

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
 Data File : BF123217.D
 Acq On : 17 Feb 2021 17:46
 Operator : JU/CG
 Sample : M1423-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-021621

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-BF021221.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123217.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	378314	419080	1.45%	0.471%
2	5.487	573	578	581	rBV	4480424	4410360	15.26%	4.955%
3	6.492	744	749	756	rBV	3027923	3292622	11.39%	3.700%
4	6.869	809	813	816	rBV	1175272	936390	3.24%	1.052%
5	7.428	899	908	911	rBV	2202264	2123529	7.35%	2.386%
6	8.151	1025	1031	1034	rBV	1570458	1333598	4.61%	1.498%
7	9.228	1210	1214	1218	rBV	4017842	3755725	12.99%	4.220%
8	9.910	1326	1330	1334	rBV	1763797	1405849	4.86%	1.580%
9	10.704	1459	1465	1468	rBV	2719225	2518315	8.71%	2.830%
10	11.404	1580	1584	1586	rBV	1525622	1426007	4.93%	1.602%
11	11.804	1647	1652	1655	rBV	9000646	8053229	27.86%	9.049%
12	11.939	1671	1675	1686	rBV3	742671	1072407	3.71%	1.205%
13	12.516	1764	1773	1774	rBV	13383207	28907630	100.00%	32.480%
14	12.539	1775	1777	1781	rVV2	14342373	15265338	52.81%	17.152%
15	12.598	1784	1787	1790	rVV	5277775	4329939	14.98%	4.865%
16	12.633	1790	1793	1804	rVB3	727091	1432762	4.96%	1.610%
17	12.998	1850	1855	1858	rBV	4007085	3439865	11.90%	3.865%
18	13.174	1880	1885	1891	rBV6	135953	322672	1.12%	0.363%
19	13.239	1891	1896	1903	rVB3	594175	812642	2.81%	0.913%
