

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
 Data File : BF123424.D
 Acq On : 24 Mar 2021 5:57
 Operator : JU/CG
 Sample : M1779-02
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3B1-(3.0-3.5)

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: BF123424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	24	31	43	rVB	1195484	1485744	22.35%	3.339%
2	2.375	45	49	55	rBV	217173	280299	4.22%	0.630%
3	5.151	517	521	528	rVB	245825	294722	4.43%	0.662%
4	5.540	581	587	590	rBV	5177260	5585794	84.03%	12.555%
5	6.534	750	756	759	rBV	5181856	5903433	88.80%	13.269%
6	6.916	817	821	824	rBV	1682725	1517300	22.82%	3.410%
7	7.475	910	916	919	rBV	3797015	3851612	57.94%	8.657%
8	8.198	1034	1039	1042	rBV	2313095	2007010	30.19%	4.511%
9	9.280	1217	1223	1226	rBV	6454277	6647702	100.00%	14.941%
10	9.669	1285	1289	1293	rBV	179561	150472	2.26%	0.338%
11	9.957	1333	1338	1342	rBV	2636986	2238307	33.67%	5.031%
12	10.745	1468	1472	1476	rBV	3761774	3338308	50.22%	7.503%
13	11.451	1588	1592	1595	rBV	2184525	1993769	29.99%	4.481%
