

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010421\
 Data File : BF122913.D
 Acq On : 4 Jan 2021 17:32
 Operator : JU/CG
 Sample : L5249-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-123120

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122913.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	13	16	24	rVB	25330	36877	1.16%	0.171%
2	5.028	497	500	513	rVB	56647	76512	2.40%	0.355%
3	5.439	566	570	595	rBV	2023228	2025203	63.55%	9.383%
4	6.457	739	743	761	rBV	2004985	2168968	68.06%	10.049%
5	6.816	801	804	814	rVB	747984	644552	20.23%	2.986%
6	7.386	896	901	913	rBV	1439539	1351532	42.41%	6.262%
7	8.104	1020	1023	1046	rBV	875340	868852	27.27%	4.026%
8	9.186	1202	1207	1217	rBV	2708745	2603149	81.69%	12.061%
9	9.580	1270	1274	1282	rBV	133713	120539	3.78%	0.558%
10	9.863	1318	1322	1333	rVB	1103933	1038967	32.60%	4.814%
11	10.657	1453	1457	1468	rBV	1752993	1856687	58.26%	8.603%
12	11.357	1572	1576	1579	rBV	1257260	1102132	34.59%	5.107%
13	11.380	1579	1580	1584	rVB	70079	41636	1.31%	0.193%
14	11.745	1639	1642	1649	rVB	213386	167708	5.26%	0.777%
15	11.886	1662	1666	1676	rBV2	115650	140704	4.42%	0.652%
16	12.433	1755	1759	1761	rBV	939178	772507	24.24%	3.579%
17	12.457	1761	1763	1769	rVB	537322	458884	14.40%	2.126%
18	12.539	1774	1777	1780	rBV	87719	70670	2.22%	0.327%
19	12.574	1780	1783	1793	rBV	90904	87692	2.75%	0.406%
20	12.674	1797	1800	1807	rBV	28428	39510	1.24%	0.183%
21	12.804	1817	1822	1826	rBV	72320	71724	2.25%	0.332%
22	12.951	1841	1847	1850	rBV	3244978	3186628	100.00%	14.765%
23	13.868	1999	2003	2019	rVB2	167519	353814	11.10%	1.639%
24	14.009	2023	2027	2038	rVB	1123609	1112479	34.91%	5.154%
25	14.521	2108	2114	2120	rBV9	15676	36850	1.16%	0.171%
26	15.056	2201	2205	2208	rBV	31247	47743	1.50%	0.221%
