

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
 Data File : BF093383.D
 Acq On : 4 Mar 2017 2:29
 Operator : SJ/MA
 Sample : I2078-11
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-6

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	3.218	96	99	109	rVB	45892	101477	2.19%	0.231%
2	4.258	187	190	209	rBV	3017270	4312477	92.86%	9.801%
3	4.944	247	250	252	rBV	2432146	3386025	72.91%	7.696%
4	5.379	286	288	304	rBV	2475084	2649031	57.04%	6.021%
5	6.430	378	380	388	rBV	3220552	3832504	82.53%	8.710%
6	6.556	388	391	393	rBV	2947781	3319033	71.47%	7.543%
7	6.784	408	411	413	rBV	1160148	1270000	27.35%	2.886%
8	6.853	415	417	419	rVB	96934	93679	2.02%	0.213%
9	6.933	422	424	427	rBV	2806139	3231208	69.58%	7.344%
10	7.127	438	441	444	rVB	36633	53517	1.15%	0.122%
11	7.356	458	461	463	rBV	2987863	2922367	62.93%	6.642%
12	7.836	500	503	511	rBV	25205	56104	1.21%	0.128%
13	8.076	521	524	526	rBV	1095672	1570143	33.81%	3.569%
14	9.150	615	618	620	rBV	4052059	4643843	100.00%	10.554%
15	9.219	622	624	626	rVB	39370	49928	1.08%	0.113%
16	9.539	650	652	656	rVB	392645	395504	8.52%	0.899%
17	9.756	669	671	674	rBV	75938	128849	2.77%	0.293%
18	9.825	674	677	679	rVV	1188835	1602523	34.51%	3.642%
19	10.248	713	714	716	rVB	156086	115585	2.49%	0.263%
20	10.465	730	733	736	rBV	52951	94987	2.05%	0.216%
21	10.613	744	746	750	rVB	426377	544244	11.72%	1.237%
22	10.716	754	755	760	rVB	152171	219706	4.73%	0.499%
23	11.162	792	794	796	rBV	103265	123971	2.67%	0.282%
24	11.299	804	806	810	rBV	1294987	1516724	32.66%	3.447%
25	11.596	830	832	834	rVV	59570	70902	1.53%	0.161%
26	11.665	836	838	840	rVB	92201	77880	1.68%	0.177%