14	11.974	1677	1681	1692	rBV	242102	234871	3.53%	0.528%
15	12.433	1756	1759	1763	rVB	82751	76455	1.15%	0.172%
16	12.716	1800	1807	1812	rBV2	67547	121901	1.83%	0.274%
17	12.763	1812	1815	1823	rVB2	86703	95010	1.43%	0.214%
18	13.045	1858	1863	1866	rBV	5291815	5039461	75.81%	11.327%
19	13.951	2013	2017	2029	rBV	577911	712839	10.72%	1.602%
20	14.098	2038	2042	2045	rBV	1155461	1054529	15.86%	2.370%
21	14.433	2094	2099	2102	rBV3	50638	81350	1.22%	0.183%
22	14.539	2109	2117	2119	rBV6	36901	84058	1.26%	0.189%
23	14.574	2119	2123	2125	rBV2	97437	121843	1.83%	0.274%
24	14.739	2147	2151	2159	rBV	170155	269126	4.05%	0.605%
25	15.604	2292	2298	2303	rBV	919835	1156897	17.40%	2.600%
26	16.180	2391	2396	2402	rBV4	70955	149179	2.24%	0.335%

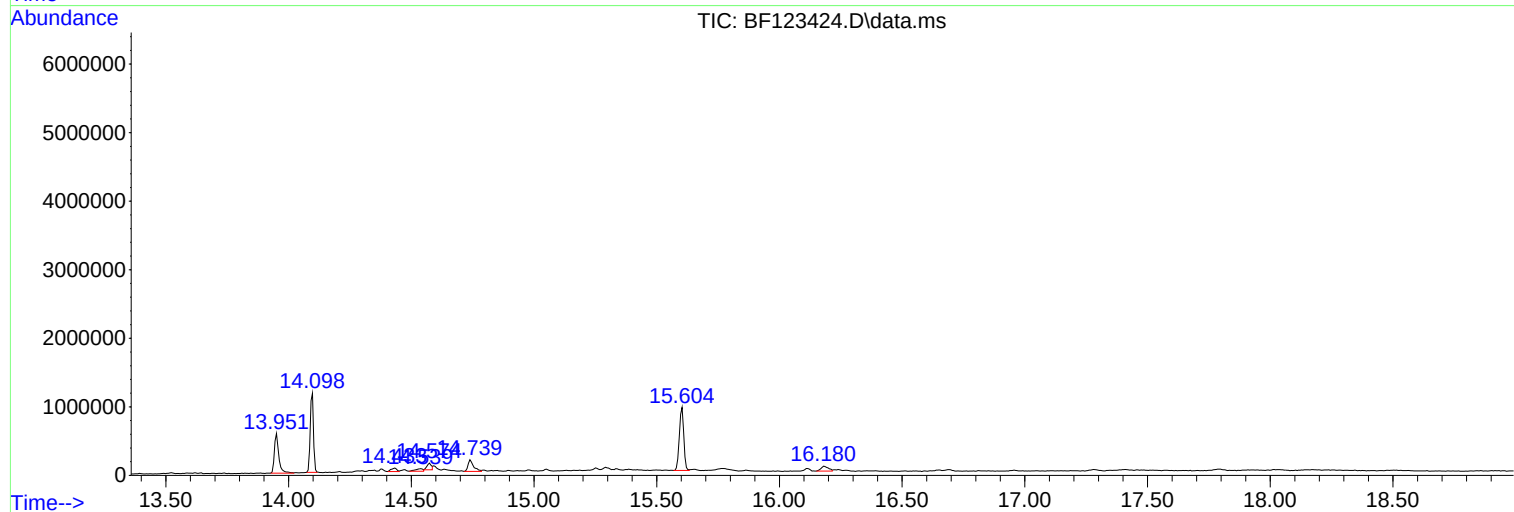
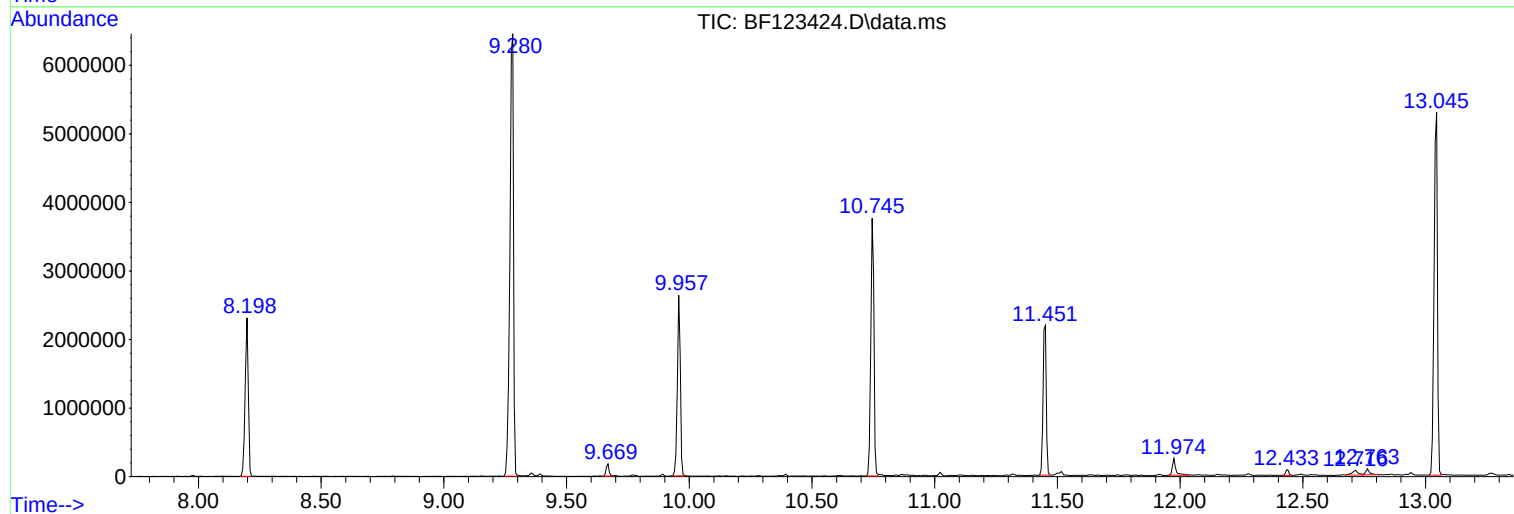
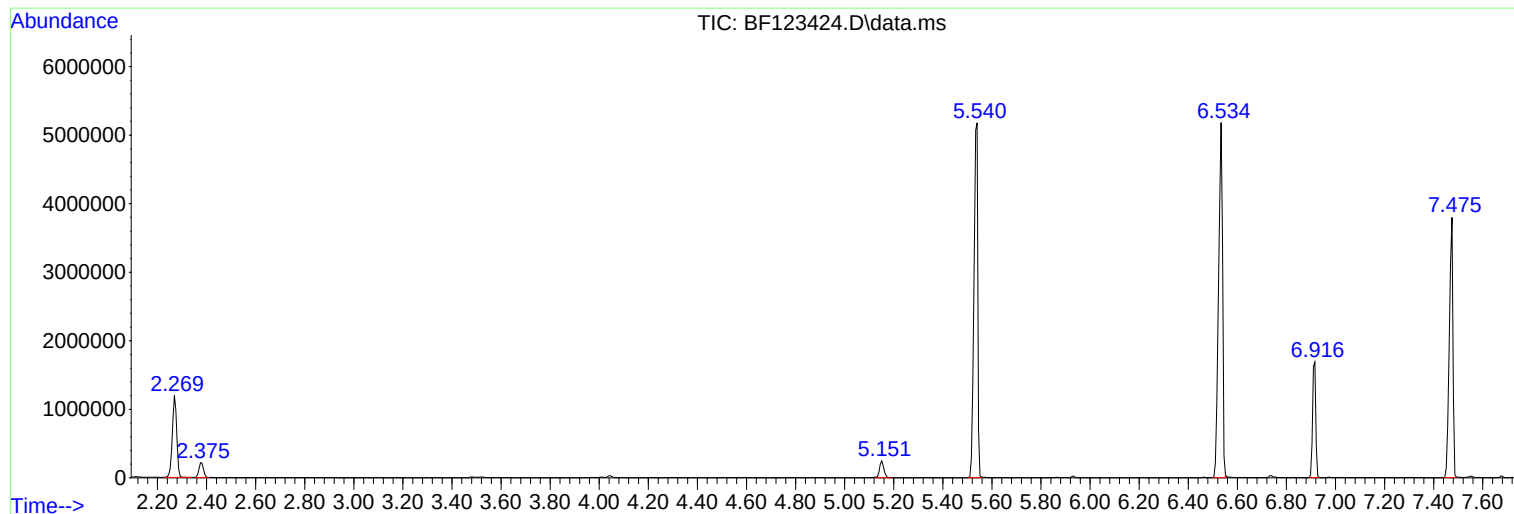
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ClientSampleId :
SB-3B1-(3.0-3.5)

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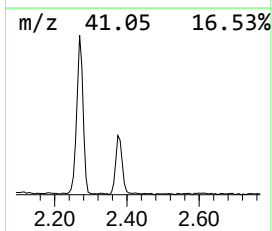
