

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
 Data File : BF093380.D
 Acq On : 4 Mar 2017 1:08
 Operator : SJ/MA
 Sample : I2078-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-3

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	4.247	187	189	205	rBV	1255182	2097322	42.08%	4.552%
2	4.944	246	250	259	rBV	1275620	2175088	43.64%	4.721%
3	5.378	286	288	302	rBV	3360845	3529896	70.83%	7.661%
4	6.430	378	380	383	rBV	3205566	4756511	95.44%	10.324%
5	6.556	388	391	393	rBV	3997677	4186402	84.00%	9.086%
6	6.784	409	411	413	rBV	1207397	1247249	25.03%	2.707%
7	6.853	415	417	419	rVB	136189	123783	2.48%	0.269%
8	6.944	422	425	427	rBV	2868178	3809976	76.45%	8.269%
9	7.356	458	461	464	rBV	2784906	3002604	60.25%	6.517%
10	7.836	500	503	512	rBV	51352	108884	2.18%	0.236%
11	8.076	521	524	526	rBV	1366875	1621864	32.54%	3.520%
12	9.002	601	605	609	rBV4	23090	58850	1.18%	0.128%
13	9.150	615	618	620	rBV	5073379	4983667	100.00%	10.817%
14	9.230	622	625	626	rVB	58852	81742	1.64%	0.177%
15	9.539	650	652	655	rBV	366520	507401	10.18%	1.101%
16	9.756	669	671	673	rBV	135796	158931	3.19%	0.345%
17	9.825	674	677	679	rVV	1611659	1634284	32.79%	3.547%
18	10.030	692	695	697	rVB3	26858	63575	1.28%	0.138%
19	10.065	697	698	701	rBV2	38183	56317	1.13%	0.122%
20	10.225	710	712	713	rBV	46386	55460	1.11%	0.120%
21	10.248	713	714	716	rVB	237887	188085	3.77%	0.408%
22	10.465	731	733	737	rBV	79813	140262	2.81%	0.304%
23	10.613	743	746	748	rBV	1156207	1195055	23.98%	2.594%
24	10.716	754	755	760	rVB	204577	351613	7.06%	0.763%
25	11.162	792	794	796	rBV	127001	187573	3.76%	0.407%
26	11.299	804	806	810	rBV	1098584	1562942	31.36%	3.392%
27	11.596	830	832	834	rBV	109714	117457	2.36%	0.255%
28	11.665	834	838	840	rVB	49284	60982	1.22%	0.132%
29	11.711	840	842	845	rBV2	47355	60708	1.22%	0.132%
30	11.859	854	855	858	rVB	166746	217420	4.36%	0.472%
31	11.928	858	861	864	rVB2	71660	125161	2.51%	0.272%
32	11.996	865	867	869	rBV	68703	60532	1.21%	0.131%
33	12.236	886	888	890	rBV2	39474	56198	1.13%	0.122%
34	12.351	896	898	900	rBV2	50388	72370	1.45%	0.157%

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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

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35	12.511	911	912	915	rBV	117835	165541	3.32%	0.359%
36	12.751	930	933	936	rBV2	96937	180284	3.62%	0.391%
37	12.888	942	945	947	rBV	3634099	3479317	69.81%	7.552%
38	13.059	958	960	962	rBV2	23638	55468	1.11%	0.120%
39	13.311	980	982	986	rBV4	27779	71919	1.44%	0.156%
40	13.459	992	995	996	rBV2	34885	51766	1.04%	0.112%
41	13.779	1020	1023	1029	rVB2	244471	353601	7.10%	0.767%
42	13.939	1035	1037	1040	rBV	1008158	1017583	20.42%	2.209%
43	14.099	1049	1051	1055	rVB	63589	90716	1.82%	0.197%
44	14.408	1076	1078	1084	rBV	78587	162112	3.25%	0.352%
45	14.694	1101	1103	1106	rBV2	69131	93853	1.88%	0.204%
46	15.357	1158	1161	1164	rBV	825532	1041115	20.89%	2.260%
47	15.757	1194	1196	1198	rBV	102429	137127	2.75%	0.298%
48	16.214	1234	1236	1242	rVB	107681	197084	3.95%	0.428%
49	16.362	1247	1249	1254	rVB3	66395	134243	2.69%	0.291%
50	16.751	1280	1283	1286	rVB	89818	185898	3.73%	0.403%

