

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
 Data File : BF093378.D
 Acq On : 4 Mar 2017 00:13
 Operator : SJ/MA
 Sample : I2078-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-1

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	4.258	187	190	207	rBV	192371	351335	6.64%	0.740%
2	4.944	247	250	262	rBV	750311	1339513	25.30%	2.820%
3	5.379	286	288	302	rBV	4133544	4458659	84.21%	9.388%
4	6.441	378	381	383	rBV	3481161	5236965	98.91%	11.026%
5	6.556	388	391	393	rBV	4620369	4754776	89.81%	10.011%
6	6.784	408	411	413	rBV	1183837	1249920	23.61%	2.632%
7	6.853	415	417	419	rVB	133640	124401	2.35%	0.262%
8	6.933	422	424	427	rBV	2793081	3700734	69.90%	7.792%
9	7.356	458	461	463	rBV	3149246	3133140	59.18%	6.597%
10	7.836	497	503	511	rBV	137719	265902	5.02%	0.560%
11	8.076	521	524	526	rBV	1248013	1679237	31.72%	3.536%
12	9.002	602	605	609	rVB	59362	84550	1.60%	0.178%
13	9.150	615	618	620	rBV	4989099	5294543	100.00%	11.148%
14	9.219	622	624	626	rVB	37379	55811	1.05%	0.118%
15	9.539	650	652	655	rBV	345375	460649	8.70%	0.970%
16	9.756	669	671	673	rBV2	93728	126172	2.38%	0.266%
17	9.825	674	677	679	rVV	1598007	1660240	31.36%	3.496%
18	10.248	713	714	716	rVB	163761	129553	2.45%	0.273%
19	10.465	731	733	737	rBV	57300	93849	1.77%	0.198%