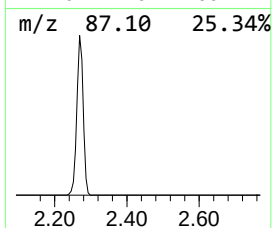
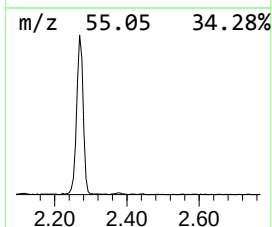
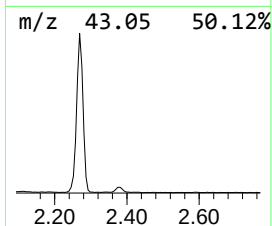
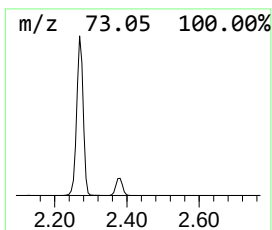
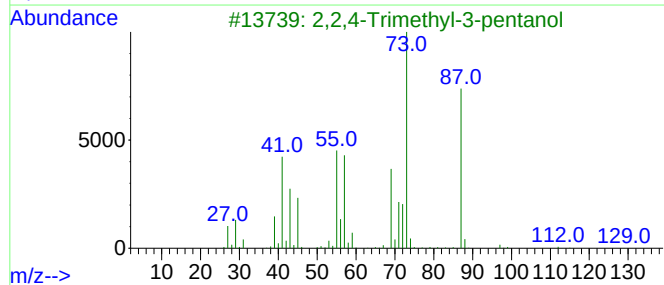
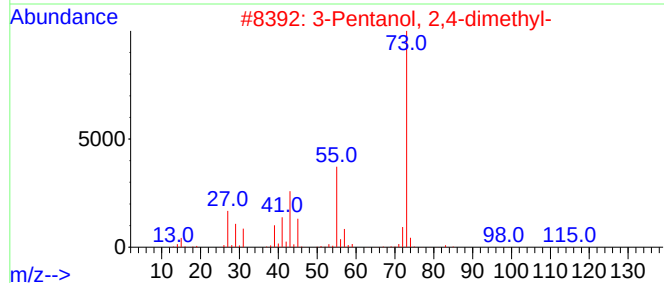
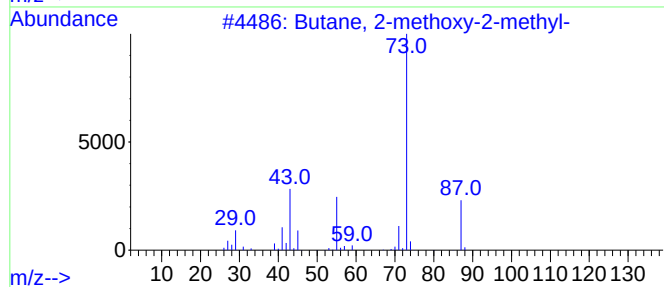
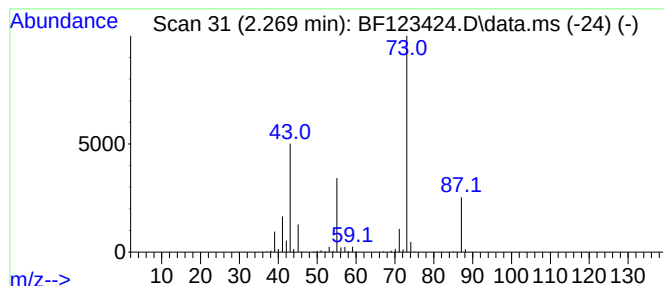
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	19.58 ng	1485740	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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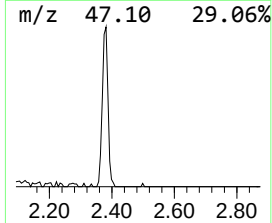
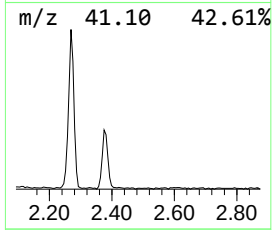
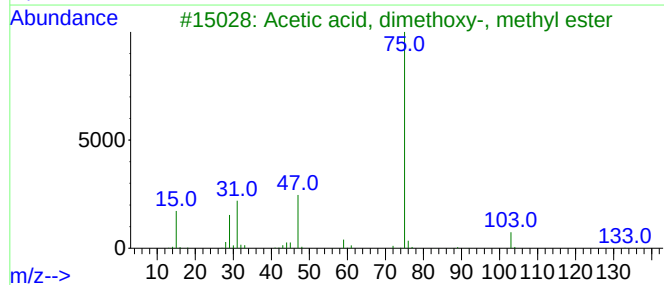
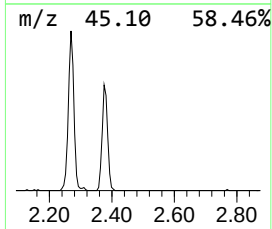
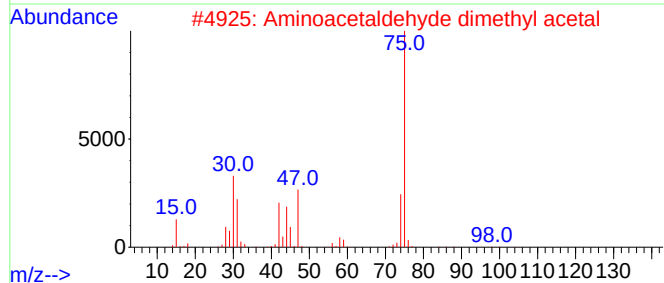
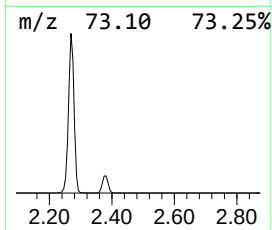
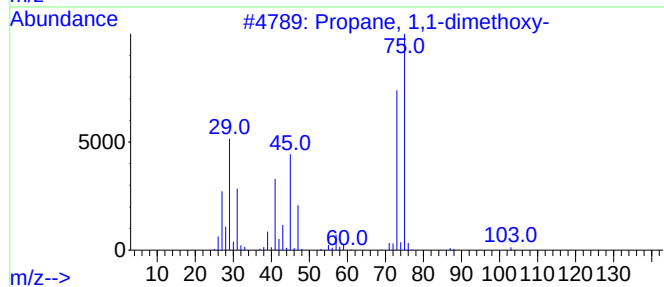
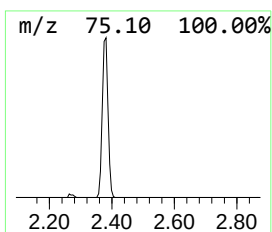
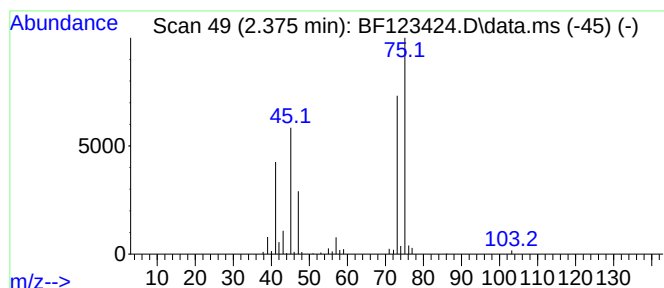
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Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.375	3.69 ng	280299	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	83
