

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013023\
 Data File : BF132230.D
 Acq On : 31 Jan 2023 01:40
 Operator : CG\JU
 Sample : 01337-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-02-012723

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-BF012723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.325	417	423	435	rVB	1088495	1276747	41.81%	5.115%
2	5.707	483	488	491	rBV	3180557	3053853	100.00%	12.234%
3	6.690	650	655	659	rBV	2788497	2843516	93.11%	11.391%
4	7.084	718	722	725	rVB	1261427	972748	31.85%	3.897%
5	7.642	813	817	820	rBV	2265016	1815054	59.43%	7.271%
6	8.366	937	940	944	rBV	1284472	1101740	36.08%	4.414%
7	9.442	1119	1123	1126	rBV	3866649	2983438	97.69%	11.952%
8	10.131	1237	1240	1244	rVB	1233042	1047303	34.29%	4.196%
9	10.842	1358	1361	1365	rVB	59442	50517	1.65%	0.202%
10	10.925	1371	1375	1378	rBV	2130281	1725621	56.51%	6.913%
11	11.025	1388	1392	1398	rBV	222186	181420	5.94%	0.727%
12	11.630	1491	1495	1498	rBV	1383486	1123738	36.80%	4.502%
13	11.654	1498	1499	1503	rVV	164078	99710	3.27%	0.399%
14	11.707	1503	1508	1510	rVV	44520	46257	1.51%	0.185%
15	12.007	1556	1559	1562	rBV	161601	120905	3.96%	0.484%
16	12.136	1578	1581	1584	rBV	332075	302337	9.90%	1.211%
17	12.701	1673	1677	1679	rBV	717547	656586	21.50%	2.630%
18	12.719	1679	1680	1687	rVB2	449294	355505	11.64%	1.424%
19	12.807	1692	1695	1698	rBV	92398	88765	2.91%	0.356%
20	12.854	1700	1703	1708	rVB	294057	257636	8.44%	1.032%
21	12.930	1713	1716	1719	rBV	75708	78734	2.58%	0.315%
22	13.089	1740	1743	1748	rVB	227774	226440	7.41%	0.907%
23	13.224	1762	1766	1769	rBV	3571029	2863861	93.78%	11.473%
24	14.295	1944	1948	1951	rBV	956588	898881	29.43%	3.601%