27	11.859	854	855	858	rVB	433803	475335	10.24%	1.080%
28	11.928	858	861	864	rVB	132688	165813	3.57%	0.377%
29	12.076	873	874	878	rVB	36700	47010	1.01%	0.107%
30	12.236	886	888	890	rBV	57643	82413	1.77%	0.187%
31	12.351	896	898	900	rBV2	31369	47372	1.02%	0.108%
32	12.511	911	912	915	rBV	99105	138840	2.99%	0.316%
33	12.739	930	932	935	rBV2	79140	141115	3.04%	0.321%
34	12.888	942	945	947	rBV	3175829	3110615	66.98%	7.070%

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Integration Parameters: rteint.p
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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.459	992	995	996	rBV2	33264	48929	1.05%	0.111%
36	13.779	1020	1023	1030	rBV2	203671	280062	6.03%	0.637%
37	13.939	1035	1037	1040	rVV	972955	988199	21.28%	2.246%
38	14.099	1049	1051	1053	rBV	63344	71964	1.55%	0.164%
39	14.408	1075	1078	1083	rBV	74917	182514	3.93%	0.415%
40	14.694	1101	1103	1106	rBV2	79403	112287	2.42%	0.255%
41	15.002	1128	1130	1133	rVB	75694	114433	2.46%	0.260%
42	15.357	1158	1161	1164	rBV	808794	1012812	21.81%	2.302%
43	15.757	1193	1196	1198	rBV	111614	185508	3.99%	0.422%
44	16.214	1233	1236	1241	rVB	108588	231303	4.98%	0.526%
45	16.751	1280	1283	1288	rVB	79318	180304	3.88%	0.410%

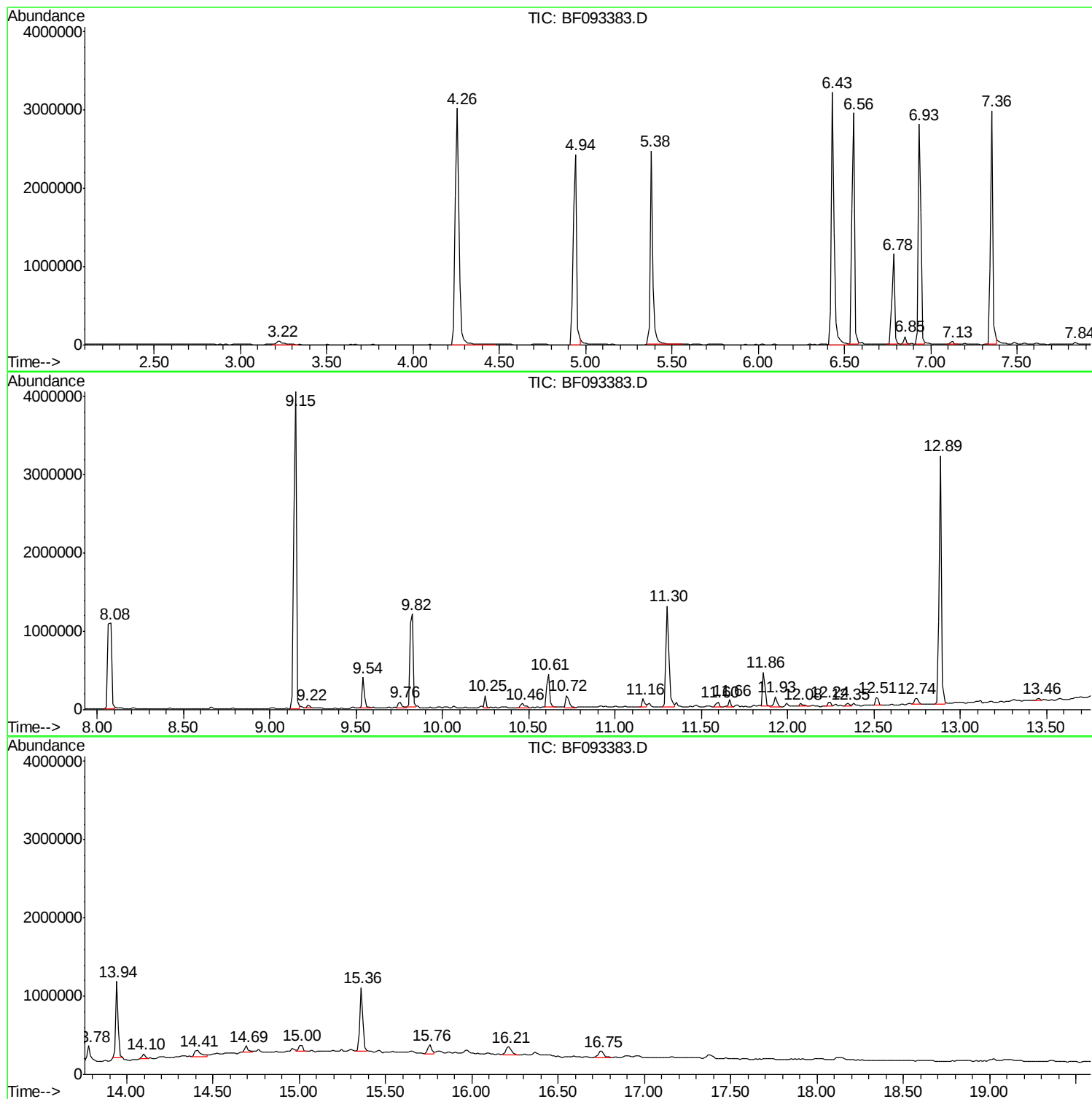
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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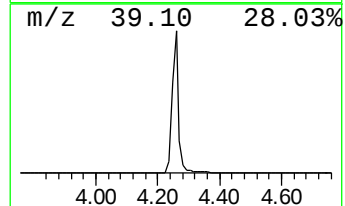
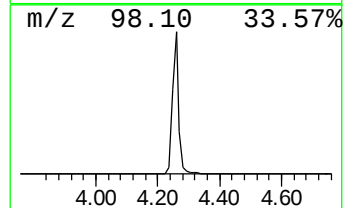
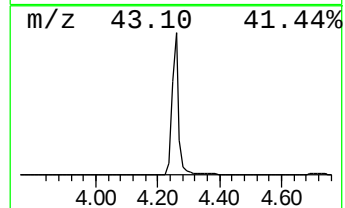
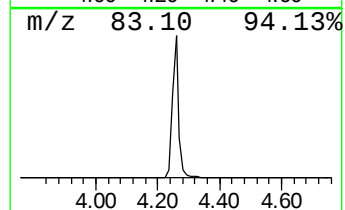
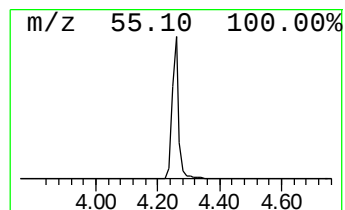
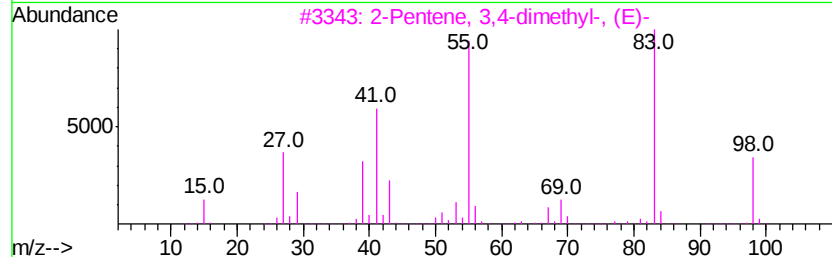