2			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
3			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
5			E-1-Methoxy-3-hexene	114	C7H14O	121441-40-5	9



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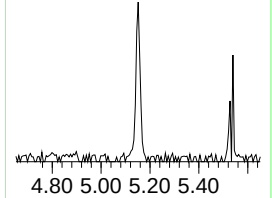
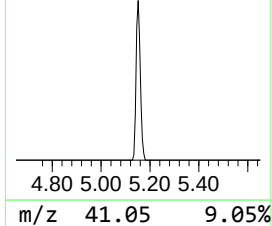
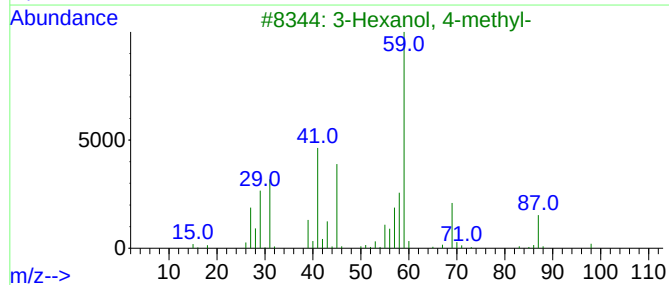
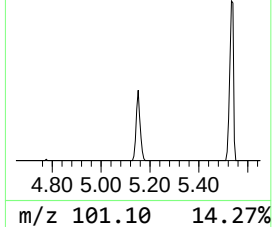
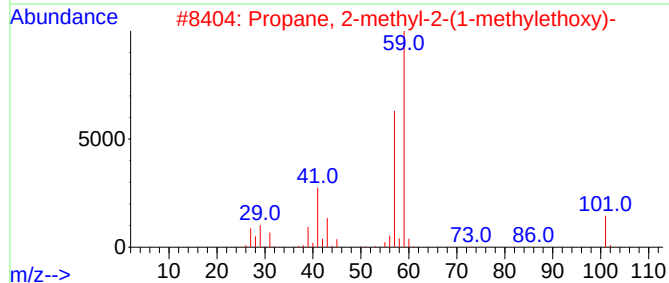
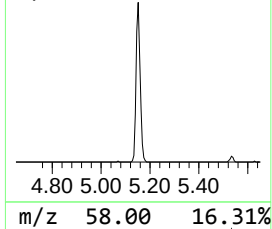
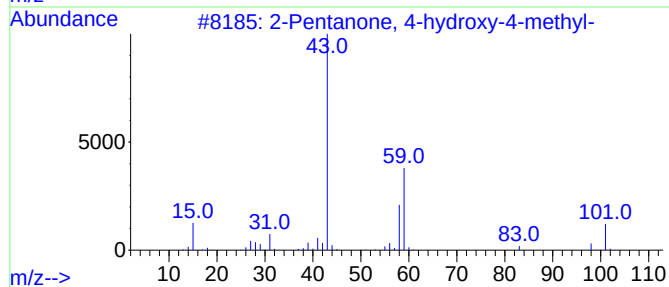
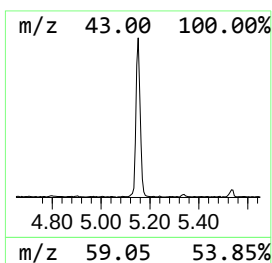
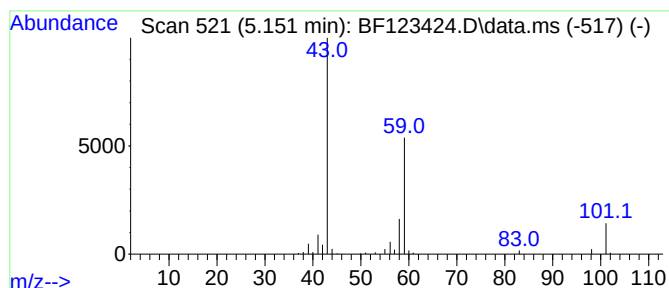
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.151	3.88 ng	294722	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	50
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	10



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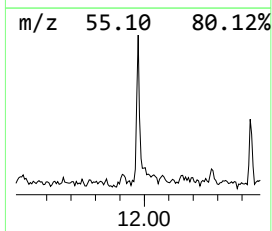
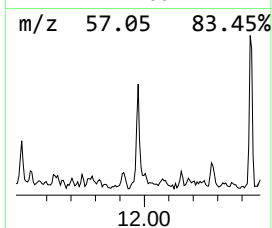
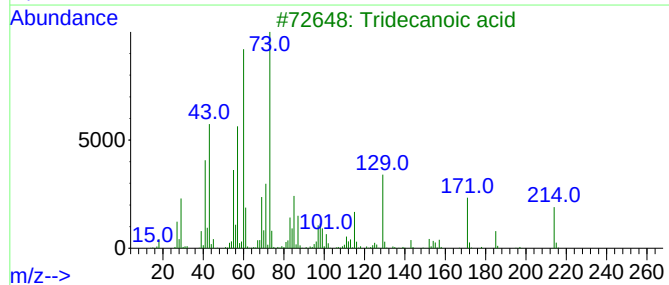