20	10.613	743	746	748	rBV	2092400	2123590	40.11%	4.471%
21	10.716	754	755	760	rVB2	176868	308619	5.83%	0.650%
22	10.785	760	761	763	rBV	57315	86149	1.63%	0.181%
23	10.819	763	764	766	rVV2	75267	103678	1.96%	0.218%
24	10.853	766	767	771	rVV2	79074	130758	2.47%	0.275%
25	10.922	771	773	776	rVV3	44386	115592	2.18%	0.243%
26	10.968	776	777	779	rVB2	60958	61120	1.15%	0.129%
27	11.002	779	780	783	rBV	82581	114263	2.16%	0.241%
28	11.162	792	794	801	rBV2	122824	219618	4.15%	0.462%
29	11.299	804	806	810	rBV	1356415	1772340	33.47%	3.732%
30	11.596	830	832	833	rBV	90461	96013	1.81%	0.202%
31	11.711	840	842	843	rBV	59891	66537	1.26%	0.140%
32	11.859	854	855	858	rVB	179414	214807	4.06%	0.452%
33	11.928	859	861	863	rVB2	69140	102642	1.94%	0.216%
34	12.351	896	898	900	rBV2	43491	61754	1.17%	0.130%

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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

35	12.522	911	913	915	rBV	149181	192267	3.63%	0.405%
36	12.751	930	933	935	rVB	110510	175585	3.32%	0.370%
37	12.888	942	945	948	rBV	3819299	3830075	72.34%	8.064%
38	13.334	980	984	985	rBV4	39222	101703	1.92%	0.214%
39	13.779	1020	1023	1028	rVB2	318959	410997	7.76%	0.865%
40	13.939	1035	1037	1040	rBV	1111181	1128071	21.31%	2.375%
41	14.408	1073	1078	1085	rBV2	189856	714318	13.49%	1.504%
