

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
 Data File : BF124247.D
 Acq On : 10 Jun 2021 23:05
 Operator : JU/CG
 Sample : M2650-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DELAWANNA-RT10-STOCKPILE-2

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	17	22	27	rBB2	24051	29321	1.70%	0.283%
2	5.075	504	508	517	rVB	52433	68899	3.99%	0.666%
3	5.481	573	577	581	rBV	1279295	1296681	75.01%	12.528%
4	6.492	744	749	752	rBV	1200054	1312728	75.94%	12.683%
5	6.675	777	780	787	rBV	29045	28195	1.63%	0.272%
6	6.845	806	809	813	rBV	305217	236665	13.69%	2.287%
7	7.416	900	906	909	rBV	987983	916637	53.02%	8.856%
8	8.127	1024	1027	1031	rBV	360058	291714	16.87%	2.818%
9	9.210	1206	1211	1214	rBV	2097505	1728732	100.00%	16.703%
10	9.598	1274	1277	1280	rBV	321470	240129	13.89%	2.320%
11	9.886	1322	1326	1329	rBV	454426	351295	20.32%	3.394%
12	10.680	1456	1461	1464	rBV	1299022	1150332	66.54%	11.114%
13	11.374	1575	1579	1582	rBV	393452	337302	19.51%	3.259%
14	11.898	1665	1668	1674	rBV2	135061	132113	7.64%	1.276%
15	12.680	1799	1801	1806	rBV3	22846	22125	1.28%	0.214%
16	12.962	1844	1849	1852	rBV	1349856	1328047	76.82%	12.831%
