

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
 Data File : BF101961.D
 Acq On : 9 Jan 2018 19:17
 Operator : SJ/JU
 Sample : J1044-10
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-COMP-D

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	368	373	382	rVB	259321	314913	5.08%	0.680%
2	4.939	476	485	492	rBV	370793	556209	8.97%	1.201%
3	5.339	547	553	556	rBV	5478514	6025333	97.18%	13.014%
4	6.363	720	727	736	rBV	5189442	6200243	100.00%	13.392%
5	6.498	745	750	753	rBV	5639870	5759701	92.89%	12.440%
6	6.557	757	760	765	rVB	70705	67451	1.09%	0.146%
7	6.728	785	789	792	rBV	1692519	1303237	21.02%	2.815%
8	6.886	811	816	819	rBV	4620848	4224749	68.14%	9.125%
9	7.292	879	885	888	rBV	3421604	3627040	58.50%	7.834%
10	8.010	1003	1007	1010	rBV	1953383	1573318	25.38%	3.398%
11	8.569	1097	1102	1105	rVB	204119	156726	2.53%	0.339%
12	9.092	1185	1191	1194	rBV	4895579	4730242	76.29%	10.217%
13	9.480	1253	1257	1261	rBV	495911	381199	6.15%	0.823%
14	9.763	1299	1305	1308	rBV2	1633211	1331834	21.48%	2.877%
15	10.474	1423	1426	1430	rBV	357402	306515	4.94%	0.662%
16	10.551	1434	1439	1442	rBV	2482211	2328114	37.55%	5.028%
17	11.245	1553	1557	1560	rBV	1356084	1108929	17.89%	2.395%
18	11.780	1644	1648	1652	rBV	238354	260145	4.20%	0.562%
19	12.451	1759	1762	1765	rBV	69052	74583	1.20%	0.161%
20	12.563	1778	1781	1787	rVB2	97789	94191	1.52%	0.203%
21	12.680	1796	1801	1803	rBV	72555	79713	1.29%	0.172%
22	12.833	1823	1827	1830	rBV	3719117	3362905	54.24%	7.264%
23	13.727	1976	1979	1987	rBV	308595	358905	5.79%	0.775%
24	13.880	2000	2005	2008	rBV	1223078	1200583	19.36%	2.593%
