

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
 Data File : BF129483.D
 Acq On : 01 Aug 2022 20:28
 Operator : CG\JU
 Sample : N3976-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP1-0729

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129483.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.104	476	479	489	rVB	237470	284800	6.67%	0.968%
2	5.516	545	549	552	rBV	4401712	3846547	90.15%	13.072%
3	6.522	716	720	723	rBV	3949239	3954142	92.67%	13.437%
4	6.875	776	780	783	rBV	1289729	1013133	23.74%	3.443%
5	7.440	871	876	879	rBV	2829090	2525193	59.18%	8.581%
6	8.157	994	998	1001	rBV	1620824	1315809	30.84%	4.472%
7	9.234	1176	1181	1184	rBV	4707528	4266845	100.00%	14.500%
8	9.492	1221	1225	1229	rBV	76572	62666	1.47%	0.213%
9	9.910	1292	1296	1300	rBV	1475586	1297757	30.41%	4.410%
10	10.704	1427	1431	1435	rBV	2107273	1749581	41.00%	5.946%
11	11.404	1546	1550	1553	rBV	1042019	973442	22.81%	3.308%
12	11.780	1611	1614	1620	rVB	146299	114461	2.68%	0.389%
13	12.439	1722	1726	1732	rBV2	73326	126295	2.96%	0.429%
14	12.486	1732	1734	1742	rVB2	139822	116546	2.73%	0.396%
15	12.575	1746	1749	1752	rVB	75626	66737	1.56%	0.227%
16	12.633	1753	1759	1762	rBV2	87998	77606	1.82%	0.264%
17	12.986	1815	1819	1822	rBV	2931596	2469053	57.87%	8.391%
18	13.639	1910	1930	1932	rBV4	743932	3032941	71.08%	10.307%
19	13.874	1967	1970	1981	rVB2	110471	173739	4.07%	0.590%
20	14.045	1995	1999	2003	rBV	975877	860113	20.16%	2.923%
21	14.133	2011	2014	2018	rVB	45385	45159	1.06%	0.153%
22	15.527	2246	2251	2259	rVB2	835842	1053702	24.70%	3.581%

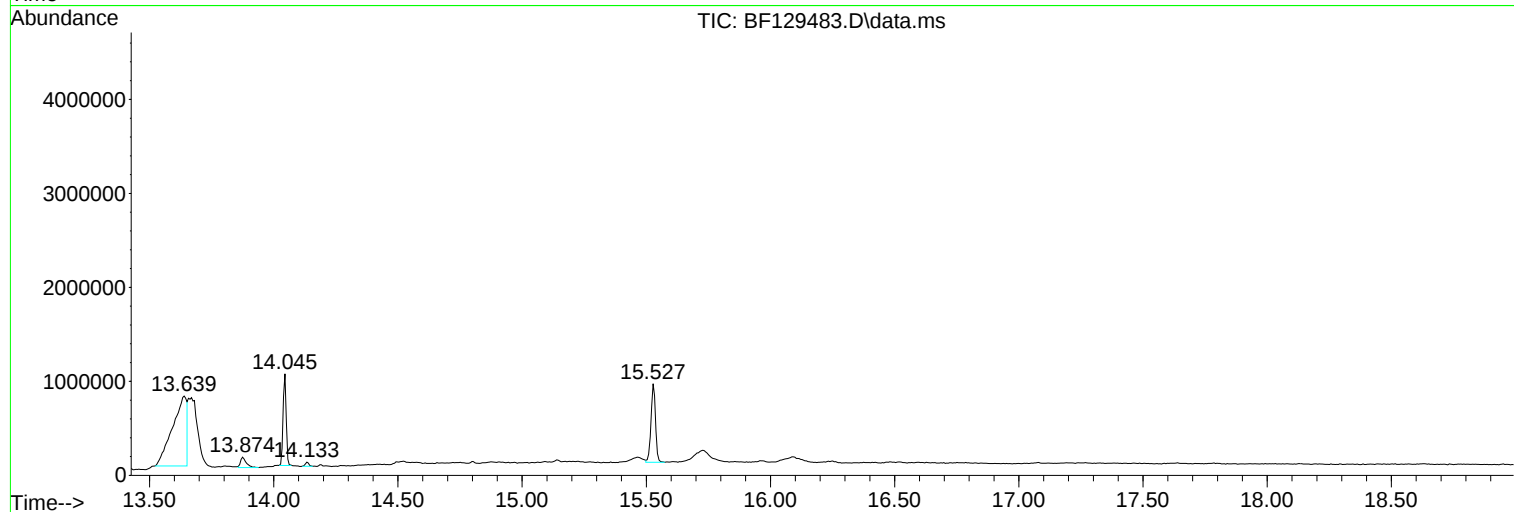
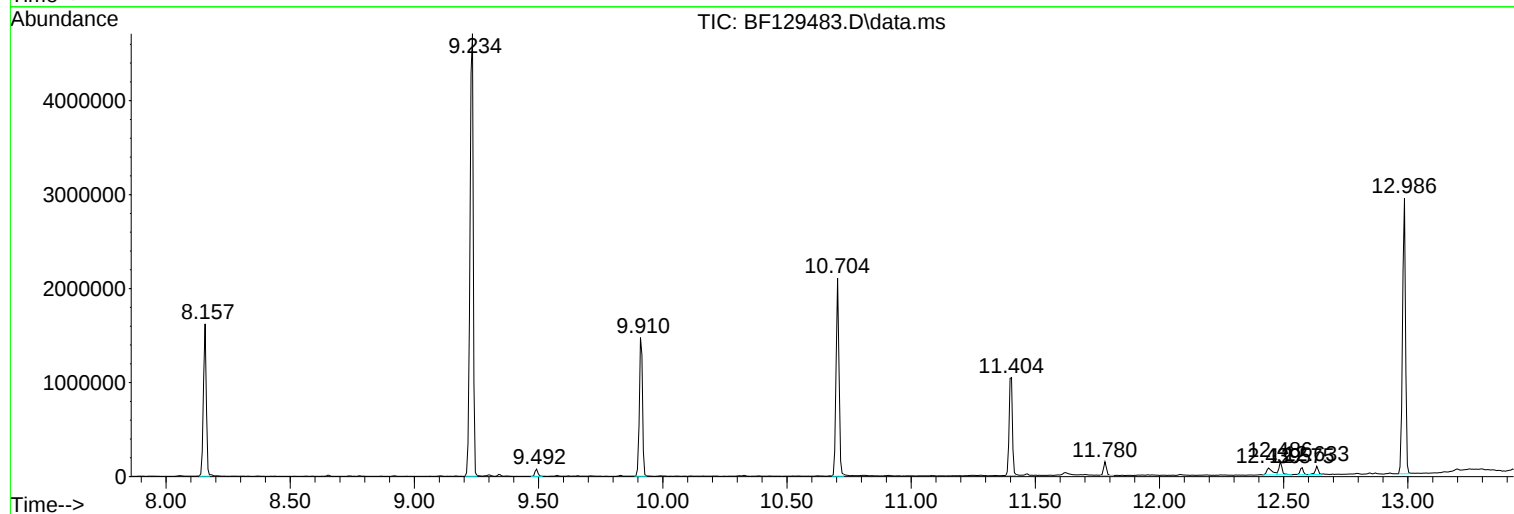
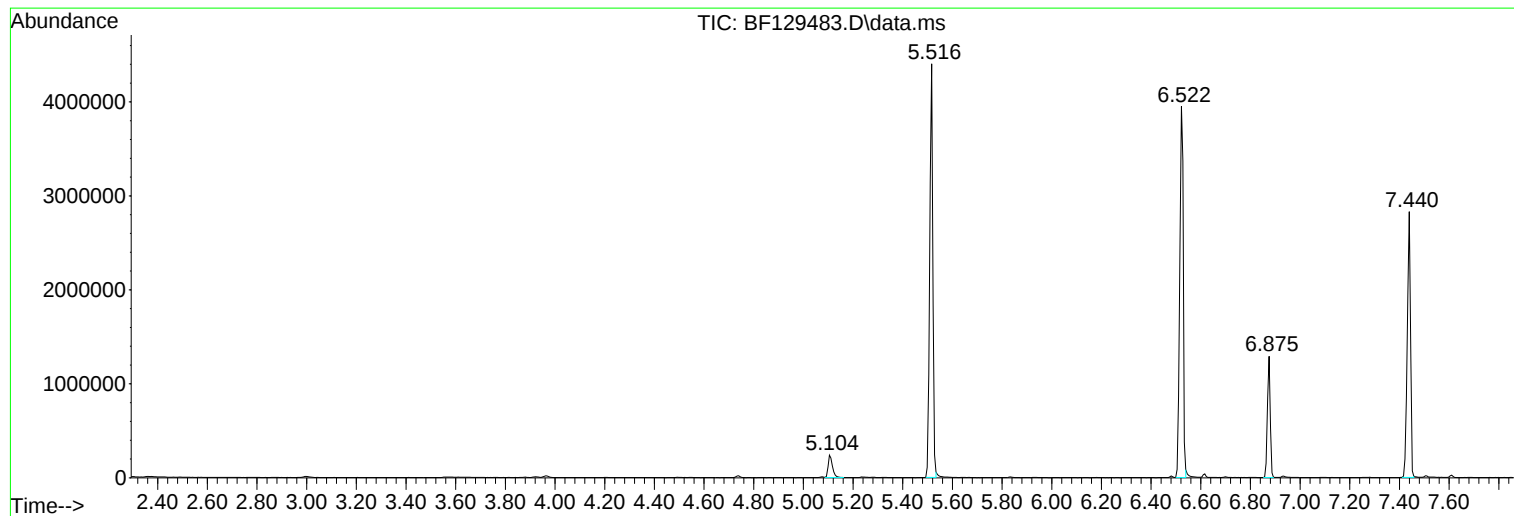
