

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
 Data File : BF098900.D
 Acq On : 28 Sep 2017 11:24
 Operator : SJ/JU
 Sample : I5418-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-119-2(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-BF092317.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	2.234	21	25	41	rVB	106442	185455	4.91%	0.532%
2	5.151	516	521	530	rVB	559864	748406	19.82%	2.146%
3	5.539	582	587	590	rBV	3178306	3464275	91.75%	9.933%
4	6.545	752	758	762	rVB	3076870	3501644	92.74%	10.041%
5	6.686	777	782	785	rBV	3602543	3509783	92.96%	10.064%
6	6.916	817	821	824	rBV	1148246	913711	24.20%	2.620%
7	7.075	843	848	851	rBV	2849403	2627280	69.58%	7.533%
8	7.481	911	917	919	rBV	2107853	2249506	59.58%	6.450%
9	7.551	925	929	932	rVB	46727	41203	1.09%	0.118%
10	8.198	1035	1039	1042	rBV	1451467	1242280	32.90%	3.562%
11	9.275	1216	1222	1225	rBV	3682514	3775763	100.00%	10.827%
12	9.663	1283	1288	1291	rBV	543297	466661	12.36%	1.338%
13	9.951	1333	1337	1341	rBV	1464807	1350737	35.77%	3.873%
14	10.139	1365	1369	1372	rBV	43761	47726	1.26%	0.137%
15	10.374	1406	1409	1411	rVB	67125	51604	1.37%	0.148%