20	13.316	1906	1909	1912	rBV	531714	500325	1.73%	0.562%
21	13.527	1942	1945	1950	rBV3	253134	321132	1.11%	0.361%
22	13.898	2005	2008	2019	rVB	366740	575611	1.99%	0.647%
23	13.986	2020	2023	2028	rVB	404094	359801	1.24%	0.404%
24	14.051	2029	2034	2037	rBV	1131154	1051959	3.64%	1.182%
25	15.527	2281	2285	2289	rBV	740740	933412	3.23%	1.049%

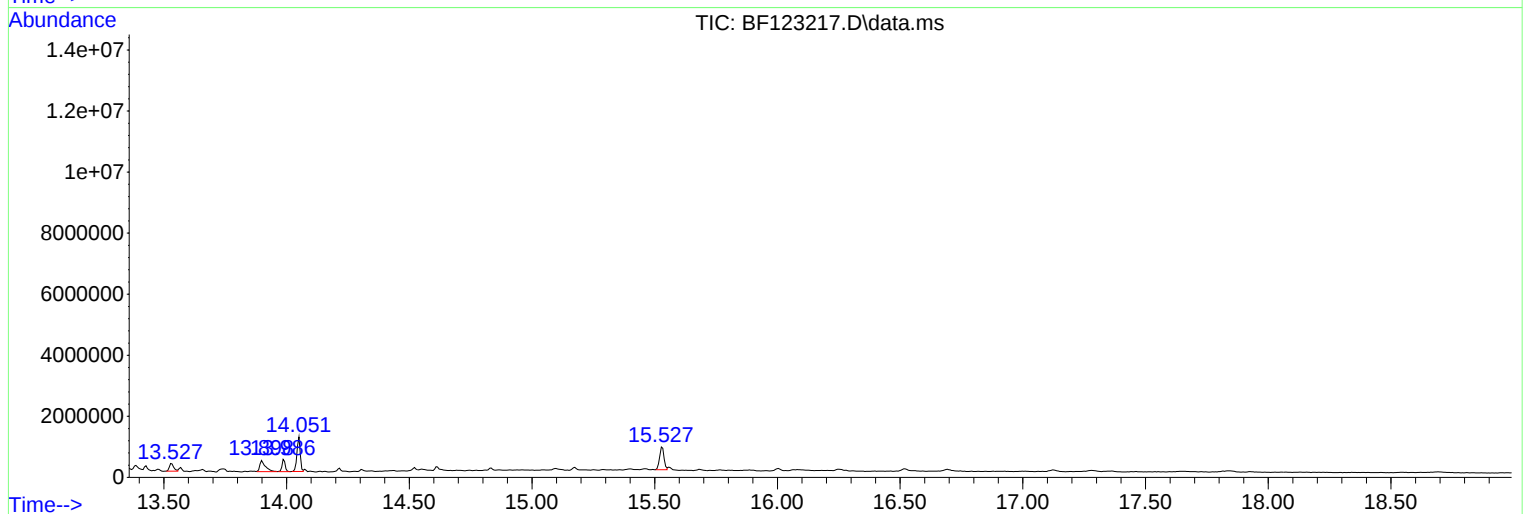
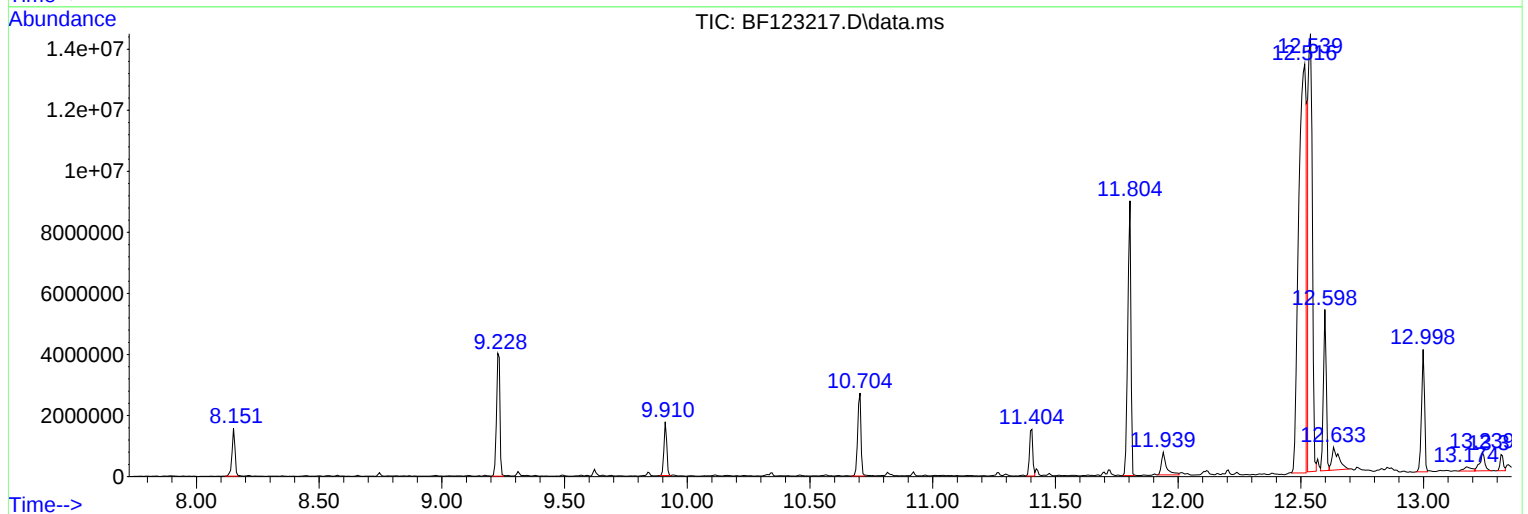
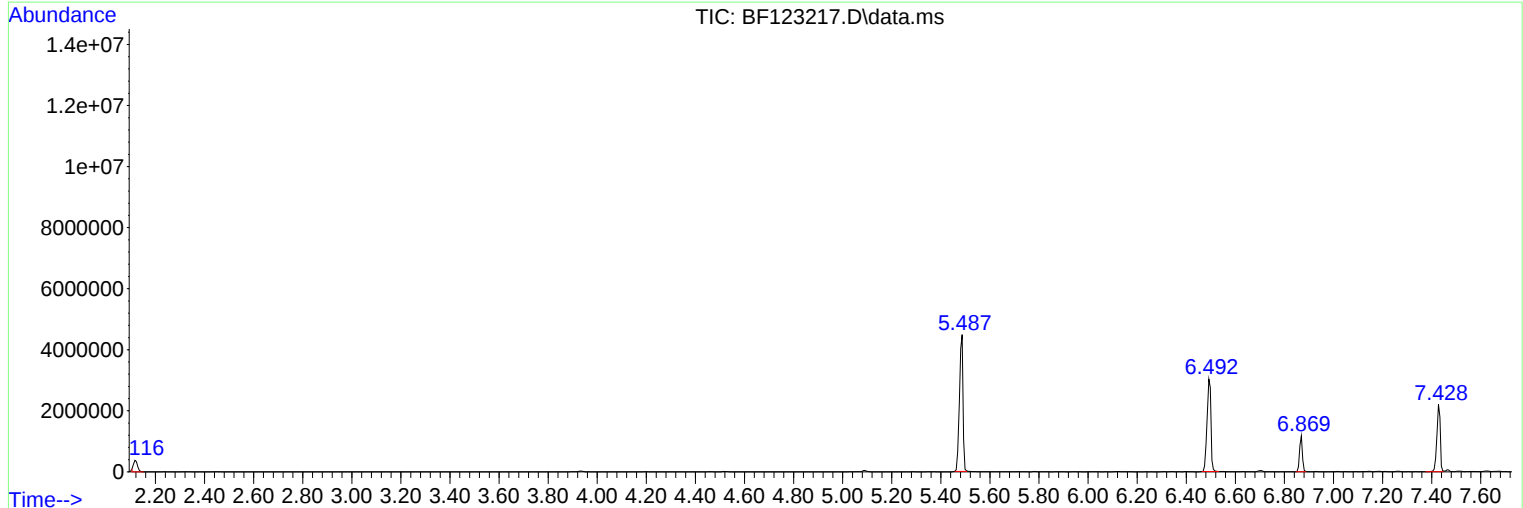
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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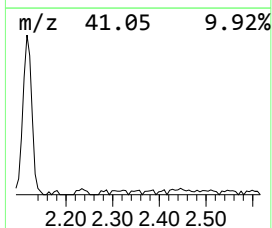
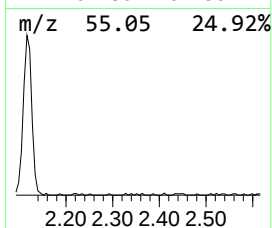
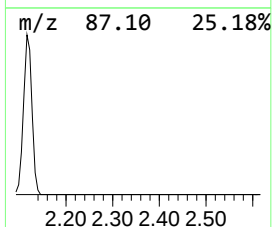
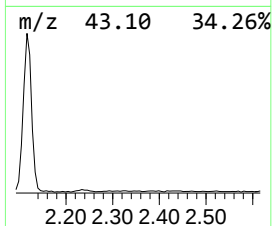
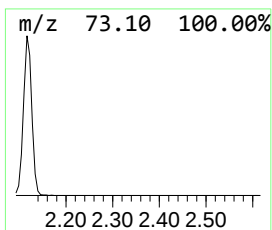
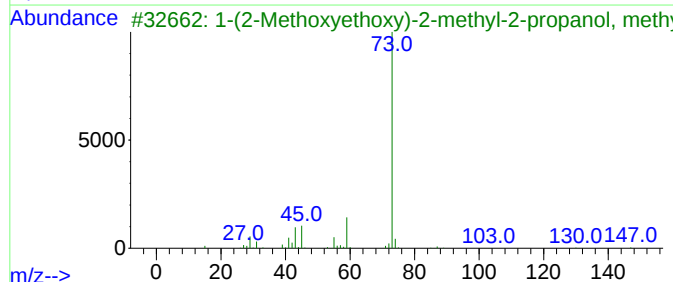
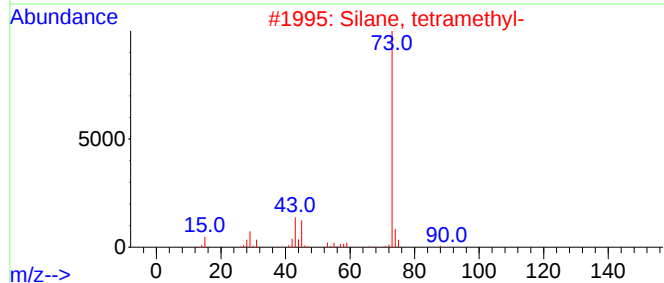
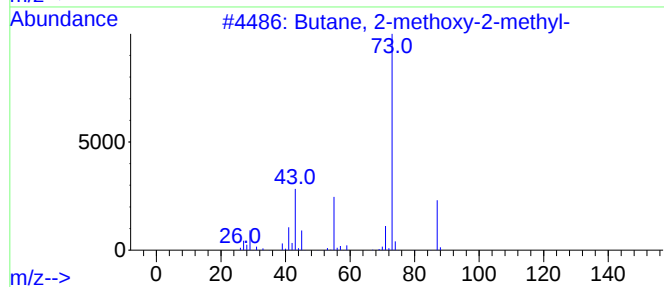
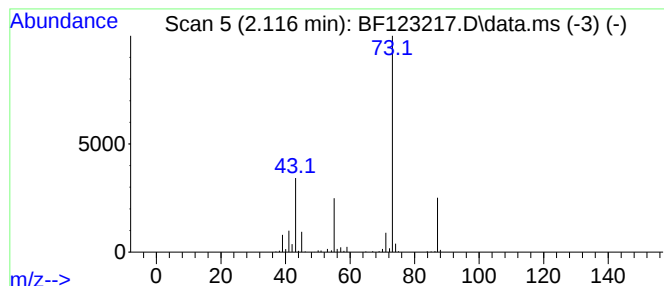
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	8.95 ng	419080	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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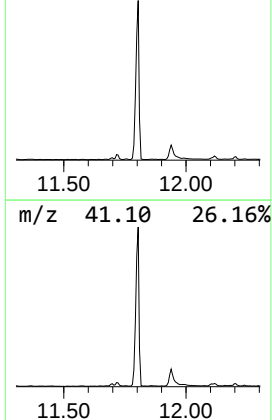
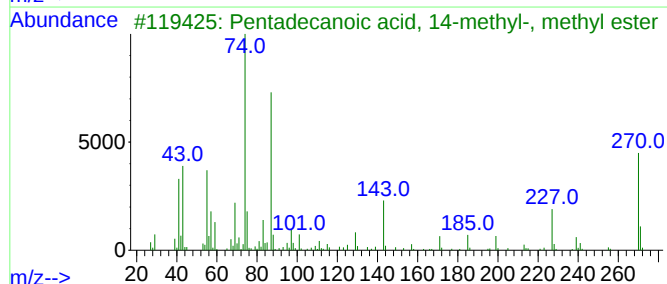
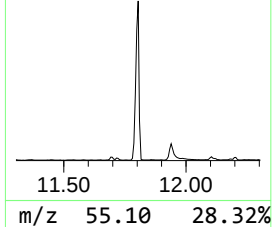
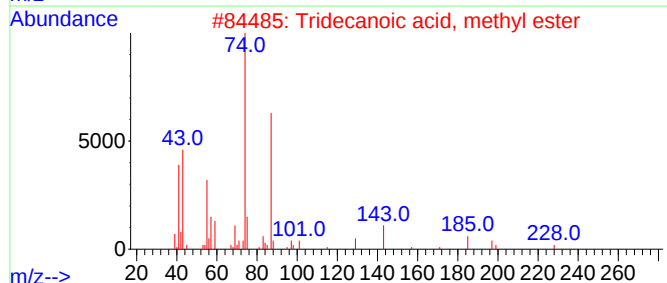
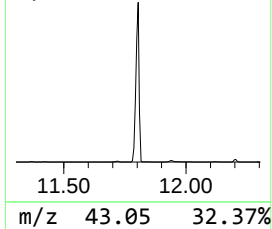
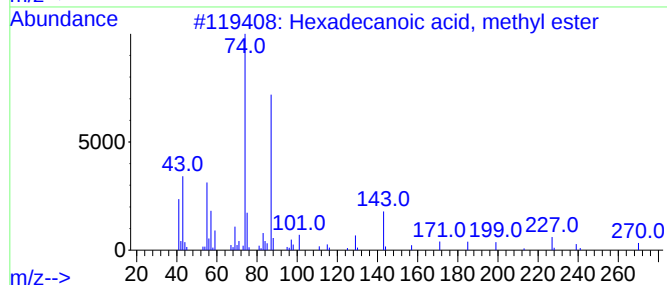
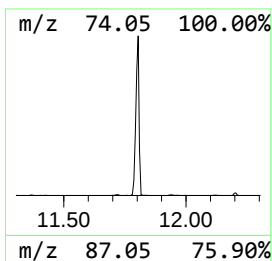
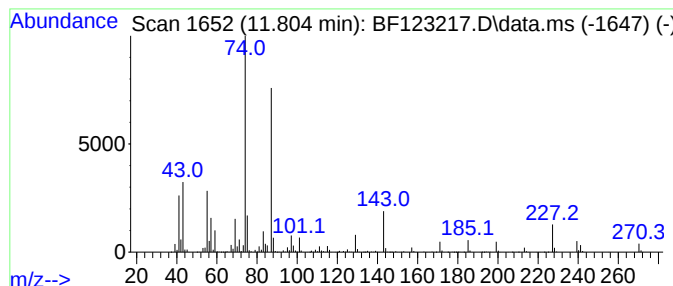