17	13.857	1997	2001	2011	rBV3	87258	158945	9.19%	1.536%
18	14.015	2024	2028	2031	rBV	282235	246477	14.26%	2.381%
19	14.474	2102	2106	2108	rBV3	21575	26057	1.51%	0.252%
20	15.056	2203	2205	2212	rBV6	14596	23383	1.35%	0.226%
21	15.127	2212	2217	2220	rVB5	22809	31025	1.79%	0.300%
22	15.492	2274	2279	2285	rBV	220105	295583	17.10%	2.856%
23	15.945	2352	2356	2360	rVB2	24257	30624	1.77%	0.296%
24	16.192	2394	2398	2402	rBV7	12547	21486	1.24%	0.208%
25	17.045	2540	2543	2547	rBV6	14016	22553	1.30%	0.218%
26	18.580	2798	2804	2806	rBV4	11372	22981	1.33%	0.222%

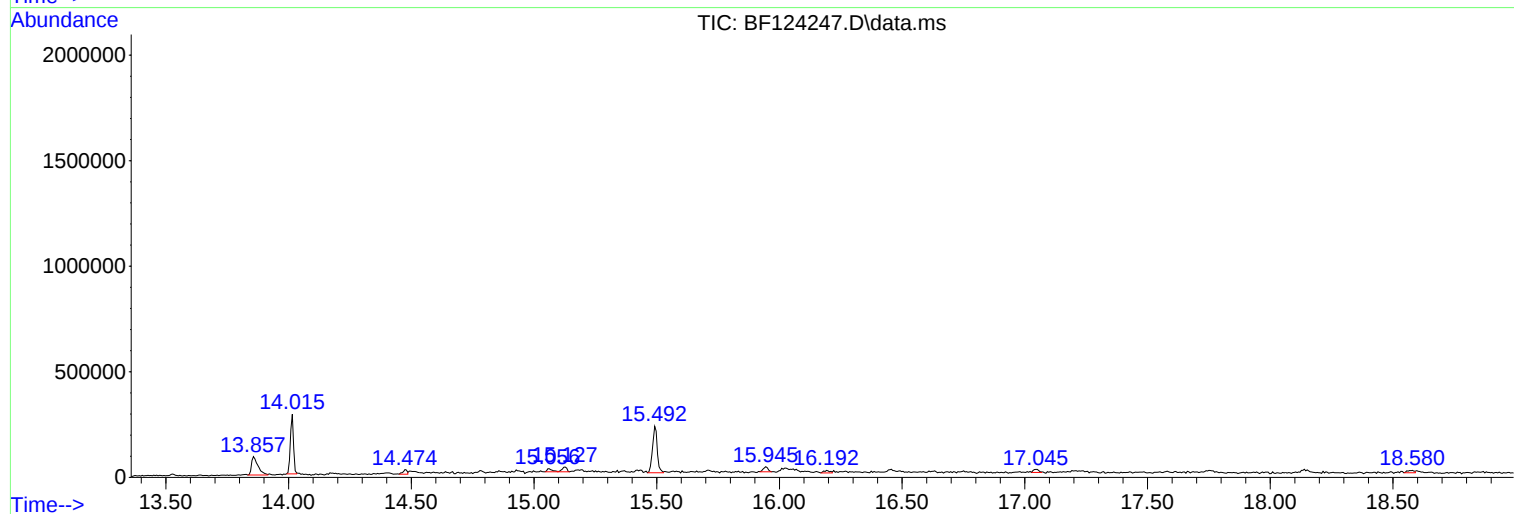
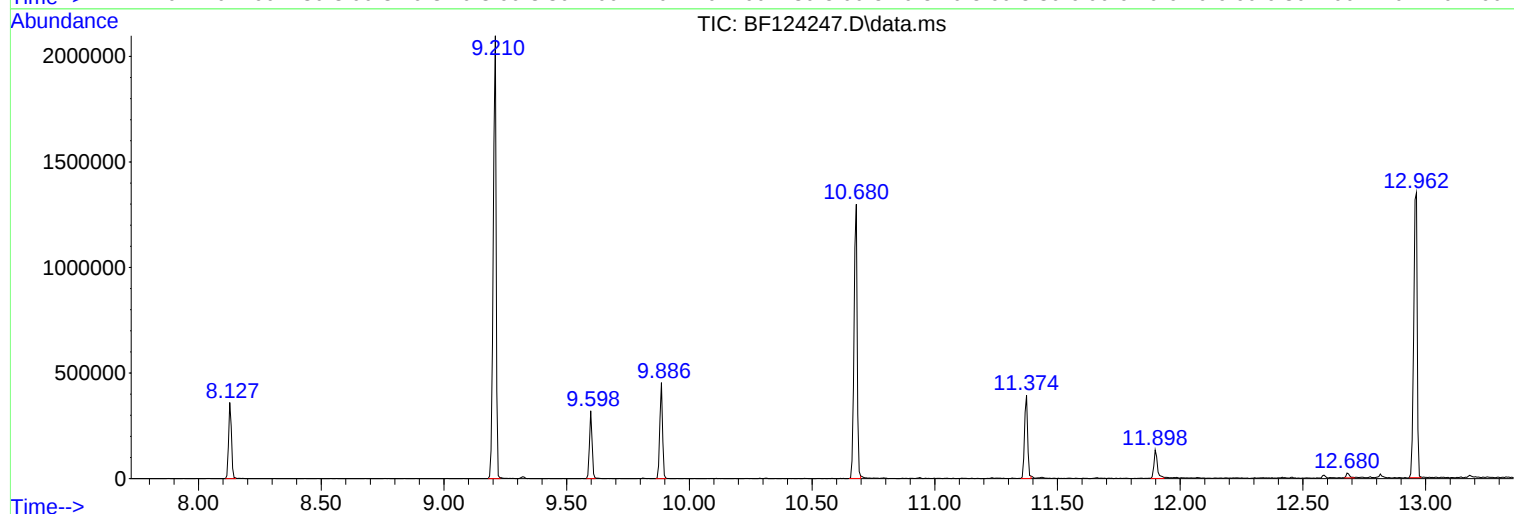
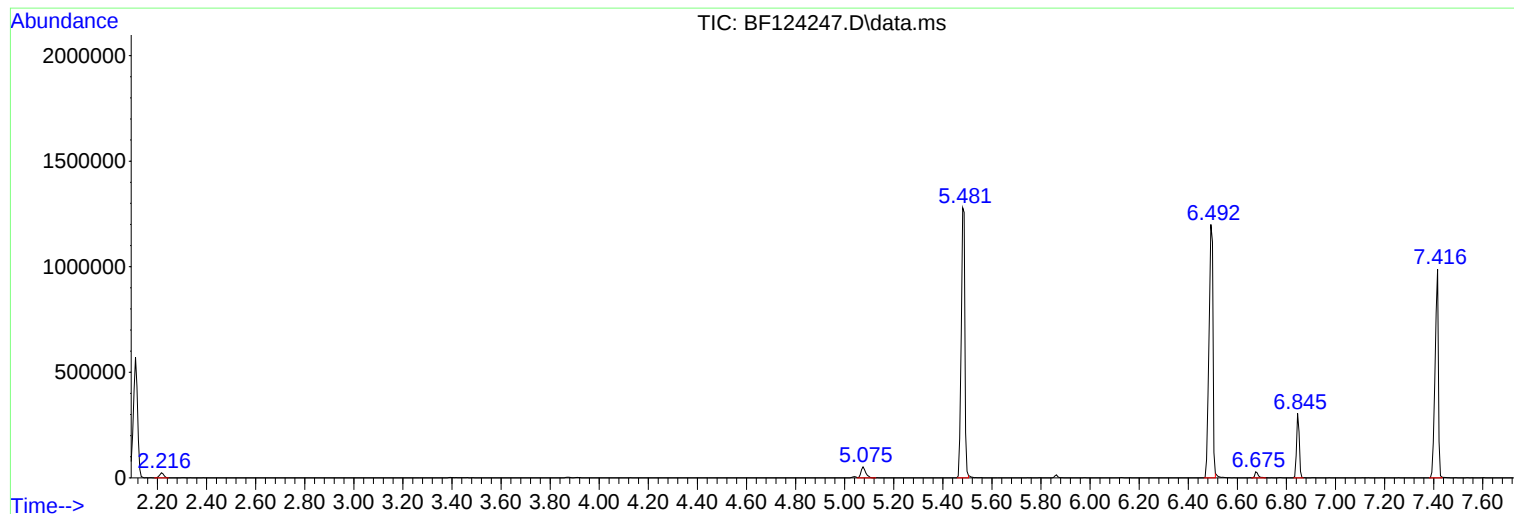
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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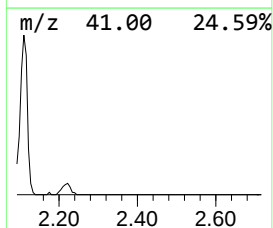
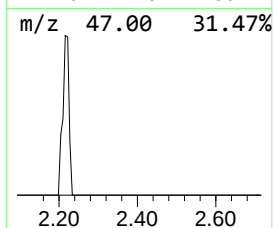
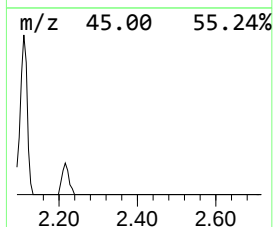
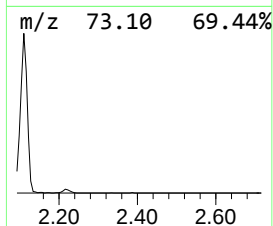
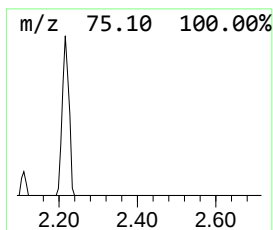
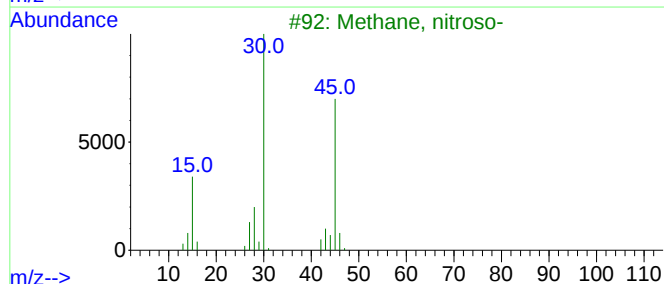
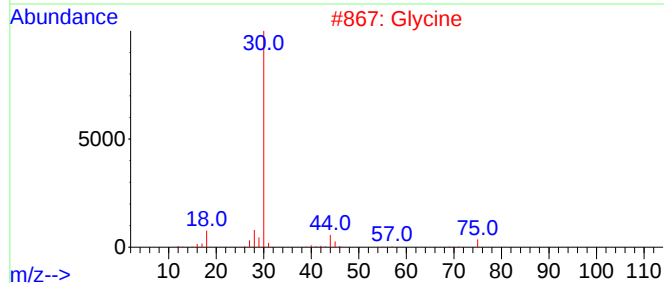