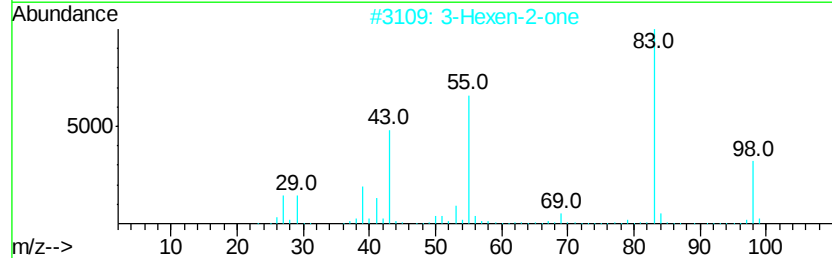
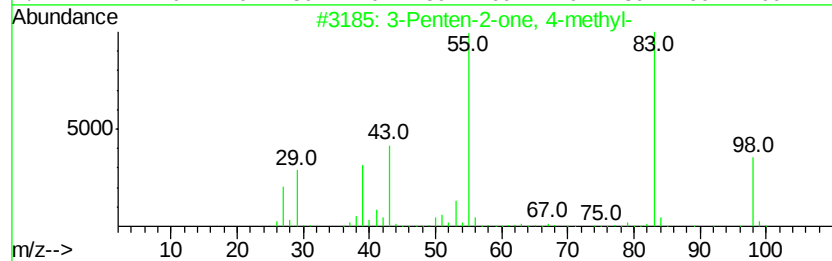
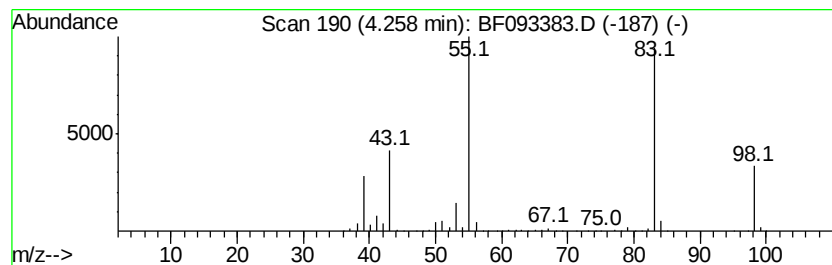
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	67.91 ng	4312480	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	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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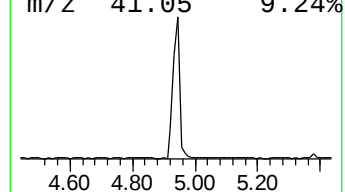
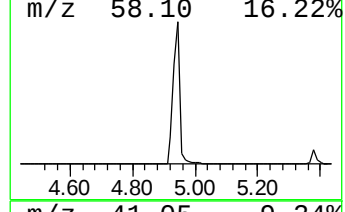
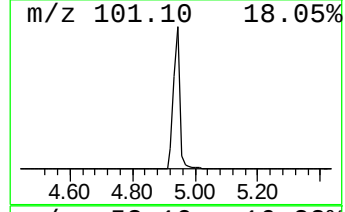
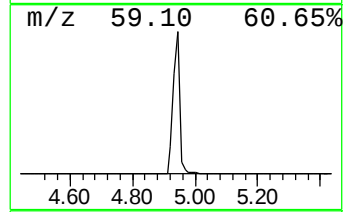
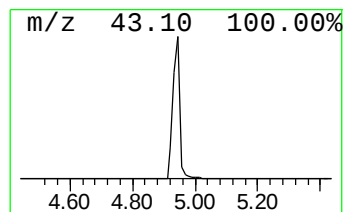
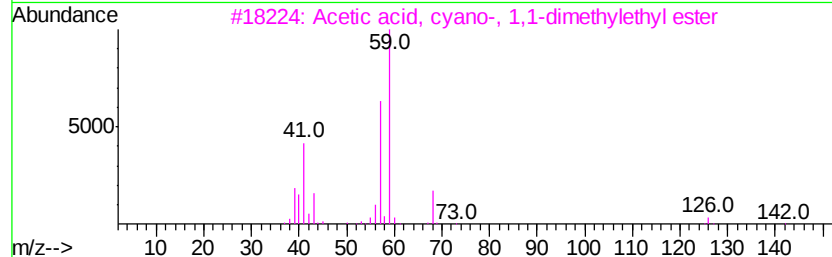
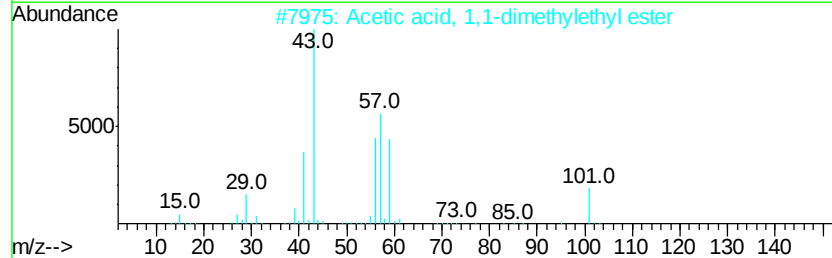
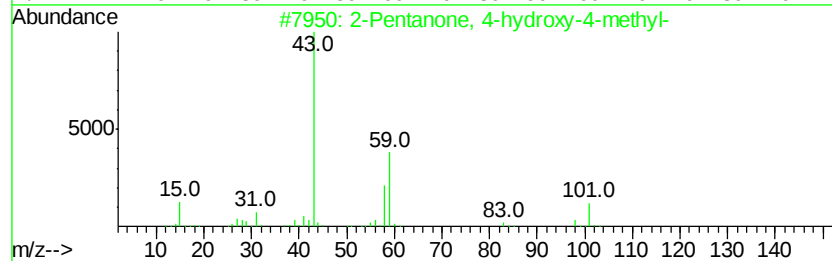
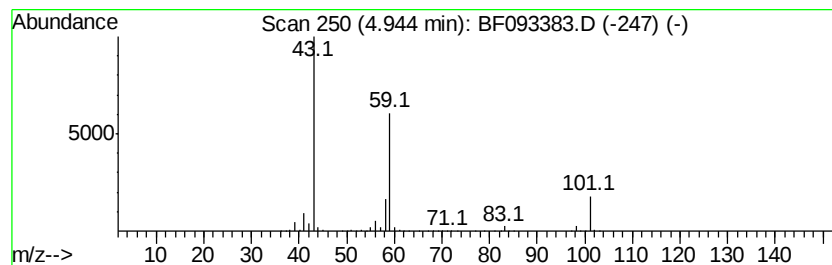
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	53.32 ng	3386030	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	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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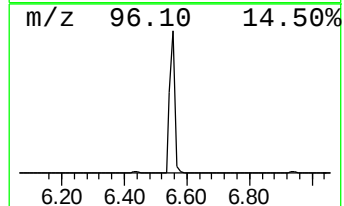
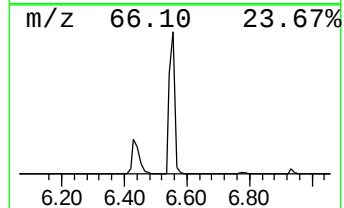
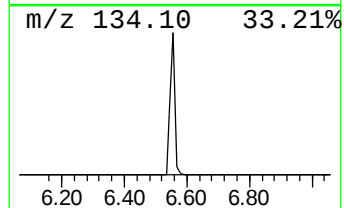
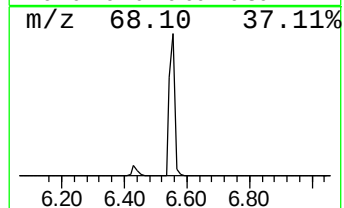
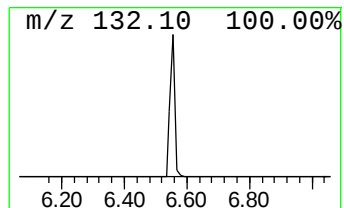
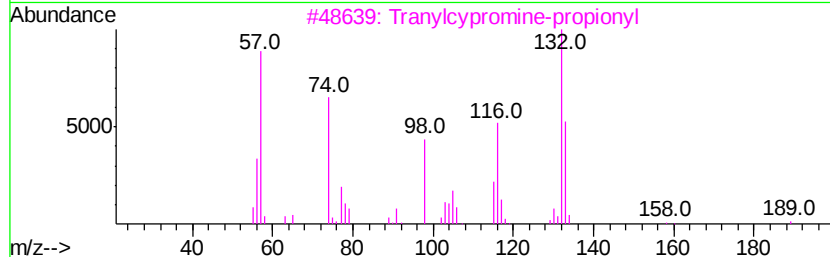
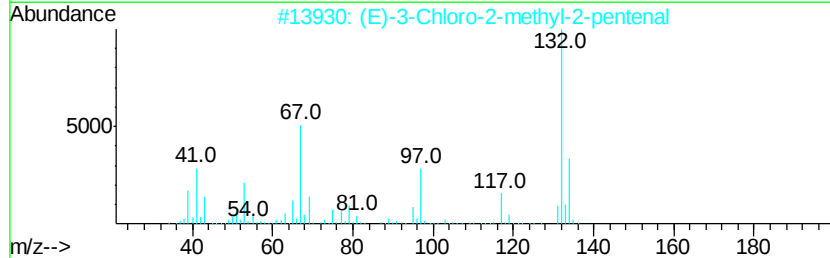
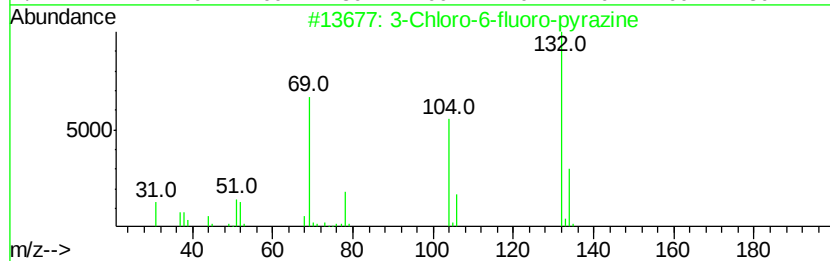
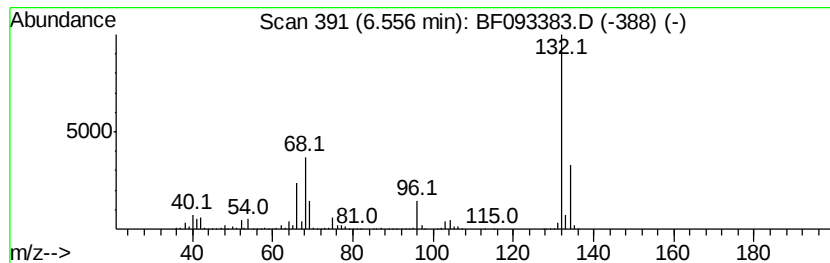
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.56 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	52.27 ng	3319030	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	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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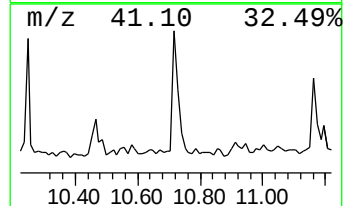