16	10.745	1464	1472	1475	rBV	2145933	2215481	58.68%	6.353%
17	10.845	1486	1489	1499	rBV	80422	81480	2.16%	0.234%
18	11.086	1526	1530	1535	rVB4	29871	44140	1.17%	0.127%
19	11.439	1586	1590	1593	rBV	1554797	1342242	35.55%	3.849%
20	11.698	1622	1634	1635	rBV6	42053	108505	2.87%	0.311%
21	11.716	1635	1637	1649	rVB2	54894	112698	2.98%	0.323%
22	11.951	1672	1677	1686	rBV	376333	452686	11.99%	1.298%
23	12.339	1734	1743	1750	rBV6	21440	66567	1.76%	0.191%
24	12.463	1756	1764	1771	rVB2	42268	105778	2.80%	0.303%
25	12.651	1792	1796	1801	rBV	44739	64169	1.70%	0.184%
26	12.739	1806	1811	1823	rVV	219094	251405	6.66%	0.721%
27	13.027	1855	1860	1863	rBV	3499106	3355047	88.86%	9.620%
28	13.421	1921	1927	1935	rBV3	51855	122845	3.25%	0.352%
29	13.568	1949	1952	1958	rVB	41435	41298	1.09%	0.118%
30	13.904	2006	2009	2013	rBV	165770	162668	4.31%	0.466%
31	14.080	2035	2039	2042	rBV	1027729	951334	25.20%	2.728%
32	14.657	2132	2137	2142	rBV2	52207	89610	2.37%	0.257%
33	14.827	2163	2166	2174	rBV2	44228	78656	2.08%	0.226%
34	15.009	2193	2197	2205	rVB9	45099	95463	2.53%	0.274%

