

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
 Data File : BF111336.D
 Acq On : 12 Dec 2018 22:01
 Operator : JU/SJ
 Sample : J6214-27 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2(0-2)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF121218.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	485	492	499	rBV	155066	185771	6.59%	0.591%
2	5.404	560	564	581	rVB	2928653	2584628	91.66%	8.220%
3	6.422	733	737	748	rBV	3016311	2819850	100.00%	8.968%
4	6.563	757	761	764	rBV	2844645	2625576	93.11%	8.351%
5	6.622	769	771	776	rVB2	58167	59270	2.10%	0.189%
6	6.792	796	800	804	rBV	1973694	1582719	56.13%	5.034%
7	6.951	823	827	830	rBV	2338702	2029063	71.96%	6.453%
8	7.345	889	894	898	rBV	1669217	1533625	54.39%	4.878%
9	8.075	1014	1018	1021	rBV	2363489	1879036	66.64%	5.976%
10	9.151	1197	1201	1204	rBV	3182112	2429828	86.17%	7.728%
11	9.245	1213	1217	1222	rBV5	35235	60889	2.16%	0.194%
12	9.539	1264	1267	1270	rBV	234731	208269	7.39%	0.662%
13	9.651	1282	1286	1290	rBV4	47806	59376	2.11%	0.189%