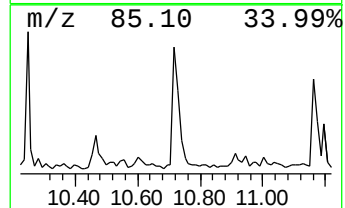
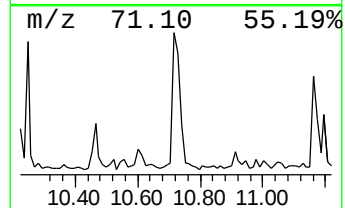
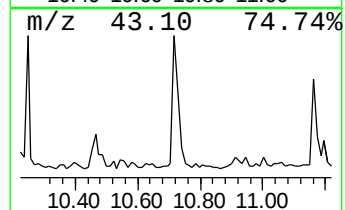
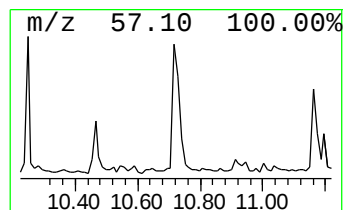
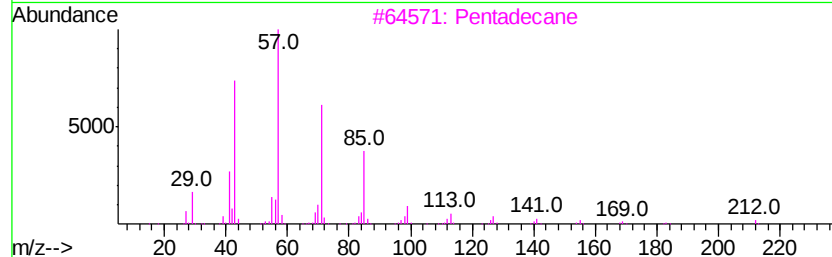
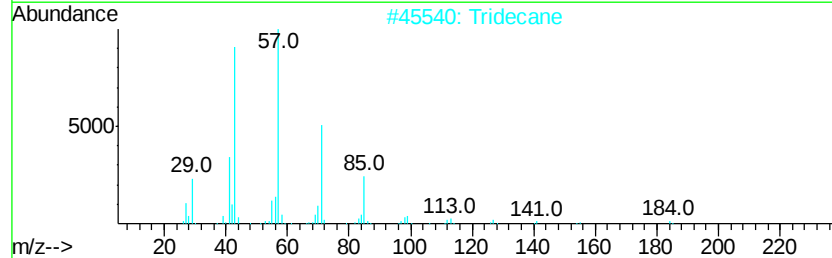
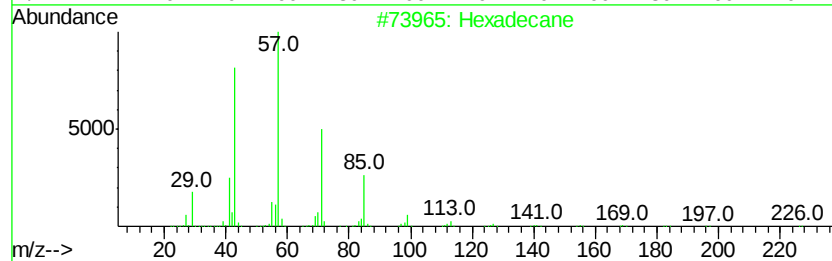
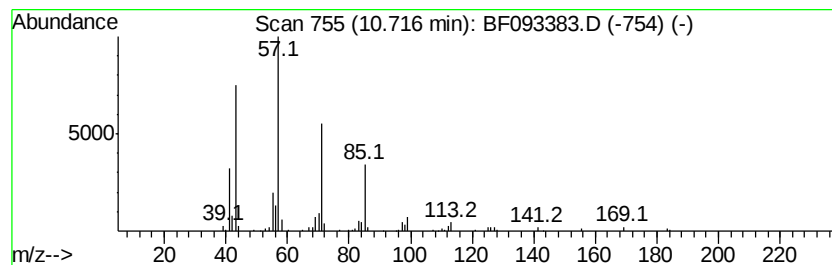
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.72	2.90 ng	219706	Phenanthrene-d10		11.30	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tridecane		184	C13H28	000629-50-5	90
3	Pentadecane		212	C15H32	000629-62-9	86
4	Nonane, 5-butyl-		184	C13H28	017312-63-9	81
5	Tetradecane		198	C14H30	000629-59-4	80



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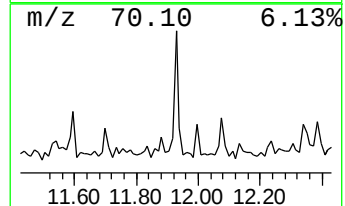
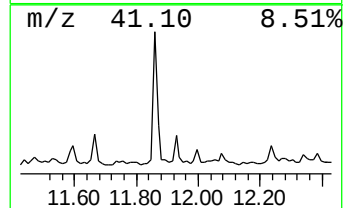
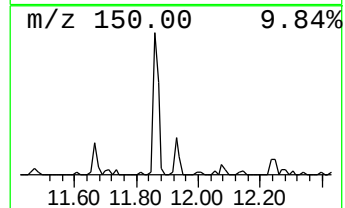
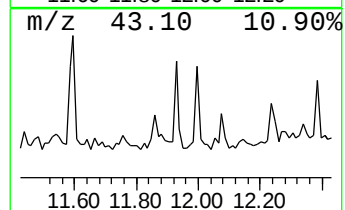
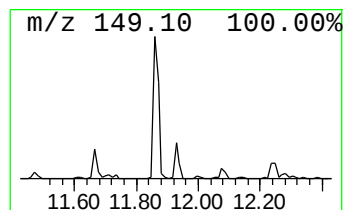
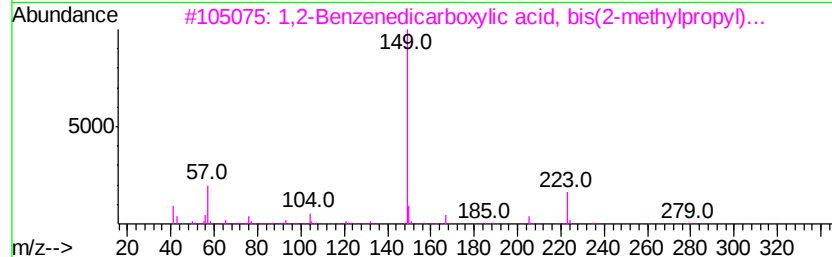
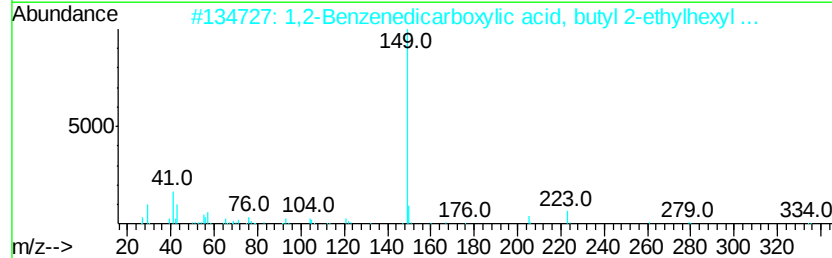
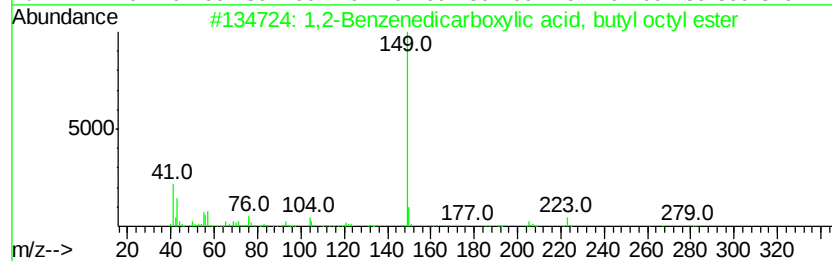
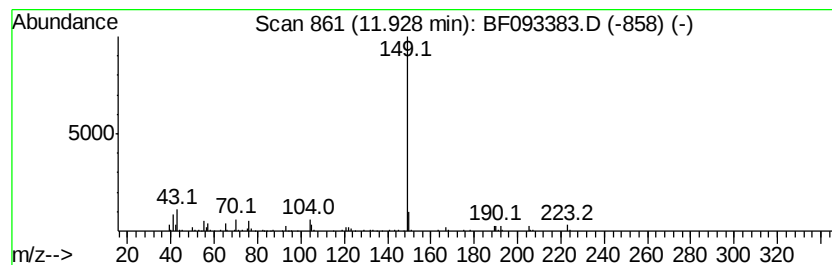
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,2-Benzenedicarboxylic aci... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.19 ng	165813	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	83
2		1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	83
3		1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	78
4		1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	78
5		1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-19-0	78



