

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
 Data File : BF093218.D
 Acq On : 27 Feb 2017 21:35
 Operator : SJ/MA
 Sample : I2013-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CR-2

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-BF013017.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	3.047	83	84	98	rBV	32639	96432	1.11%	0.262%
2	3.287	102	105	115	rVB	63458	126283	1.45%	0.343%
3	4.316	191	195	198	rBV	3513601	5423944	62.43%	14.728%
4	5.013	250	256	259	rBV	3880234	8687880	100.00%	23.591%
5	5.424	290	292	302	rVB	57124	94983	1.09%	0.258%
6	6.464	381	383	391	rBV	553046	607301	6.99%	1.649%
7	6.590	391	394	396	rVV	128343	150458	1.73%	0.409%
8	6.807	411	413	416	rBV	810209	917213	10.56%	2.491%
9	6.967	425	427	430	rBV	2725361	2440110	28.09%	6.626%
10	7.379	461	463	466	rBV	1803598	2036772	23.44%	5.531%
11	8.099	524	526	529	rBV	1364721	1254611	14.44%	3.407%
12	9.185	617	621	623	rBV	3153636	3854710	44.37%	10.467%
13	9.573	653	655	658	rBV	592886	665788	7.66%	1.808%
14	9.859	677	680	682	rVV	1515785	1426762	16.42%	3.874%
15	10.282	713	717	719	rVB2	56528	96586	1.11%	0.262%
16	10.762	757	759	762	rBV	117812	154678	1.78%	0.420%
17	11.208	796	798	799	rBV	139751	117784	1.36%	0.320%
18	11.345	807	810	811	rBV	1488806	1356893	15.62%	3.684%
19	11.368	811	812	813	rVV	137173	104975	1.21%	0.285%
20	11.562	827	829	833	rBV3	156149	244949	2.82%	0.665%
21	11.631	833	835	838	rBV	132606	120585	1.39%	0.327%
22	12.385	899	901	903	rBV2	91877	113857	1.31%	0.309%
23	12.556	914	916	918	rBV	240061	204023	2.35%	0.554%
24	12.785	931	936	939	rBV	224985	333544	3.84%	0.906%