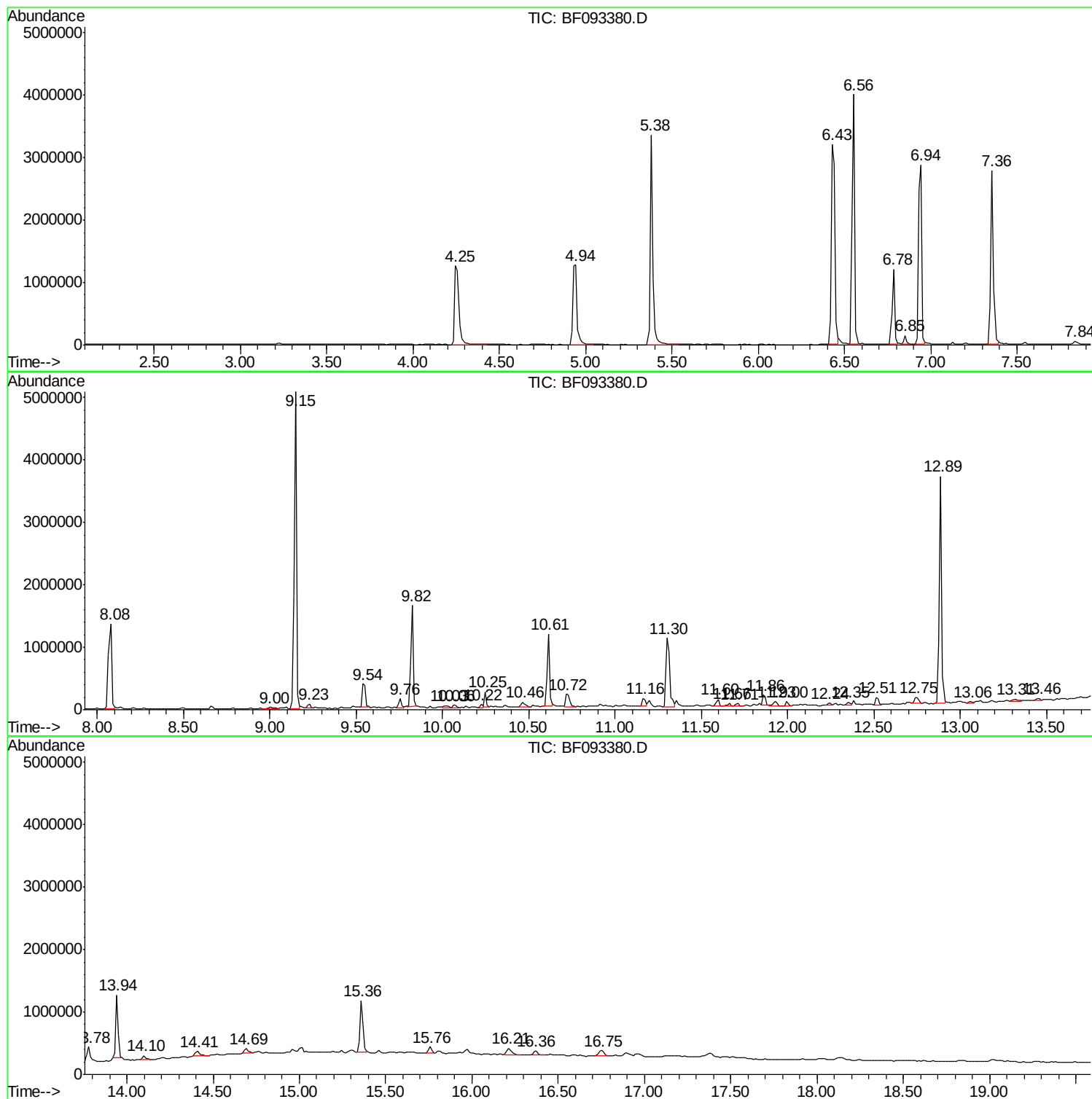
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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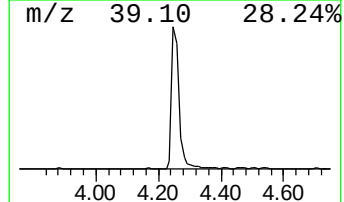
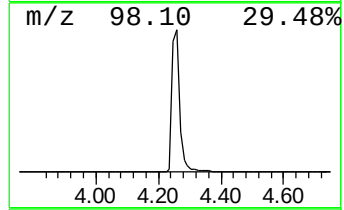
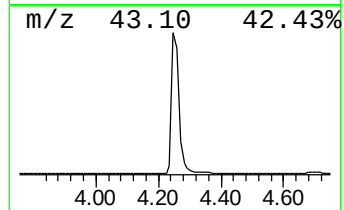
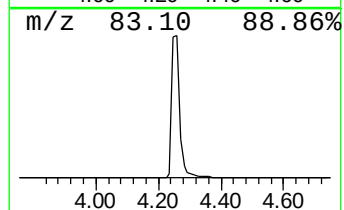
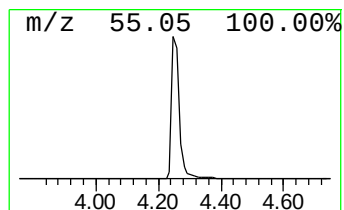
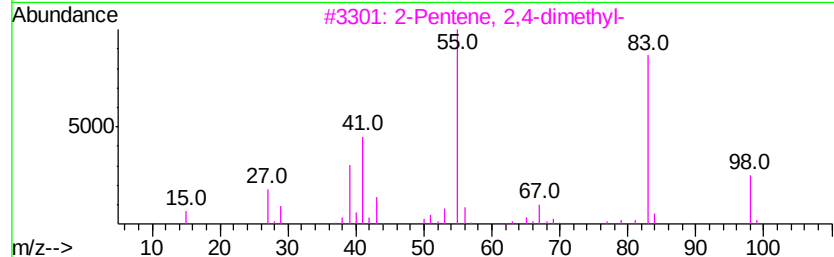
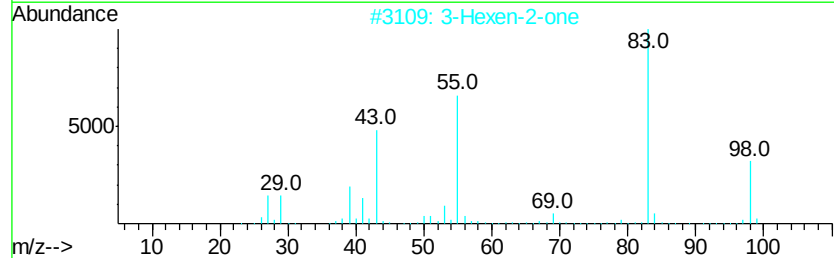
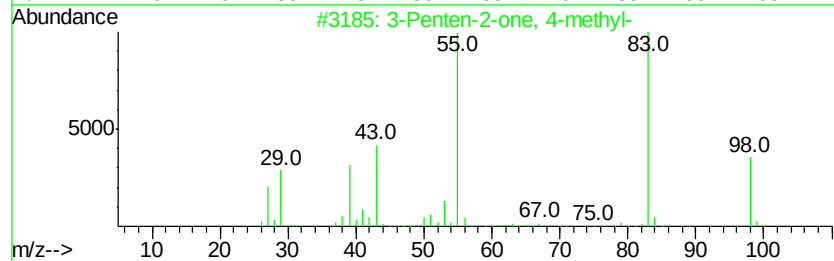
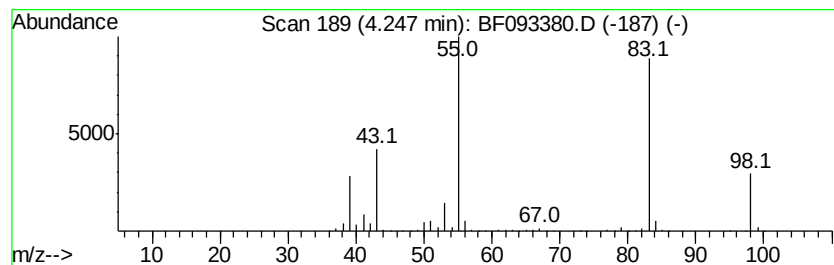
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	33.63 ng	2097320	1,4-Dichlorobenzene-d4	6.78

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	87
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