27	15.115	2212	2215	2221	rVB2	34363	42659	1.34%	0.198%
28	15.486	2272	2278	2289	rBV	698826	918900	28.84%	4.258%
29	15.921	2348	2352	2358	rVB2	41461	59373	1.86%	0.275%
30	16.427	2434	2438	2441	rVB2	25858	39077	1.23%	0.181%
31	17.009	2533	2537	2545	rVB4	21178	40384	1.27%	0.187%

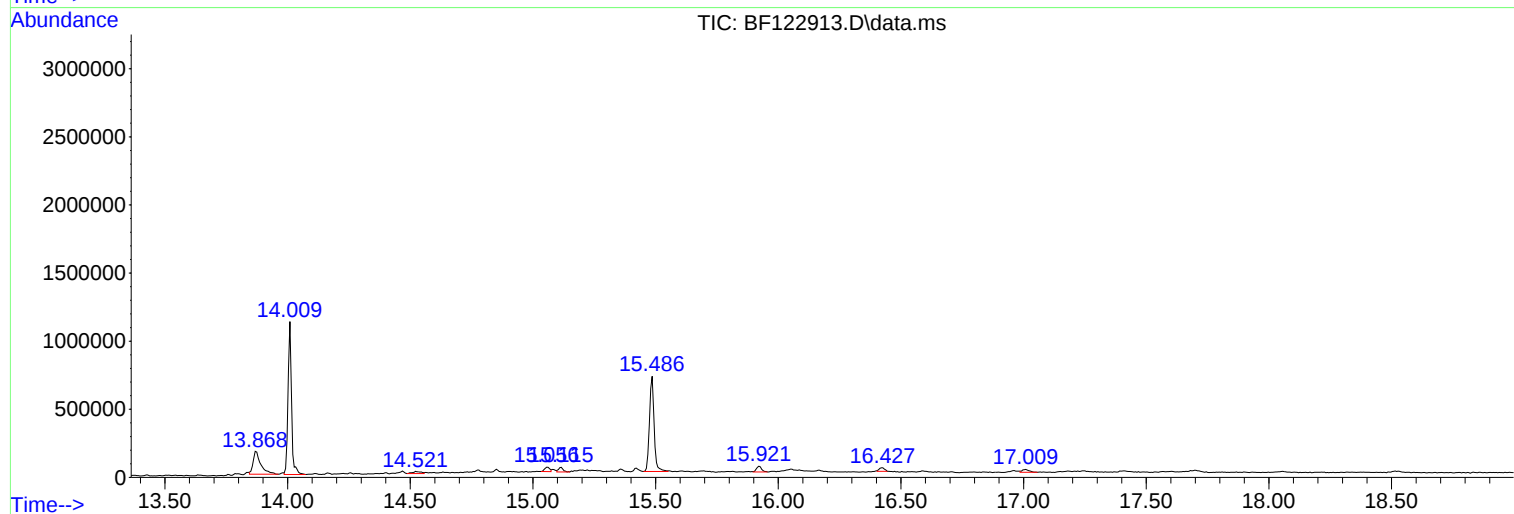
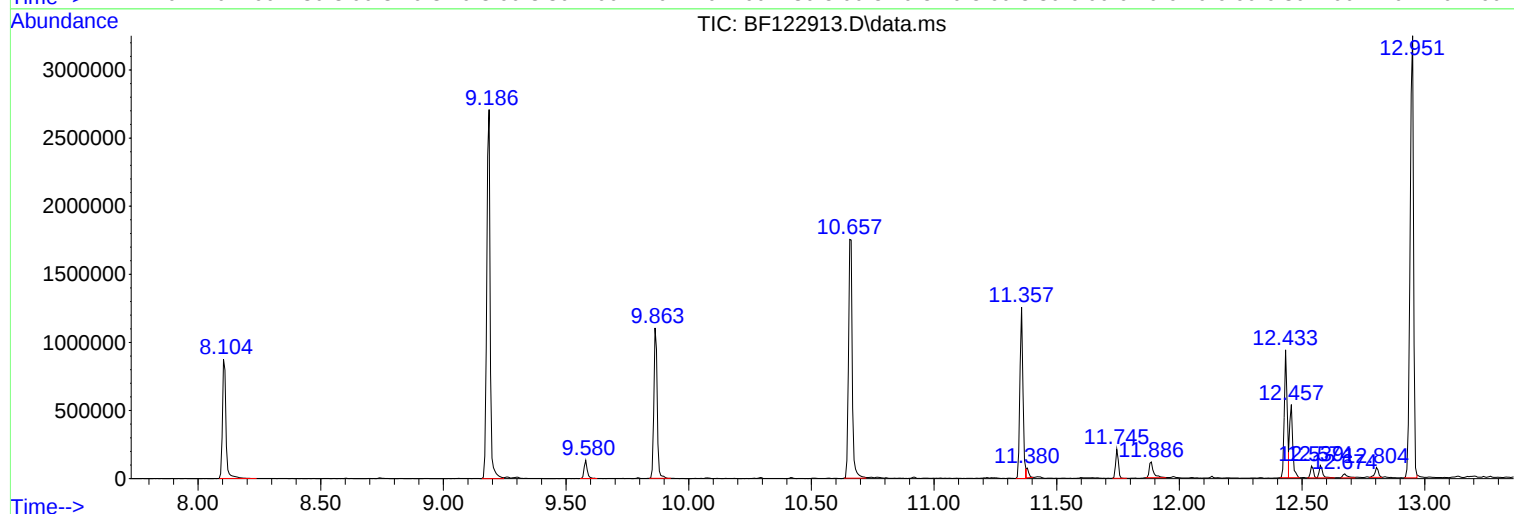
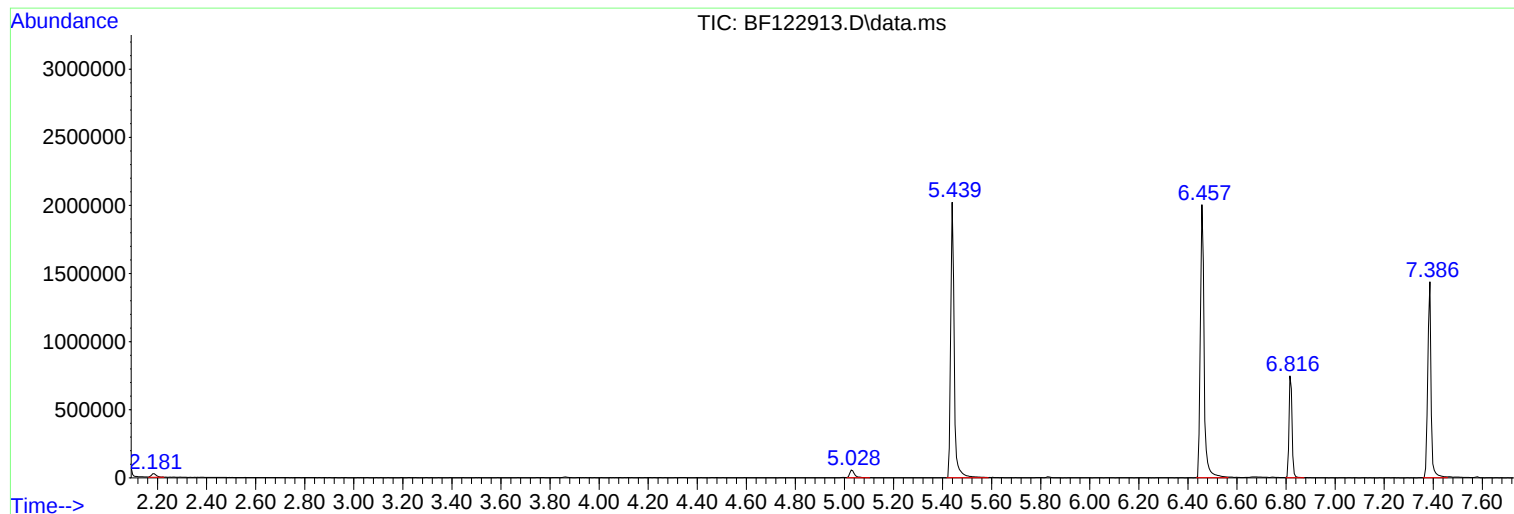
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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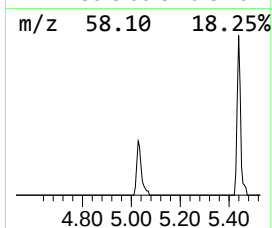
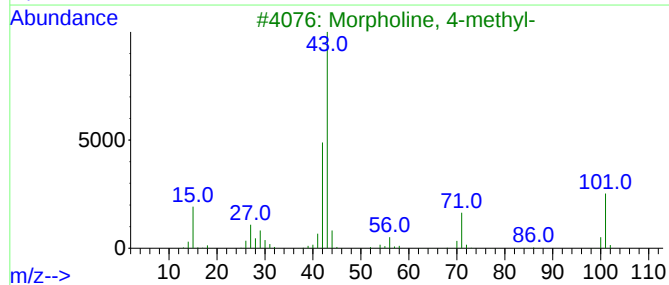
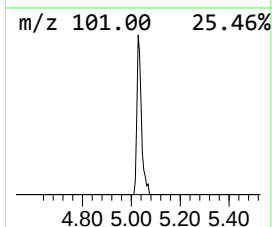
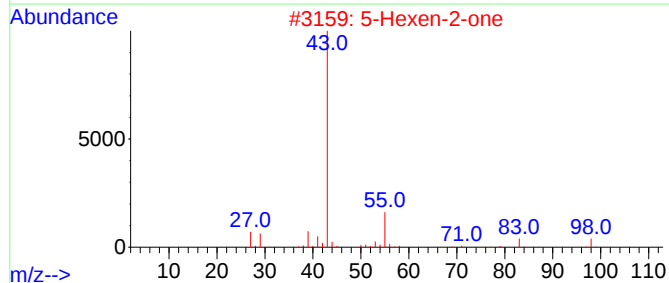
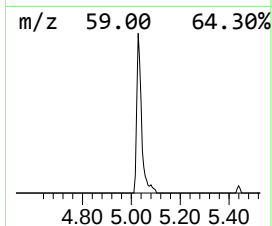
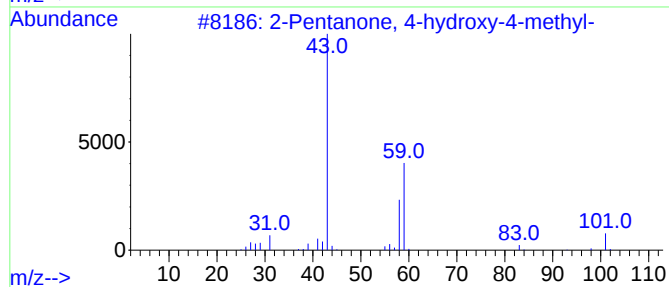
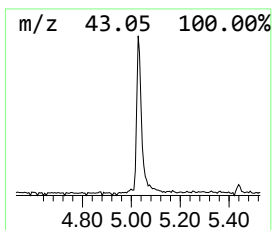
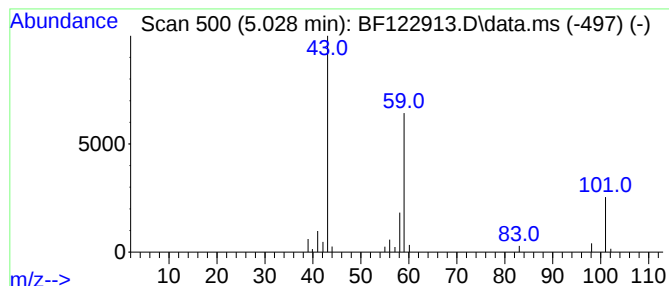
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.	
