

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
 Data File : BF135017.D
 Acq On : 30 Aug 2023 22:06
 Operator : CG\JU
 Sample : 04197-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-309-OK-370-COMP-20

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135017.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	8	12	18	rVB	41730	56275	2.00%	0.258%
2	5.004	492	496	503	rVB	86159	97367	3.47%	0.446%
3	5.404	559	564	567	rBV	2815343	2511796	89.43%	11.503%
4	6.410	730	735	738	rBV	2613461	2477078	88.20%	11.344%
5	6.598	764	767	779	rBV	125542	121352	4.32%	0.556%
6	6.769	792	796	800	rBV	1103591	876279	31.20%	4.013%
7	7.334	886	892	895	rBV	1698372	1596275	56.84%	7.310%
8	8.051	1009	1014	1017	rBV	1303941	1172017	41.73%	5.367%
9	9.128	1192	1197	1200	rBV	3073753	2808580	100.00%	12.862%
10	9.245	1213	1217	1221	rBV	300124	287108	10.22%	1.315%
11	9.398	1240	1243	1247	rVB2	29463	29461	1.05%	0.135%
12	9.804	1307	1312	1316	rBV	1341878	1278130	45.51%	5.853%
13	10.016	1342	1348	1356	rBV	23649	36062	1.28%	0.165%
14	10.598	1441	1447	1450	rBV	1922318	1684960	59.99%	7.716%
15	11.298	1562	1566	1569	rBV	1485109	1242562	44.24%	5.690%
16	11.322	1569	1570	1573	rVB	151080	89613	3.19%	0.410%
17	11.704	1632	1635	1639	rVB	43629	34809	1.24%	0.159%
18	11.839	1653	1658	1668	rVB	547156	587305	20.91%	2.690%
19	12.416	1753	1756	1759	rVB2	57430	46463	1.65%	0.213%
20	12.516	1768	1773	1777	rBV	186065	180478	6.43%	0.827%
21	12.628	1787	1792	1802	rBV2	148633	194406	6.92%	0.890%
22	12.745	1807	1812	1815	rVV	124222	134630	4.79%	0.617%
23	12.898	1834	1838	1841	rBV	2519748	2150027	76.55%	9.846%
24	13.810	1989	1993	2002	rVB2	166359	222162	7.91%	1.017%
25	13.957	2013	2018	2021	rBV	760842	762078	27.13%	3.490%
