

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
 Data File : BF101960.D
 Acq On : 9 Jan 2018 18:50
 Operator : SJ/JU
 Sample : J1044-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-COMP-C

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	4.287	368	374	381	rVB	193300	247478	3.54%	0.474%
2	4.939	479	485	493	rVB	396436	594962	8.51%	1.141%
3	5.339	547	553	556	rBV	5707903	6567544	93.95%	12.590%
4	6.363	720	727	740	rBV	5247440	6990436	100.00%	13.401%
5	6.498	744	750	753	rVV	5921227	6362394	91.02%	12.197%
6	6.728	785	789	792	rBV	1911660	1486308	21.26%	2.849%
7	6.886	811	816	819	rBV	4840882	4557871	65.20%	8.737%
8	7.298	879	886	889	rBV	3759068	4118849	58.92%	7.896%
9	8.010	1002	1007	1010	rBV	2331356	1904288	27.24%	3.650%
10	8.569	1097	1102	1105	rBV	281402	221760	3.17%	0.425%
11	9.092	1185	1191	1194	rVB	5435003	5195609	74.32%	9.960%
12	9.480	1253	1257	1261	rBV	622420	517736	7.41%	0.992%
13	9.763	1299	1305	1309	rBV2	2068670	1740068	24.89%	3.336%
14	10.474	1422	1426	1430	rBV	509766	471705	6.75%	0.904%