25	14.362	2085	2087	2093	rVB2	76925	96356	1.55%	0.208%
26	15.298	2242	2246	2252	rVB	682651	775276	12.50%	1.675%

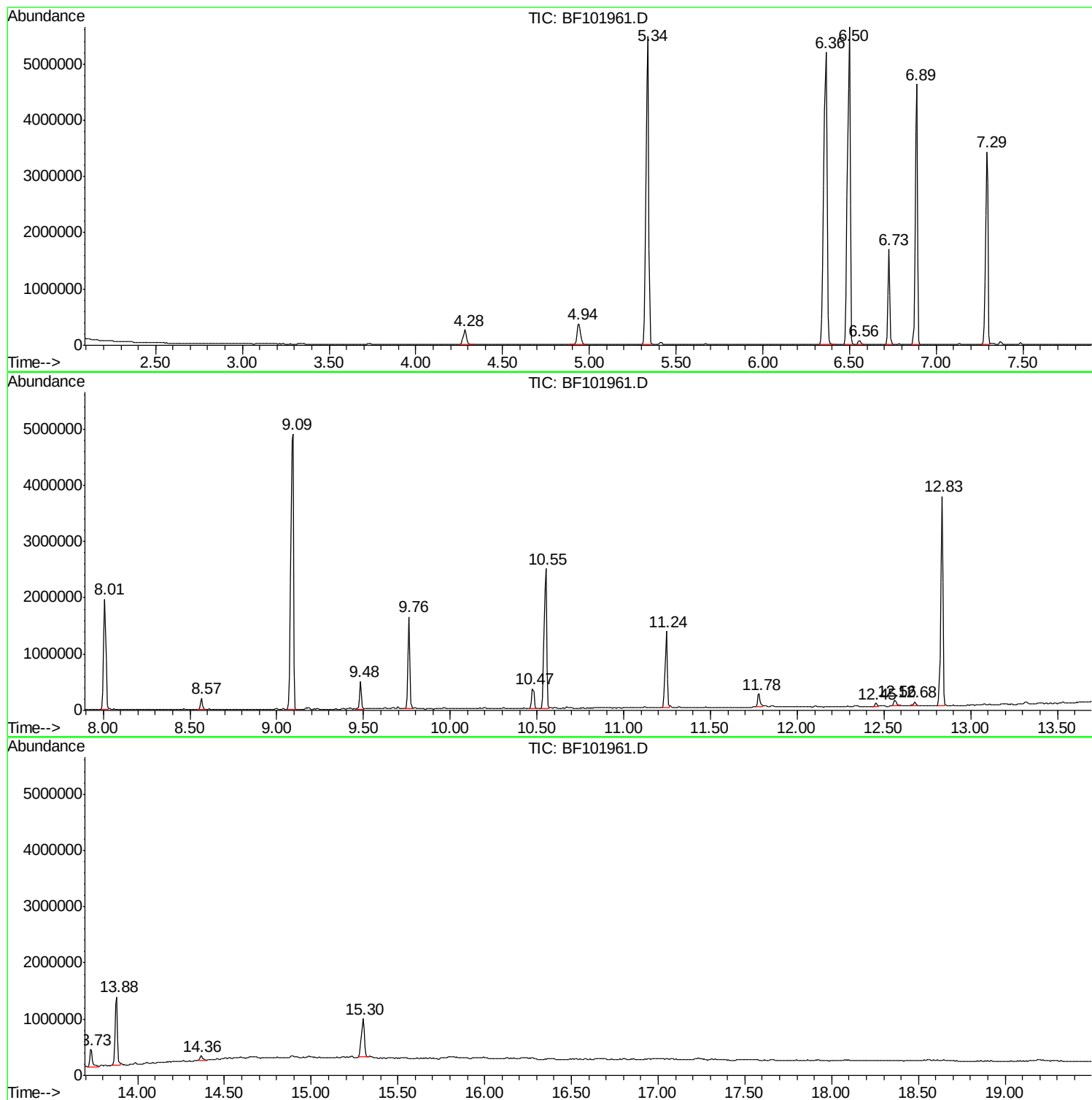
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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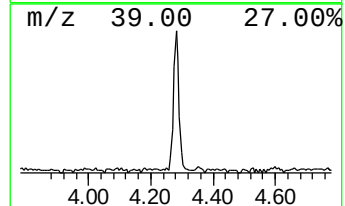
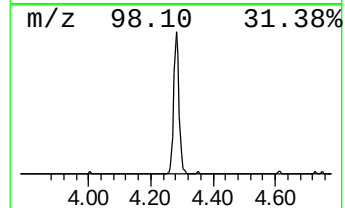
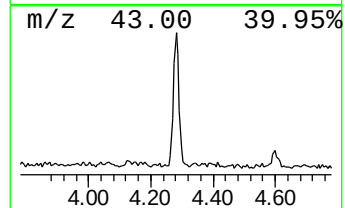
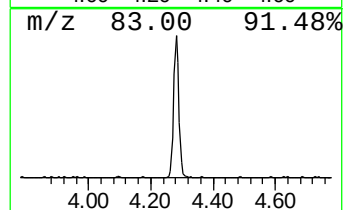
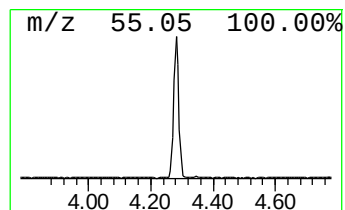
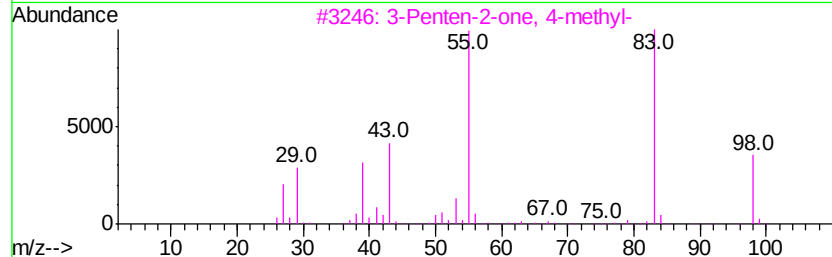
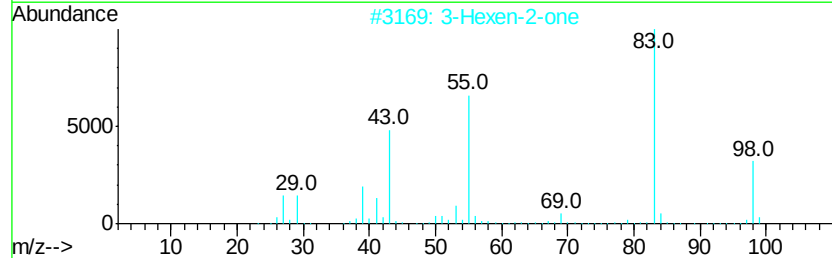
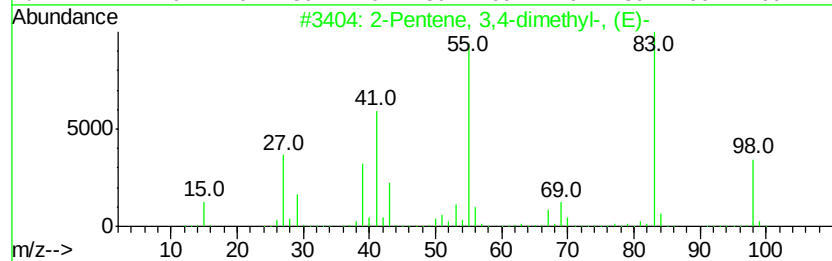
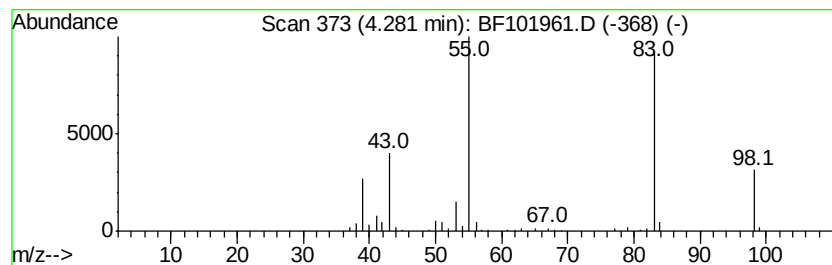
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentene, 3,4-dimethyl-, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	4.83 ng	314913	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	87
