

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
 Data File : BF136121.D
 Acq On : 03 Nov 2023 13:38
 Operator : CG\JU
 Sample : 05143-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-1

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-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136121.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	29	34	42	rVB	51711	71811	3.51%	0.584%
2	2.910	133	140	147	rVB2	45334	76535	3.74%	0.623%
3	4.416	392	396	402	rVB	33235	39548	1.93%	0.322%
4	5.034	497	501	506	rVB	92152	93309	4.56%	0.759%
5	5.440	566	570	574	rBV	572728	479087	23.43%	3.897%
6	6.410	727	735	737	rBV2	17744	23239	1.14%	0.189%
7	6.440	737	740	749	rVB	425344	342081	16.73%	2.783%
8	6.645	772	775	785	rBV	75948	83250	4.07%	0.677%
9	6.816	801	804	808	rVB	688486	539281	26.37%	4.387%
10	7.381	895	900	903	rBV	1342775	1151691	56.32%	9.369%
11	8.098	1018	1022	1025	rVB	904196	693955	33.93%	5.645%
12	9.175	1201	1205	1208	rBV	2413567	2045036	100.00%	16.636%
13	9.857	1317	1321	1324	rBV	867398	744118	36.39%	6.053%
14	10.057	1351	1355	1361	rBV3	21211	24379	1.19%	0.198%
