

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100590.D
 Acq On : 15 Nov 2017 16:11
 Operator : SJ/JU
 Sample : I6422-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EPE-120-2(0-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	2.187	14	17	23	rVB2	18287	26984	1.21%	0.119%
2	4.492	405	409	418	rBV	146663	158103	7.10%	0.698%
3	5.104	509	513	526	rVB	457785	571431	25.65%	2.522%
4	5.504	576	581	584	rBV	1948743	1908217	85.64%	8.423%
5	6.504	746	751	756	rBV	1831296	2071780	92.98%	9.145%
6	6.651	771	776	779	rBV	2216974	1992249	89.41%	8.794%
7	6.881	812	815	819	rBV	854485	761185	34.16%	3.360%
8	7.039	838	842	845	rVB	1921279	1644925	73.83%	7.261%
9	7.445	906	911	914	rBV	1439302	1281584	57.52%	5.657%
10	8.163	1029	1033	1036	rBV	1144997	959414	43.06%	4.235%
11	8.186	1036	1037	1040	rVB	66248	31916	1.43%	0.141%
12	8.716	1123	1127	1130	rBV	137344	103654	4.65%	0.458%
13	9.239	1211	1216	1219	rBV	2616459	2228116	100.00%	9.835%
14	9.310	1225	1228	1231	rBV	29759	26909	1.21%	0.119%
15	9.627	1279	1282	1285	rBV	238607	181153	8.13%	0.800%
16	9.780	1305	1308	1311	rBV	31722	28515	1.28%	0.126%
17	9.839	1312	1318	1323	rVB	29681	28038	1.26%	0.124%
18	9.922	1327	1332	1335	rVB	971216	901014	40.44%	3.977%
19	10.627	1447	1452	1455	rBV	312558	240882	10.81%	1.063%
20	10.704	1461	1465	1468	rBV	981063	791088	35.50%	3.492%
21	10.816	1480	1484	1485	rBV2	28722	31129	1.40%	0.137%
