

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
 Data File : BF101959.D
 Acq On : 9 Jan 2018 18:23
 Operator : SJ/JU
 Sample : J1044-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-COMP-B

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-BF010918.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	4.281	366	373	378	rBV	133676	162921	2.62%	0.326%
2	4.934	477	484	494	rVB	356896	531334	8.54%	1.063%
3	5.340	547	553	556	rBV	5305566	5845297	93.96%	11.698%
4	6.363	720	727	737	rBV	5210260	6221084	100.00%	12.450%
5	6.498	744	750	753	rBV	5656259	5793255	93.12%	11.594%
6	6.557	757	760	766	rVB	66394	64025	1.03%	0.128%
7	6.728	785	789	792	rBV	1992768	1551690	24.94%	3.105%
8	6.887	811	816	819	rBV	4582943	4189457	67.34%	8.384%
9	7.292	879	885	888	rBV	3498025	3729713	59.95%	7.464%
10	8.010	1002	1007	1010	rBV	2477021	2046050	32.89%	4.095%
11	8.569	1097	1102	1105	rBV	236887	184374	2.96%	0.369%
12	9.092	1185	1191	1194	rBV	5636876	5221966	83.94%	10.451%
13	9.169	1201	1204	1209	rBV2	60614	82590	1.33%	0.165%
14	9.480	1253	1257	1261	rBV	503313	437925	7.04%	0.876%
15	9.698	1292	1294	1299	rVB	104451	89945	1.45%	0.180%
16	9.763	1299	1305	1309	rVV2	2230272	1969803	31.66%	3.942%
17	9.792	1309	1310	1315	rVB	94901	70086	1.13%	0.140%
18	10.198	1376	1379	1382	rVB2	106539	92380	1.48%	0.185%
19	10.310	1395	1398	1402	rBV	70513	65104	1.05%	0.130%
20	10.480	1422	1427	1429	rBV	522731	439194	7.06%	0.879%
21	10.551	1434	1439	1442	rBV	3039512	2780191	44.69%	5.564%
22	10.675	1457	1460	1469	rVB2	78478	102678	1.65%	0.205%
23	11.245	1553	1557	1560	rBV	1858670	1648216	26.49%	3.299%
24	11.269	1560	1561	1564	rVB	183281	96447	1.55%	0.193%
25	11.780	1644	1648	1656	rBV2	352482	403749	6.49%	0.808%
26	11.857	1659	1661	1669	rVB3	53757	68715	1.10%	0.138%
27	12.451	1759	1762	1766	rBV	148532	156725	2.52%	0.314%