25	15.889	2216	2219	2230	rVB	499931	791014	25.90%	3.169%

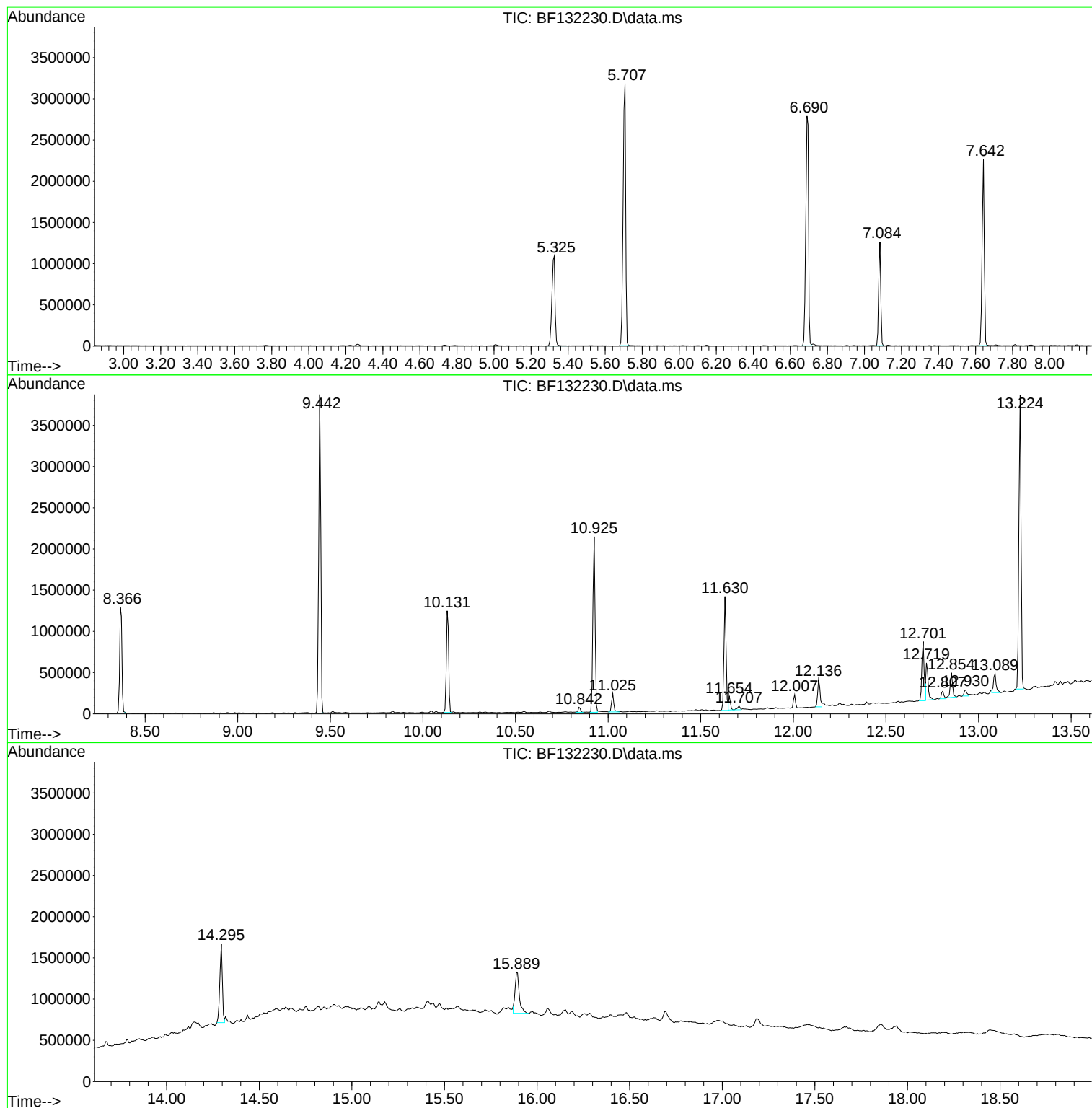
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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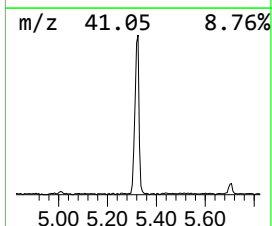
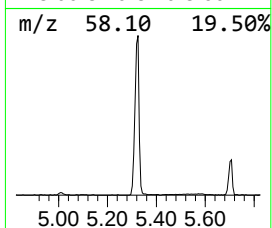
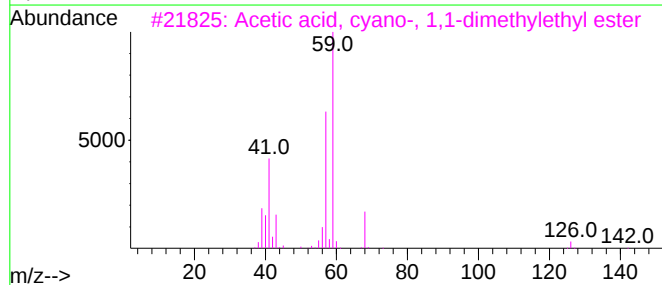
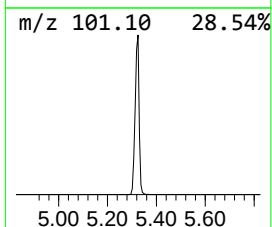
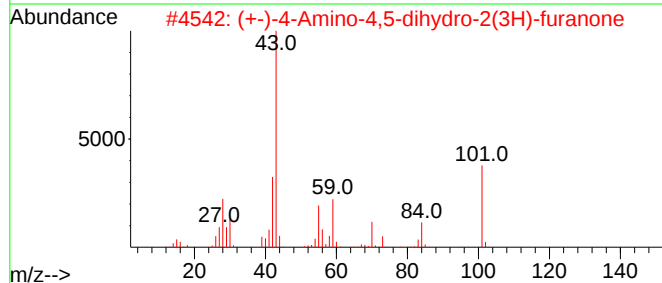
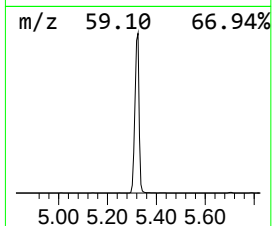
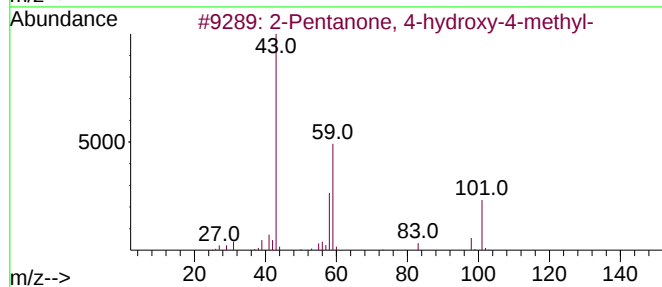
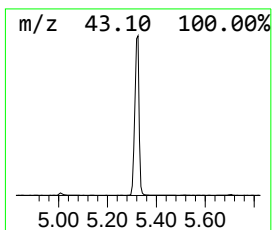
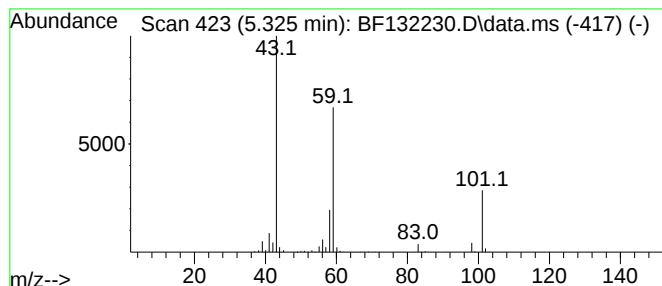
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.325	26.25 ng	1276750	1,4-Dichlorobenzene-d4	7.084

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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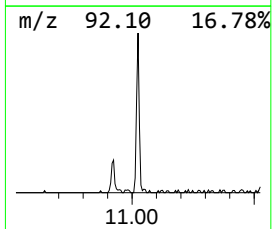
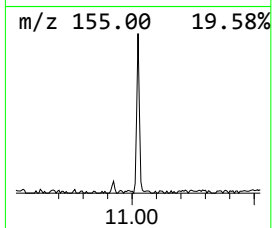
