

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
 Data File : BF123425.D
 Acq On : 24 Mar 2021 6:29
 Operator : JU/CG
 Sample : M1779-04
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4B2-(4.0-4.5)

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-BF032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123425.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	22	30	36	rBV	1180013	1493306	24.29%	3.501%
2	2.375	44	49	54	rVB	209946	268166	4.36%	0.629%
3	5.151	512	521	526	rBV	221954	287825	4.68%	0.675%
4	5.534	581	586	589	rBV	5080646	5296353	86.13%	12.417%
5	6.533	750	756	760	rBV	5091714	5726062	93.12%	13.424%
6	6.916	817	821	824	rBV	1721843	1503542	24.45%	3.525%
7	7.475	910	916	919	rBV	3589203	3645403	59.28%	8.546%
8	8.198	1034	1039	1042	rBV	2294428	1975254	32.12%	4.631%
9	9.274	1217	1222	1226	rBV	5947821	6149087	100.00%	14.416%
10	9.669	1285	1289	1293	rBV	268232	230158	3.74%	0.540%
11	9.957	1333	1338	1342	rBV	2630489	2216974	36.05%	5.197%
12	10.745	1468	1472	1476	rBV	3493241	3185265	51.80%	7.467%
13	11.451	1588	1592	1595	rBV	2152698	1980776	32.21%	4.644%
14	11.974	1675	1681	1684	rBV	188515	180871	2.94%	0.424%
15	12.433	1756	1759	1763	rBV	106364	101077	1.64%	0.237%
16	12.715	1800	1807	1812	rBV2	47178	87822	1.43%	0.206%
17	13.039	1858	1862	1866	rBV	4557747	4487067	72.97%	10.519%
18	13.598	1951	1957	1963	rBV	216797	219520	3.57%	0.515%
19	13.951	2013	2017	2031	rBV	473029	592661	9.64%	1.389%
20	14.098	2038	2042	2045	rBV	1162529	1089189	17.71%	2.553%
21	14.433	2094	2099	2102	rBV4	50739	92834	1.51%	0.218%
22	14.527	2109	2115	2119	rBV7	30165	77921	1.27%	0.183%
23	14.574	2119	2123	2125	rBV	98719	136068	2.21%	0.319%
24	14.739	2147	2151	2158	rBV	200125	319569	5.20%	0.749%
25	15.603	2292	2298	2302	rBV	941612	1188911	19.33%	2.787%
26	16.180	2391	2396	2402	rBV4	55137	123907	2.02%	0.290%

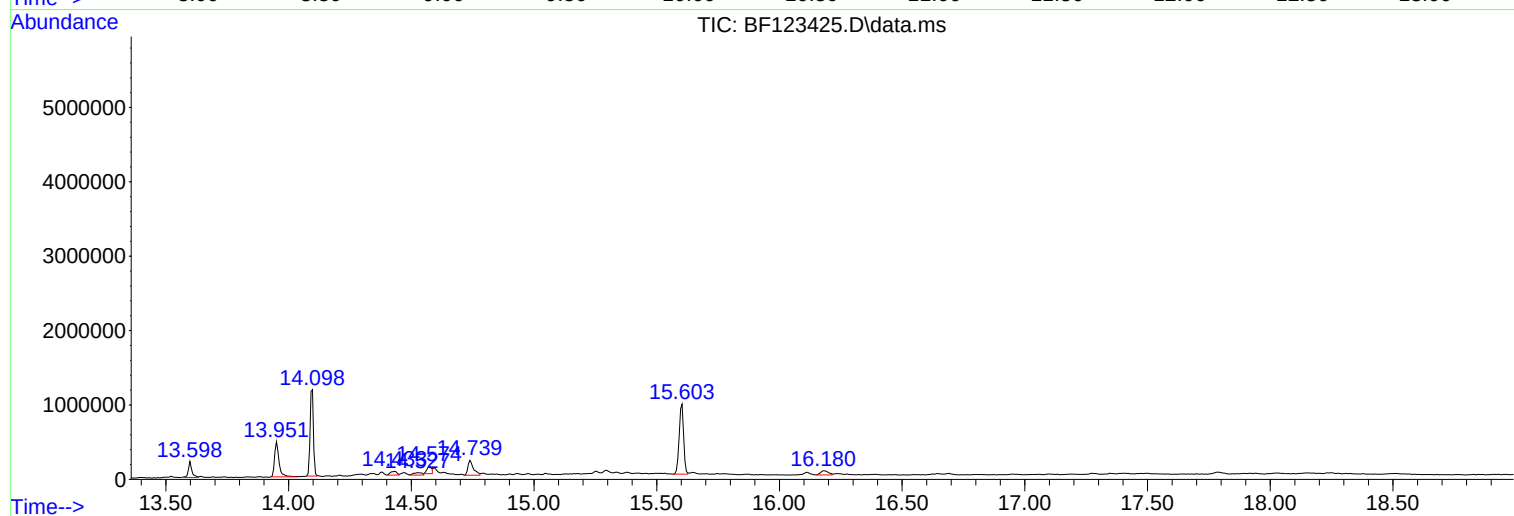
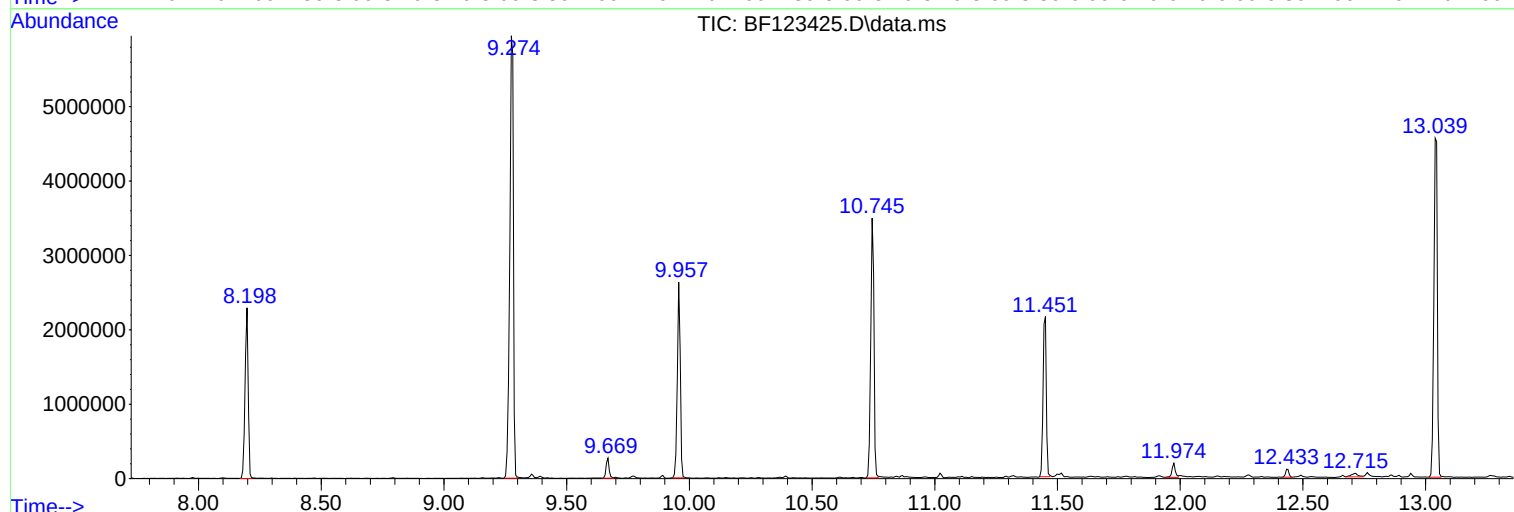
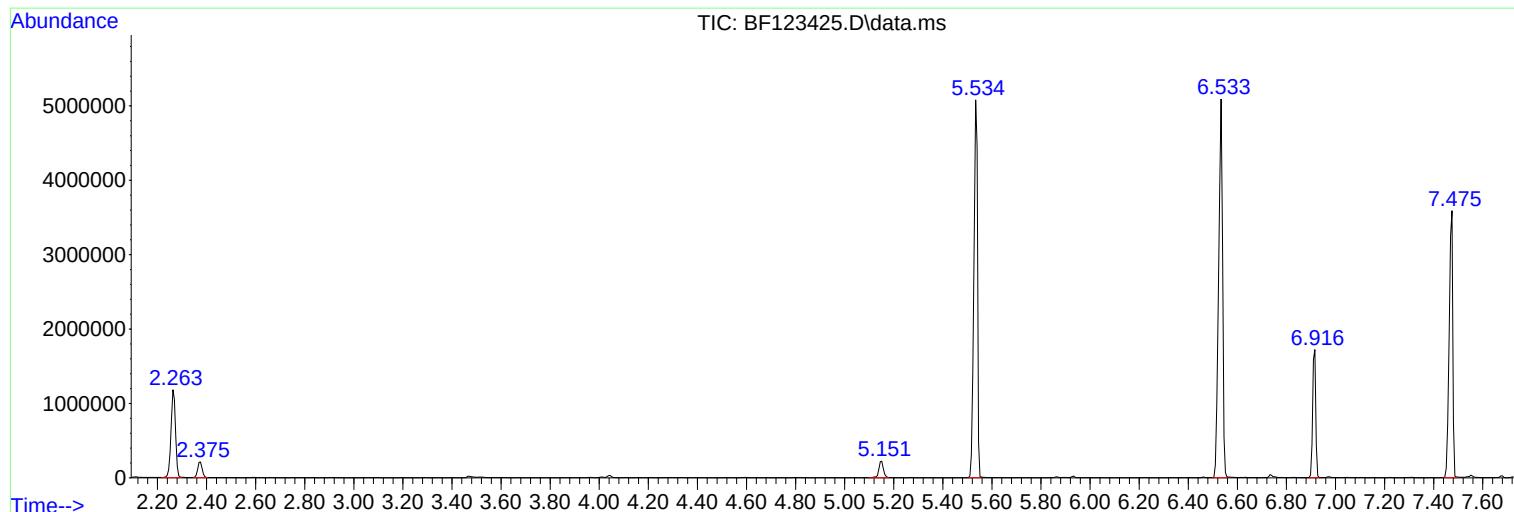
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ClientSampleId :
SB-4B2-(4.0-4.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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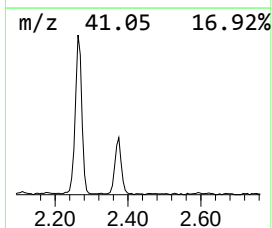