26	14.439	2097	2100	2107	rVB4	31817	42408	1.51%	0.194%
27	14.821	2162	2165	2170	rVB	63563	60021	2.14%	0.275%
28	14.992	2190	2194	2197	rBV	46107	66165	2.36%	0.303%
29	15.092	2207	2211	2215	rBV4	23244	38696	1.38%	0.177%
30	15.298	2242	2246	2252	rVB	29103	36787	1.31%	0.168%
31	15.357	2252	2256	2260	rBV	35237	50438	1.80%	0.231%
32	15.421	2262	2267	2273	rBV	627106	805321	28.67%	3.688%
33	18.068	2712	2717	2724	rVB	26340	58821	2.09%	0.269%

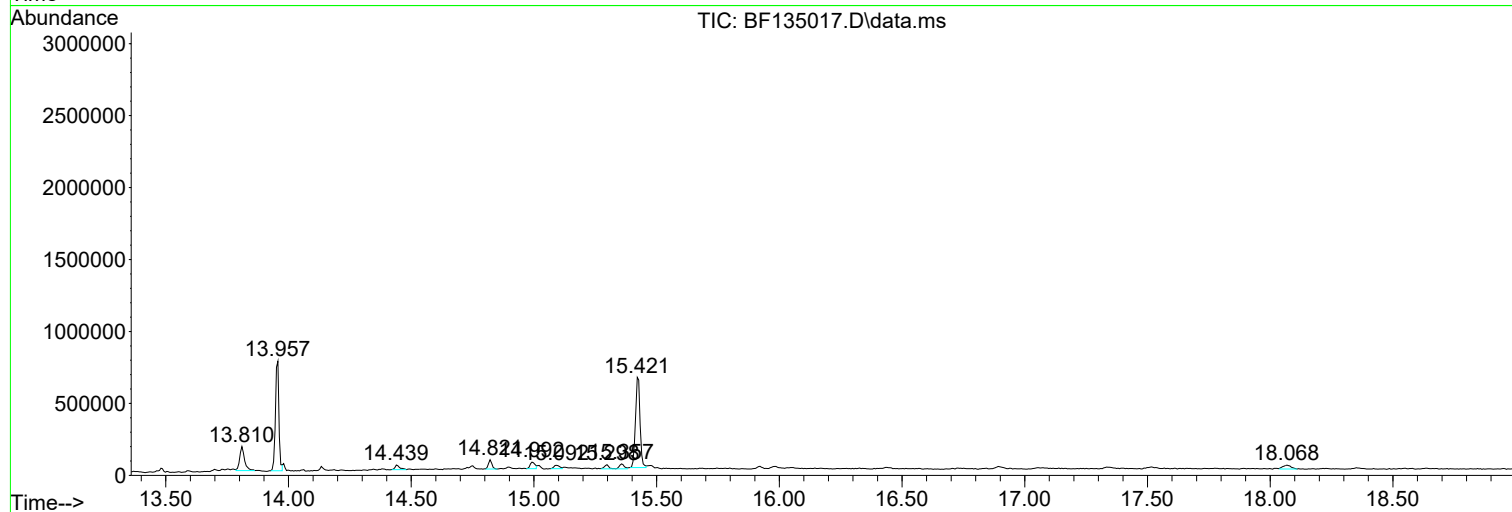
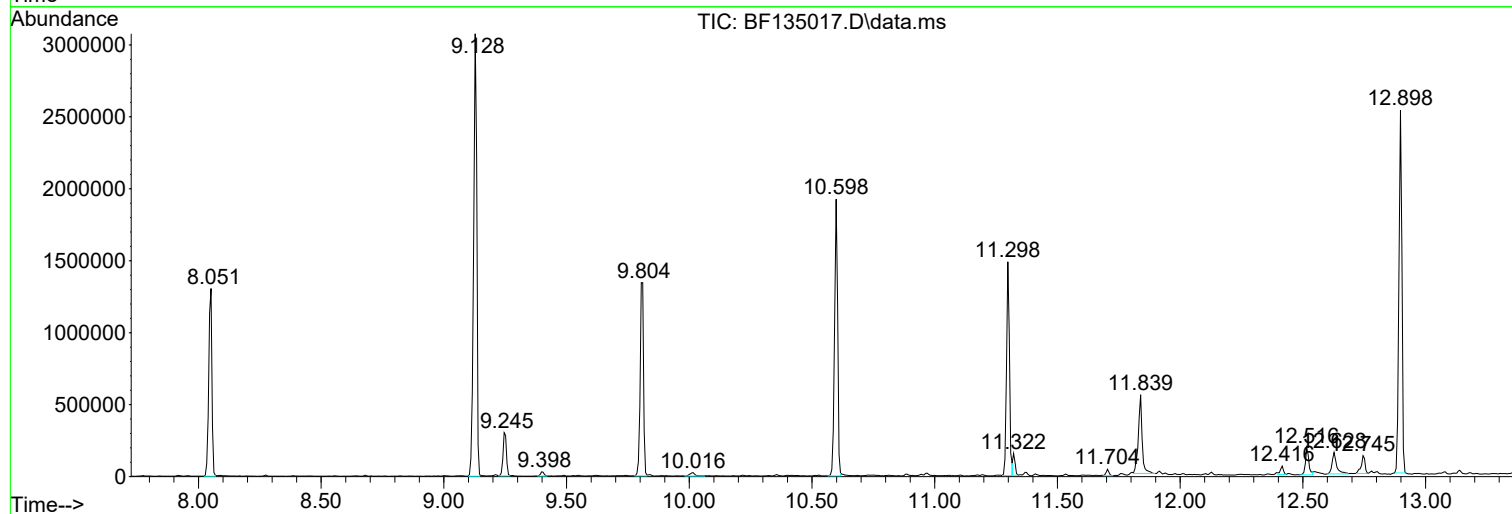
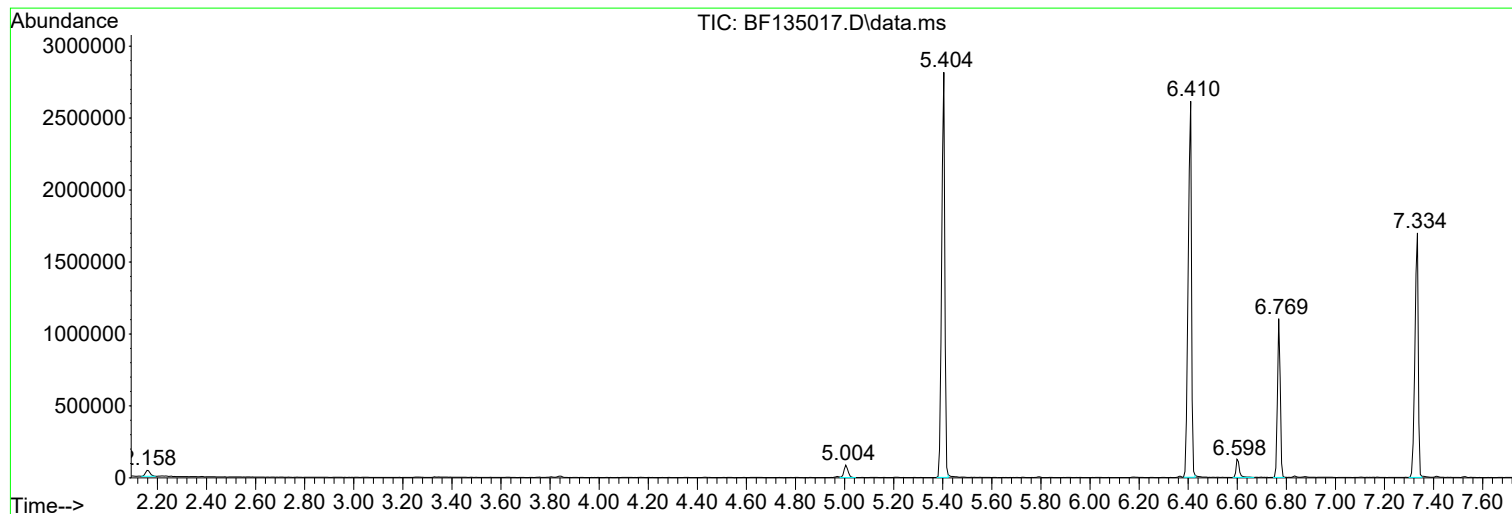
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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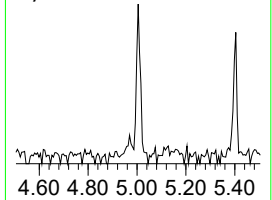
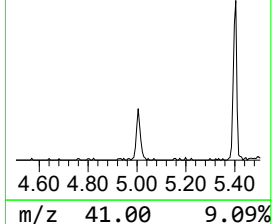
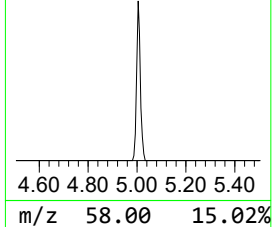
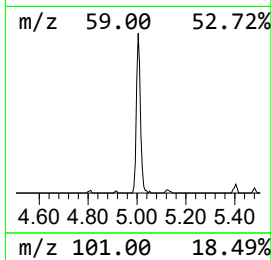