15	10.551	1434	1439	1442	rBV	2876065	2663263	38.10%	5.105%
16	11.245	1553	1557	1560	rBV	1647033	1360735	19.47%	2.609%
17	11.780	1644	1648	1652	rBV	494356	457649	6.55%	0.877%
18	11.857	1658	1661	1669	rVB2	57305	81701	1.17%	0.157%
19	12.451	1759	1762	1766	rBV	179450	162640	2.33%	0.312%
20	12.563	1778	1781	1787	rBV	170413	178059	2.55%	0.341%
21	12.680	1796	1801	1804	rBV	163459	165442	2.37%	0.317%
22	12.833	1823	1827	1830	rBV	3452709	3281131	46.94%	6.290%
23	13.727	1976	1979	1987	rBV	634147	639194	9.14%	1.225%
24	13.880	2000	2005	2008	rBV	1289627	1256664	17.98%	2.409%
25	14.362	2085	2087	2093	rVB3	118978	124035	1.77%	0.238%
26	15.298	2242	2246	2251	rBV	677392	817725	11.70%	1.568%

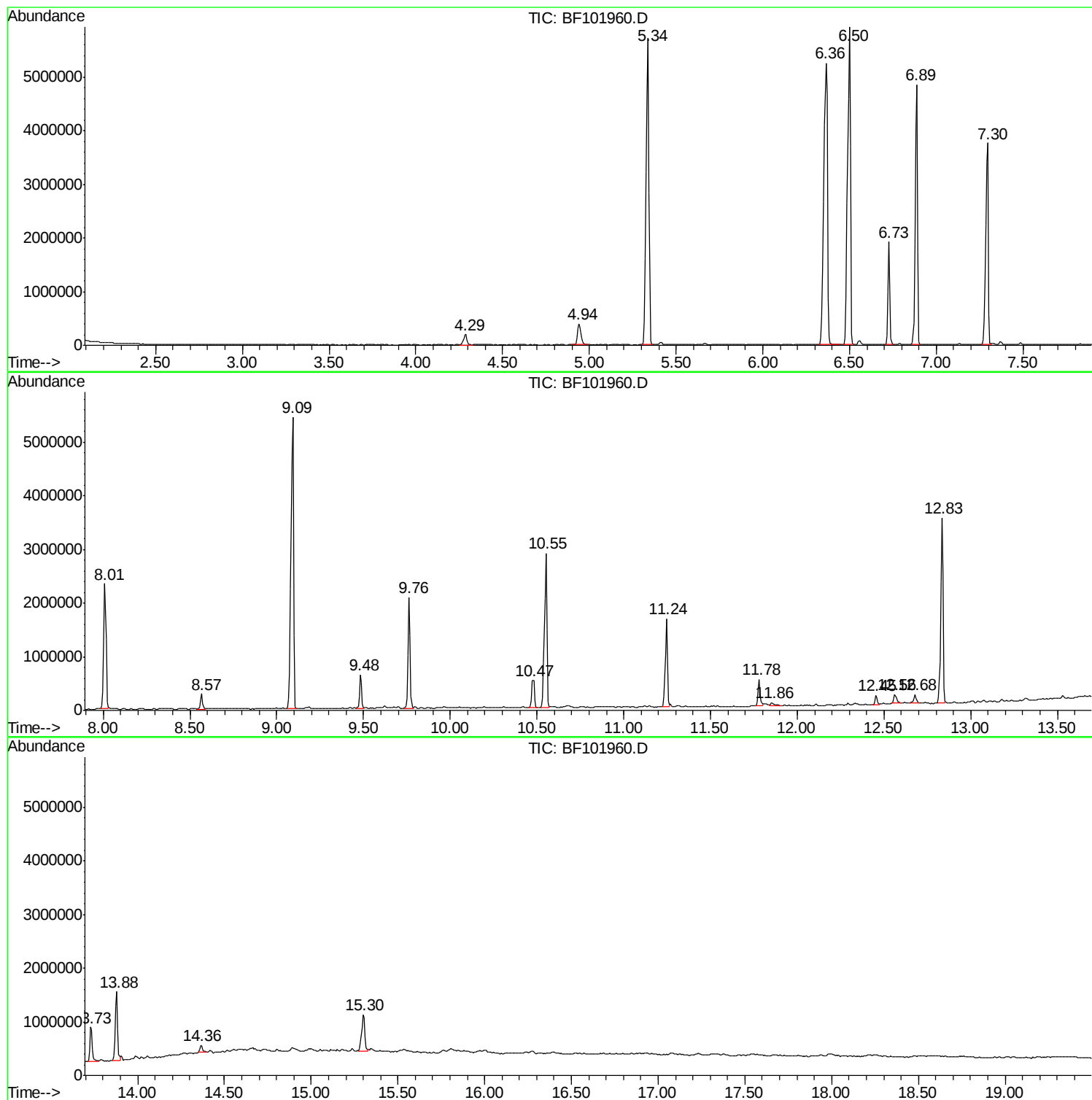
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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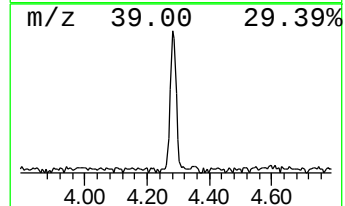
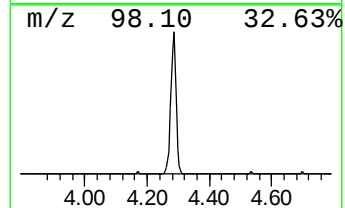
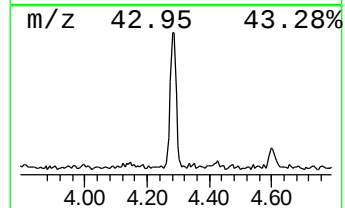
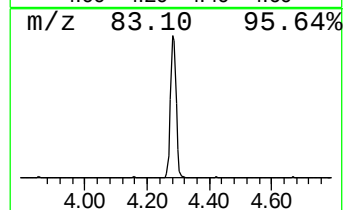