14	9.828	1311	1316	1320	rBV	2002713	1727540	61.26%	5.494%
15	10.033	1348	1351	1358	rVB8	58039	61792	2.19%	0.197%
16	10.245	1383	1387	1390	rBV	94828	104876	3.72%	0.334%
17	10.422	1414	1417	1422	rBV	139117	138000	4.89%	0.439%
18	10.504	1426	1431	1435	rBV	372138	342543	12.15%	1.089%
19	10.610	1446	1449	1453	rBV	1327075	1171570	41.55%	3.726%
20	10.757	1469	1474	1478	rBV	144312	157020	5.57%	0.499%
21	11.063	1523	1526	1531	rBV	120655	111678	3.96%	0.355%
22	11.222	1550	1553	1556	rVB	200227	175608	6.23%	0.559%
23	11.310	1565	1568	1571	rBV	1759002	1514030	53.69%	4.815%
24	11.333	1571	1572	1575	rVB	227589	128649	4.56%	0.409%
25	11.845	1656	1659	1662	rBV2	640197	638697	22.65%	2.031%
26	11.880	1662	1665	1668	rVB	231207	236418	8.38%	0.752%
27	12.521	1771	1774	1777	rBV	720224	744186	26.39%	2.367%
28	12.633	1791	1793	1796	rBV2	365216	403739	14.32%	1.284%
29	12.898	1835	1838	1842	rBV	2338548	2242731	79.53%	7.133%
30	13.951	2015	2017	2024	rVB	1175170	1571528	55.73%	4.998%
31	14.592	2124	2126	2132	rVB	1757367	1913221	67.85%	6.085%

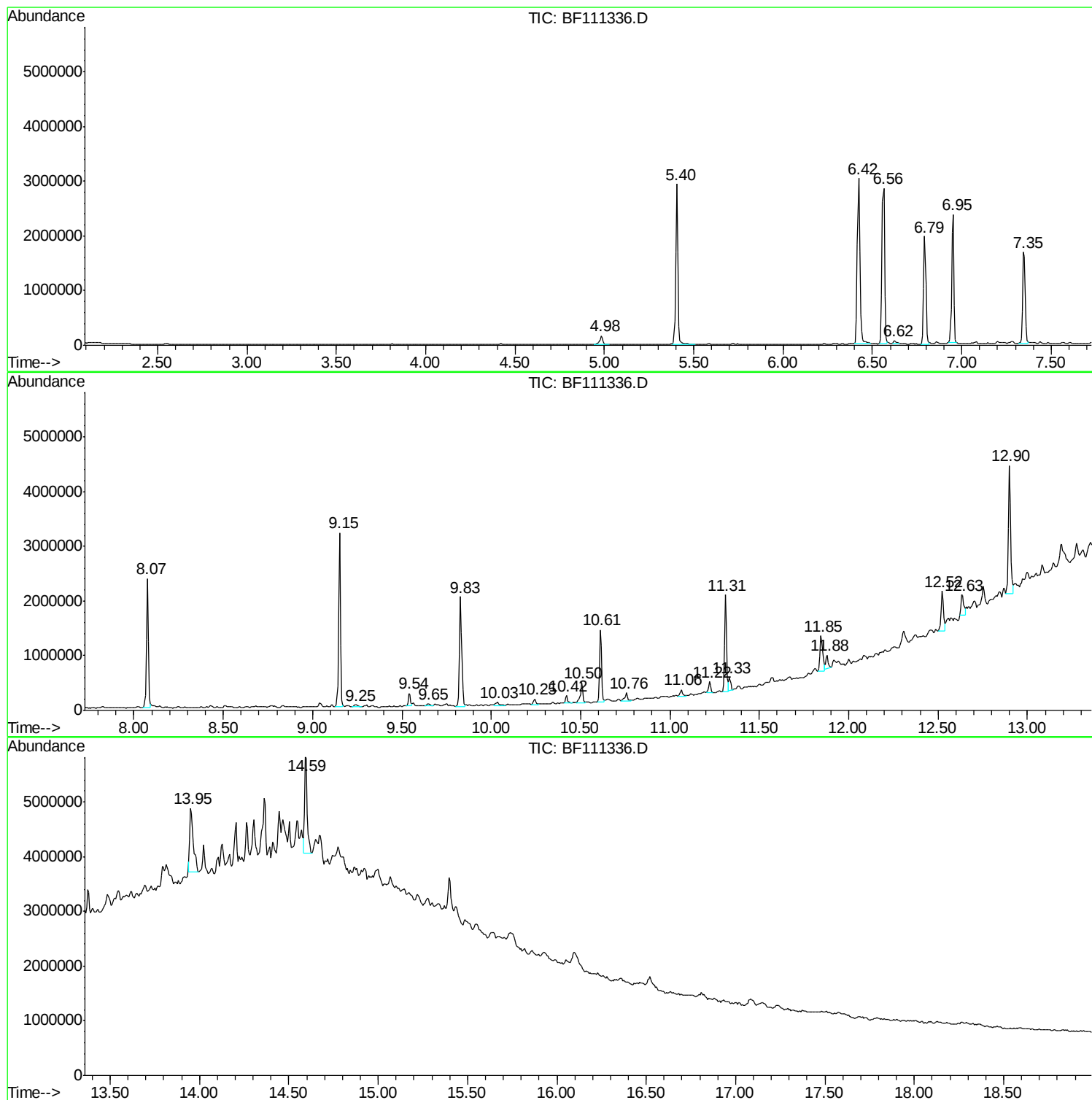