28	12.563	1778	1781	1785	rBV2	154854	179296	2.88%	0.359%
29	12.680	1799	1801	1804	rVB	125664	110600	1.78%	0.221%
30	12.833	1823	1827	1831	rBV	3487043	3335317	53.61%	6.675%
31	13.733	1977	1980	1983	rBV	295331	270223	4.34%	0.541%
32	13.880	2001	2005	2008	rBV	1284464	1177283	18.92%	2.356%
33	15.298	2243	2246	2251	rVB	714472	849840	13.66%	1.701%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

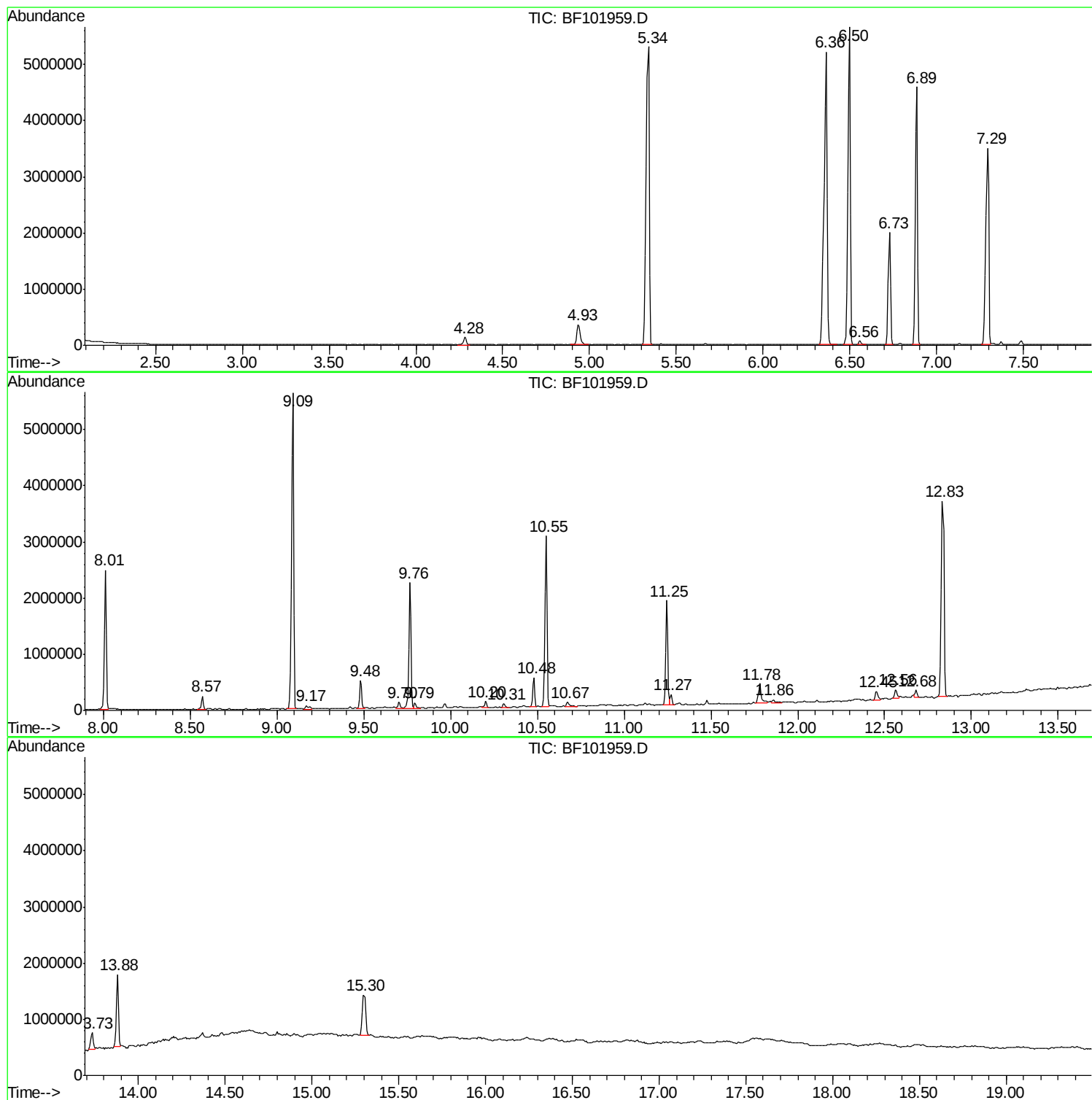
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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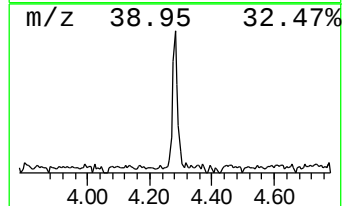
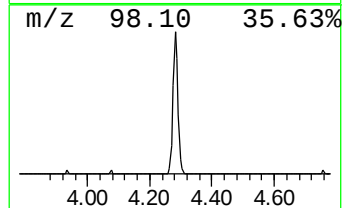
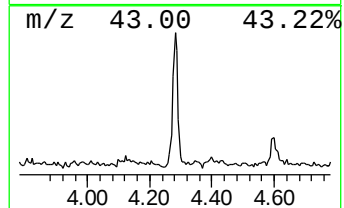
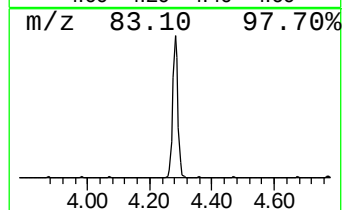
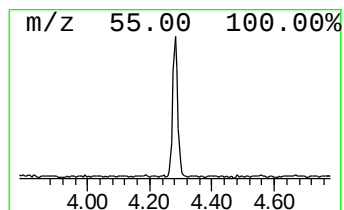
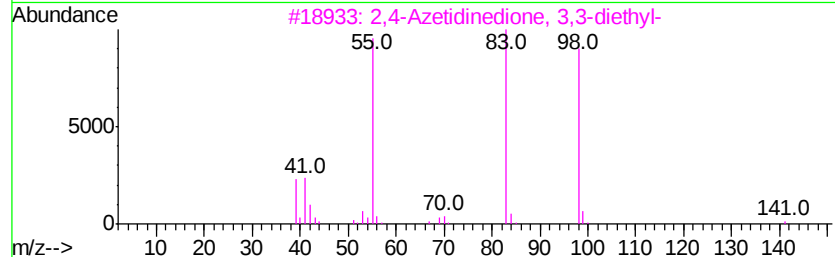
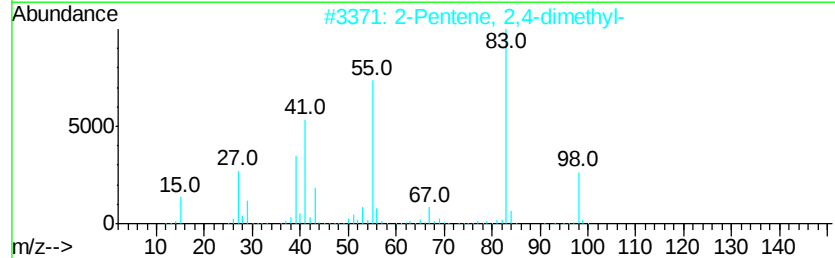
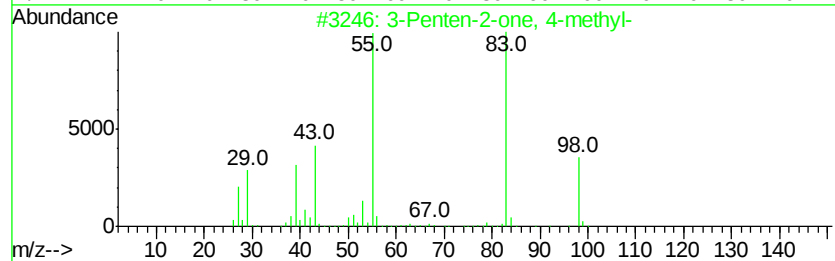