42	15.357	1158	1161	1164	rBV	830372	1038251	19.61%	2.186%
43	16.751	1280	1283	1286	rBV2	59967	125930	2.38%	0.265%

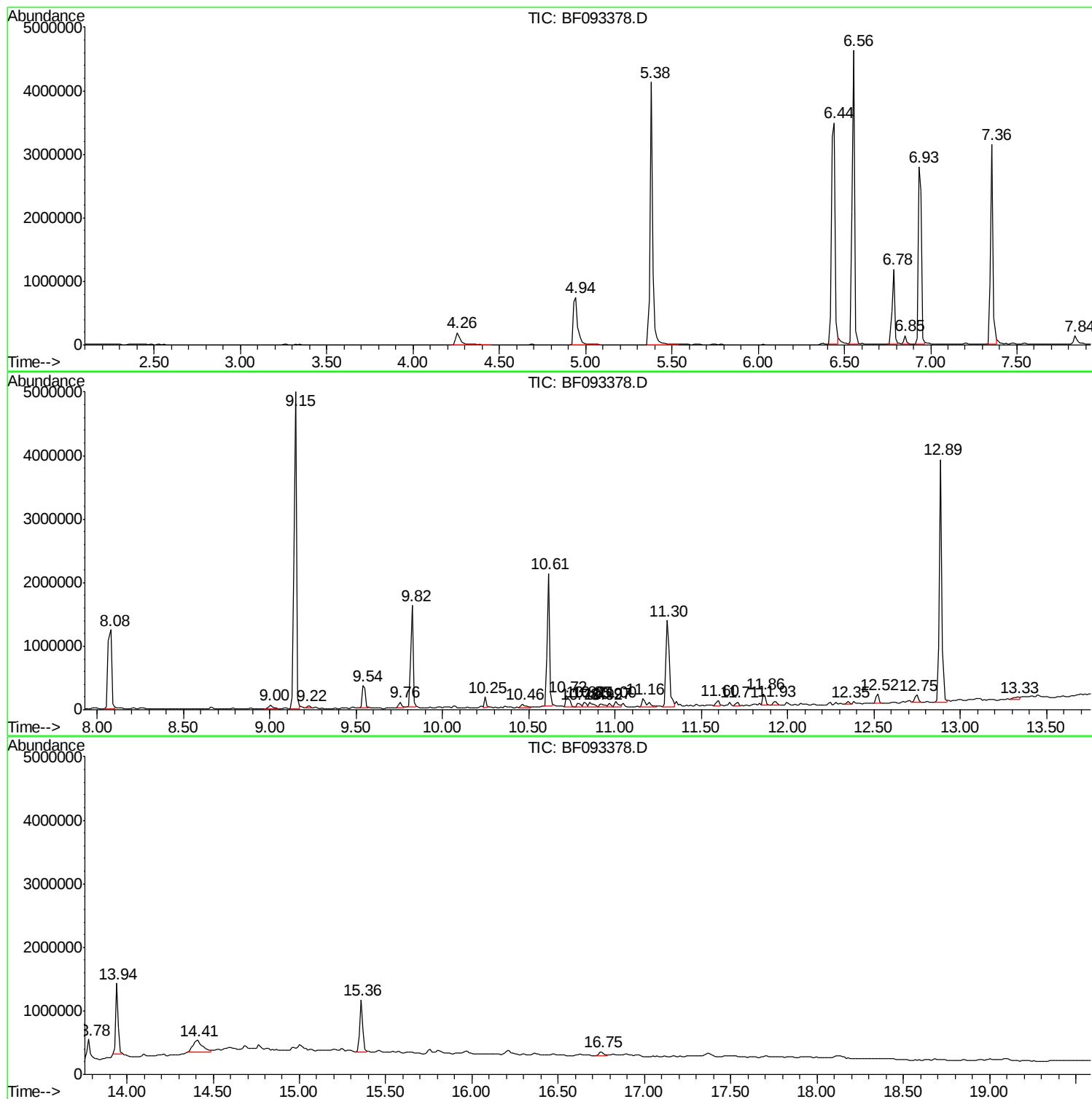
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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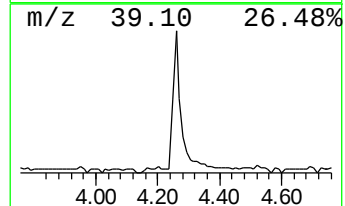
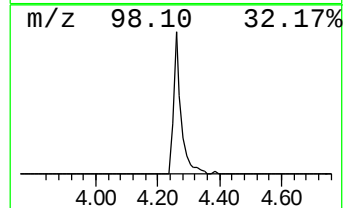
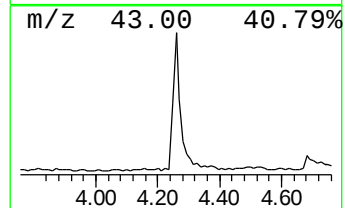
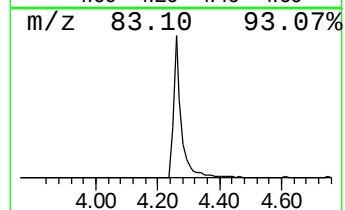
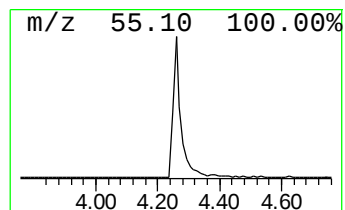
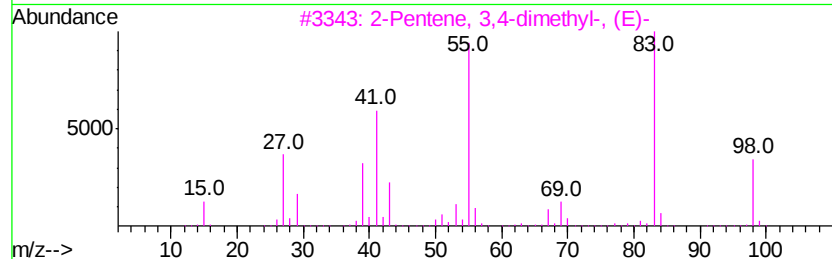
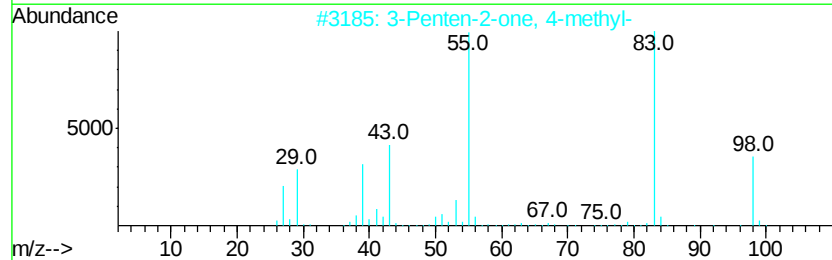
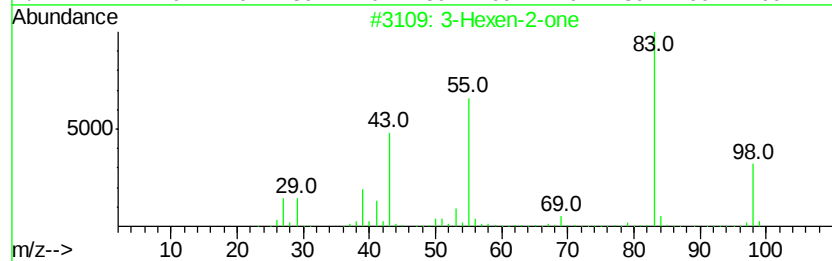
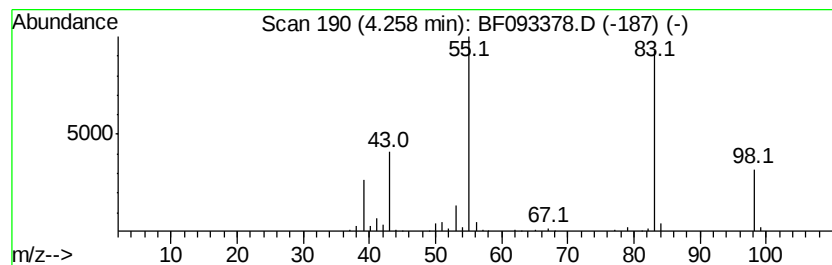
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	5.62 ng	351335	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	90
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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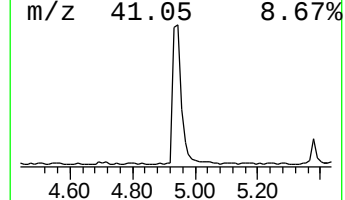
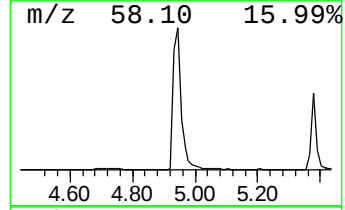
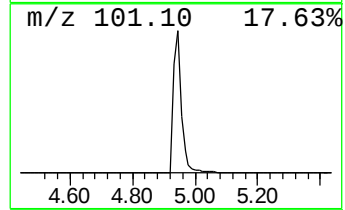
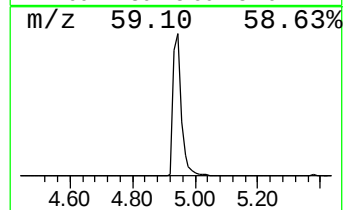
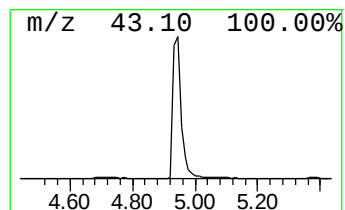
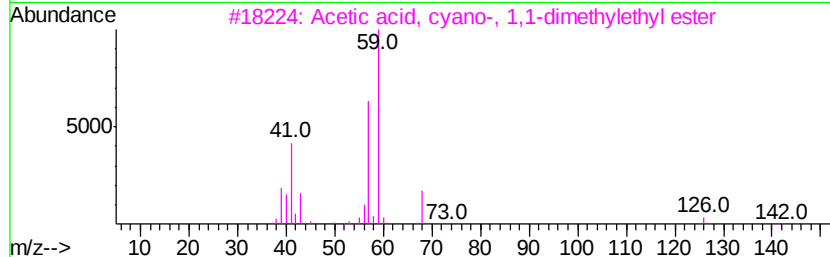
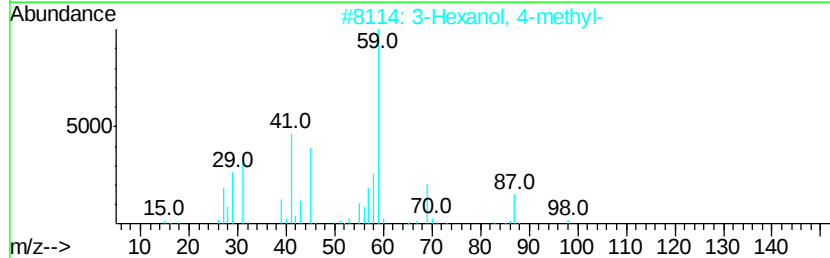
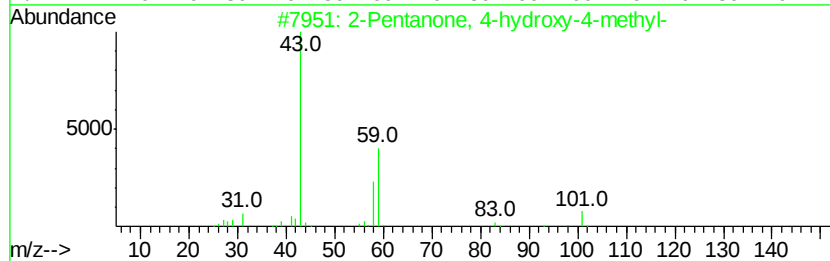
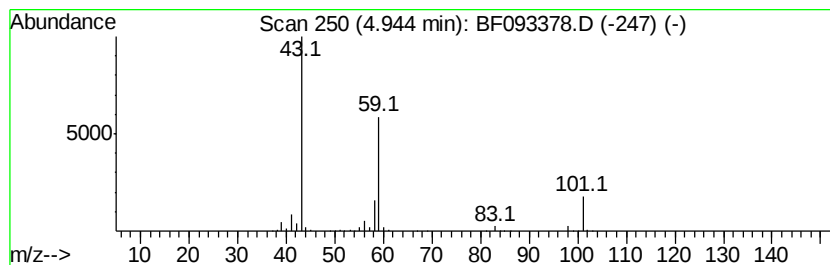