5.028	2.37 ng	76512	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	56
2	5-Hexen-2-one		98	C6H10O	000109-49-9	9
3	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-		102	C6H14O	000628-81-9	9
5	(+) -4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	9



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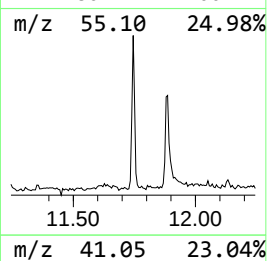
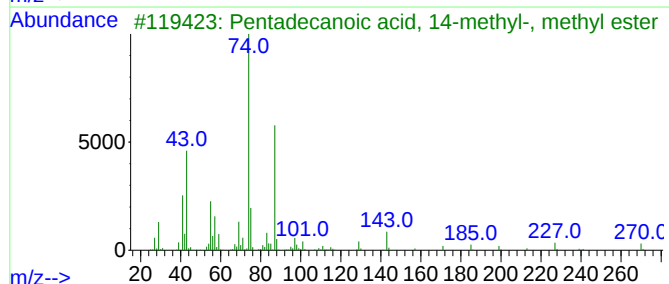
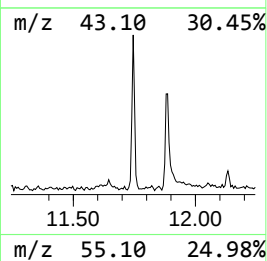
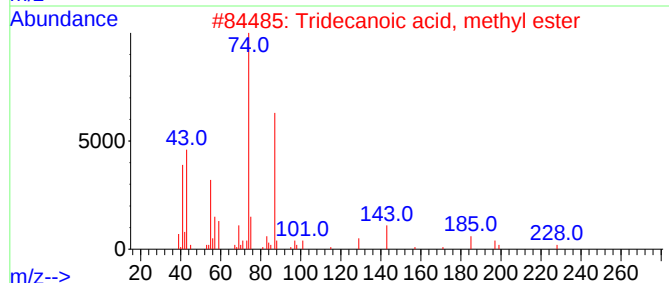
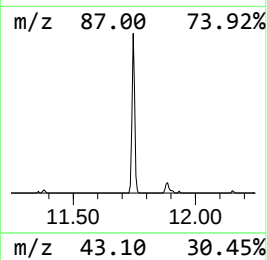
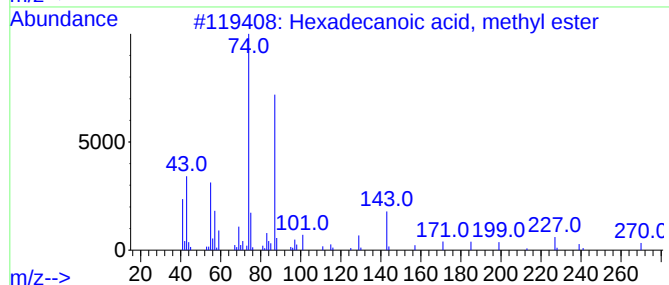
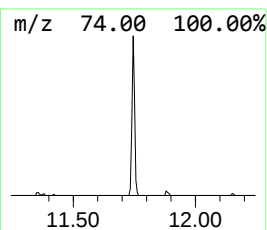
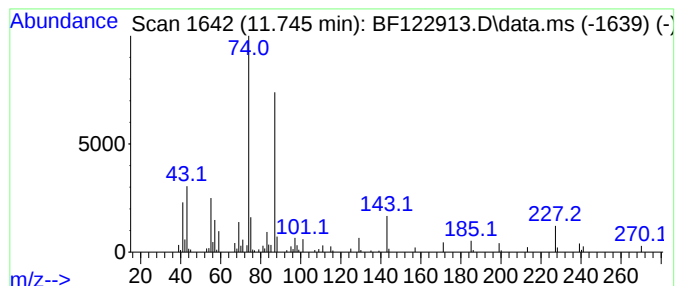
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	3.04 ng	167708	Phenanthrene-d10	11.357

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	92