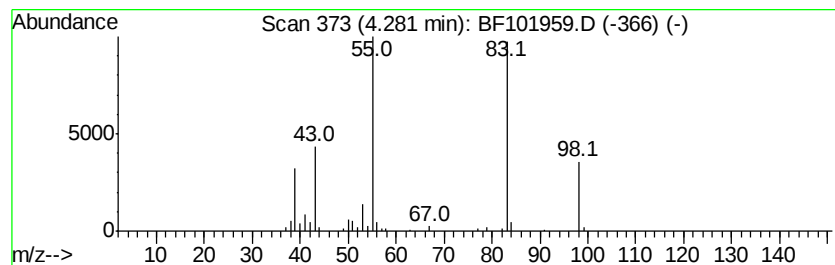
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	2.10 ng	162921	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
3			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N2O2	042282-85-9	78
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72



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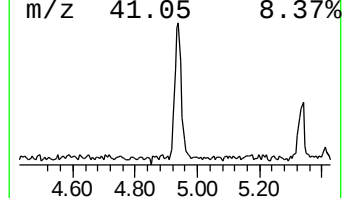
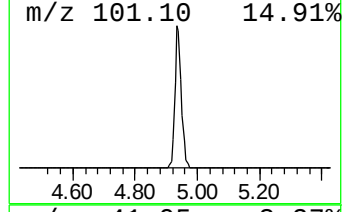
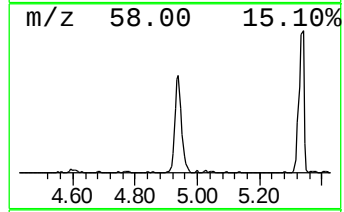
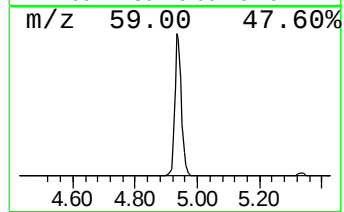
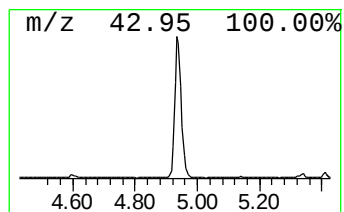
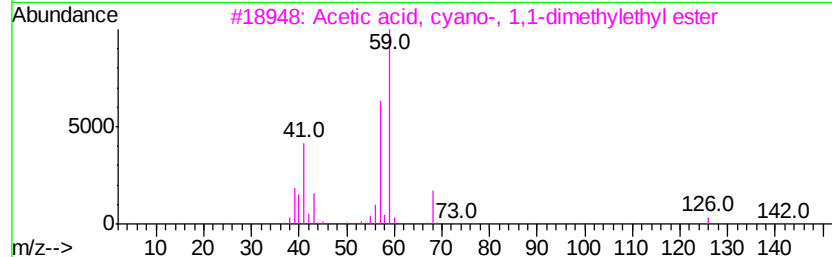
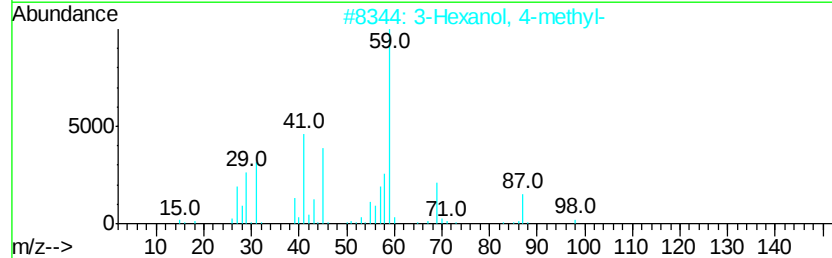
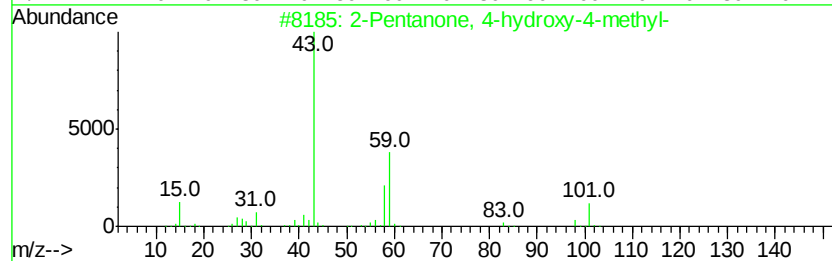
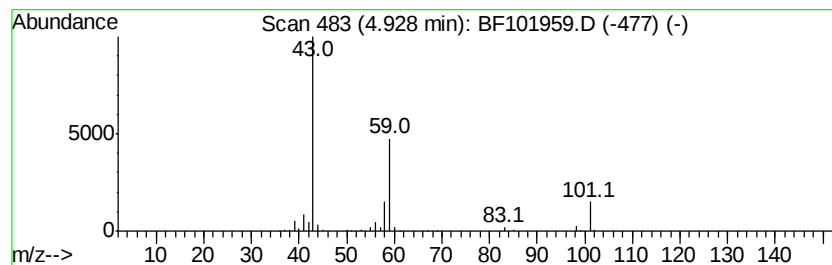
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	6.85 ng	531334	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9



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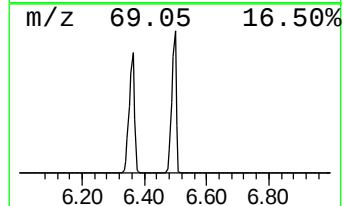