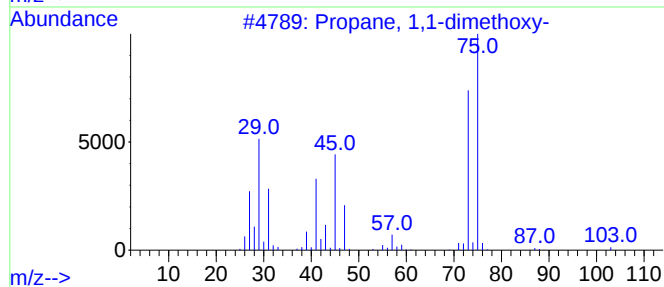
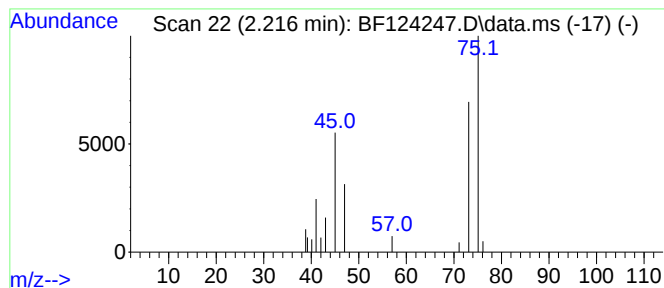
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	2.48 ng	29321	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Glycine	75	C2H5NO2	000056-40-6	4
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	4
5			Methanamine, N,N-dimethyl-, N-oxide	75	C3H9NO	001184-78-7	4



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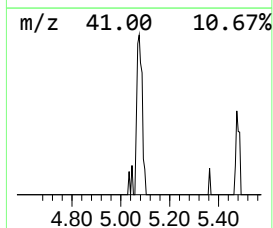
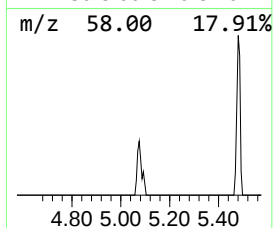
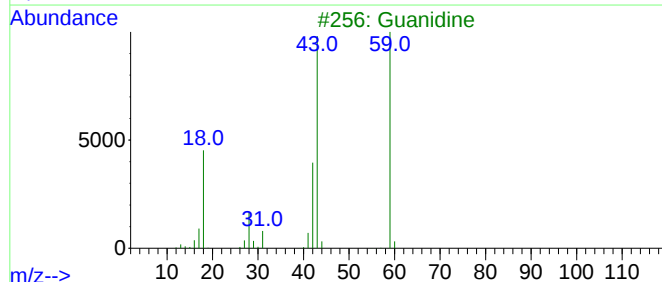
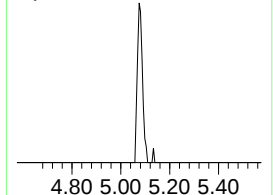
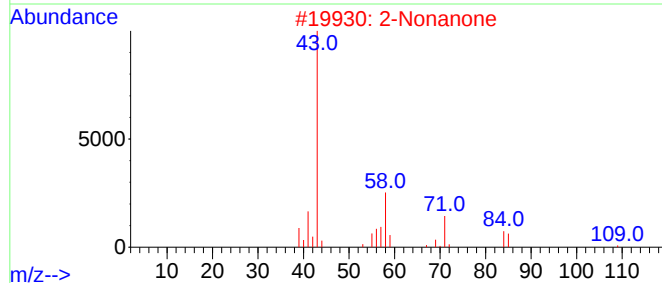
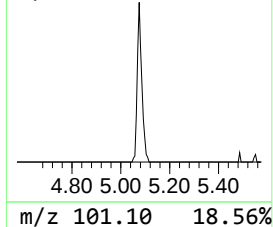
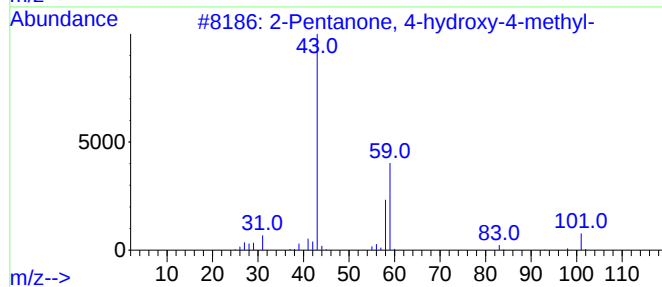
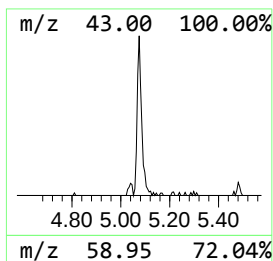
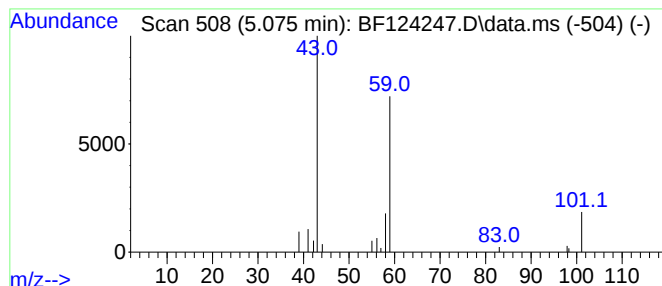
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.82 ng	68899	1,4-Dichlorobenzene-d4	6.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Nonanone	142	C9H18O	000821-55-6	23
3		Guanidine	59	CH5N3	000113-00-8	9
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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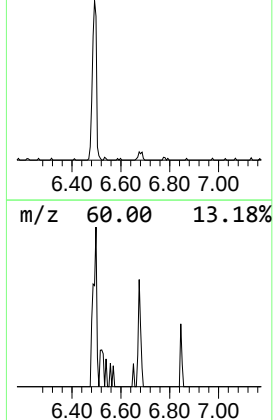