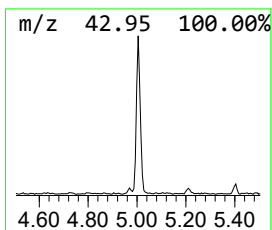
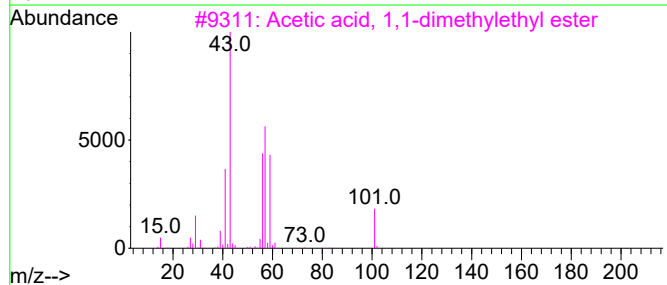
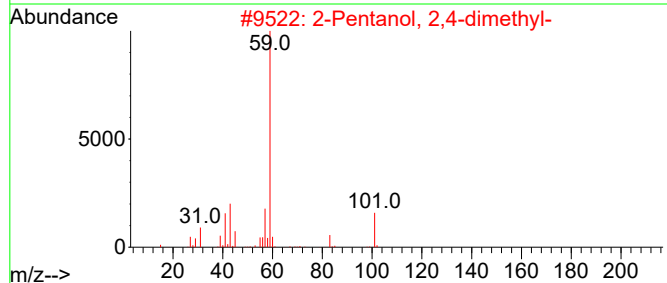
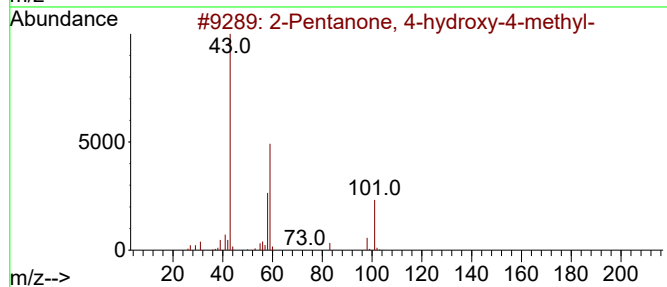
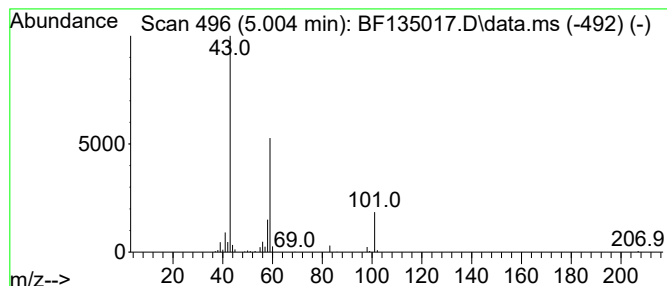
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.22 ng	97367	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	3-Octanol	130	C8H18O	000589-98-0	28		



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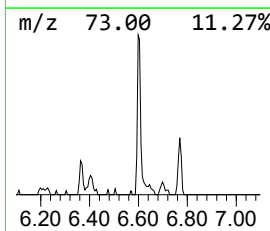
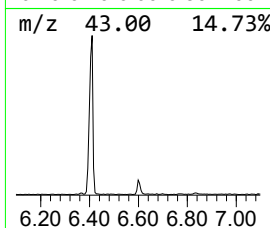
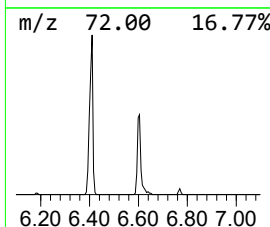
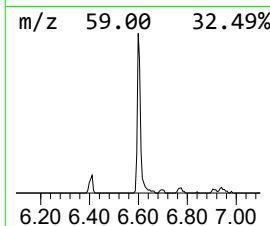
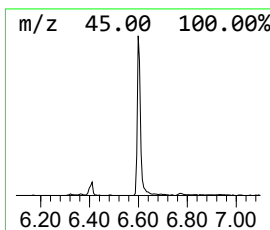
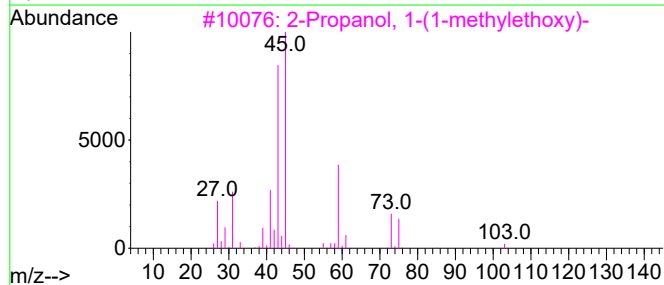
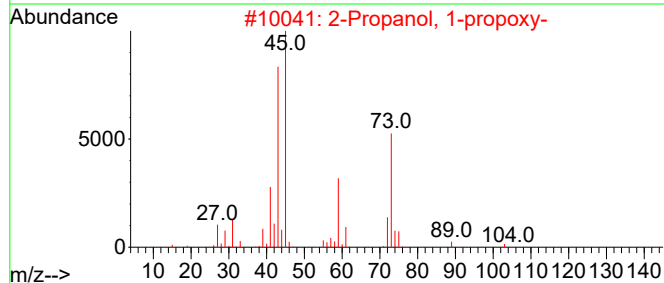
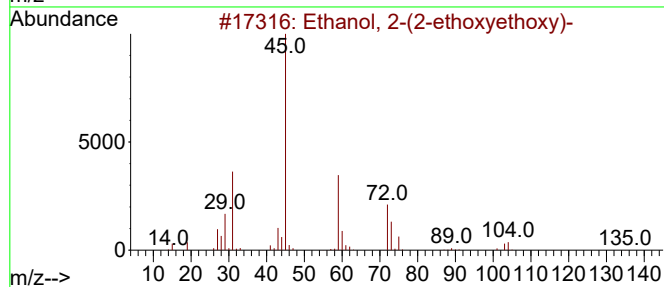
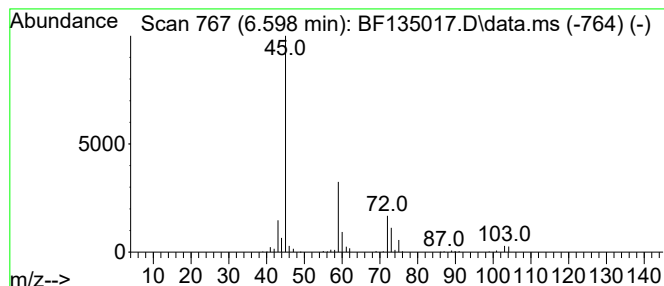