25	12.934	946	949	951	rBV	2812310	3120943	35.92%	8.474%
26	13.825	1024	1027	1032	rVB3	193199	305441	3.52%	0.829%
27	13.985	1038	1041	1043	rBV	1051248	1160677	13.36%	3.152%
28	14.499	1084	1086	1088	rBV	81332	121101	1.39%	0.329%
29	14.808	1111	1113	1115	rBV	80803	97674	1.12%	0.265%
30	15.002	1128	1130	1134	rVB	85337	149859	1.72%	0.407%
31	15.414	1163	1166	1171	rVB	700689	955569	11.00%	2.595%
32	15.825	1200	1202	1204	rBV	71835	100952	1.16%	0.274%
33	16.294	1241	1243	1250	rVB3	75252	184528	2.12%	0.501%

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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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

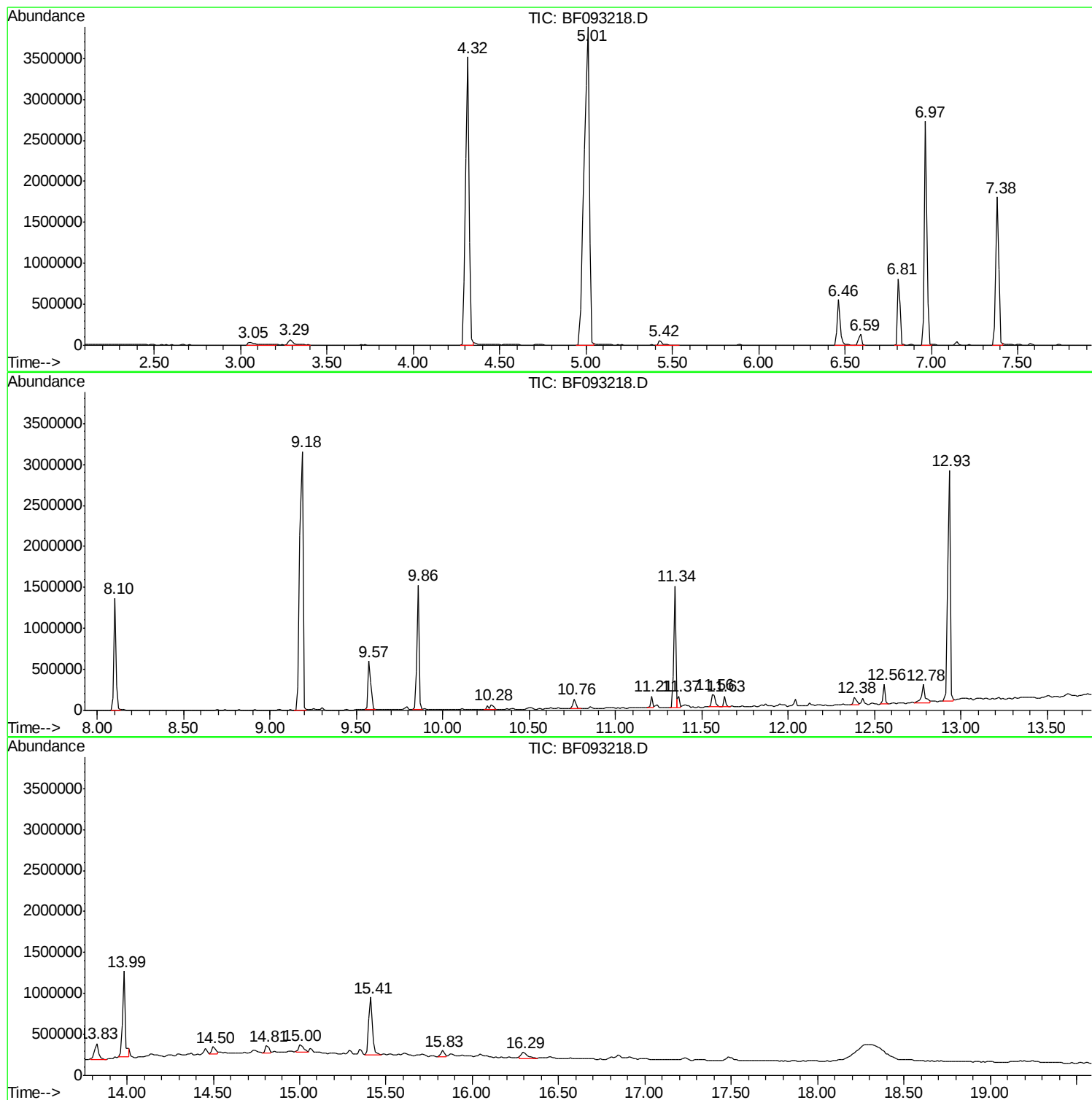
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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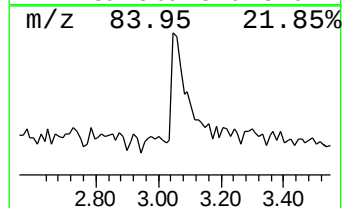
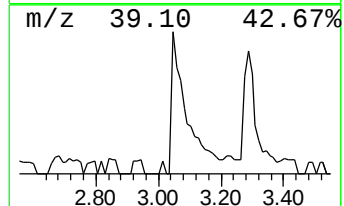
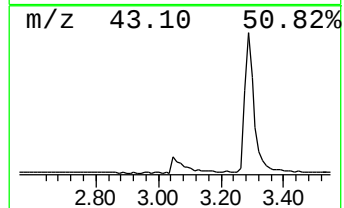
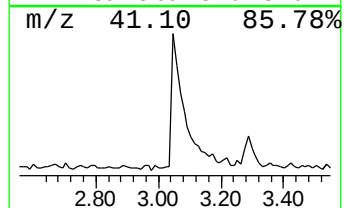
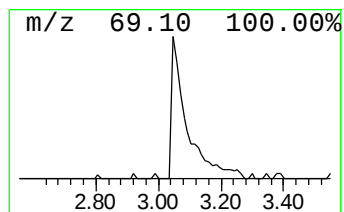
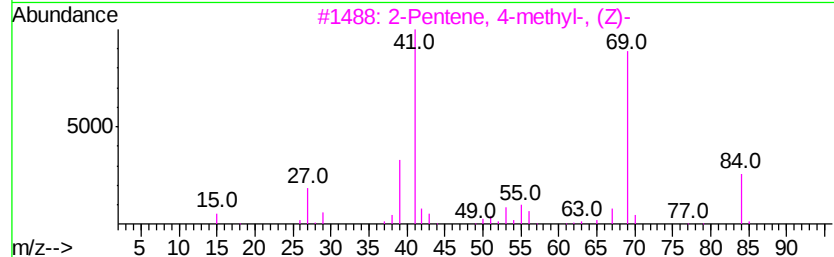
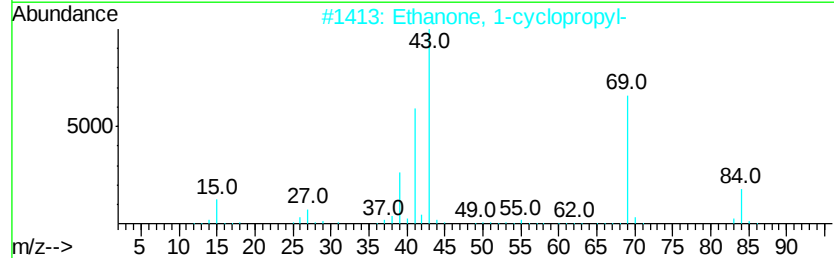
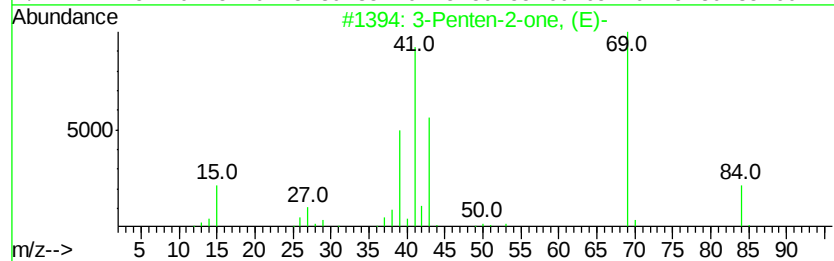
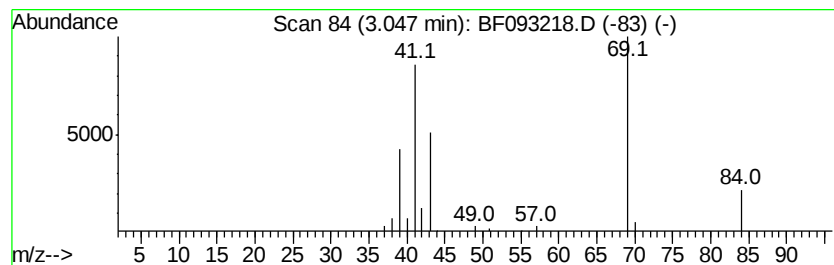
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	2.10 ng	96432	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	91
2			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	53
3			2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	53
4			2-Pentene, 4-methyl-	84	C6H12	004461-48-7	53
5			Cyclopropane, 1,1,2-trimethyl-	84	C6H12	004127-45-1	53