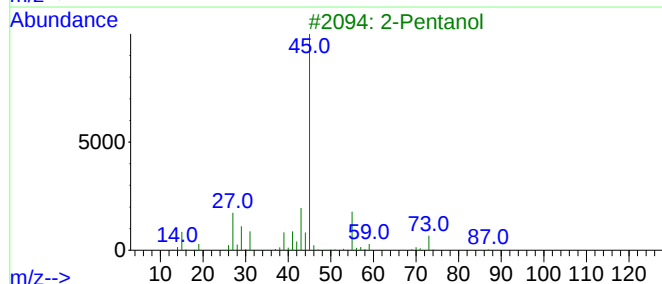
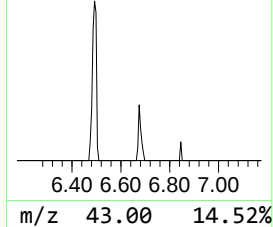
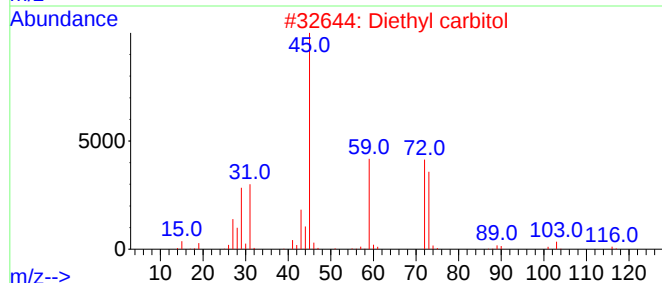
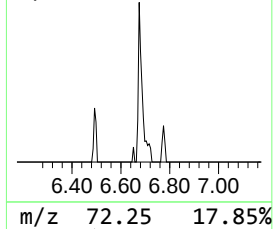
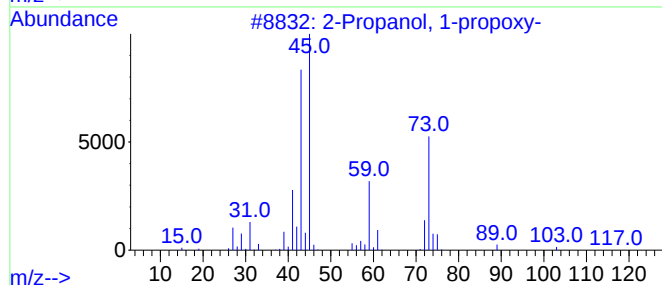
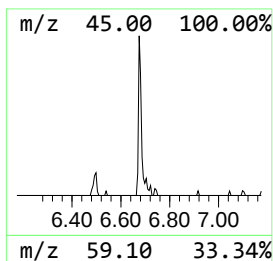
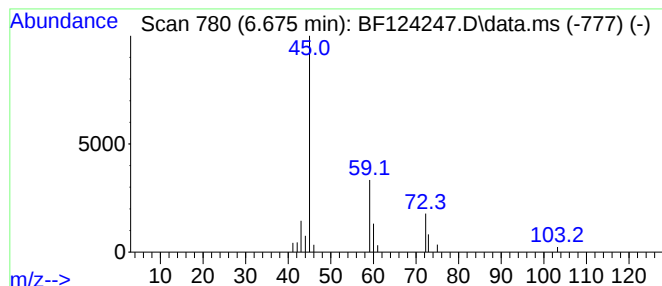
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.675 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.675	2.38 ng	28195	1,4-Dichlorobenzene-d4	6.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	40
2		Diethyl carbitol	162	C8H18O3	000112-36-7	39
3		2-Pentanol	88	C5H12O	006032-29-7	33
4		Ethanol, 2-ethoxy-	90	C4H10O2	000110-80-5	9
5		2,3-Butanediol	90	C4H10O2	000513-85-9	9



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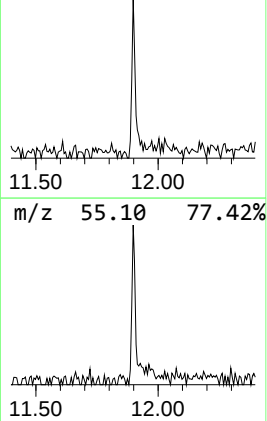
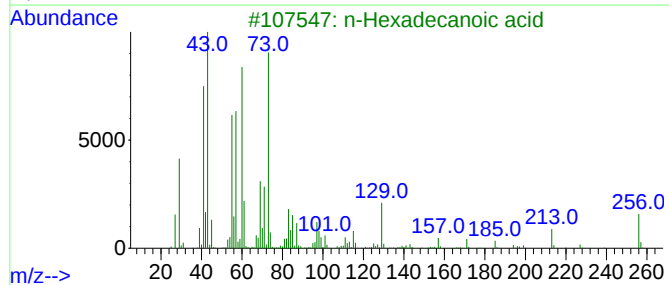
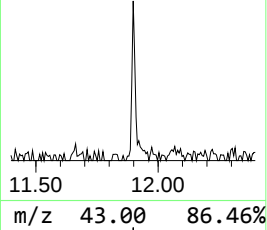
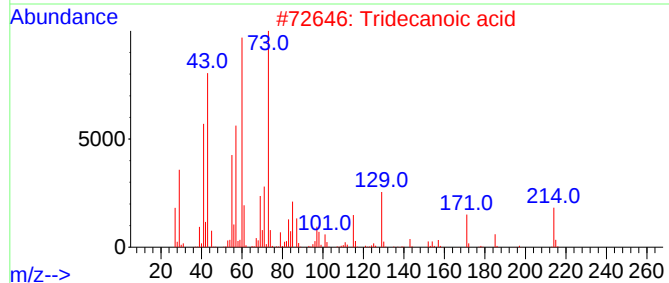
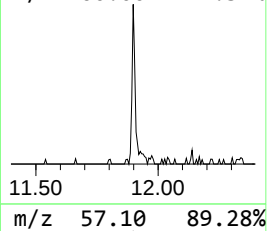
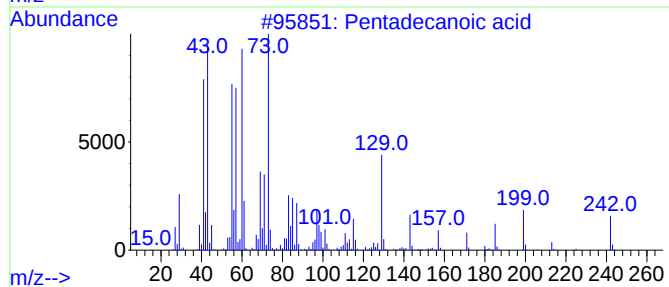
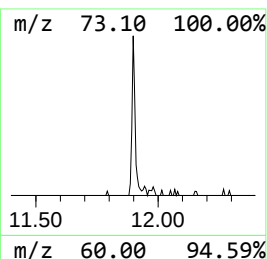
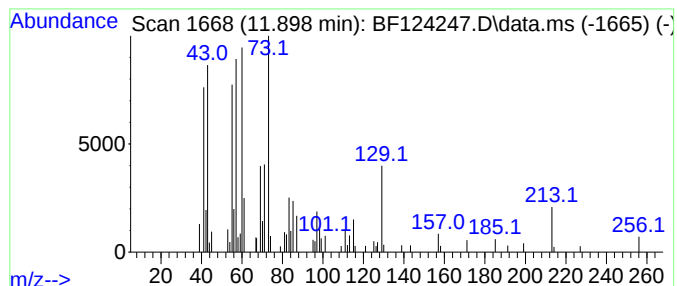