3		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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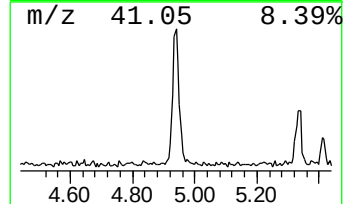
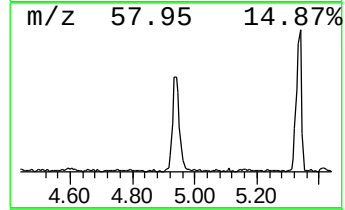
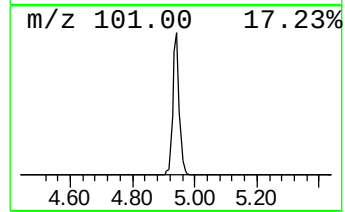
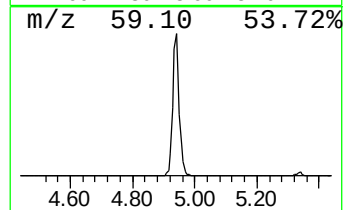
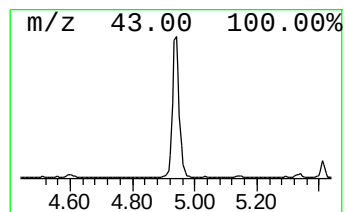
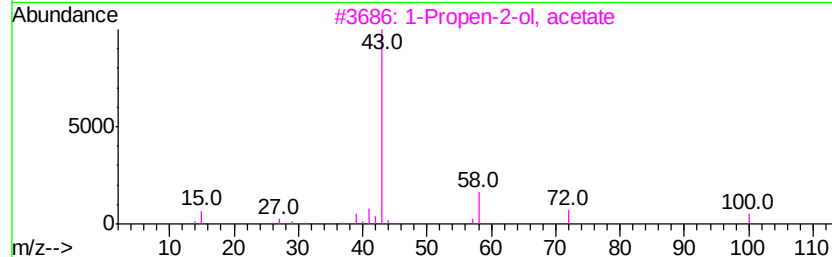
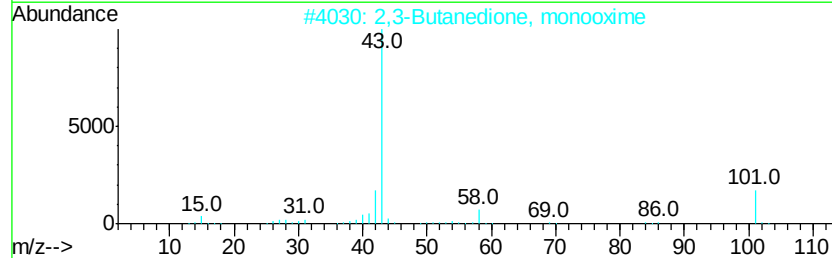
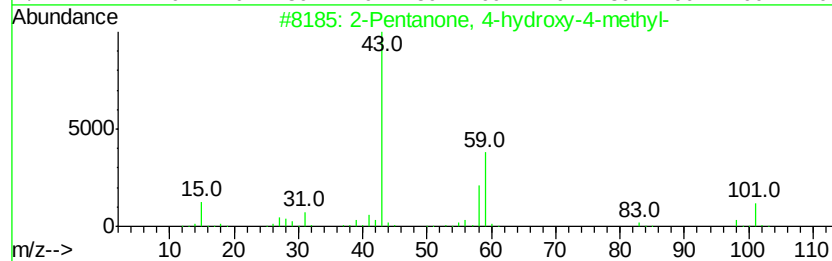
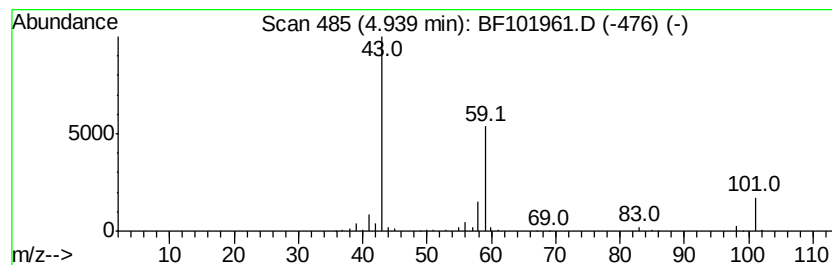
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	8.54 ng	556209	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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Allyl acetate	100	C5H8O2	000591-87-7	9
5			1,2-Butanediol	90	C4H10O2	000584-03-2	9