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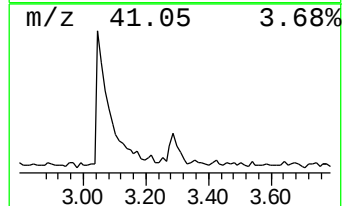
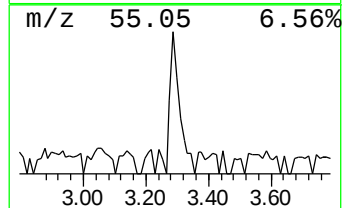
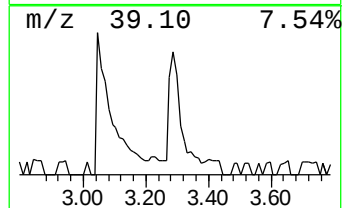
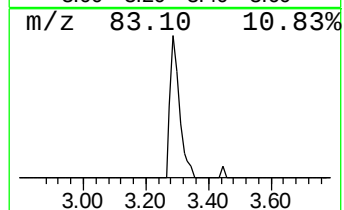
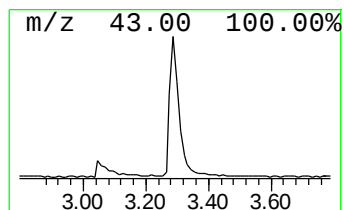
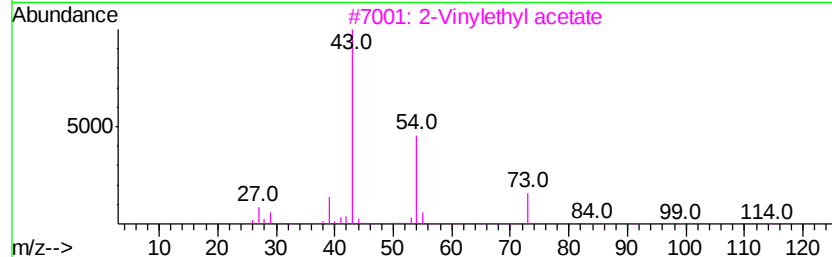
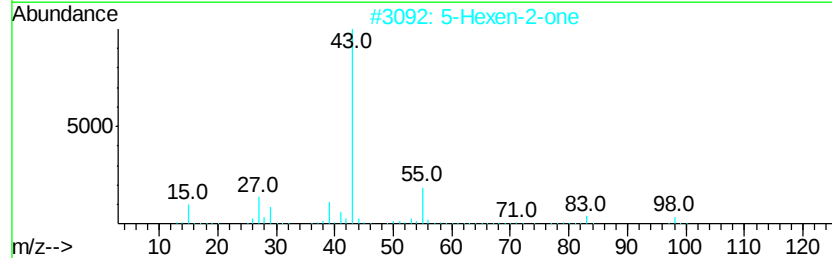
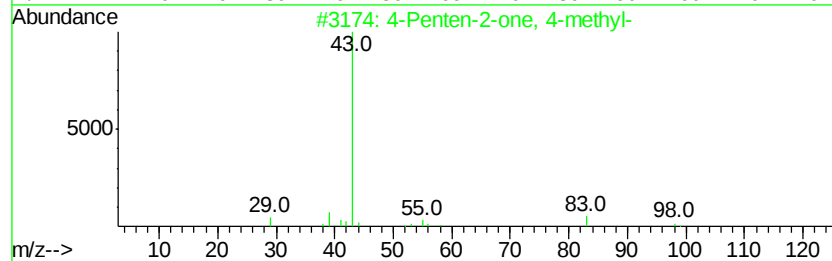
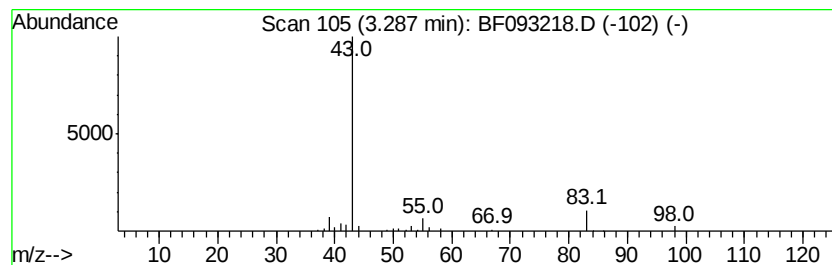
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	2.75 ng	126283	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2			5-Hexen-2-one	98	C6H10O	000109-49-9	38
3			2-Vinylethyl acetate	114	C6H10O2	001576-84-7	28
4			Pent-3-enylamine	85	C5H11N	087156-70-5	9
5			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9



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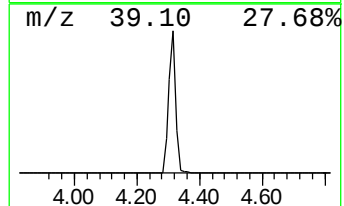
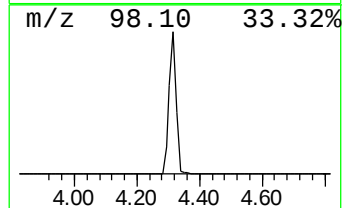
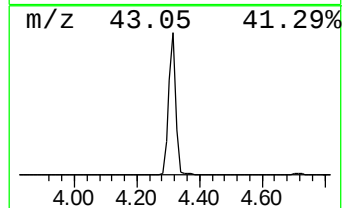
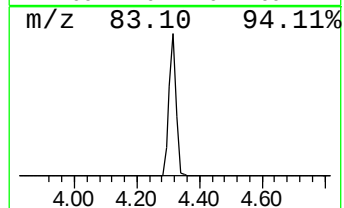
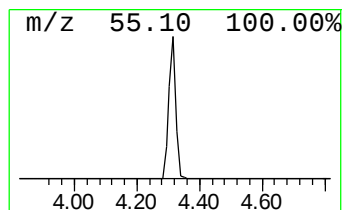
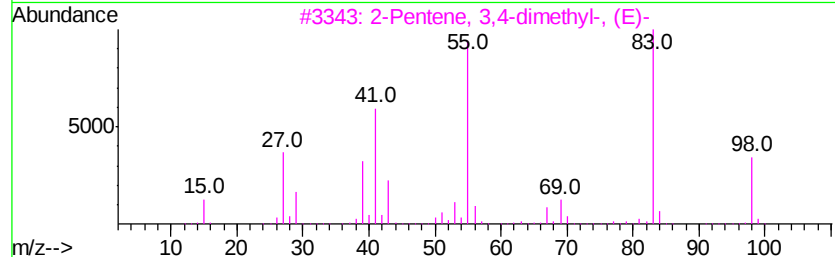
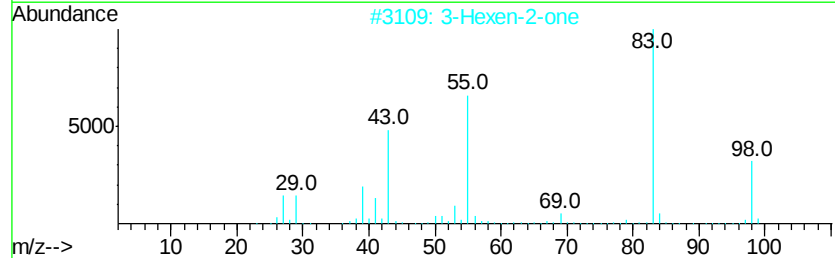
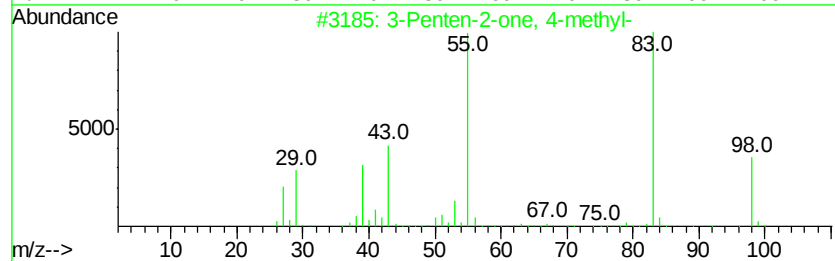
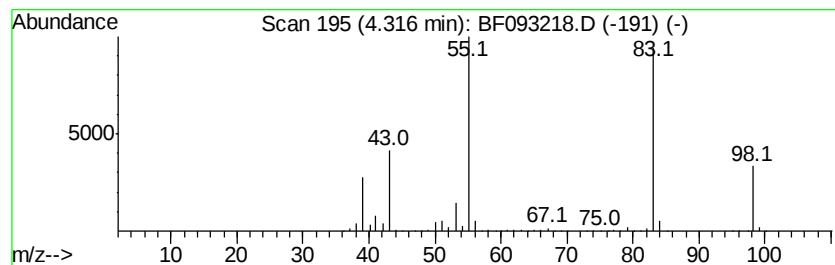
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	118.27 ng	5423940	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
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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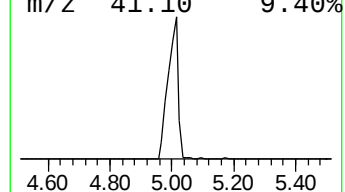
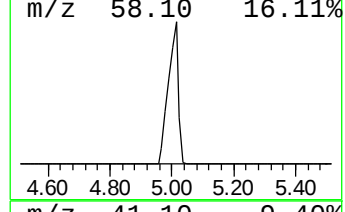
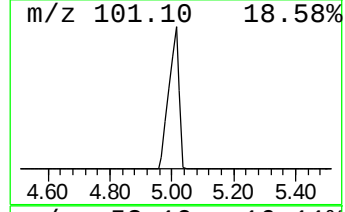
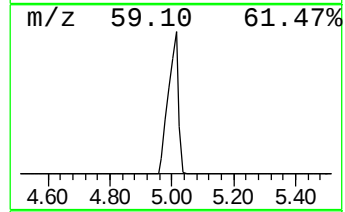
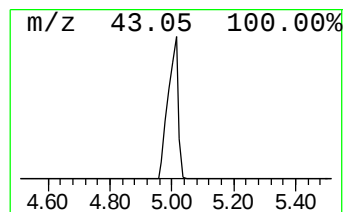