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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
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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

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35	15.233	2231	2235	2239	rVB2	36391	53691	1.42%	0.154%
36	15.574	2287	2293	2305	rVB	570968	845656	22.40%	2.425%
37	16.545	2456	2458	2465	rVB3	32311	57545	1.52%	0.165%

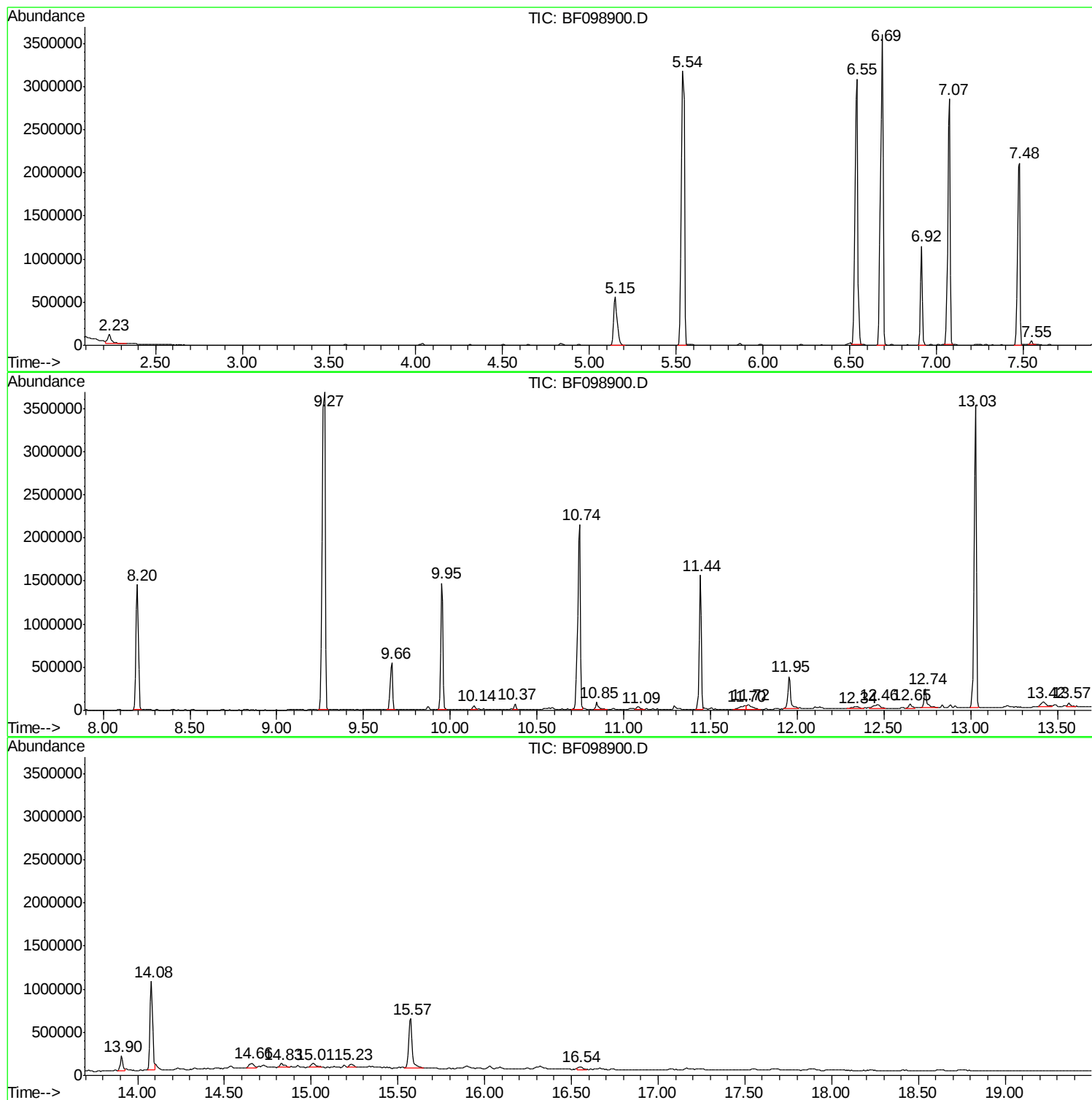
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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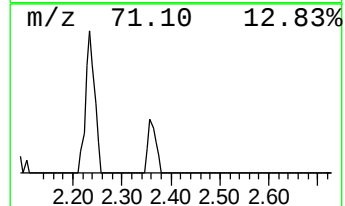
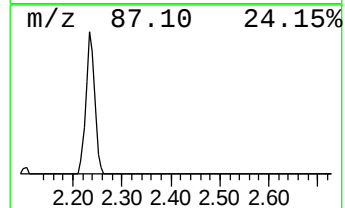
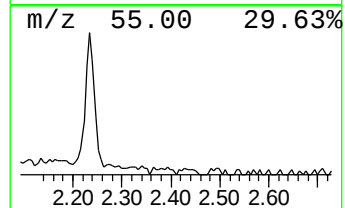
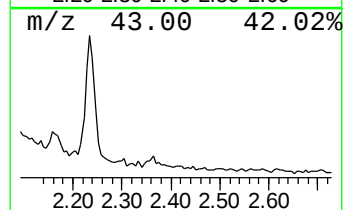
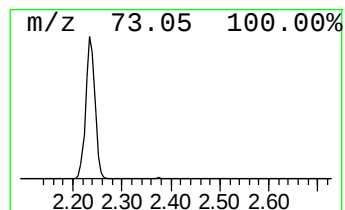
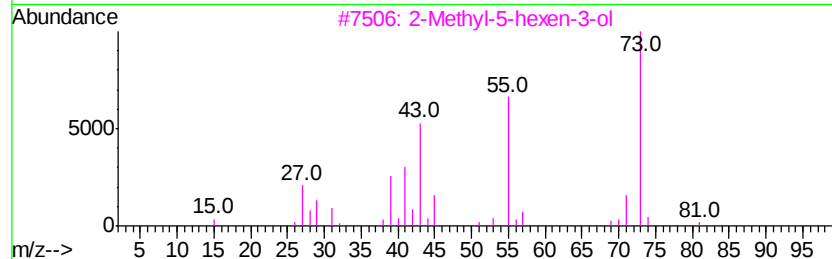
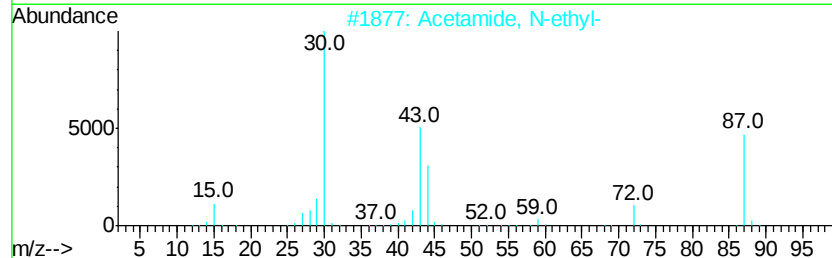
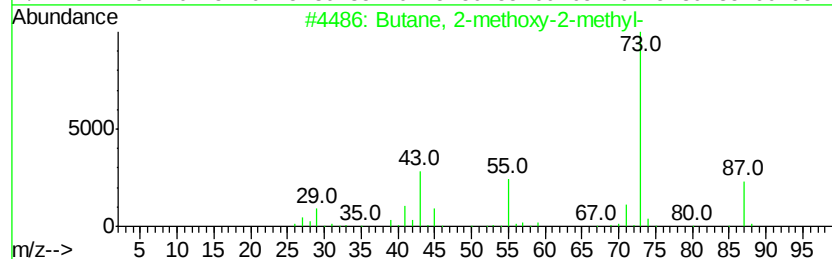
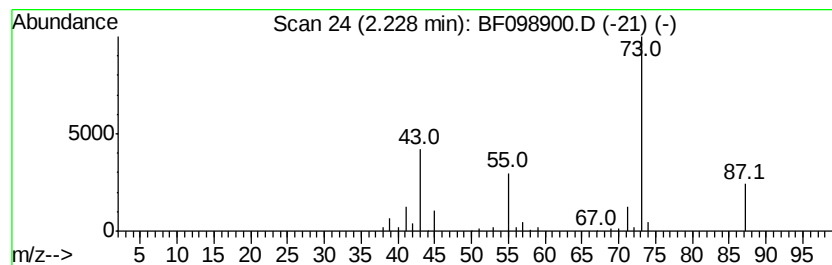
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	4.06 ng	185455	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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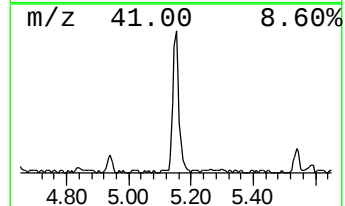
