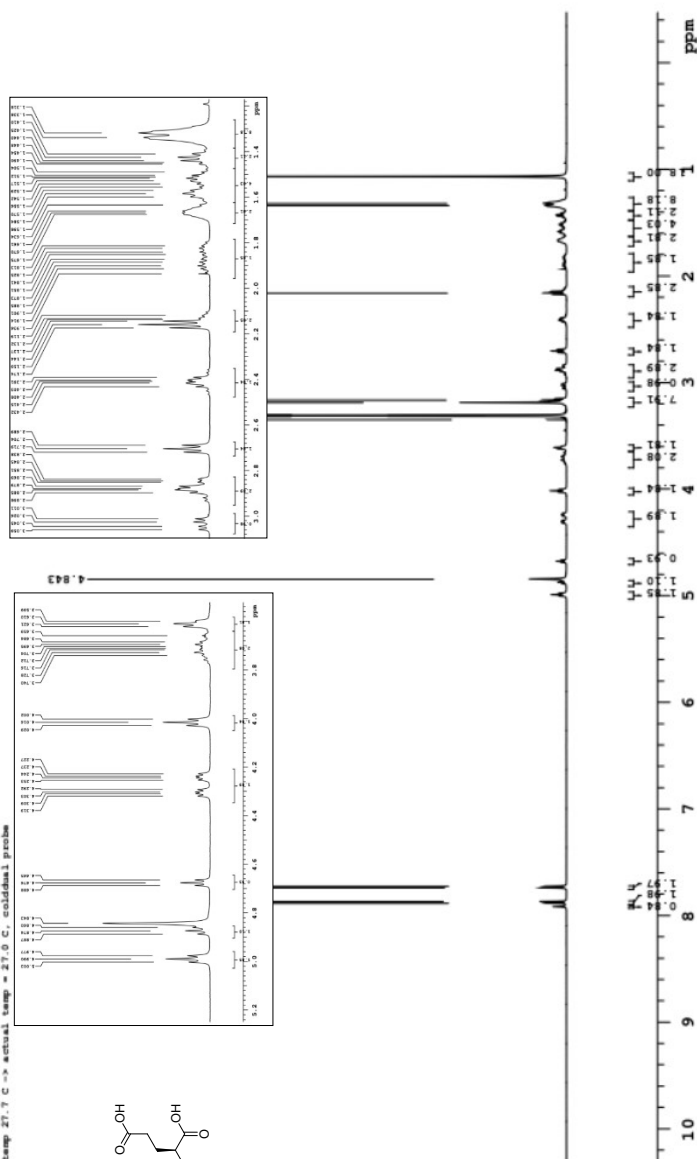


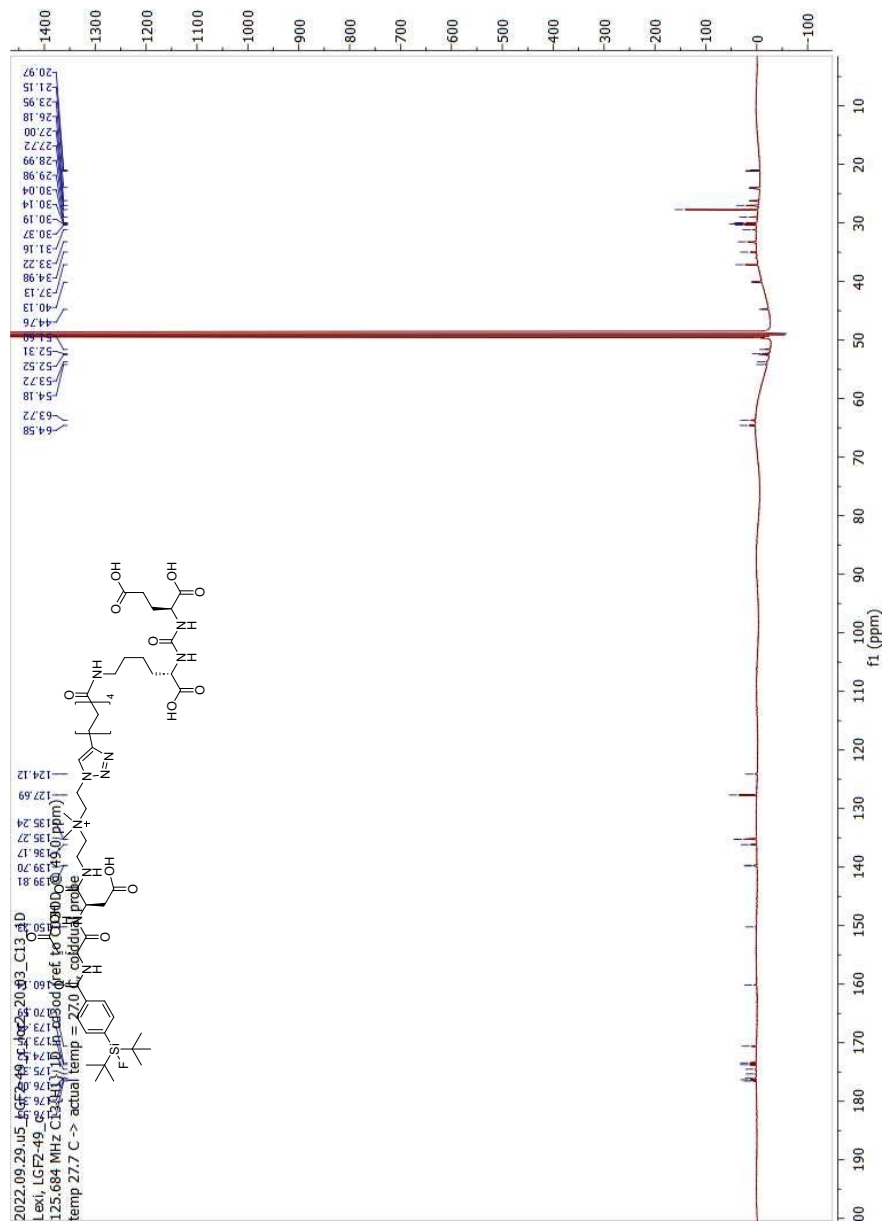
[illegible]