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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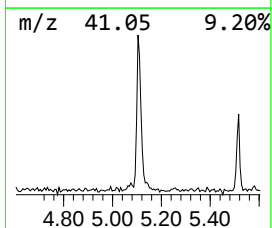
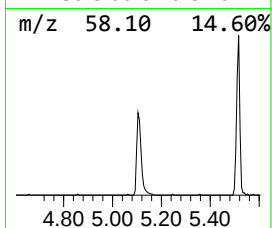
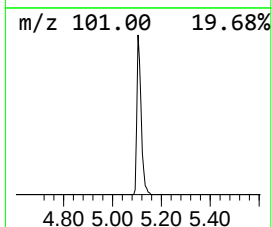
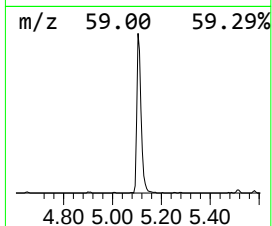
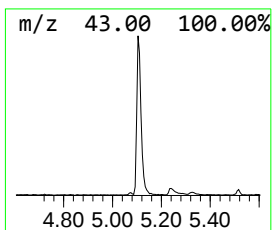
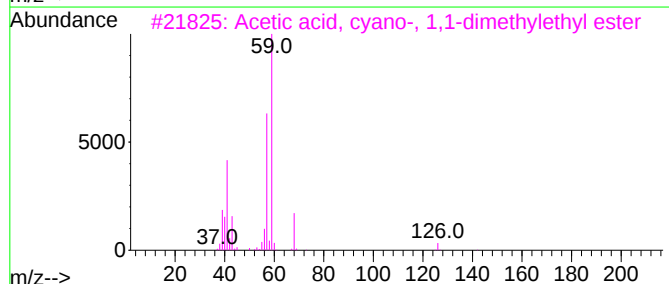
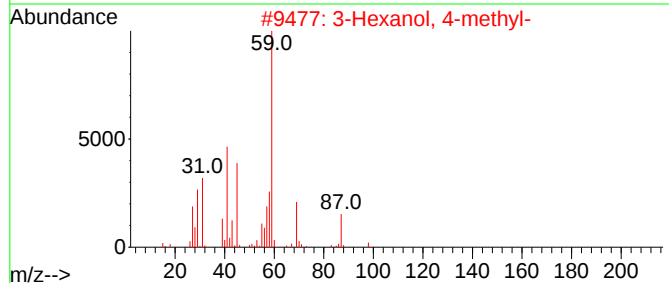
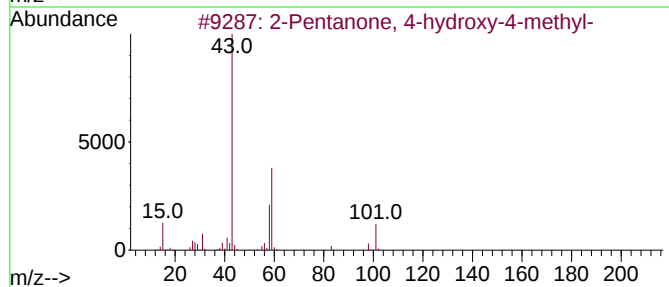
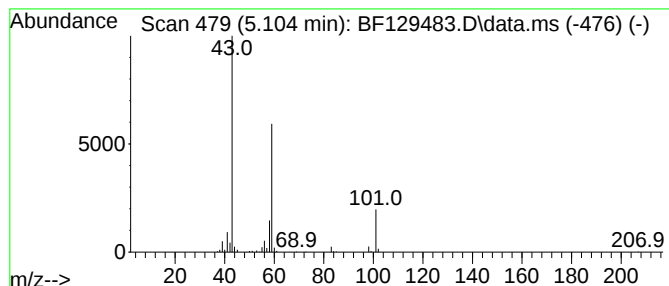
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.62 ng	284800	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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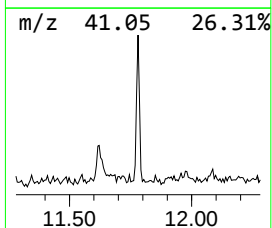
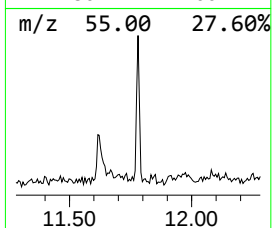
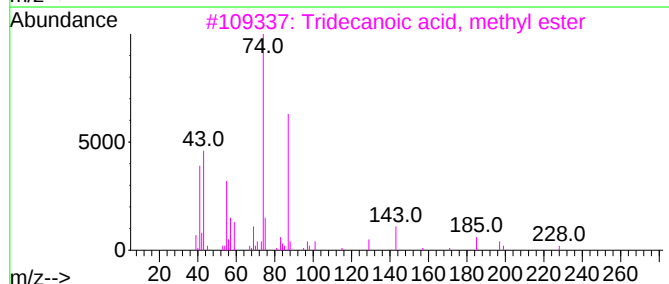
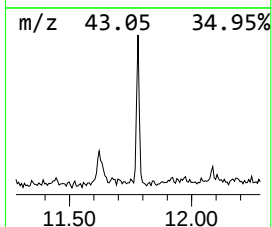