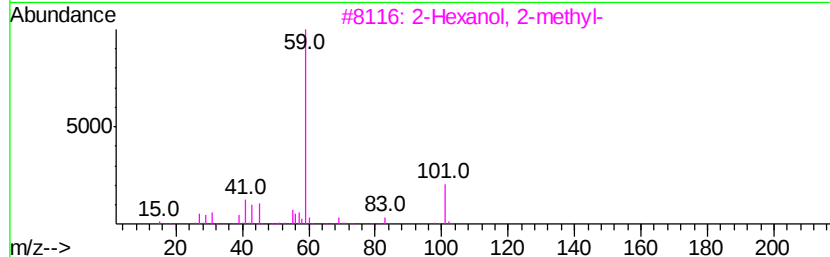
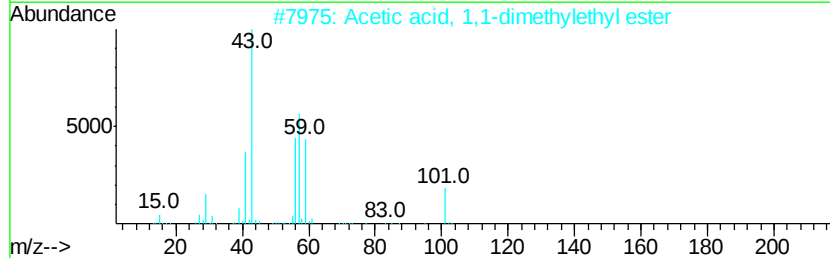
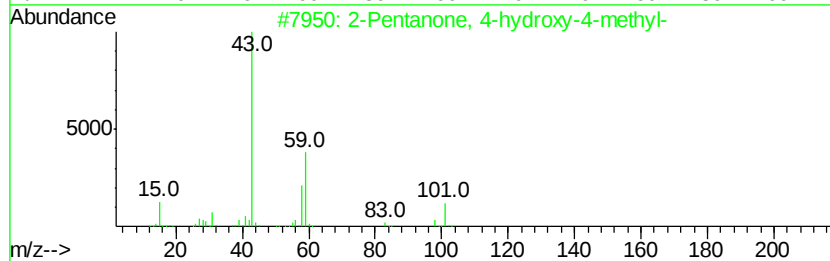
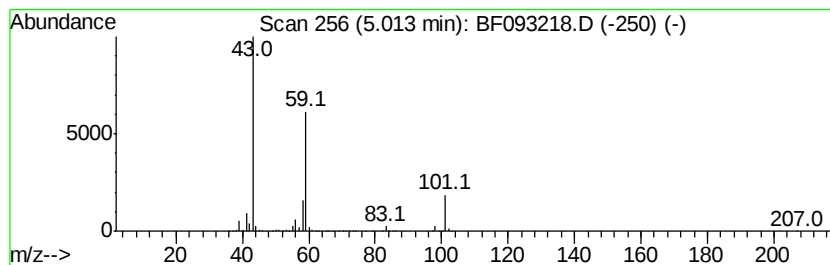
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	189.44 ng	8687880	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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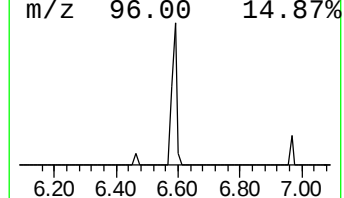
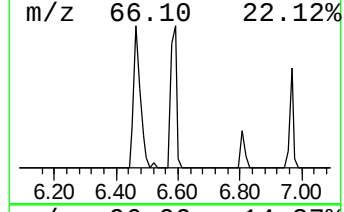
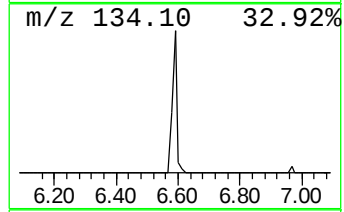
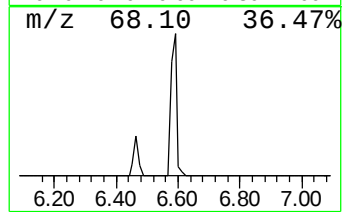
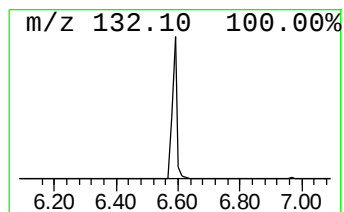
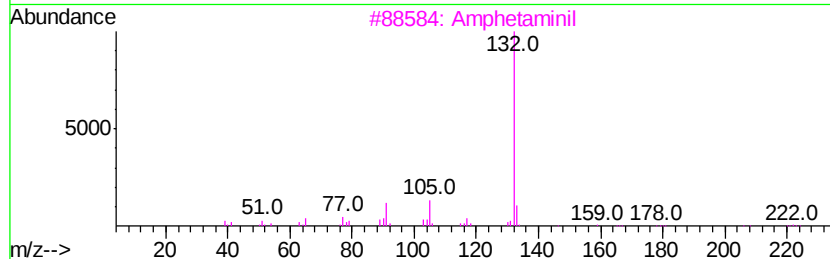
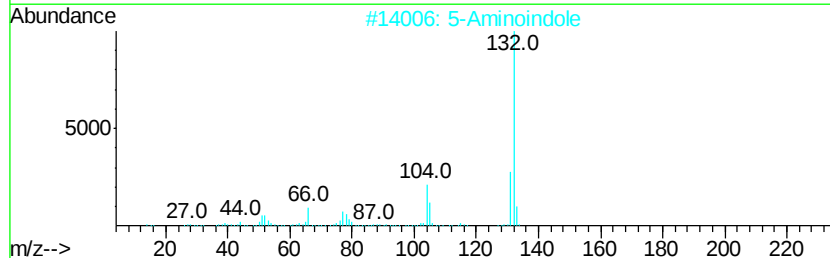
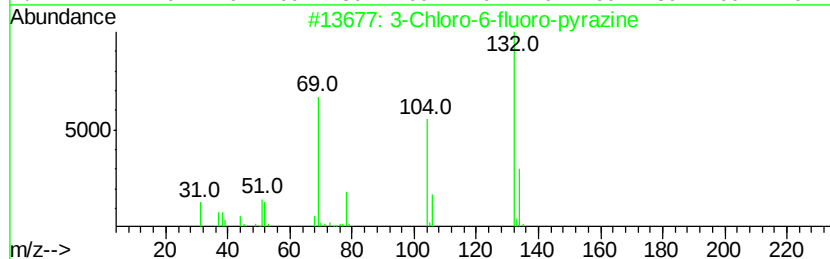
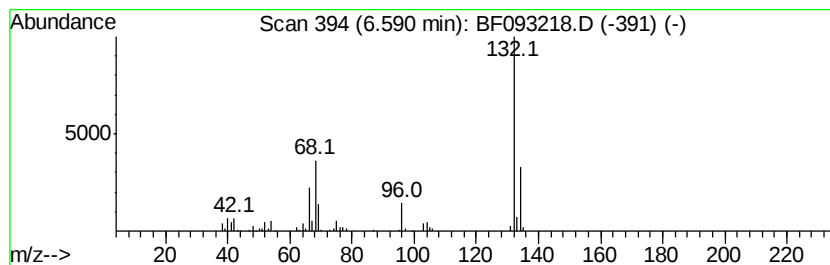
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.59 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	3.28 ng	150458	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Amphetaminil	250	C17H18N2	017590-01-1	12	
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12	
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	



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ClientSampleId :
CR-2

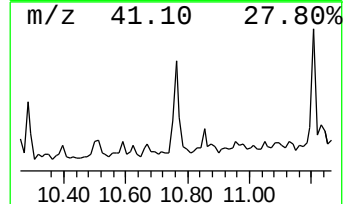
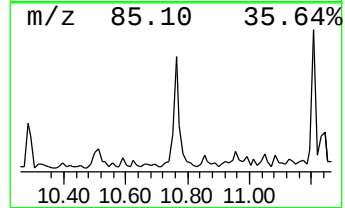
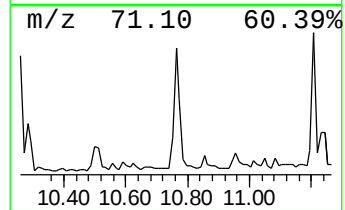
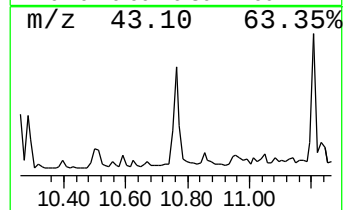
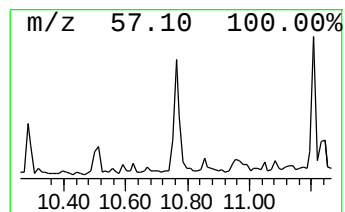
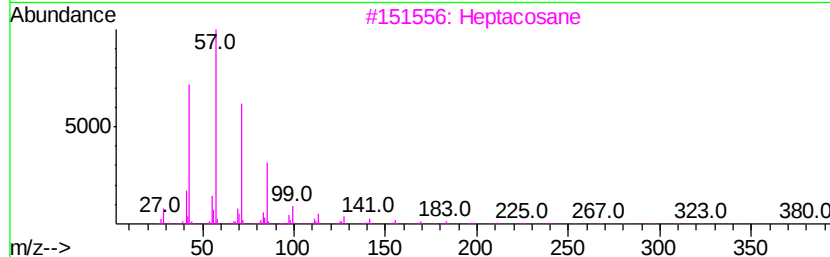
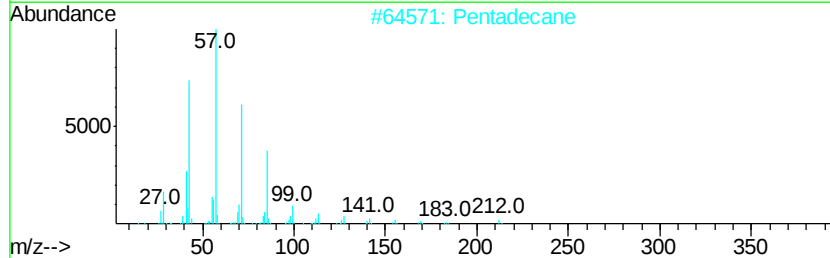
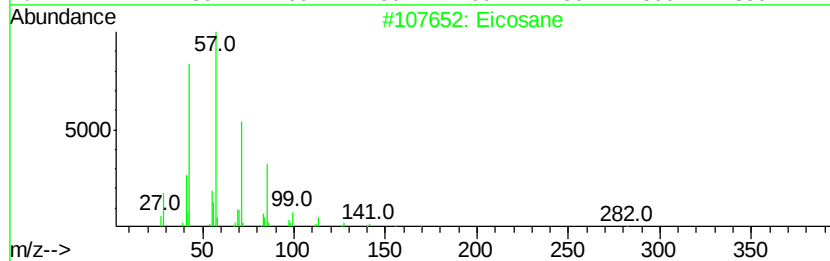
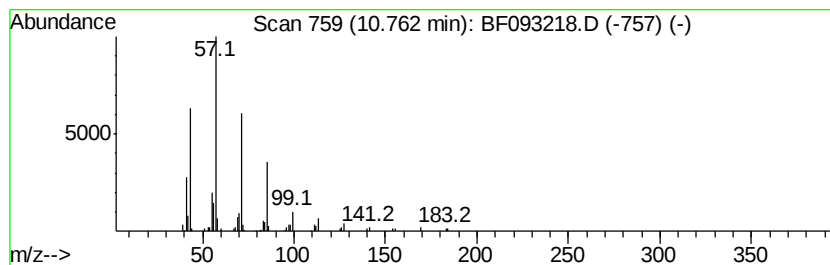
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.28 ng	154678	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Pentadecane		212	C15H32	000629-62-9	91