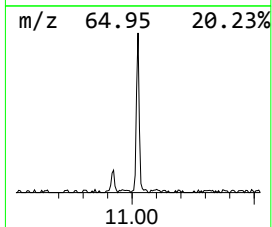
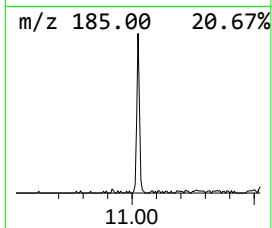
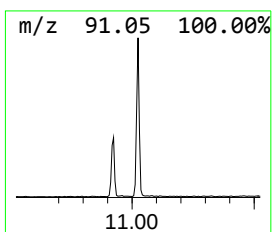
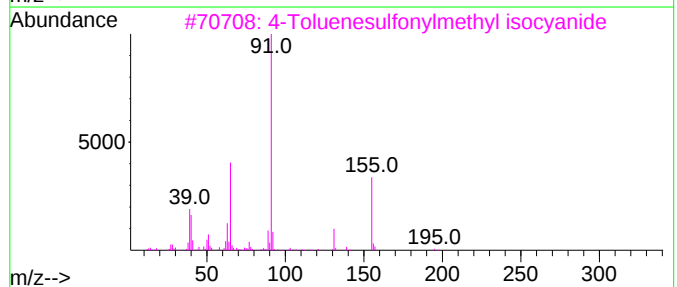
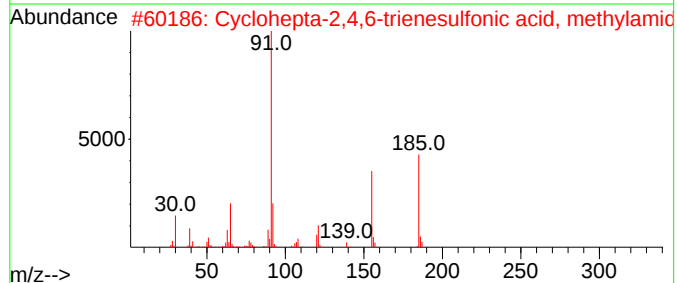
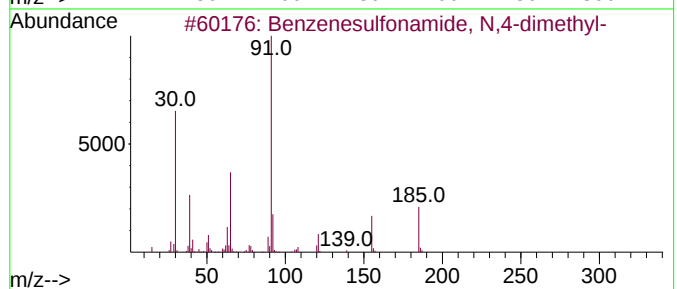
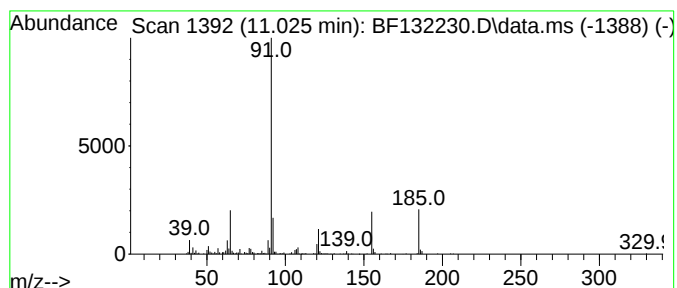
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Peak Number 2 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.025	3.23 ng	181420	Phenanthrene-d10			11.630
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-		185	C8H11NO2S	000640-61-9	95
2	Cyclohepta-2,4,6-trienesulfonic ...		185	C8H11NO2S	1000187-28-7	70
3	4-Toluenesulfonylmethyl isocyanide		195	C9H9NO2S	036635-61-7	47
4	Benzene, 1-[(chloromethyl)sulfon...		204	C8H9ClO2S	007569-26-8	47
5	(O-p-Tosylisonitroso)malononitrile		249	C10H7N3O3S	020893-01-0	47