22	11.292	1562	1565	1571	rVB4	27606	33077	1.48%	0.146%
23	11.404	1580	1584	1586	rBV	861932	710911	31.91%	3.138%
24	11.427	1586	1588	1591	rVB	173453	128897	5.79%	0.569%
25	11.916	1666	1671	1672	rBV2	43099	51465	2.31%	0.227%
26	12.451	1758	1762	1764	rBV4	27894	29019	1.30%	0.128%
27	12.480	1764	1767	1770	rVV2	36433	33443	1.50%	0.148%
28	12.616	1787	1790	1793	rBV	170332	143765	6.45%	0.635%
29	12.704	1802	1805	1809	rBV5	26143	41628	1.87%	0.184%
30	12.792	1817	1820	1823	rVB	212187	168192	7.55%	0.742%
31	12.845	1823	1829	1834	rBV	171505	226413	10.16%	0.999%
32	12.986	1847	1853	1861	rBV	1665727	1642346	73.71%	7.249%
33	13.515	1940	1943	1946	rBV	217145	193156	8.67%	0.853%
34	13.551	1947	1949	1952	rVV2	38570	38428	1.72%	0.170%

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ClientSampleId :
EPE-120-2(0-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.874	2001	2004	2010	rVB3	203876	233888	10.50%	1.032%
36	14.010	2025	2027	2029	rBV	95818	96402	4.33%	0.426%
37	14.039	2029	2032	2035	rVB	783952	709813	31.86%	3.133%
38	14.662	2134	2138	2142	rVB	1468323	1344383	60.34%	5.934%
39	15.145	2218	2220	2225	rVB	104201	116321	5.22%	0.513%
40	15.521	2280	2284	2292	rVB	532544	745749	33.47%	3.292%

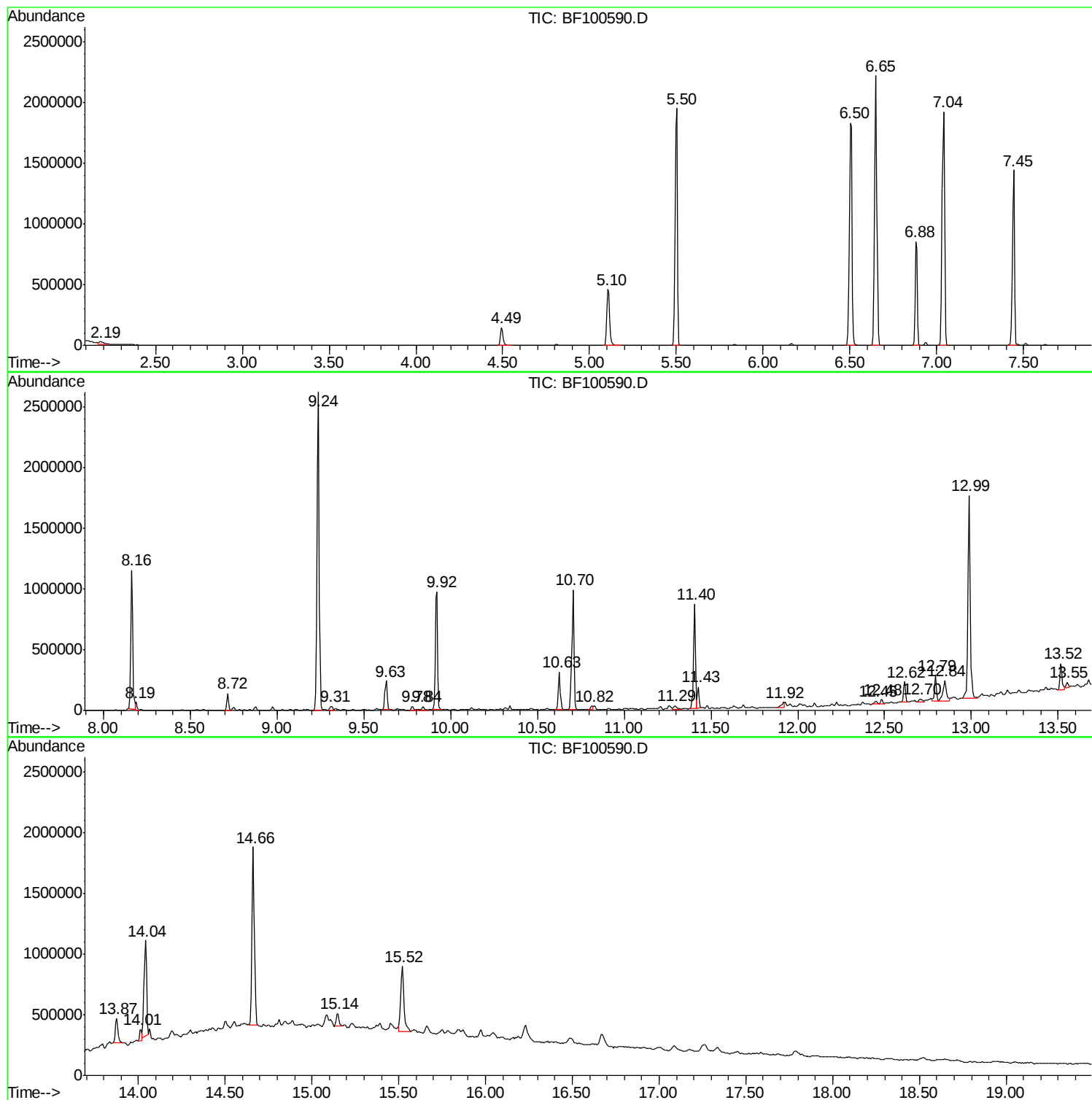
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Instrument :
BNA_F
ClientSampled :
EPE-120-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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Instrument :