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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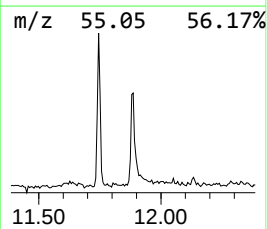
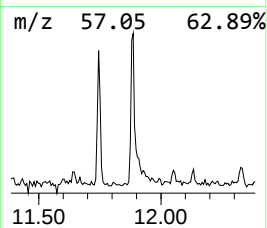
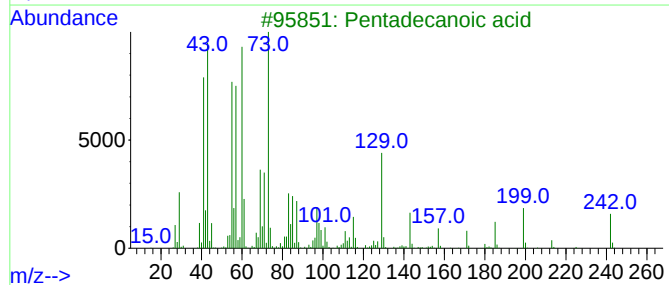
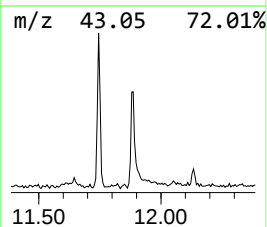
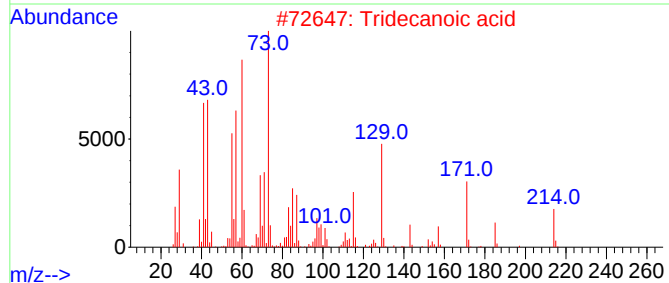
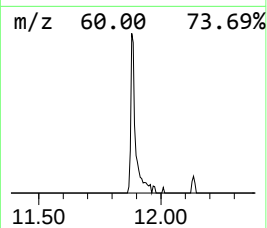
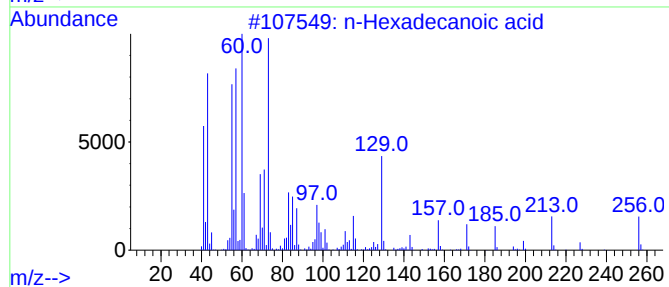
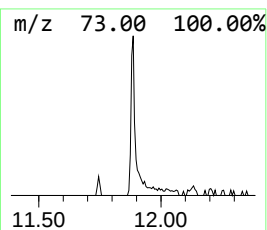
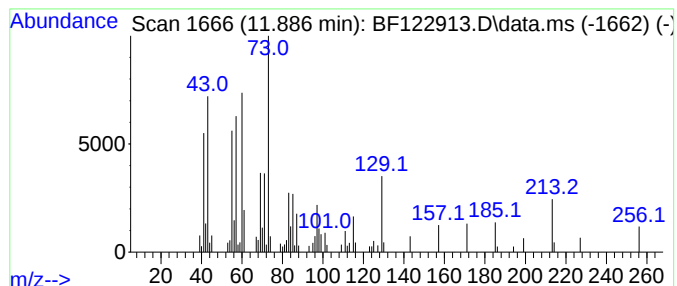
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.55 ng	140704	Phenanthrene-d10	11.357

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	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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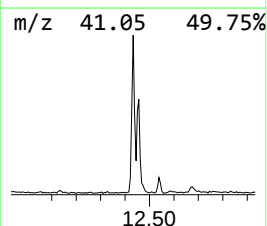
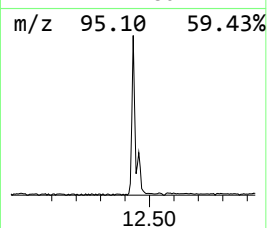
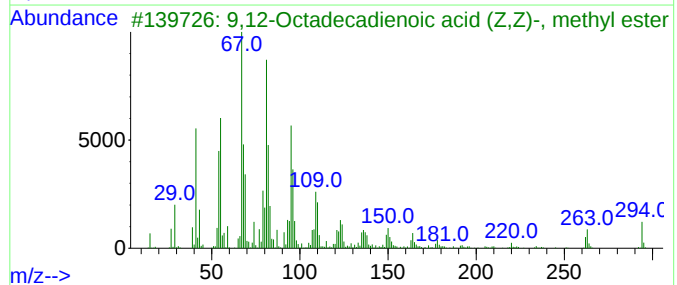
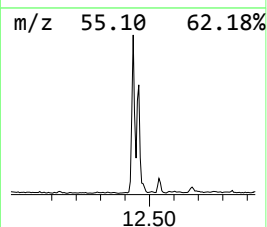