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ClientSampleId :
SB-2(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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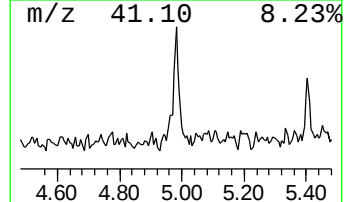
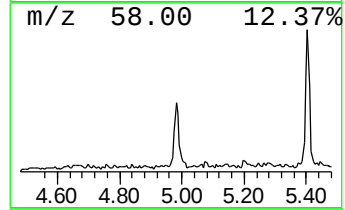
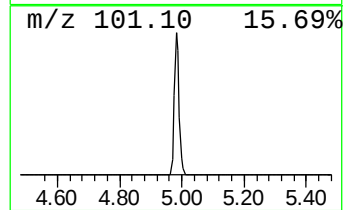
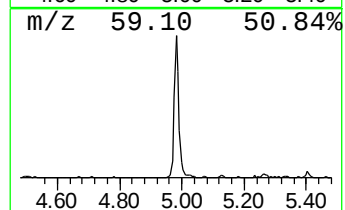
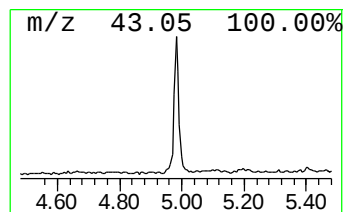
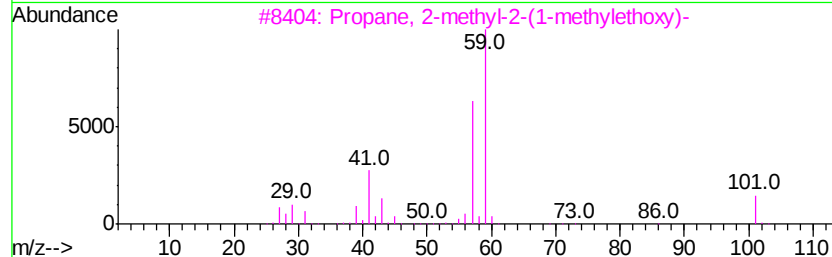
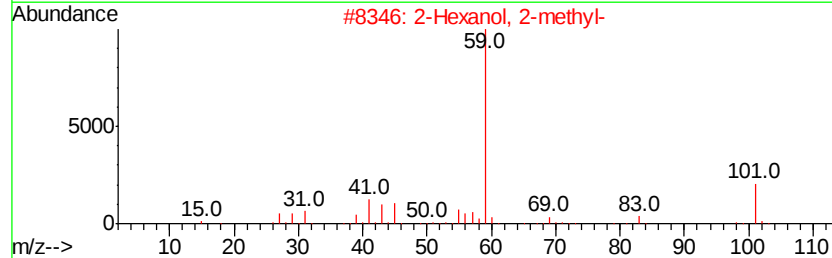
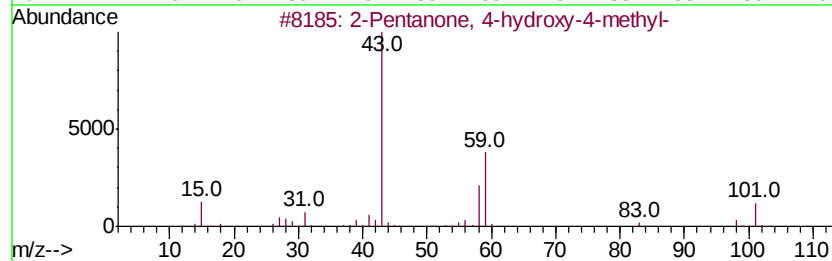
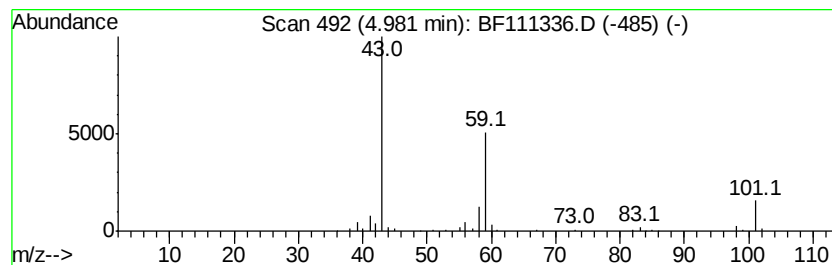
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	2.35 ng	185771	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	36
4			1,2-Butanediol	90	C4H10O2	000584-03-2	28
5			3-Pentanol	88	C5H12O	000584-02-1	28



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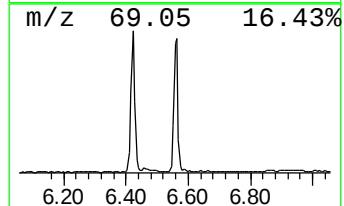
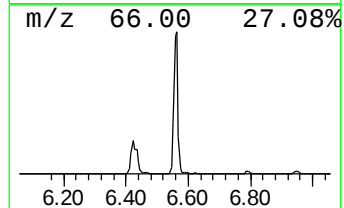
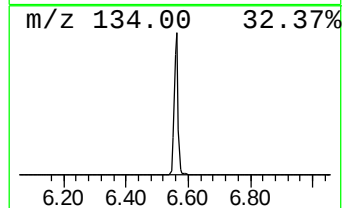
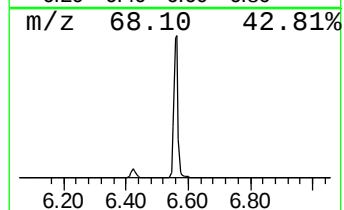
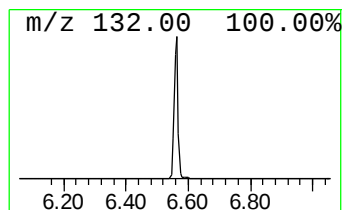