3	Heptacosane		380	C27H56	000593-49-7	90
4	Tridecane		184	C13H28	000629-50-5	87
5	Octadecane		254	C18H38	000593-45-3	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022717\
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Acq On : 27 Feb 2017 21:35
Operator : SJ/MA
Sample : I2013-02
Misc :
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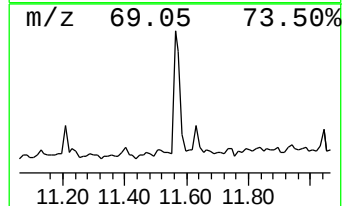
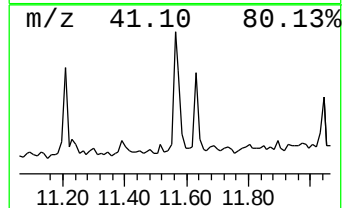
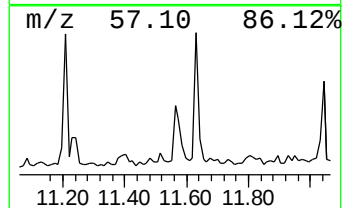
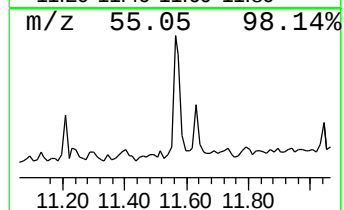
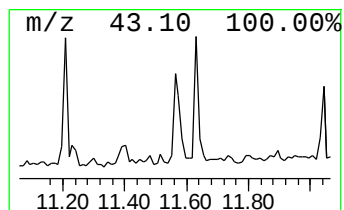
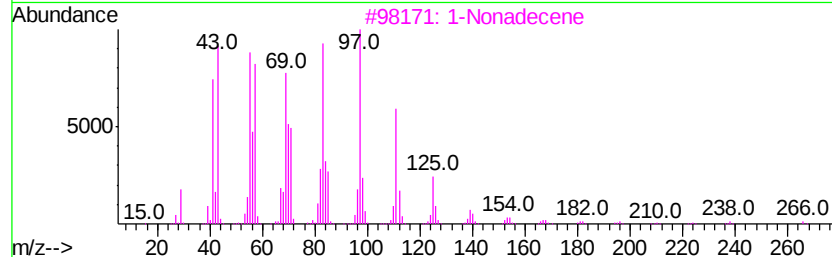
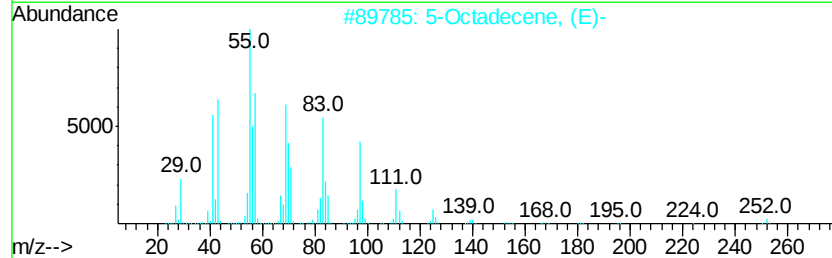
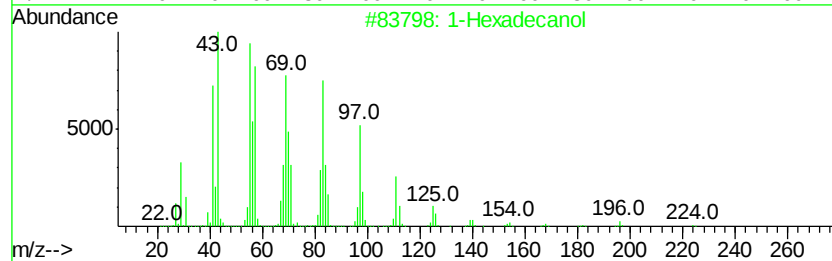
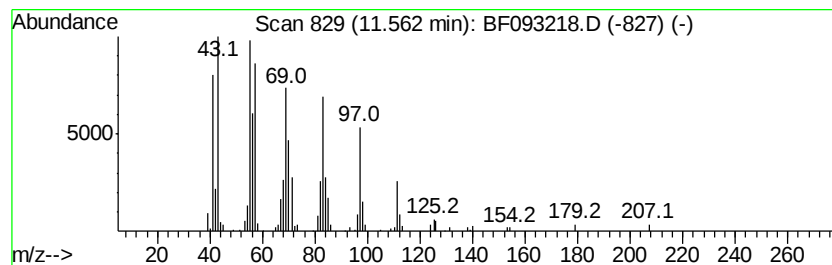
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Hexadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.56	3.61 ng	244949	Phenanthrene-d10		11.34
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	91
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	90
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	1-Pentadecanol	228	C15H32O	000629-76-5	87
5	1-Tetradecanol	214	C14H30O	000112-72-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
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Instrument :
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ClientSampleId :
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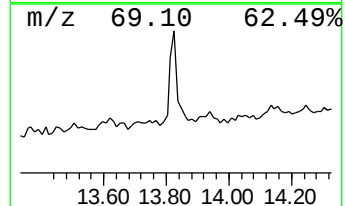
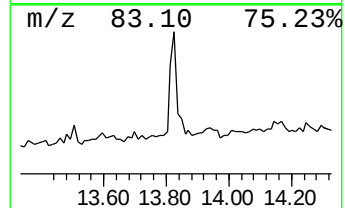
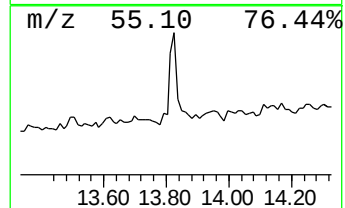
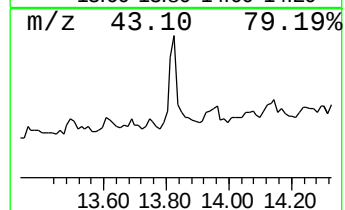