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	2.77 ng	121352	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
4			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	38
5			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	38



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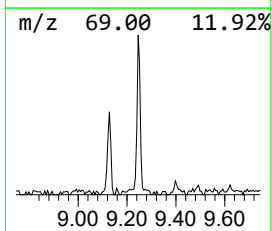
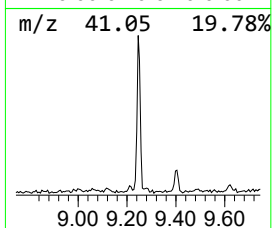
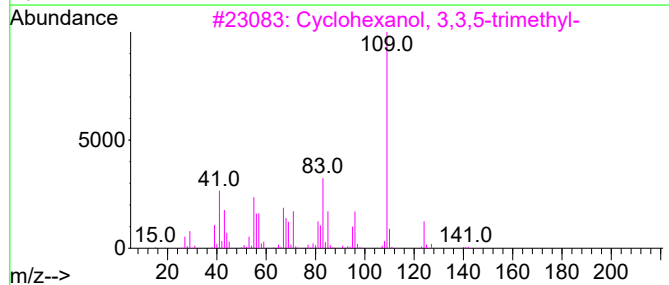
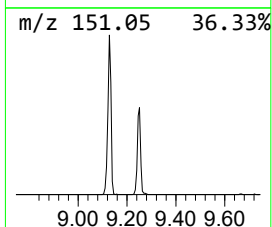
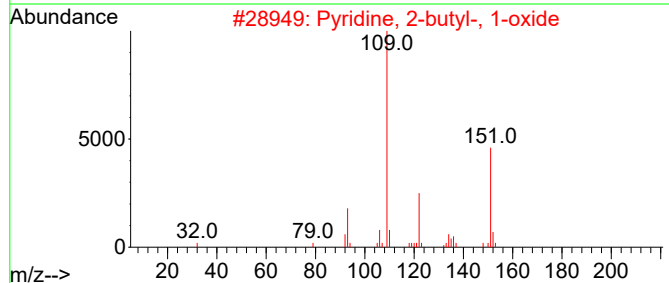
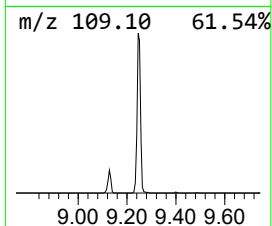
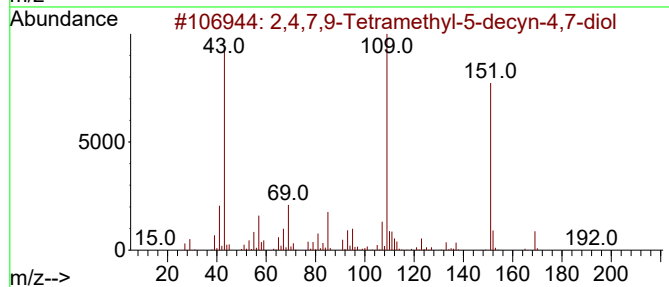
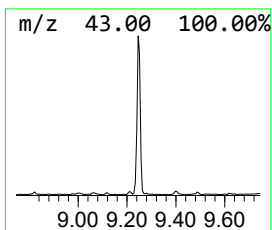
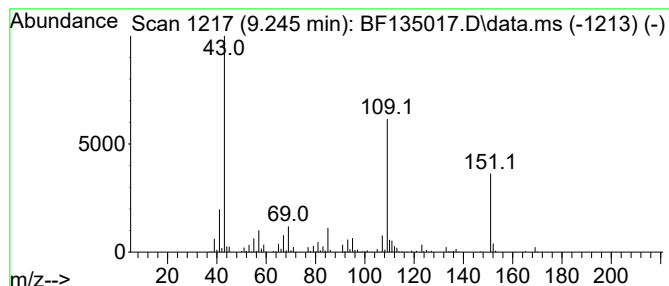
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.245	4.49 ng	287108	Acenaphthene-d10		9.810	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	53
3	Cyclohexanol, 3,3,5-trimethyl-		142	C9H18O	000116-02-9	47