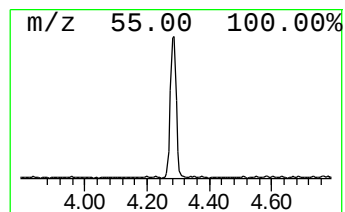
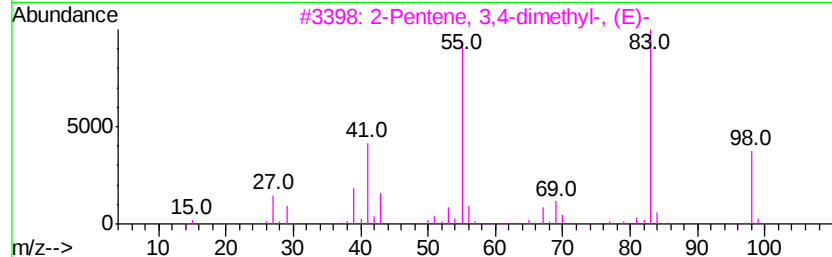
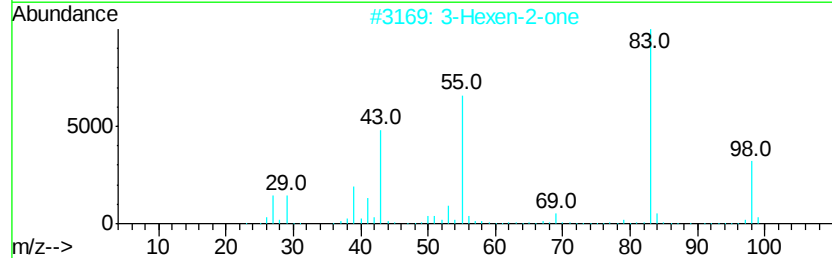
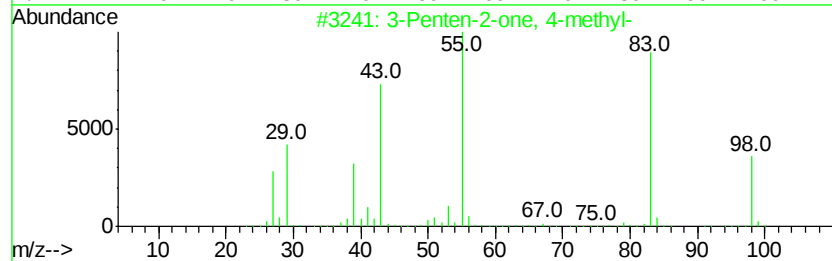
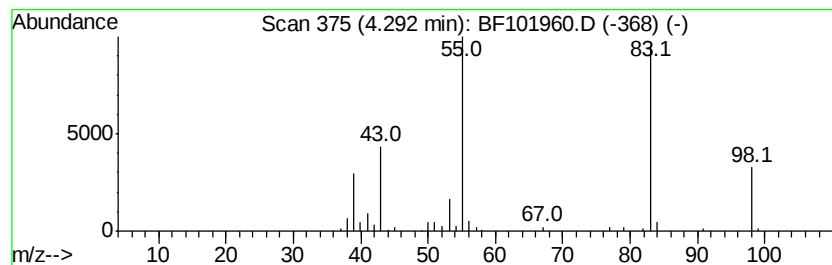
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	3.33 ng	247478	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	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	87
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78



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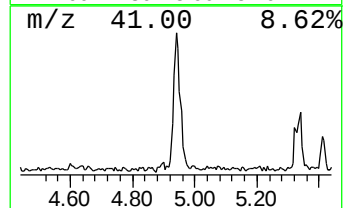
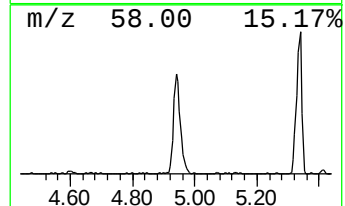
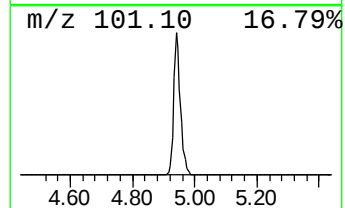
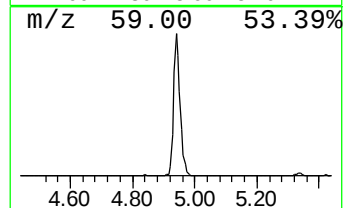
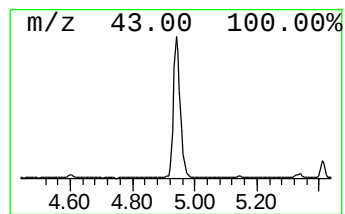
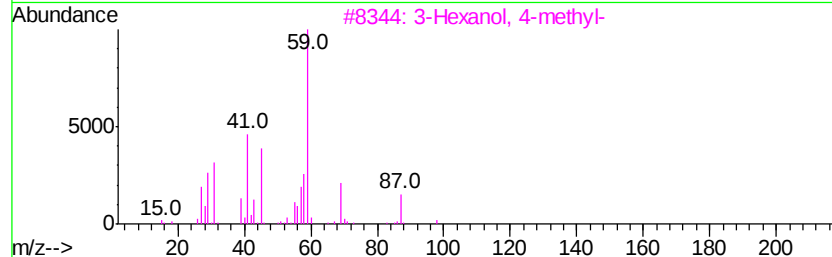
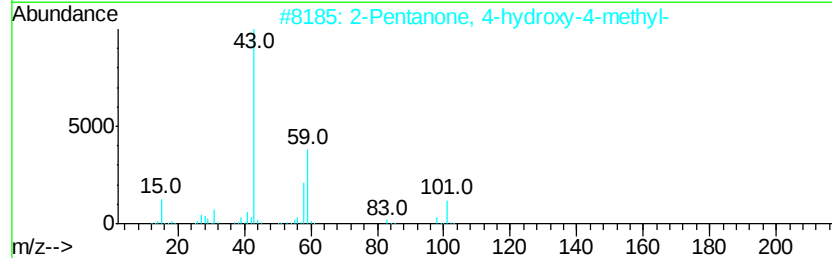
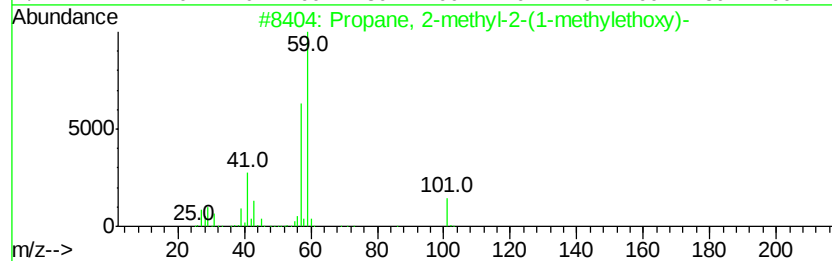
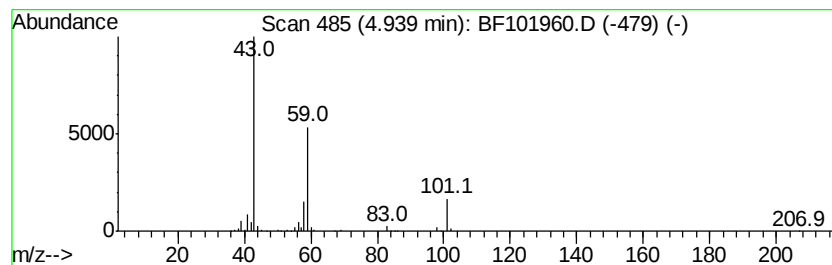
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown4.94 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	8.01 ng	594962	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