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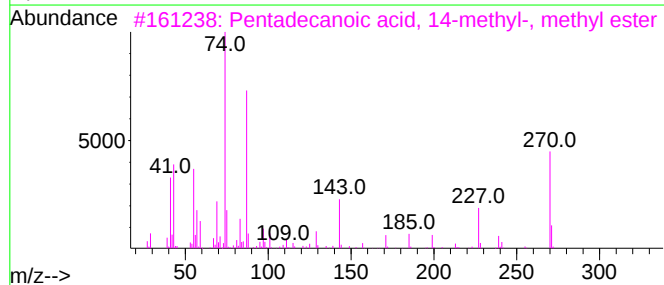
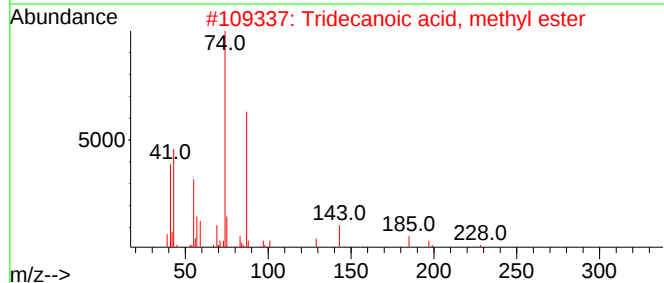
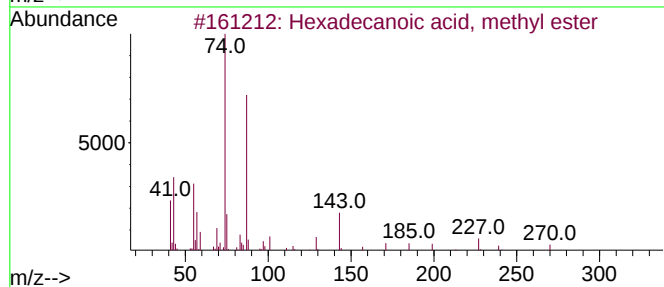
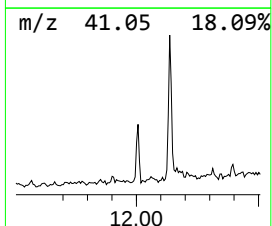
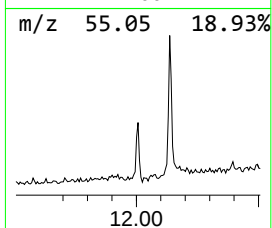
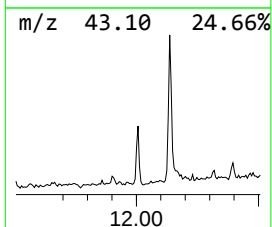
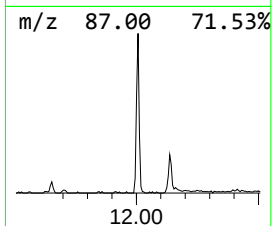
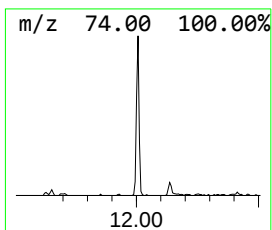
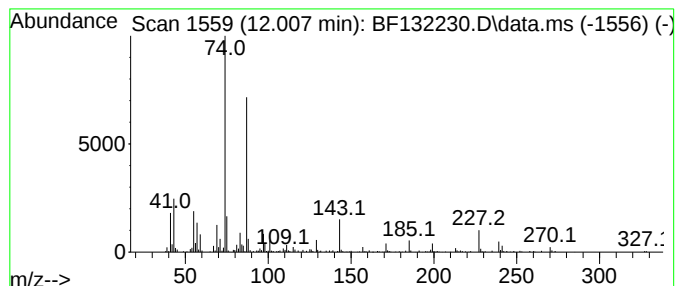
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Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.007	2.15 ng	120905	Phenanthrene-d10		11.630	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	98
2	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	87
3	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	86
4	Heptadecanoic acid, methyl ester		284	C18H36O2	001731-92-6	83
5	Hexadecanoic acid, 2-methyl-		270	C17H34O2	027147-71-3	83