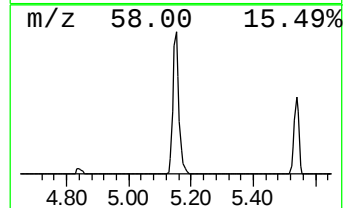
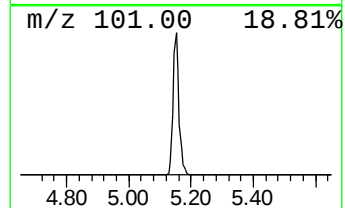
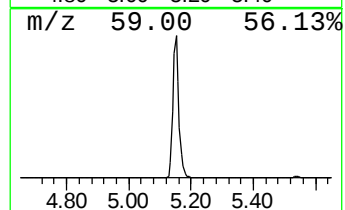
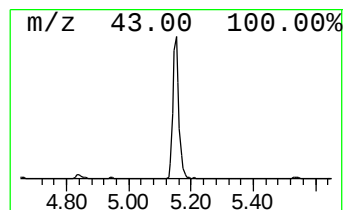
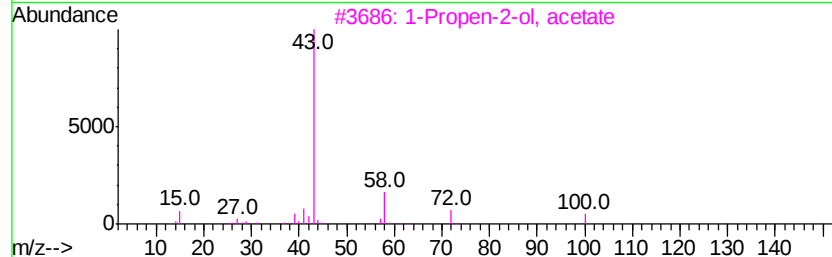
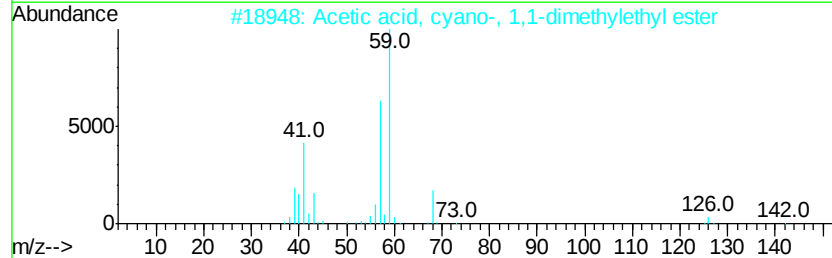
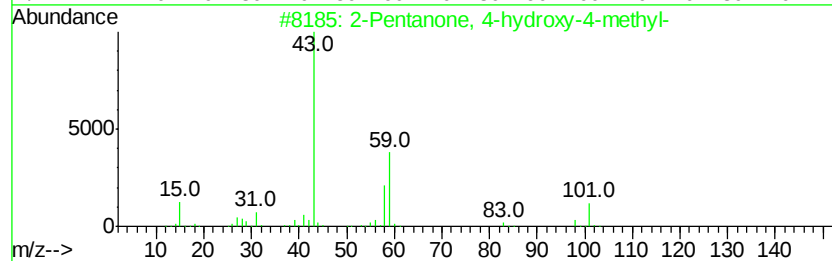
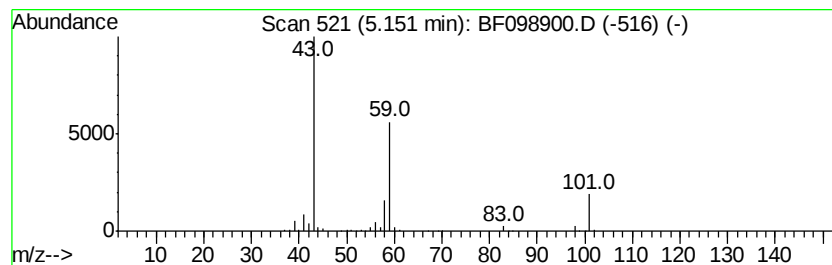
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	16.38 ng	748406	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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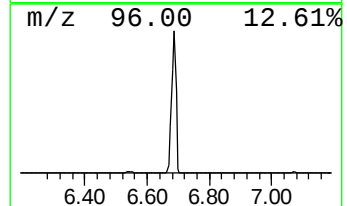
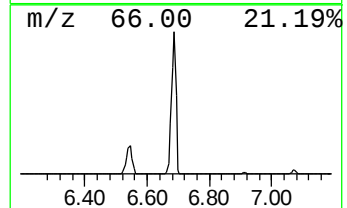
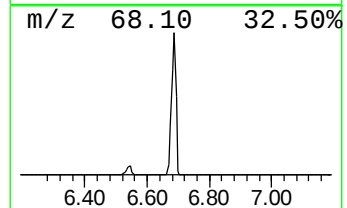
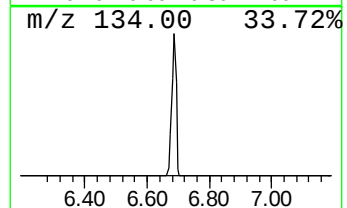
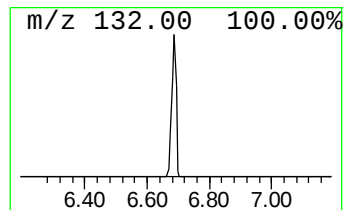
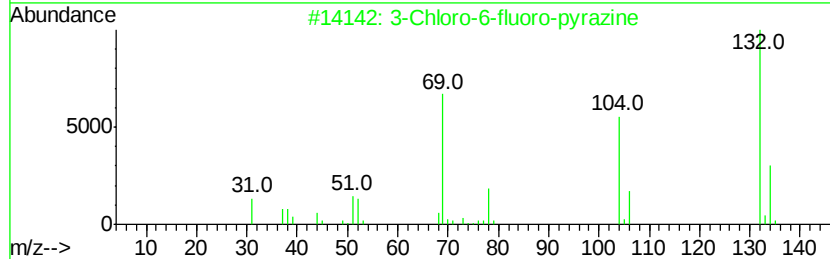
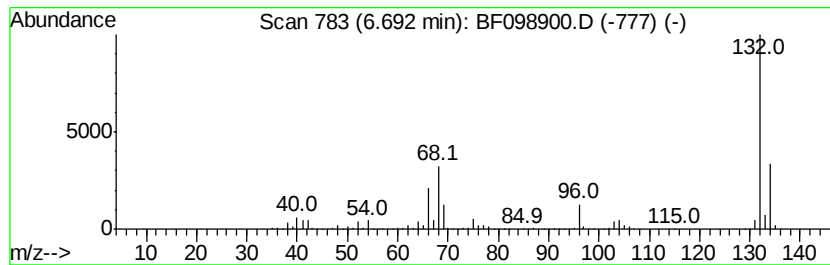
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	76.82 ng	3509780	1,4-Dichlorobenzene-d4	6.92

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	16
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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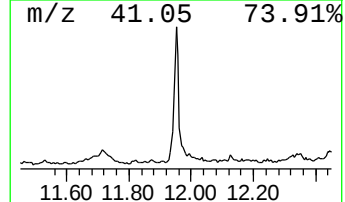