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	21.43 ng	1339510	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	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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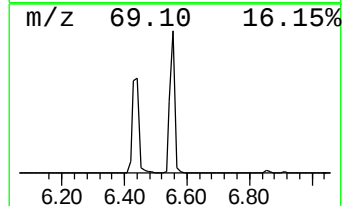
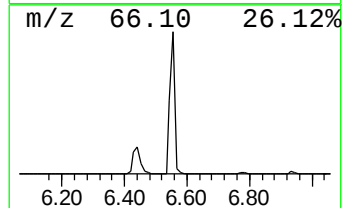
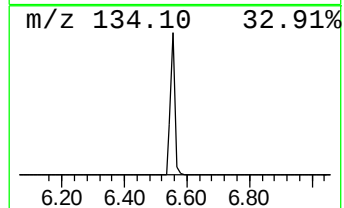
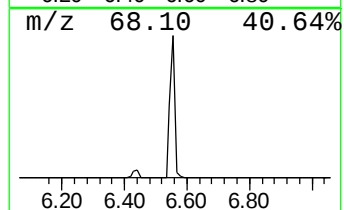
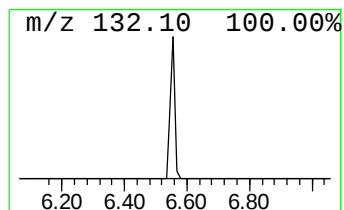
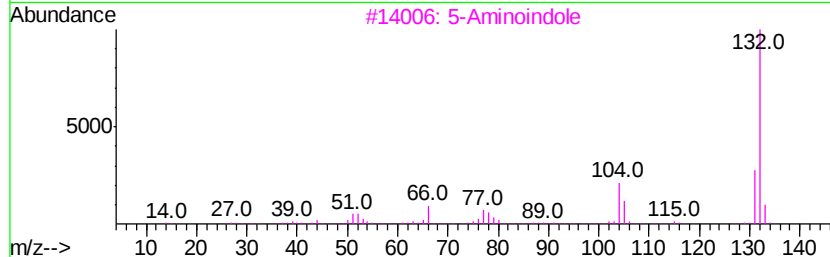
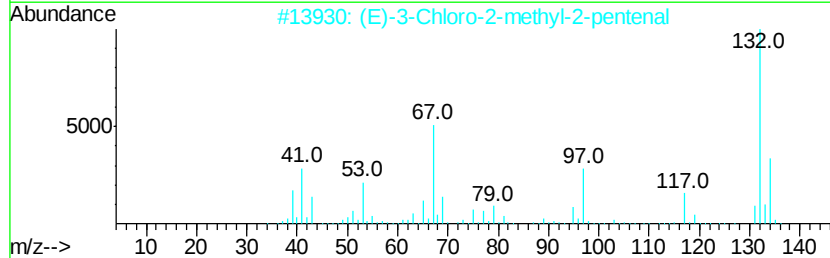
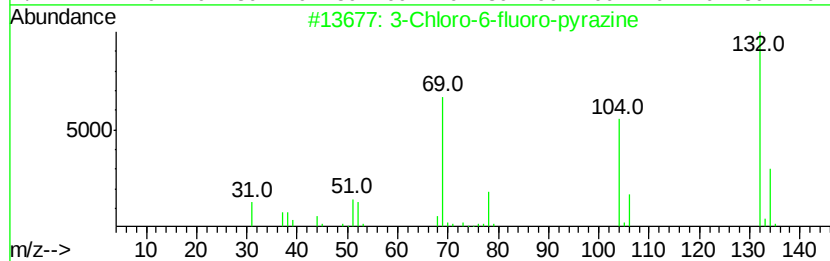
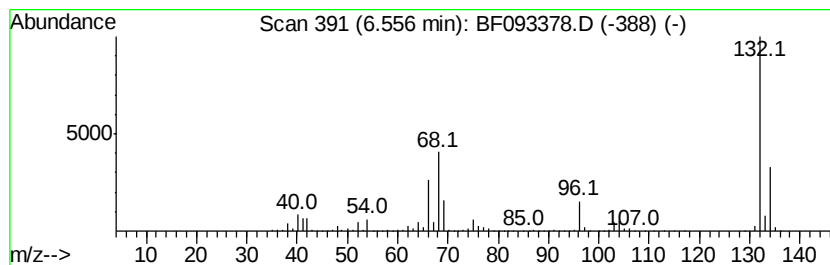
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	76.08 ng	4754780	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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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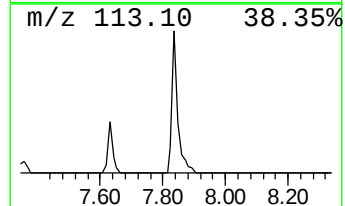
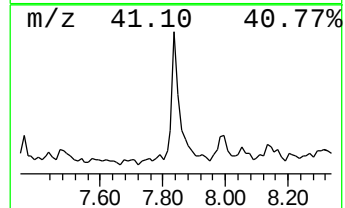
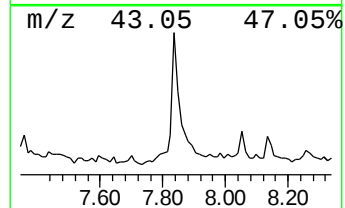
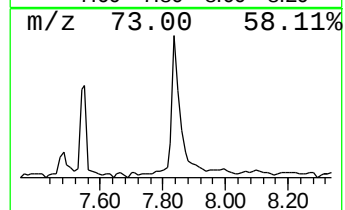
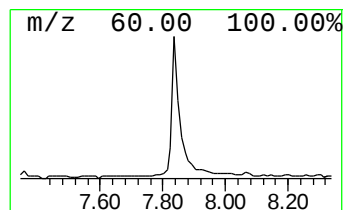
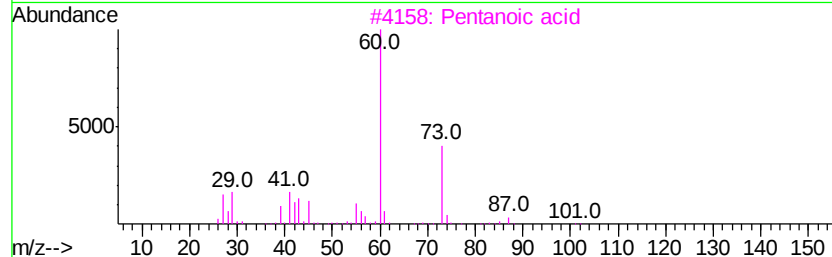
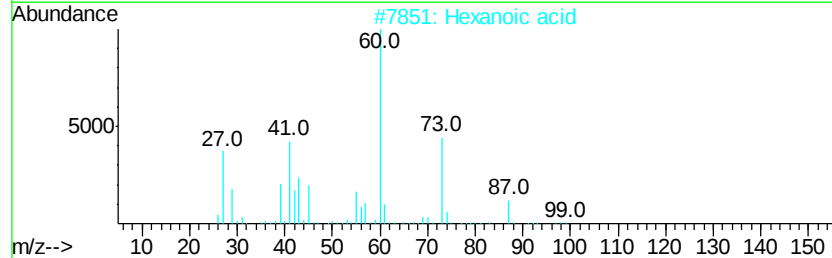
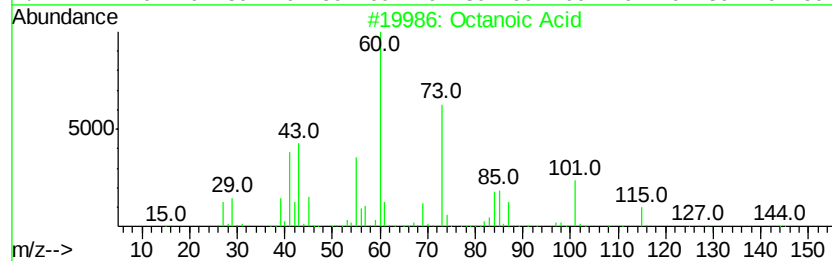
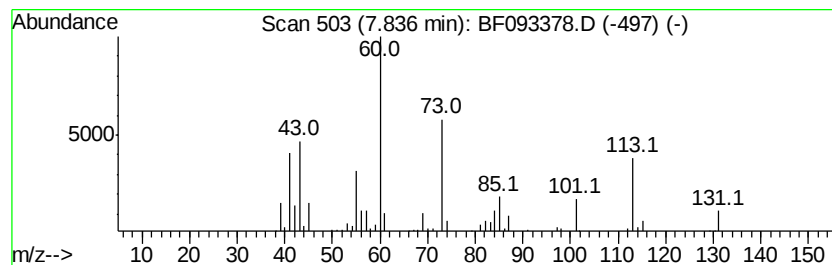
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octanoic Acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	3.17 ng	265902	Naphthalene-d8	8.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic Acid		144	C8H16O2	000124-07-2	58