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	10



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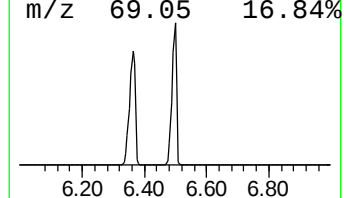
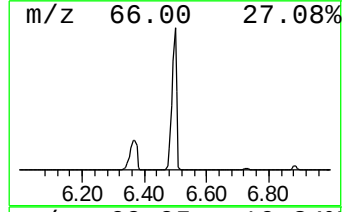
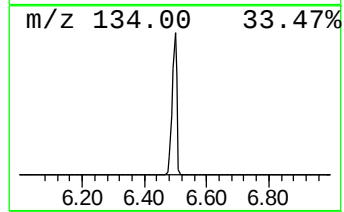
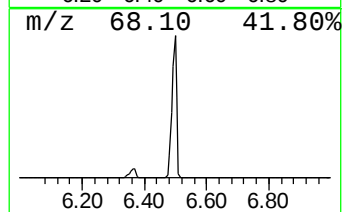
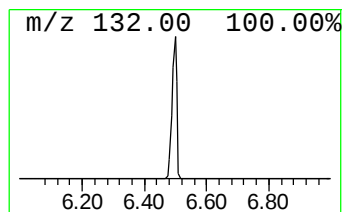
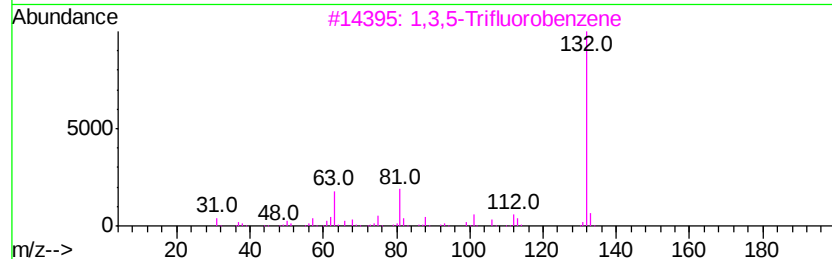
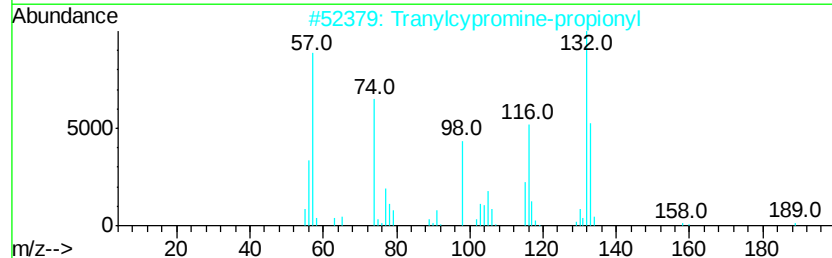
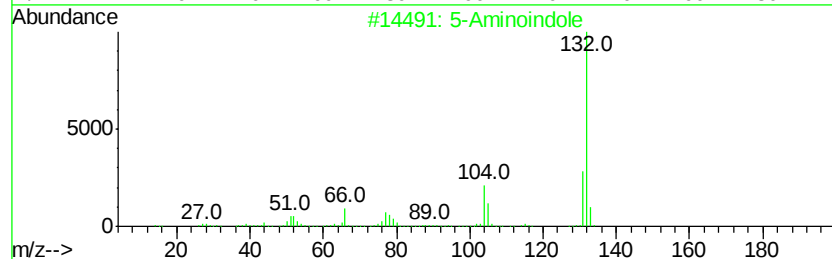
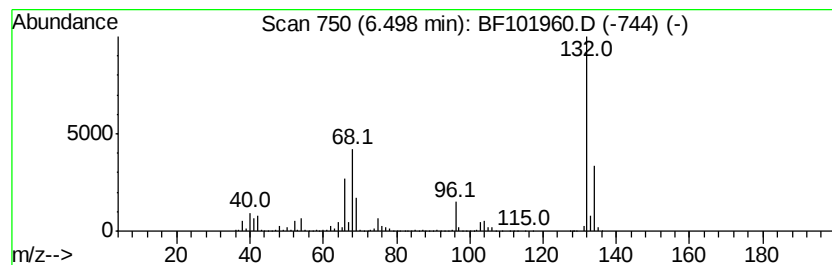
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Peak Number 3 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	85.61 ng	6362390	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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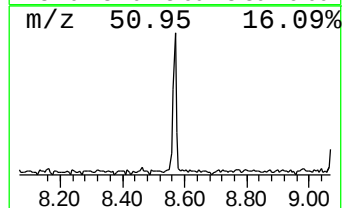
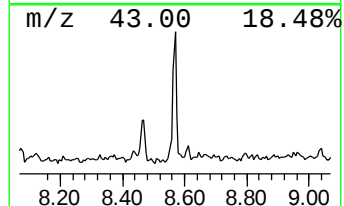
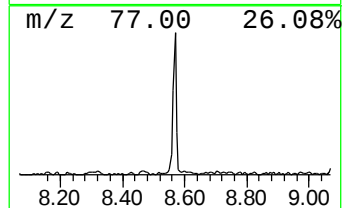
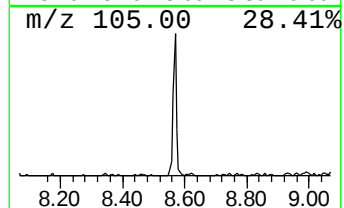
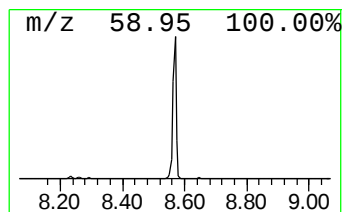
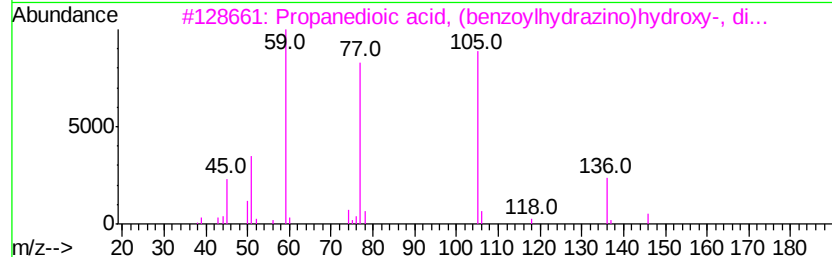