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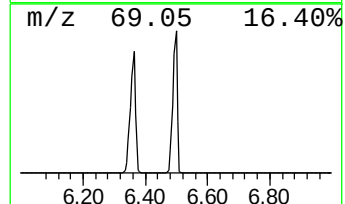
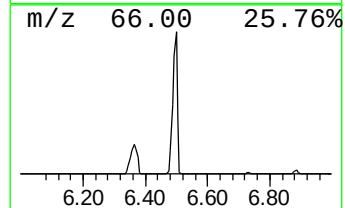
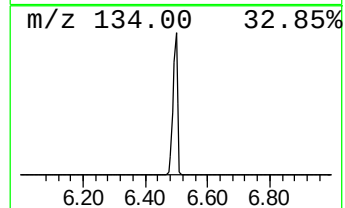
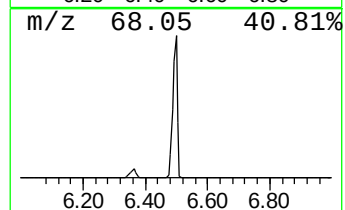
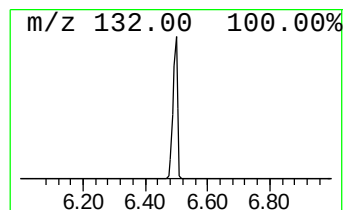
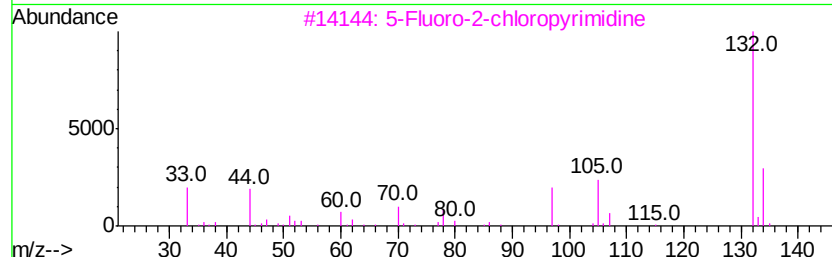
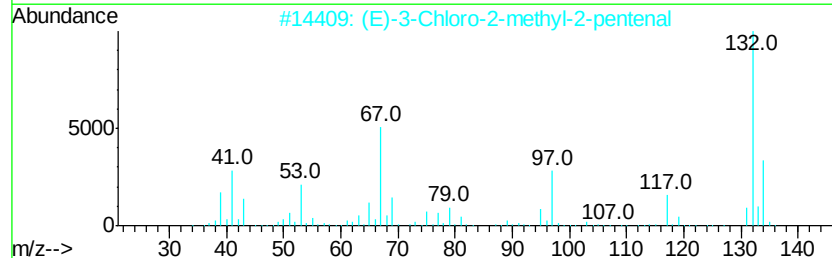
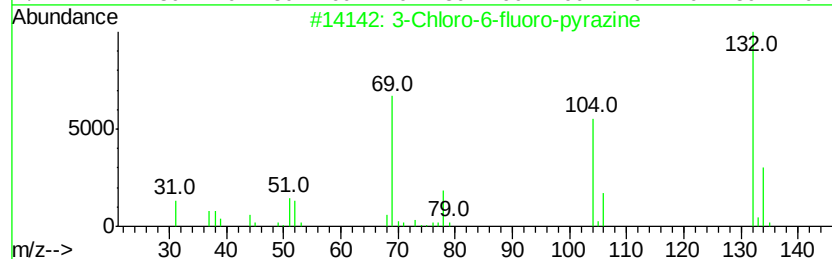
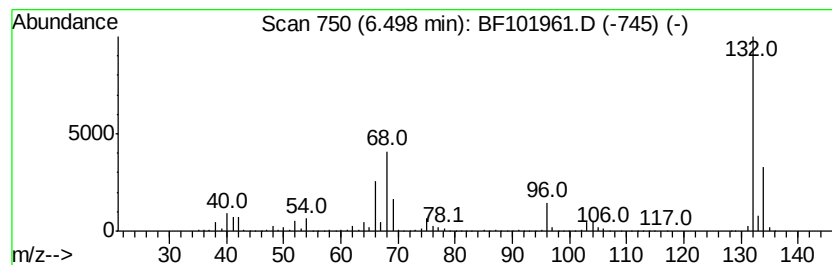
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Peak Number 3 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	88.39 ng	5759700	1,4-Dichlorobenzene-d4	6.73

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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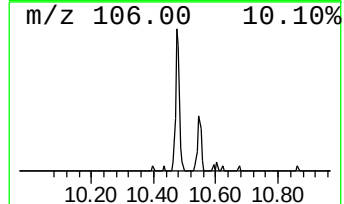
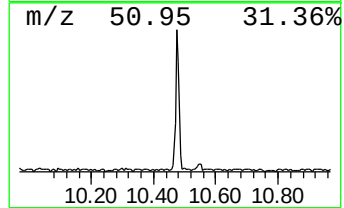