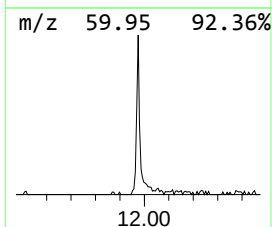
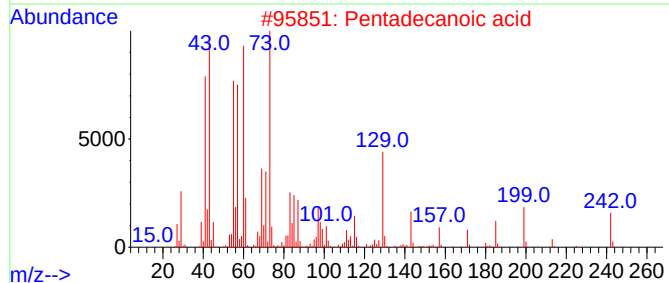
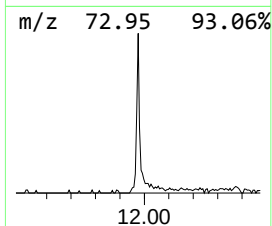
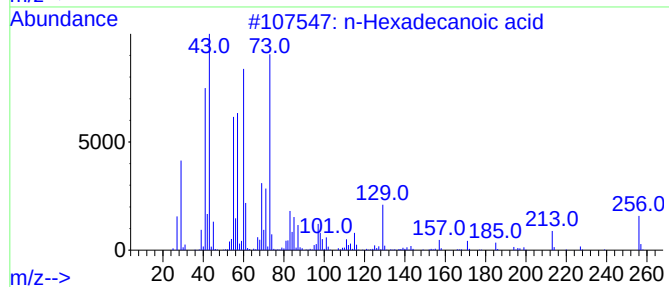
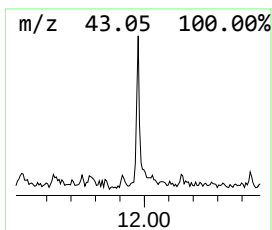
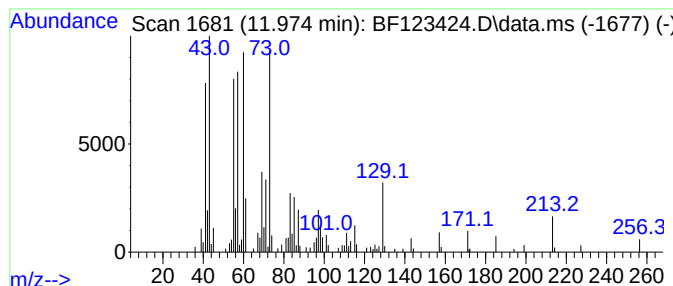
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	2.36 ng	234871	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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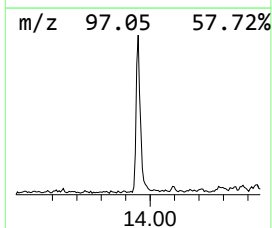
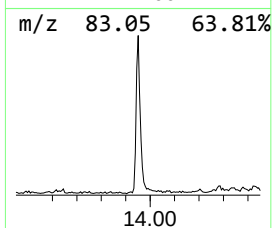
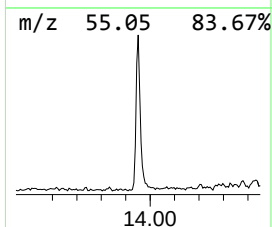
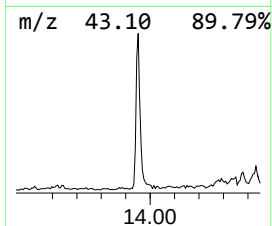
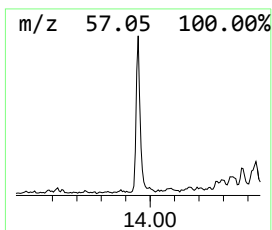
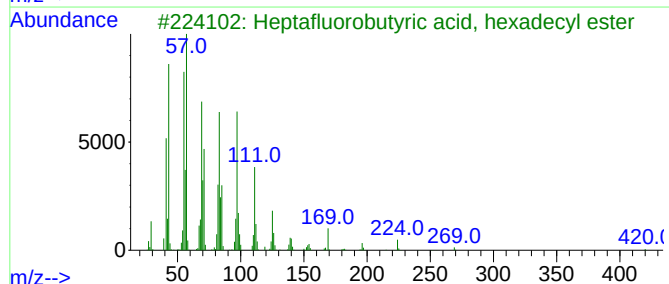
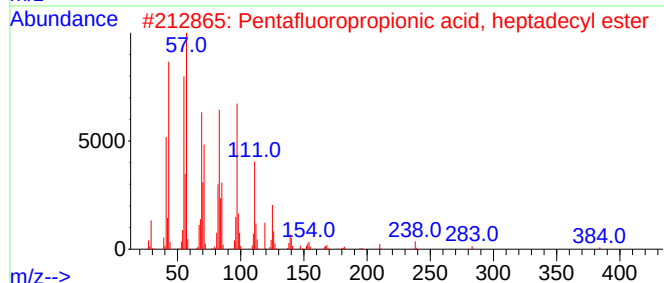
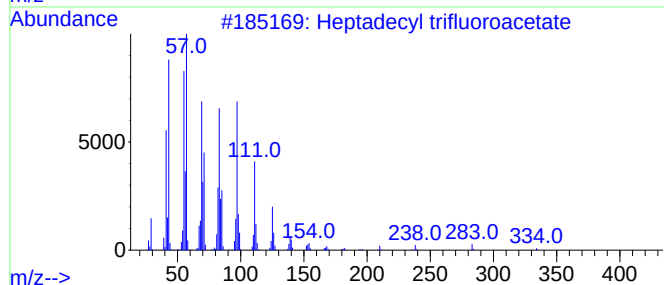
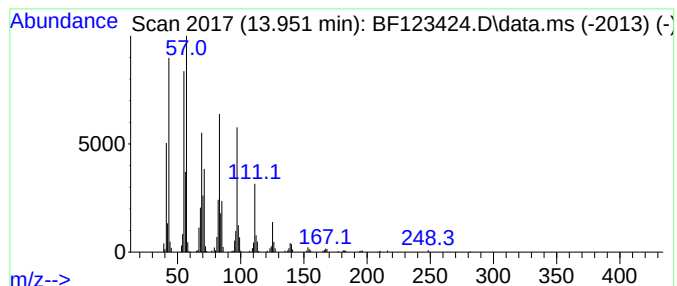
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	13.52 ng	712839	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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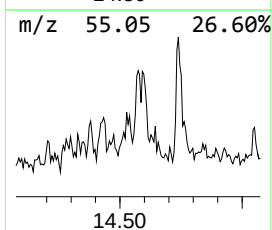