BNA_F
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EPE-120-2(0-5)

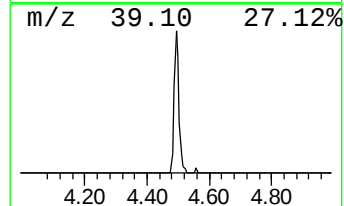
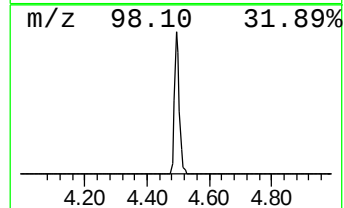
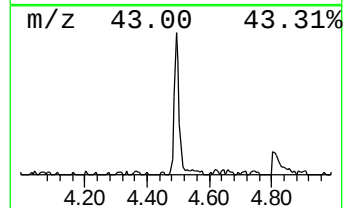
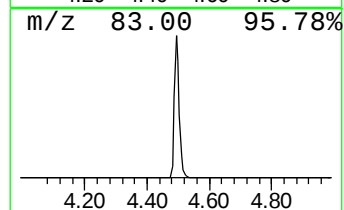
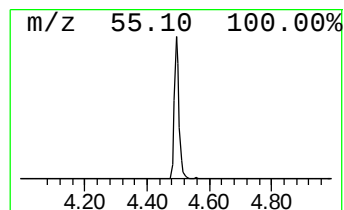
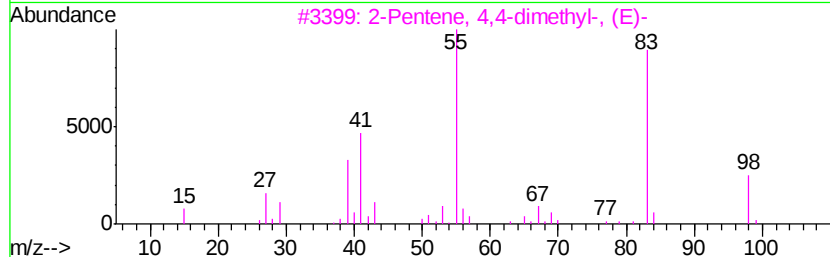
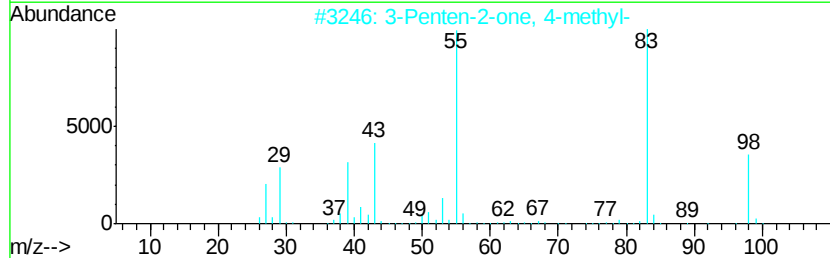
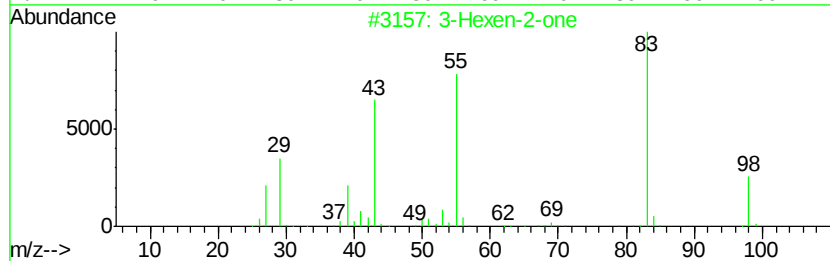
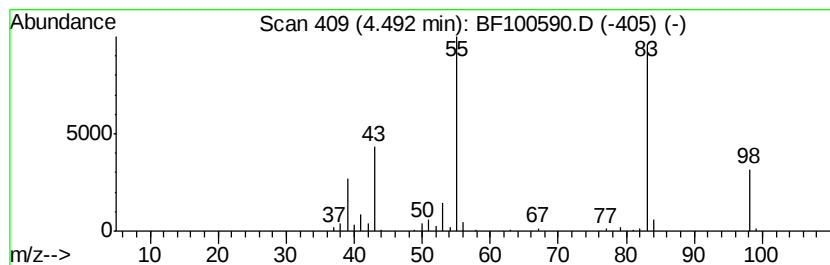
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	4.15 ng	158103	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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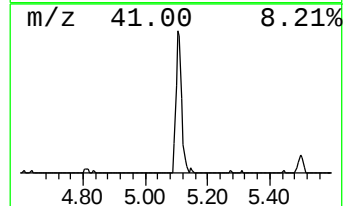
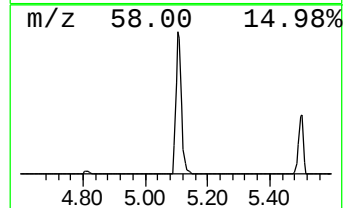
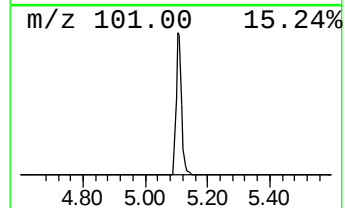
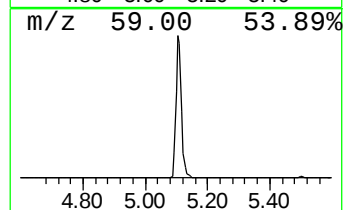
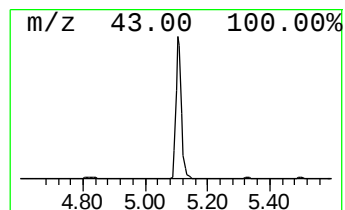
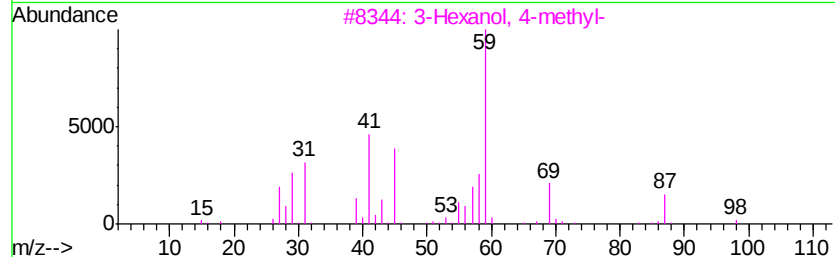
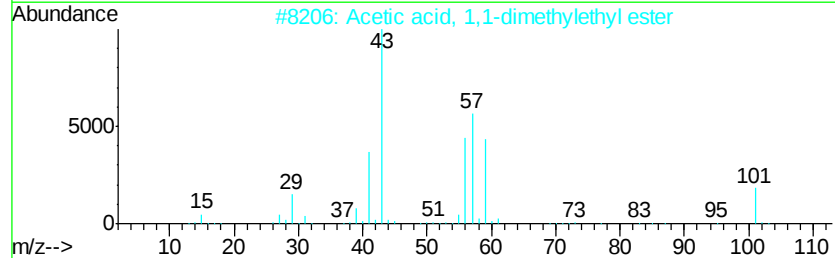
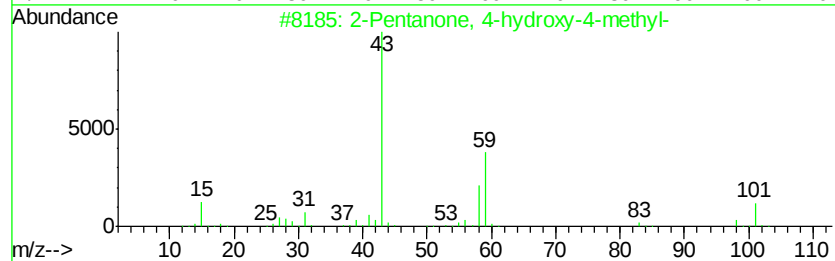
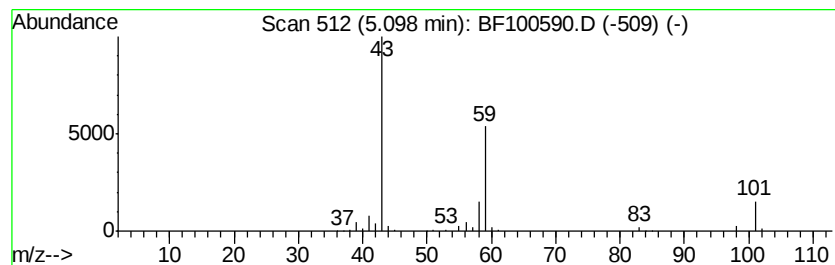
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	15.01 ng	571431	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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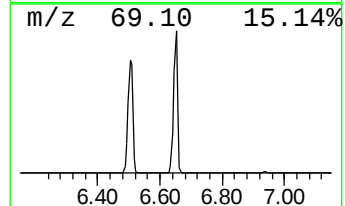
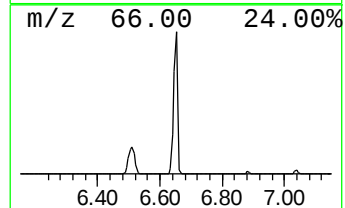
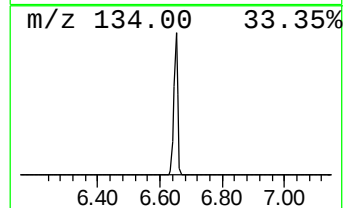
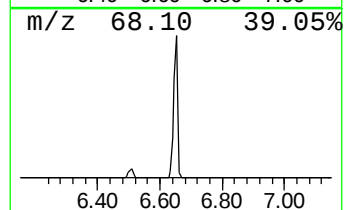
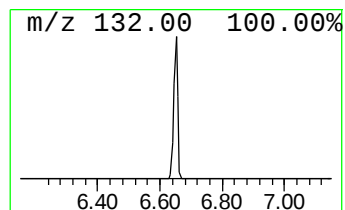