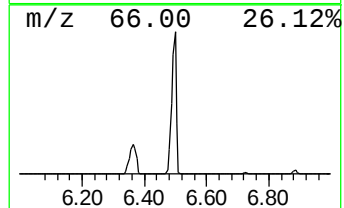
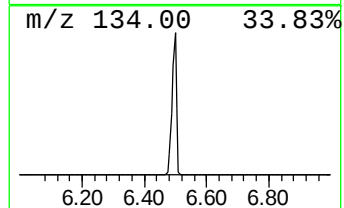
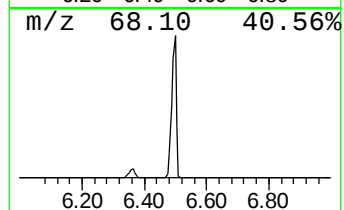
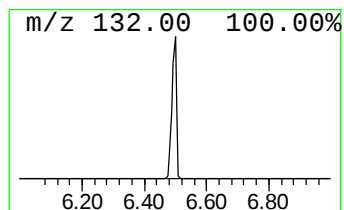
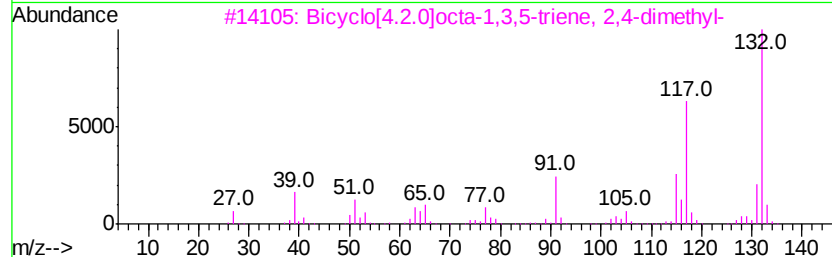
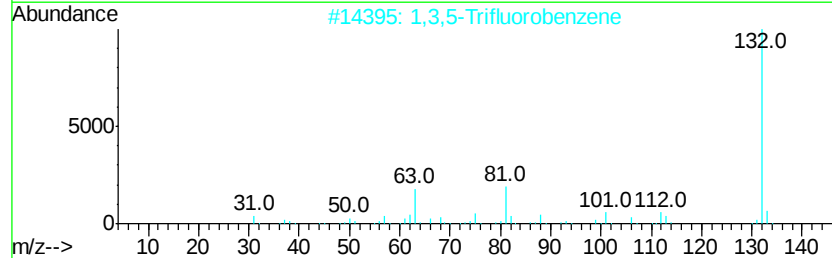
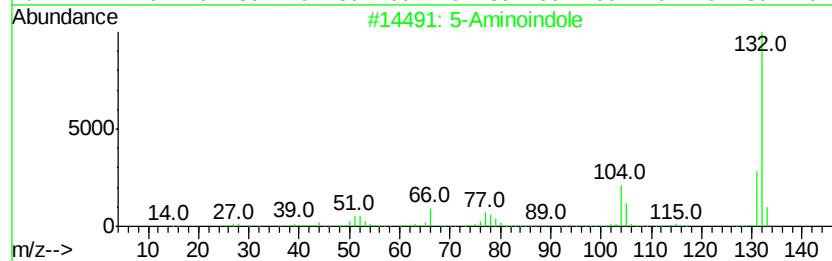
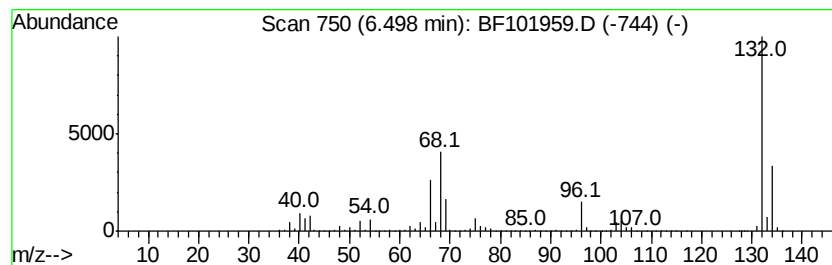
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	74.67 ng	5793260	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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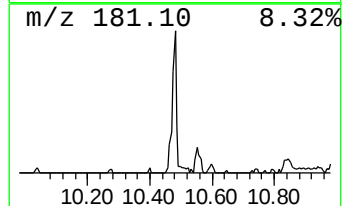
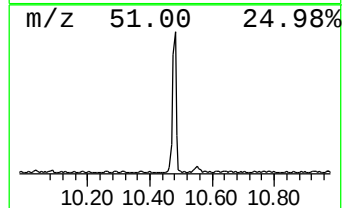
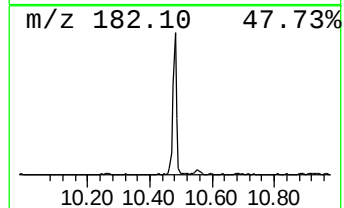
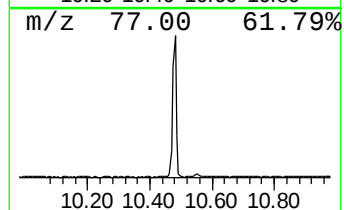
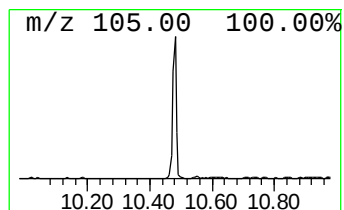
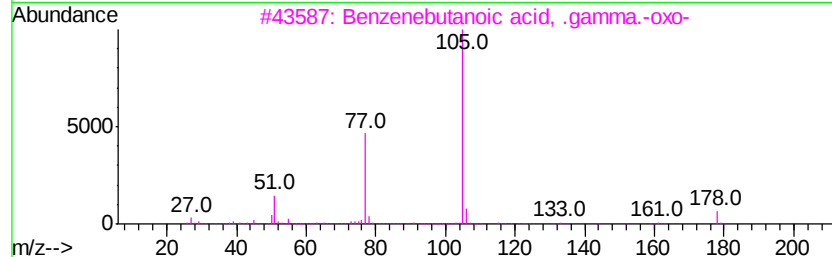
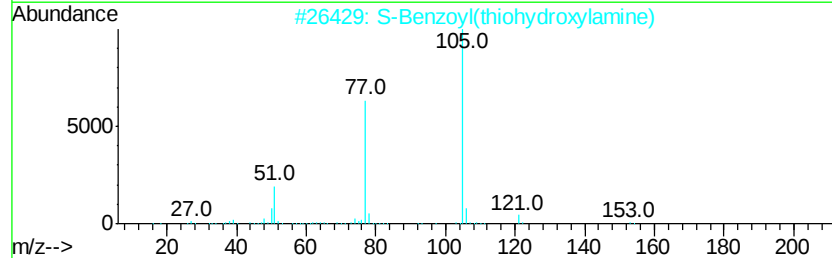
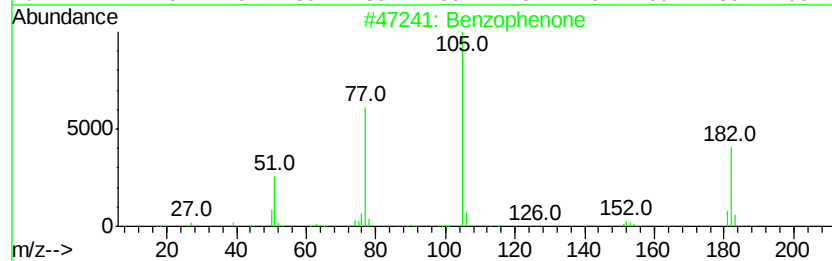