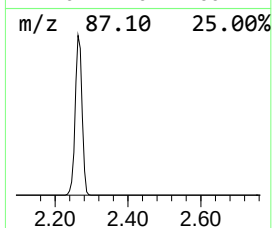
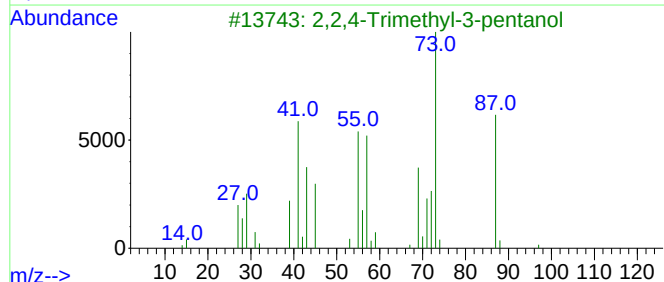
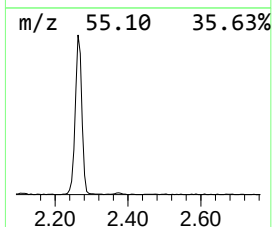
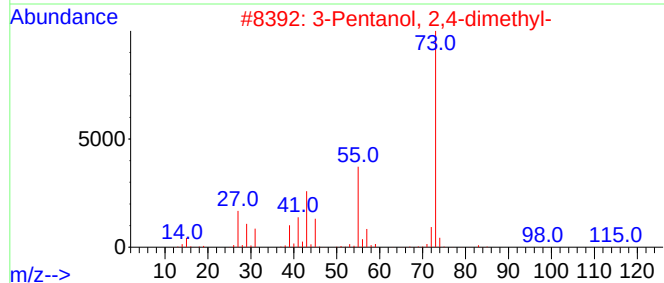
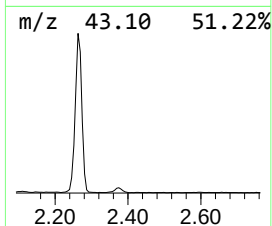
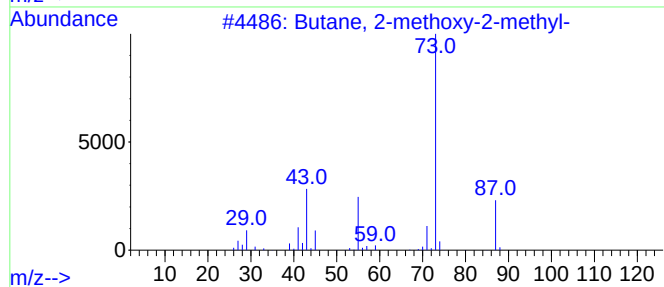
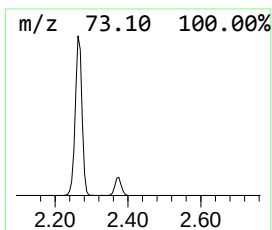
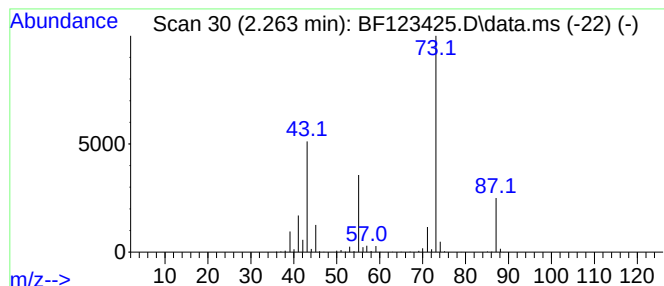
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	19.86 ng	1493310	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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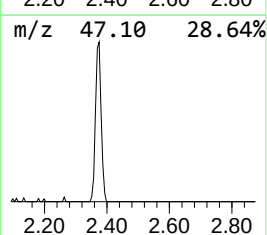
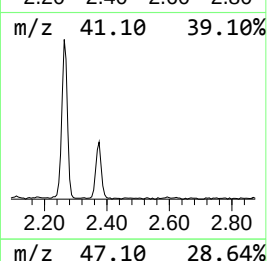
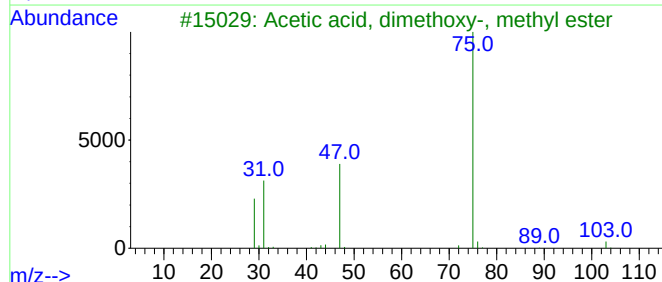
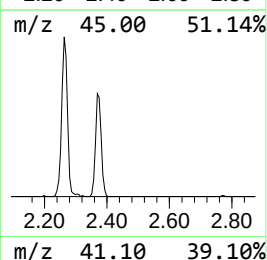
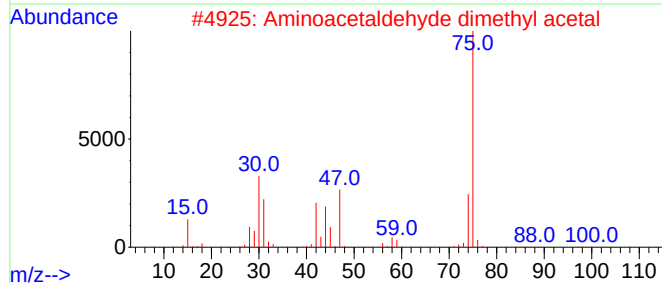
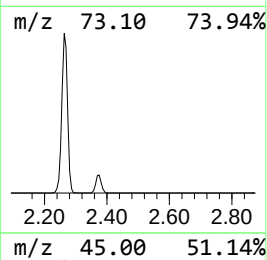
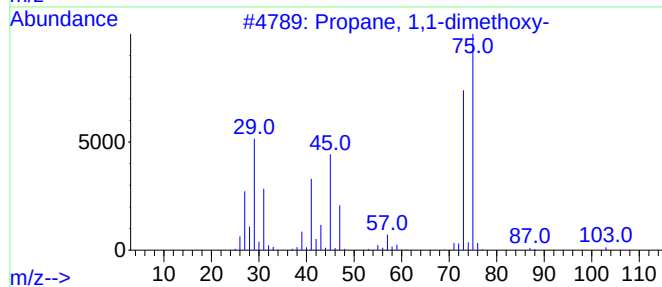
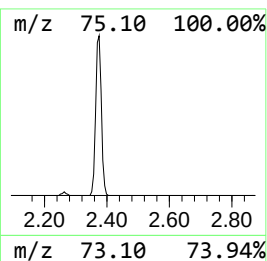
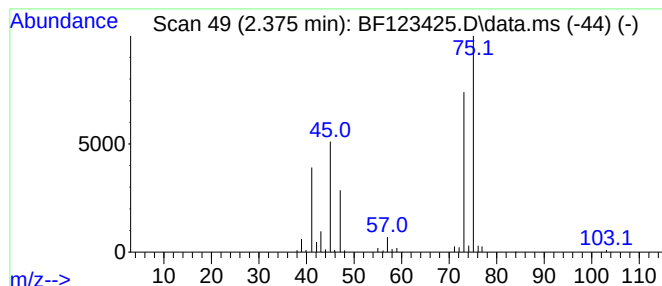
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.375	3.57 ng	268166	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