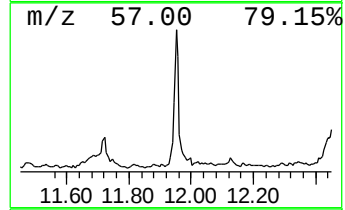
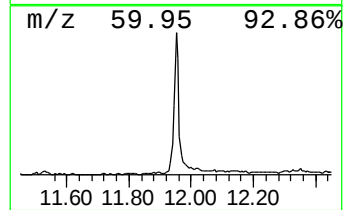
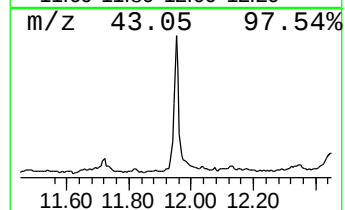
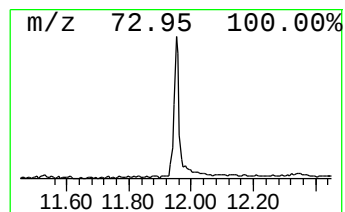
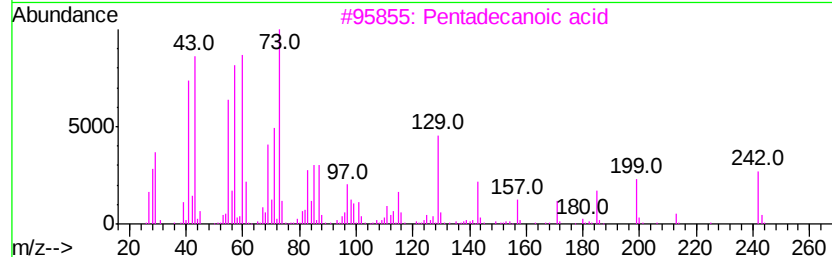
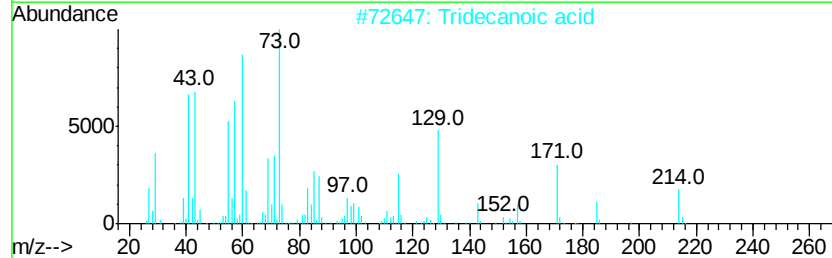
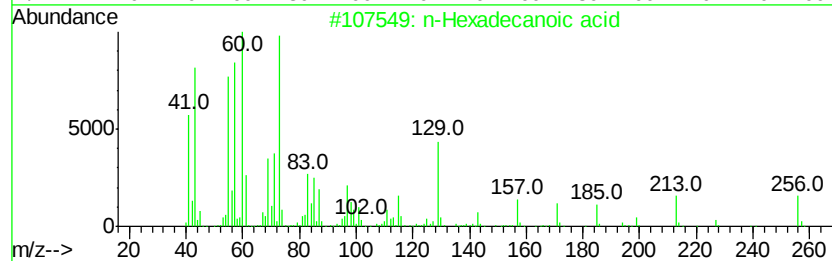
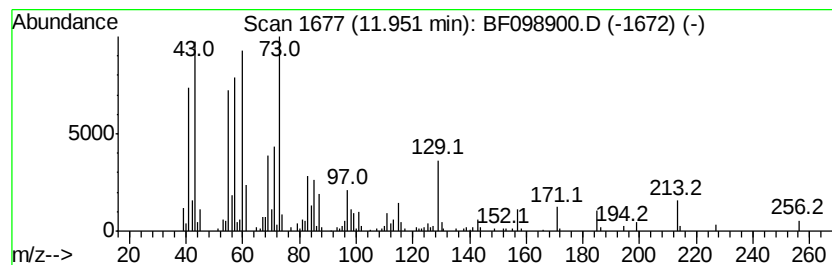
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.95	6.75 ng	452686	Phenanthrene-d10		11.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25



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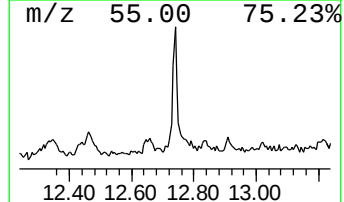
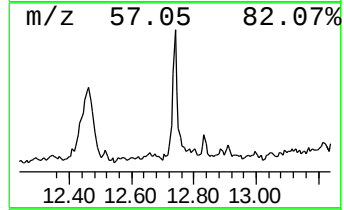
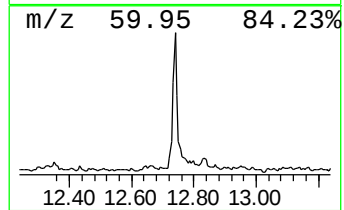
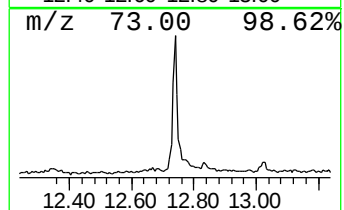
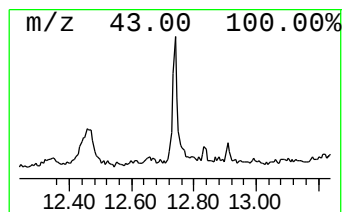
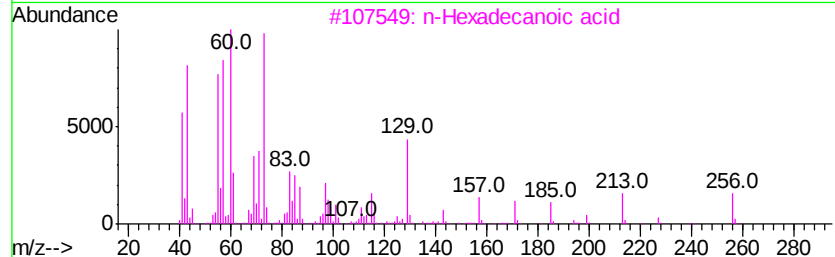
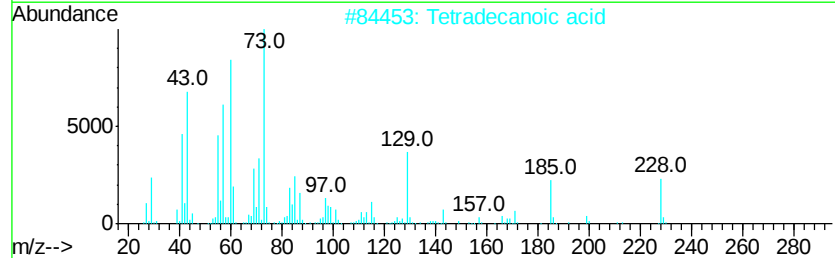
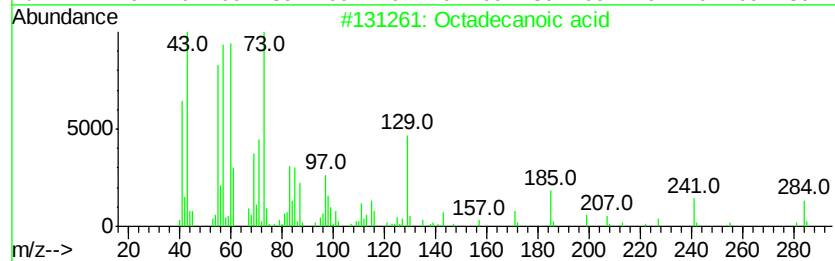
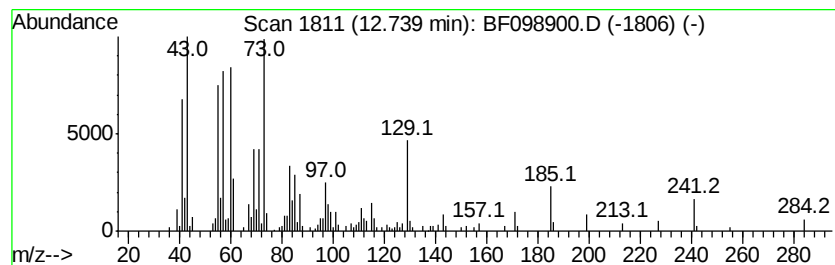
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.75 ng	251405	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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BNA_F
ClientSampleId :