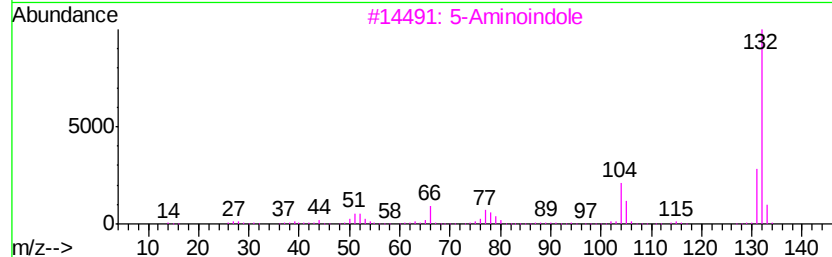
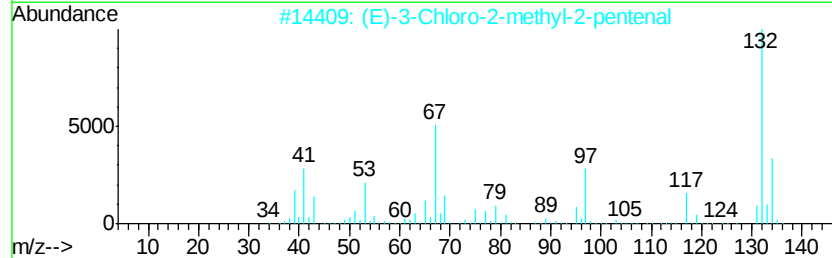
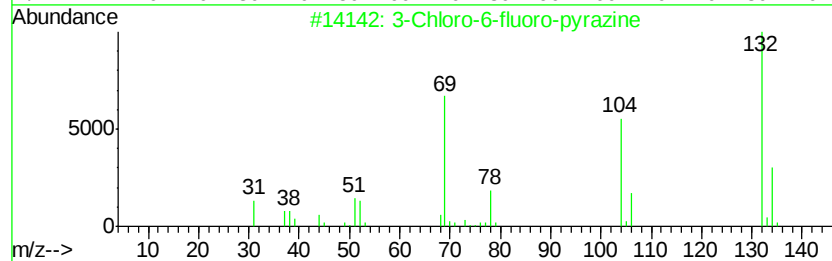
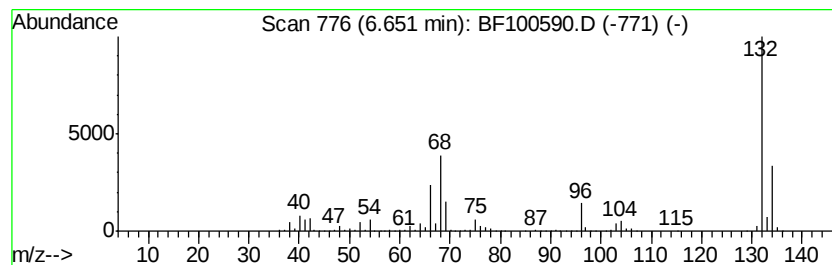
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	52.35 ng	1992250	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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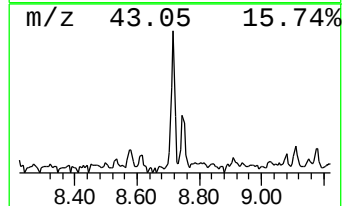
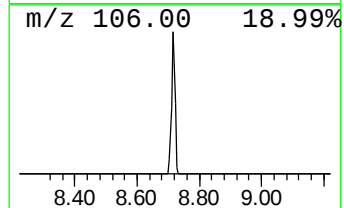
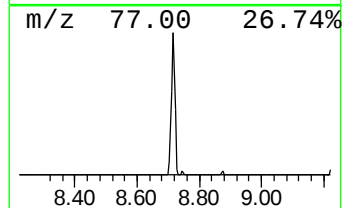
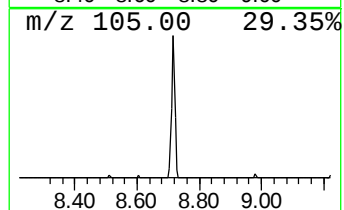
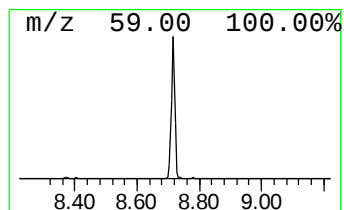
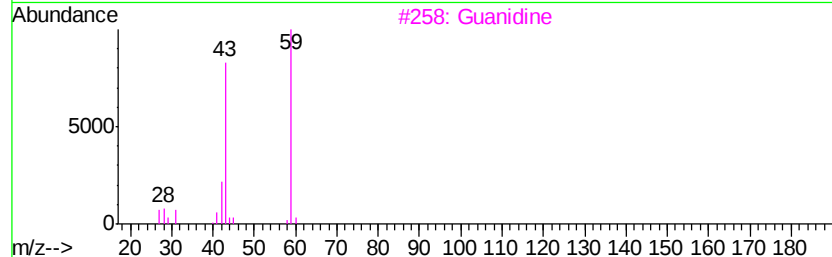
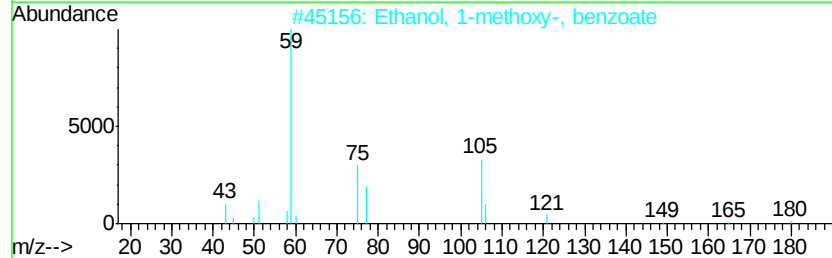
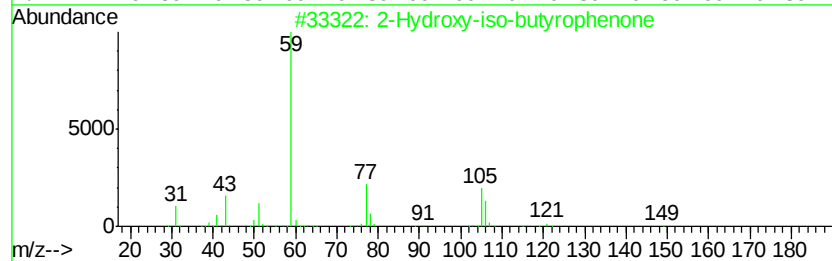
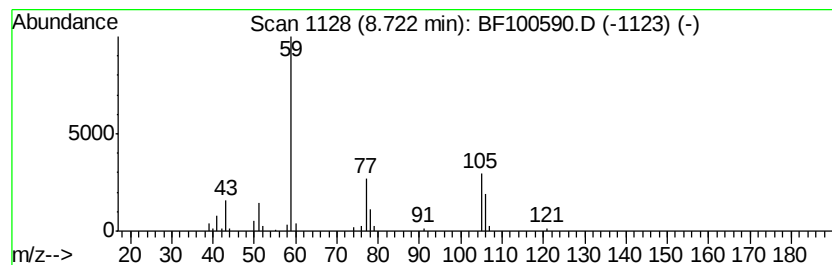
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.16 ng	103654	Napthalene-d8	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	86
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
3		Guanidine	59	CH5N3	000113-00-8	7
4		Acetamide	59	C2H5NO	000060-35-5	5
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	4



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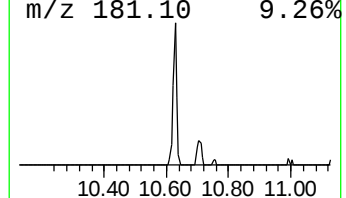
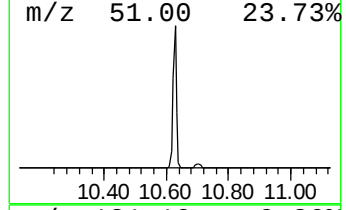
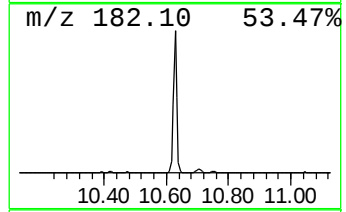
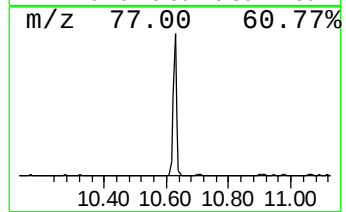
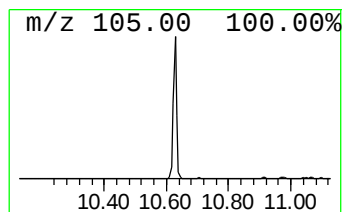
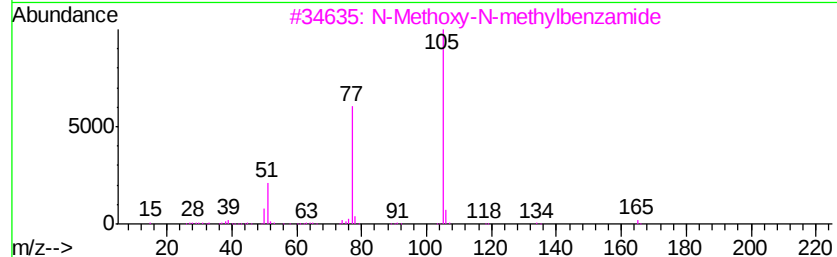
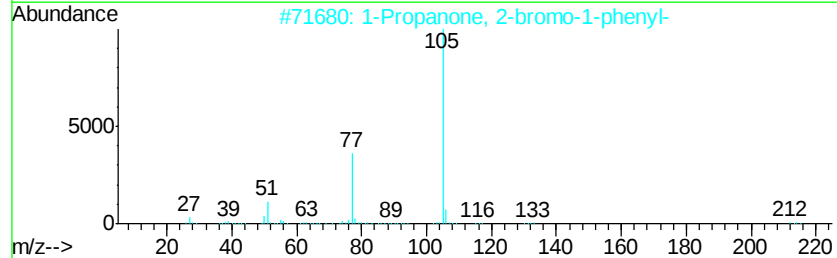
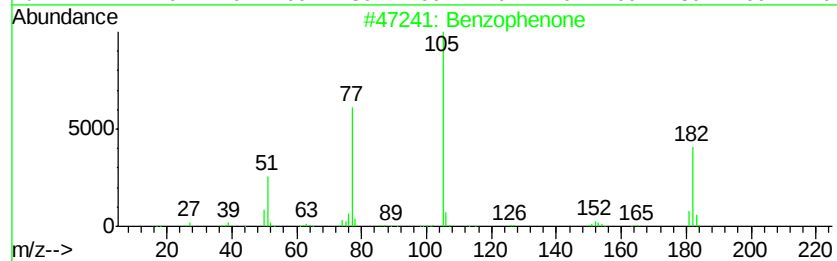