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	112.95 ng	8053230	Phenanthrene-d10	11.404

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	90
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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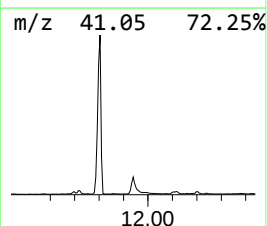
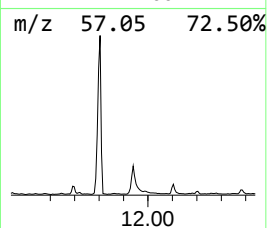
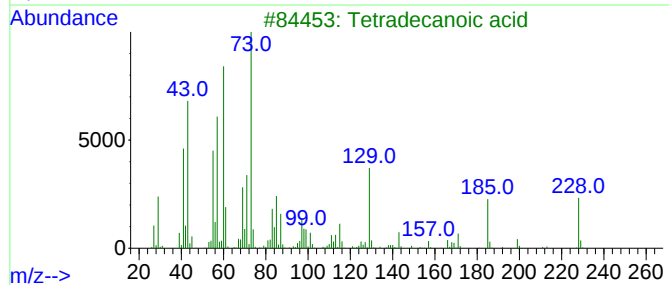
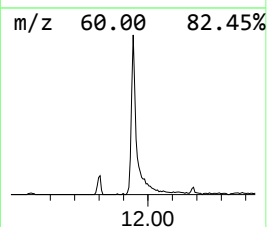
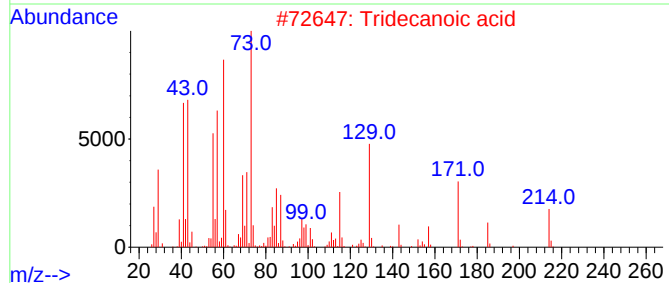
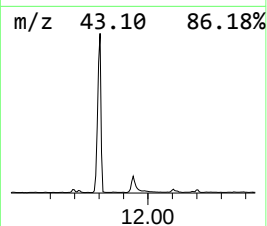
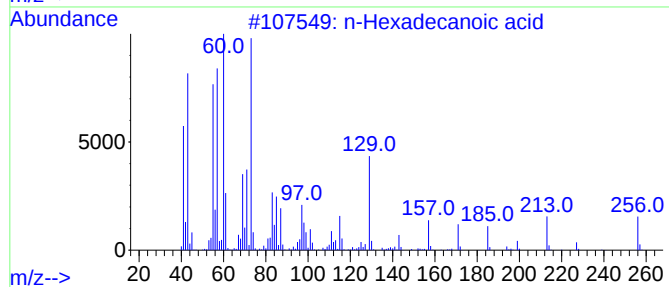
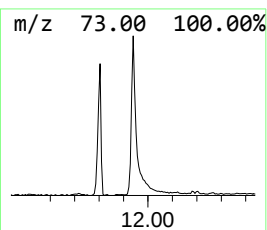
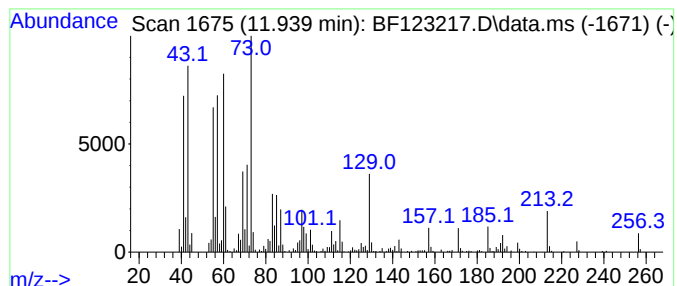
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.939	15.04 ng	1072410	Phenanthrene-d10	11.404	
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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25



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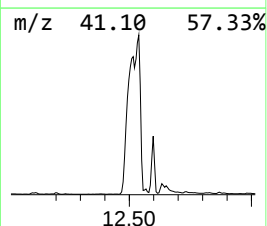
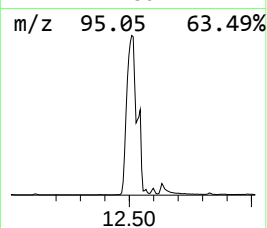
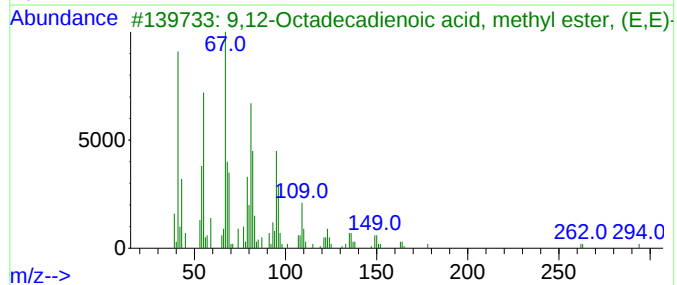
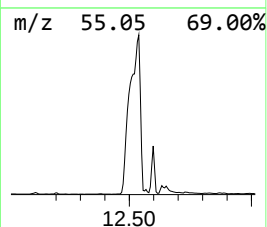
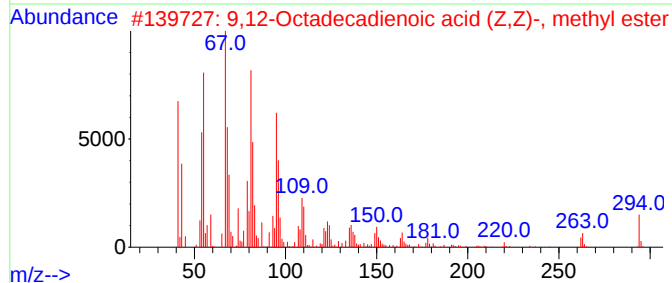
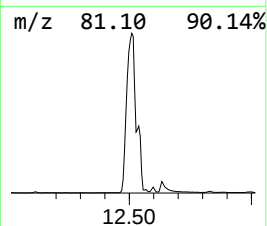
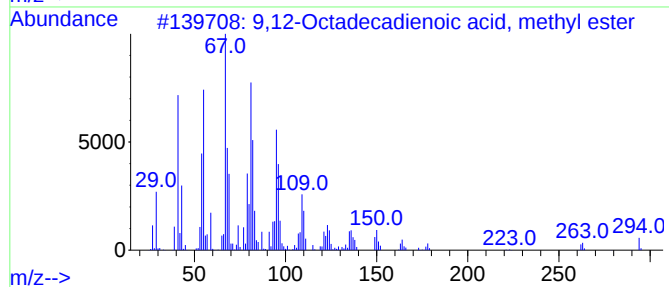
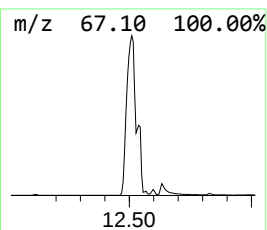
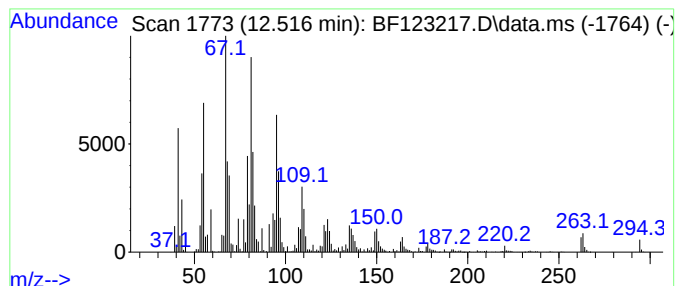
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.516	405.44 ng	28907600	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99