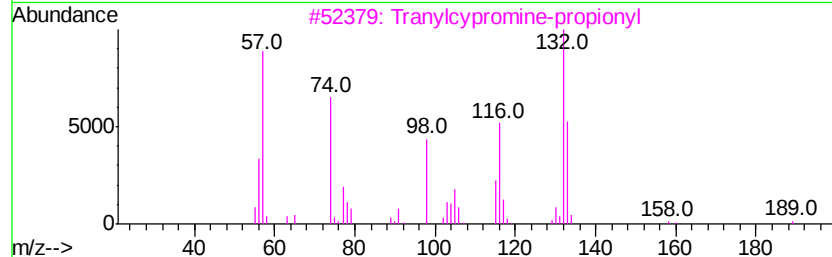
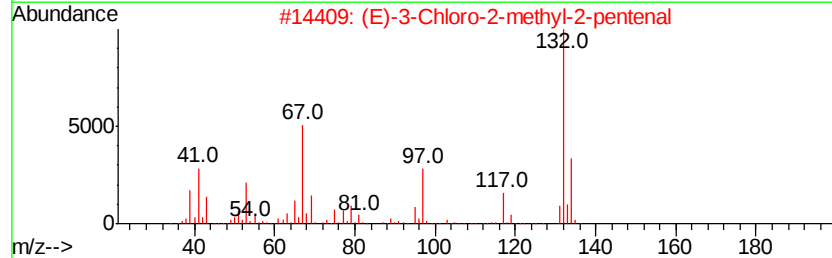
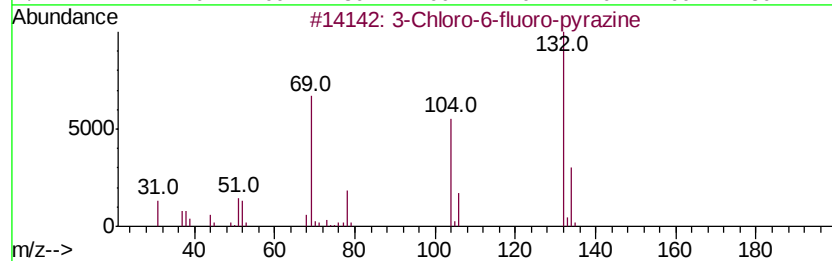
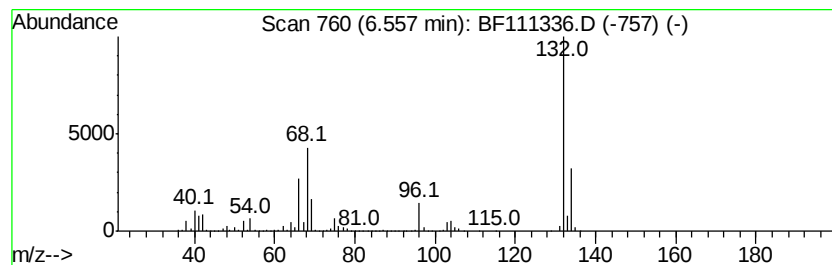
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	33.18 ng	2625580	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	16
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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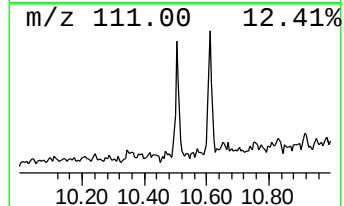
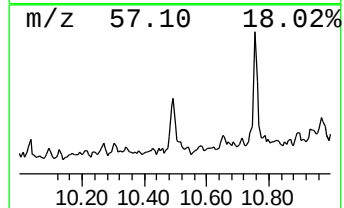
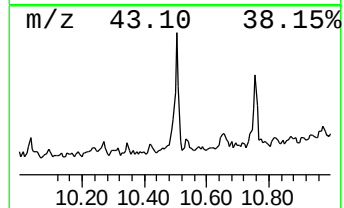
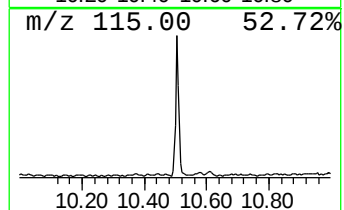
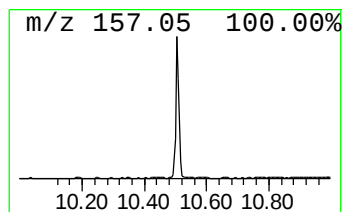
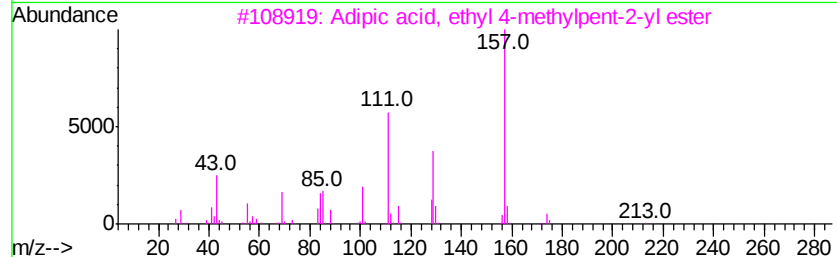
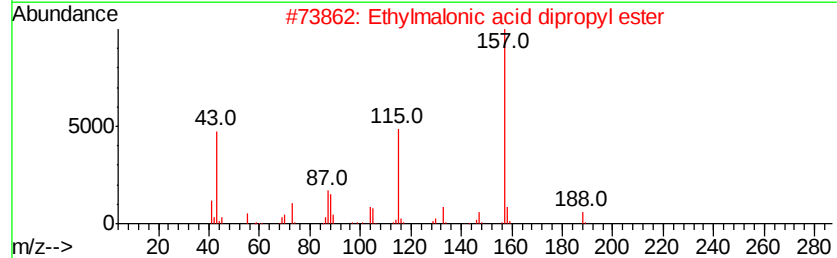
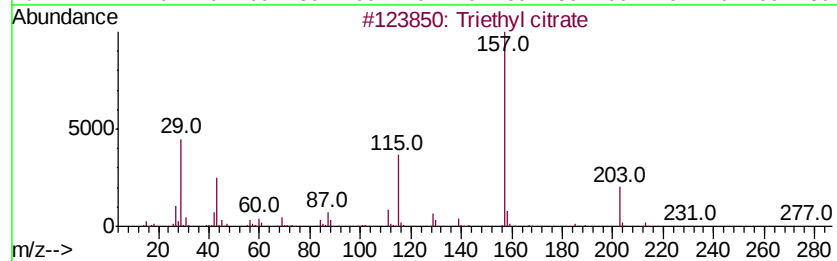
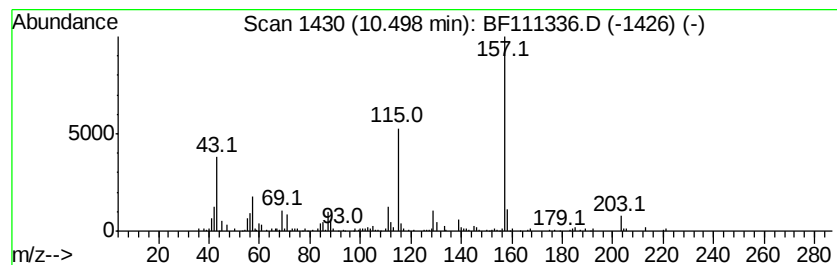
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	3.97 ng	342543	Acenaphthene-d10	9.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triethyl citrate	276 C12H20O7	000077-93-0 90
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 64
3		Adipic acid, ethyl 4-methylpent-...	258 C14H26O4	1000353-49-9 47