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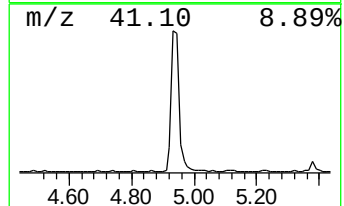
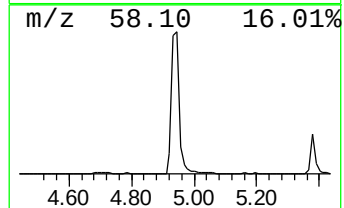
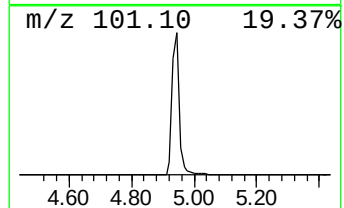
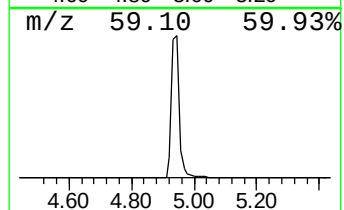
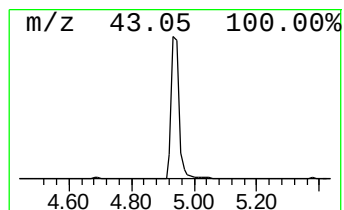
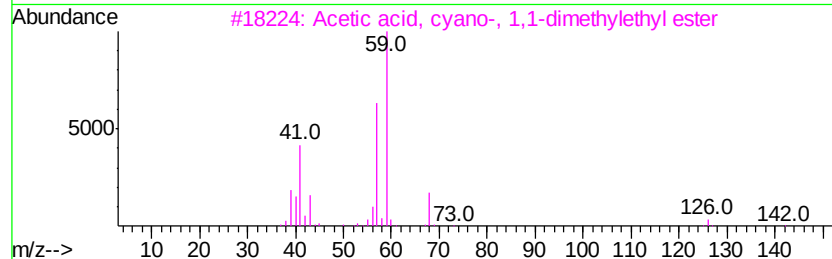
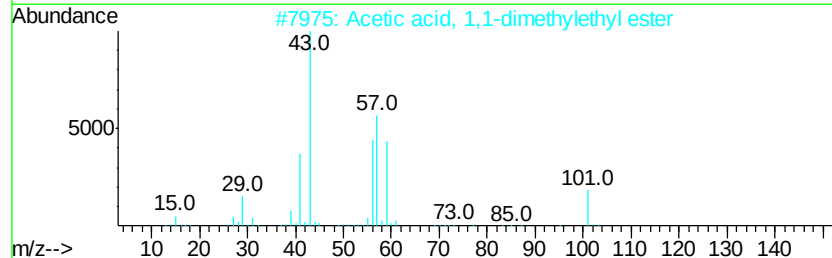
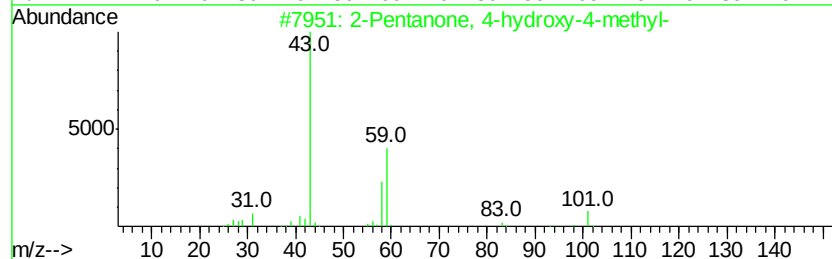
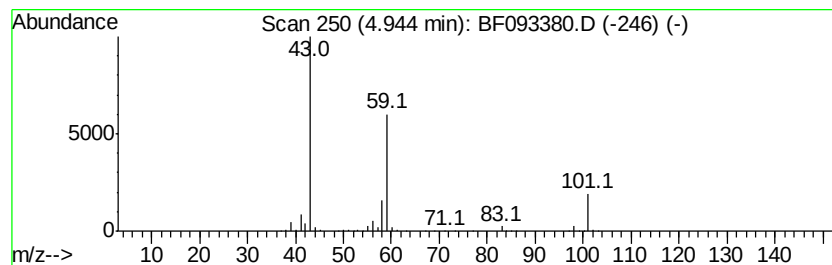
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	34.88 ng	2175090	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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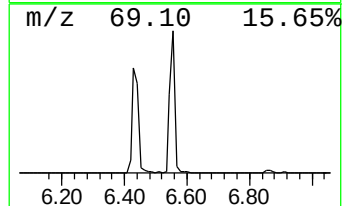
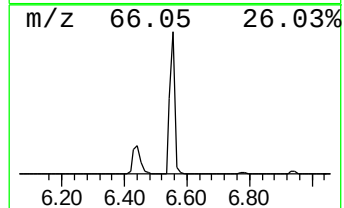
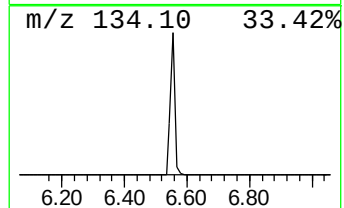
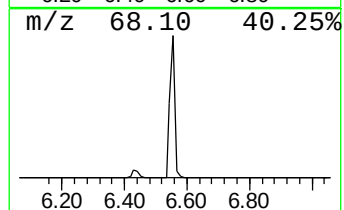
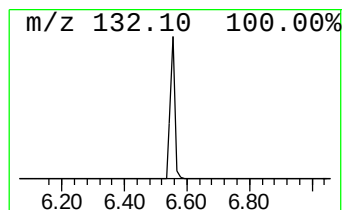
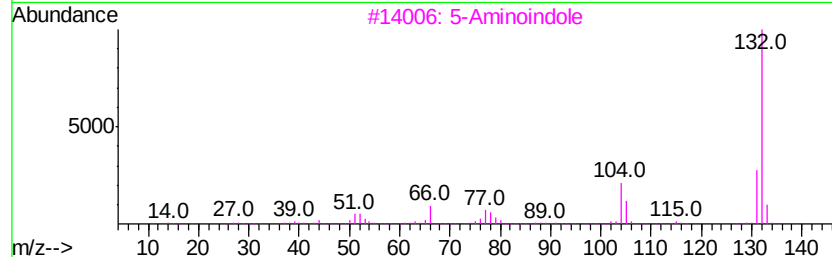
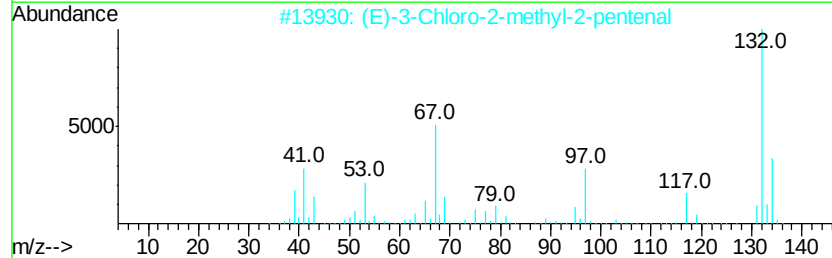
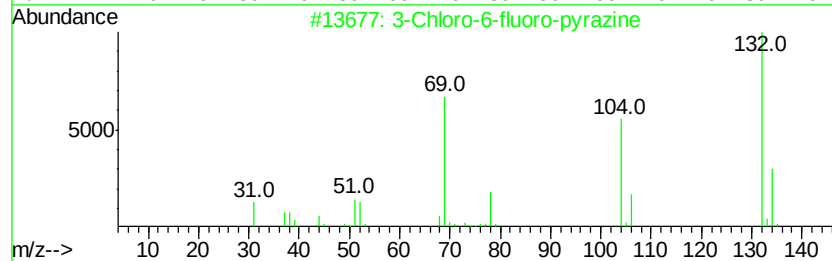
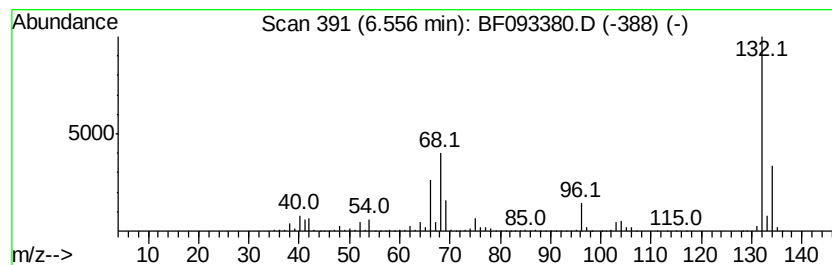
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	67.13 ng	4186400	1,4-Dichlorobenzene-d4	6.78

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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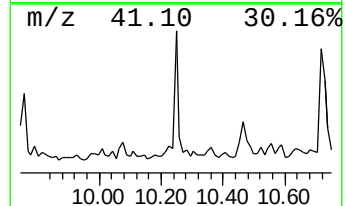
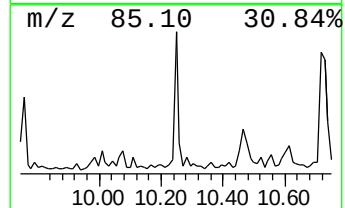
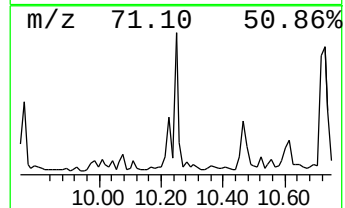
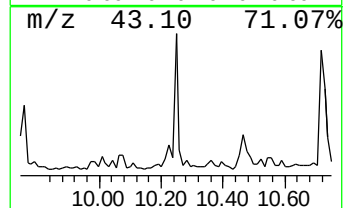
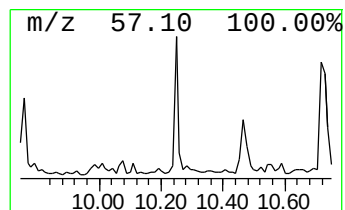
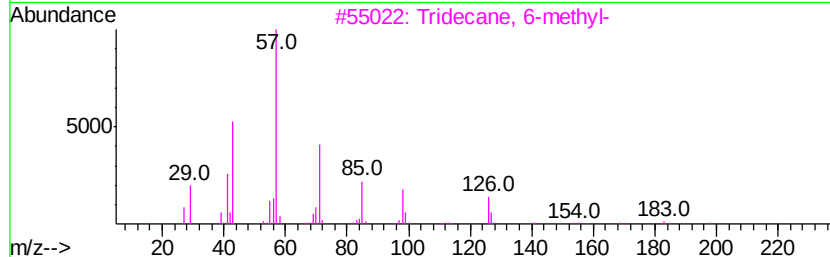
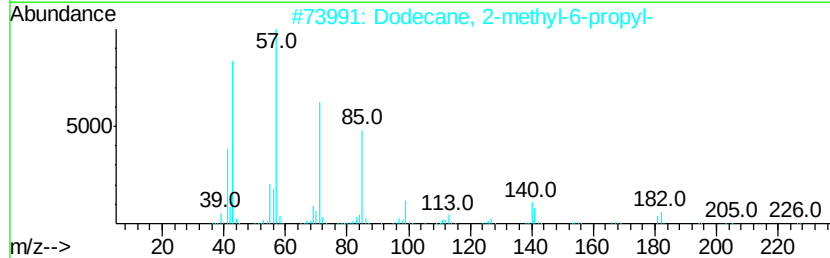
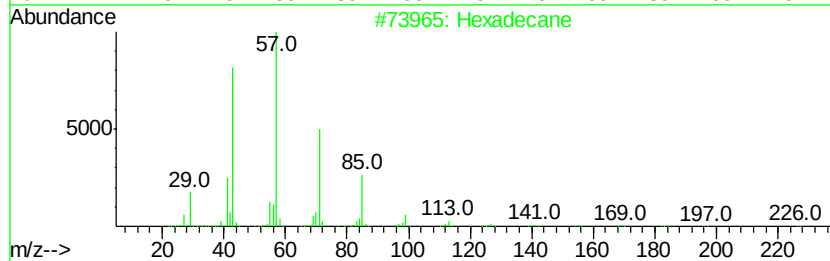
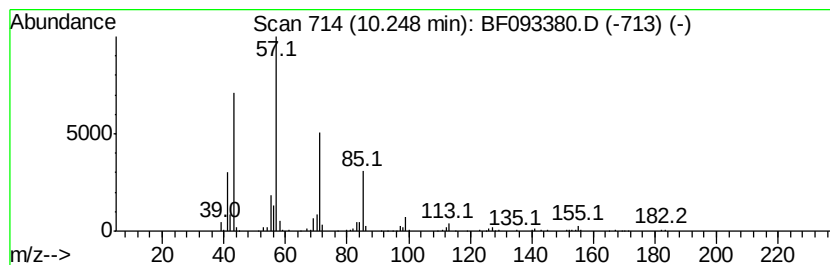
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.25	2.30 ng	188085	Acenaphthene-d10	9.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
4	Undecane, 2-methyl-	170	C12H26	007045-71-8	72
5	Pentadecane	212	C15H32	000629-62-9	72