15	10.569	1439	1442	1446	rBV	133230	107024	5.23%	0.871%
16	10.645	1451	1455	1461	rBV	676853	605012	29.58%	4.922%
17	10.804	1480	1482	1486	rVB	48161	36345	1.78%	0.296%
18	11.204	1546	1550	1552	rBV	37475	38250	1.87%	0.311%
19	11.345	1571	1574	1578	rBV	843723	676747	33.09%	5.505%
20	11.751	1639	1643	1646	rVB	38861	33852	1.66%	0.275%
21	11.892	1661	1667	1688	rBV	549877	606184	29.64%	4.931%
22	12.680	1797	1801	1809	rVB	115960	123187	6.02%	1.002%
23	12.945	1842	1846	1850	rBV	1907898	1674388	81.88%	13.621%
24	13.904	2004	2009	2021	rBV5	97323	375790	18.38%	3.057%
25	14.004	2022	2026	2032	rVB	570349	573158	28.03%	4.663%
26	14.492	2105	2109	2113	rBV	23382	27298	1.33%	0.222%
27	14.592	2121	2126	2129	rBV6	10726	23208	1.13%	0.189%
28	14.651	2133	2136	2141	rVB	30568	34659	1.69%	0.282%
29	14.810	2157	2163	2168	rVB	21406	27194	1.33%	0.221%
30	14.886	2173	2176	2180	rVB	34423	35526	1.74%	0.289%
31	15.157	2218	2222	2228	rVB	27383	36743	1.80%	0.299%
32	15.492	2273	2279	2286	rBV	498982	610847	29.87%	4.969%
33	15.557	2286	2290	2296	rVB2	20014	30262	1.48%	0.246%
34	16.021	2363	2369	2374	rVB3	21191	34835	1.70%	0.283%