4		Hexanedioic acid, 3-ethyl-, bis(...	286 C16H30O4	057983-54-7 40
5		N-(5-[3-(2-Oxo-benzooxazol-3-yl)...	318 C14H14N4O3S	1000300-11-5 38



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Misc :
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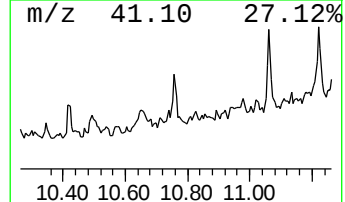
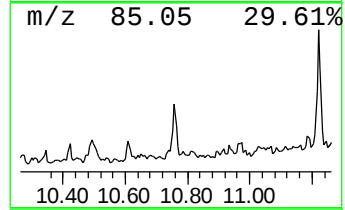
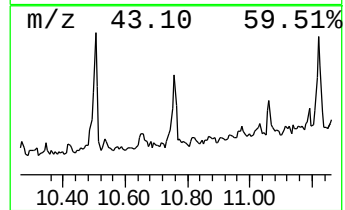
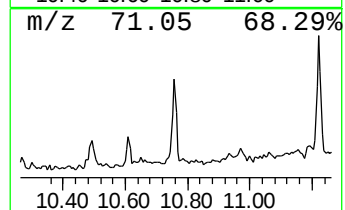
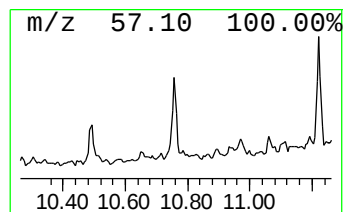
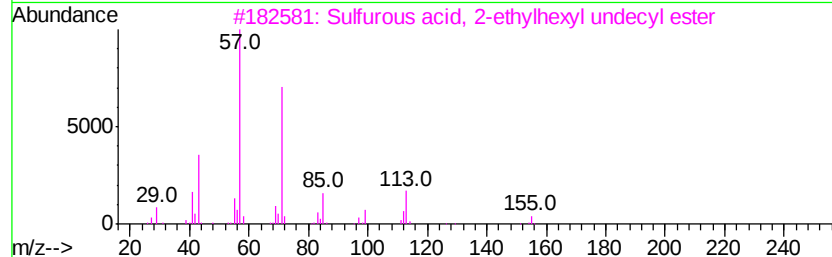
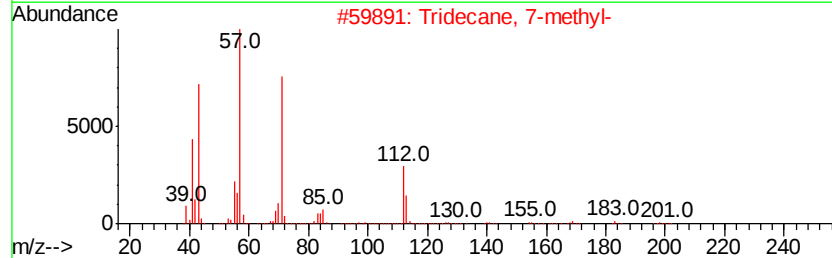
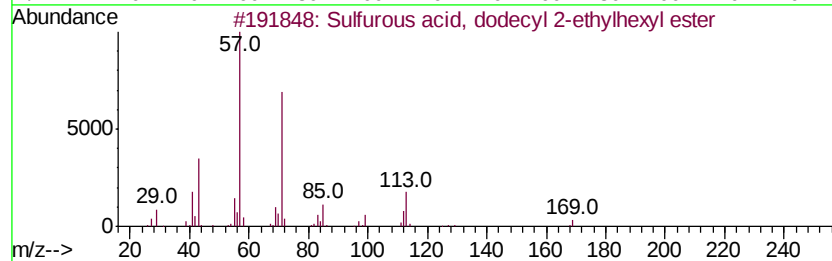
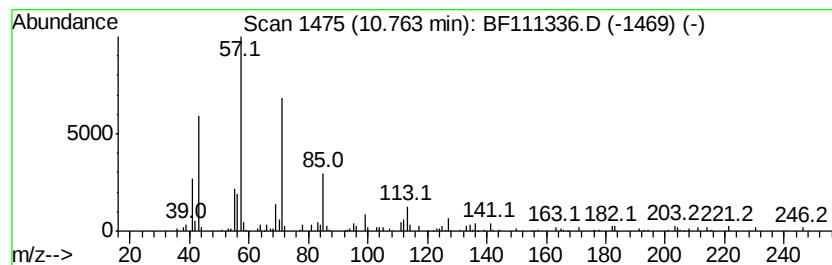
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Peak Number 5 Sulfurous acid, dodecyl 2-e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.07 ng	157020	Phenanthrene-d10	11.31
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Sulfurous acid, dodecyl 2-ethylh...	362 C20H42O3S	1000309-19-5 74
2		Tridecane, 7-methyl-	198 C14H30	026730-14-3 62
3		Sulfurous acid, 2-ethylhexyl und...	348 C19H40O3S	1000309-19-4 59