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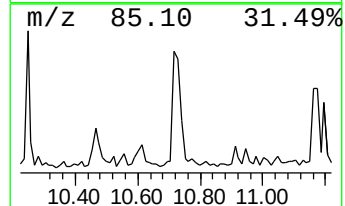
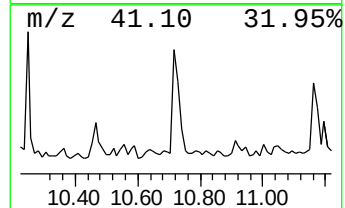
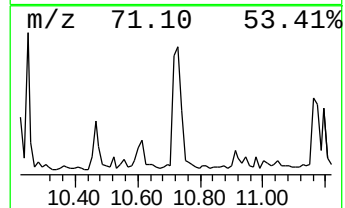
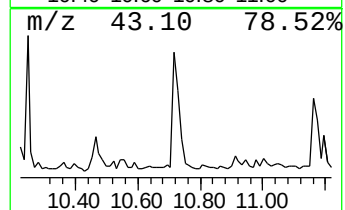
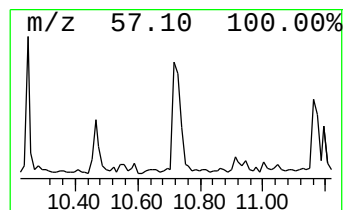
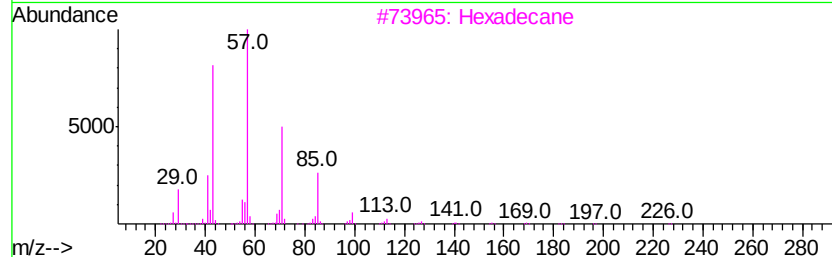
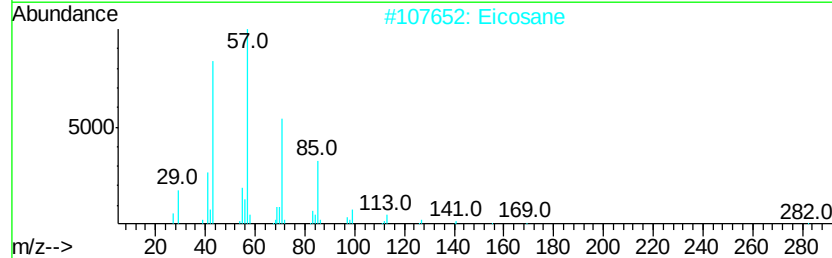
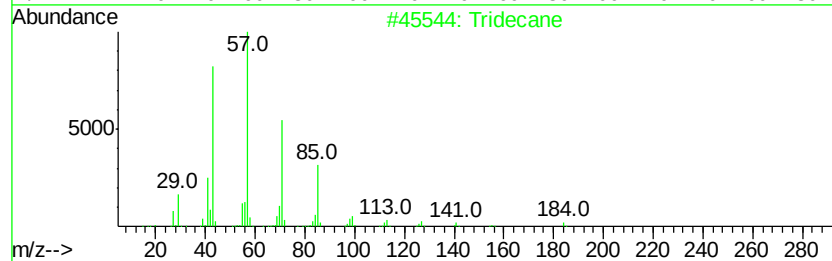
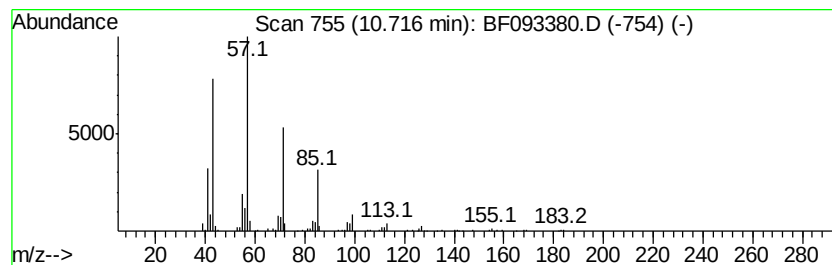
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C-3

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 6 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.72	4.50 ng	351613	Phenanthrene-d10		11.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Eicosane	282	C20H42	000112-95-8	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	90
5	Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093380.D
Acq On : 4 Mar 2017 1:08
Operator : SJ/MA
Sample : I2078-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