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Pentadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	7.83 ng	132113	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2			Tridecanoic acid	214	C13H26O2	000638-53-9	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	38



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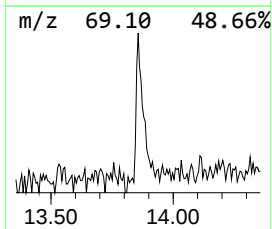
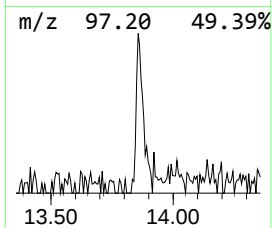
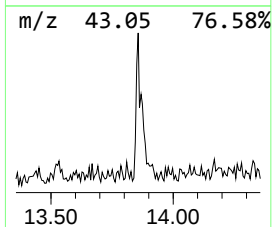
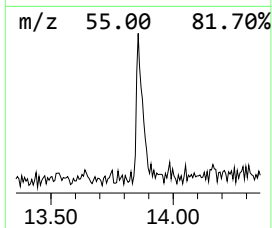
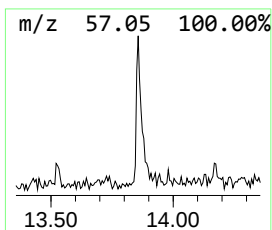
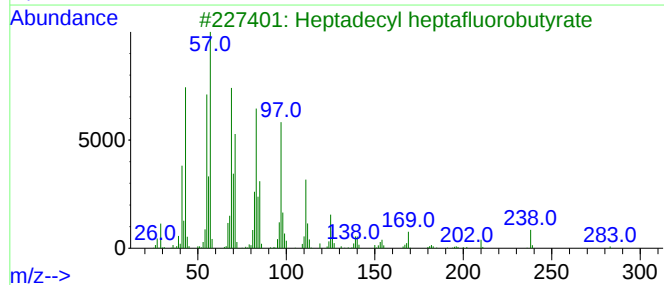
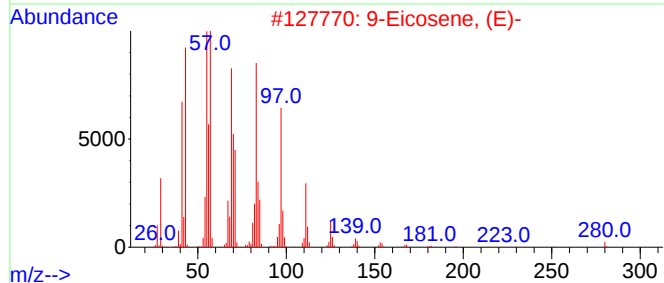
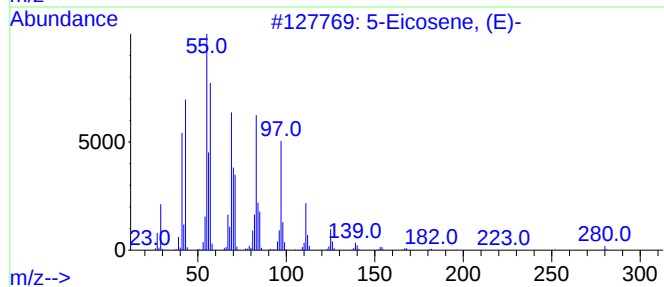
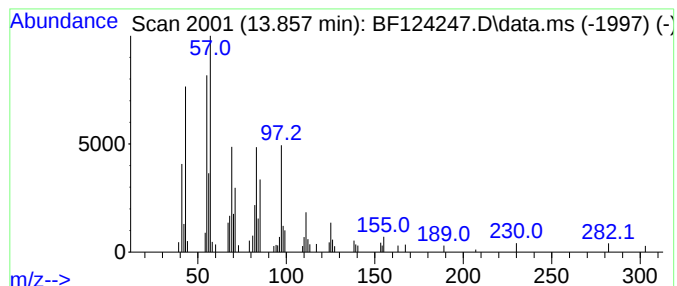
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	12.90 ng	158945	Chrysene-d12	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	74
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	64
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
4	1-Eicosanol	298	C20H42O	000629-96-9	58
5	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	53



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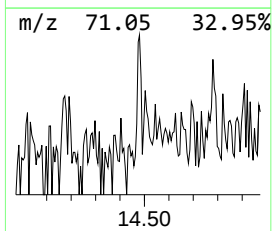