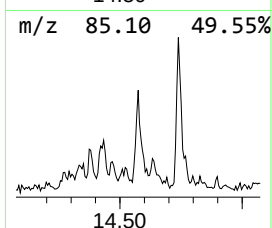
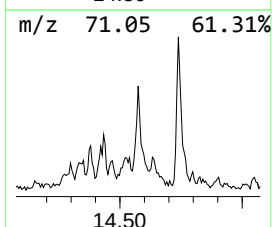
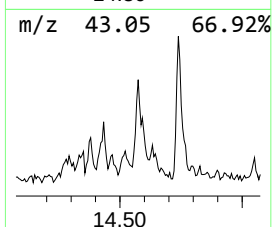
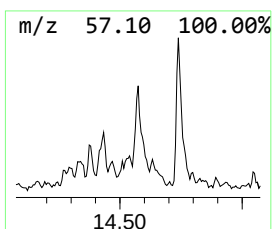
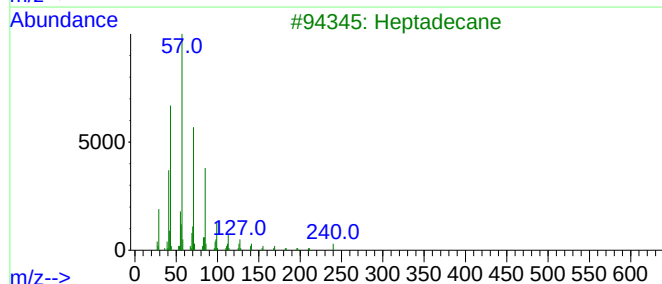
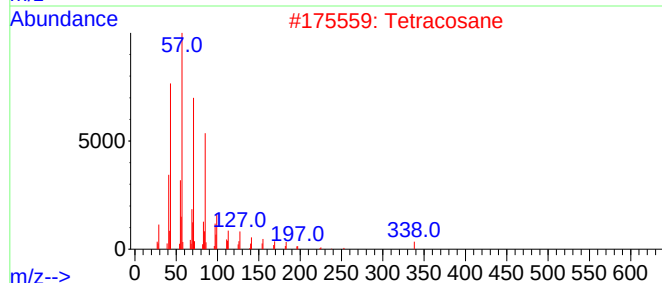
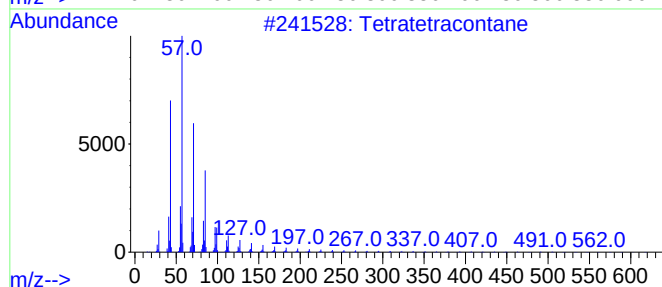
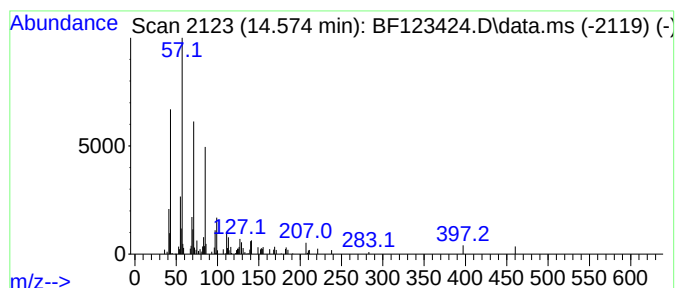
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	2.31 ng	121843	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	86
2			Tetracosane	338	C24H50	000646-31-1	83
3			Heptadecane	240	C17H36	000629-78-7	72
4			Docosane	310	C22H46	000629-97-0	72
5			Eicosane	282	C20H42	000112-95-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
Data File : BF123424.D
Acq On : 24 Mar 2021 5:57
Operator : JU/CG
Sample : M1779-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3B1-(3.0-3.5)

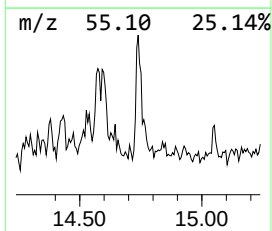
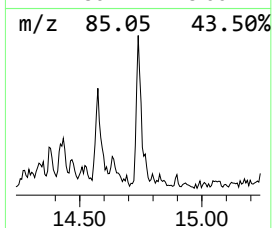
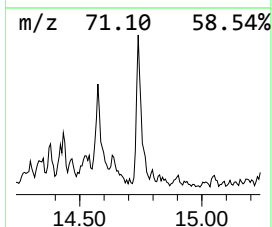
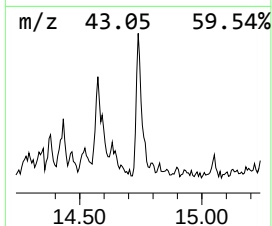
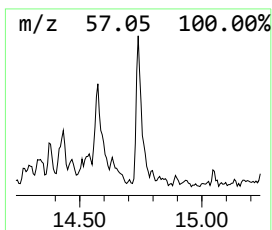