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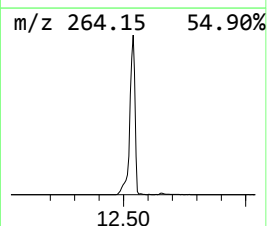
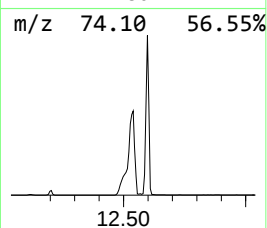
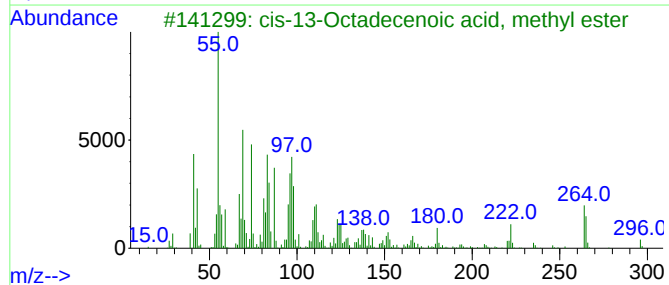
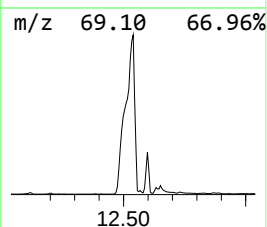
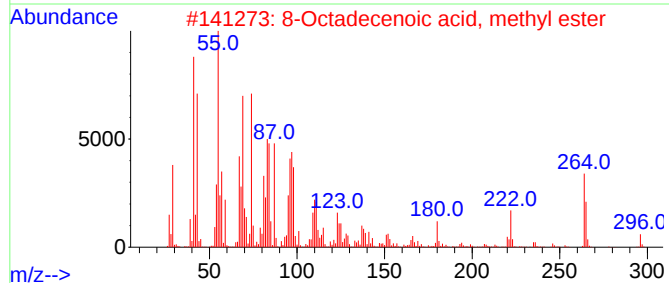
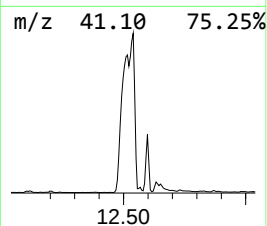
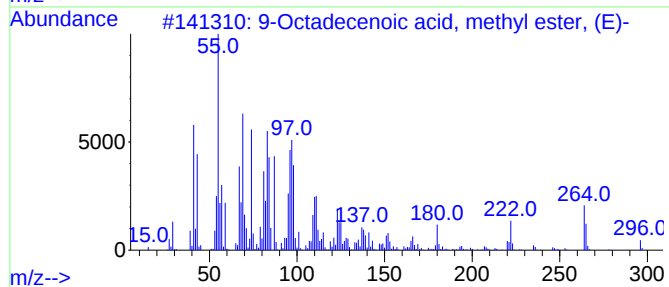
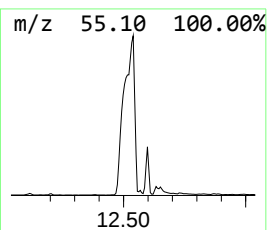
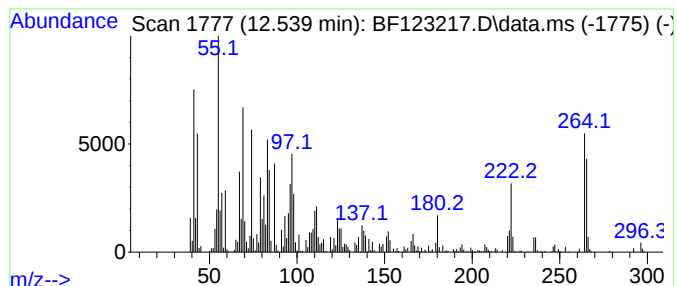
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	214.10 ng	15265300	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2			8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
3			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
4			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
5			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	98



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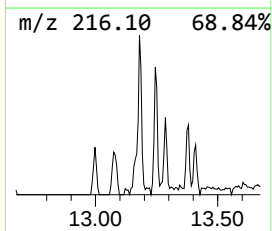
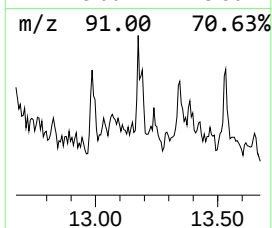
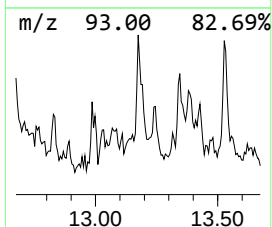
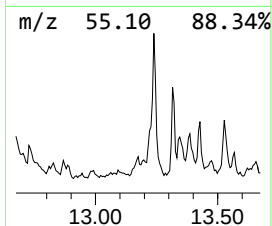
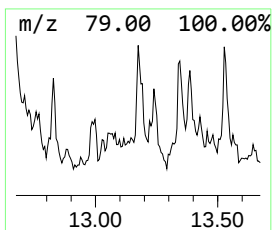
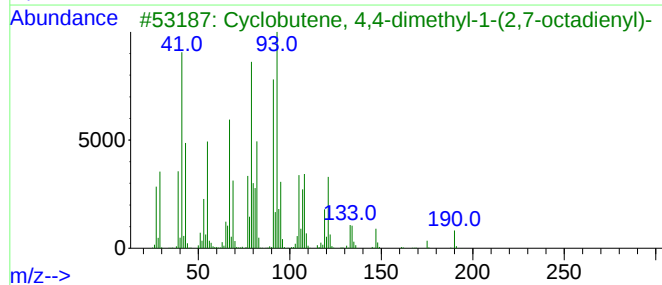
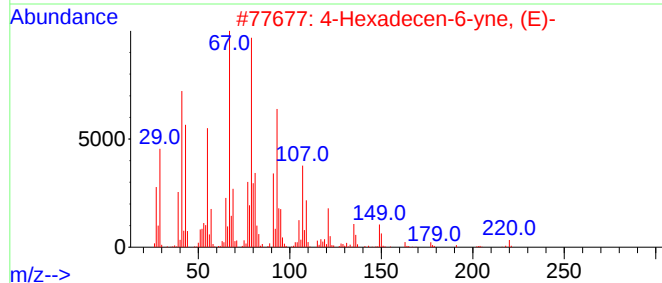
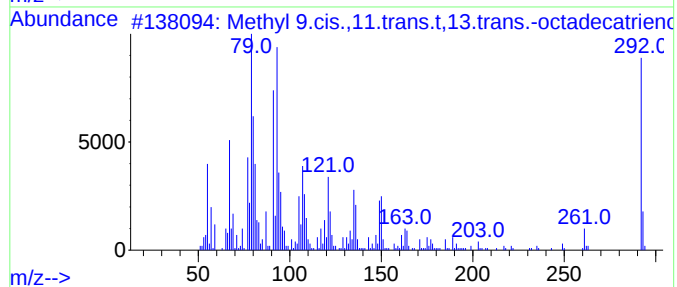
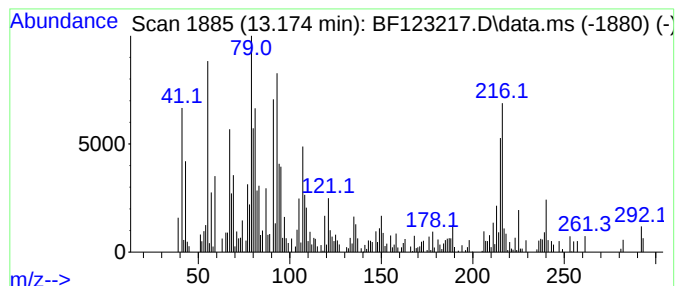
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl 9.cis.,11.trans.t,13... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.174	6.13 ng	322672	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	90
2			4-Hexadecen-6-yne, (E)-	220	C16H28	074744-51-7	70