3			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
4			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22



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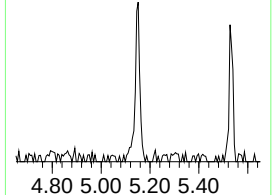
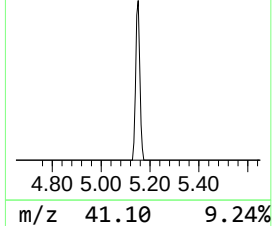
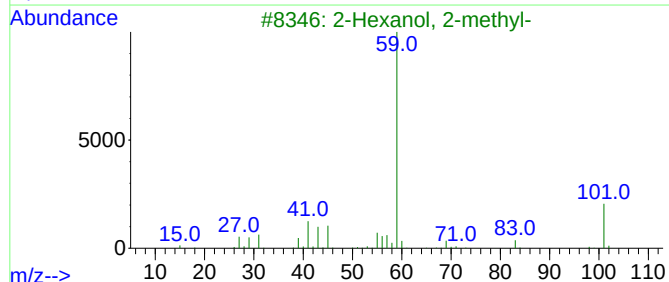
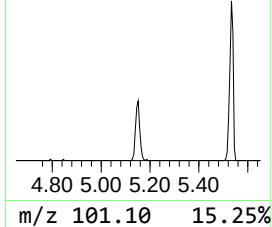
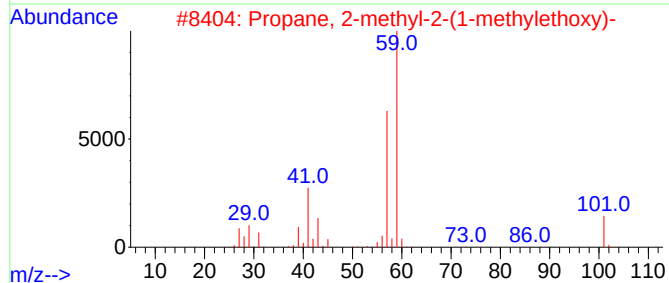
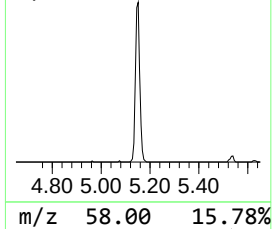
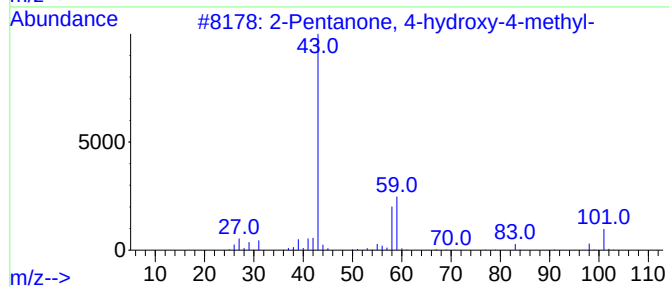
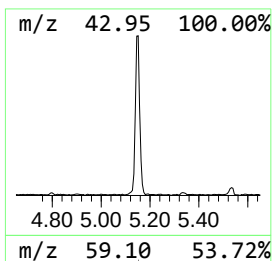
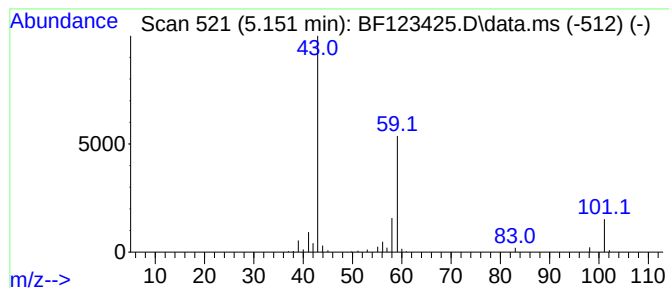
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BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.151	3.83 ng	287825	1,4-Dichlorobenzene-d4			6.916
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10



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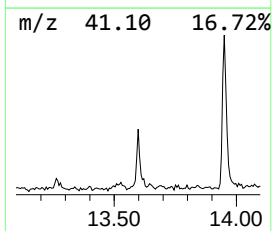
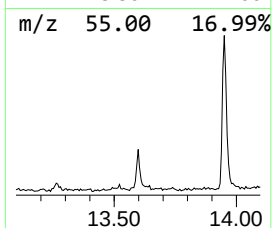
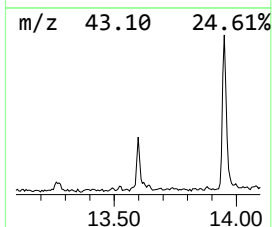
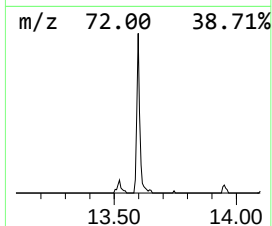
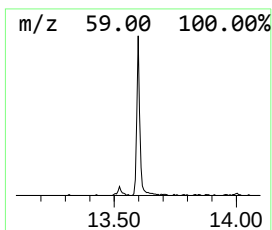
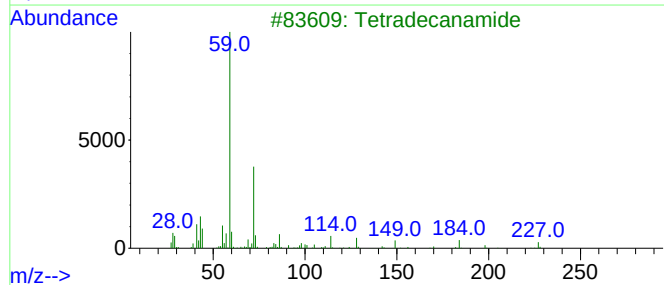