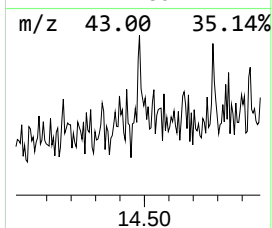
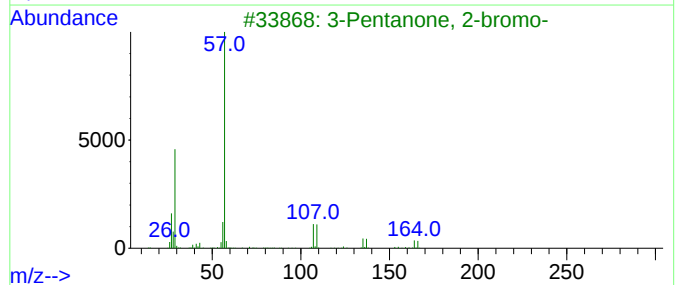
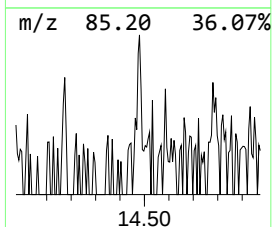
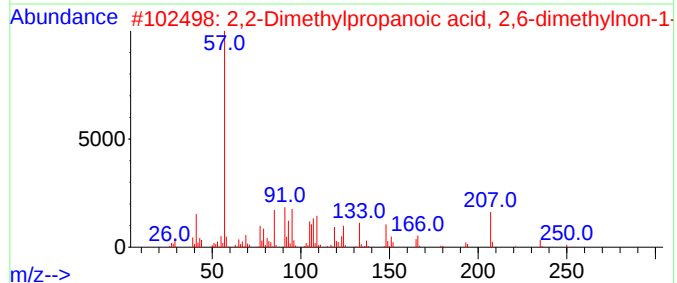
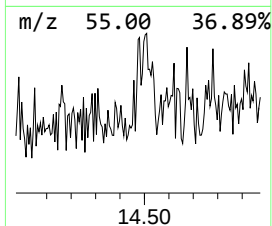
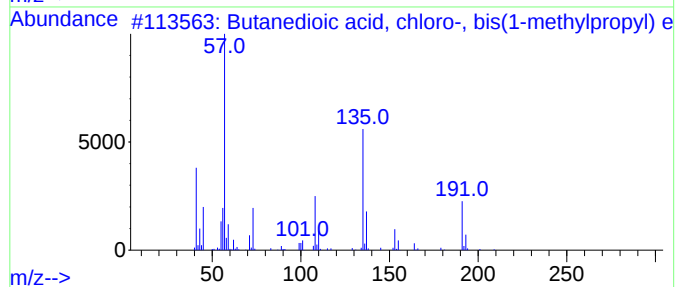
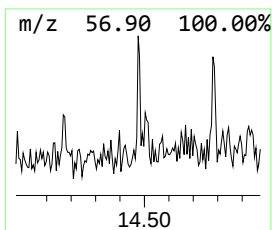
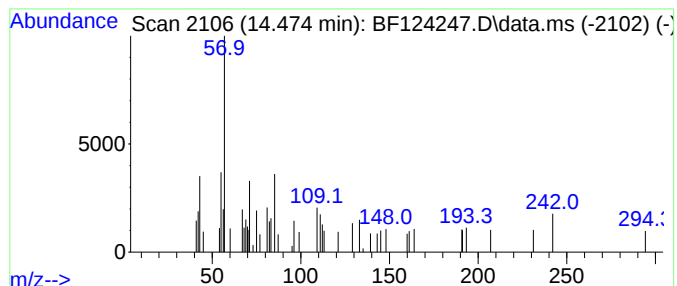
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.474 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	2.11 ng	26057	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanedioic acid, chloro-, bis(1-methylpropyl) ester	264	C12H21ClO4	057983-51-4	9
2			2,2-Dimethylpropanoic acid, 2,6-dimethylnon-1-yl ester	250	C16H26O2	1000299-33-6	9
3			3-Pentanone, 2-bromo-	164	C5H9BrO	000815-52-1	5
4			Propanamide, 2,2-dimethyl-N-(3-methylbutyl)-	191	C12H17NO	032597-29-8	4
5			2-tert-Butyl-5-chloromethyl-3-methylbenzofuran	304	C14H25ClN2O3	1000192-88-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124247.D
Acq On : 10 Jun 2021 23:05
Operator : JU/CG
Sample : M2650-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-2

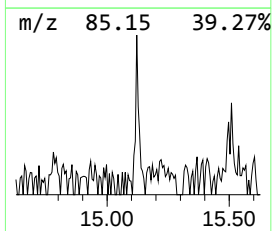
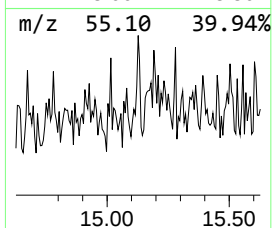