35	16.151	2381	2391	2394	rBV7	25076	59381	2.90%	0.483%
36	16.557	2455	2460	2474	rVB6	11952	33873	1.66%	0.276%

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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-BF103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.686	2476	2482	2488	rVV3	20837	38332	1.87%	0.312%
38	16.815	2497	2504	2510	rBV6	20608	43409	2.12%	0.353%

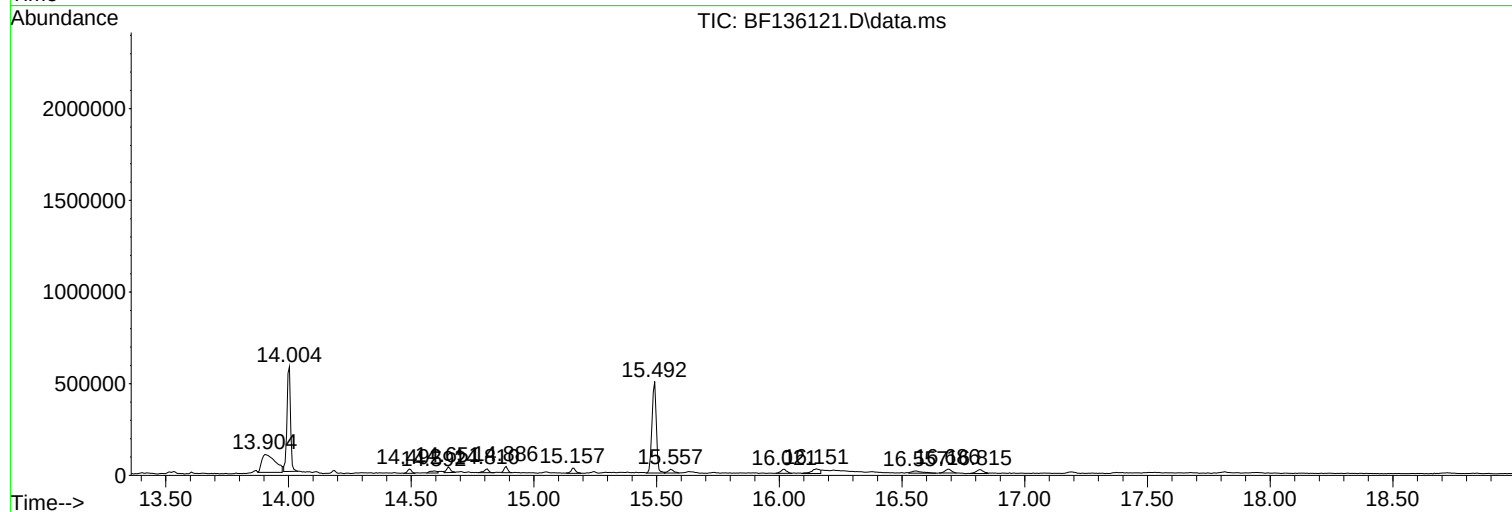
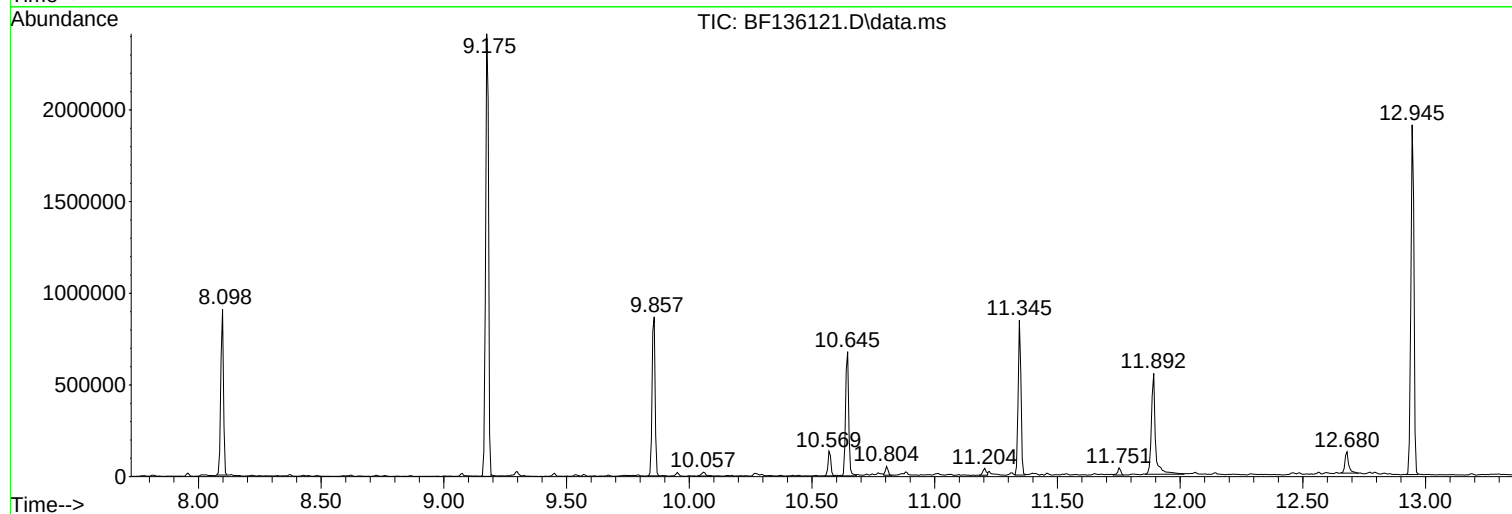
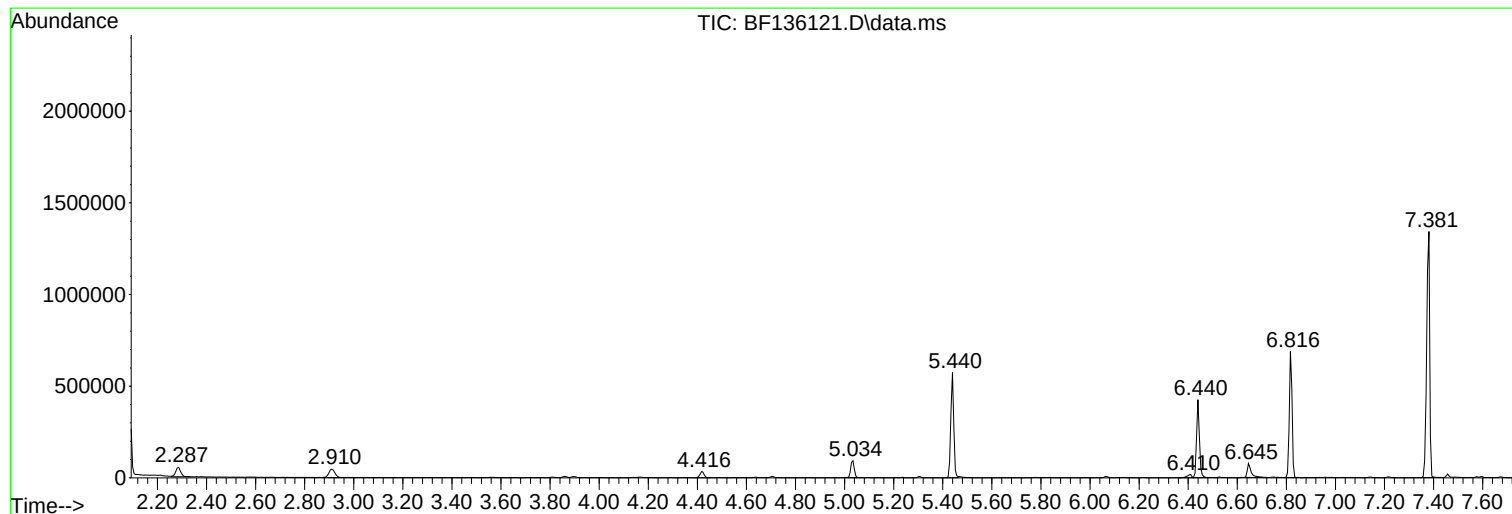
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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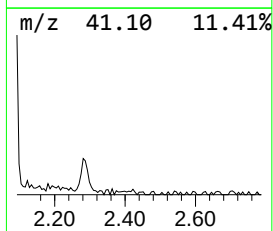
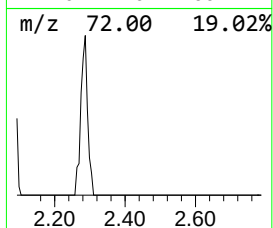
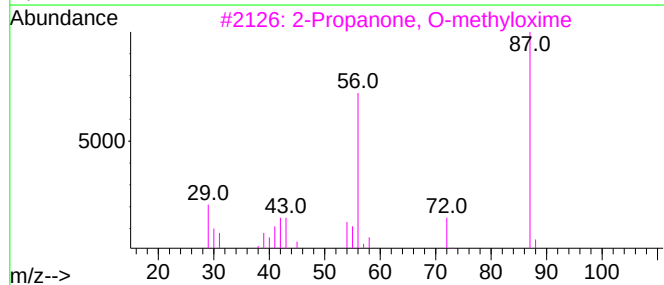
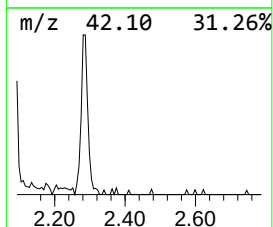
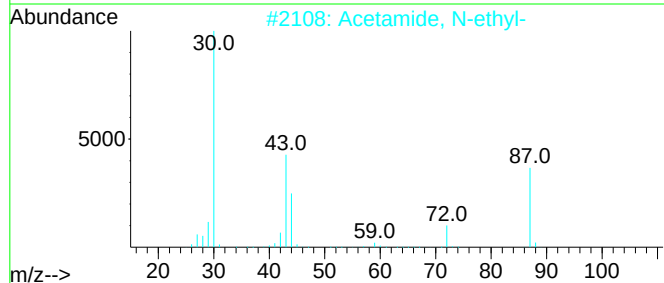
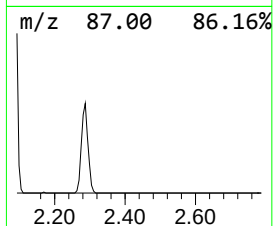
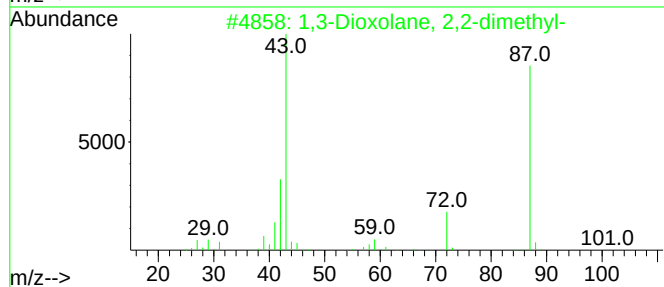
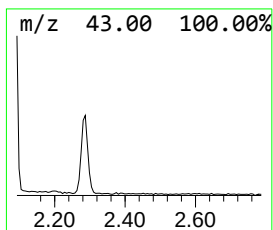
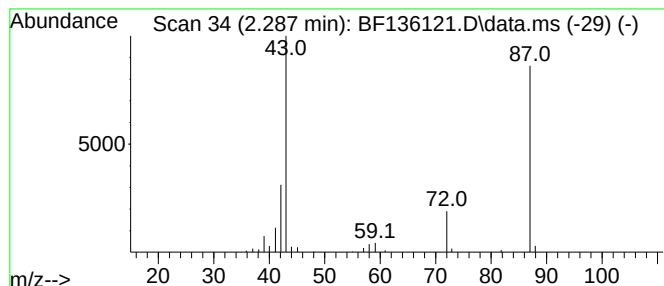
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	2.66 ng	71811	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	83