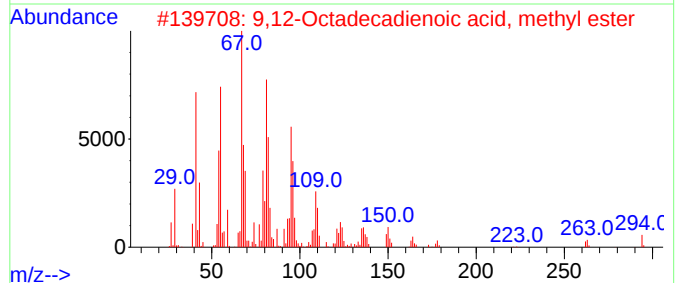
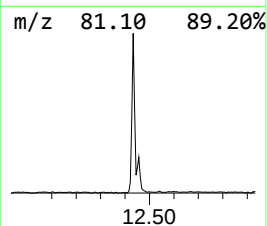
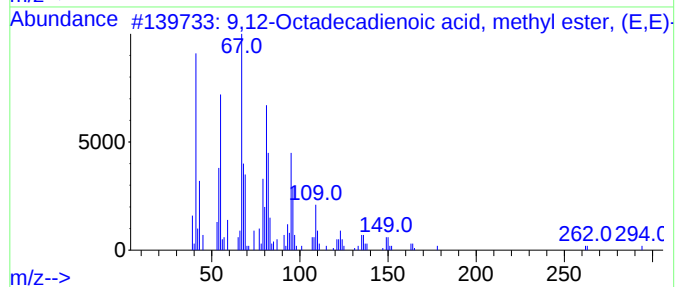
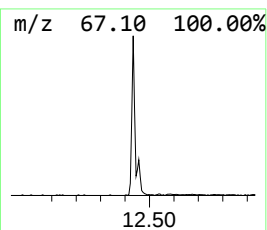
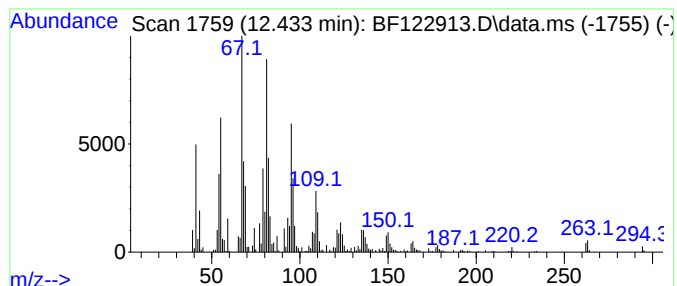
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	14.02 ng	772507	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99		
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99		
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98		
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98		



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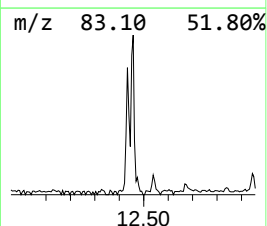
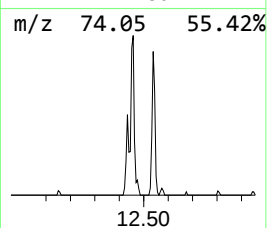
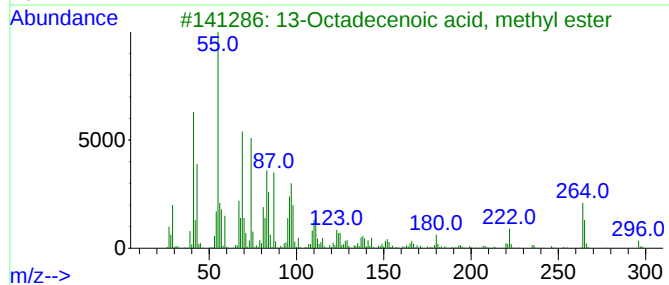
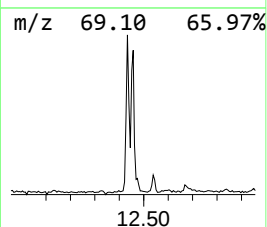
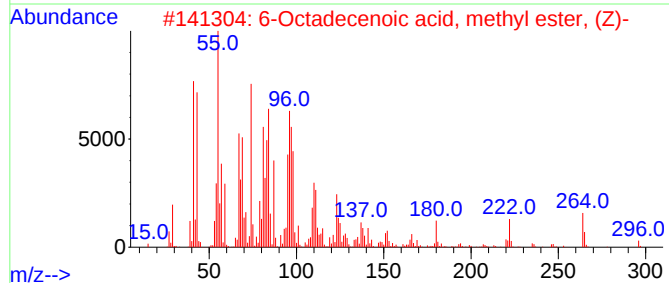
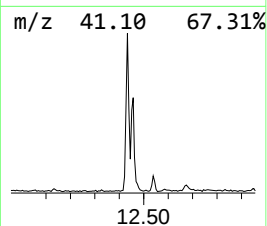
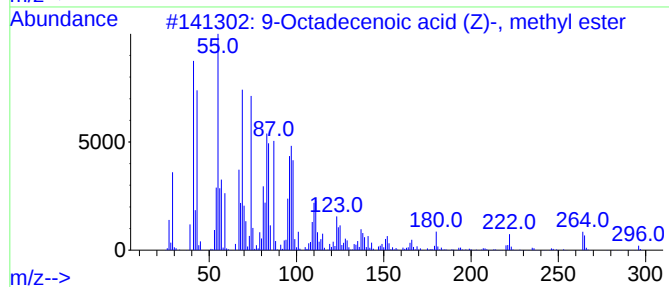