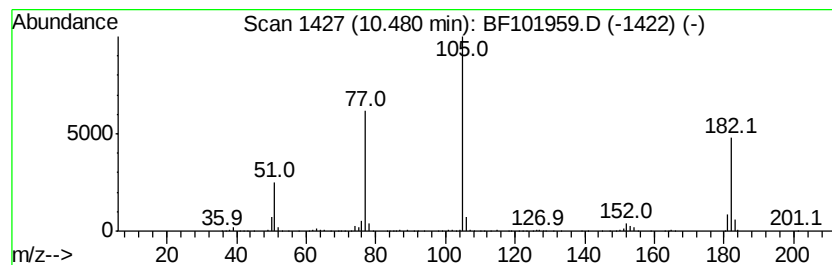
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.48	4.46 ng	439194	Acenaphthene-d10	9.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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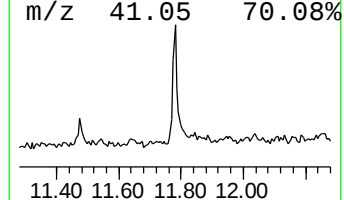
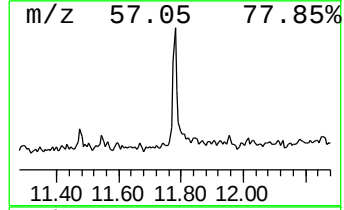
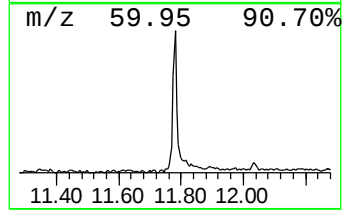
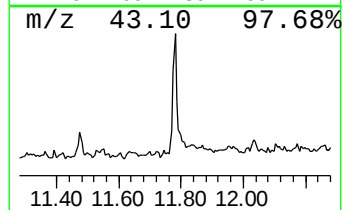
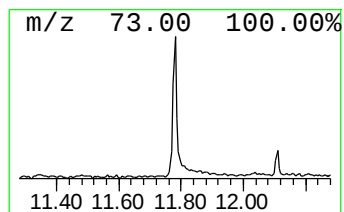
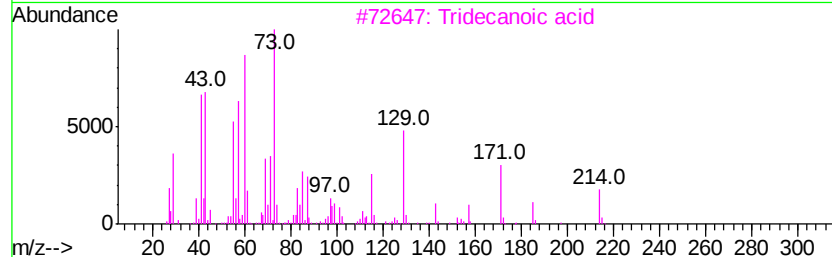
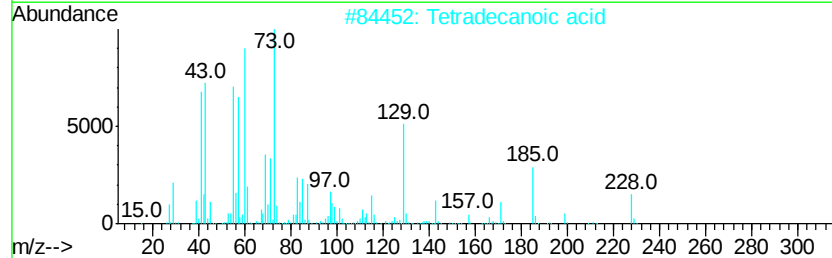
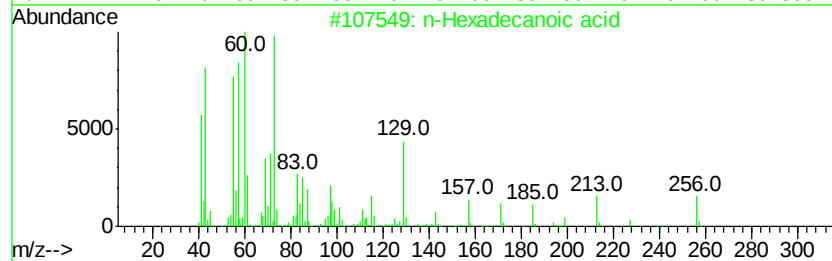
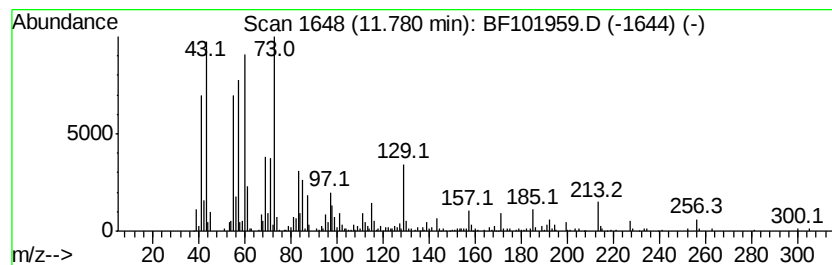
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	4.90 ng	403749	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90



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ClientSampleId :
SP-COMP-B

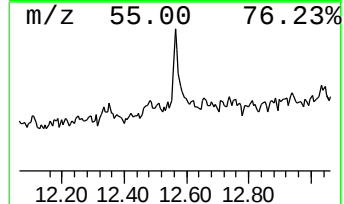
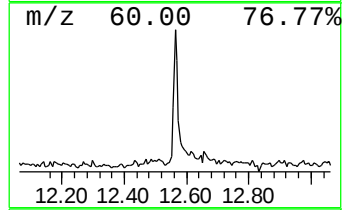