2	Hexanoic acid		116	C6H12O2	000142-62-1	47
3	Pentanoic acid		102	C5H10O2	000109-52-4	43
4	Propanedioic acid, propyl-		146	C6H10O4	000616-62-6	38
5	Heptanoic acid		130	C7H14O2	000111-14-8	37



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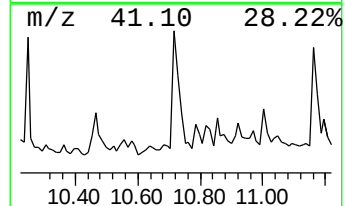
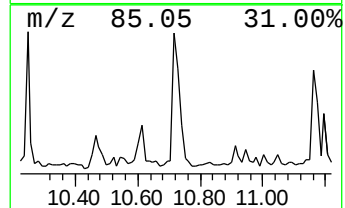
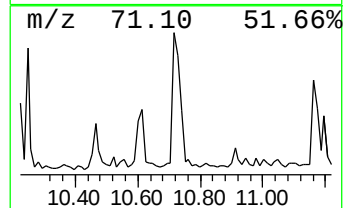
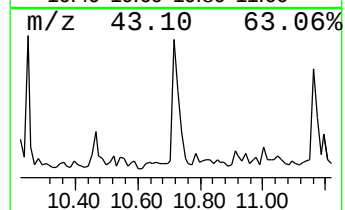
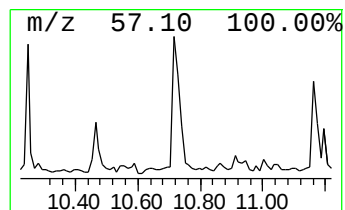
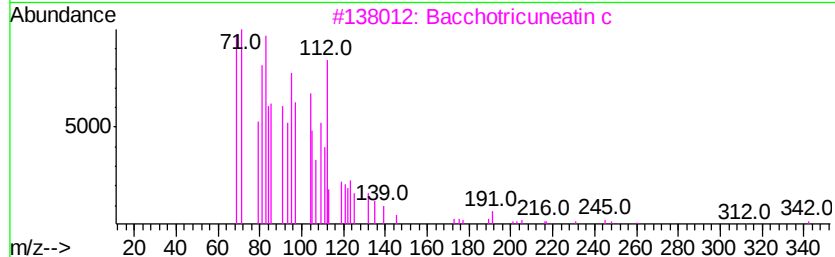
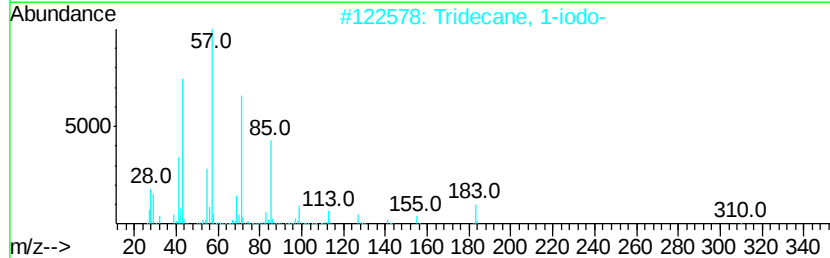
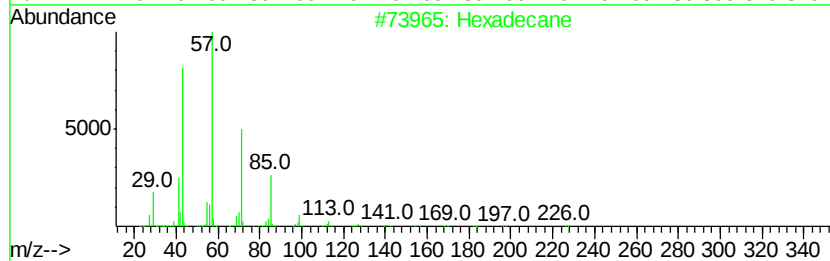
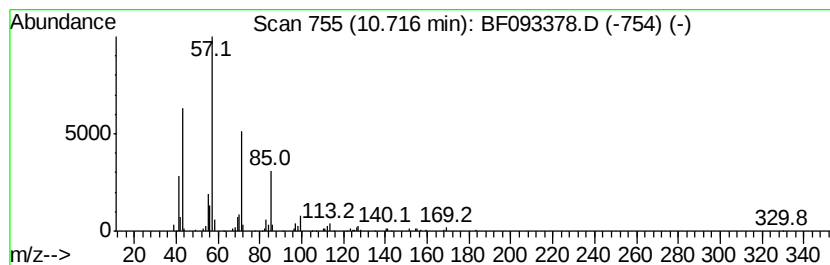
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.72	3.48 ng	308619	Phenanthrene-d10		11.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	78
3	Bacchotricuneatin c	342	C20H22O5	066563-30-2	72
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
5	triacontane	422	C30H62	000638-68-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093378.D
Acq On : 4 Mar 2017 00:13
Operator : SJ/MA
Sample : I2078-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-1

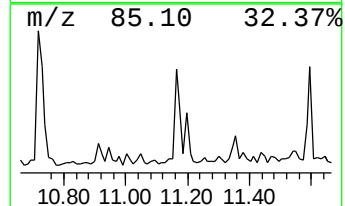
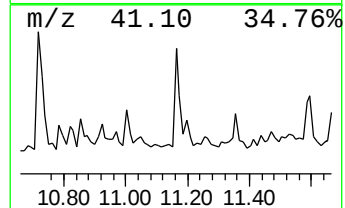
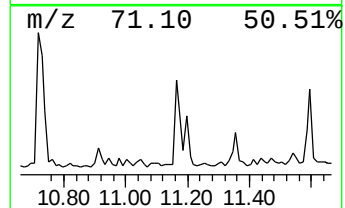