3			Cyclobutene, 4,4-dimethyl-1-(2,7...	190	C14H22	062338-42-5	64
4			Spiro[2.4]heptane, 1,5-dimethyl-...	136	C10H16	062238-24-8	60
5			Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1000336-37-7	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123217.D
Acq On : 17 Feb 2021 17:46
Operator : JU/CG
Sample : M1423-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-021621

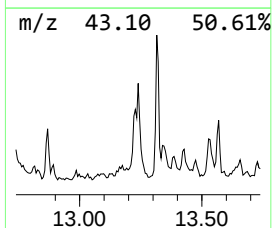
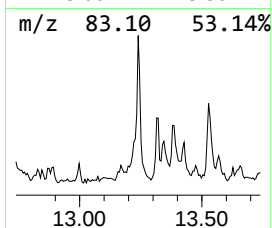
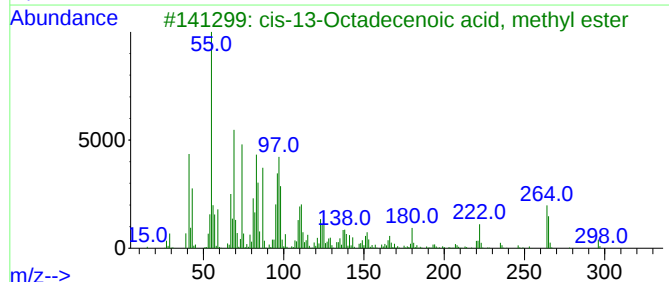
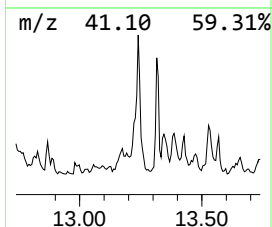
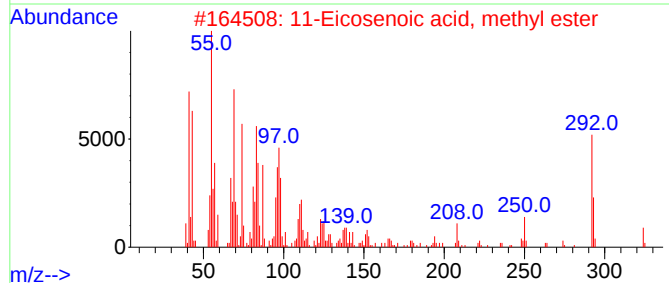
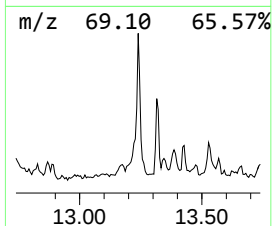
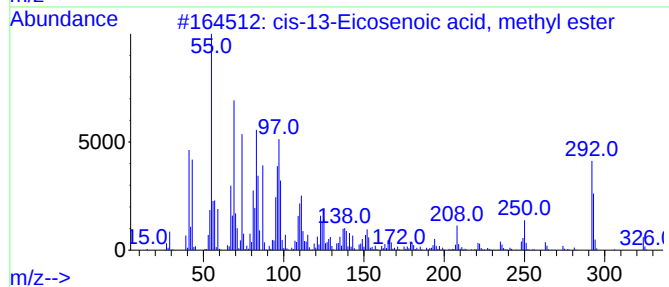
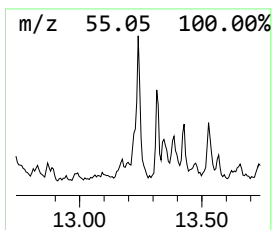
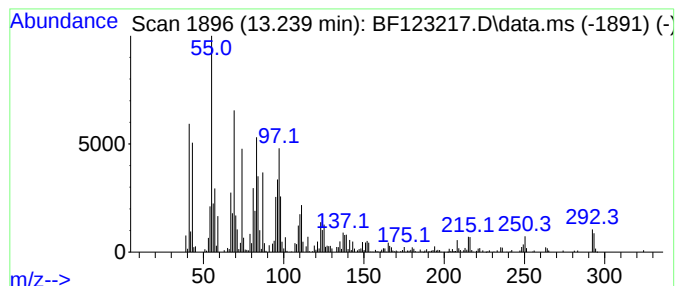
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 cis-13-Eicosenoic acid, met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	15.45 ng	812642	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-52-1	99
2			11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	94
3			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	91
4			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
5			Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123217.D
Acq On : 17 Feb 2021 17:46
Operator : JU/CG
Sample : M1423-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-021621

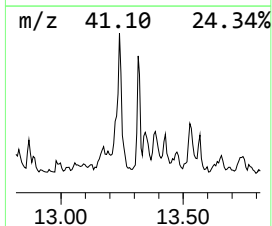
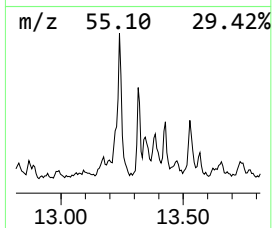