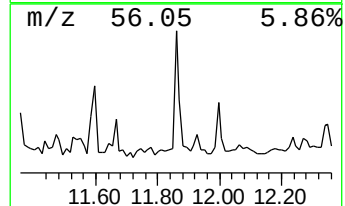
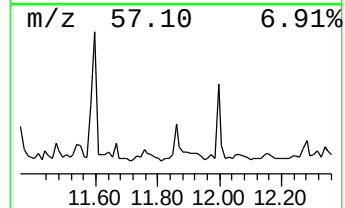
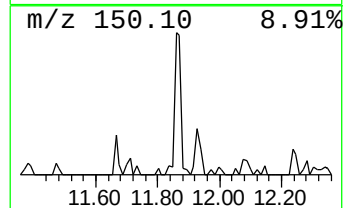
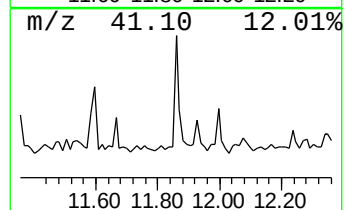
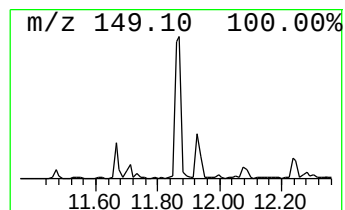
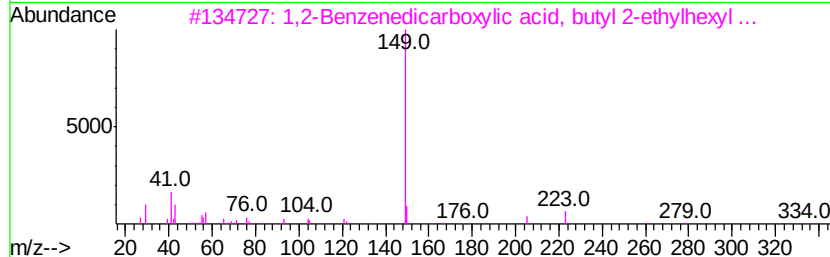
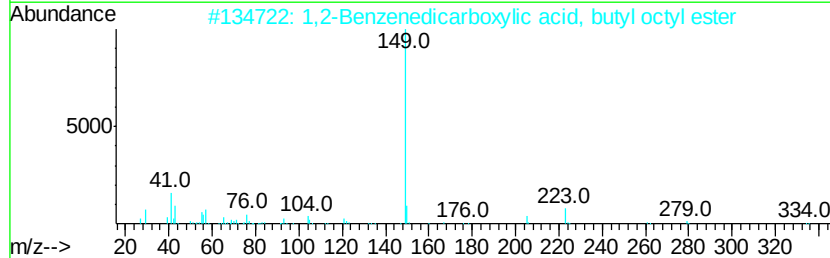
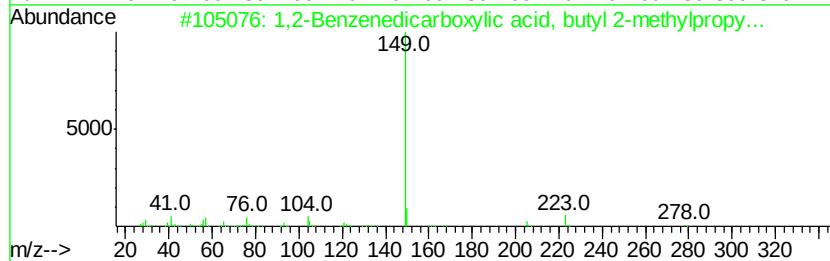
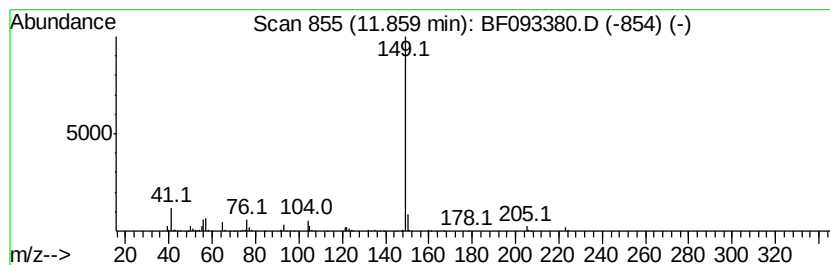
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.86	2.78 ng	217420	Phenanthrene-d10	11.30		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	90	
2	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	83	
3	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	83	
4	Dibutyl phthalate	278	C16H22O4	000084-74-2	83	
5	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	78	



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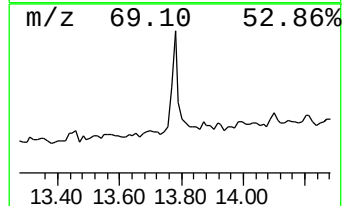
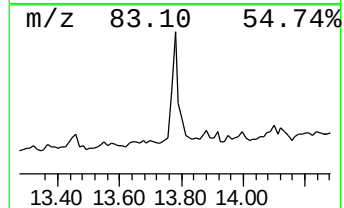
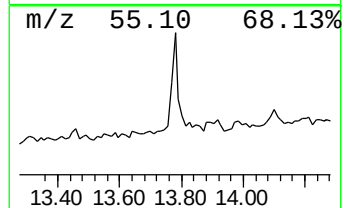
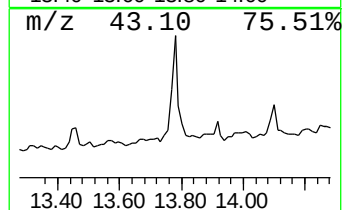
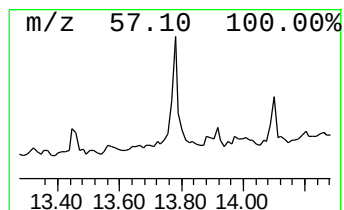
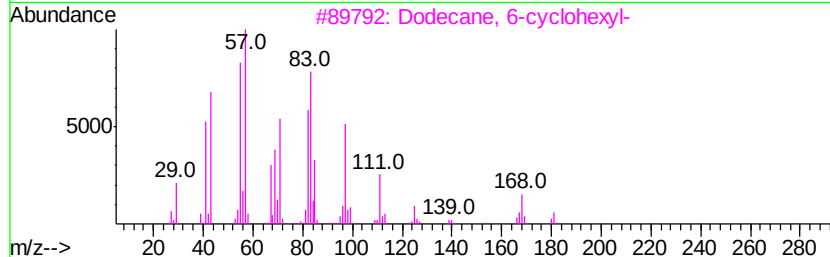
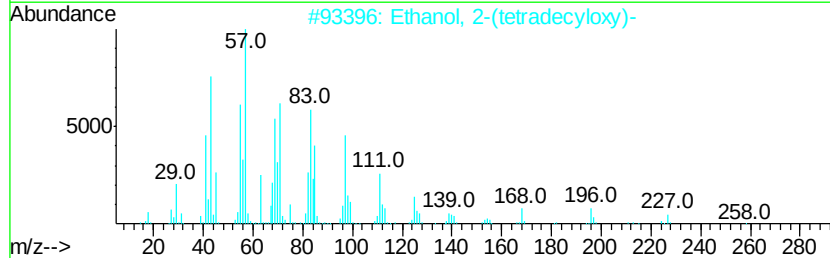
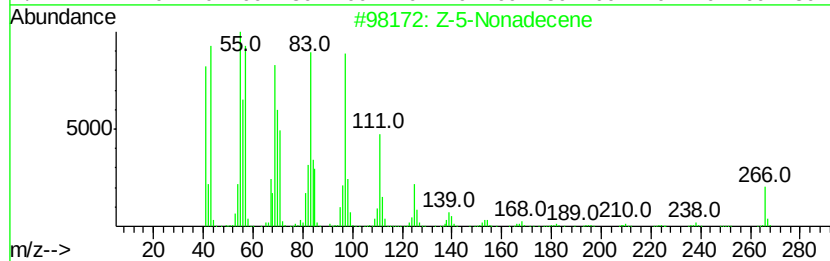
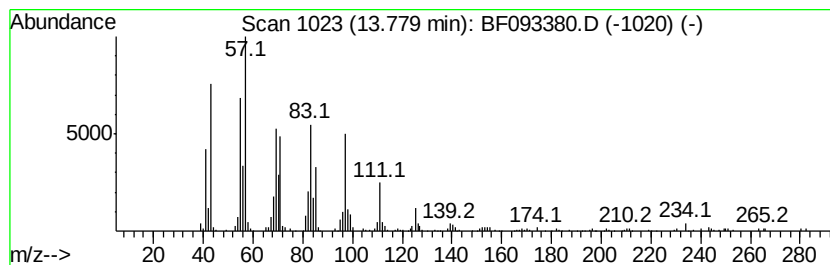
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Z-5-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.78	6.95 ng	353601	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	93
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	91
4	Heptafluorobutanoic acid, heptadecyl-	452	C21H35F7O2	1000282-97-3	91
5	Heptafluorobutyric acid, n-octadecyl-	466	C22H37F7O2	000400-57-7	91