SASP2P-ENV-119-2(0-5)

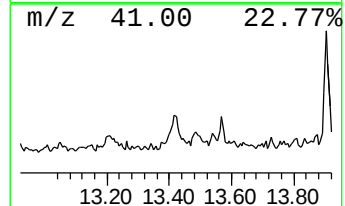
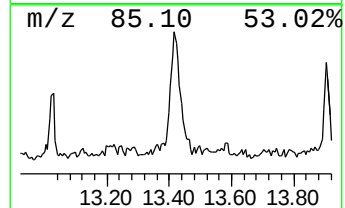
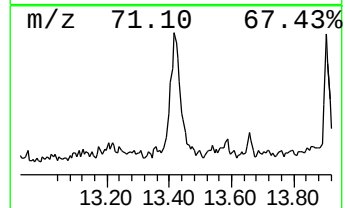
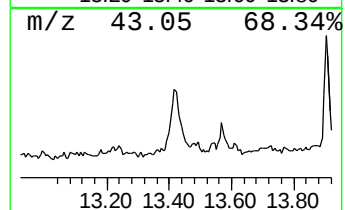
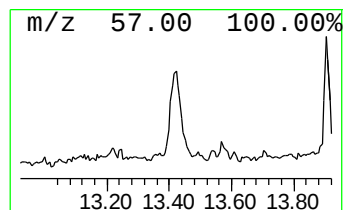
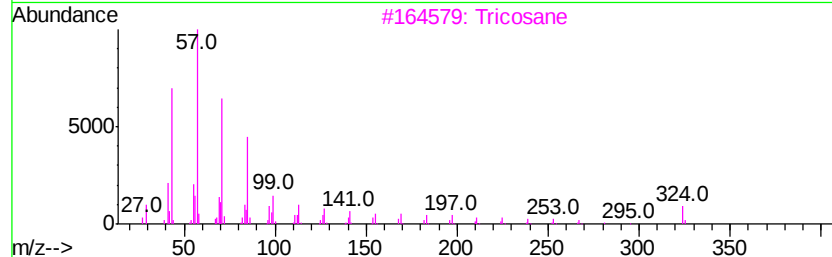
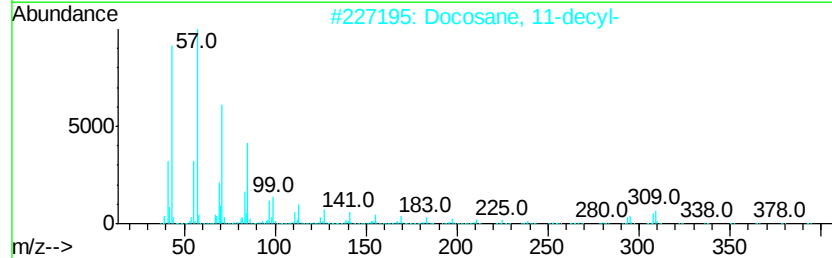
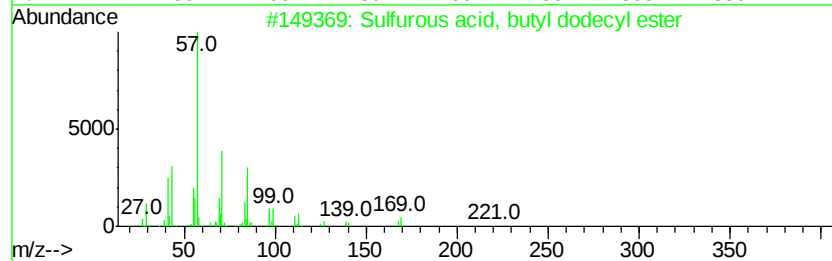
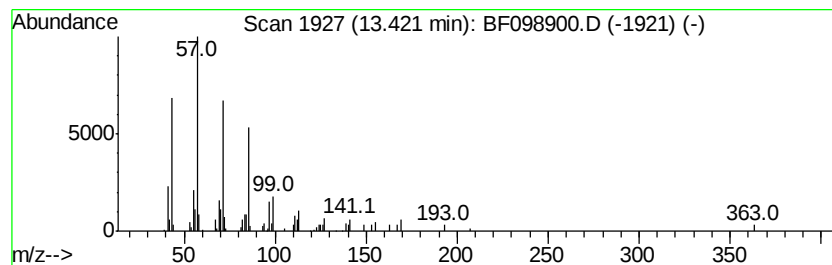
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl dodec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	2.58 ng	122845	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
2		Docosane, 11-decyl-	451	C32H66	055401-55-3	86
3		Tricosane	324	C23H48	000638-67-5	86
4		Tetracosane	338	C24H50	000646-31-1	86
5		Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098900.D
Acq On : 28 Sep 2017 11:24
Operator : SJ/JU
Sample : I5418-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

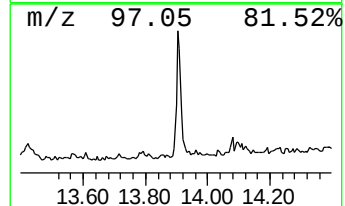
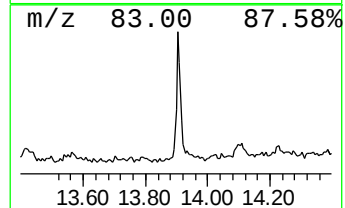
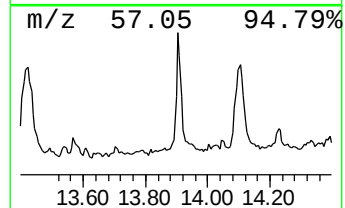
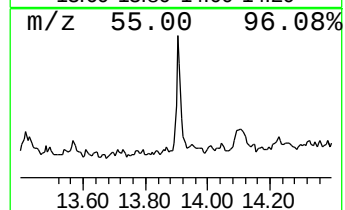
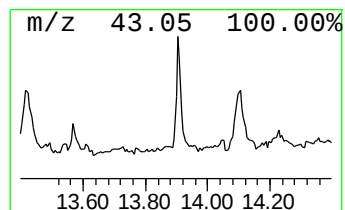
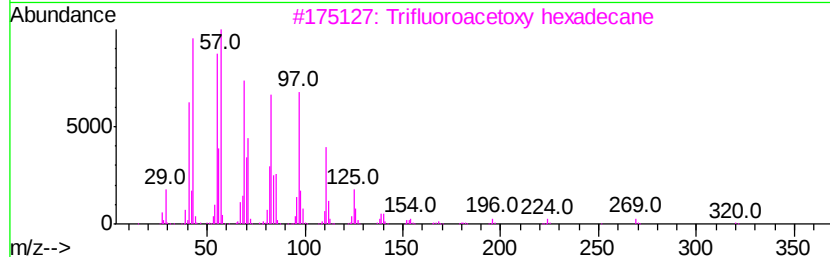