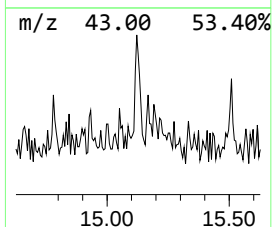
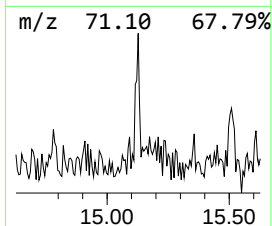
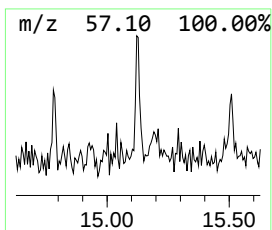
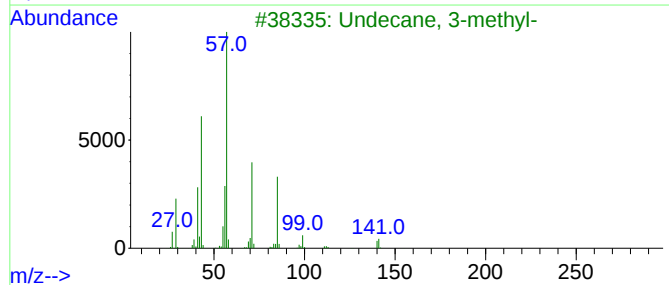
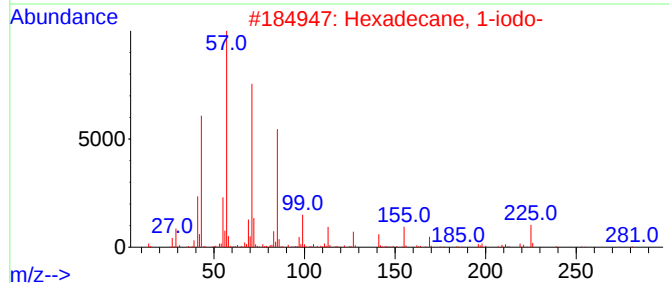
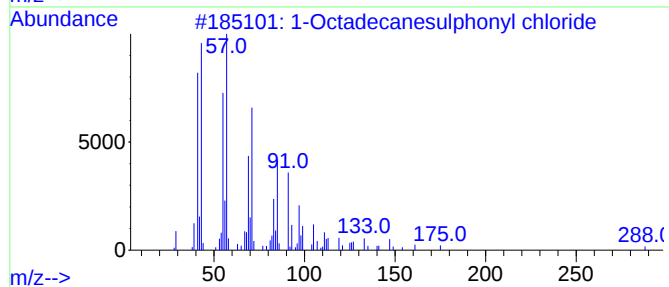
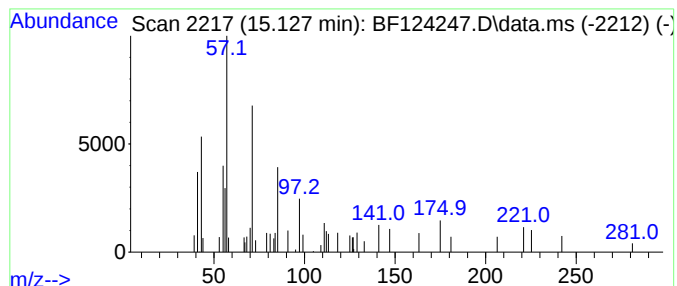
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Octadecanesulphonyl chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.10 ng	31025	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	50
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	47
3			Undecane, 3-methyl-	170	C12H26	001002-43-3	43
4			Tridecane	184	C13H28	000629-50-5	38
5			Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124247.D
Acq On : 10 Jun 2021 23:05
Operator : JU/CG
Sample : M2650-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-2

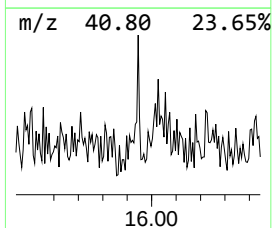
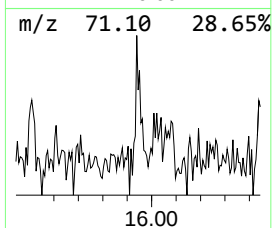
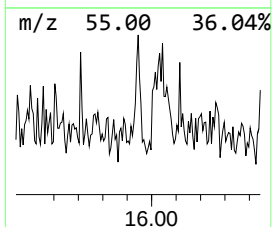
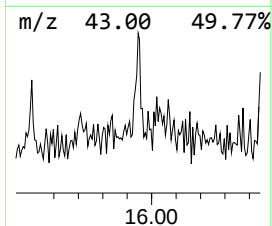
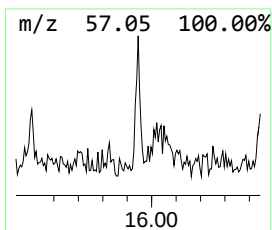
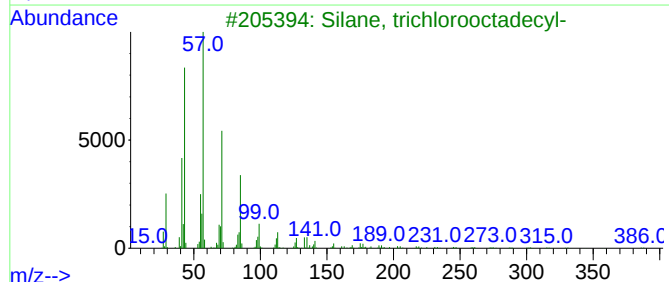
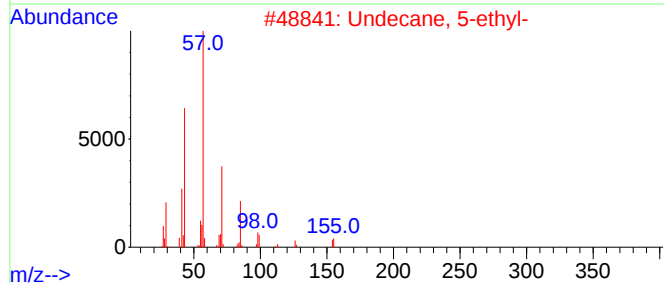