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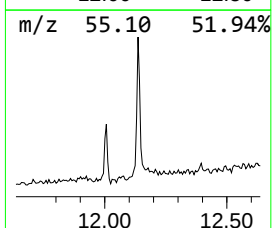
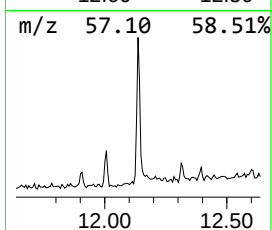
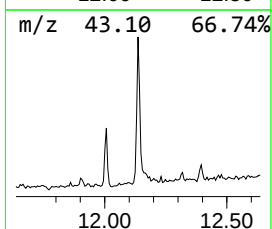
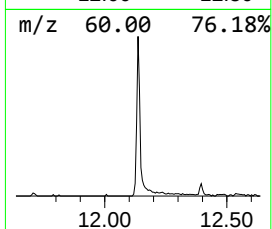
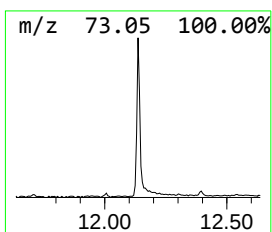
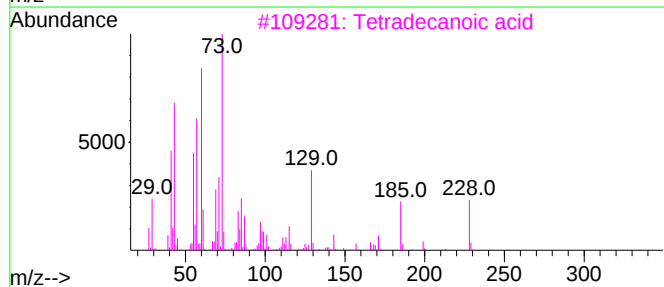
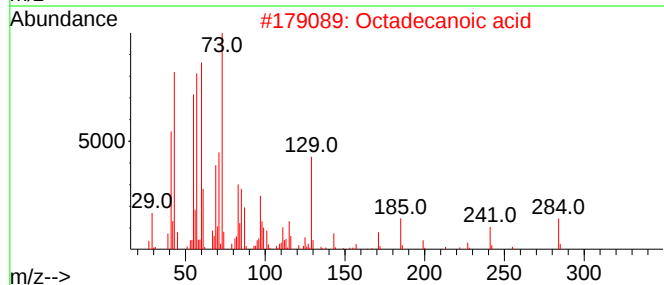
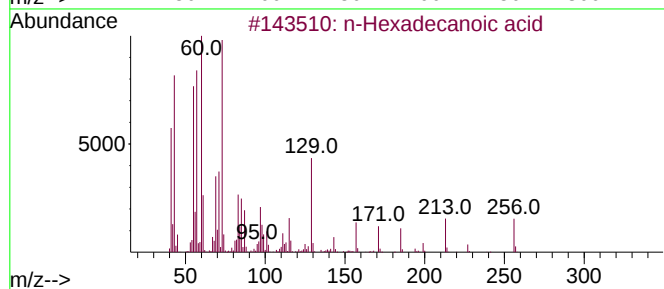
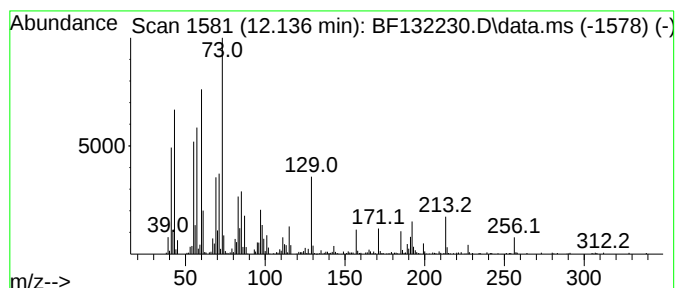
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.136	5.38 ng	302337	Phenanthrene-d10	11.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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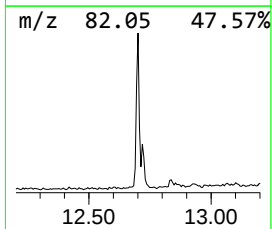
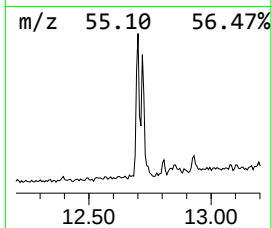
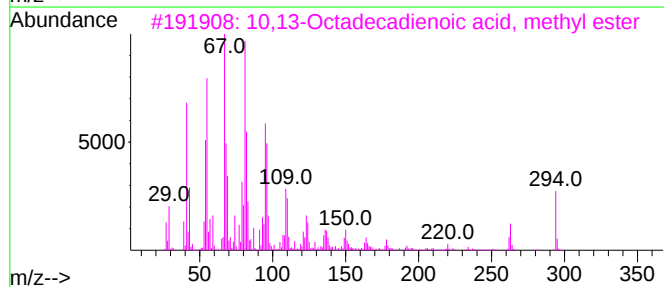
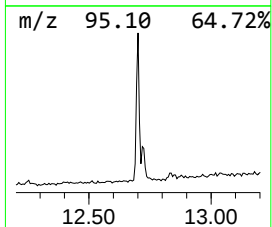
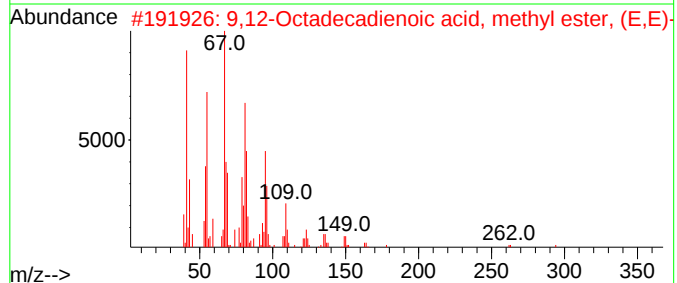
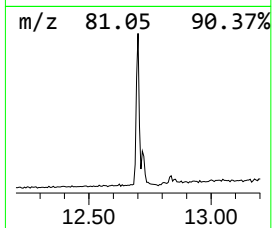