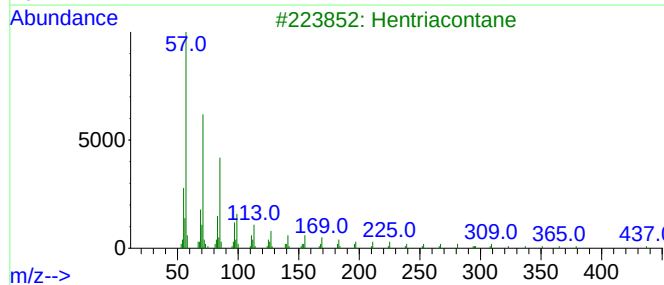
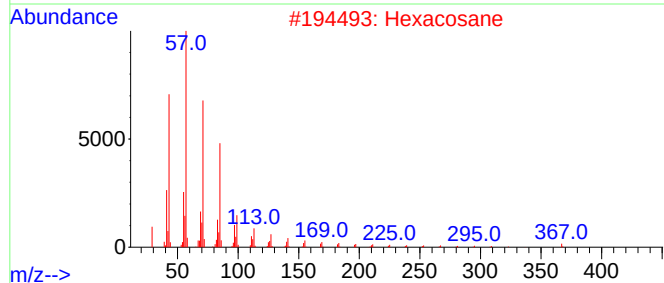
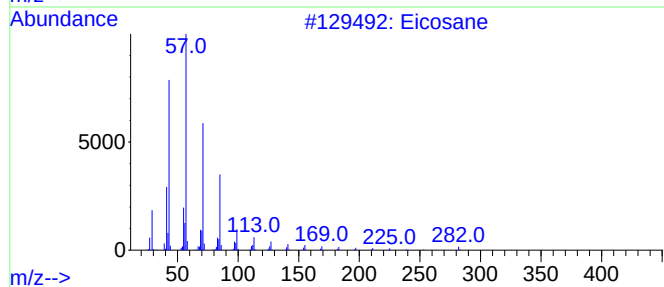
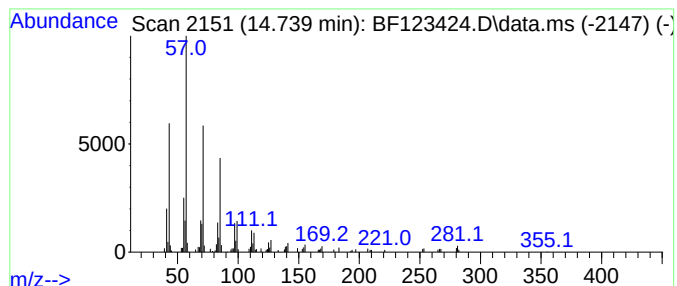
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	5.10 ng	269126	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Hexacosane	366	C26H54	000630-01-3	90
3			Hentriacontane	437	C31H64	000630-04-6	90
4			Tetratetracontane	619	C44H90	007098-22-8	90
5			Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
Data File : BF123424.D
Acq On : 24 Mar 2021 5:57
Operator : JU/CG
Sample : M1779-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3B1-(3.0-3.5)

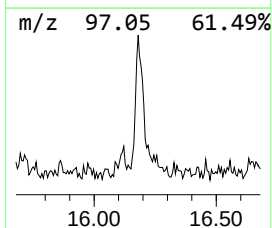
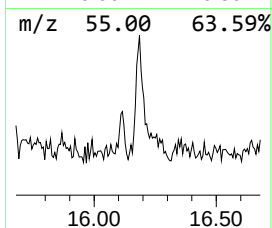
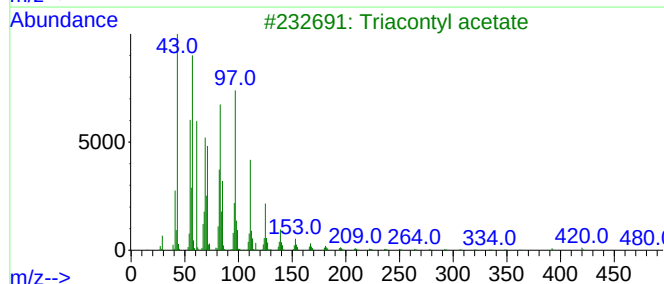
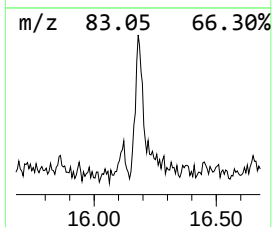
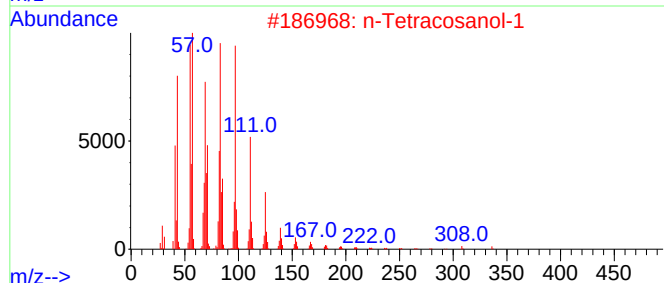
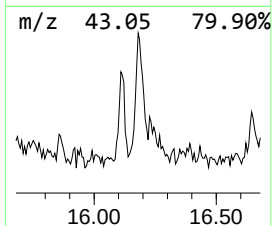
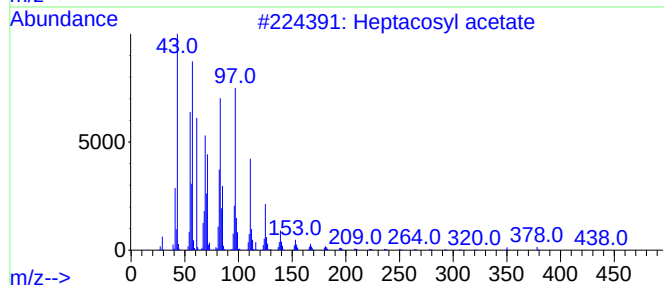
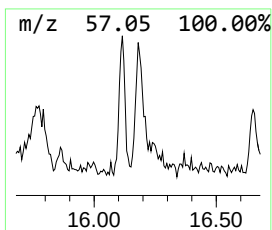
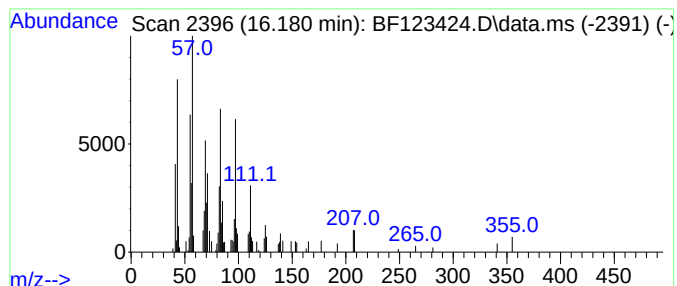
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.180	2.58 ng	149179	Perylene-d12	15.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	76
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
3			Triacontyl acetate	480	C32H64O2	041755-58-2	76
4			1-Heptacosanol	396	C27H56O	002004-39-9	76
5			Octacosanol	410	C28H58O	000557-61-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032321\
Data File : BF123424.D
Acq On : 24 Mar 2021 5:57
Operator : JU/CG
Sample : M1779-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3B1-(3.0-3.5)

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...	2.269	19.6	ng	1485740	1	6.916	1517300	20.0
Propane, 1,1-di...	2.375	3.7	ng	280299	1	6.916	1517300	20.0
2-Pentanone, 4-...	5.151	3.9	ng	294722	1	6.916	1517300	20.0
n-Hexadecanoic ...	11.974	2.4	ng	234871	4	11.451	1993770	20.0
Heptadecyl trif...	13.951	13.5	ng	712839	5	14.098	1054530	20.0
Tetratetracontane	14.574	2.3	ng	121843	5	14.098	1054530	20.0
Eicosane	14.739	5.1	ng	269126	5	14.098	1054530	20.0
Heptacosyl acetate	16.180	2.6	ng	149179	6	15.604	1156900	20.0