4		Sulfurous acid, 2-ethylhexyl hep...	432 C25H52O3S	1000309-20-0 53
5		Pentadecane, 7-methyl-	226 C16H34	006165-40-8 53



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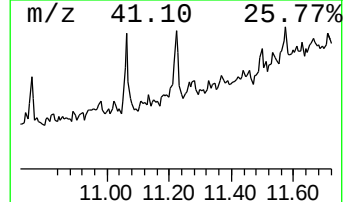
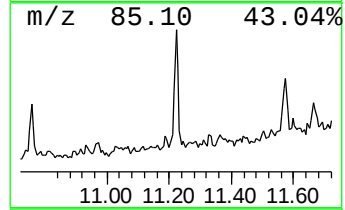
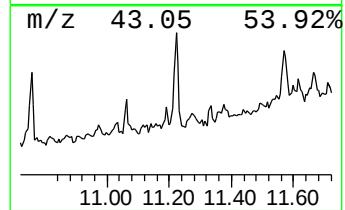
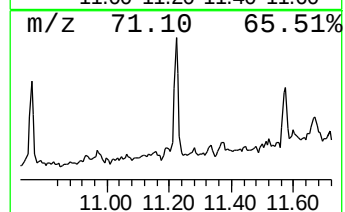
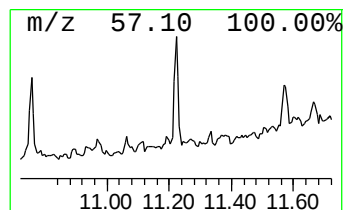
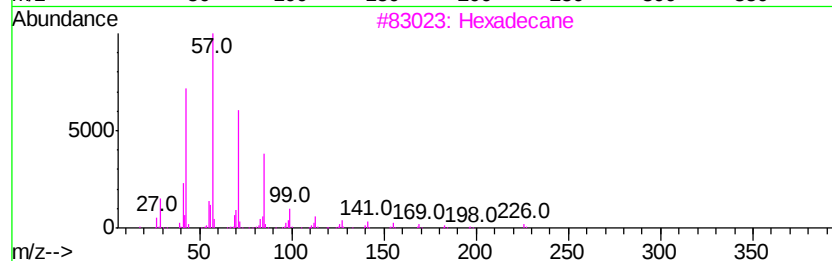
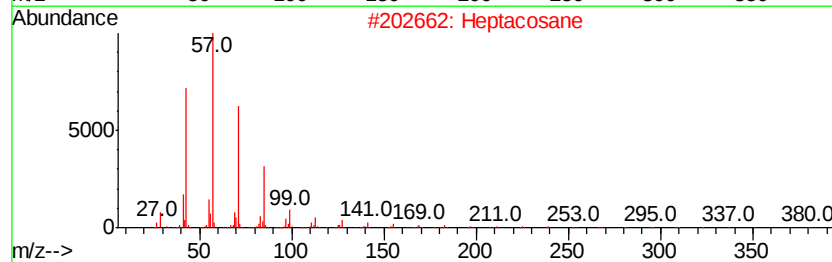
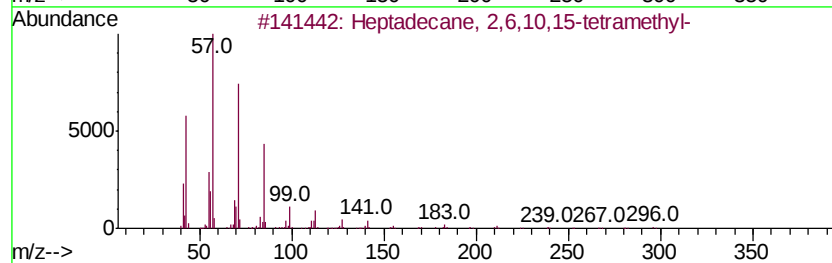
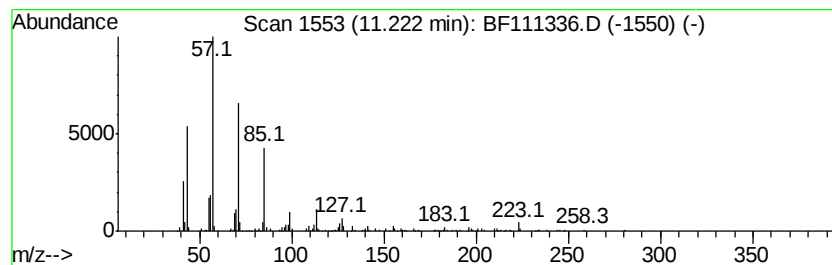
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.22	2.32 ng	175608	Phenanthrene-d10		11.31
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
2	Heptacosane	380	C27H56	000593-49-7	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Eicosane	282	C20H42	000112-95-8	80
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	74



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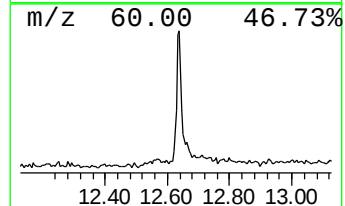
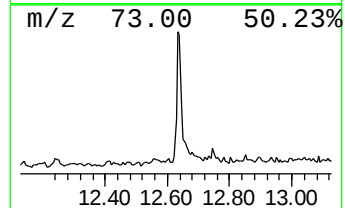