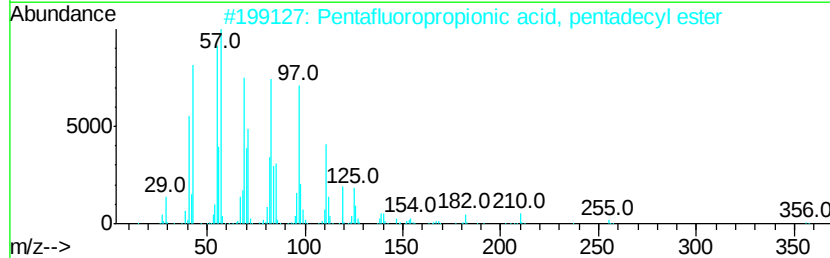
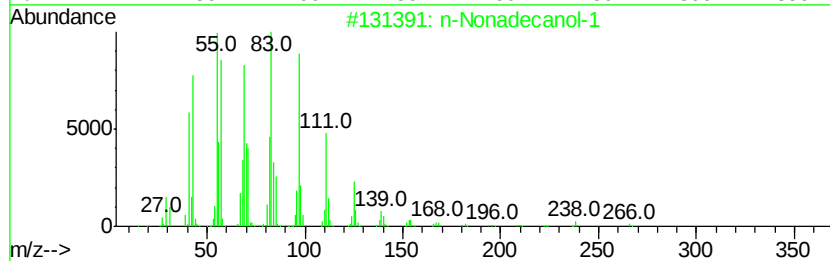
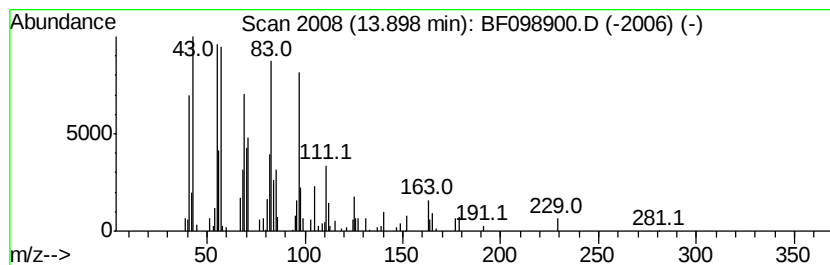
Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-119-2(0-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Nonadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	3.42 ng	162668	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	93
4	Heptafluorobutvric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098900.D
Acq On : 28 Sep 2017 11:24
Operator : SJ/JU
Sample : I5418-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

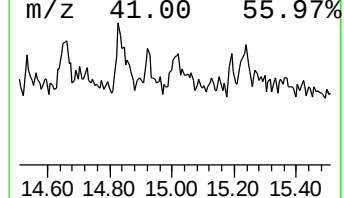
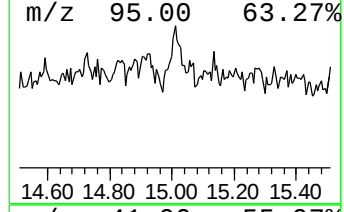
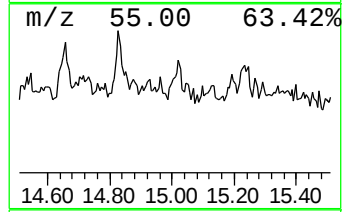
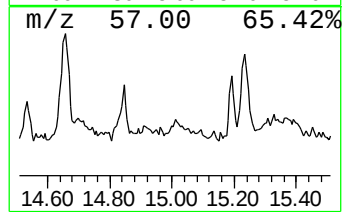
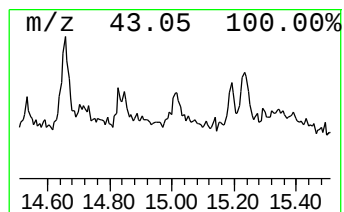
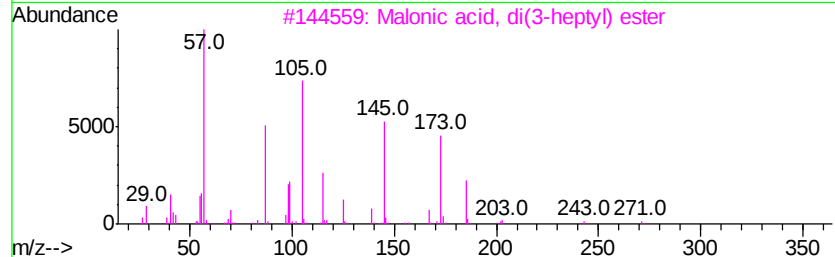
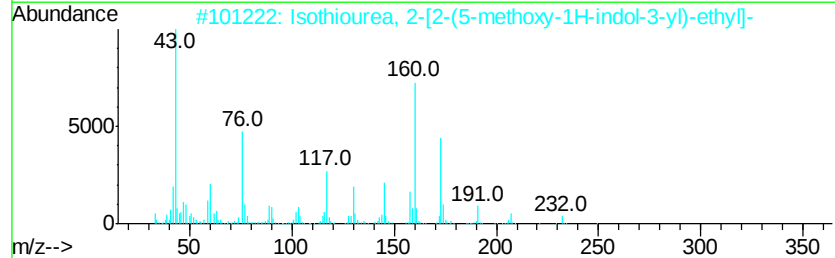
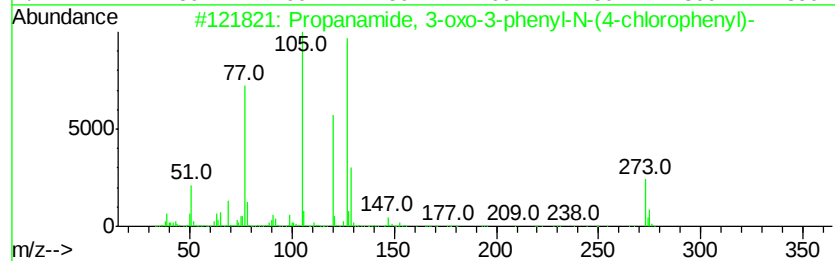
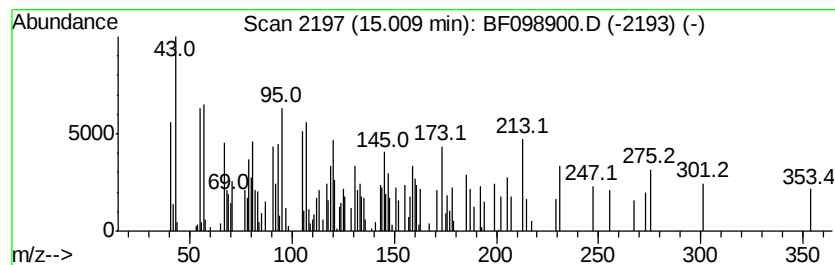
Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-119-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	2.26 ng	95463	Perylene-d12	15.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Propanamide, 3-oxo-3-phenyl-N-(4...	273 C15H12ClN02	000962-08-3 9