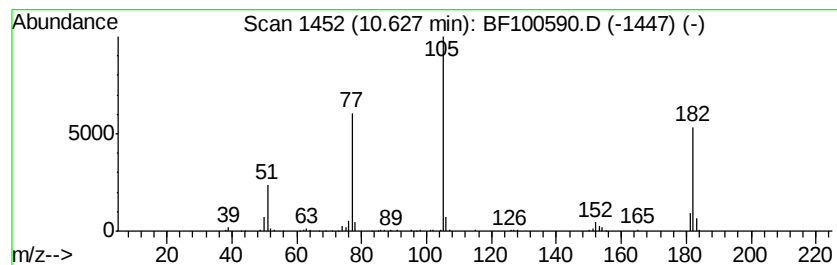
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	5.35 ng	240882	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		1-Propanone, 2-bromo-1-phenyl-	212 C9H9BrO	002114-00-3 47
3		N-Methoxy-N-methylbenzamide	165 C9H11NO2	006919-61-5 47
4		Vinyl benzoate	148 C9H8O2	000769-78-8 47
5		Benzoic acid, phenyl ester	198 C13H10O2	000093-99-2 47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100590.D
Acq On : 15 Nov 2017 16:11
Operator : SJ/JU
Sample : I6422-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

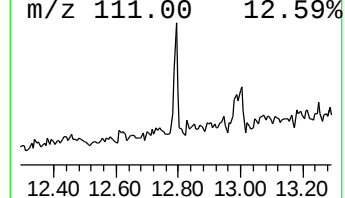
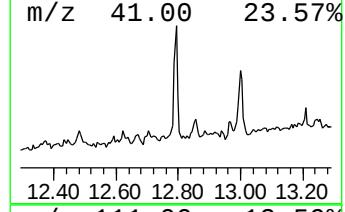
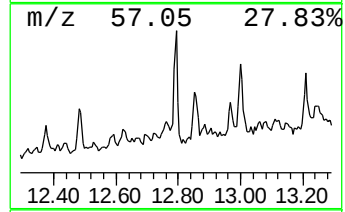
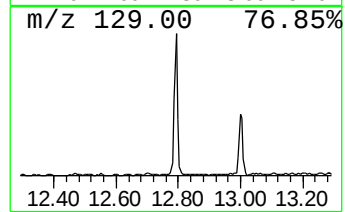
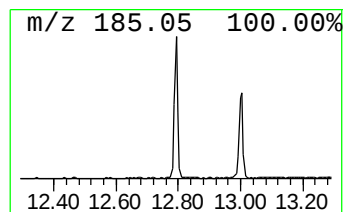
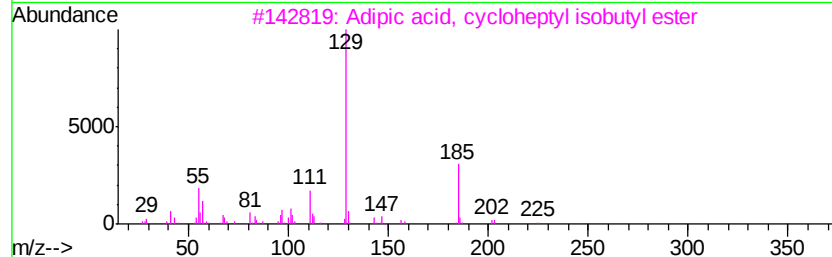
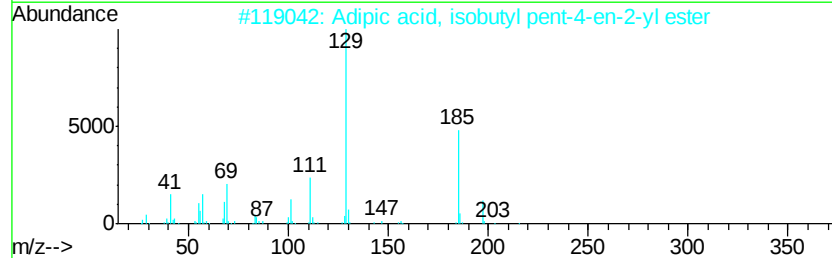
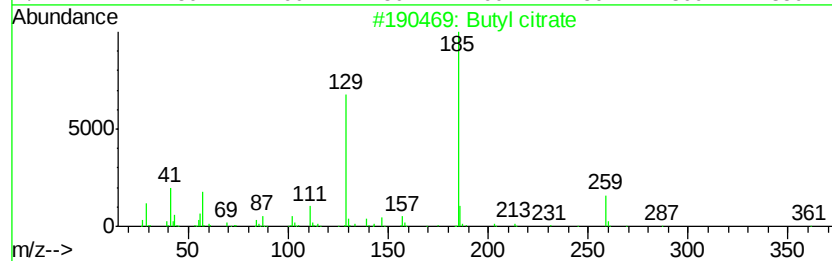
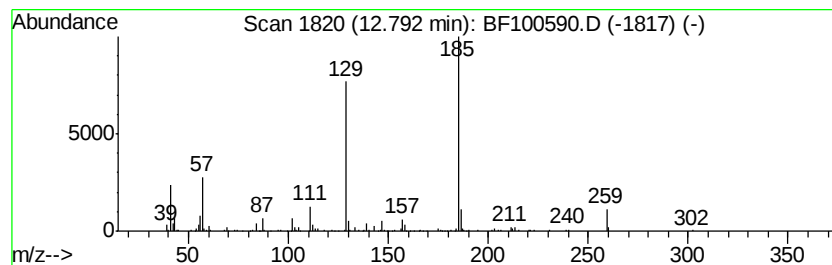
Instrument :
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ClientSampleId :
EPE-120-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Butyl citrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	4.74 ng	168192	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1 91	
2	Adipic acid, isobutyl pent-4-en-...	270 C15H26O4	1000354-11-8 78	
3	Adipic acid, cycloheptyl isobuty...	298 C17H30O4	1000324-71-5 72	
4	Adipic acid, cyclopentylmethyl i...	284 C16H28O4	1000324-77-3 72	