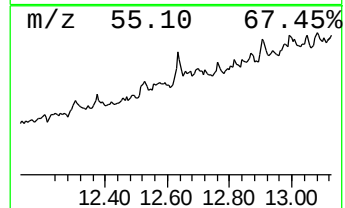
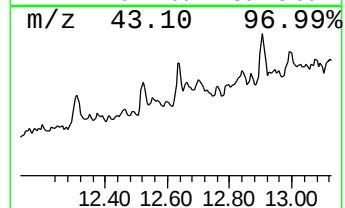
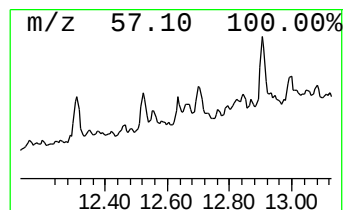
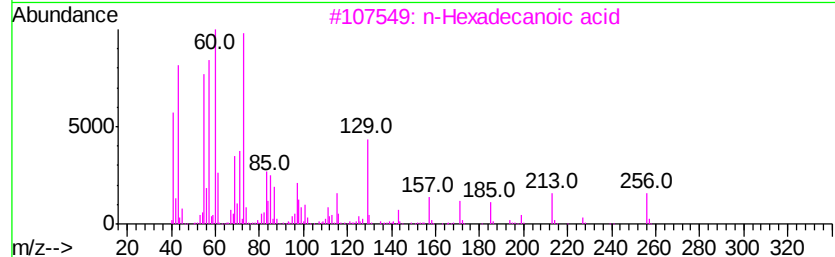
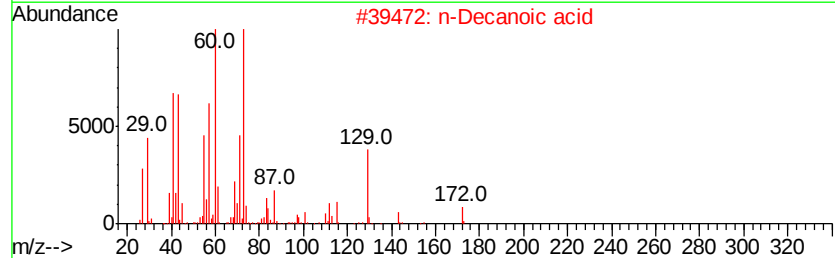
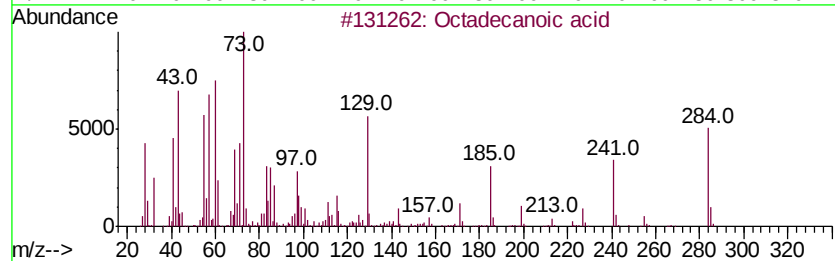
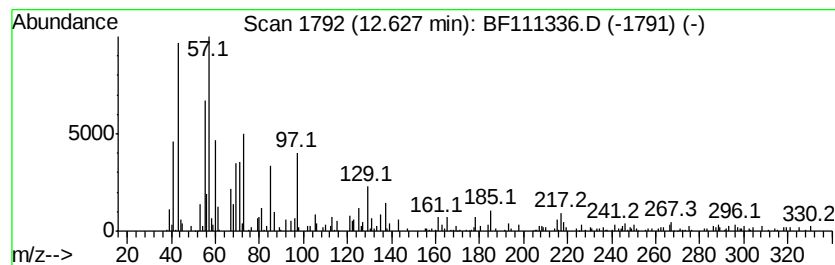
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	5.33 ng	403739	Phenanthrene-d10	11.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		n-Decanoic acid	172	C10H20O2	000334-48-5	52
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
4		Eicosane	282	C20H42	000112-95-8	35
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111336.D
Acq On : 12 Dec 2018 22:01
Operator : JU/SJ
Sample : J6214-27 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-2)

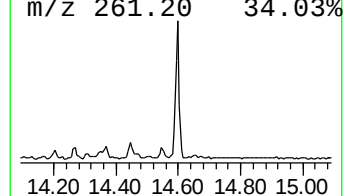
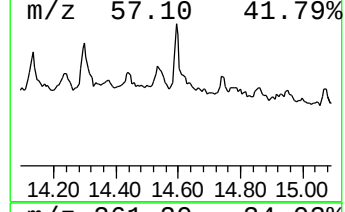
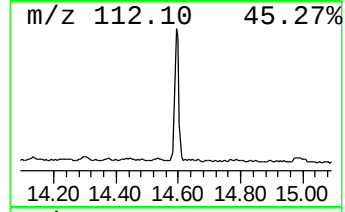
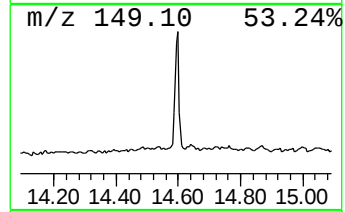
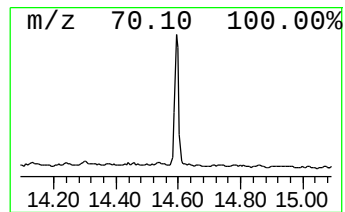
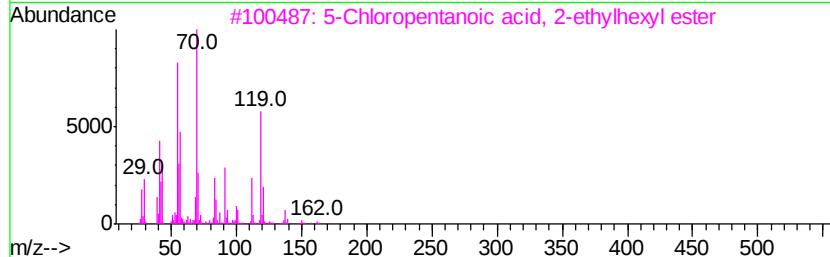
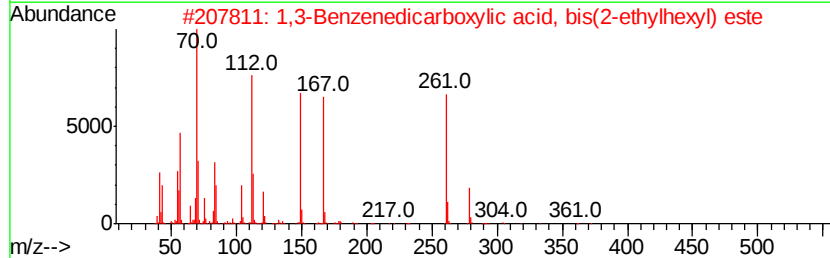