2			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	72
3			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	53
4			2-Butanone	72	C4H8O	000078-93-3	10
5			Isobutane	58	C4H10	000075-28-5	10



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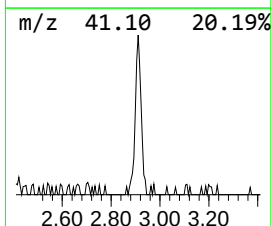
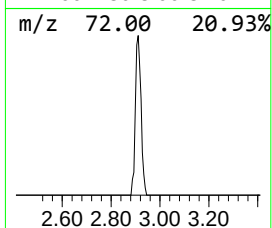
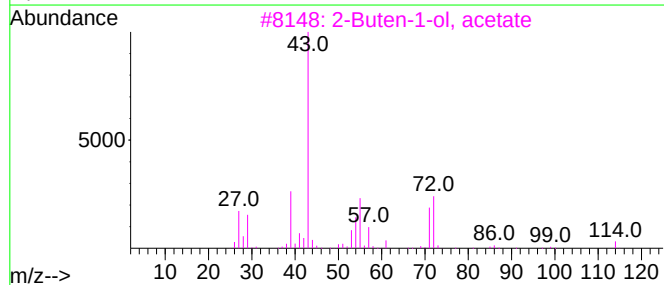
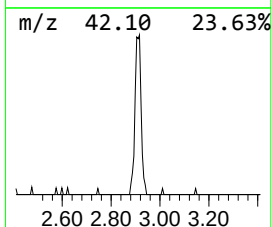
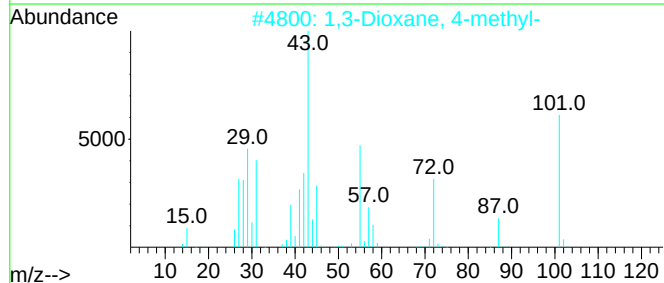
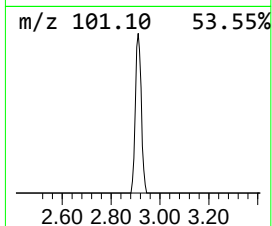
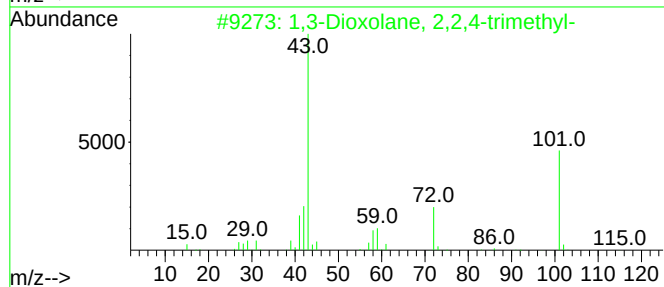
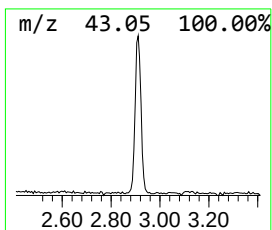
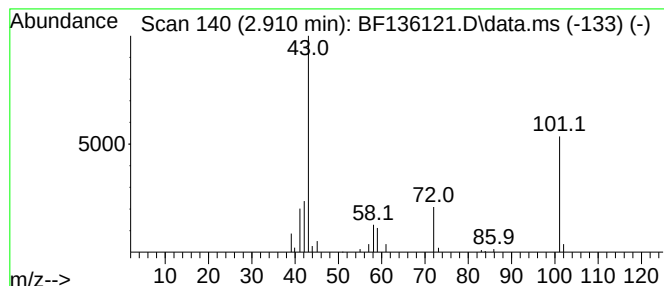
Instrument :
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COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.910	2.84 ng	76535	1,4-Dichlorobenzene-d4	6.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
3	2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	12
4	Butane	58	C4H10	000106-97-8	9
5	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	9



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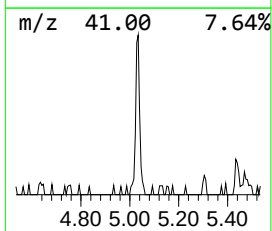
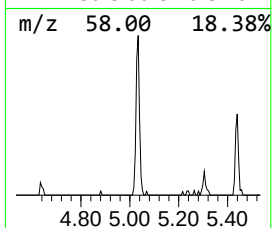