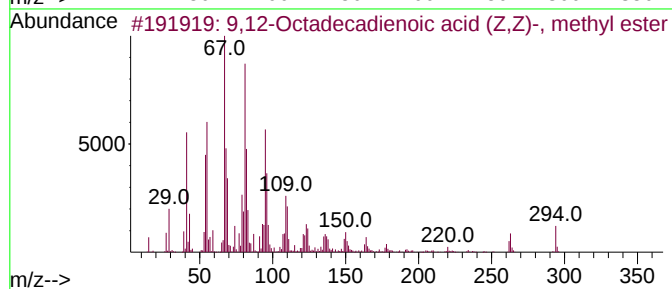
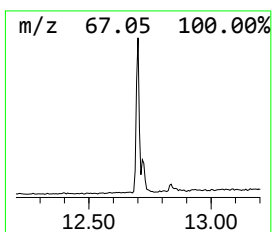
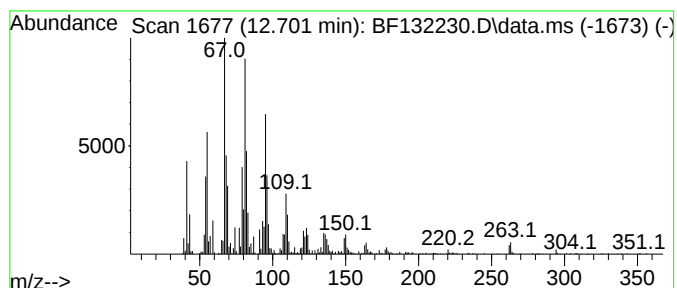
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TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.701	11.69 ng	656586	Phenanthrene-d10	11.630	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	9,12-Octadecadienoic acid, ethyl...	308	C20H36O2	007619-08-1	99
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98



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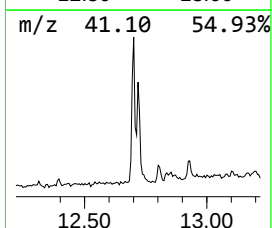
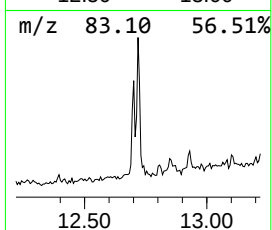
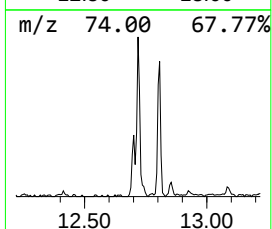
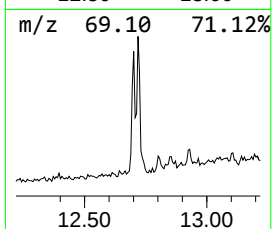
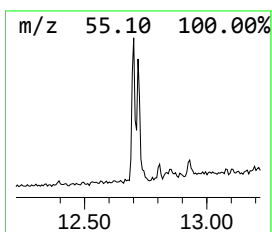
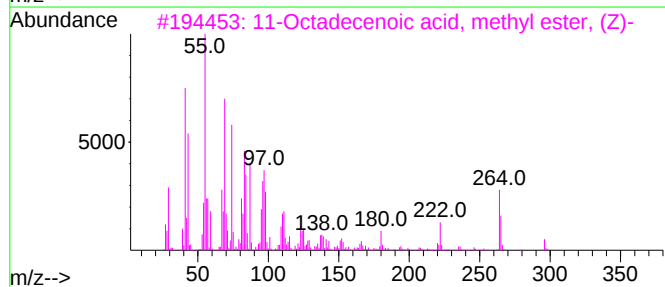
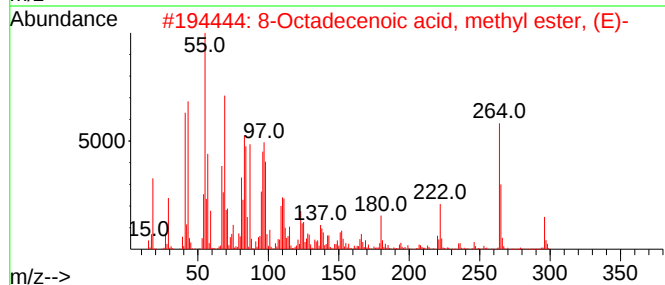
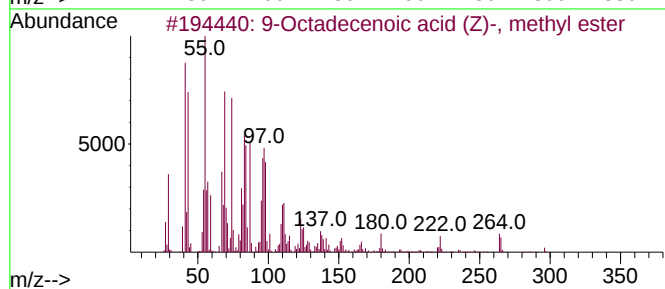