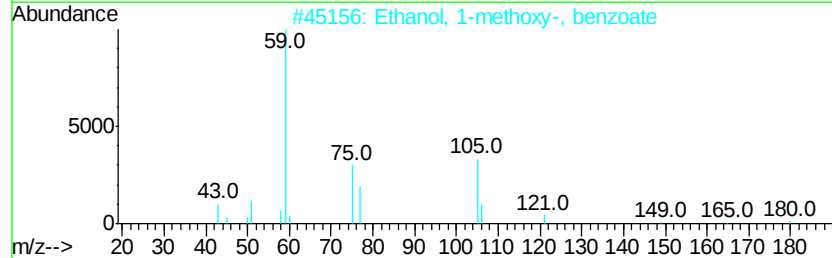
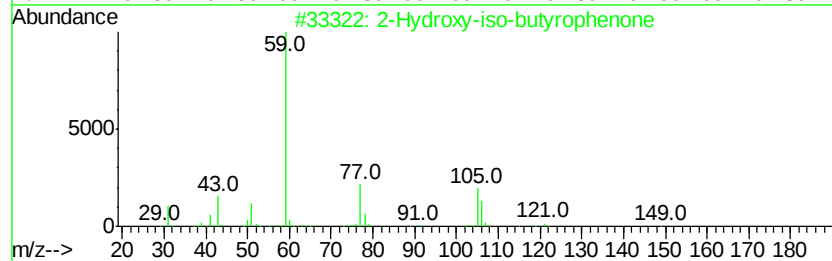
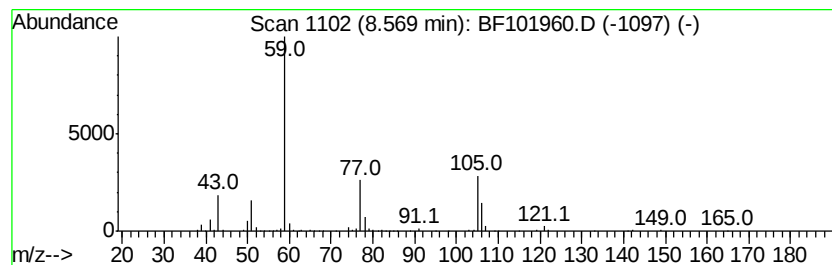
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Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	2.33 ng	221760	Napthalene-d8	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone			164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate			180	C10H12O3	051835-44-0	72
3	Propanedioic acid, (benzoylhydrazino)hydroxy-, di...			282	C12H14N2O6	1000142-99-9	23
4	3-Ethoxy-2-bromo-1-propanol			182	C5H11BrO2	133532-45-3	23
5	Propanoic acid, 2-hydroxy-2-meth...			132	C6H12O3	000080-55-7	23



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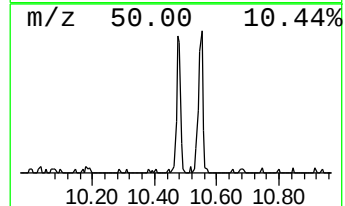
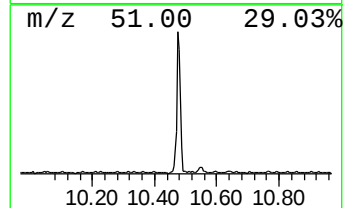
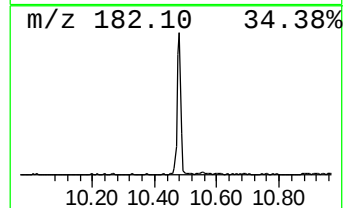
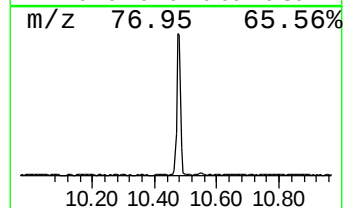
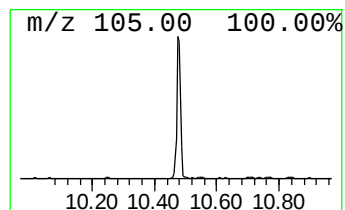
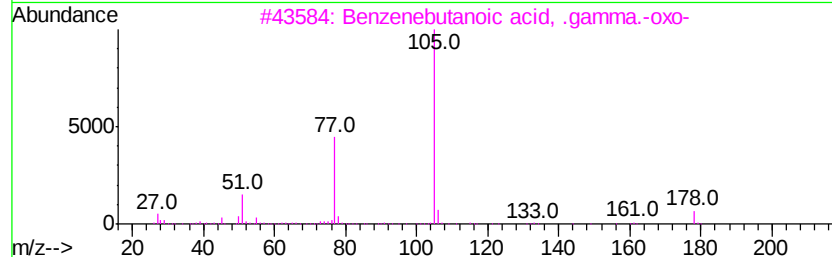
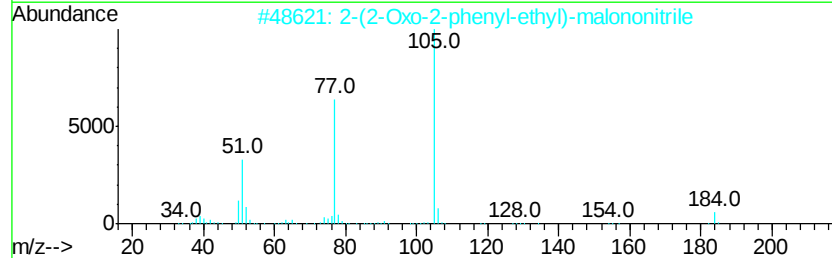
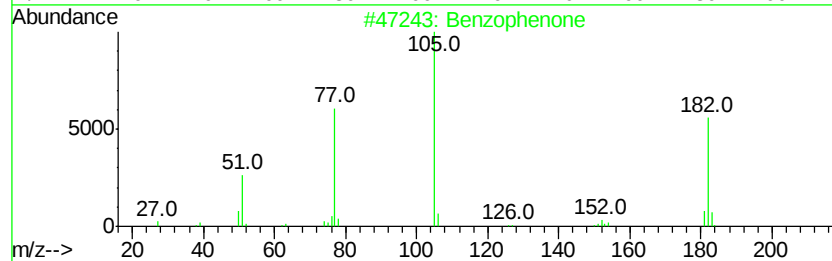