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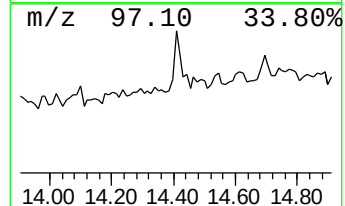
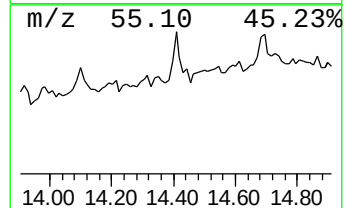
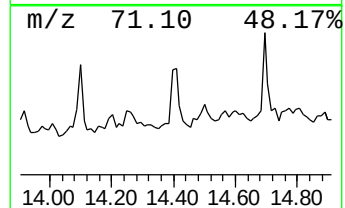
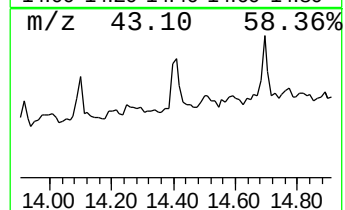
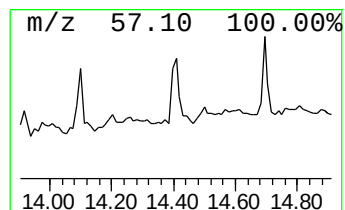
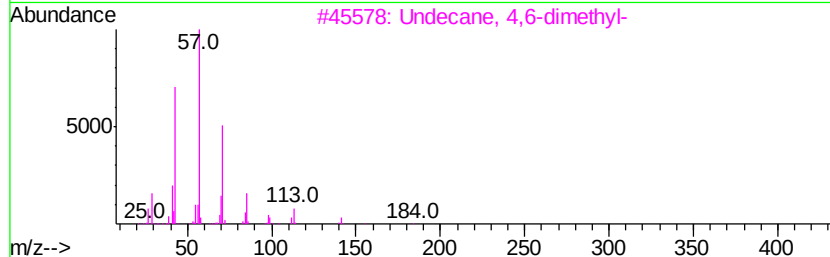
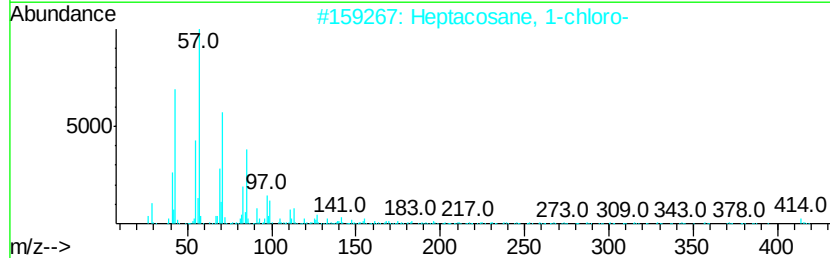
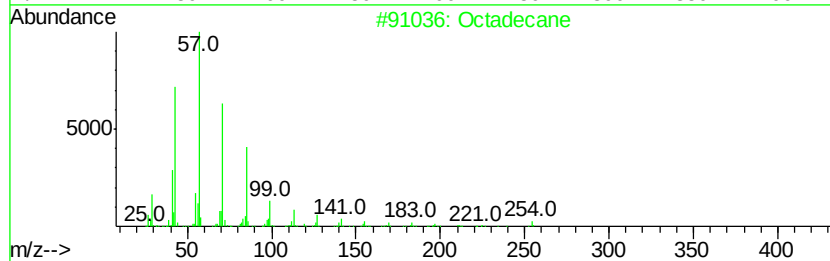
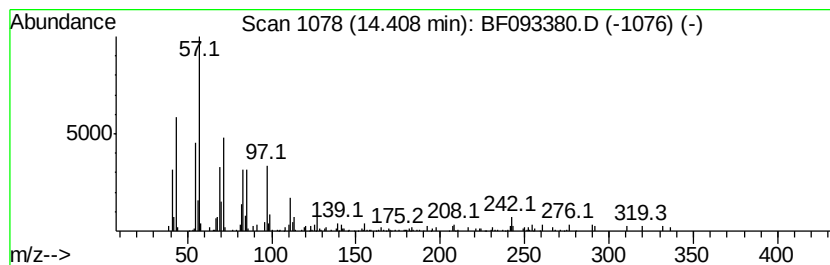
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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Peak Number 12 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	3.19 ng	162112	Chrysene-d12	13.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane		254 C18H38	000593-45-3 90
2	Heptacosane, 1-chloro-		414 C27H55Cl	062016-79-9 58
3	Undecane, 4,6-dimethyl-		184 C13H28	017312-82-2 50
4	Eicosane		282 C20H42	000112-95-8 46
5	Tetradecane		198 C14H30	000629-59-4 46



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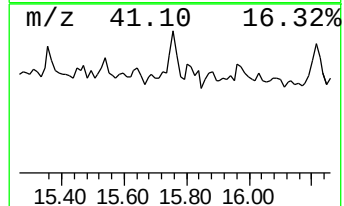
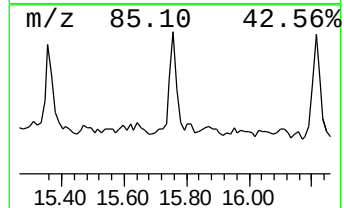
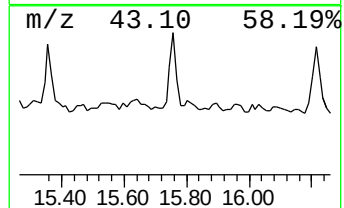
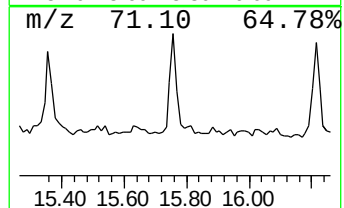
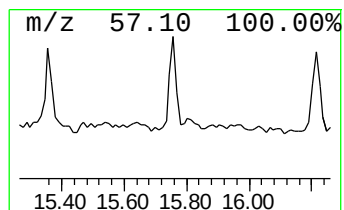
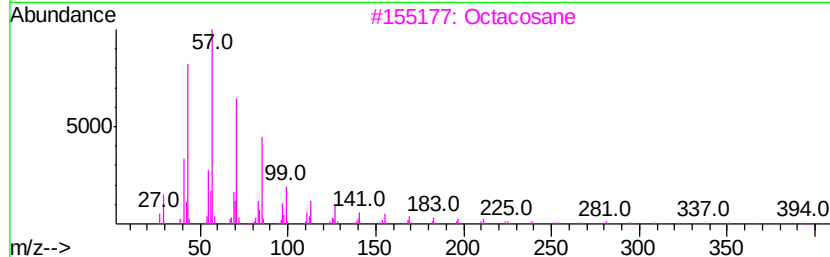
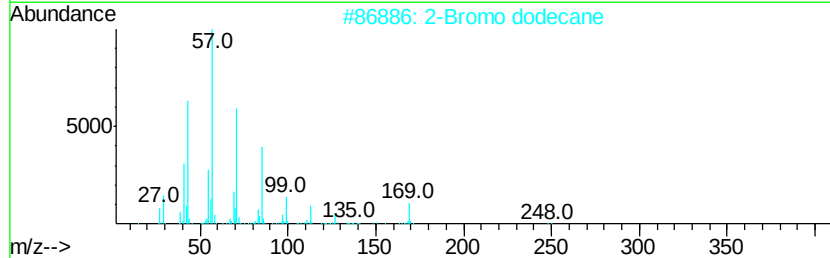
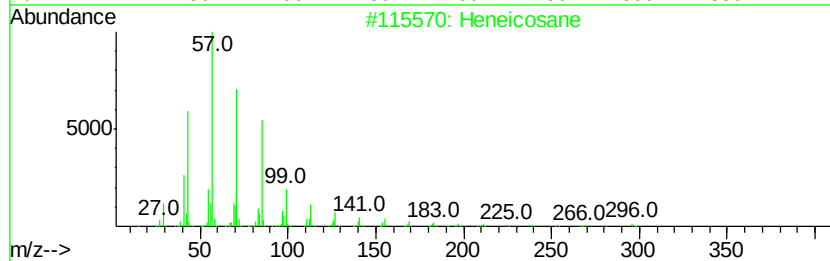
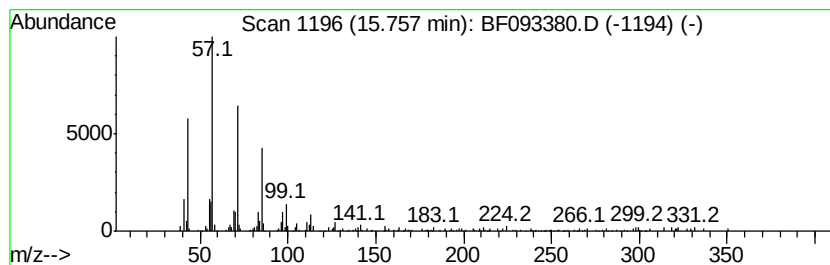
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 13 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	2.63 ng	137127	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	94
2		2-Bromo dodecane	248	C12H25Br	013187-99-0	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Tetratetracontane	619	C44H90	007098-22-8	86
5		Tetracosane	338	C24H50	000646-31-1	86