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Data File : BF093383.D
Acq On : 4 Mar 2017 2:29
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Sample : I2078-11
Misc :
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Instrument :
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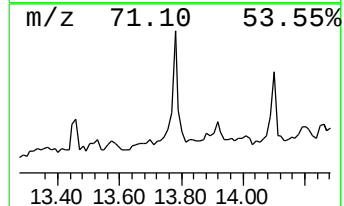
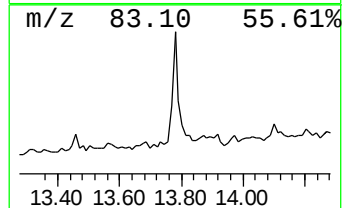
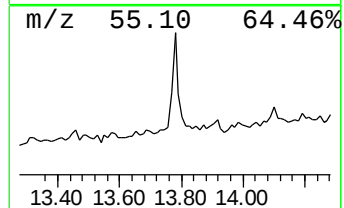
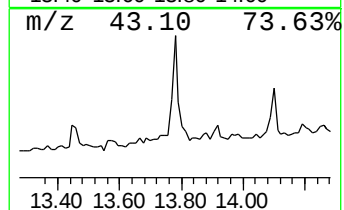
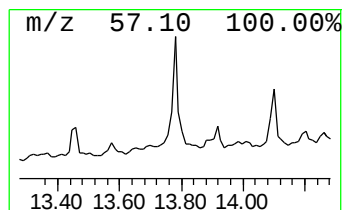
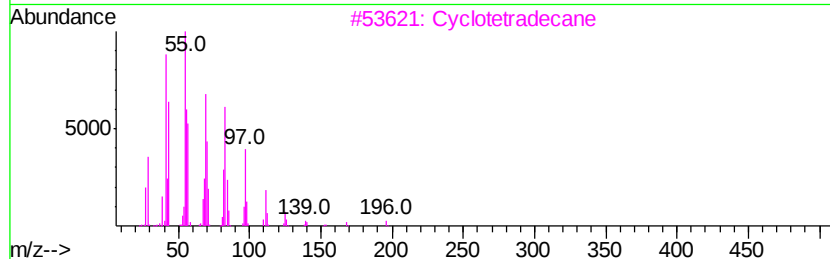
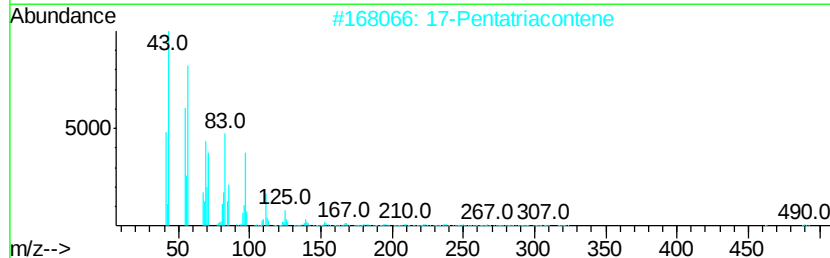
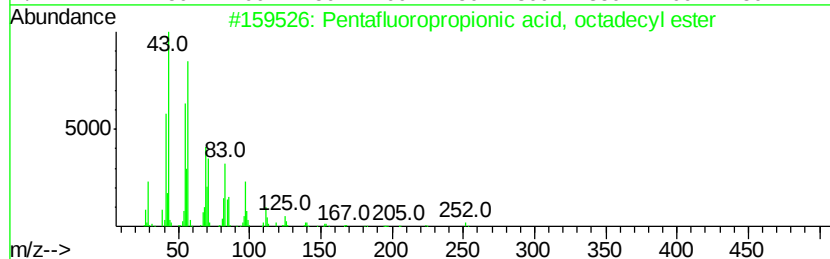
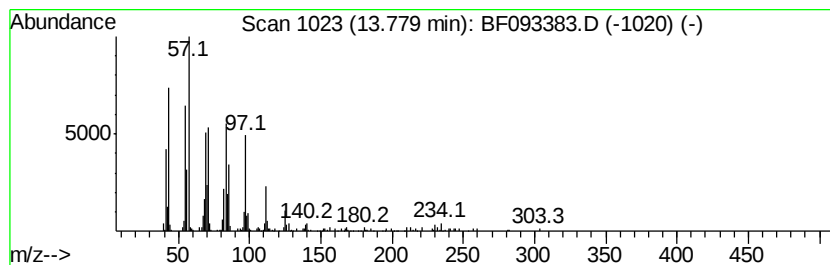
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	5.67 ng	280062	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	90
2		17-Pentatriacontene	491	C35H70	006971-40-0	83
3		Cyclotetradecane	196	C14H28	000295-17-0	74
4		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	72
5		1-Eicosanol	298	C20H42O	000629-96-9	58



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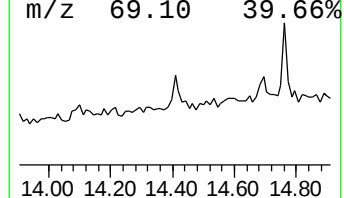
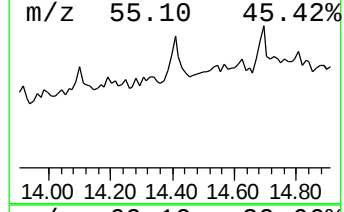
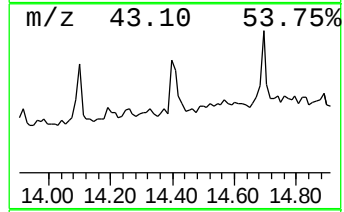
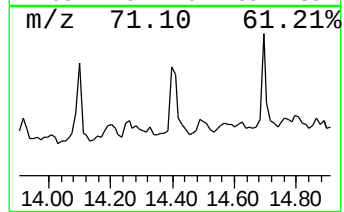
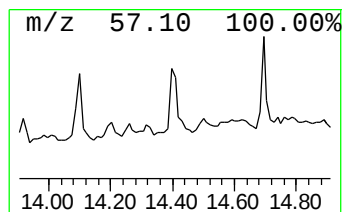
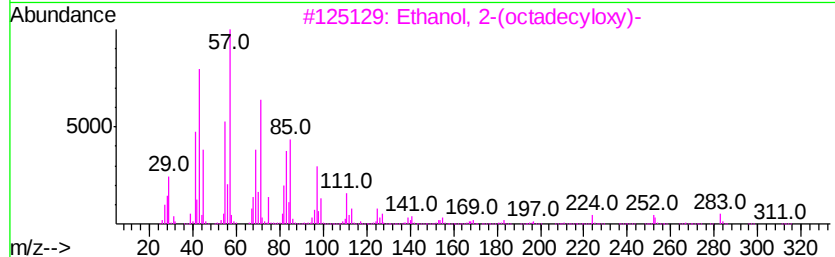
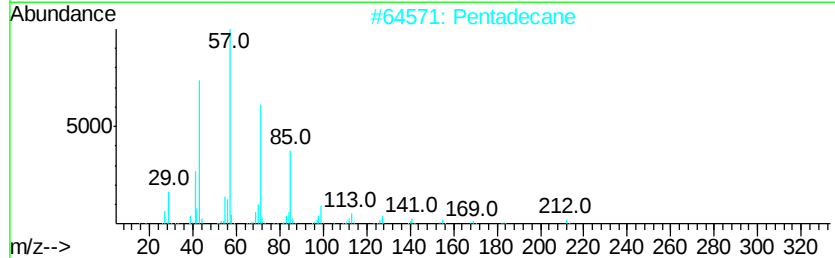
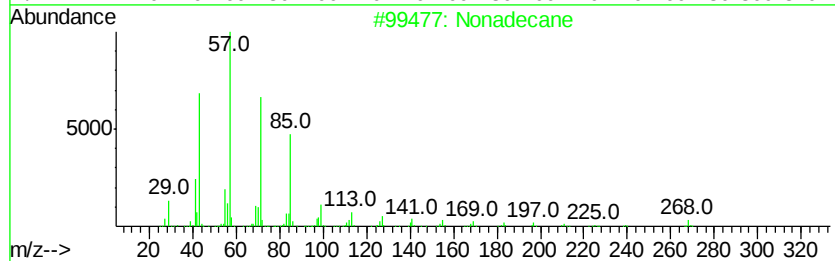
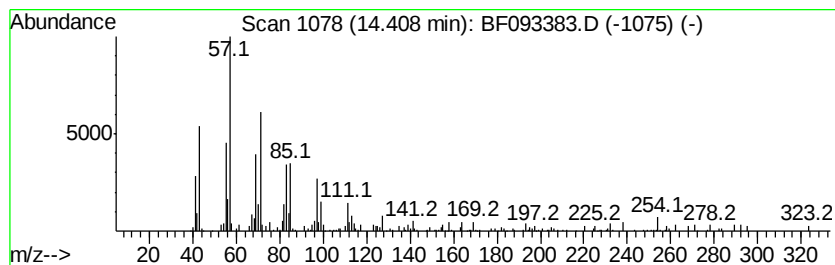
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	3.69 ng	182514	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	95
2	Pentadecane		212	C15H32	000629-62-9	90
3	Ethanol, 2-(octadecyl)-		314	C20H42O2	002136-72-3	83