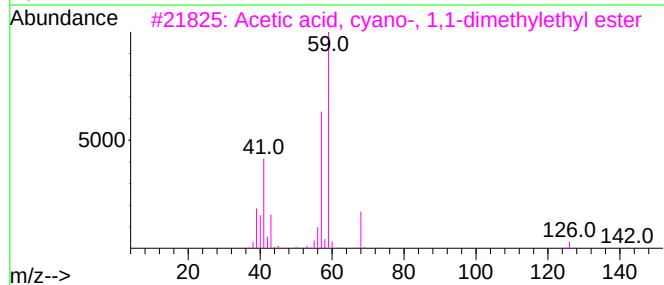
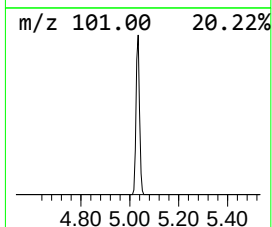
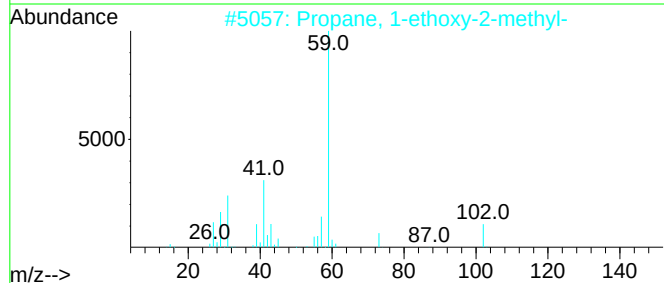
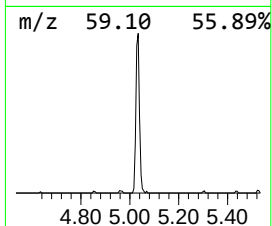
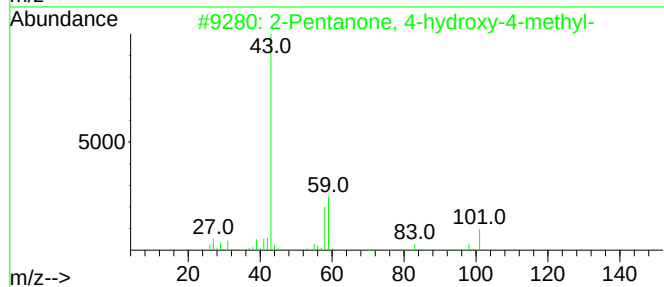
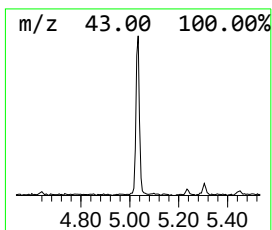
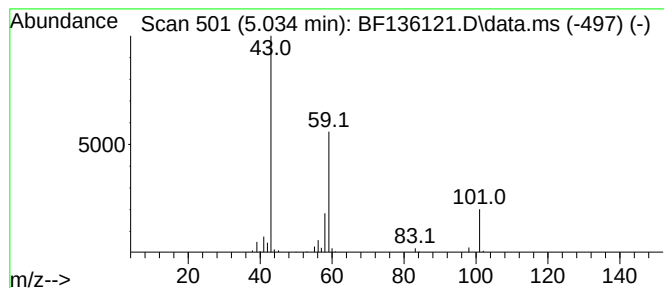
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	3.46 ng	93309	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17		



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Instrument :
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ClientSampleId :
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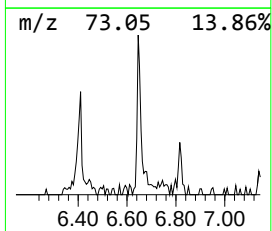
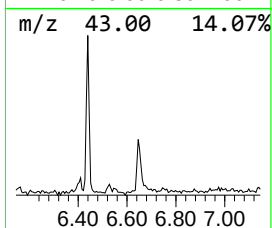
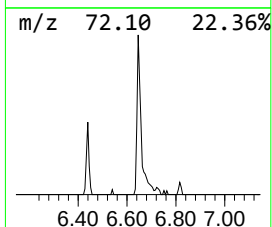
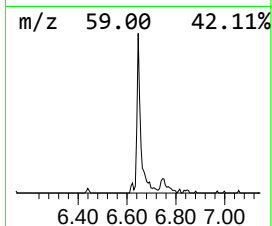
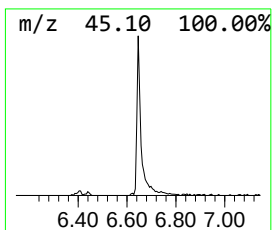
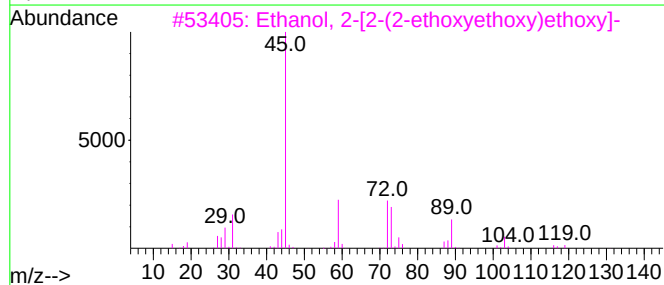
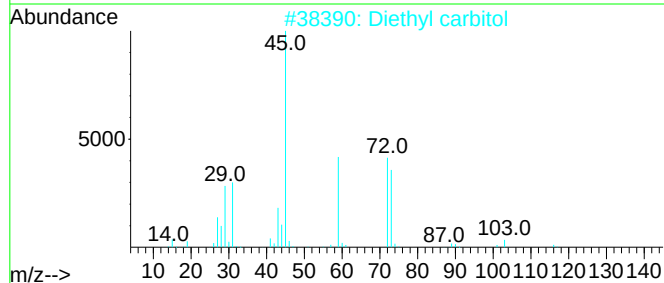
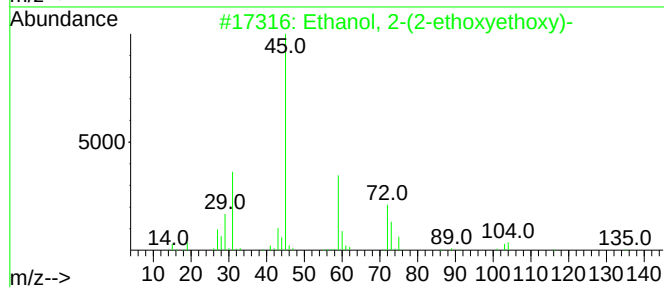
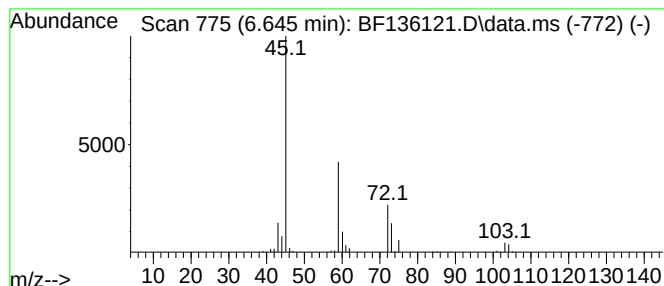
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.645	3.09 ng	83250	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	53