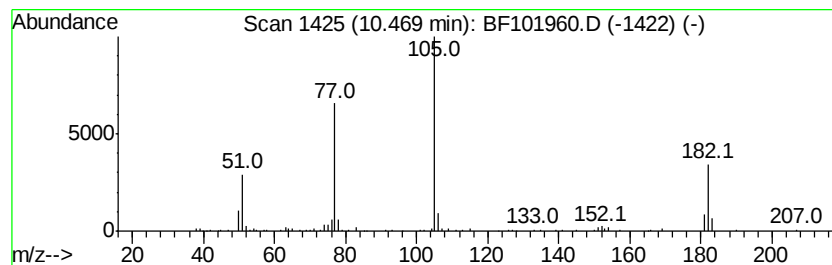
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Peak Number 6 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	5.42 ng	471705	Acenaphthene-d10	9.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184 C11H8N2O	1000296-76-9 47
3		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
4		1-Propanone, 3-chloro-1-phenyl-	168 C9H9ClO	000936-59-4 47
5		1-Butanone, 1-phenyl-	148 C10H12O	000495-40-9 47



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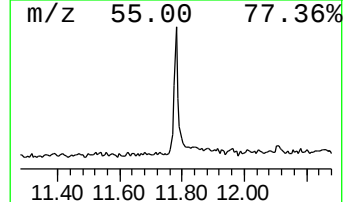
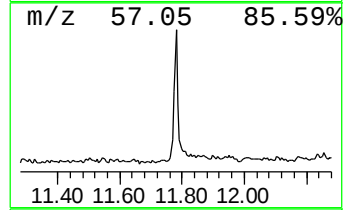
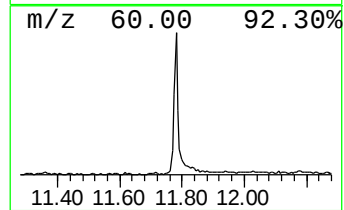
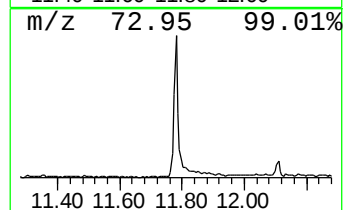
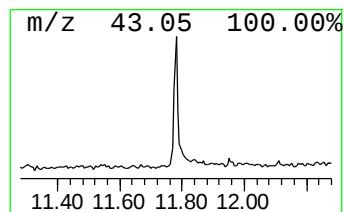
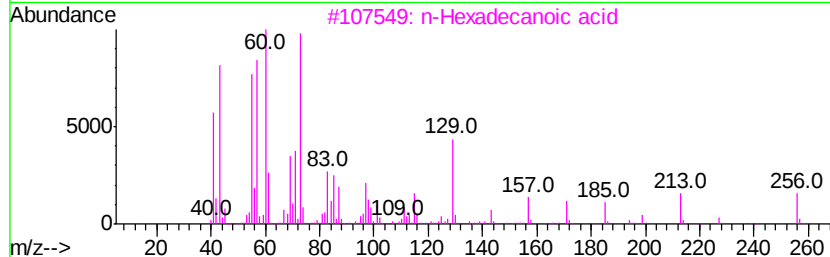
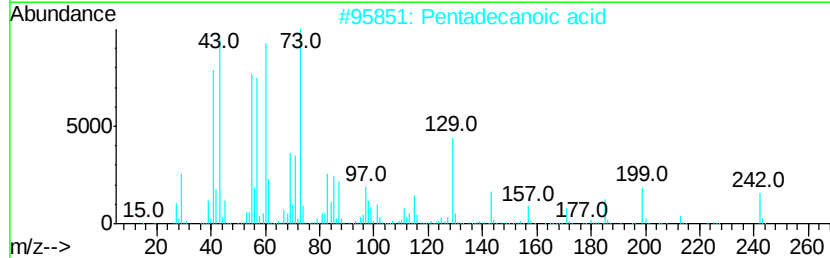
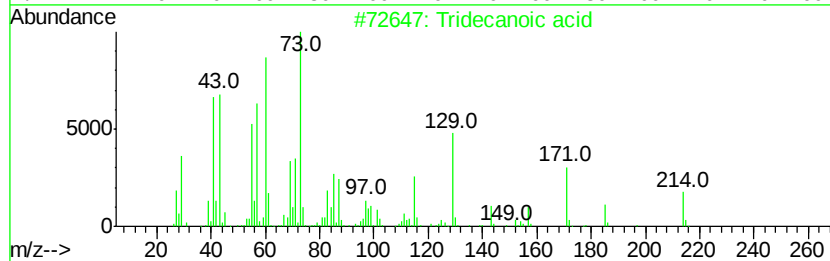
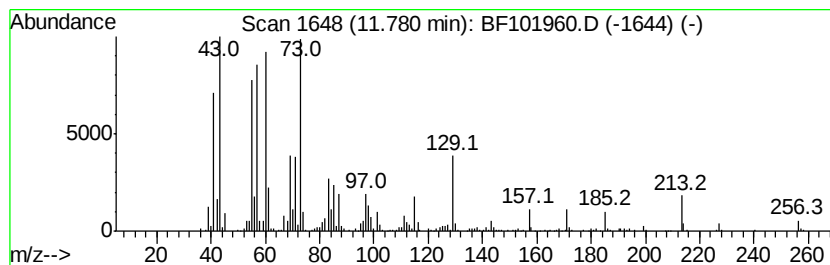
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	6.73 ng	457649	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF01960.D
Acq On : 9 Jan 2018 18:50