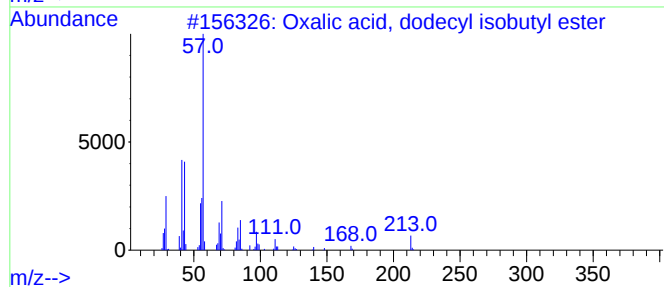
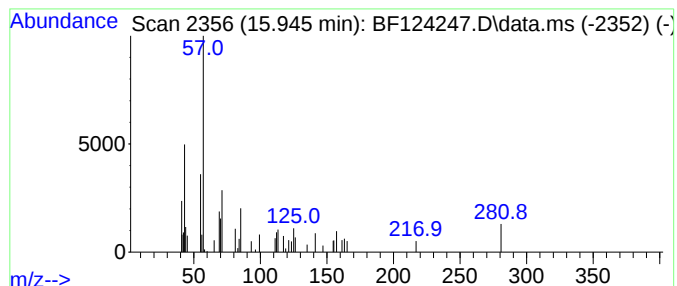
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.945 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.07 ng	30624	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	43
2			Undecane, 5-ethyl-	184	C13H28	017453-94-0	38
3			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	35
4			Eicosane, 10-methyl-	296	C21H44	054833-23-7	35
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124247.D
Acq On : 10 Jun 2021 23:05
Operator : JU/CG
Sample : M2650-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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
Propane, 1,1-di...	2.216	2.5	ng	29321	1	6.845	236665	20.0
2-Pentanone, 4-...	5.075	5.8	ng	68899	1	6.845	236665	20.0
unknown6.675	6.675	2.4	ng	28195	1	6.845	236665	20.0
Pentadecanoic acid	11.898	7.8	ng	132113	4	11.374	337302	20.0
5-Eicosene, (E)-	13.857	12.9	ng	158945	5	14.015	246477	20.0
unknown14.474	14.474	2.1	ng	26057	5	14.015	246477	20.0
1-Octadecanesul...	15.127	2.1	ng	31025	6	15.492	295583	20.0
unknown15.945	15.945	2.1	ng	30624	6	15.492	295583	20.0