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38



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ClientSampleId :
COMPOSITE-1

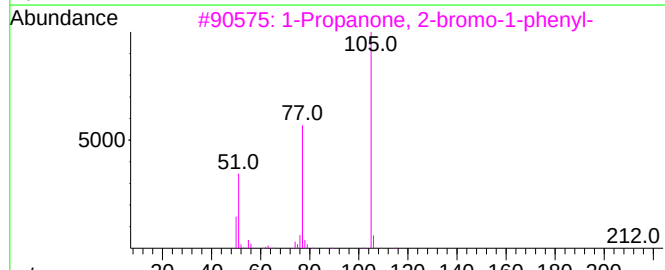
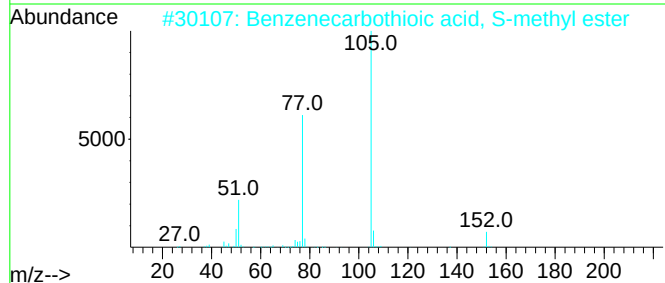
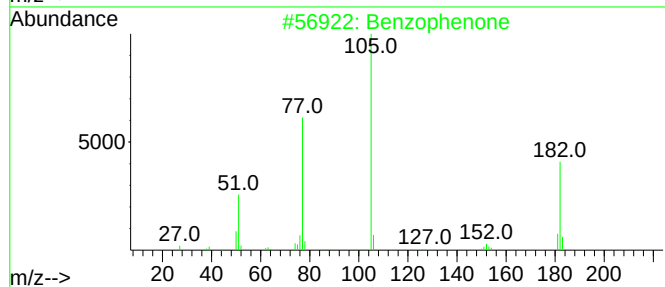
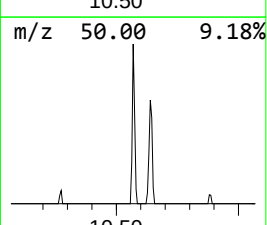
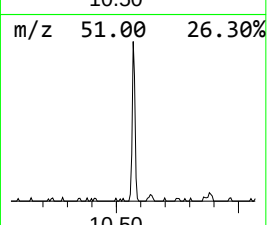
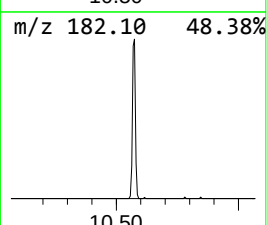
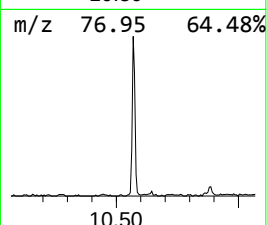
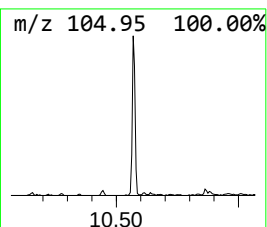
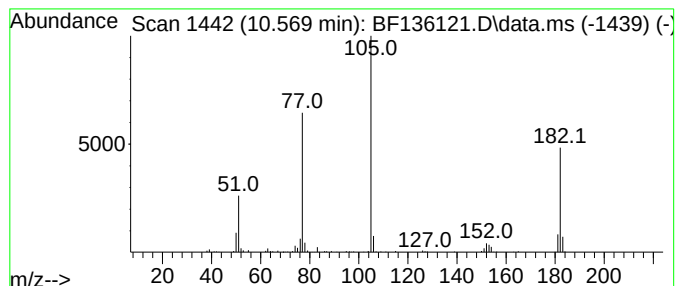
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	2.88 ng	107024	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
Data File : BF136121.D
Acq On : 03 Nov 2023 13:38
Operator : CG\JU
Sample : 05143-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

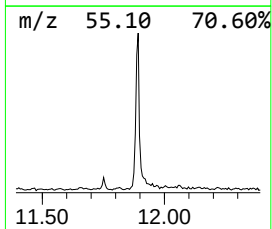
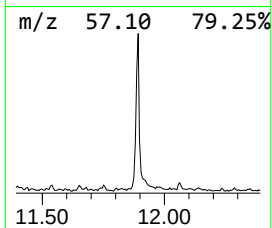
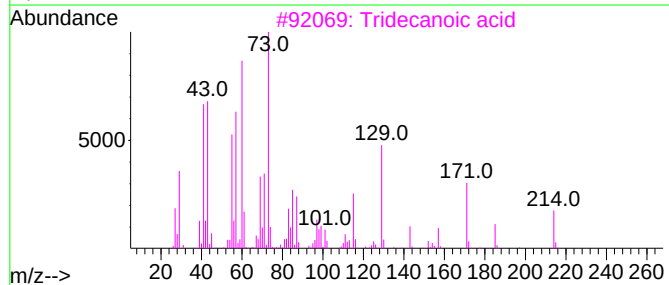
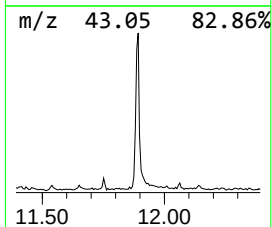
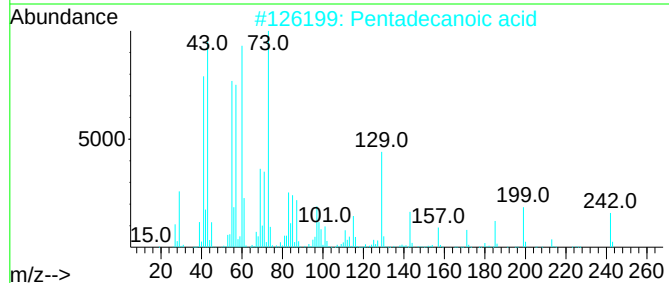
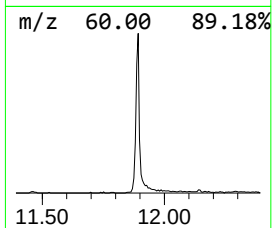
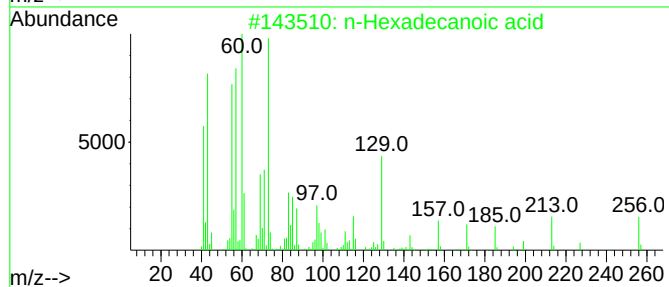
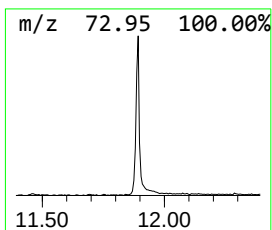
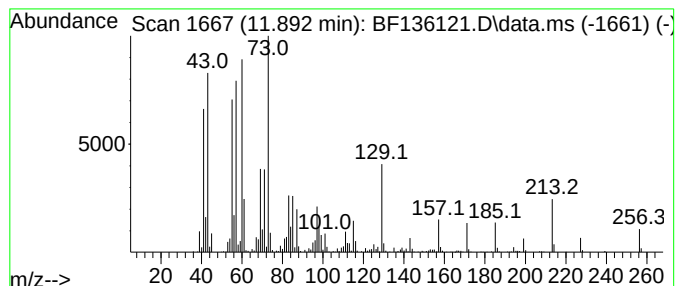