4	3-Pyridinol, 4-methyl-, acetate ...		151	C8H9NO2	001006-96-8	47
5	Metacetamol		151	C8H9NO2	000621-42-1	47



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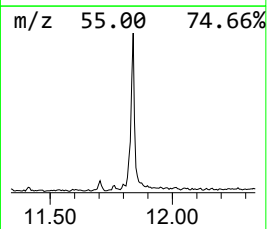
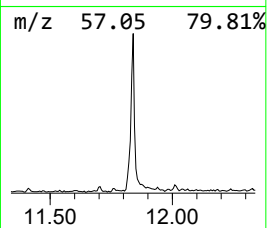
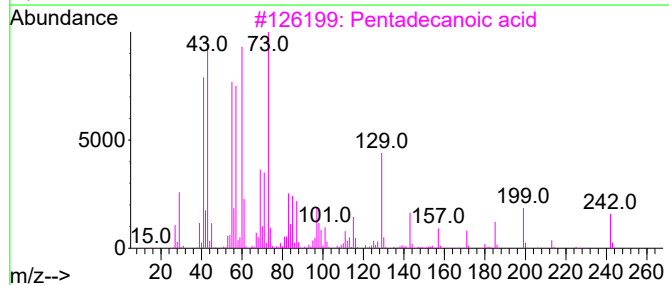
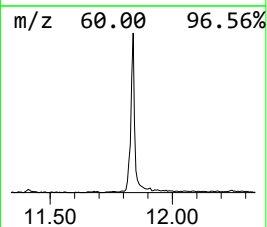
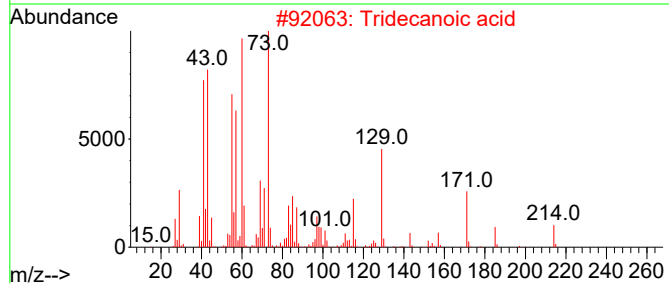
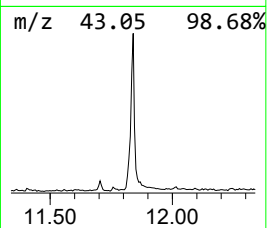
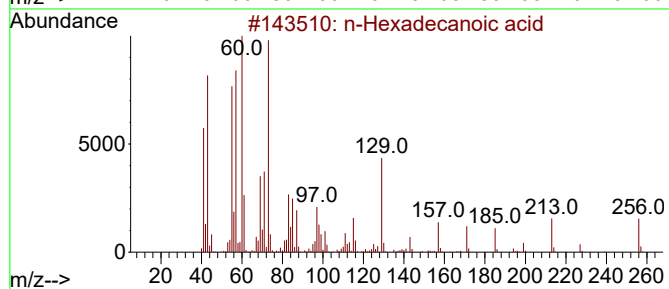
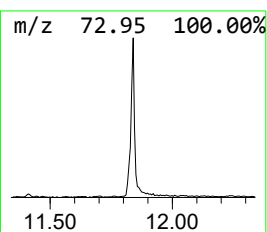
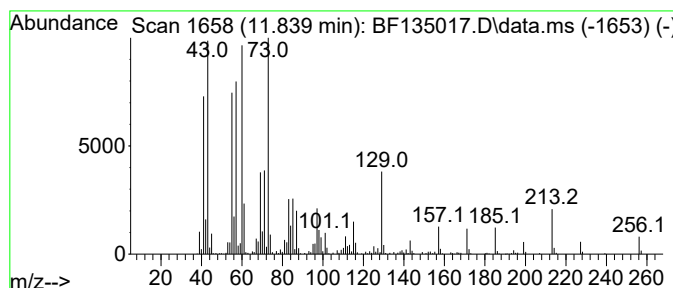
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.839	9.45 ng	587305	Phenanthrene-d10	11.298	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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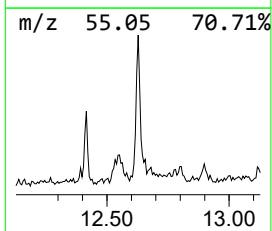
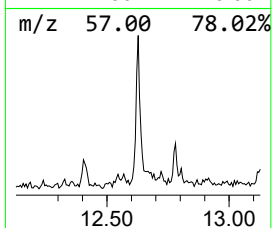