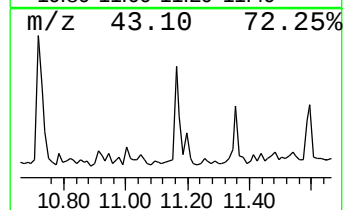
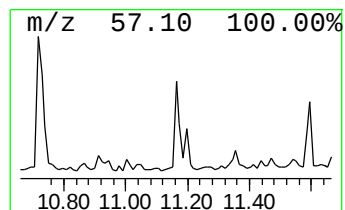
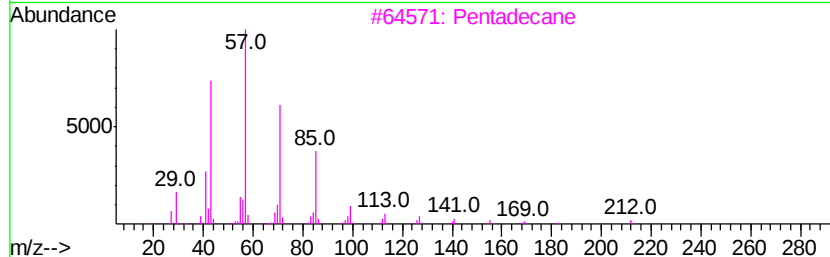
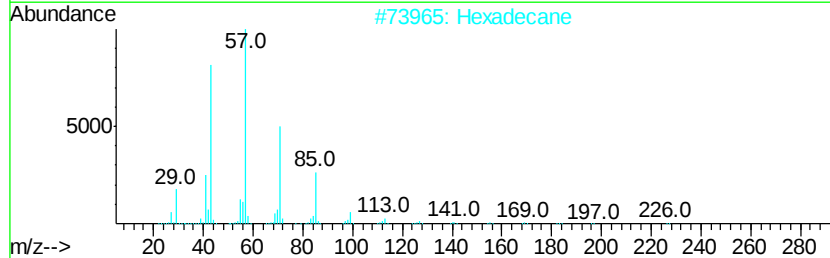
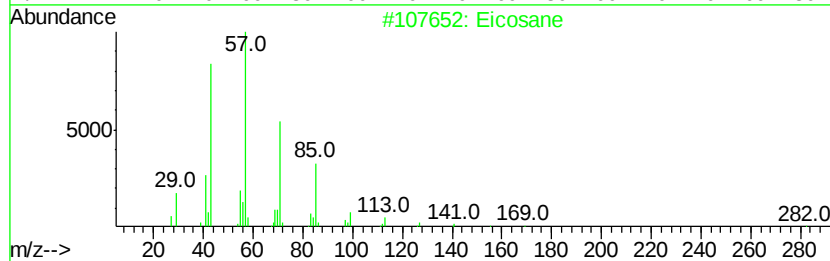
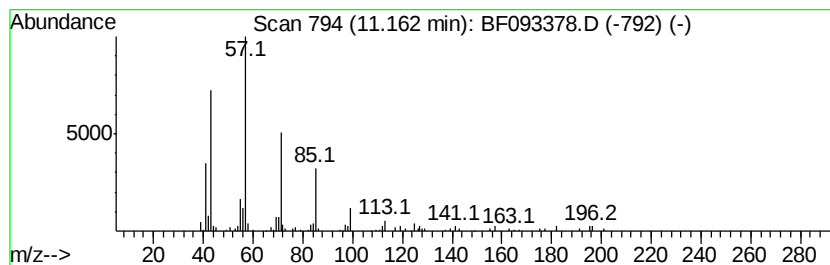
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	2.48 ng	219618	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	87
2		Hexadecane	226	C16H34	000544-76-3	86
3		Pentadecane	212	C15H32	000629-62-9	80
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5		Tridecane, 7-hexyl-	268	C19H40	007225-66-3	78



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Sample : I2078-01
Misc :
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Instrument :
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ClientSampleId :
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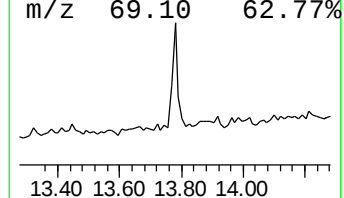
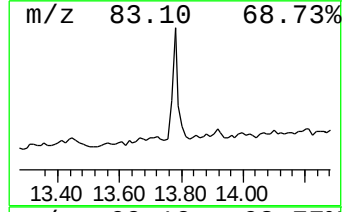
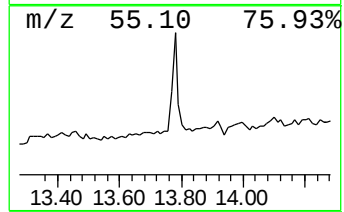
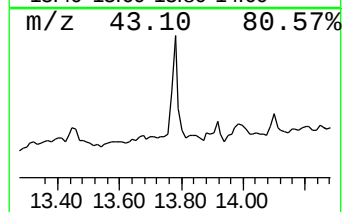
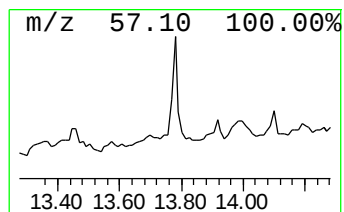
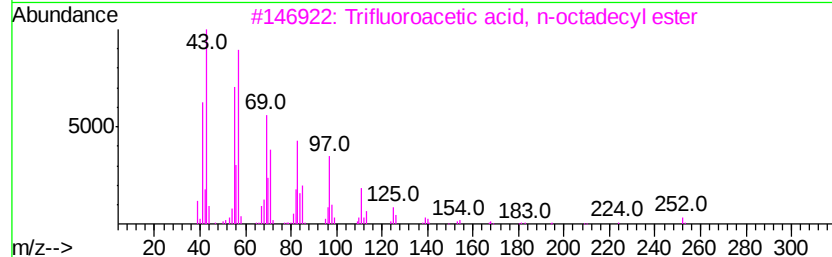
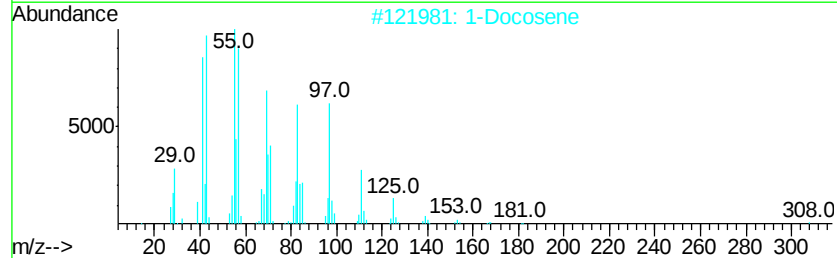
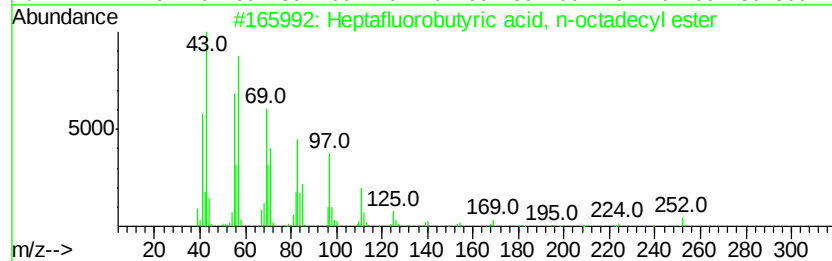
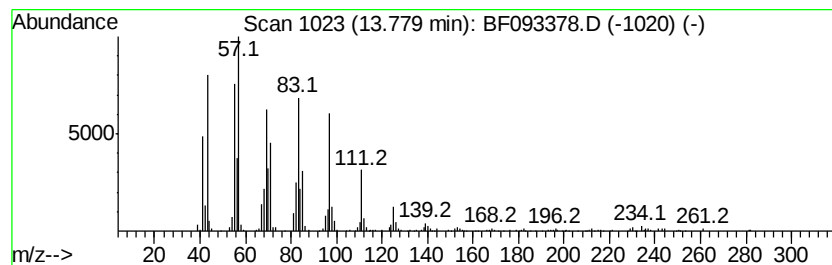