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	17.91 ng	606184	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
Data File : BF136121.D
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Operator : CG\JU
Sample : 05143-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

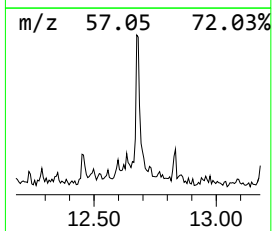
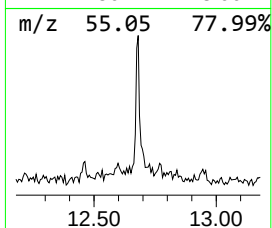
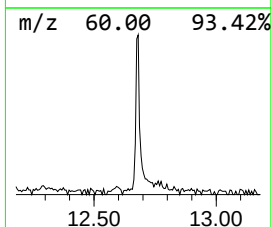
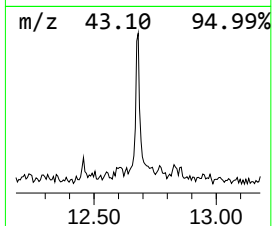
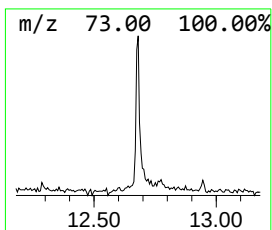
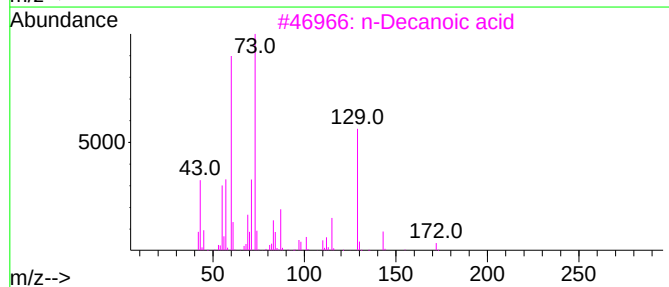
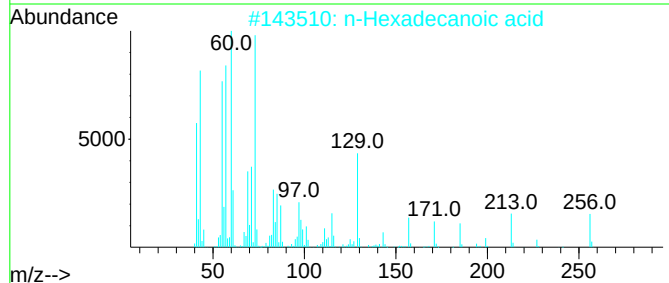
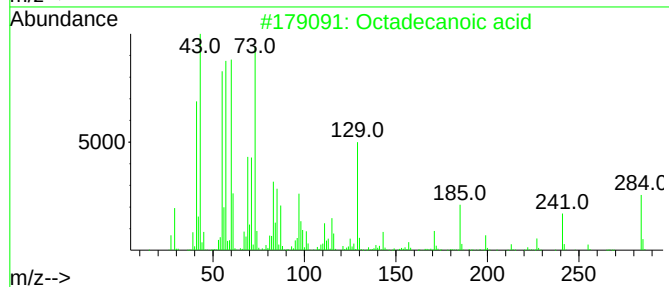
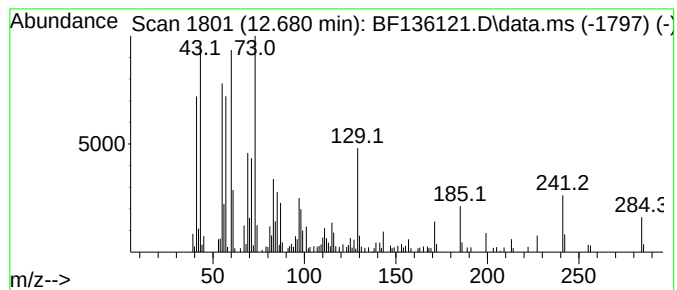
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	4.30 ng	123187	Chrysene-d12	14.004

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	94
3			n-Decanoic acid	172	C10H20O2	000334-48-5	91
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

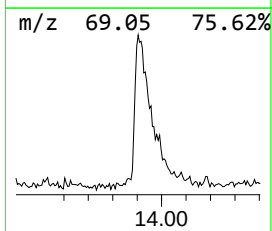
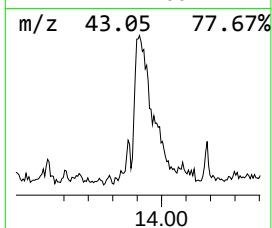
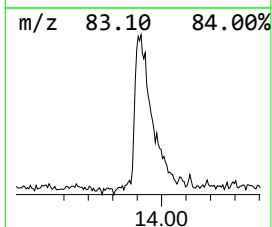
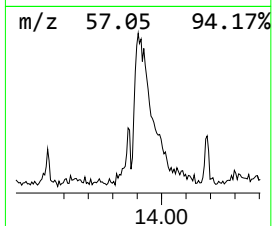
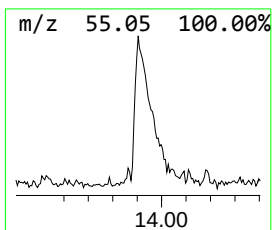