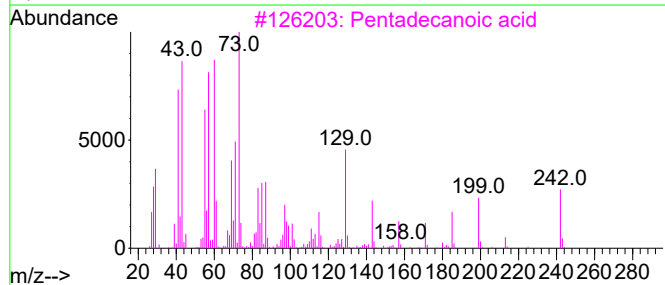
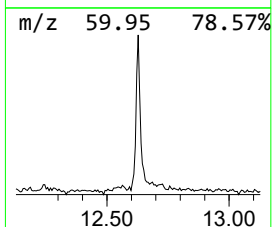
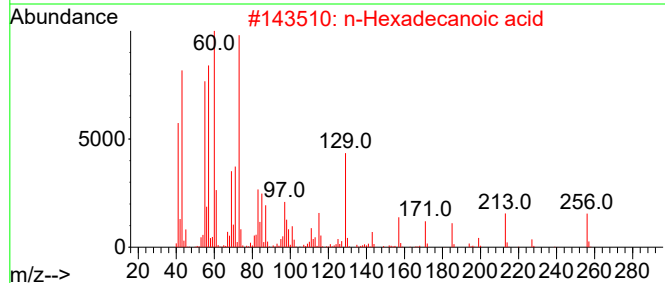
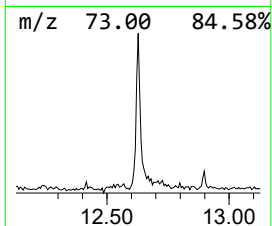
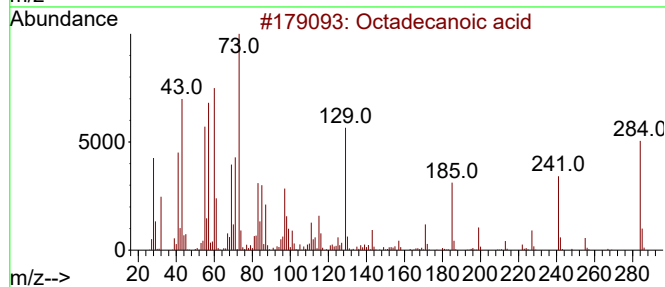
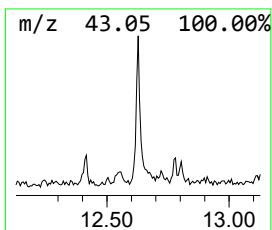
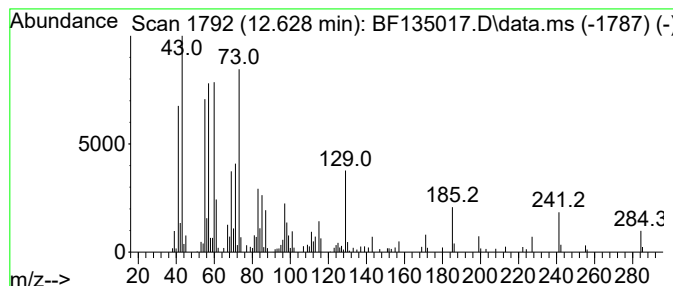
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.628	5.10 ng	194406	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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ClientSampleId :
OR-309-OK-370-COMP-20

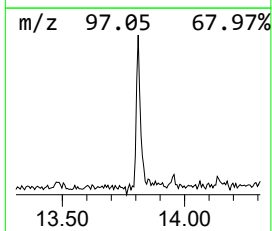
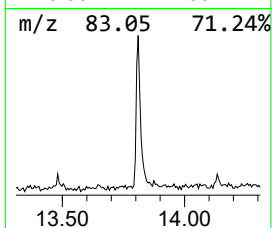
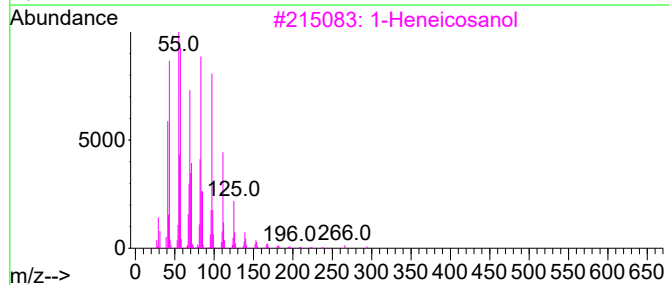
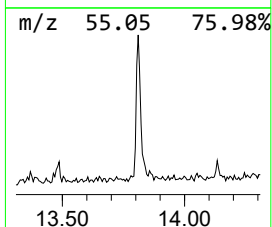
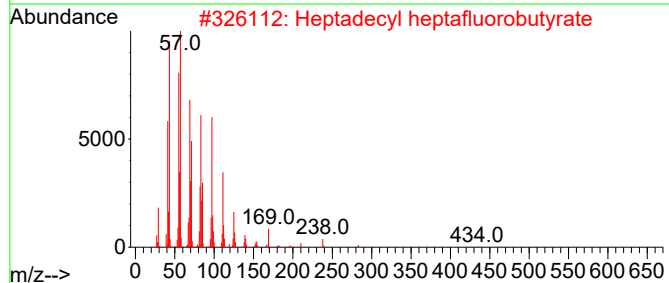
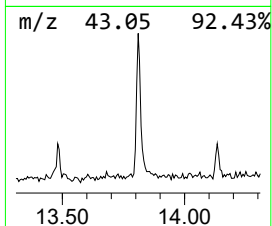
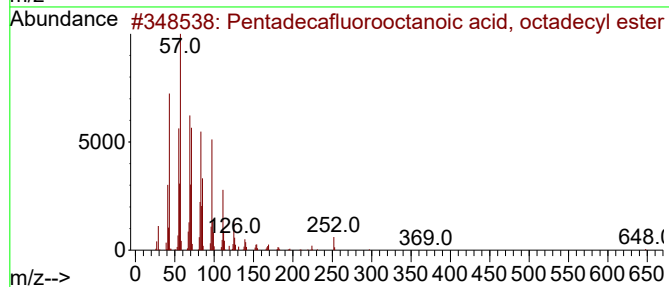
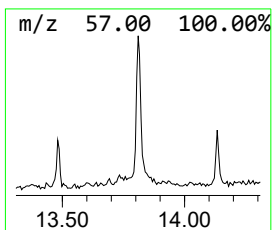