Operator : SJ/JU
Sample : J1044-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP-C

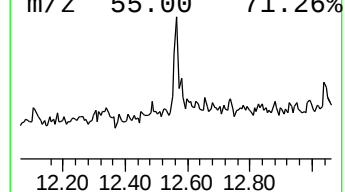
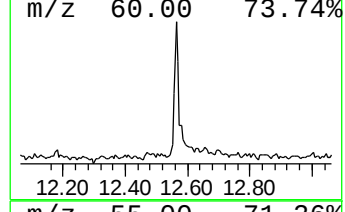
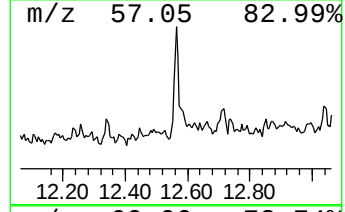
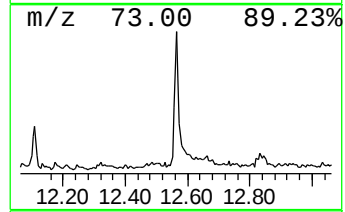
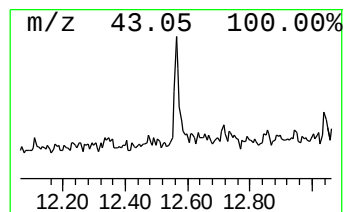
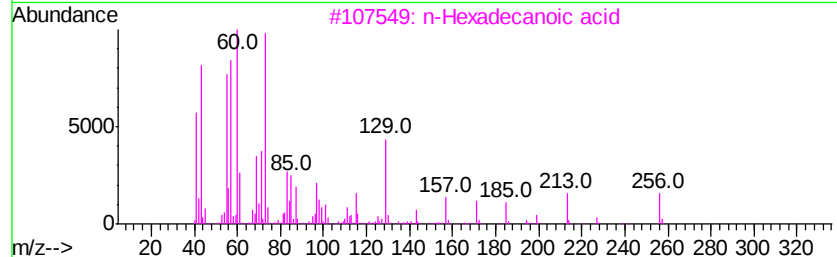
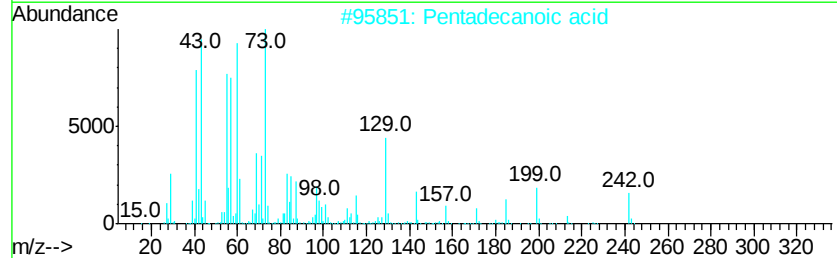
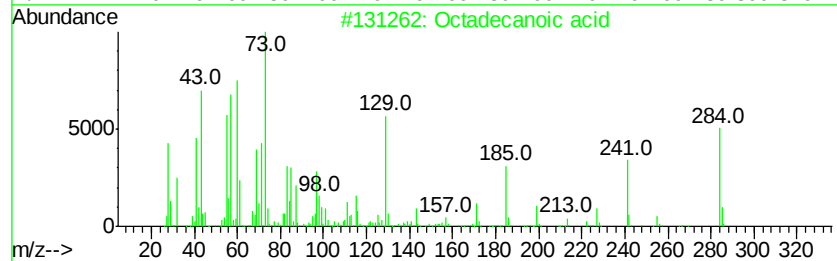
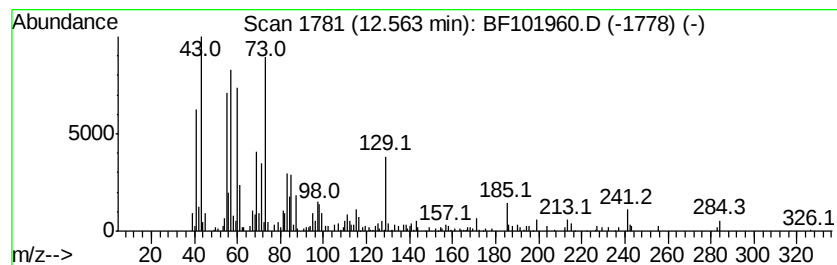
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.83 ng	178059	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF01960.D
Acq On : 9 Jan 2018 18:50
Operator : SJ/JU
Sample : J1044-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP-C

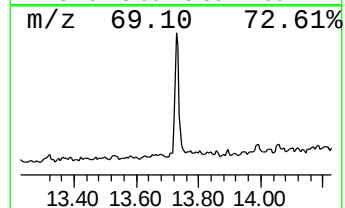
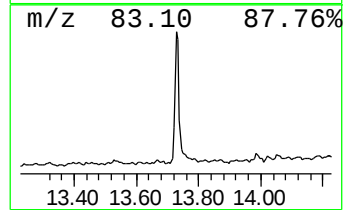
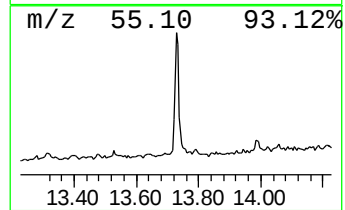
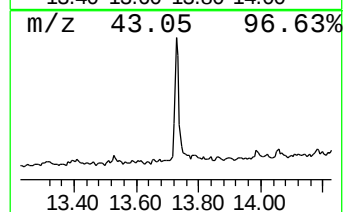
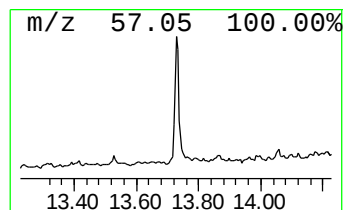
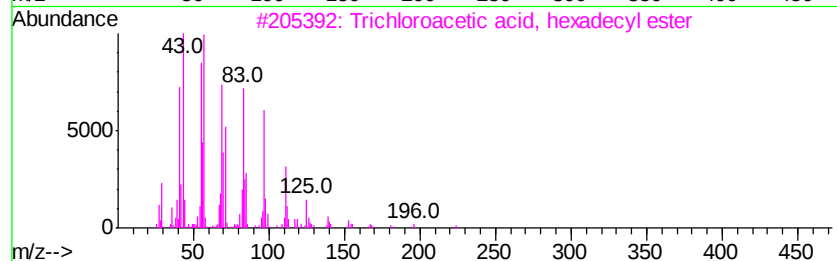
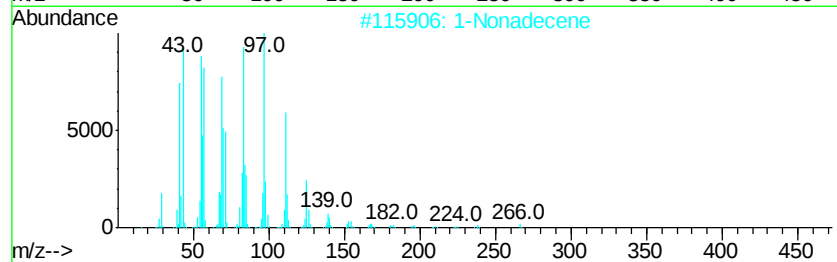