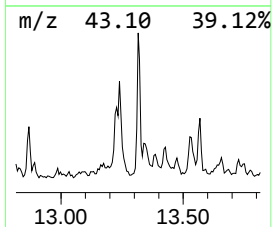
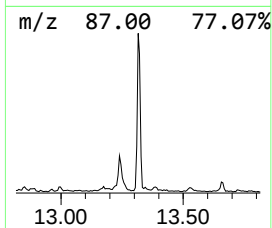
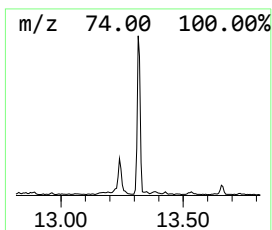
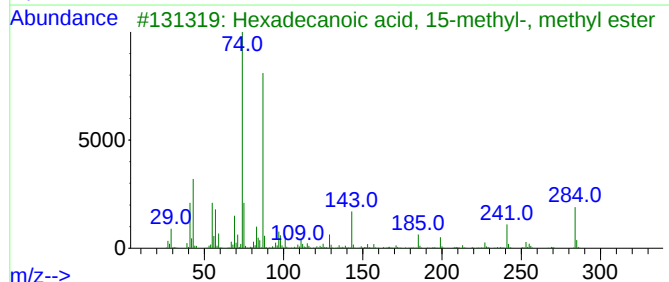
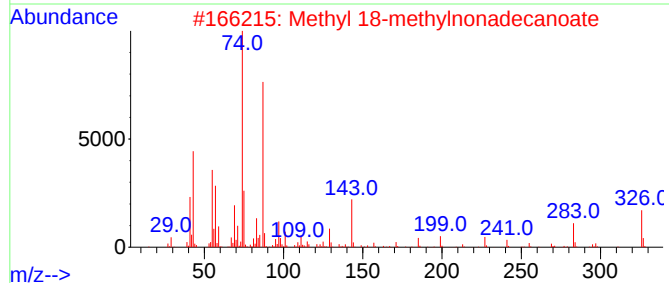
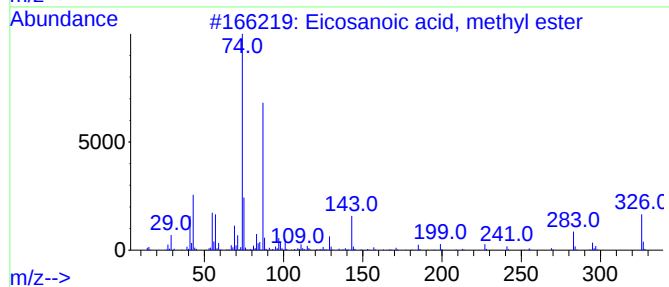
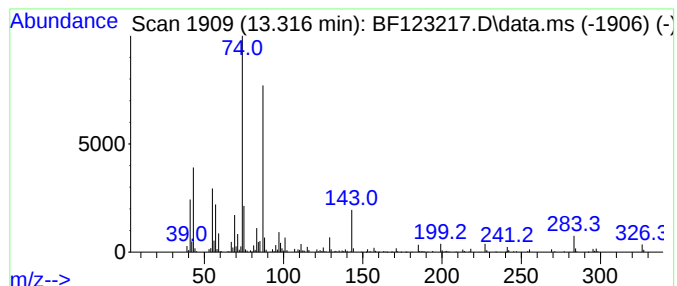
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.316	9.51 ng	500325	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2			Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	98
3			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	94
4			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
5			Methyl stearate	298	C19H38O2	000112-61-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123217.D
Acq On : 17 Feb 2021 17:46
Operator : JU/CG
Sample : M1423-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-021621

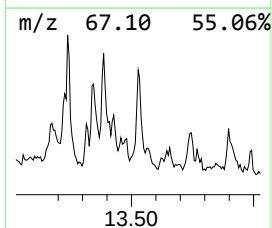
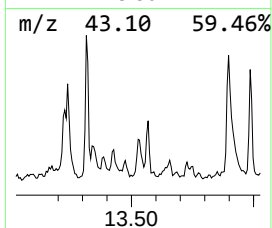
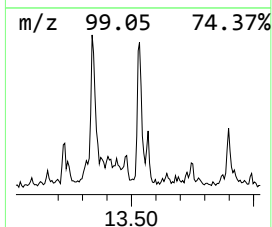
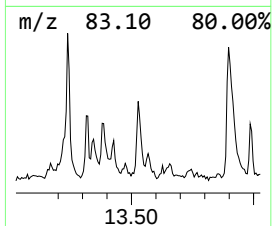
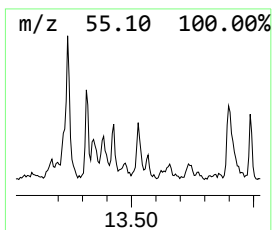
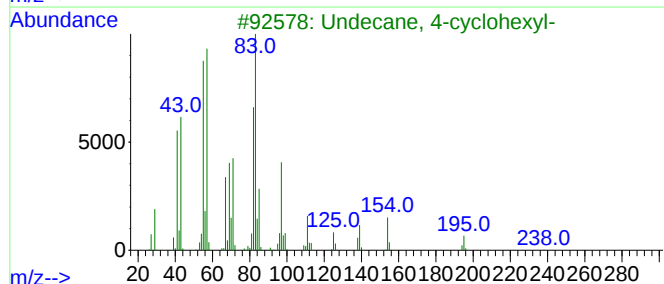
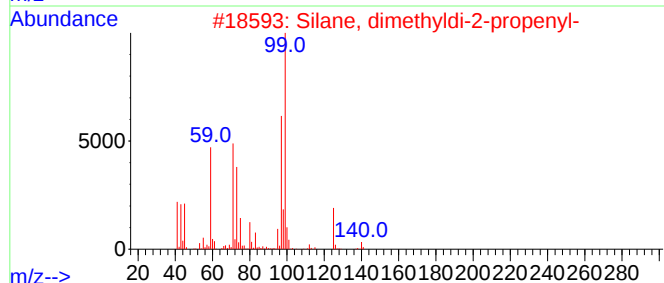
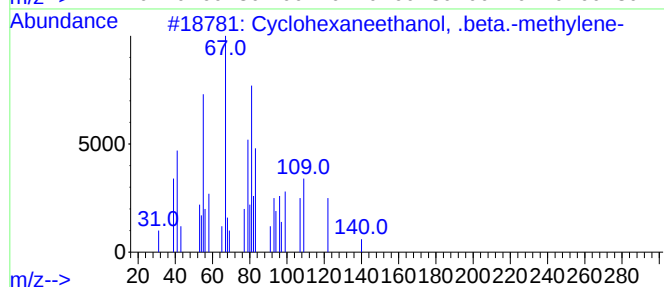
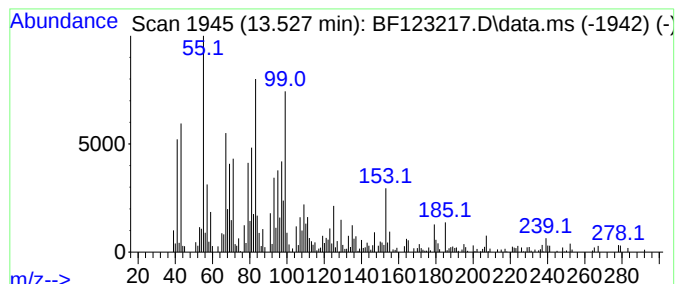
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.527 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.527	6.11 ng	321132	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexaneethanol, .beta.-methy...	140	C9H16O	007697-55-4	45