5	Adipic acid, 3-heptyl isobutyl e...	300 C17H32O4	1000353-64-8 72	



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Acq On : 15 Nov 2017 16:11
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Sample : I6422-05
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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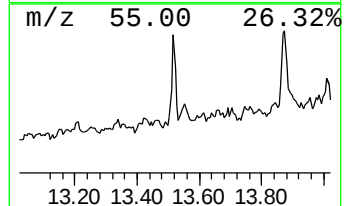
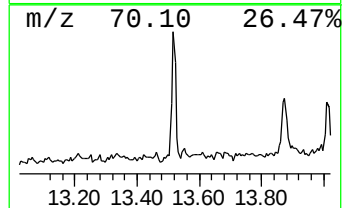
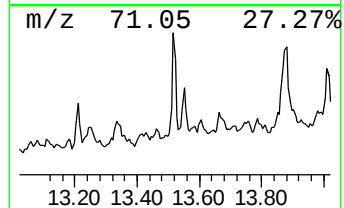
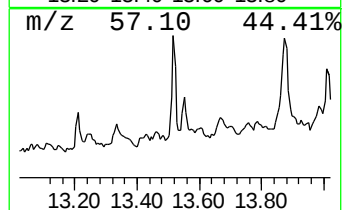
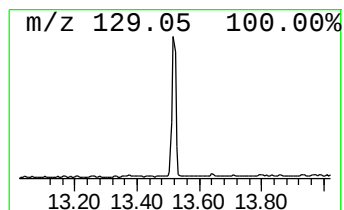
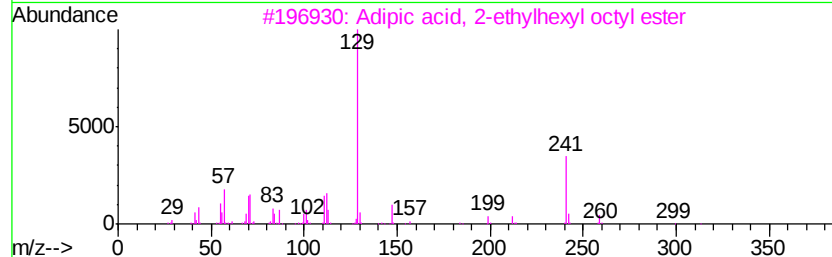
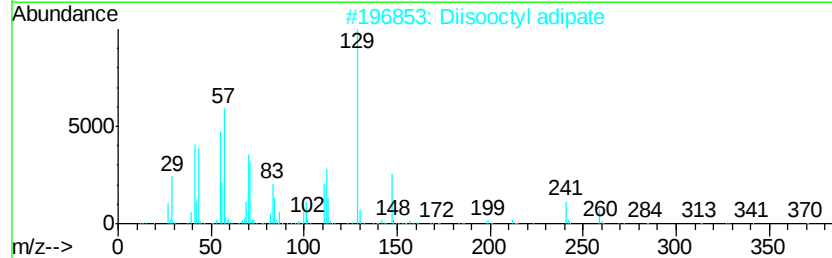
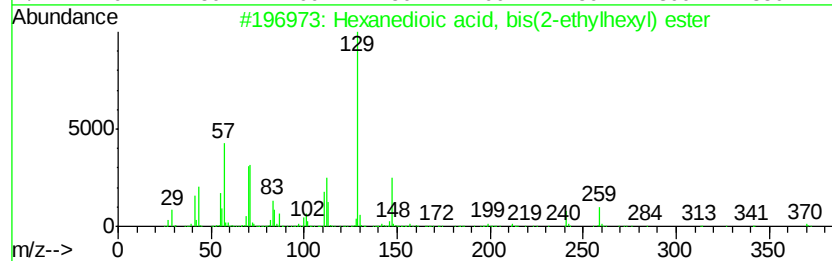
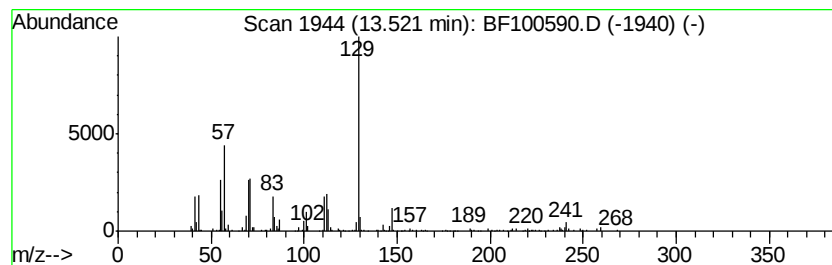
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	5.44 ng	193156	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
2		Diisooctyl adipate	370	C22H42O4	001330-86-5	87
3		Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	86
4		Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	58
5		Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	50



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Acq On : 15 Nov 2017 16:11
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Sample : I6422-05
Misc :
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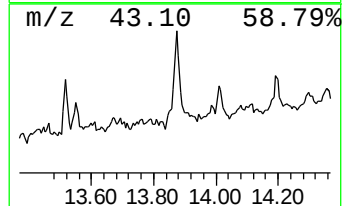
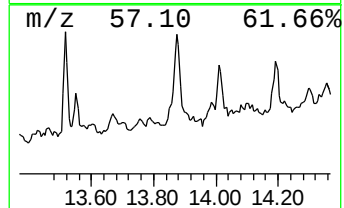
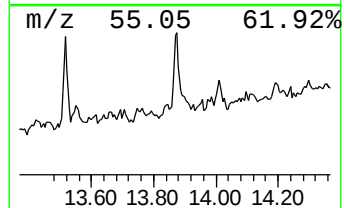