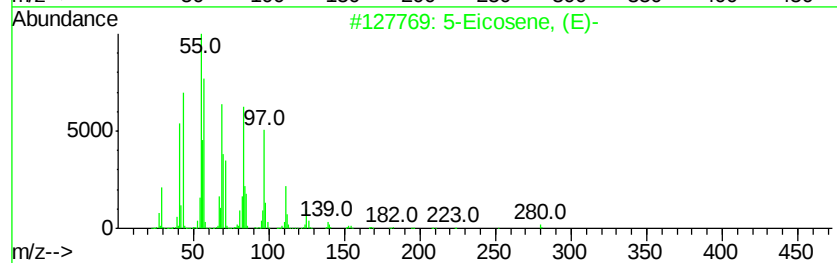
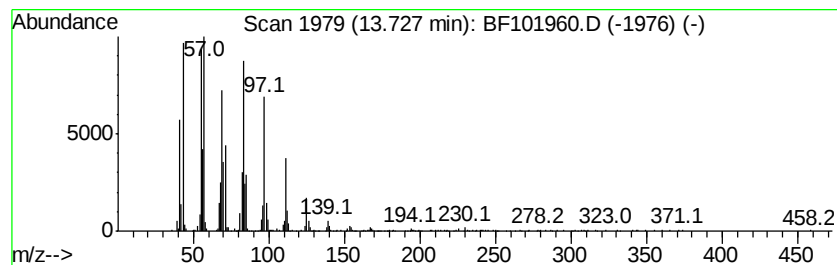
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	10.17 ng	639194	Chrysene-d12	13.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2			1-Nonadecene	266	C19H38	018435-45-5	95
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			1-Docosene	308	C22H44	001599-67-3	92



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF101960.D
Acq On : 9 Jan 2018 18:50
Operator : SJ/JU
Sample : J1044-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP-C

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...	4.29	3.3	ng	247478	1	6.73	1486310	20.0
unknown4.94	4.94	8.0	ng	594962	1	6.73	1486310	20.0
unknown6.50	6.50	85.6	ng	6362390	1	6.73	1486310	20.0
2-Hydroxy-iso-but...	8.57	2.3	ng	221760	2	8.01	1904290	20.0
Benzophenone	10.47	5.4	ng	471705	3	9.76	1740070	20.0
Tridecanoic acid	11.78	6.7	ng	457649	4	11.24	1360740	20.0
Octadecanoic acid	12.56	2.8	ng	178059	5	13.88	1256660	20.0
5-Eicosene, (E)-	13.73	10.2	ng	639194	5	13.88	1256660	20.0