4	Eicosane		282	C20H42	000112-95-8	64
5	Octadecane		254	C18H38	000593-45-3	64



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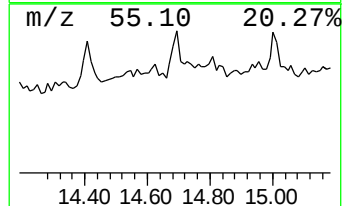
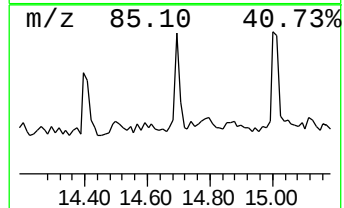
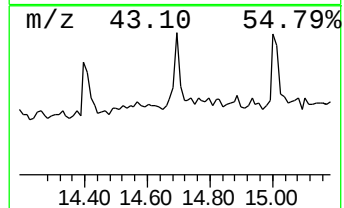
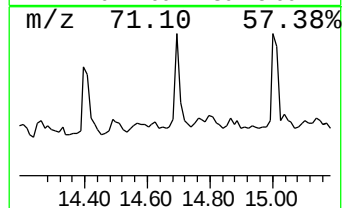
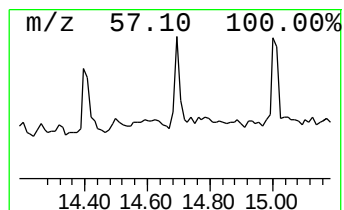
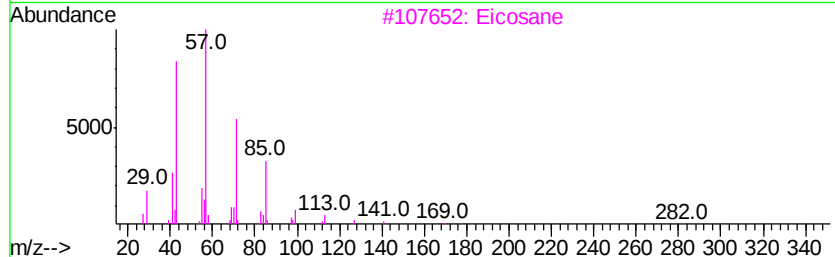
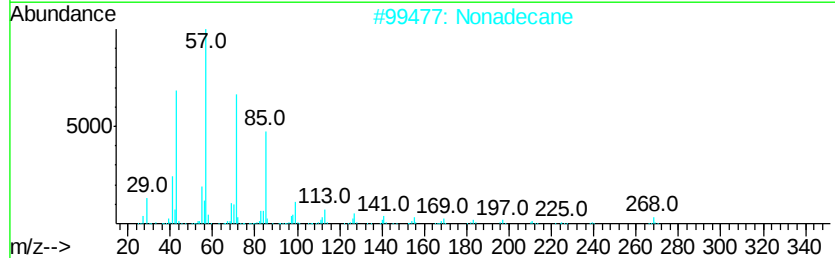
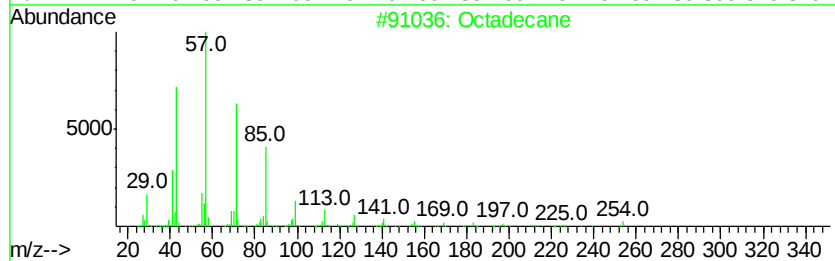
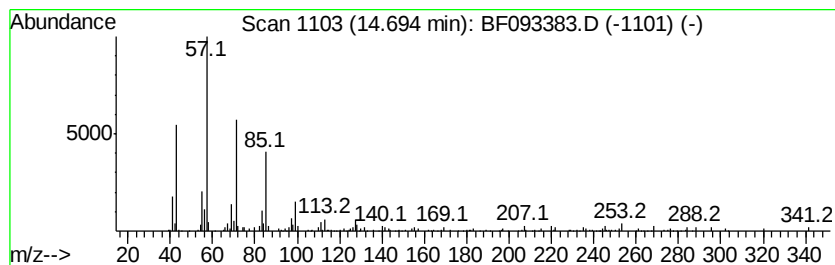
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 10 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.22 ng	112287	Perylene-d12	15.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	80
2			Nonadecane	268	C19H40	000629-92-5	80
3			Eicosane	282	C20H42	000112-95-8	72
4			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	72
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72



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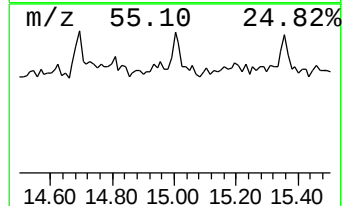
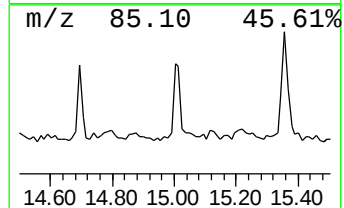
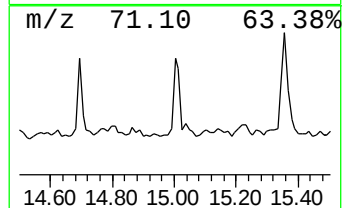
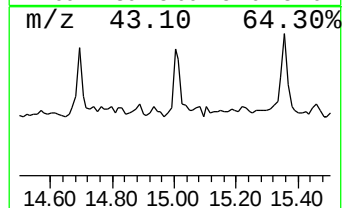
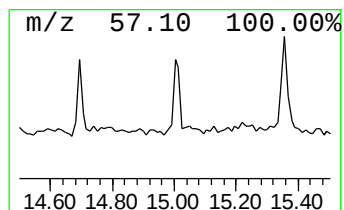
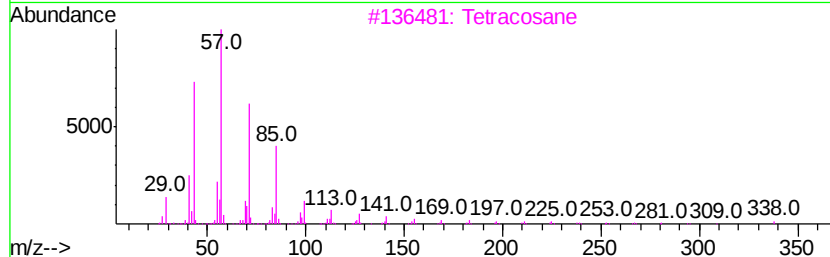
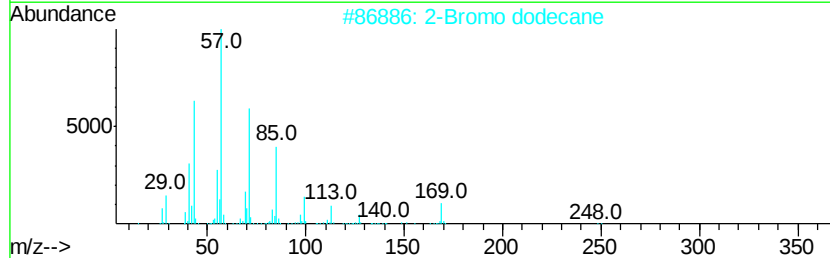
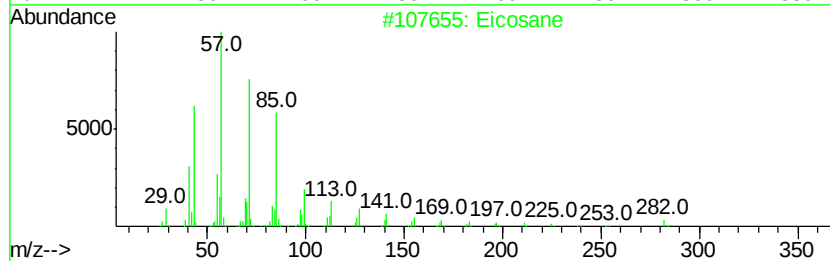
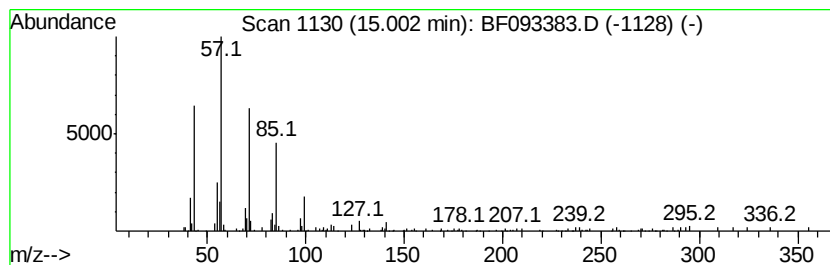
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.26 ng	114433	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	83
2	2-Bromo dodecane	248 C12H25Br	013187-99-0	80
3	Tetracosane	338 C24H50	000646-31-1	72
4	Pentadecane, 2,6,10-trimethyl-	254 C18H38	003892-00-0	72
5	Heptacosane	380 C27H56	000593-49-7	72