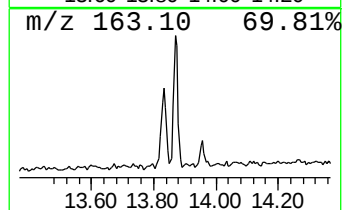
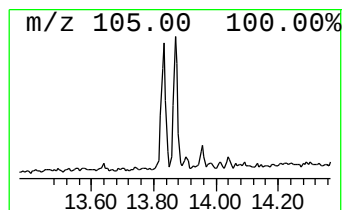
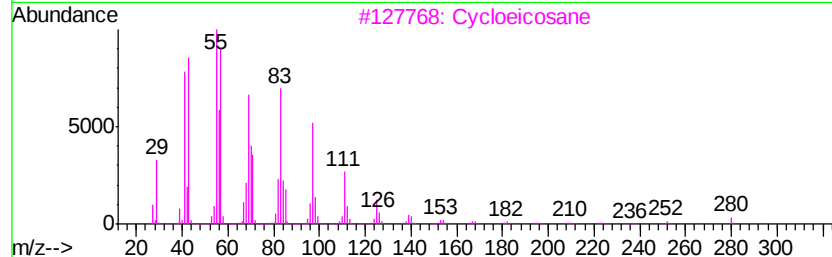
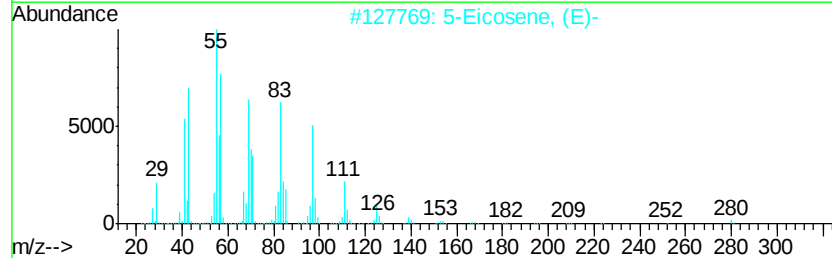
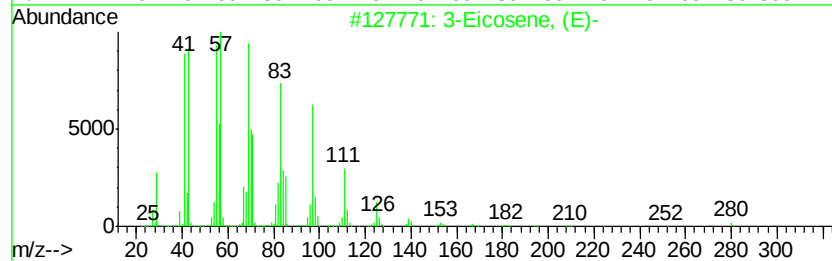
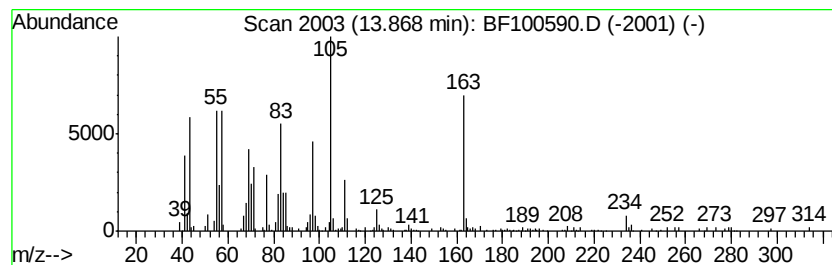
Instrument :
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ClientSampleId :
EPE-120-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.87	6.59 ng	233888	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	Cycloeicosane	280	C20H40	000296-56-0	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	87



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Sample : I6422-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EPE-120-2(0-5)

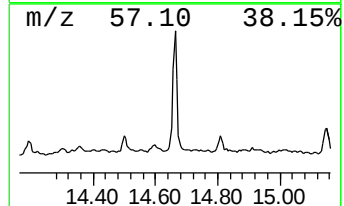
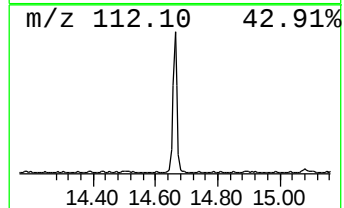
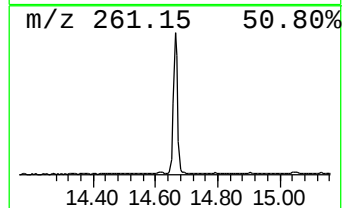
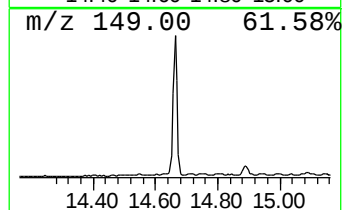
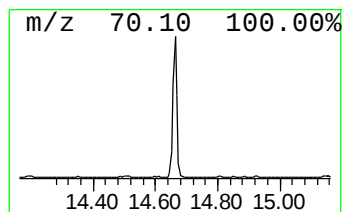
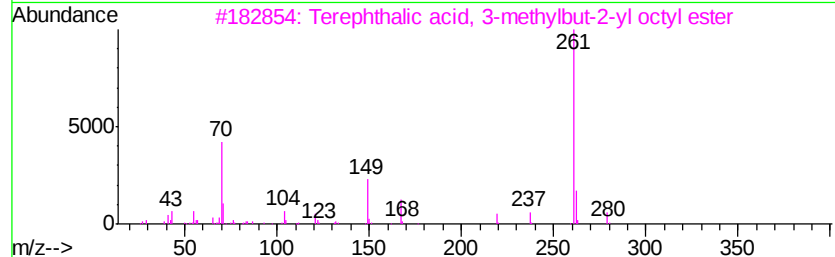
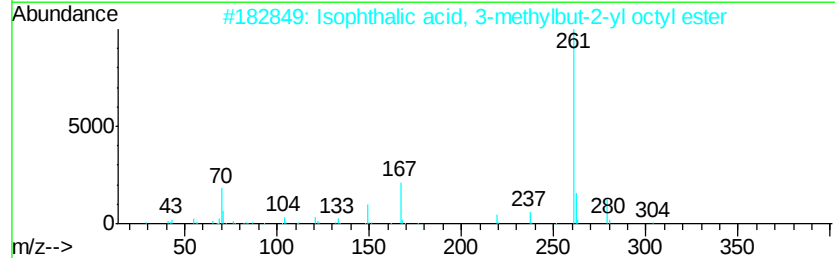
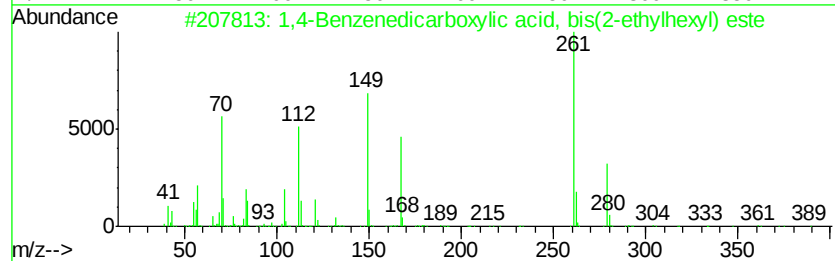
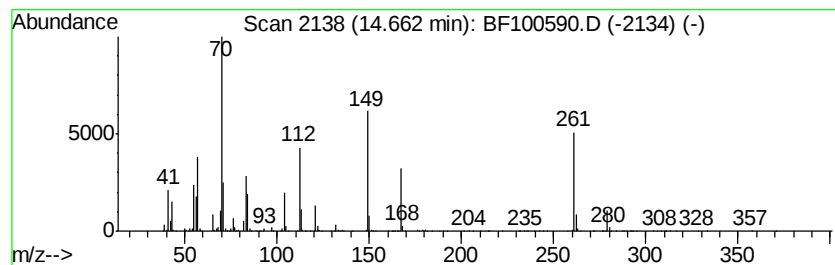
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	37.88 ng	1344380	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2		Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	50
3		Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
4		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
5		Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38