Department of Chemistry, University of Alberta

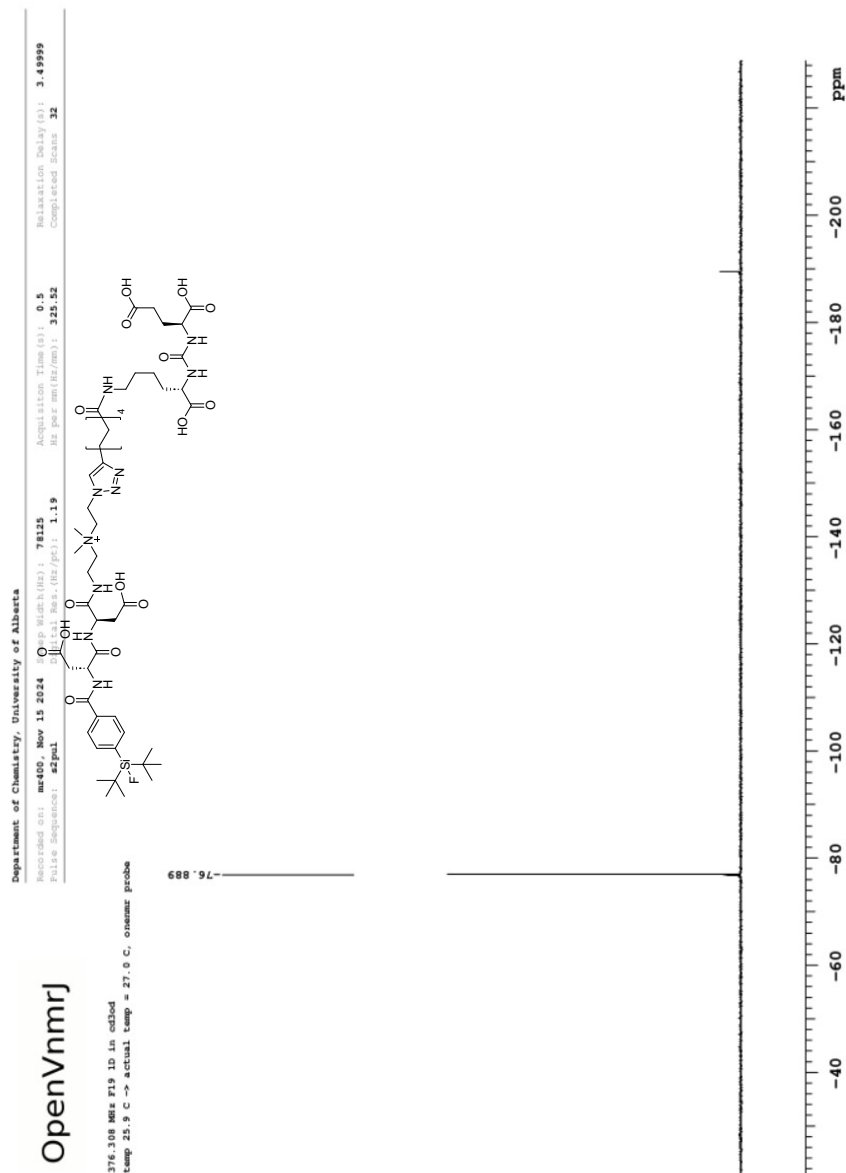
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Recorded on: 05/09, Sep 26 2022      Jump Width (Hz): 6009.62      Acquisition Time (s): 3      Relaxation Delay (s): 2
D 3.1 Hz: 0.09                      Fix per cent (Hz/ms): 22.43      Completed: 8
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Lexi, Ig22-49
499.769 MHz H1 ID in cd3od (ref. to CD3OD @ 3.30 ppm)
temp 27.7 C -> actual temp = 27.0 C, coldwall probe