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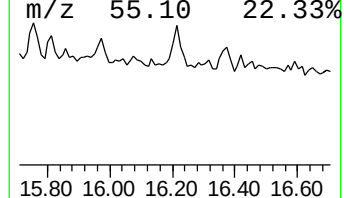
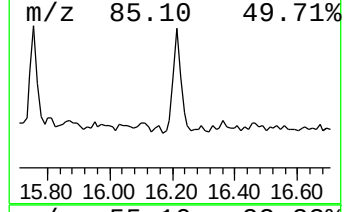
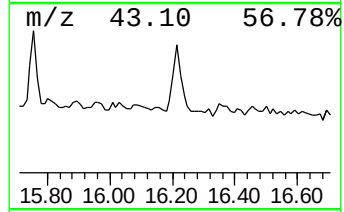
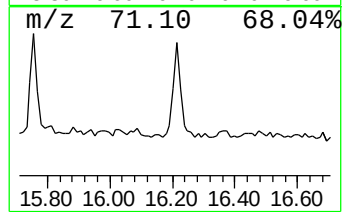
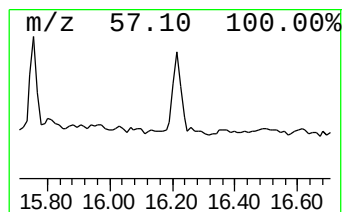
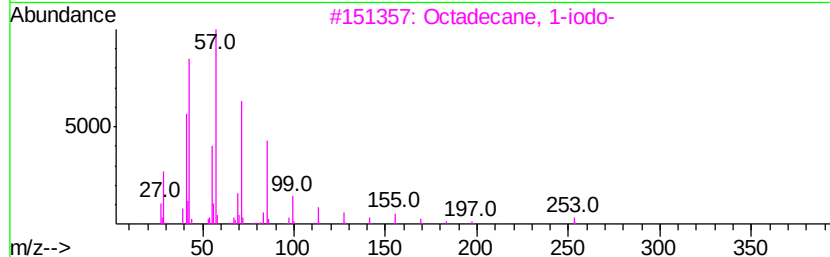
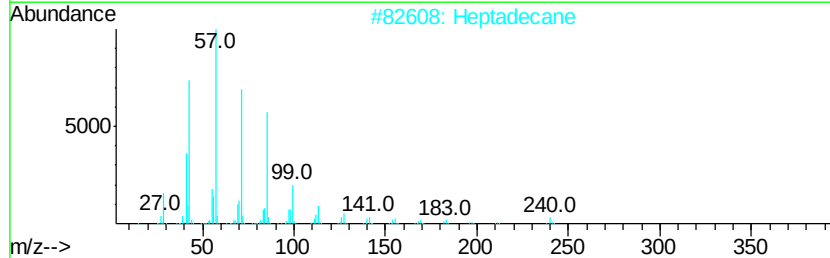
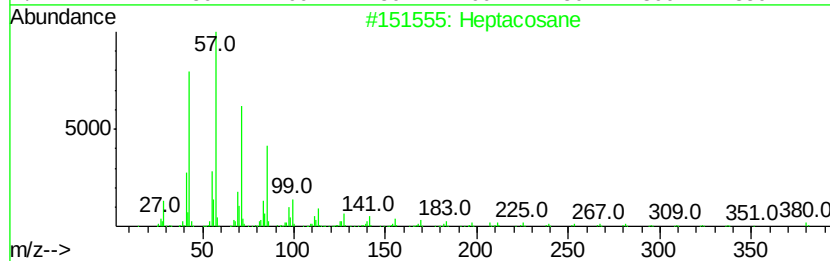
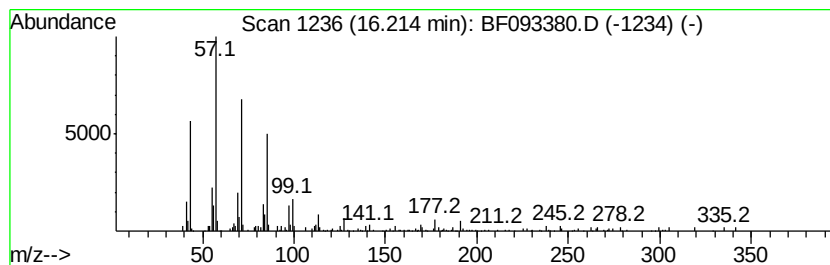
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	3.79 ng	197084	Perylene-d12	15.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	86
2			Heptadecane	240	C17H36	000629-78-7	80
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
5			2-Bromo dodecane	248	C12H25Br	013187-99-0	80