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	7.29 ng	410997	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-octadecyl...	466	C22H37F7O2	000400-57-7	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
4		17-Pentatriacontene	491	C35H70	006971-40-0	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	90



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Operator : SJ/MA
Sample : I2078-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-1

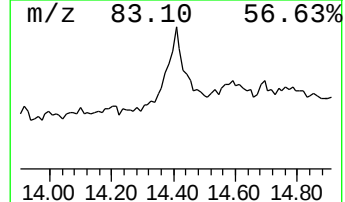
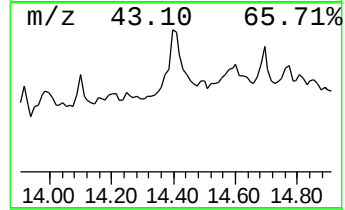
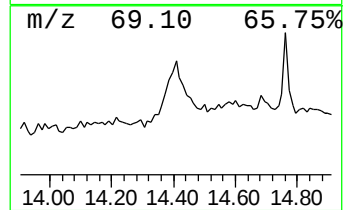
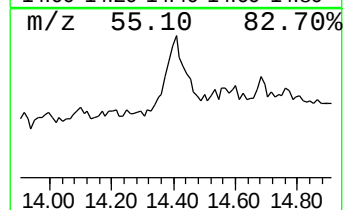
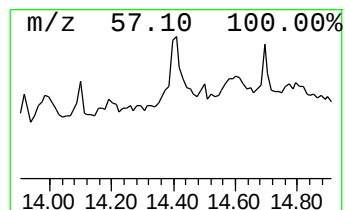
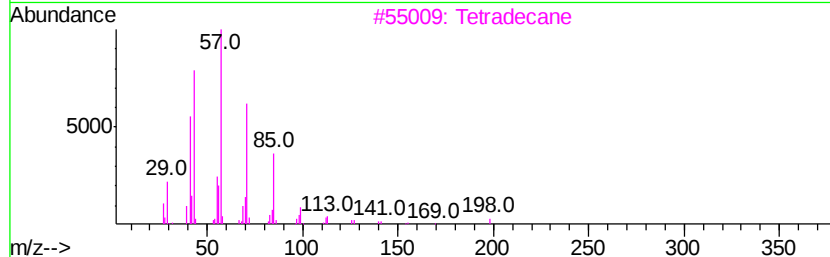
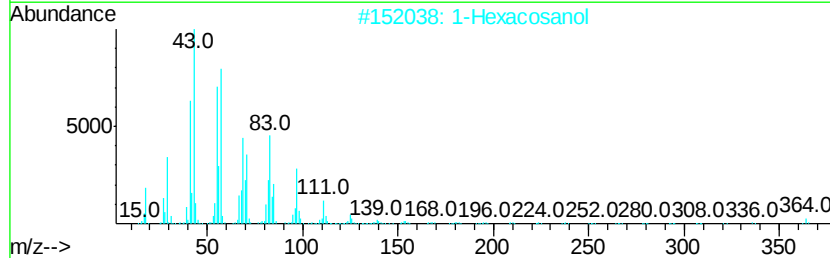
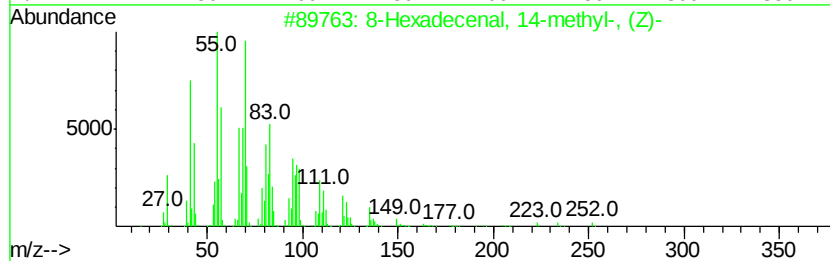
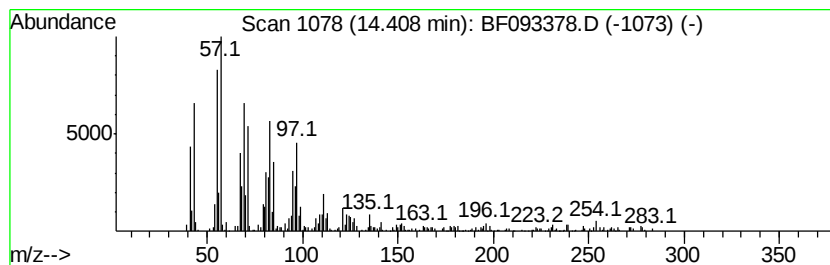
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 8-Hexadecenal, 14-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	12.66 ng	714318	Chrysene-d12	13.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Hexadecenal, 14-methyl-, (Z)-	252	C17H32O	060609-53-2	70
2			1-Hexacosanol	382	C26H54O	000506-52-5	58
3			Tetradecane	198	C14H30	000629-59-4	56
4			1,19-Eicosadiene	278	C20H38	014811-95-1	55
5			Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