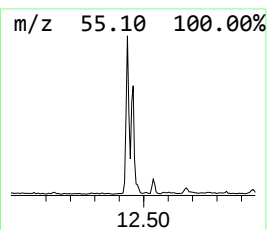
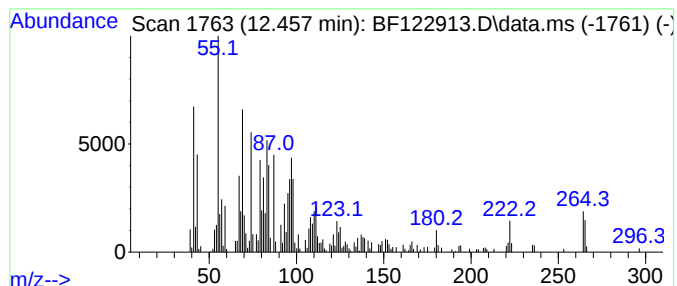
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	8.33 ng	458884	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99



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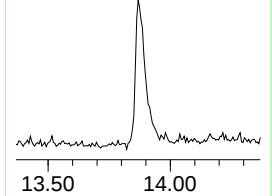
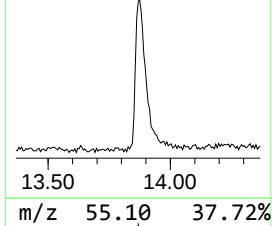
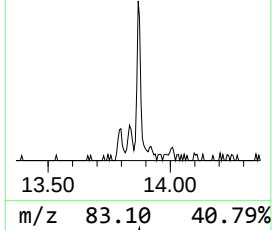
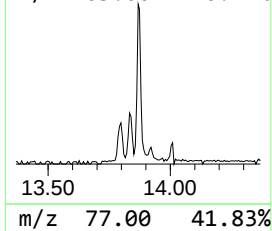
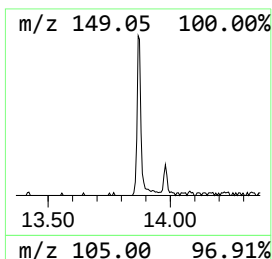
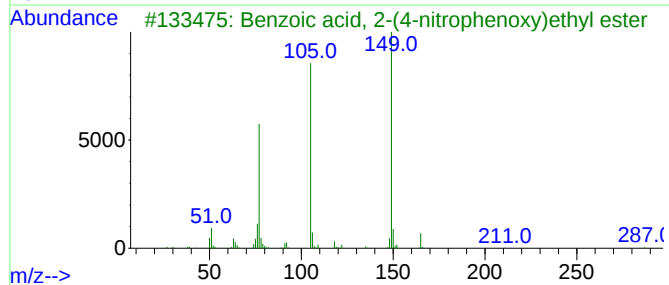
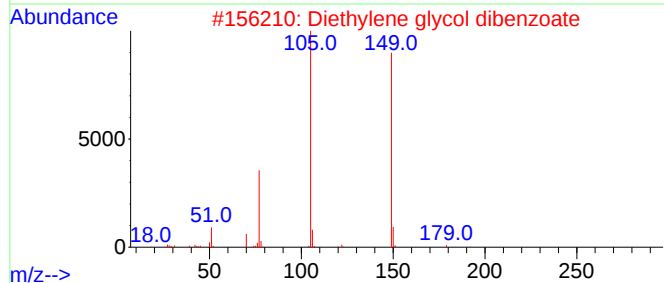
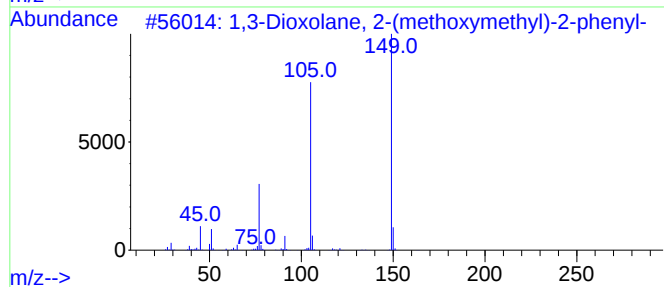
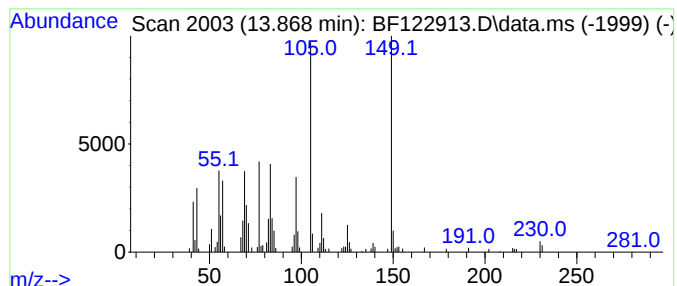
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown13.868 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	6.36 ng	353814	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	47
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	47
3			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	47
4			2-(2-(2-Ethoxyethoxy)ethoxy)ethy...	282	C15H22O5	1000366-98-8	47
5			Phthalic acid, 4,4-dimethylpent-...	320	C19H28O4	1000371-14-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010421\
Data File : BF122913.D
Acq On : 4 Jan 2021 17:32
Operator : JU/CG
Sample : L5249-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-123120

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.028	2.4	ng	76512	1	6.816	644552	20.0
Hexadecanoic ac...	11.745	3.0	ng	167708	4	11.357	1102130	20.0
n-Hexadecanoic ...	11.886	2.5	ng	140704	4	11.357	1102130	20.0
9,12-Octadecadi...	12.433	14.0	ng	772507	4	11.357	1102130	20.0
9-Octadecenoic ...	12.457	8.3	ng	458884	4	11.357	1102130	20.0
unknown13.868	13.868	6.4	ng	353814	5	14.009	1112480	20.0