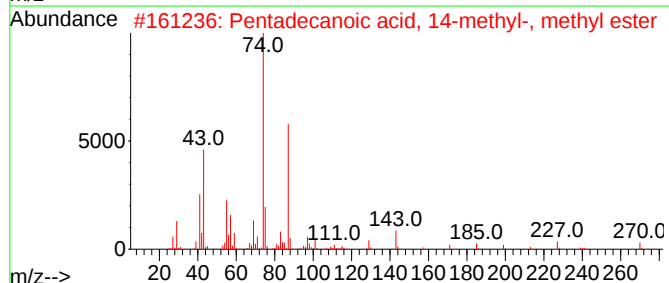
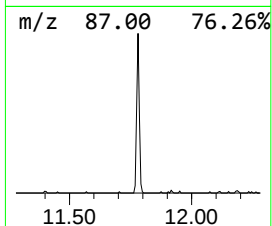
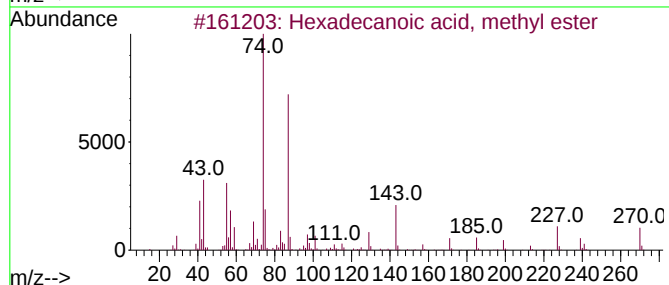
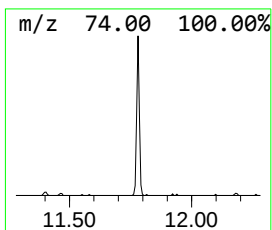
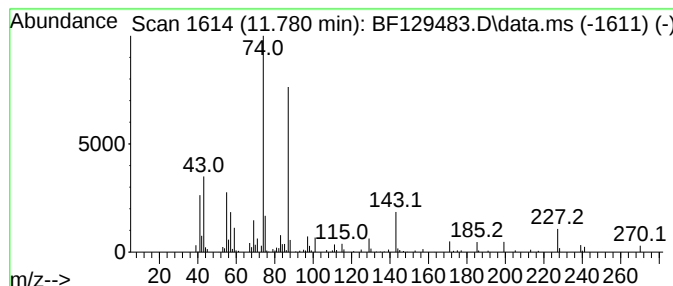
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.781	2.35 ng	114461	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



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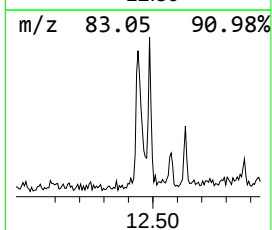
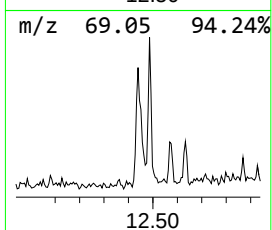
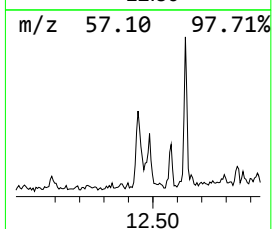
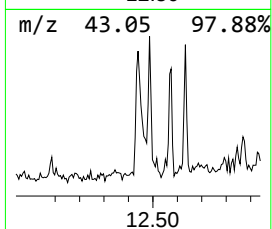
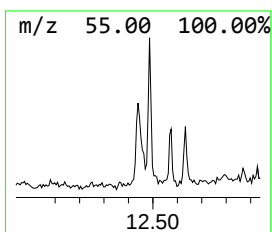
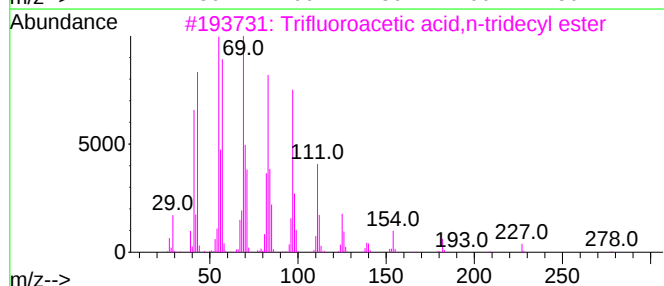
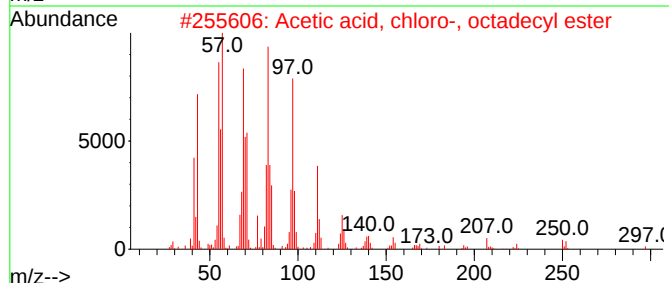
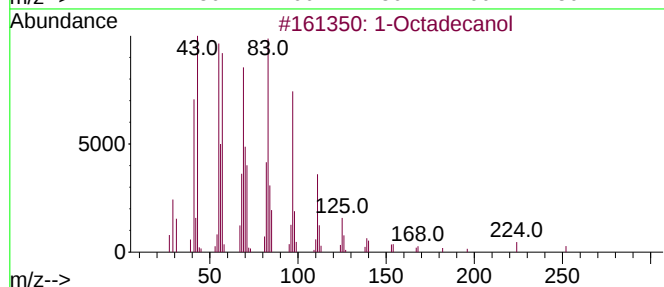
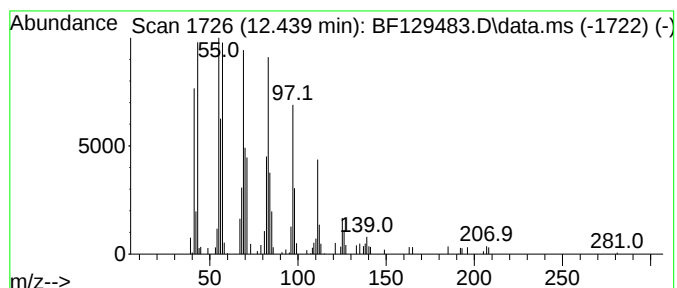
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Octadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.439	2.59 ng	126295	Phenanthrene-d10	11.404