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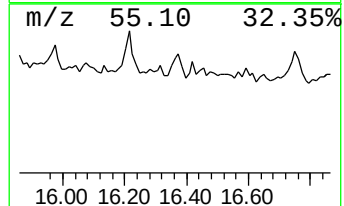
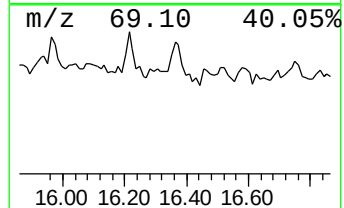
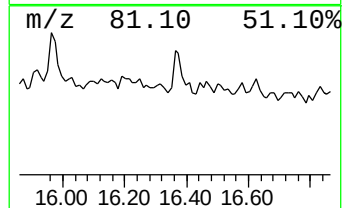
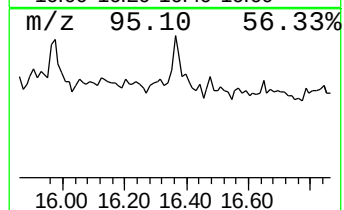
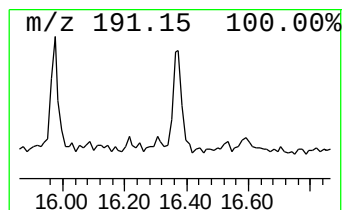
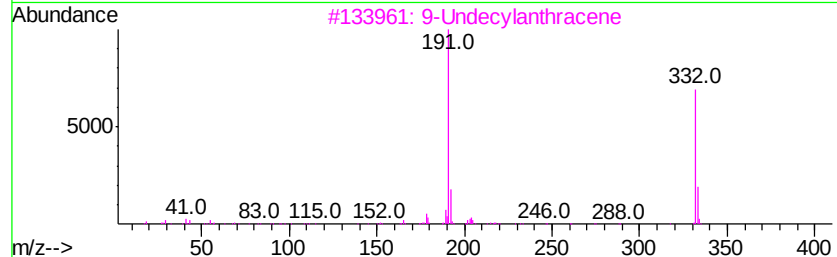
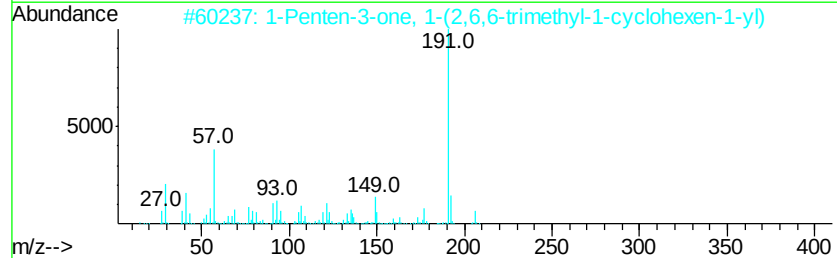
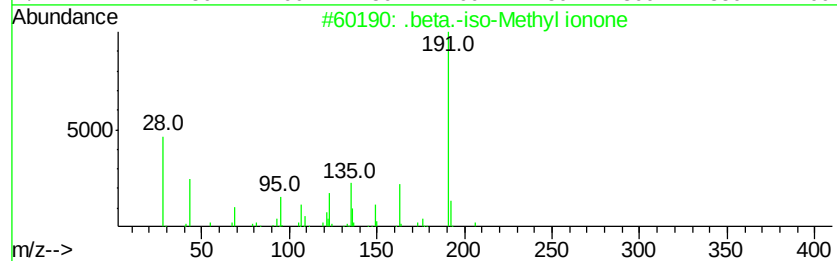
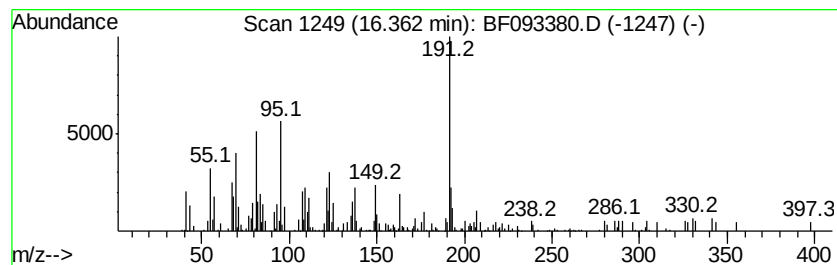
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown16.36 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	2.58 ng	134243	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	40
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
3		9-Undecylantracene	332	C25H32	132034-75-4	27
4		Amiphenazole	191	C9H9N3S	000490-55-1	27
5		2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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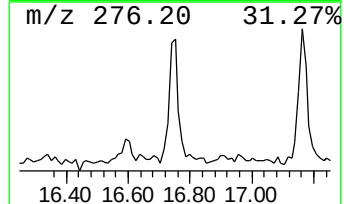
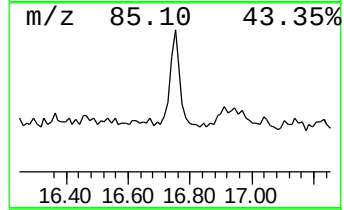
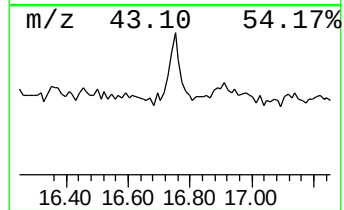
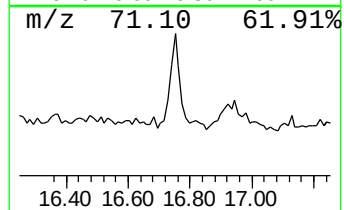
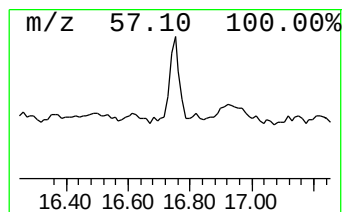
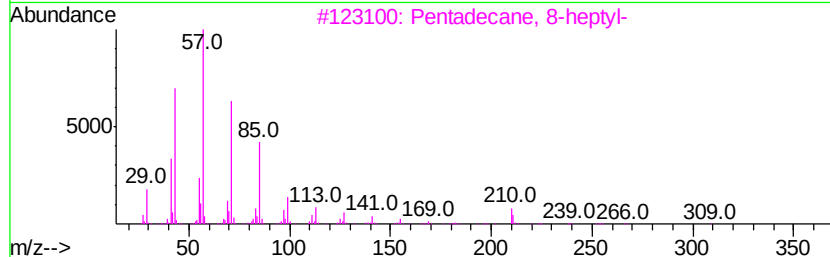
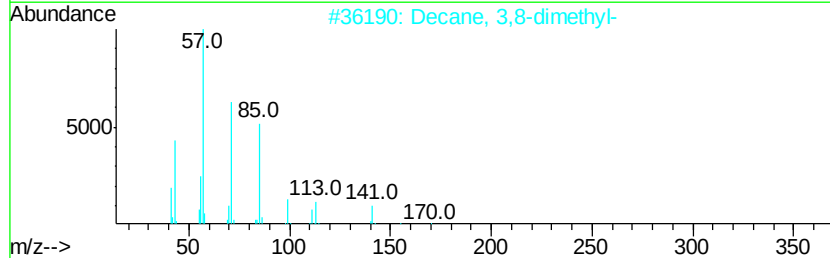
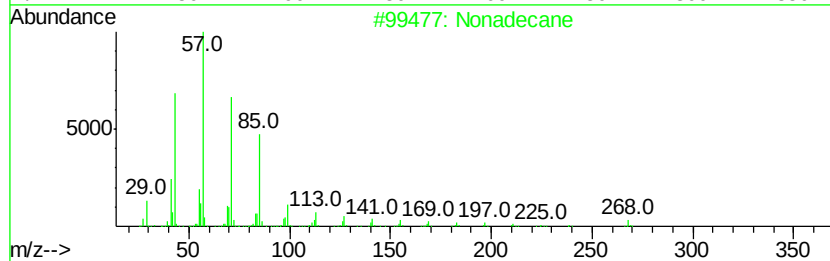
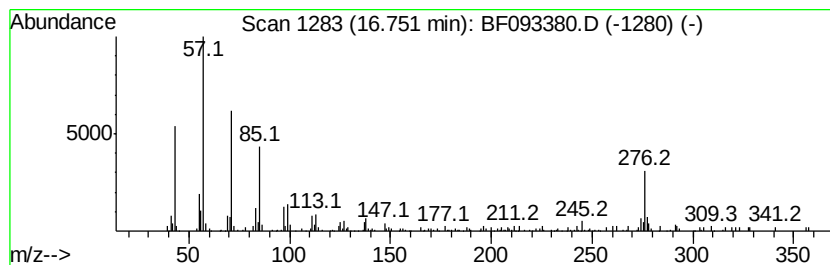
Instrument :
BNA_F
ClientSampleId :
C-3

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 16 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	3.57 ng	185898	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane	268 C19H40	000629-92-5	78
2	Decane, 3,8-dimethyl-	170 C12H26	017312-55-9	60
3	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	52
4	Tricosane, 2-methyl-	338 C24H50	001928-30-9	50
5	Tetratriacontane	479 C34H70	014167-59-0	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
 Data File : BF093380.D
 Acq On : 4 Mar 2017 1:08
 Operator : SJ/MA
 Sample : I2078-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-3

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, 4...	4.25	33.6	ng	2097320	1	6.78	1247250	20.0
2-Pentanone, 4-hy...	4.94	34.9	ng	2175090	1	6.78	1247250	20.0
unknown6.56	6.56	67.1	ng	4186400	1	6.78	1247250	20.0
Hexadecane	10.25	2.3	ng	188085	3	9.82	1634280	20.0
Tridecane	10.72	4.5	ng	351613	4	11.30	1562940	20.0
1,2-Benzenedicarb...	11.86	2.8	ng	217420	4	11.30	1562940	20.0
Z-5-Nonadecene	13.78	7.0	ng	353601	5	13.94	1017580	20.0
Octadecane	14.41	3.2	ng	162112	5	13.94	1017580	20.0
Heneicosane	15.76	2.6	ng	137127	6	15.36	1041120	20.0
Heptacosane	16.21	3.8	ng	197084	6	15.36	1041120	20.0
unknown16.36	16.36	2.6	ng	134243	6	15.36	1041120	20.0
Nonadecane	16.75	3.6	ng	185898	6	15.36	1041120	20.0