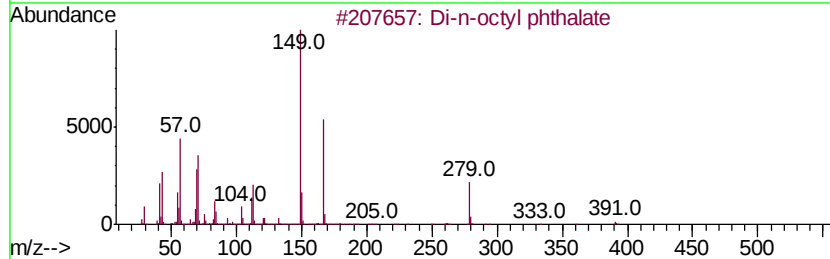
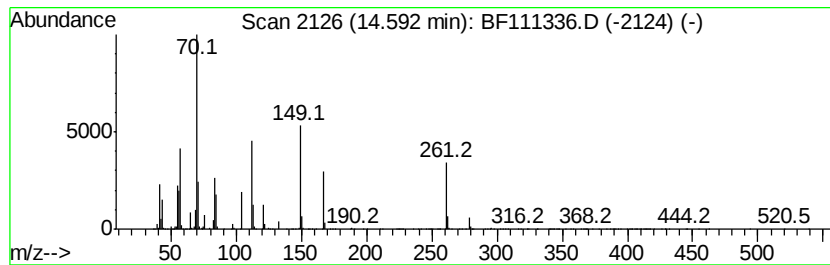
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	24.35 ng	1913220	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	42
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
3		5-Chloropentanoic acid, 2-ethylh...	248	C13H25ClO2	1000293-48-9	22
4		9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	22
5		Fumaric acid, 2-ethylhexyl hexyl...	312	C18H32O4	1000339-14-1	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121218\
Data File : BF111336.D
Acq On : 12 Dec 2018 22:01
Operator : JU/SJ
Sample : J6214-27 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.98	2.4	ng	185771	1	6.79	1582720	20.0
unknown6.56	6.56	33.2	ng	2625580	1	6.79	1582720	20.0
Triethyl citrate	10.50	4.0	ng	342543	3	9.83	1727540	20.0
Sulfurous acid, d...	10.76	2.1	ng	157020	4	11.31	1514030	20.0
Heptadecane, 2,6,...	11.22	2.3	ng	175608	4	11.31	1514030	20.0
Octadecanoic acid	12.63	5.3	ng	403739	4	11.31	1514030	20.0
unknown14.59	14.59	24.4	ng	1913220	5	13.96	1571530	20.0