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Sample : I2078-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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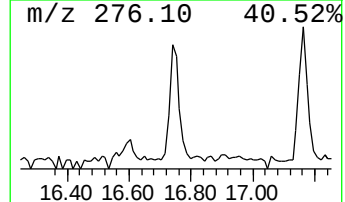
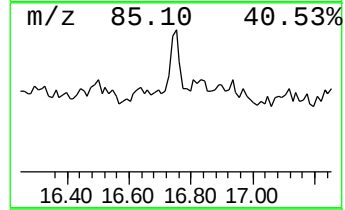
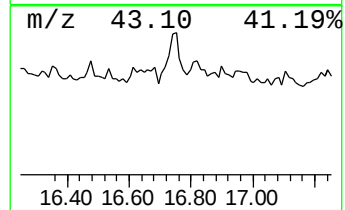
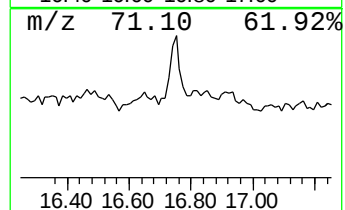
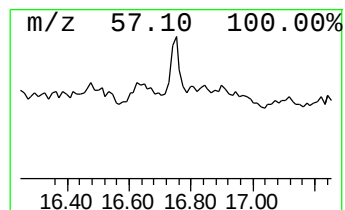
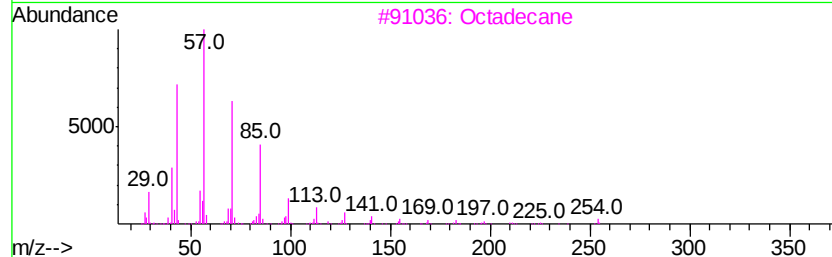
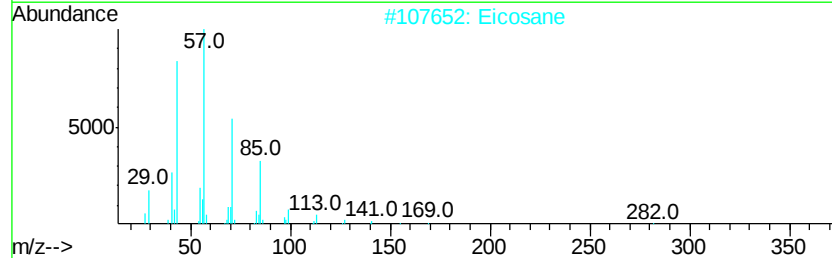
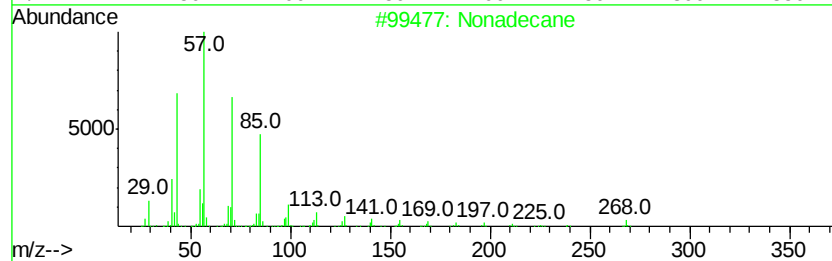
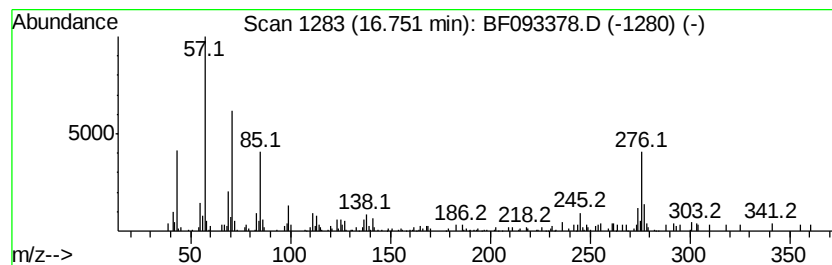
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	2.43 ng	125930	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	86
2		Eicosane	282	C20H42	000112-95-8	83
3		Octadecane	254	C18H38	000593-45-3	62
4		Docosane	310	C22H46	000629-97-0	60
5		Hexadecane	226	C16H34	000544-76-3	46



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.26	5.6 ng		351335	1	6.78	1249920	20.0
2-Pentanone, 4-hy...	4.94	21.4 ng		1339510	1	6.78	1249920	20.0
unknown6.56	6.56	76.1 ng		4754780	1	6.78	1249920	20.0
Octanoic Acid	7.84	3.2 ng		265902	2	8.08	1679240	20.0
Hexadecane	10.72	3.5 ng		308619	4	11.30	1772340	20.0
Eicosane	11.16	2.5 ng		219618	4	11.30	1772340	20.0
Heptafluorobutyri...	13.78	7.3 ng		410997	5	13.94	1128070	20.0
8-Hexadecenal, 14...	14.41	12.7 ng		714318	5	13.94	1128070	20.0
Nonadecane	16.75	2.4 ng		125930	6	15.36	1038250	20.0