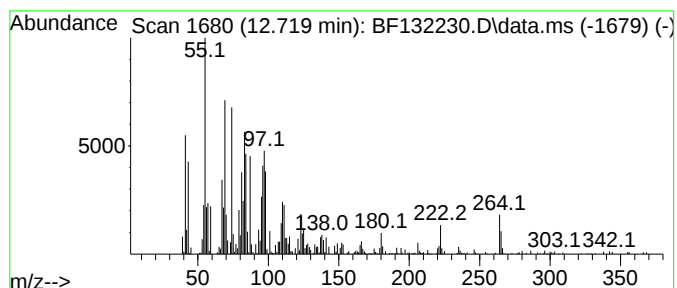
Instrument :
BNA_F
ClientSampleId :
SU-02-012723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.719	6.33 ng	355505	Phenanthrene-d10	11.630	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013023\
Data File : BF132230.D
Acq On : 31 Jan 2023 01:40
Operator : CG\JU
Sample : 01337-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-012723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012723.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-...	5.325	26.3	ng	1276750	1	7.084	972748	20.0
Benzenesulfonam...	11.025	3.2	ng	181420	4	11.630	1123740	20.0
Hexadecanoic ac...	12.007	2.1	ng	120905	4	11.630	1123740	20.0
n-Hexadecanoic ...	12.136	5.4	ng	302337	4	11.630	1123740	20.0
9,12-Octadecadi...	12.701	11.7	ng	656586	4	11.630	1123740	20.0
9-Octadecenoic ...	12.719	6.3	ng	355505	4	11.630	1123740	20.0