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecanol	270	C18H38O	000112-92-5	95
2		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	94
3		Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	91
4		n-Pentadecanol	228	C15H32O	000629-76-5	91
5		Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	91



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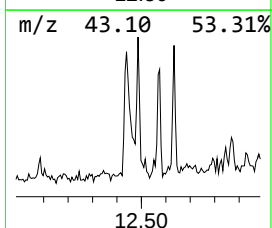
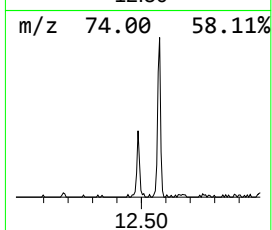
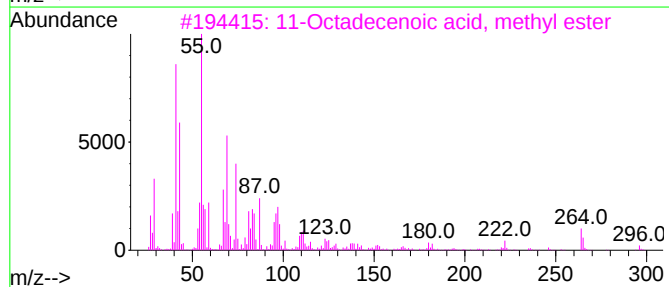
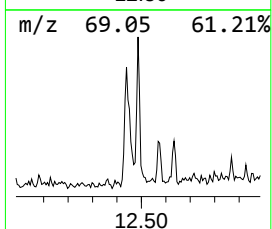
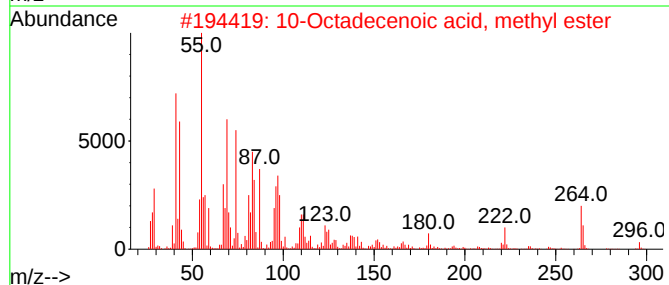
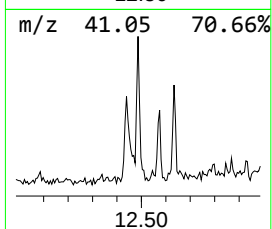
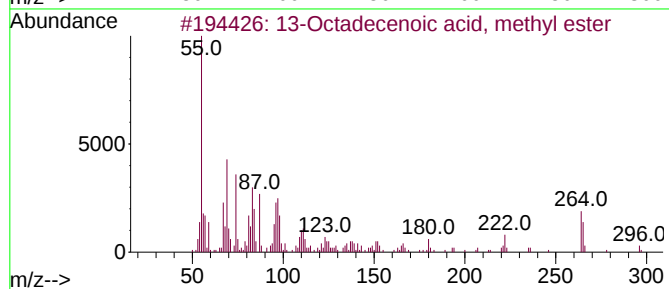
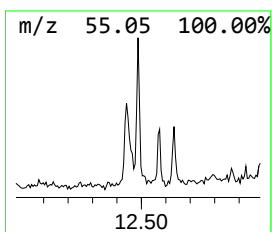
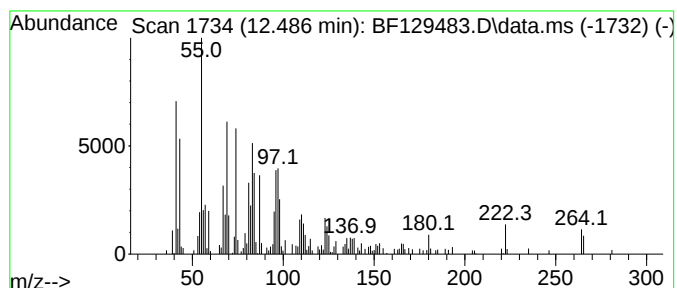