2		Isothiourea, 2-[2-(5-methoxy-1H-...	249 C12H15N3OS	1000310-63-3 9
3		Malonic acid, di(3-heptyl) ester	300 C17H32O4	1000349-16-3 9
4		2-Furancarboxamide, N-[2-(5,5-di...	301 C17H19N04	1000337-74-9 9
5		6-Azaspiro[2.5]octa-4,7-diene-6-...	207 C12H17N02	034995-40-9 9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098900.D
Acq On : 28 Sep 2017 11:24
Operator : SJ/JU
Sample : I5418-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-119-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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-methoxy...	2.23	4.1 ng		185455	1	6.92	913711	20.0
2-Pentanone, 4-hy...	5.15	16.4 ng		748406	1	6.92	913711	20.0
unknown6.69	6.69	76.8 ng		3509780	1	6.92	913711	20.0
n-Hexadecanoic acid	11.95	6.8 ng		452686	4	11.44	1342240	20.0
Octadecanoic acid	12.74	3.8 ng		251405	4	11.44	1342240	20.0
Sulfurous acid, b...	13.42	2.6 ng		122845	5	14.08	951334	20.0
n-Nonadecanol-1	13.90	3.4 ng		162668	5	14.08	951334	20.0
unknown15.01	15.01	2.3 ng		95463	6	15.57	845656	20.0