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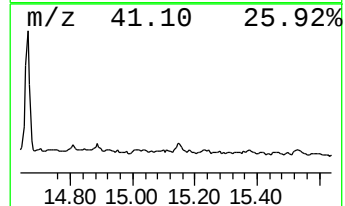
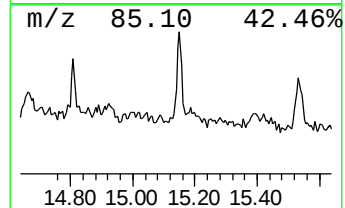
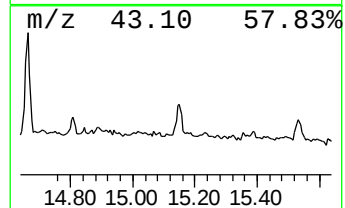
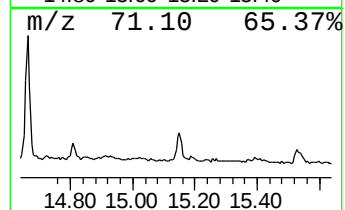
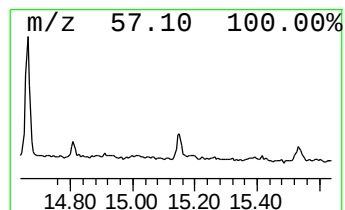
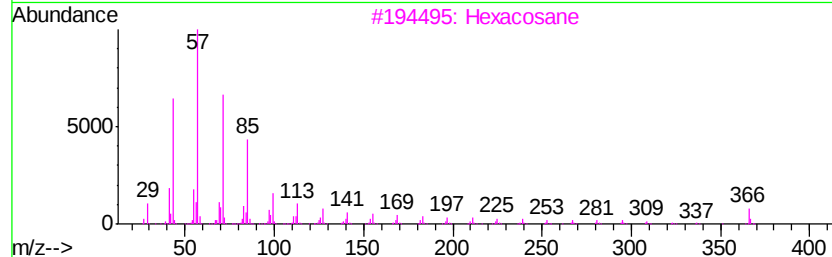
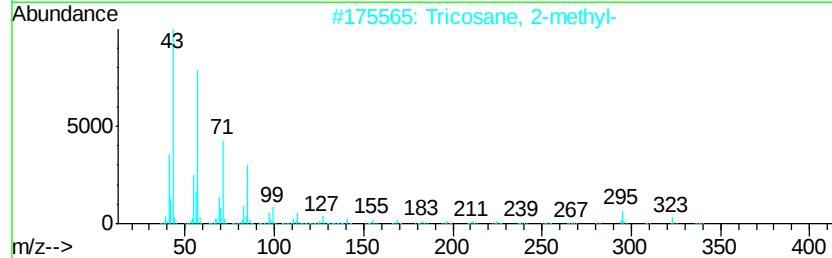
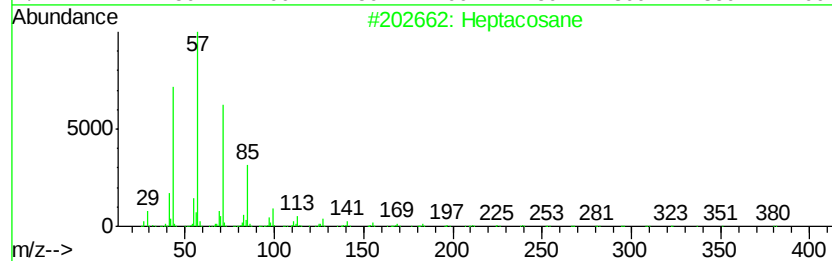
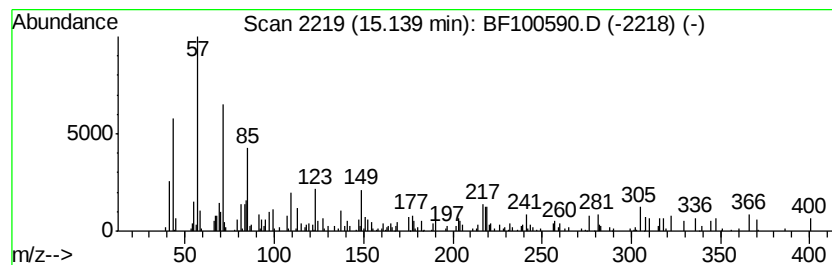
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	3.12 ng	116321	Perylene-d12	15.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Hexatriacontane	507	C36H74	000630-06-8	86
5			Tetracosane	338	C24H50	000646-31-1	80



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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EPE-120-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
3-Hexen-2-one	4.49	4.2	ng	158103	1	6.88	761185	20.0
2-Pentanone, 4-hy...	5.10	15.0	ng	571431	1	6.88	761185	20.0
unknown6.65	6.65	52.4	ng	1992250	1	6.88	761185	20.0
2-Hydroxy-iso-but...	8.72	2.2	ng	103654	2	8.16	959414	20.0
Benzophenone	10.63	5.3	ng	240882	3	9.92	901014	20.0
Butyl citrate	12.79	4.7	ng	168192	5	14.04	709813	20.0
Hexanedioic acid, ...	13.52	5.4	ng	193156	5	14.04	709813	20.0
3-Eicosene, (E)-	13.87	6.6	ng	233888	5	14.04	709813	20.0
1,4-Benzenedicarb...	14.66	37.9	ng	1344380	5	14.04	709813	20.0
Heptacosane	15.14	3.1	ng	116321	6	15.52	745749	20.0