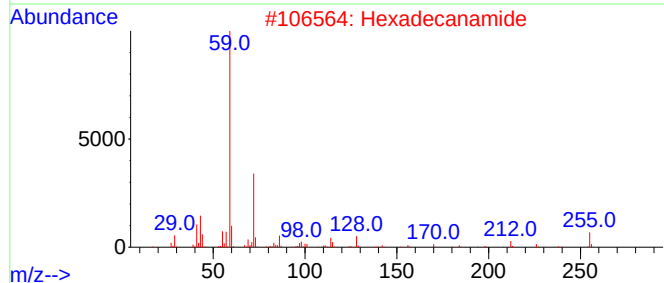
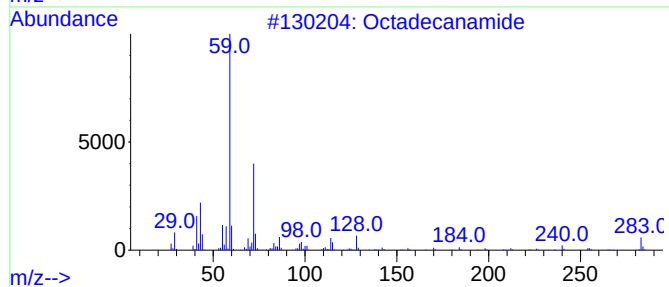
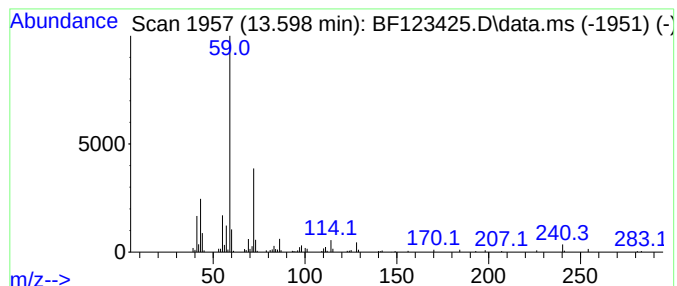
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Peak Number 4 Octadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.598	4.03 ng	219520	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanamide	283	C18H37NO	000124-26-5	90
2			Hexadecanamide	255	C16H33NO	000629-54-9	86
3			Tetradecanamide	227	C14H29NO	000638-58-4	86
4			Dodecanamide	199	C12H25NO	001120-16-7	78
5			Nonanamide	157	C9H19NO	001120-07-6	72



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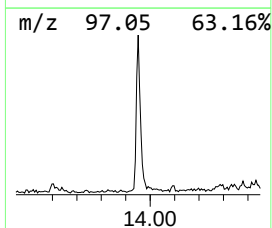
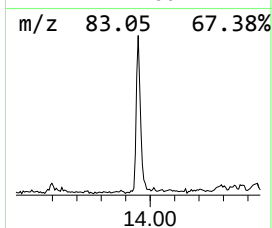
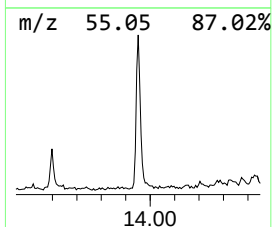
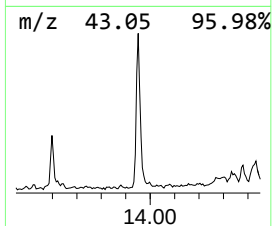
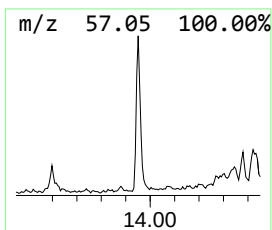
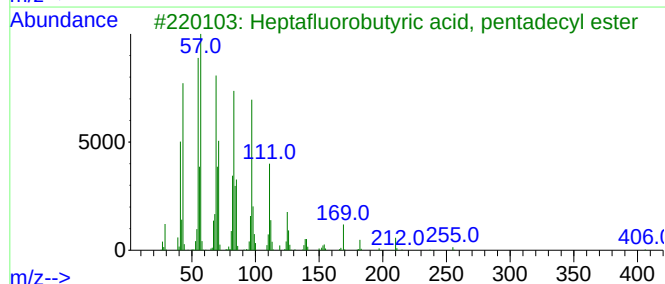
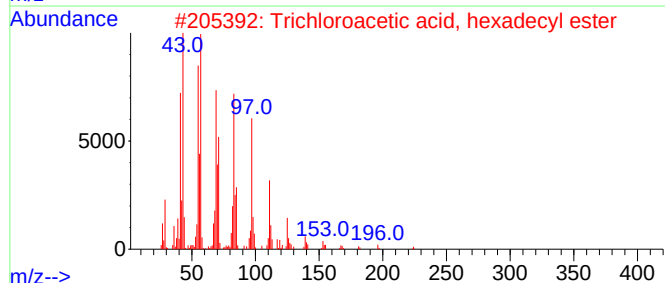
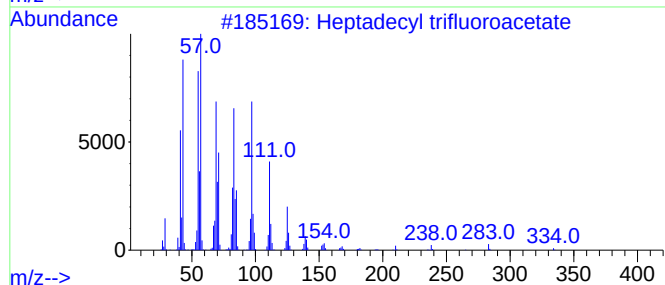
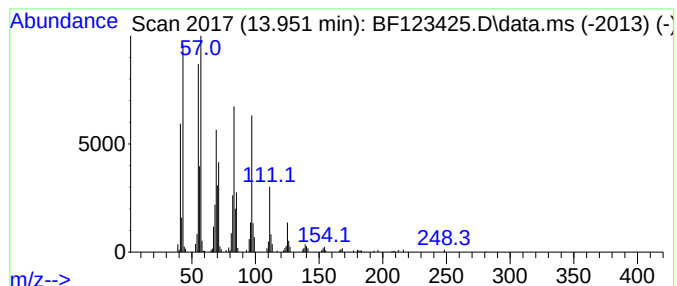