2			Silane, dimethyldi-2-propenyl-	140	C8H16Si	001113-12-8	38
3			Undecane, 4-cyclohexyl-	238	C17H34	013151-79-6	30
4			4-Chloro-3-n-hexyltetrahydropyran	204	C11H21ClO	066555-66-6	30
5			3-Decen-5-one	154	C10H18O	032064-73-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123217.D
Acq On : 17 Feb 2021 17:46
Operator : JU/CG
Sample : M1423-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-021621

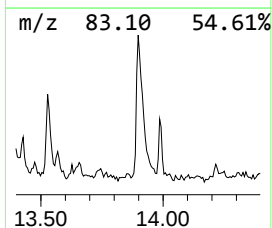
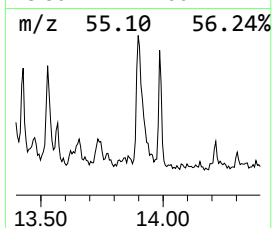
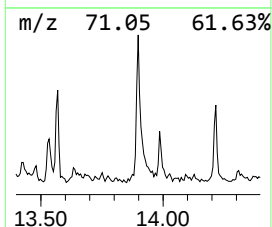
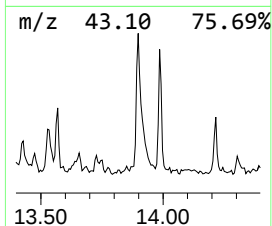
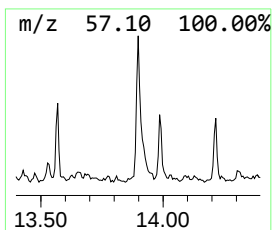
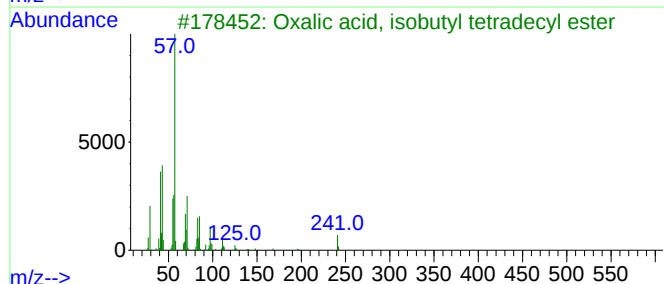
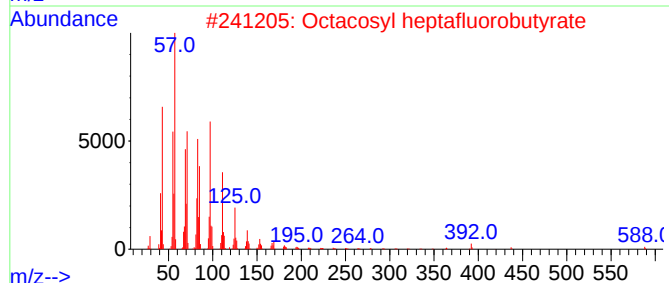
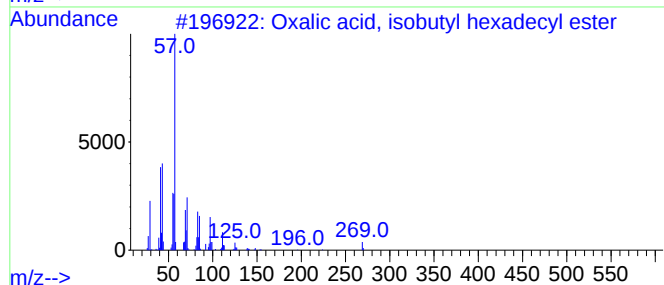
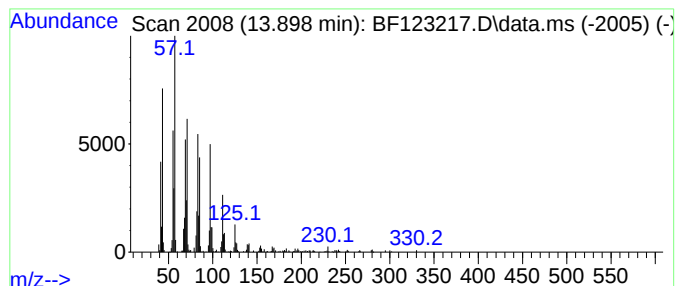
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxalic acid, isobutyl hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	10.94 ng	575611	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91
3			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	86
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123217.D
Acq On : 17 Feb 2021 17:46
Operator : JU/CG
Sample : M1423-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-021621

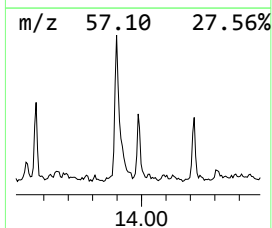
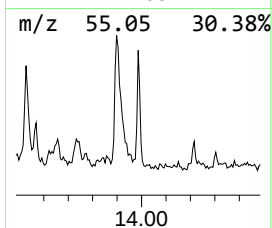
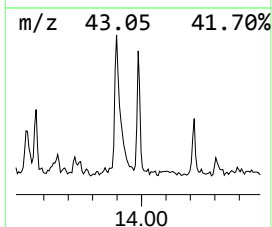
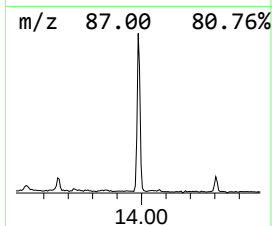
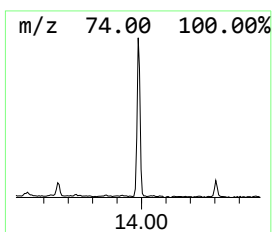