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Peak Number 4 13-Octadecenoic acid, methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.486	2.39 ng	116546	Phenanthrene-d10	11.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	87
4	(Z)-Methyl hexadec-11-enoate	268	C17H32O2	000822-05-9	87
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87



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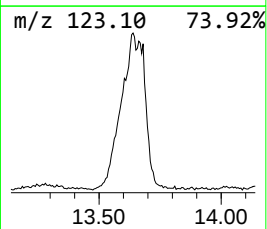
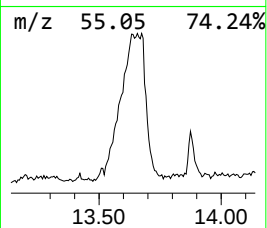
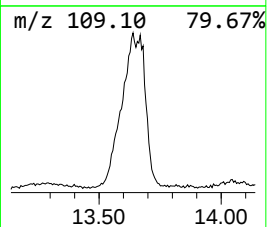
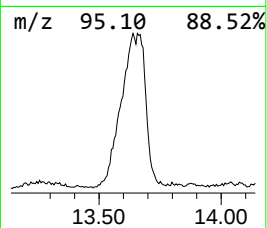
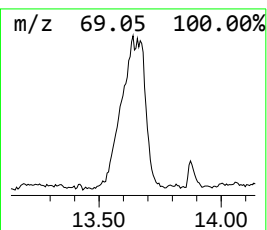
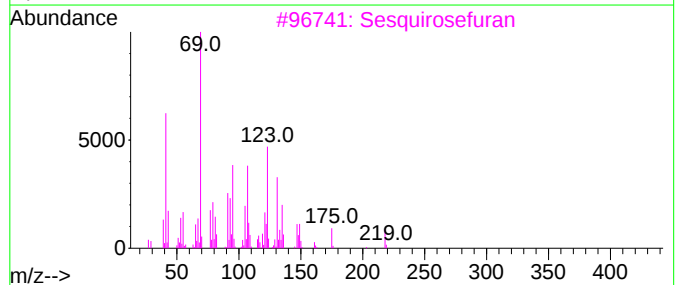
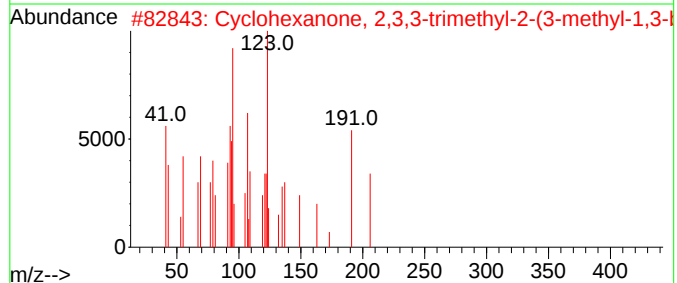
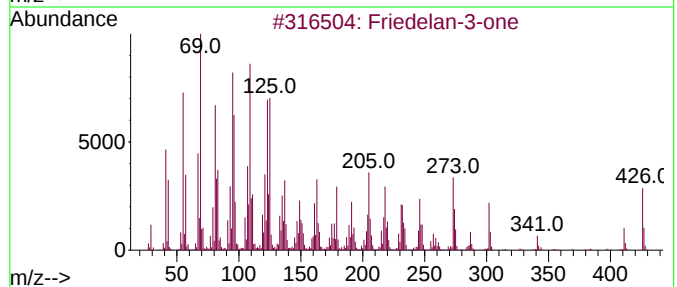
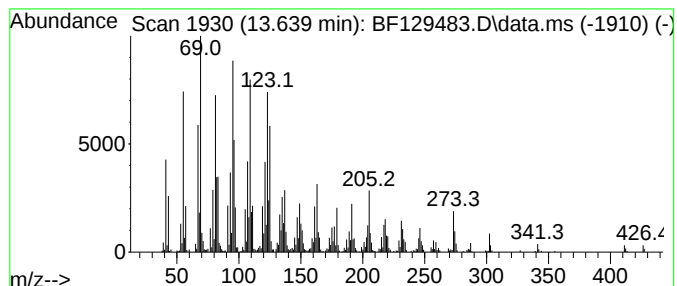