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	10.88 ng	592661	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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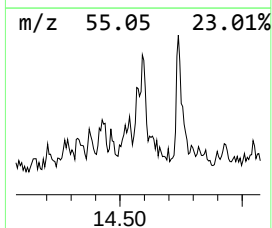
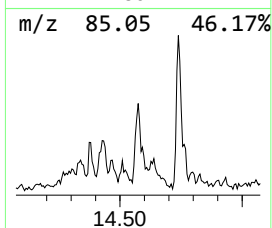
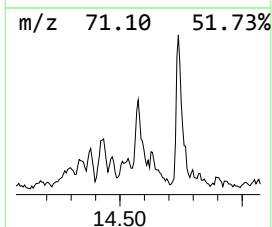
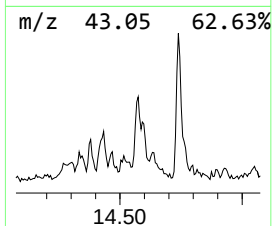
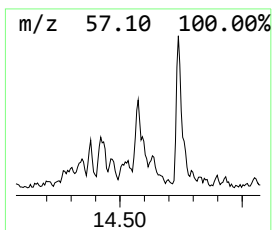
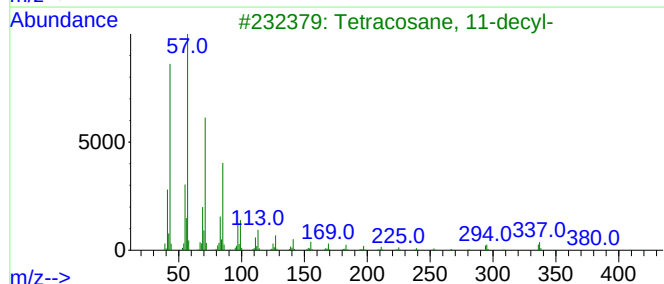
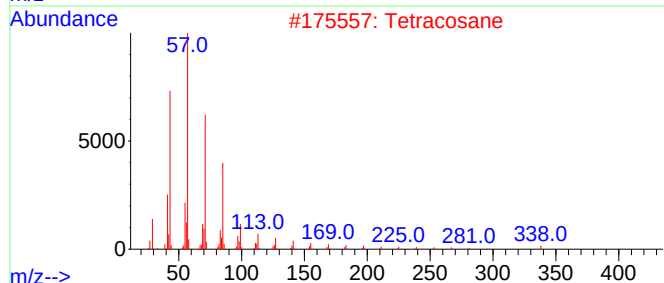
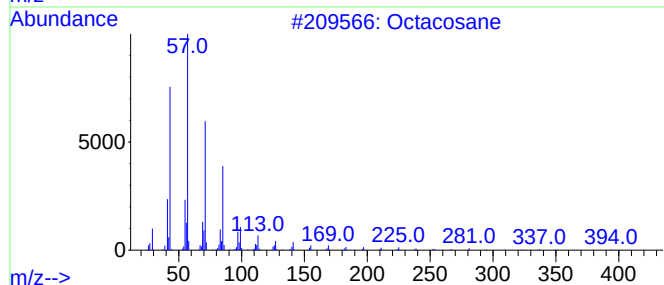
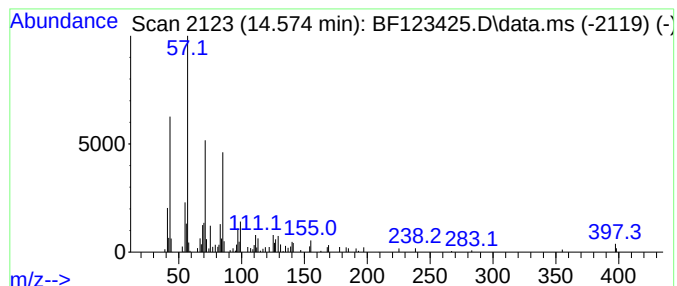
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	2.50 ng	136068	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Tetracosane	338	C24H50	000646-31-1	87
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4			9-methylheptadecane	254	C18H38	026741-18-4	83
5			Docosane	310	C22H46	000629-97-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
Data File : BF123425.D
Acq On : 24 Mar 2021 6:29
Operator : JU/CG
Sample : M1779-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4B2-(4.0-4.5)

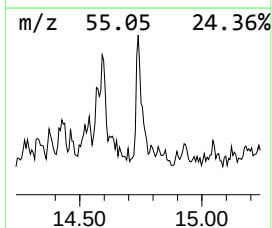
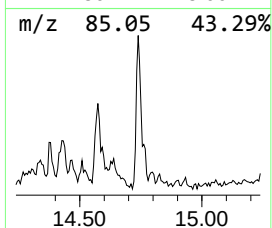
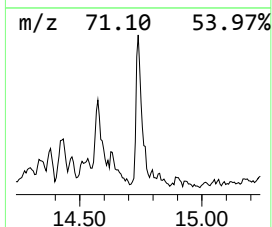