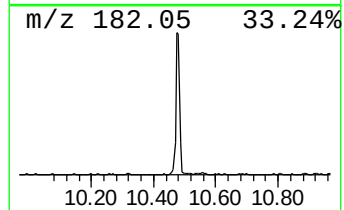
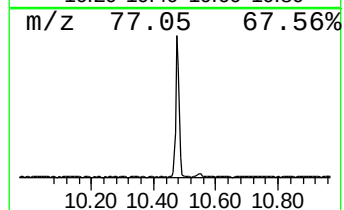
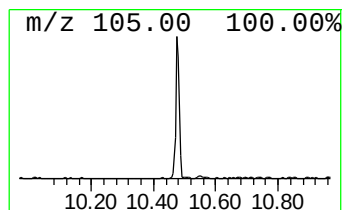
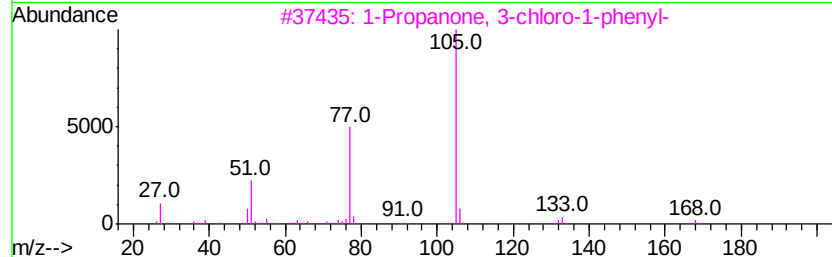
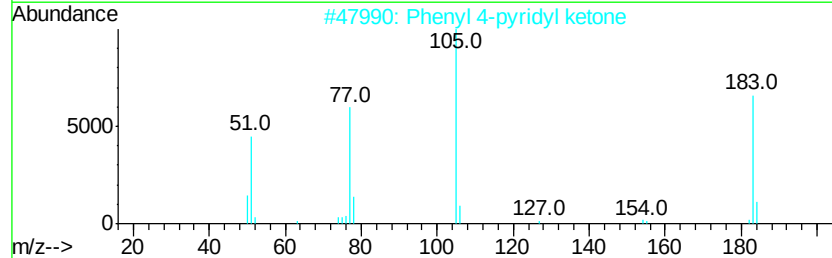
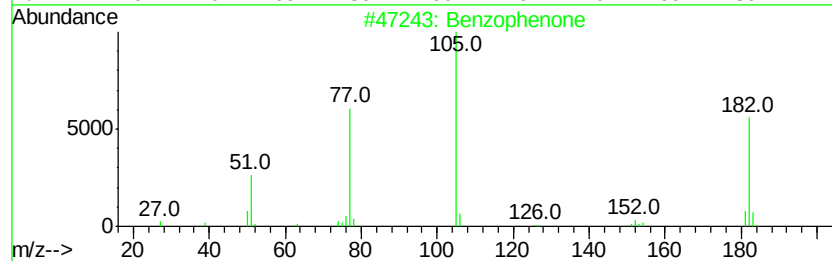
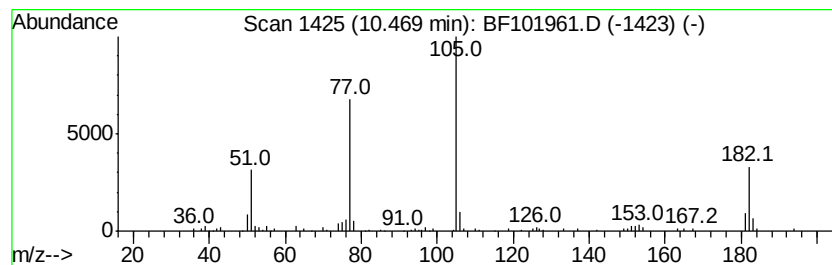
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	4.60 ng	306515	Acenaphthene-d10	9.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3		1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4		Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5		N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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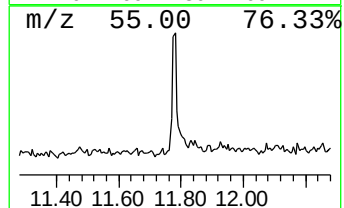
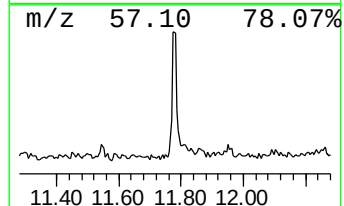
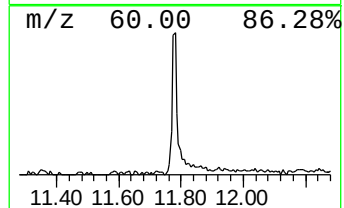