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Friedelan-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	70.52 ng	3032940	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	94
2			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	64
3			Sesquirosefuran	218	C15H22O	039007-93-7	59
4			3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	51
5			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	49



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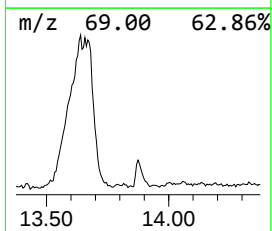
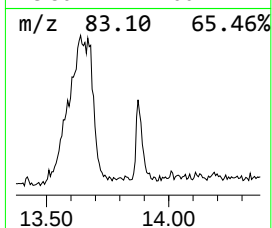
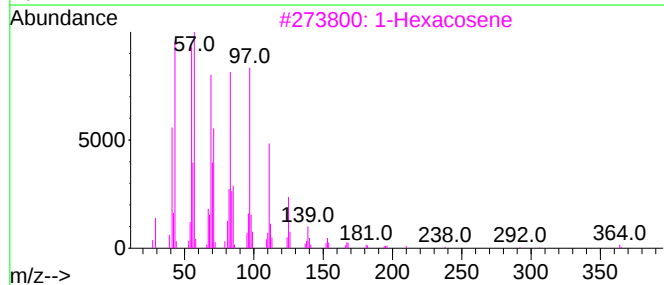
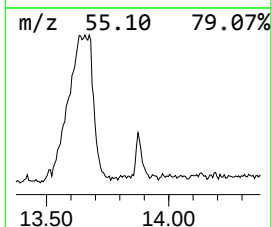
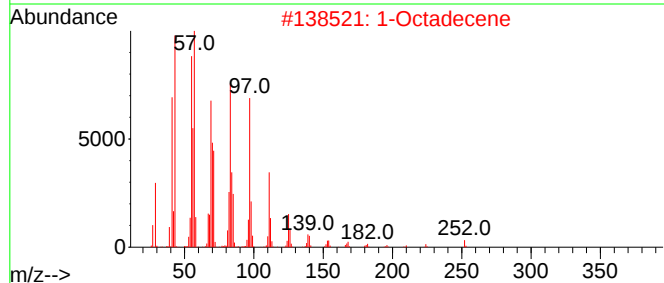
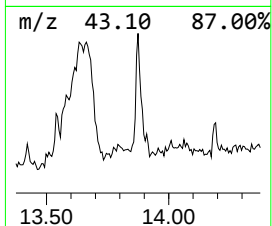
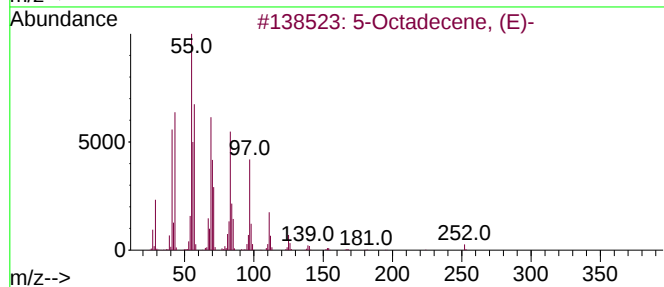
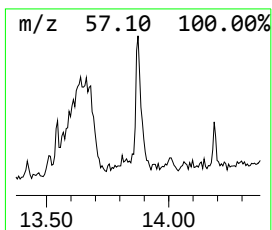
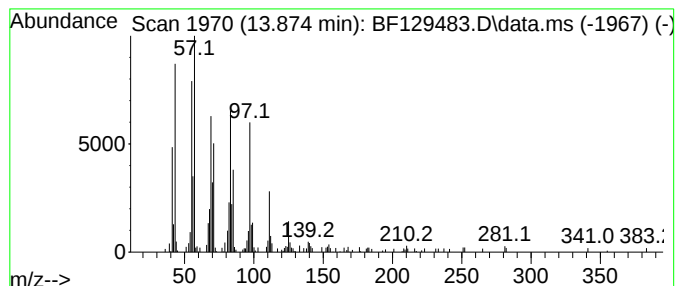
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	4.04 ng	173739	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2			1-Octadecene	252	C18H36	000112-88-9	94
3			1-Hexacosene	364	C26H52	018835-33-1	93
4			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	93
5			3-Octadecene, (E)-	252	C18H36	007206-19-1	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129483.D
Acq On : 01 Aug 2022 20:28
Operator : CG\JU
Sample : N3976-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0729

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.104	5.6	ng	284800	1	6.875	1013130	20.0
Hexadecanoic ac...	11.781	2.4	ng	114461	4	11.404	973442	20.0
1-Octadecanol	12.439	2.6	ng	126295	4	11.404	973442	20.0
13-Octadecenoic...	12.486	2.4	ng	116546	4	11.404	973442	20.0
Friedelan-3-one	13.639	70.5	ng	3032940	5	14.045	860113	20.0
5-Octadecene, (E)-	13.874	4.0	ng	173739	5	14.045	860113	20.0