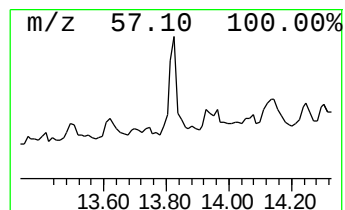
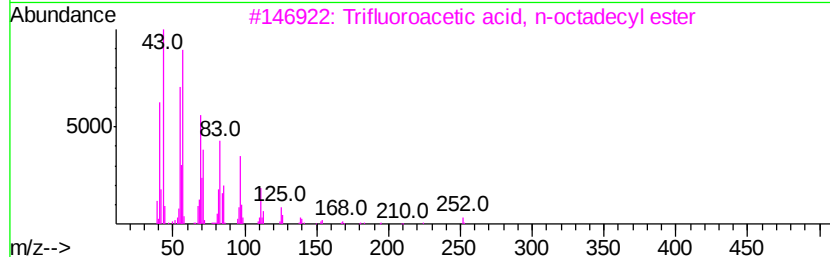
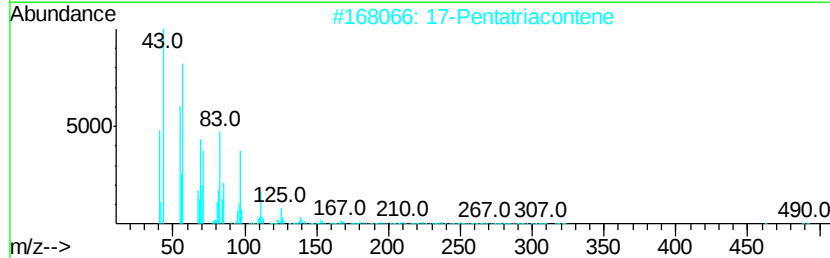
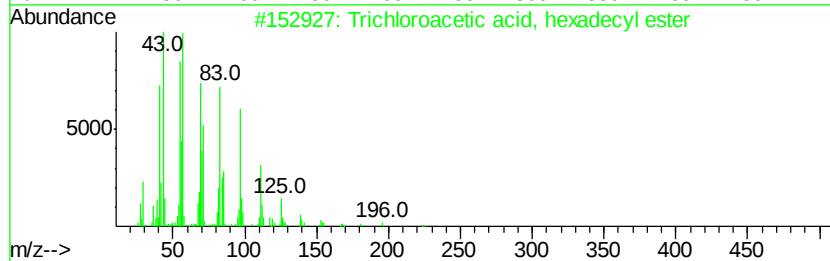
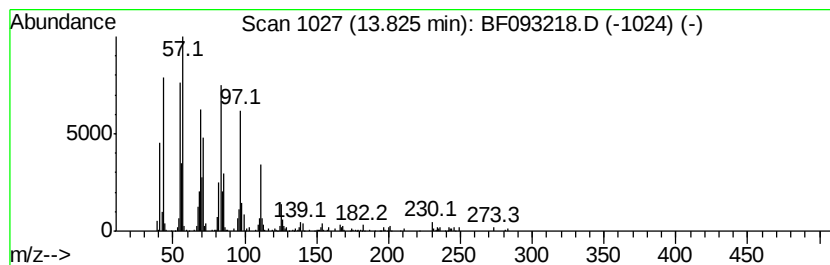
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.26 ng	305441	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	81
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	64
5		1-Docosene	308	C22H44	001599-67-3	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
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Acq On : 27 Feb 2017 21:35
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Sample : I2013-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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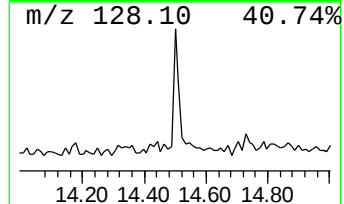
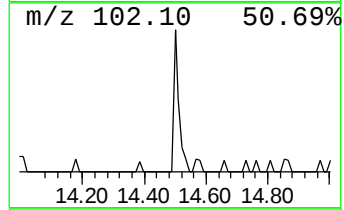
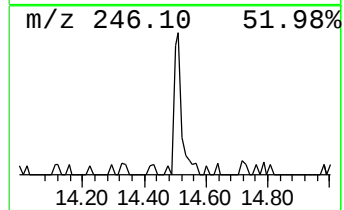
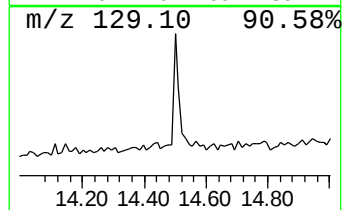
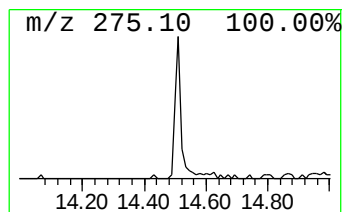
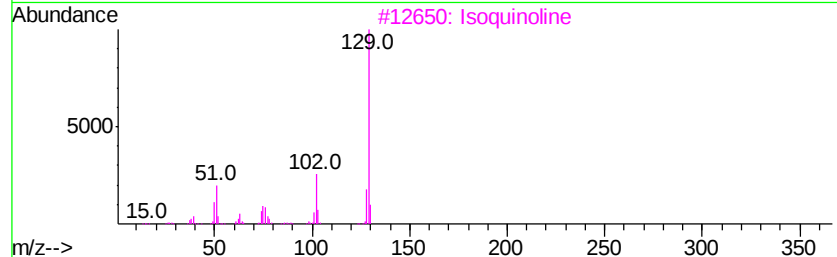
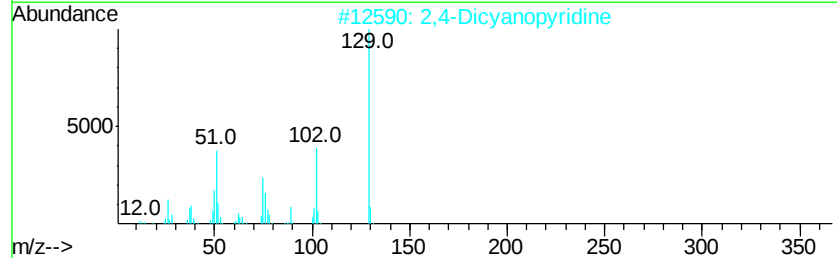
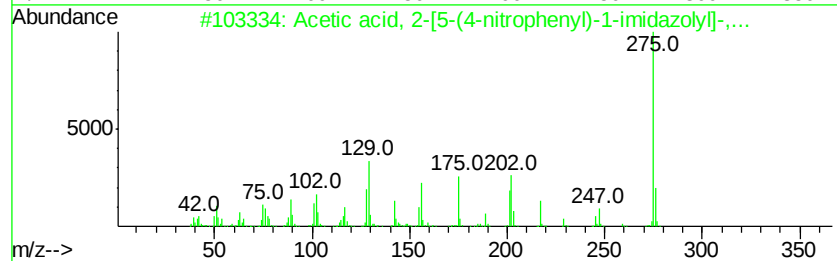
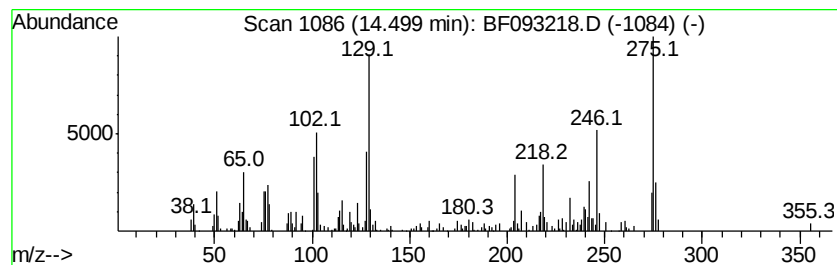
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.09 ng	121101	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 2-[5-(4-nitrophenyl)-1-imidazolyl]-...	275	C13H13N3O4	351064-45-4	58
2		2,4-Dicyanopyridine	129	C7H3N3	029181-50-8	35
3		Isoquinoline	129	C9H7N	000119-65-3	30
4		Quinoline	129	C9H7N	000091-22-5	30
5		Benzonitrile, 4-ethenyl-	129	C9H7N	003435-51-6	30



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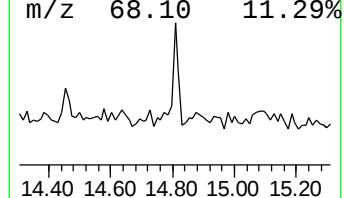