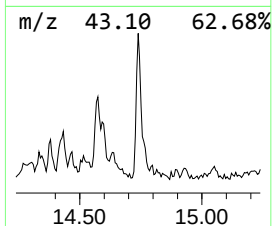
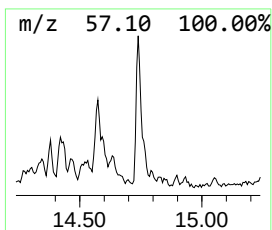
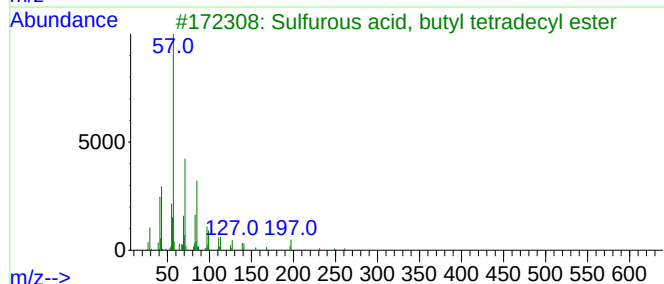
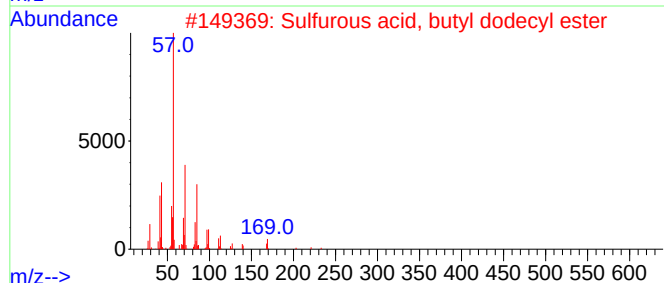
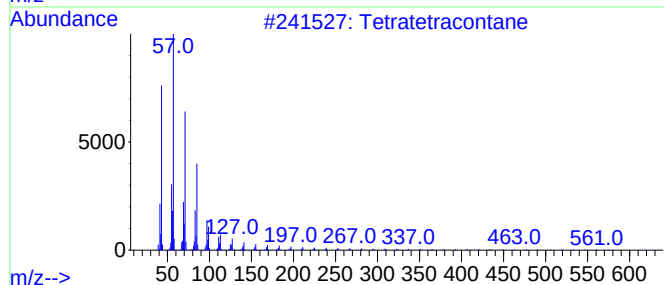
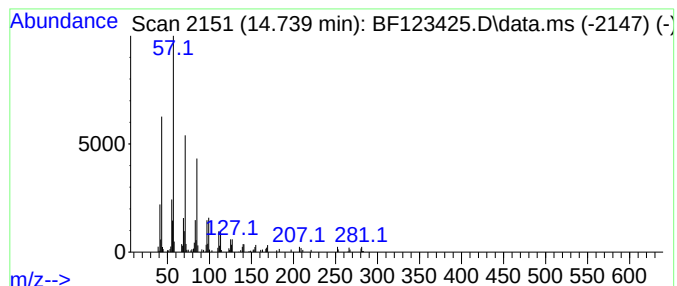
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	5.87 ng	319569	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	91
3			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
Data File : BF123425.D
Acq On : 24 Mar 2021 6:29
Operator : JU/CG
Sample : M1779-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4B2-(4.0-4.5)

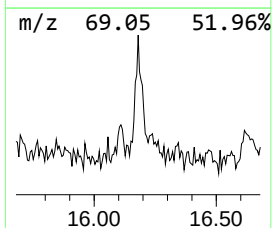
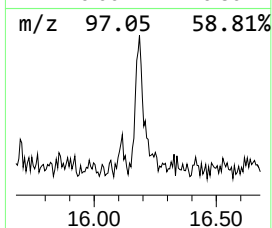
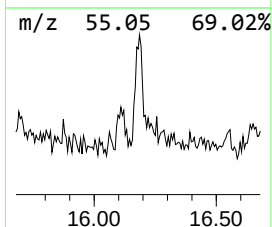
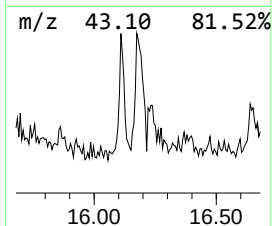
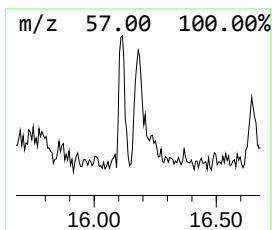
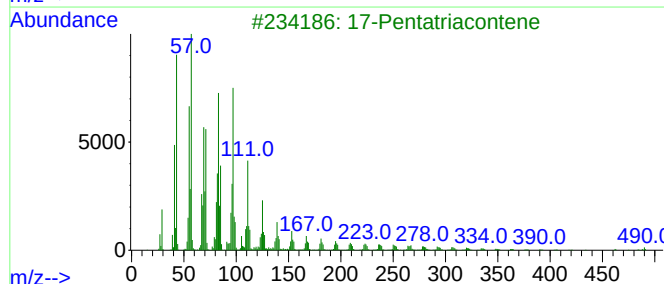
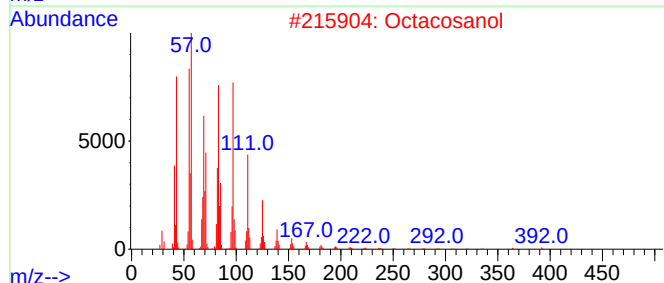
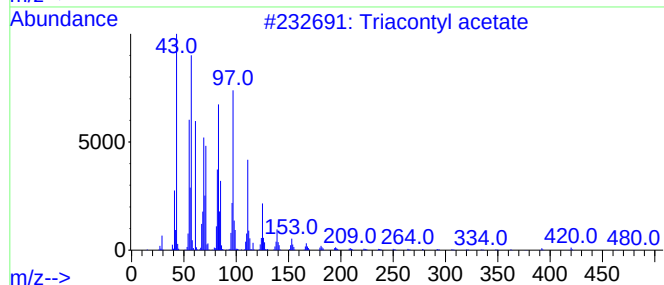
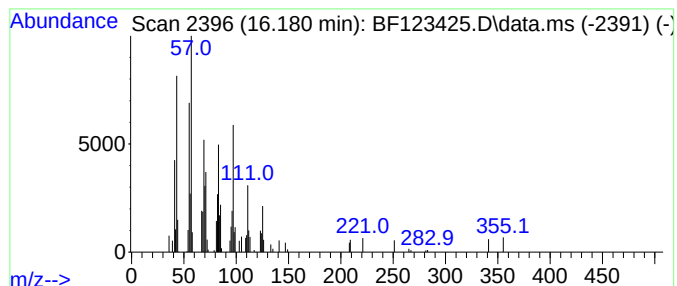
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacetyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.180	2.08 ng	123907	Perylene-d12	15.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacetyl acetate	480	C32H64O2	041755-58-2	87
2			Octacosanol	410	C28H58O	000557-61-9	87
3			17-Pentatriacontene	491	C35H70	006971-40-0	81
4			1-Heptacosanol	396	C27H56O	002004-39-9	76
5			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
Data File : BF123425.D
Acq On : 24 Mar 2021 6:29
Operator : JU/CG
Sample : M1779-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4B2-(4.0-4.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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
Butane, 2-metho...	2.263	19.9	ng	1493310	1	6.916	1503540	20.0
Propane, 1,1-di...	2.375	3.6	ng	268166	1	6.916	1503540	20.0
2-Pentanone, 4-...	5.151	3.8	ng	287825	1	6.916	1503540	20.0
Octadecanamide	13.598	4.0	ng	219520	5	14.098	1089190	20.0
Heptadecyl trif...	13.951	10.9	ng	592661	5	14.098	1089190	20.0
Octacosane	14.574	2.5	ng	136068	5	14.098	1089190	20.0
Tetratetracontane	14.739	5.9	ng	319569	5	14.098	1089190	20.0
Triacetyl acetate	16.180	2.1	ng	123907	6	15.604	1188910	20.0