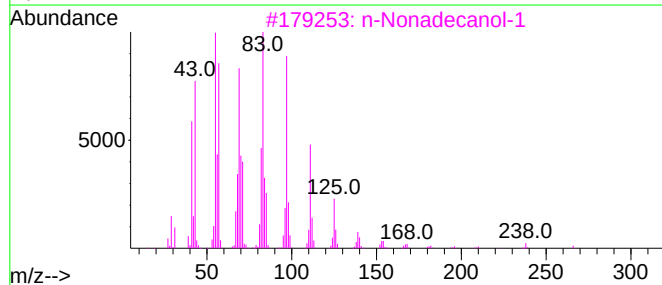
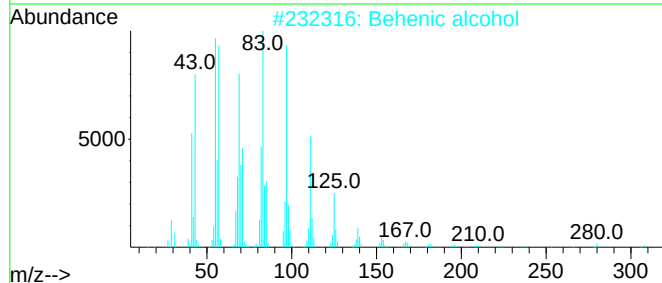
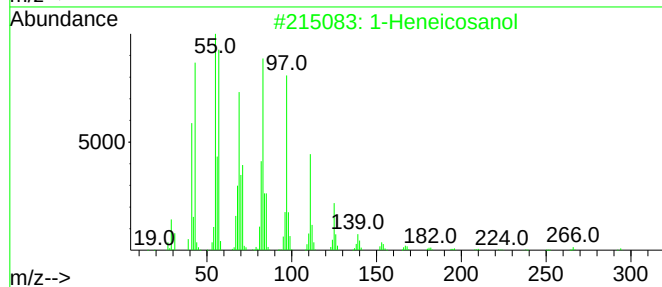
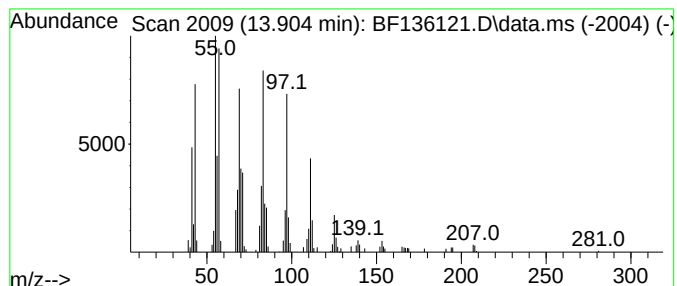
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	13.11 ng	375790	Chrysene-d12	14.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	91
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		1-Tetracosene	336	C24H48	010192-32-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
Data File : BF136121.D
Acq On : 03 Nov 2023 13:38
Operator : CG\JU
Sample : 05143-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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
1,3-Dioxolane, ...	2.287	2.7	ng	71811	1	6.816	539281	20.0
1,3-Dioxolane, ...	2.910	2.8	ng	76535	1	6.816	539281	20.0
2-Pentanone, 4-...	5.034	3.5	ng	93309	1	6.816	539281	20.0
Ethanol, 2-(2-e...	6.645	3.1	ng	83250	1	6.816	539281	20.0
Benzophenone	10.569	2.9	ng	107024	3	9.857	744118	20.0
n-Hexadecanoic ...	11.892	17.9	ng	606184	4	11.345	676747	20.0
Octadecanoic acid	12.680	4.3	ng	123187	5	14.004	573158	20.0
1-Heneicosanol	13.904	13.1	ng	375790	5	14.004	573158	20.0