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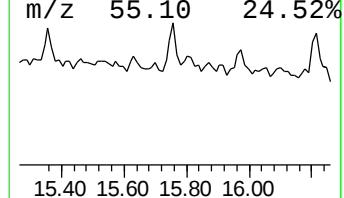
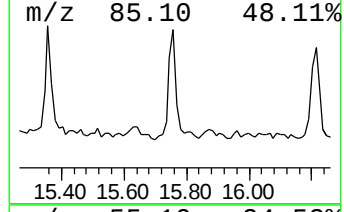
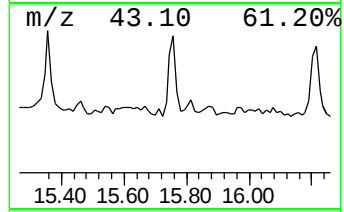
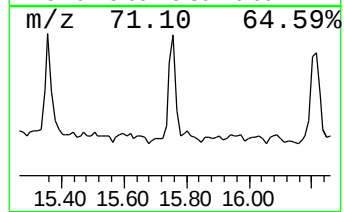
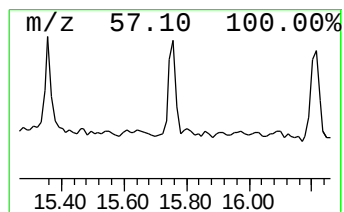
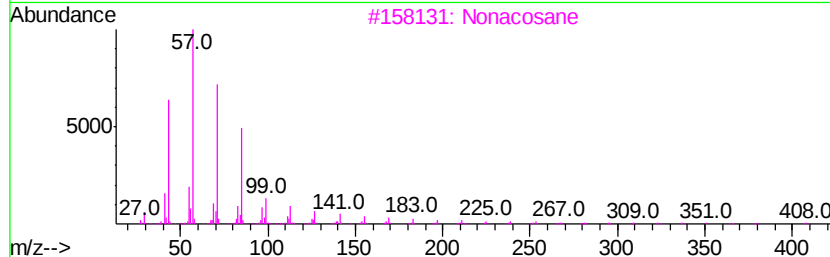
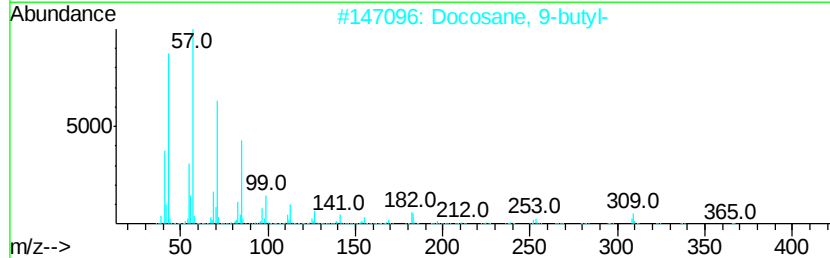
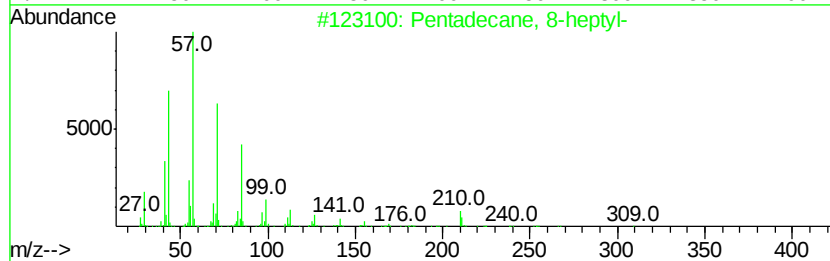
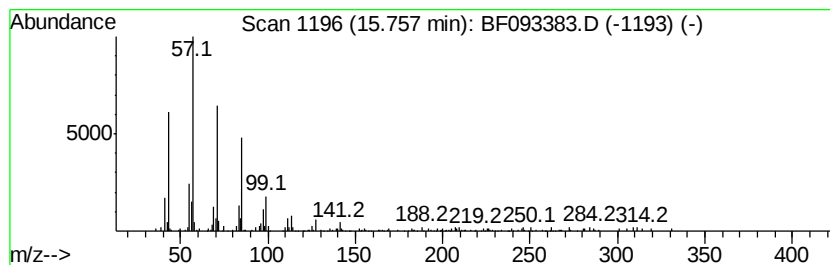
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 12 Pentadecane, 8-heptyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	3.66 ng	185508	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
2		Docosane, 9-butyl-	366	C26H54	055282-14-9	86
3		Nonacosane	408	C29H60	000630-03-5	86
4		Docosane, 11-decyl-	451	C32H66	055401-55-3	86
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	83



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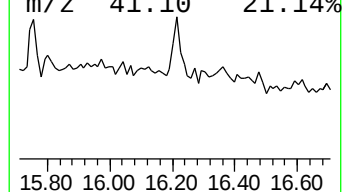
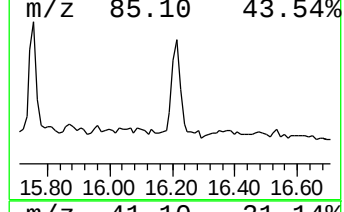
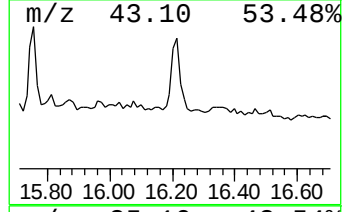
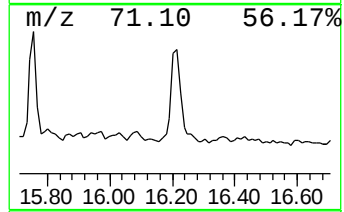
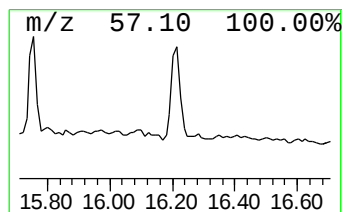
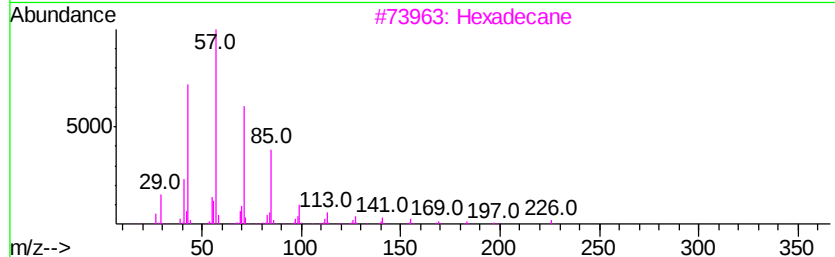
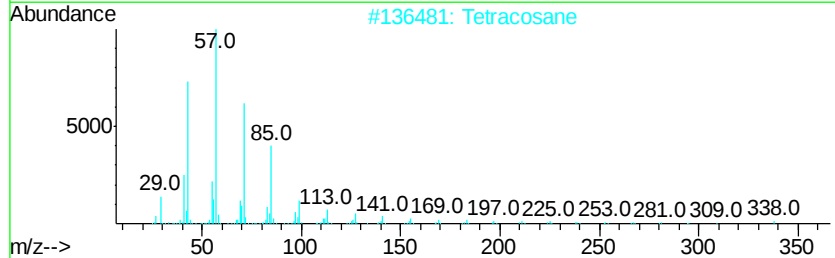
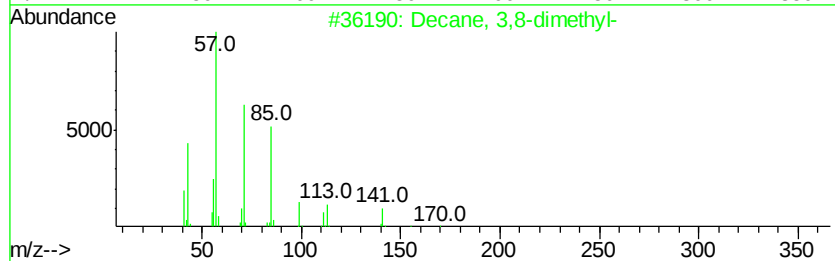
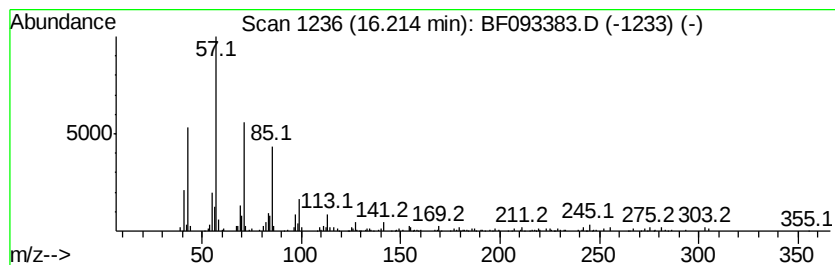
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Decane, 3,8-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	4.57 ng	231303	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
2		Tetracosane	338	C24H50	000646-31-1	87
3		Hexadecane	226	C16H34	000544-76-3	80
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5		Heneicosane	296	C21H44	000629-94-7	80