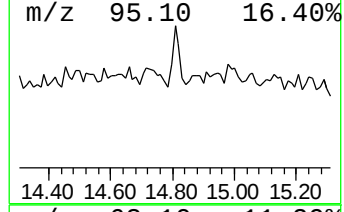
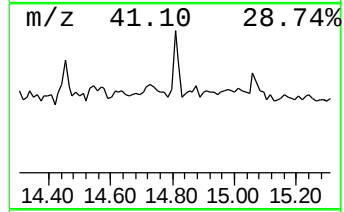
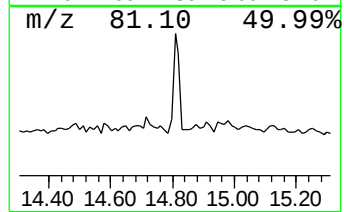
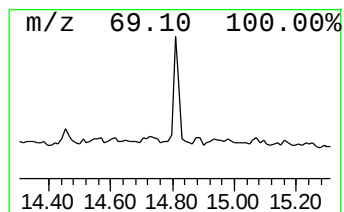
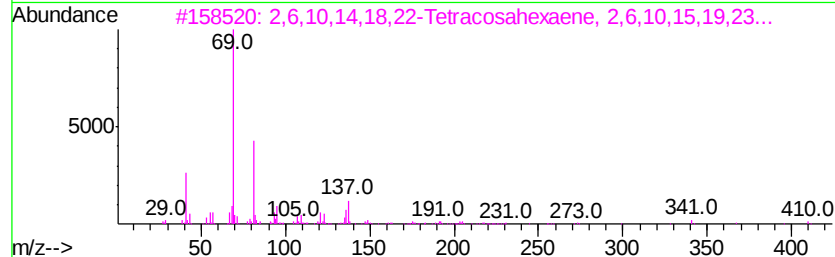
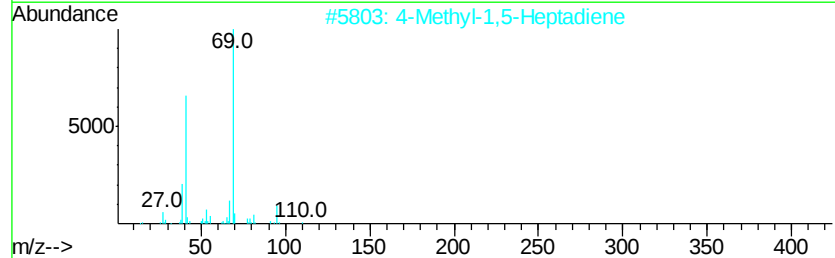
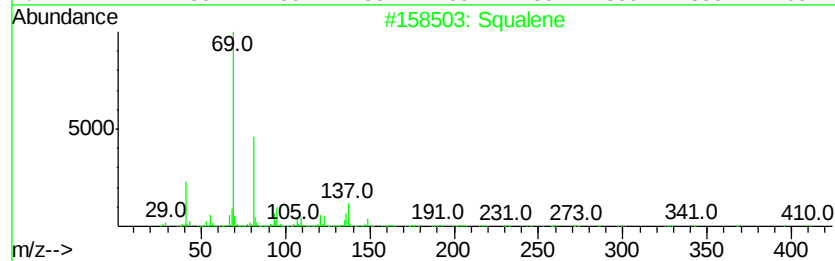
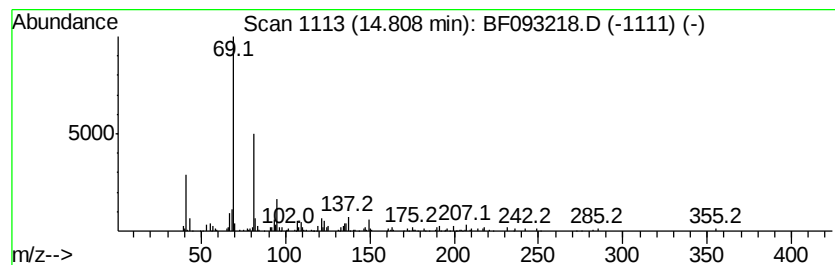
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Squalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.04 ng	97674	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	80
2		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64
3		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64
4		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	64
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022717\
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Sample : I2013-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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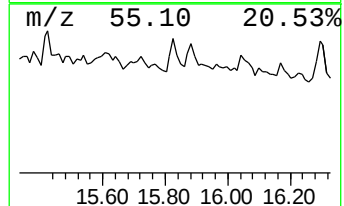
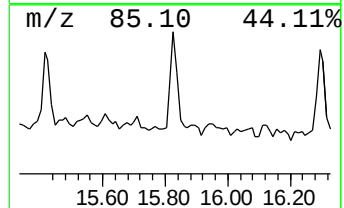
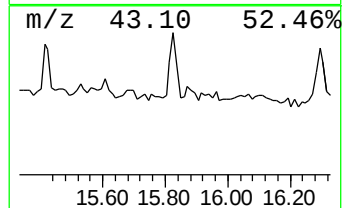
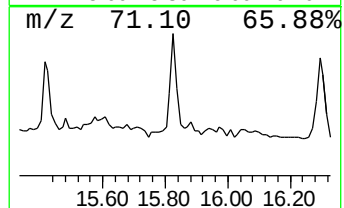
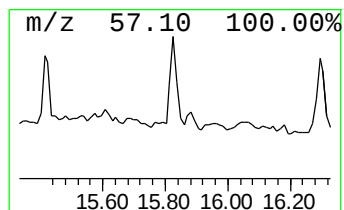
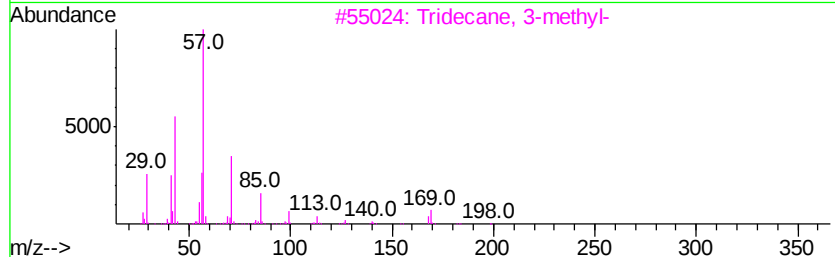
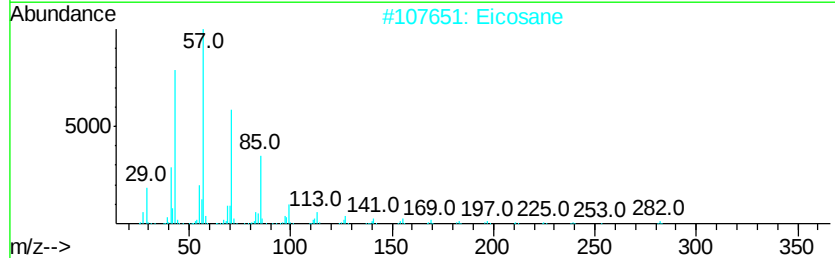
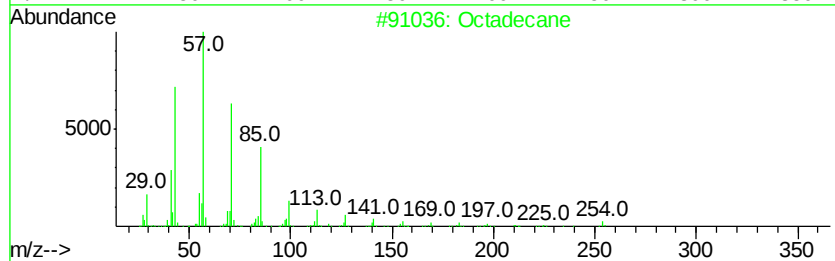
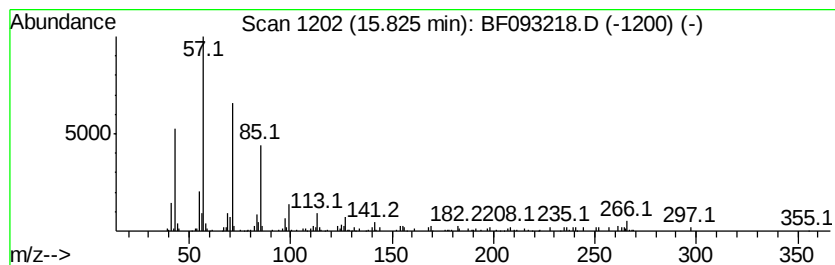
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	2.11 ng	100952	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	83
2		Eicosane	282	C20H42	000112-95-8	80
3		Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
4		Tetradecane	198	C14H30	000629-59-4	72
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022717\