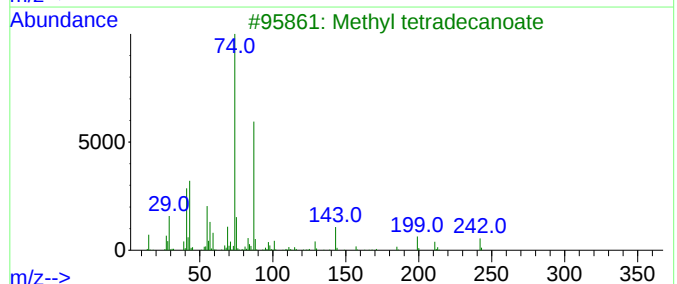
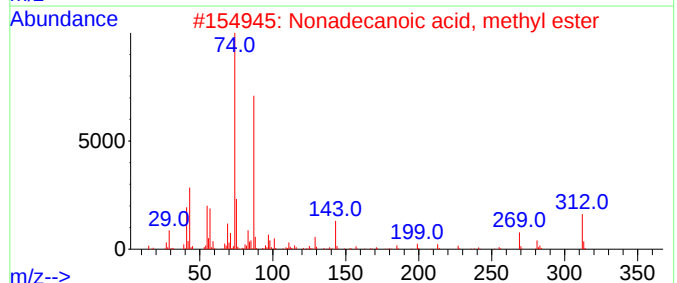
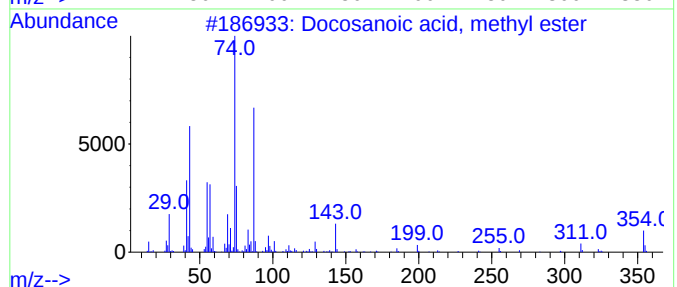
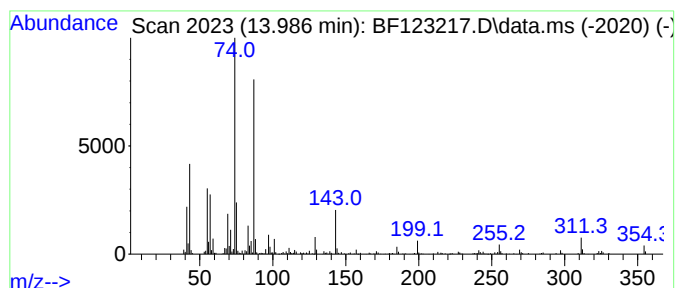
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Docosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	6.84 ng	359801	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	93
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4			Methyl stearate	298	C19H38O2	000112-61-8	87
5			Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123217.D
Acq On : 17 Feb 2021 17:46
Operator : JU/CG
Sample : M1423-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-021621

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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
Butane, 2-metho...	2.116	8.9	ng	419080	1	6.869	936390	20.0
Hexadecanoic ac...	11.804	113.0	ng	8053230	4	11.404	1426010	20.0
n-Hexadecanoic ...	11.939	15.0	ng	1072410	4	11.404	1426010	20.0
9,12-Octadecadi...	12.516	405.4	ng	28907600	4	11.404	1426010	20.0
9-Octadecenoic ...	12.539	214.1	ng	15265300	4	11.404	1426010	20.0
Methyl 9.cis.,1...	13.174	6.1	ng	322672	5	14.051	1051960	20.0
cis-13-Eicoseno...	13.239	15.4	ng	812642	5	14.051	1051960	20.0
Eicosanoic acid...	13.316	9.5	ng	500325	5	14.051	1051960	20.0
unknown13.527	13.527	6.1	ng	321132	5	14.051	1051960	20.0
Oxalic acid, is...	13.898	10.9	ng	575611	5	14.051	1051960	20.0
Docosanoic acid...	13.986	6.8	ng	359801	5	14.051	1051960	20.0