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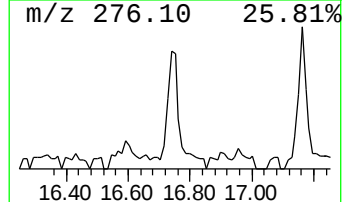
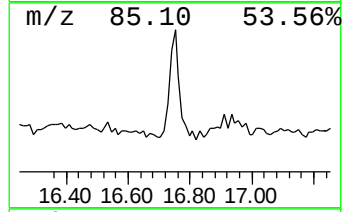
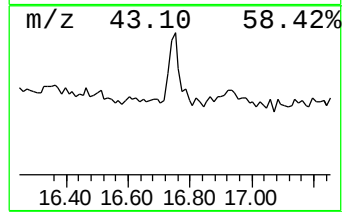
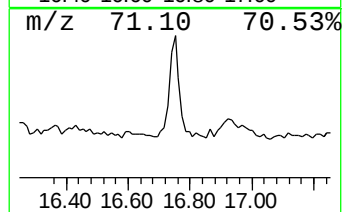
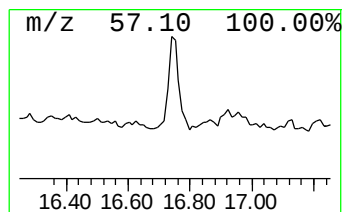
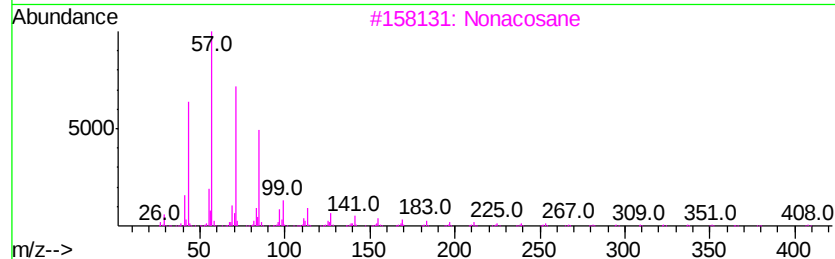
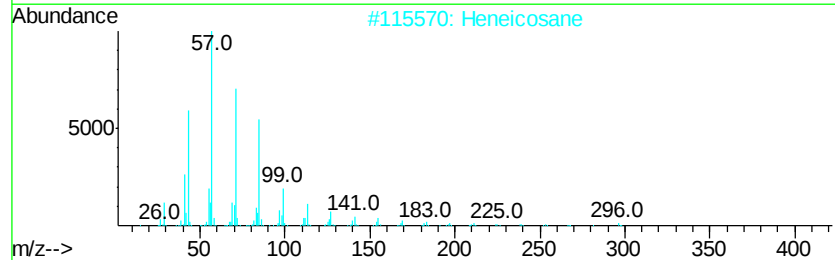
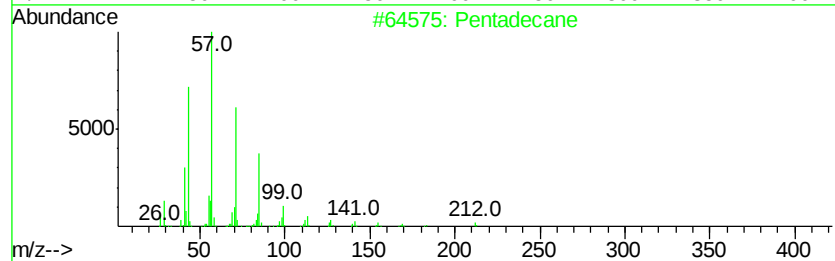
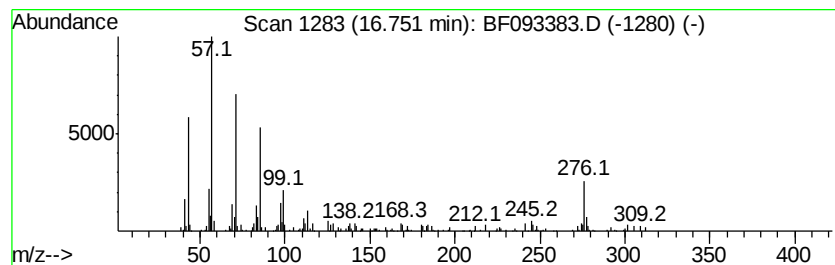
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	3.56 ng	180304	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	58
2		Heneicosane	296	C21H44	000629-94-7	58
3		Nonacosane	408	C29H60	000630-03-5	50
4		Hexadecane	226	C16H34	000544-76-3	46
5		Tridecane	184	C13H28	000629-50-5	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
Data File : BF093383.D
Acq On : 4 Mar 2017 2:29
Operator : SJ/MA
Sample : I2078-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-6

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...	4.26	67.9	ng	4312480	1	6.78	1270000	20.0
2-Pentanone, 4-hy...	4.94	53.3	ng	3386030	1	6.78	1270000	20.0
unknown6.56	6.56	52.3	ng	3319030	1	6.78	1270000	20.0
Hexadecane	10.72	2.9	ng	219706	4	11.30	1516720	20.0
1,2-Benzenedicarb...	11.93	2.2	ng	165813	4	11.30	1516720	20.0
Pentafluoropropio...	13.78	5.7	ng	280062	5	13.94	988199	20.0
Nonadecane	14.41	3.7	ng	182514	5	13.94	988199	20.0
Octadecane	14.69	2.2	ng	112287	6	15.36	1012810	20.0
Eicosane	15.00	2.3	ng	114433	6	15.36	1012810	20.0
Pentadecane, 8-he...	15.76	3.7	ng	185508	6	15.36	1012810	20.0
Decane, 3,8-dimet...	16.21	4.6	ng	231303	6	15.36	1012810	20.0
Pentadecane	16.75	3.6	ng	180304	6	15.36	1012810	20.0