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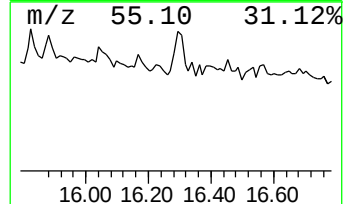
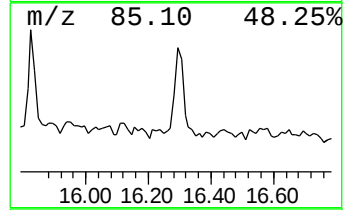
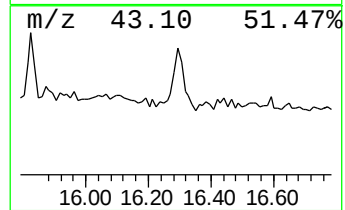
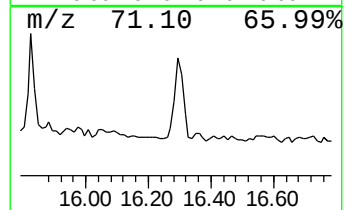
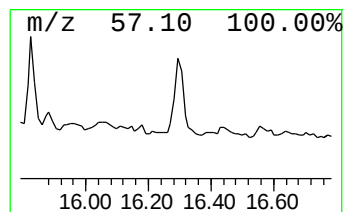
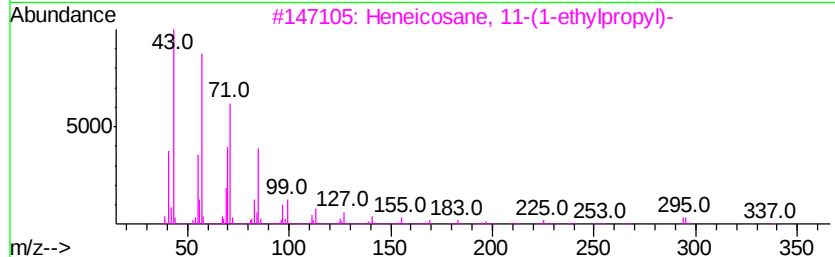
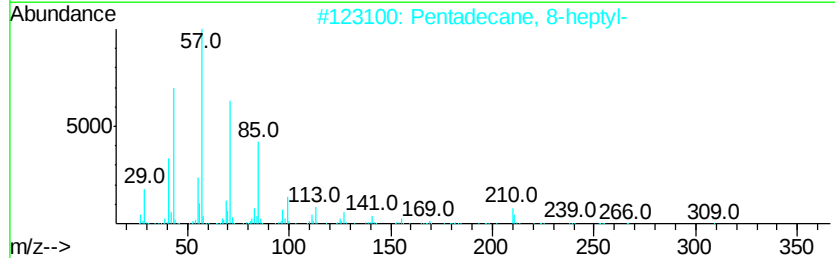
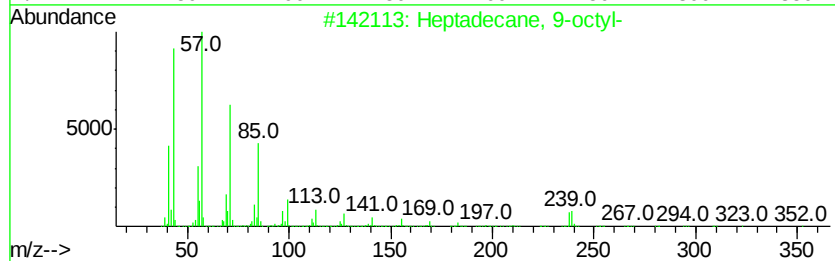
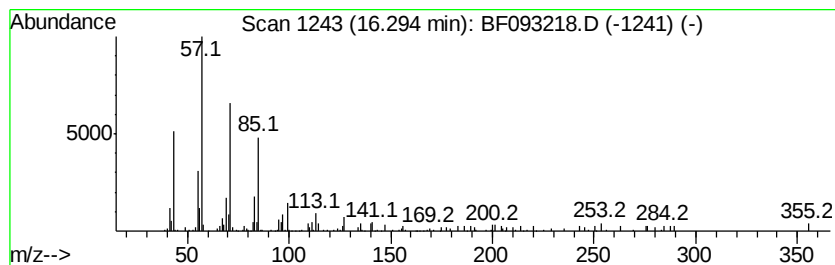
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	3.86 ng	184528	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
2		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	72
5		triacontane	422	C30H62	000638-68-6	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
 Data File : BF093218.D
 Acq On : 27 Feb 2017 21:35
 Operator : SJ/MA
 Sample : I2013-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CR-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, (E)-	3.05	2.1	ng	96432	1	6.81	917213	20.0
4-Penten-2-one, 4...	3.29	2.8	ng	126283	1	6.81	917213	20.0
3-Penten-2-one, 4...	4.32	118.3	ng	5423940	1	6.81	917213	20.0
2-Pentanone, 4-hy...	5.01	189.4	ng	8687880	1	6.81	917213	20.0
unknown6.59	6.59	3.3	ng	150458	1	6.81	917213	20.0
Eicosane	10.76	2.3	ng	154678	4	11.34	1356890	20.0
1-Hexadecanol	11.56	3.6	ng	244949	4	11.34	1356890	20.0
Trichloroacetic a...	13.83	5.3	ng	305441	5	13.99	1160680	20.0
Acetic acid, 2-[5...	14.50	2.1	ng	121101	5	13.99	1160680	20.0
Squalene	14.81	2.0	ng	97674	6	15.41	955569	20.0
Octadecane	15.83	2.1	ng	100952	6	15.41	955569	20.0
Heptadecane, 9-oc...	16.29	3.9	ng	184528	6	15.41	955569	20.0