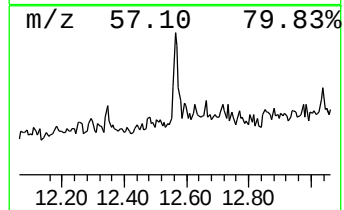
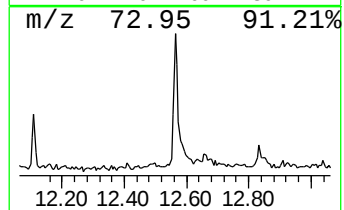
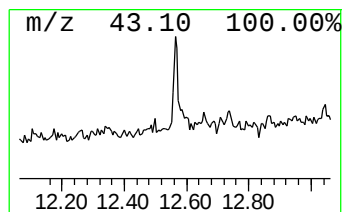
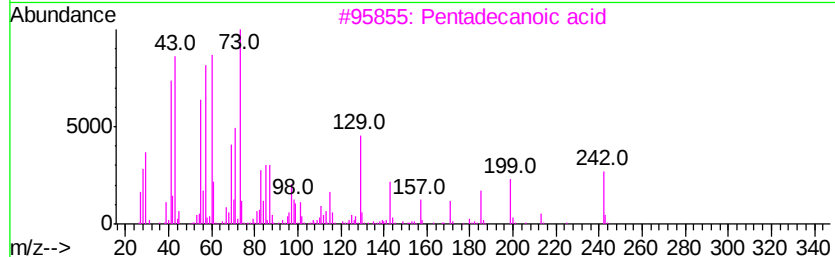
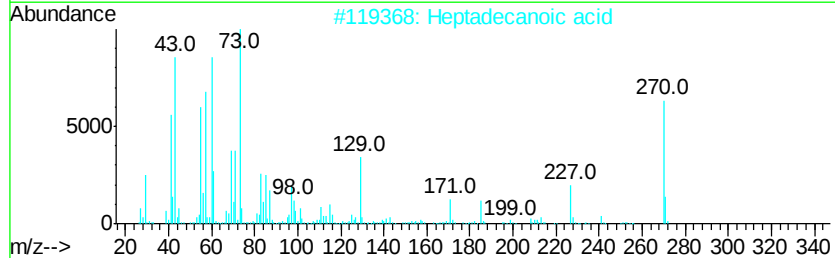
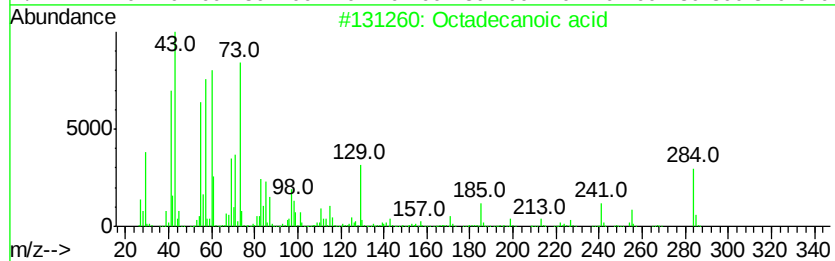
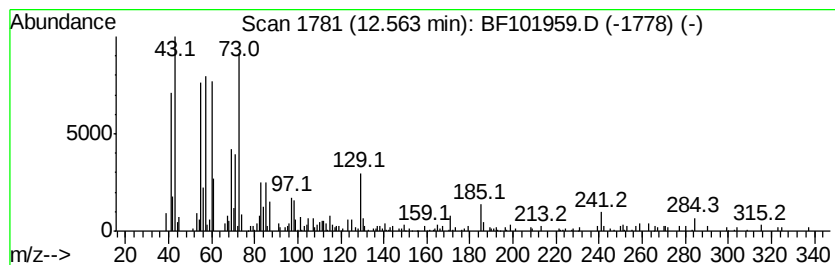
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	3.05 ng	179296	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Heptadecanoic acid	270	C17H34O2	000506-12-7	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101959.D
Acq On : 9 Jan 2018 18:23
Operator : SJ/JU
Sample : J1044-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP-B

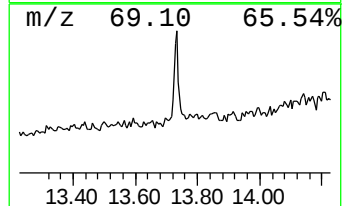
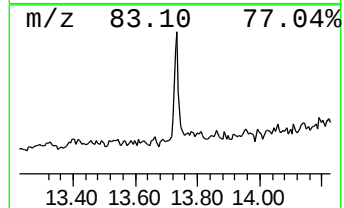
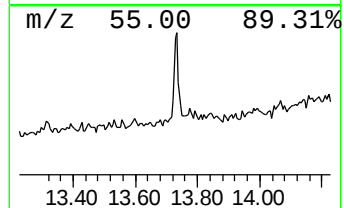
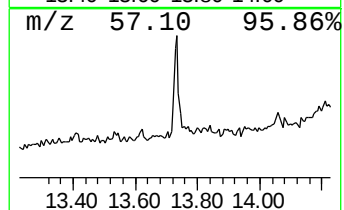
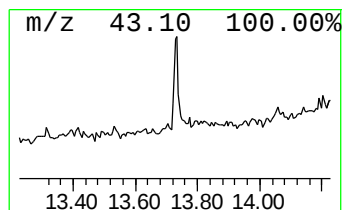
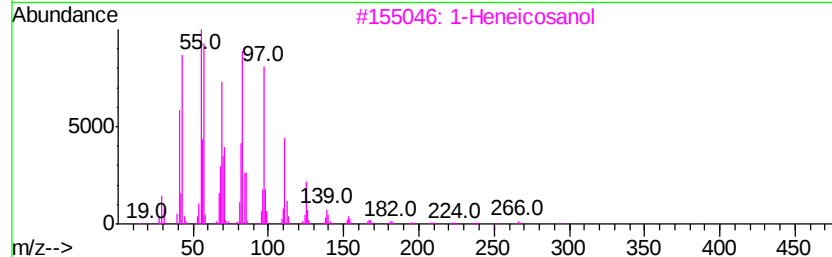
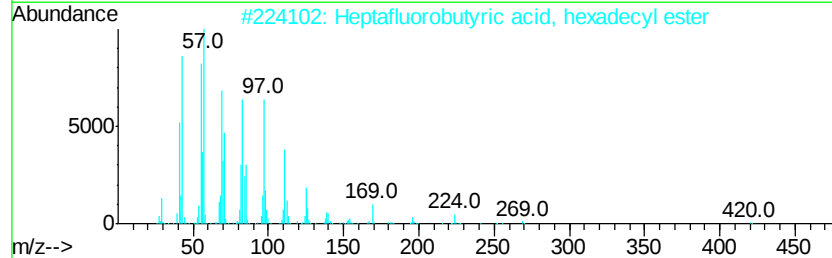
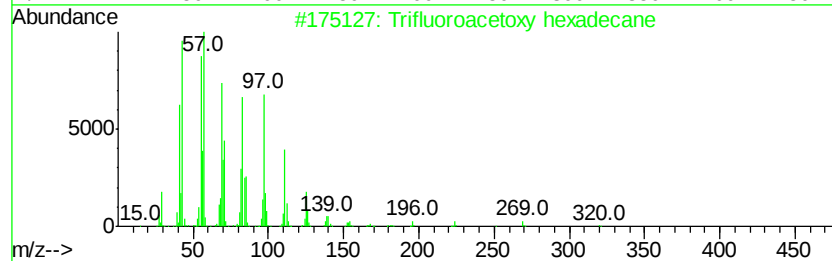
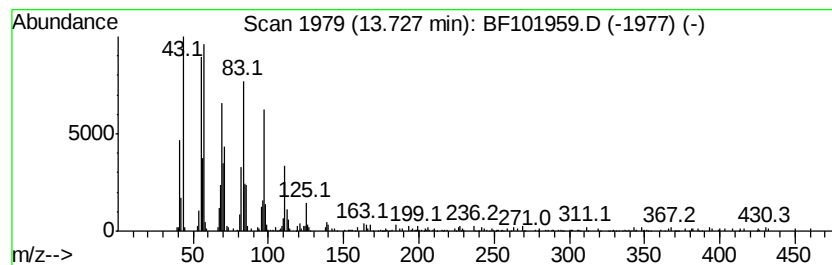
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.59 ng	270223	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	91
5		1-Eicosene	280	C20H40	003452-07-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF101959.D
Acq On : 9 Jan 2018 18:23
Operator : SJ/JU
Sample : J1044-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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-Penten-2-one, 4...	4.28	2.1 ng		162921	1	6.73	1551690	20.0
2-Pentanone, 4-hy...	4.93	6.8 ng		531334	1	6.73	1551690	20.0
unknown6.50	6.50	74.7 ng		5793260	1	6.73	1551690	20.0
Benzophenone	10.48	4.5 ng		439194	3	9.76	1969800	20.0
n-Hexadecanoic acid	11.78	4.9 ng		403749	4	11.25	1648220	20.0
Octadecanoic acid	12.56	3.0 ng		179296	5	13.88	1177280	20.0
Trifluoroacetoxy ...	13.73	4.6 ng		270223	5	13.88	1177280	20.0