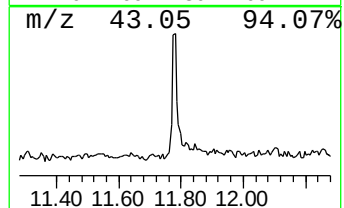
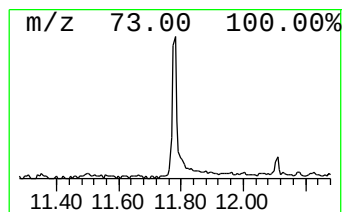
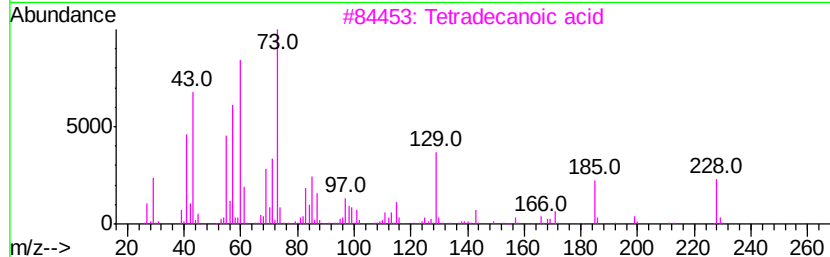
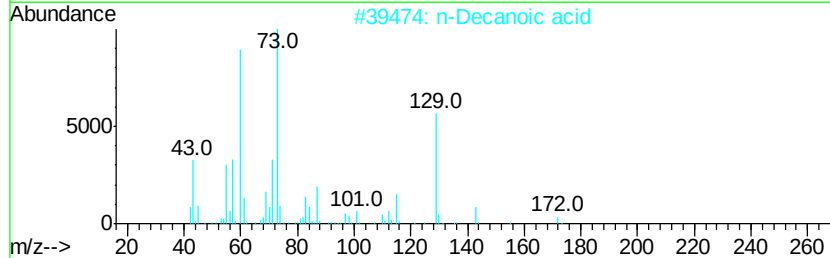
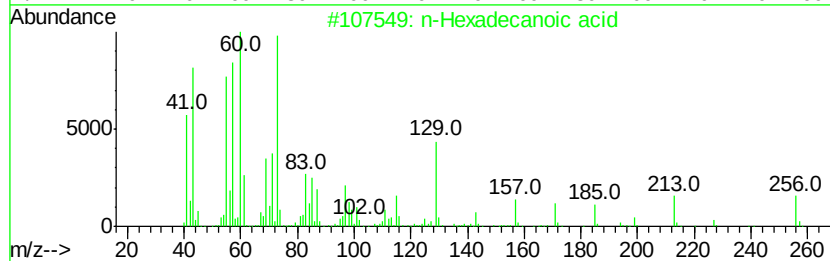
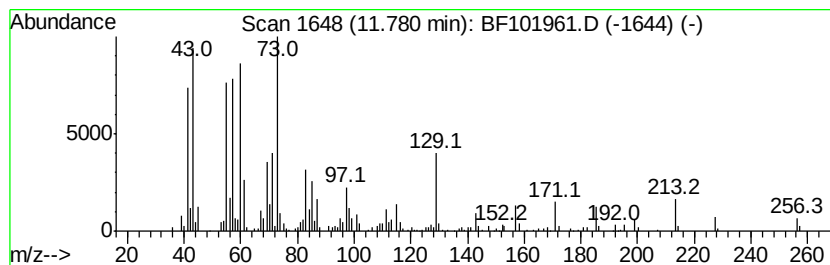
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.78	4.69 ng	260145	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74



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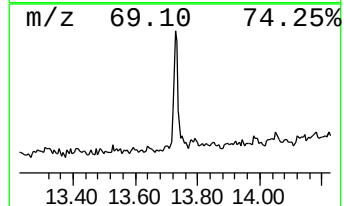
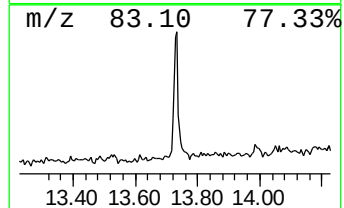
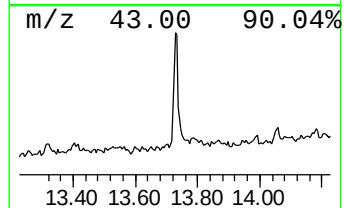
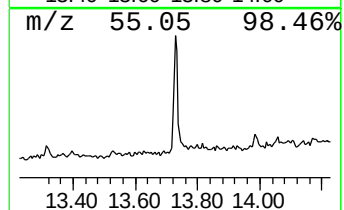
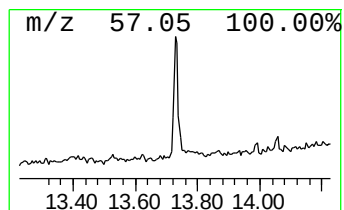
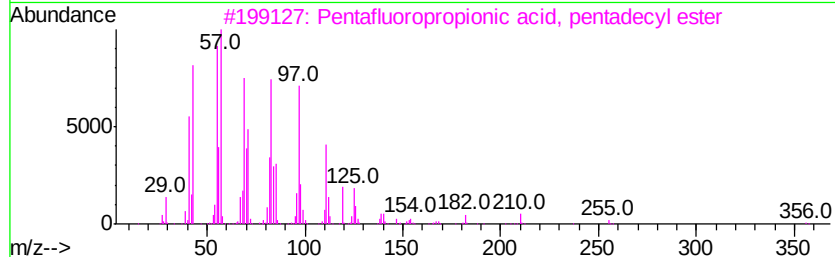
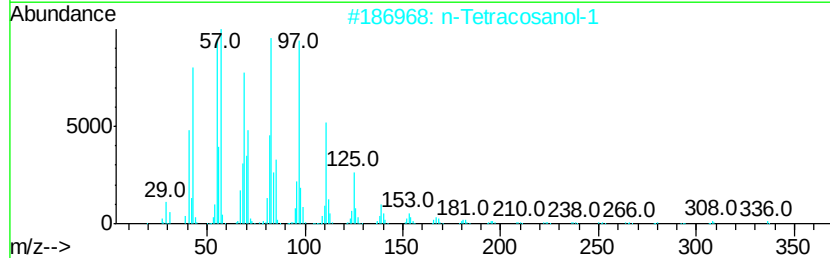
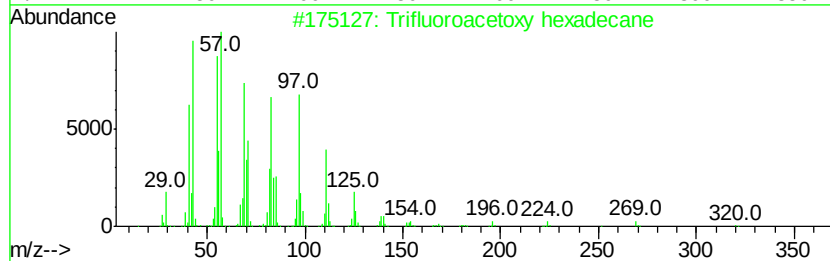
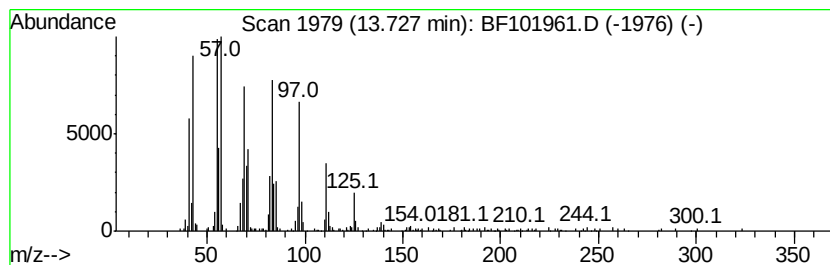
Instrument :
BNA_F
ClientSampleId :
SP-COMP-D

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 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	5.98 ng	358905	Chrysene-d12	13.88	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF101961.D
Acq On : 9 Jan 2018 19:17
Operator : SJ/JU
Sample : J1044-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP-D

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
2-Pentene, 3,4-di...	4.28	4.8	ng	314913	1	6.73	1303240	20.0
2-Pentanone, 4-hy...	4.94	8.5	ng	556209	1	6.73	1303240	20.0
unknown6.50	6.50	88.4	ng	5759700	1	6.73	1303240	20.0
Benzophenone	10.47	4.6	ng	306515	3	9.76	1331830	20.0
n-Hexadecanoic acid	11.78	4.7	ng	260145	4	11.24	1108930	20.0
Trifluoroacetoxy ...	13.73	6.0	ng	358905	5	13.88	1200580	20.0