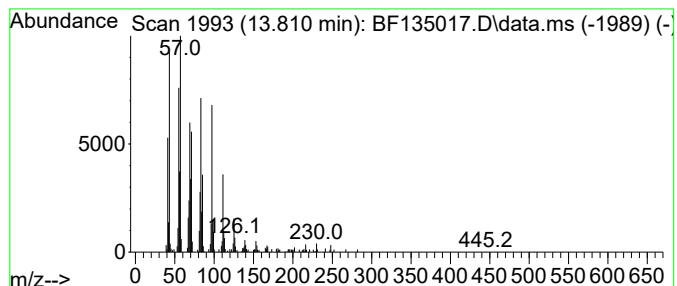
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	5.83 ng	222162	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			1-Hexacosene	364	C26H52	018835-33-1	93
5			Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135017.D
Acq On : 30 Aug 2023 22:06
Operator : CG\JU
Sample : 04197-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-309-OK-370-COMP-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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-...	5.004	2.2	ng	97367	1	6.769	876279	20.0
Ethanol, 2-(2-e...	6.598	2.8	ng	121352	1	6.769	876279	20.0
2,4,7,9-Tetrame...	9.245	4.5	ng	287108	3	9.810	1278130	20.0
n-Hexadecanoic ...	11.839	9.4	ng	587305	4	11.298	1242560	20.0
Octadecanoic acid	12.628	5.1	ng	194406	5	13.957	762078	20.0
Pentadecafluoro...	13.810	5.8	ng	222162	5	13.957	762078	20.0