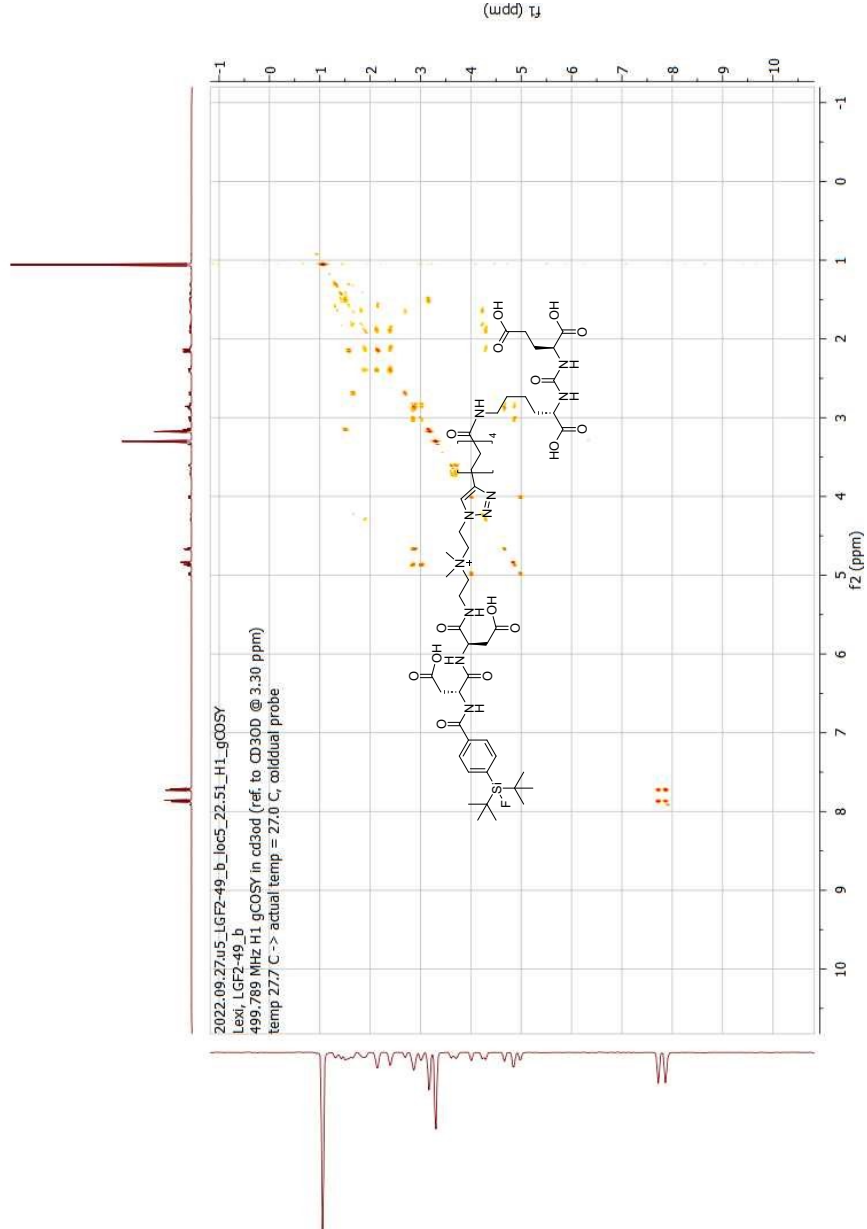




Compound 14, ¹⁹F NMR



Compound 14, COSY:



Compound 14, HSQC:

