

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061716\
 Data File : BF088099.D
 Acq On : 17 Jun 2016 18:08
 Operator : UM/SJ
 Sample : H3558-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-11

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-BF060716.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	1.667	6	7	16	rVB	189133	334328	9.22%	1.535%
2	1.793	16	18	86	rVB	1439095	3624248	100.00%	16.635%
3	4.136	221	223	233	rVB	370890	485180	13.39%	2.227%
4	4.833	281	284	287	rBV	453543	690347	19.05%	3.169%
5	5.279	321	323	333	rVB	676267	621650	17.15%	2.853%
6	5.690	357	359	361	rBV	111096	94897	2.62%	0.436%
7	6.330	414	415	421	rBV2	331950	415151	11.45%	1.905%
8	6.456	424	426	429	rBV	963867	1061198	29.28%	4.871%
9	6.696	445	447	449	rBV	637343	595755	16.44%	2.734%
10	6.765	452	453	457	rVB	43907	45215	1.25%	0.208%
11	6.845	458	460	463	rVB	1144693	1460264	40.29%	6.702%
12	7.267	494	497	499	rBV	1049320	1288045	35.54%	5.912%
13	7.976	557	559	562	rBV	725838	797090	21.99%	3.658%
14	9.062	651	654	656	rBV	2426718	2383369	65.76%	10.939%
15	9.462	686	689	690	rBV	86326	112202	3.10%	0.515%
16	9.679	705	708	710	rVB	44023	47709	1.32%	0.219%
17	9.736	710	713	715	rVB	739117	995091	27.46%	4.567%
18	10.159	748	750	753	rBV2	167630	229967	6.35%	1.056%
19	10.388	767	770	774	rBV	24348	45280	1.25%	0.208%
20	10.513	779	781	784	rBV	896032	934760	25.79%	4.290%
21	10.639	790	792	796	rBV2	70534	102524	2.83%	0.471%
22	11.211	840	842	844	rBV	1132620	991326	27.35%	4.550%
23	11.759	887	890	903	rBV2	63647	118024	3.26%	0.542%
24	12.537	955	958	964	rBV	40129	54865	1.51%	0.252%
25	12.799	978	981	983	rBV	1943533	2244155	61.92%	10.300%
26	13.702	1057	1060	1069	rBV2	43239	90204	2.49%	0.414%
27	13.840	1069	1072	1074	rBV	855510	811586	22.39%	3.725%
28	14.697	1143	1147	1150	rBV2	27042	36475	1.01%	0.167%
29	15.074	1177	1180	1183	rBV	43394	64356	1.78%	0.295%
30	15.223	1190	1193	1204	rVB	520308	597985	16.50%	2.745%
31	15.508	1215	1218	1222	rBV	57490	102848	2.84%	0.472%
32	16.023	1259	1263	1266	rBV	51273	99984	2.76%	0.459%
33	16.640	1310	1317	1324	rBV	30075	76772	2.12%	0.352%
34	17.383	1377	1382	1391	rVB3	17370	52968	1.46%	0.243%

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.297	1456	1462	1467	rBV2	10654	40568	1.12%	0.186%
36	19.440	1555	1562	1570	rvB4	7652	41014	1.13%	0.188%

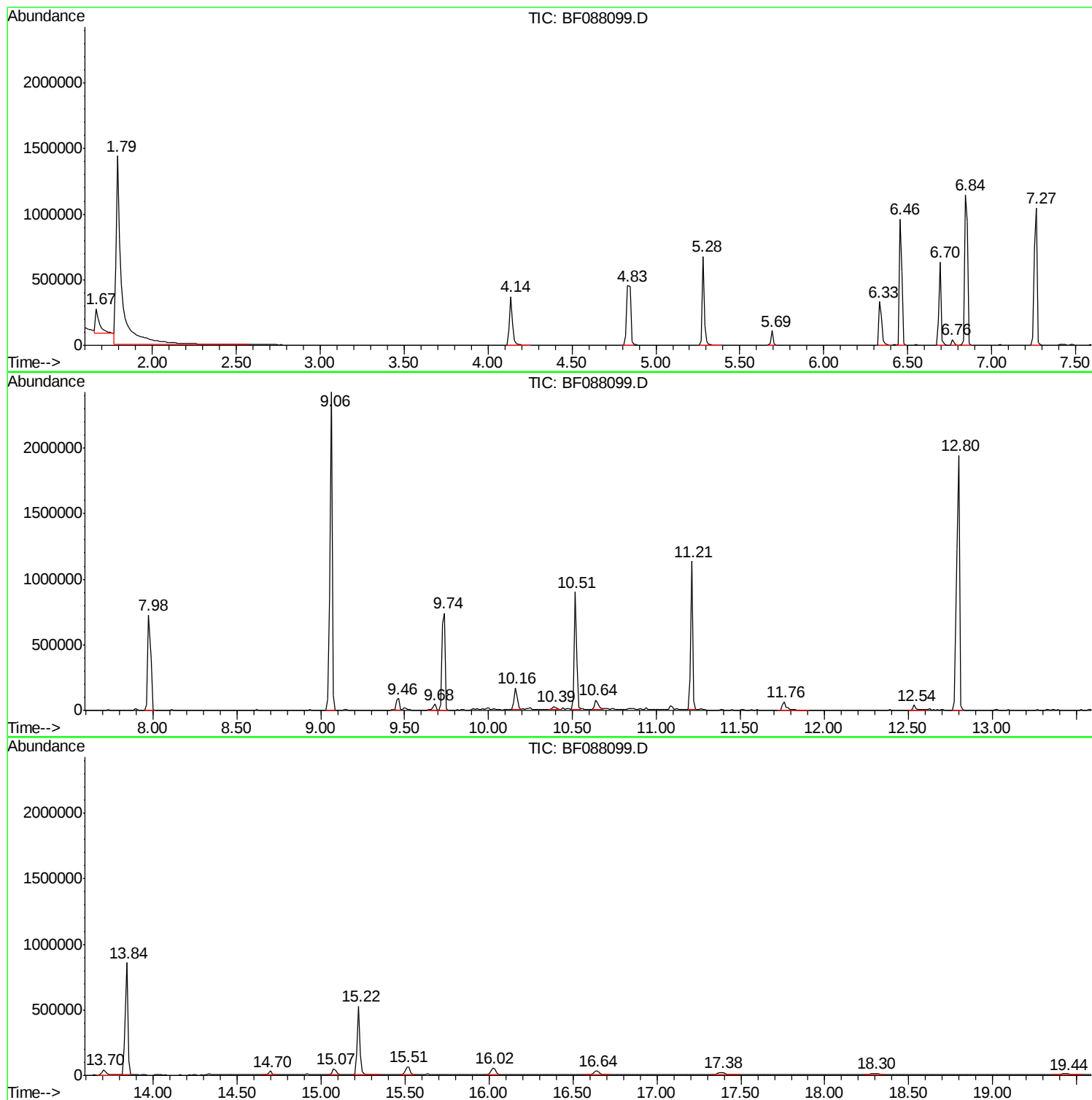
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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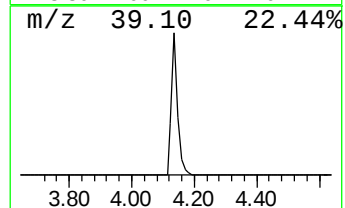
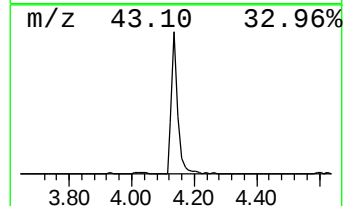
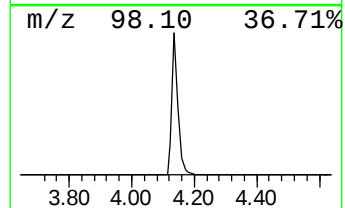
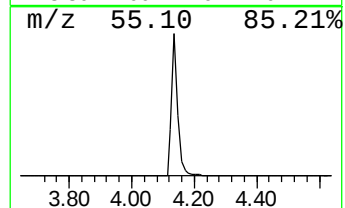
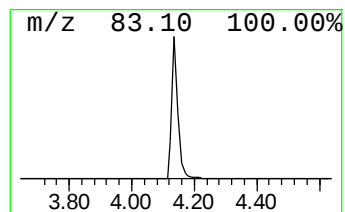
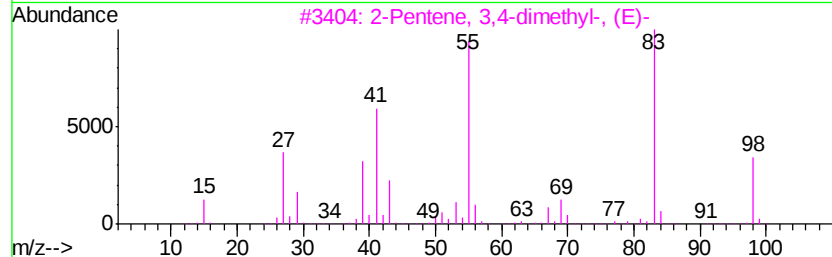
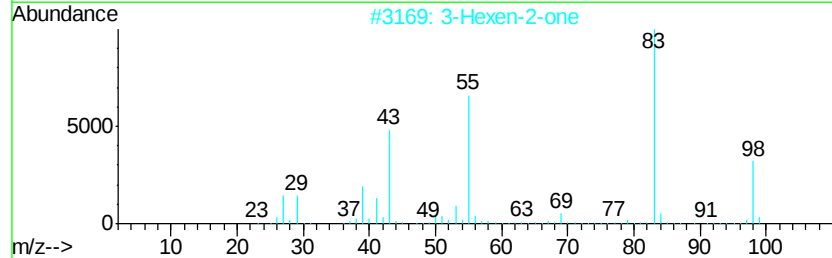
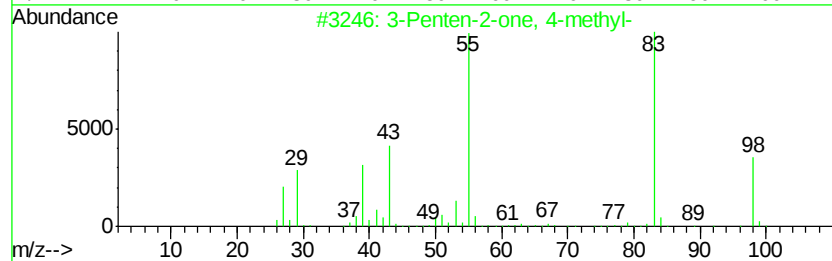
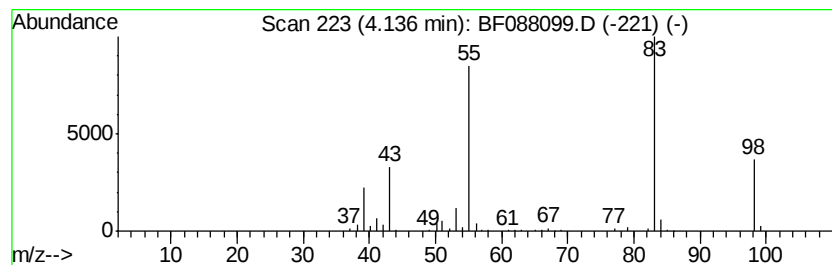
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	16.29 ng	485180	1,4-Dichlorobenzene-d4	6.70

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	91
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		2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N2O2	042282-85-9	78



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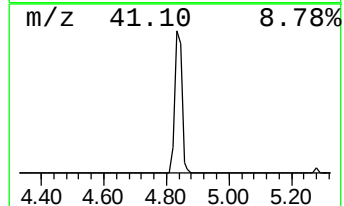
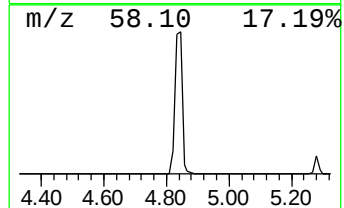
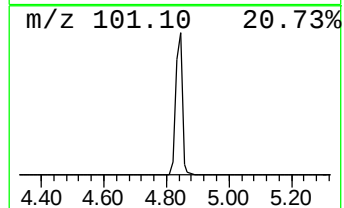
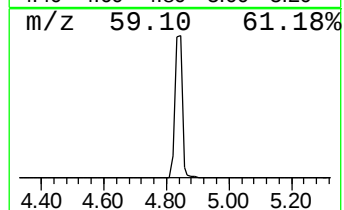
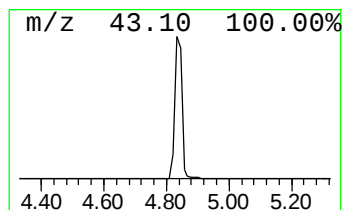
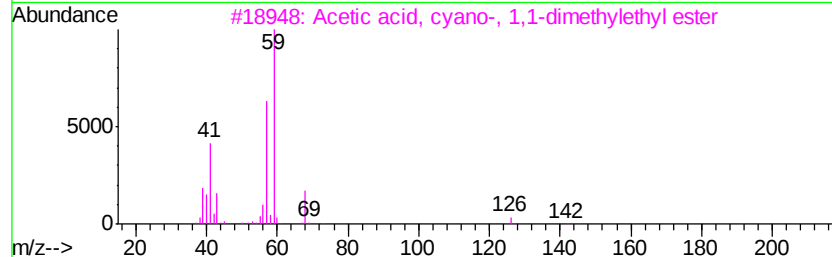
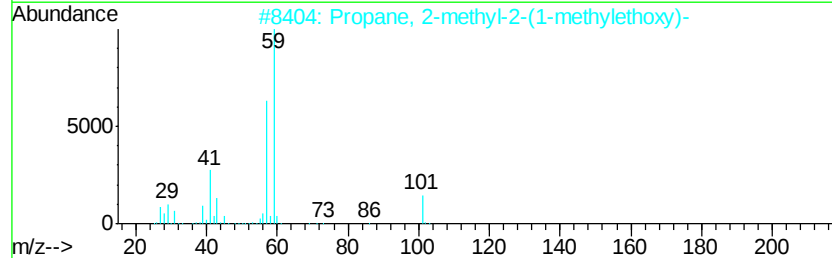
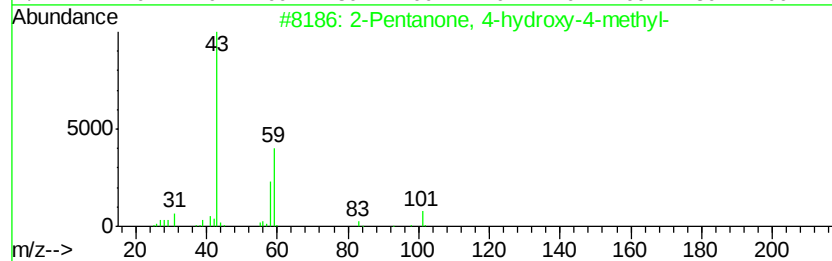
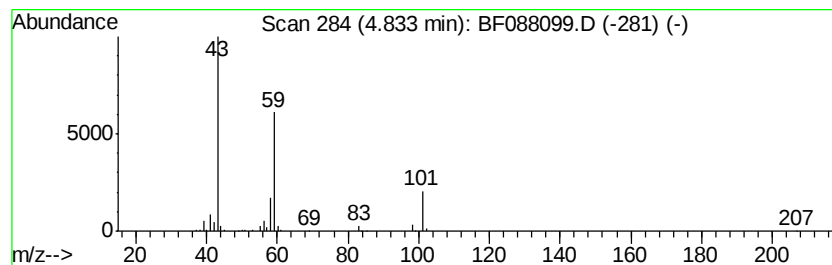
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	23.18 ng	690347	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Acetone	58	C3H6O	000067-64-1	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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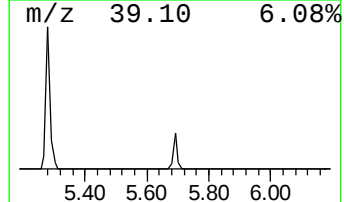
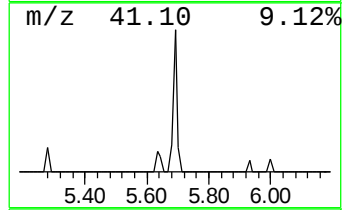
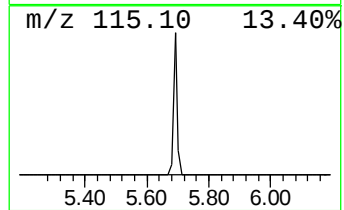
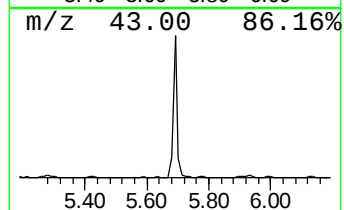
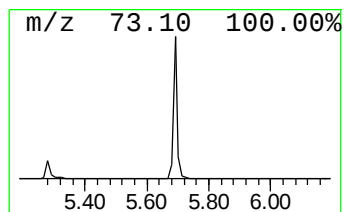
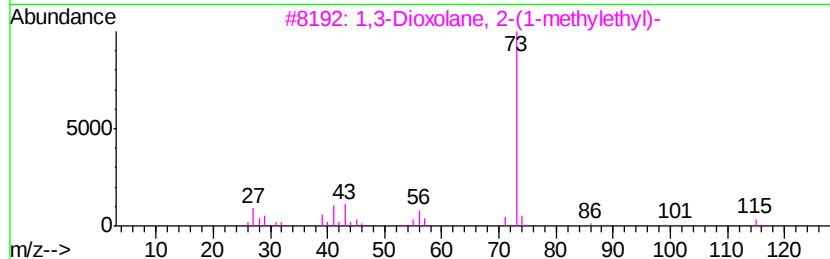
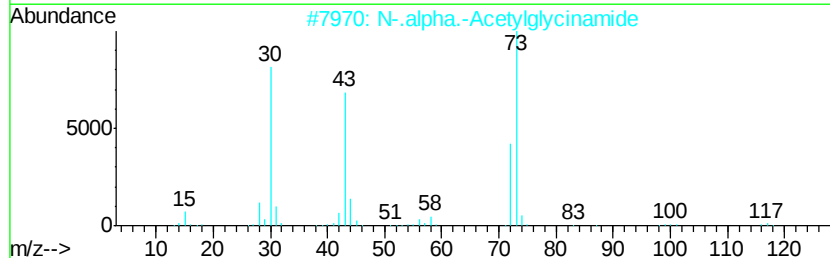
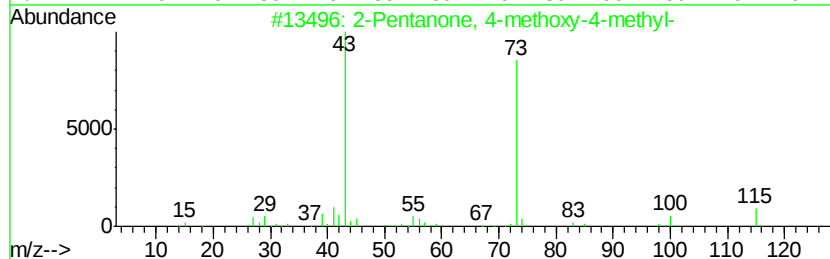
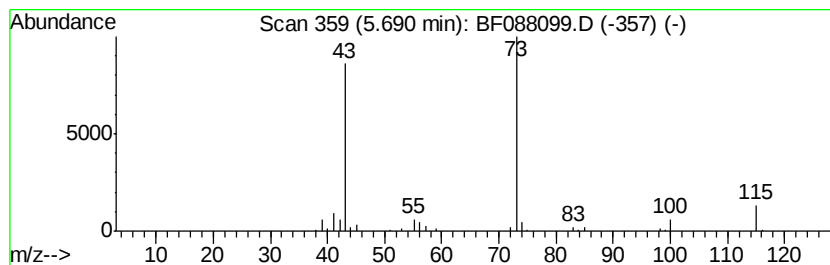
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	3.19 ng	94897	1,4-Dichlorobenzene-d4	6.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglutcinamide	116	C4H8N2O2	002620-63-5	33
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
4		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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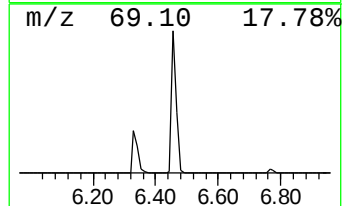
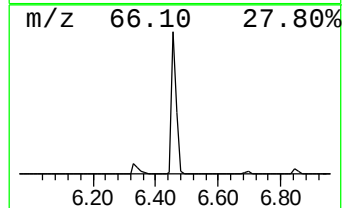
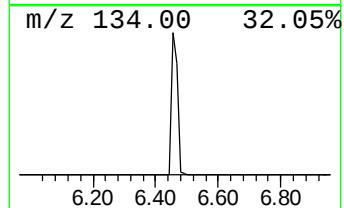
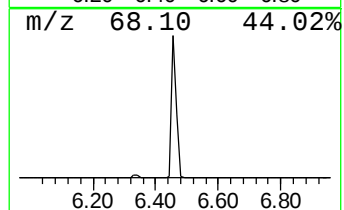
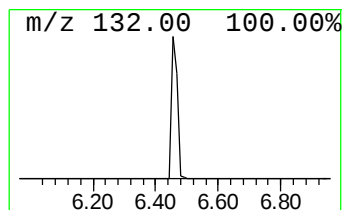
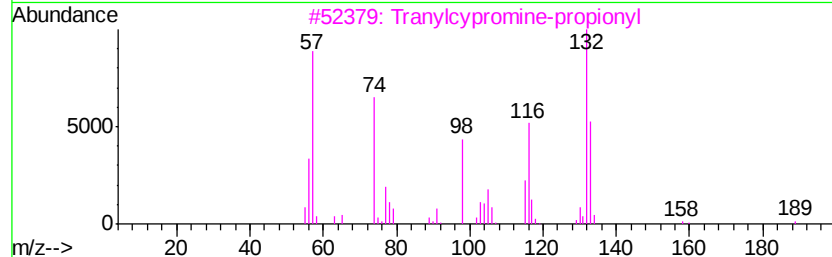
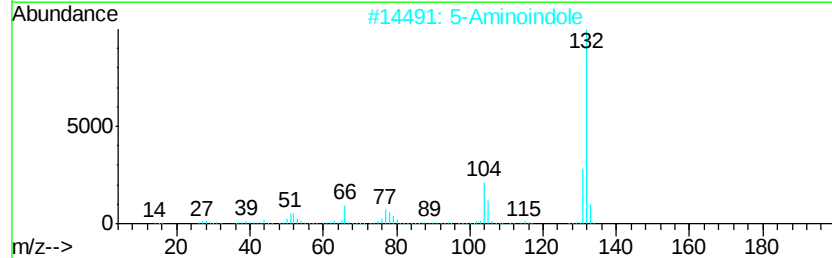
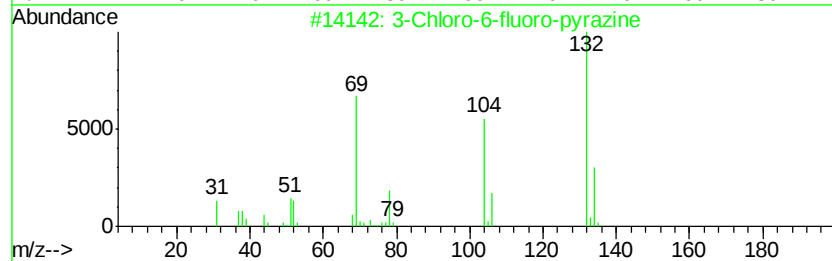
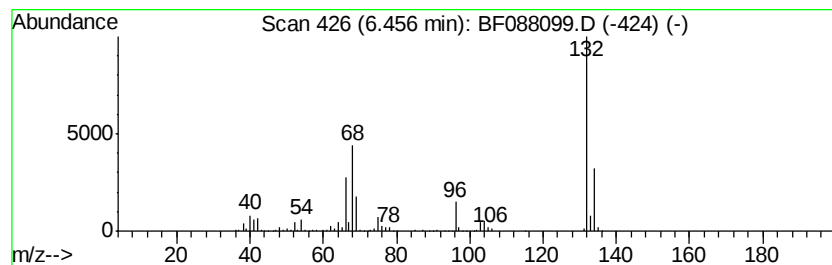
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown6.46 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	35.63 ng	1061200	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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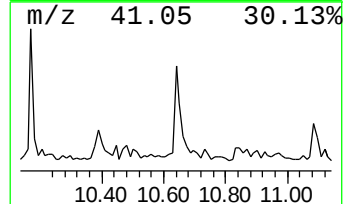
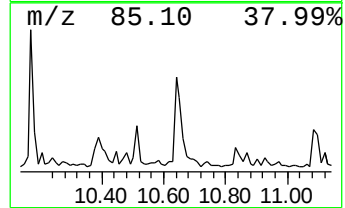
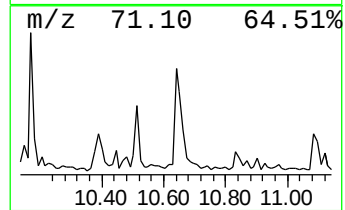
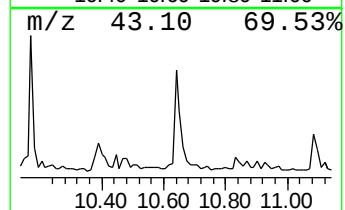
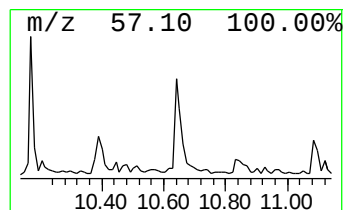
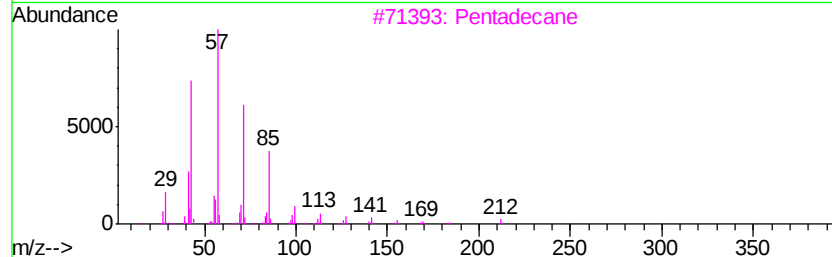
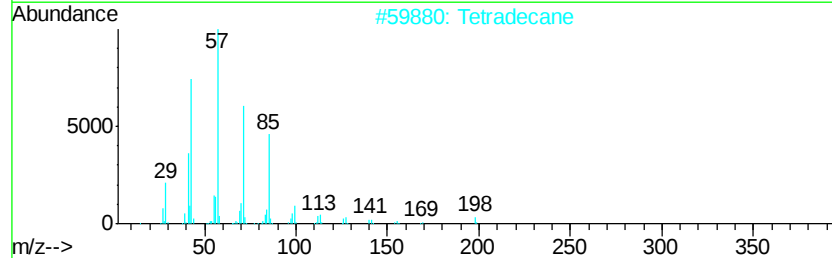
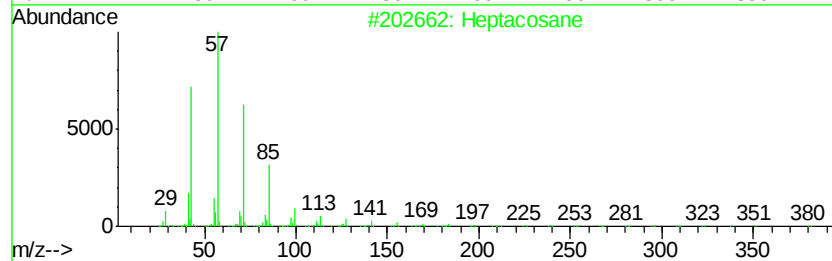
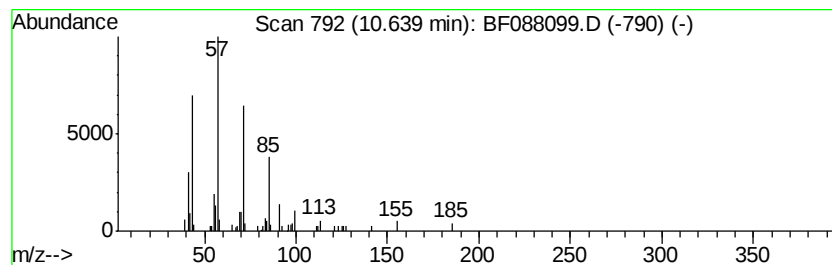
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Peak Number 8 Heptacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	2.07 ng	102524	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	72
2		Tetradecane	198	C14H30	000629-59-4	72
3		Pentadecane	212	C15H32	000629-62-9	72
4		Octacosane	394	C28H58	000630-02-4	72
5		Octadecane	254	C18H38	000593-45-3	64



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ClientSampleId :
TWP-11

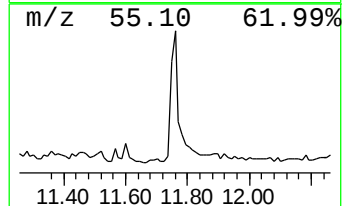
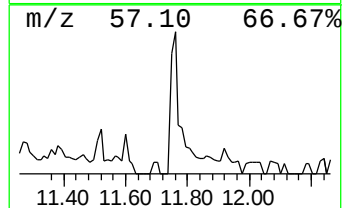
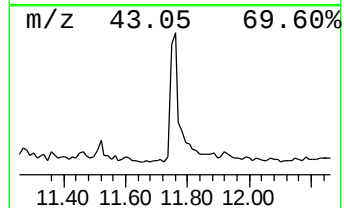
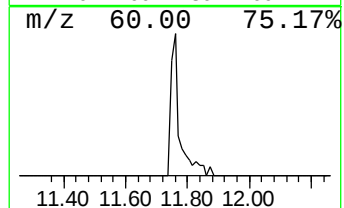
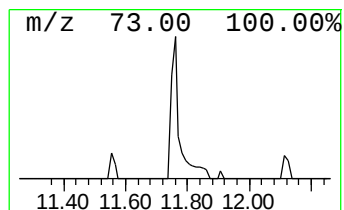
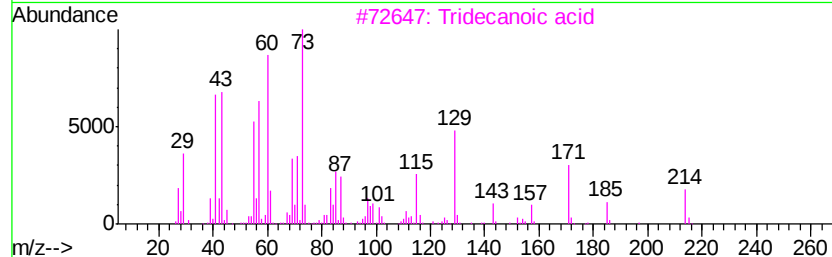
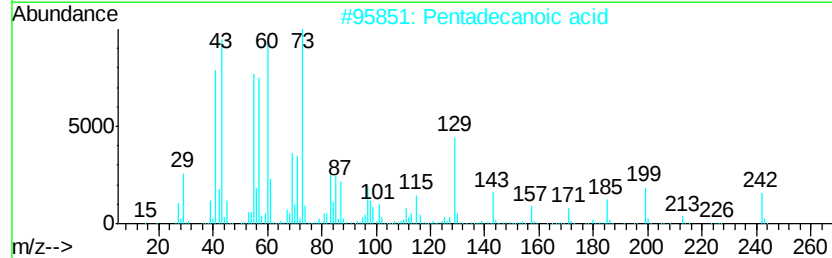
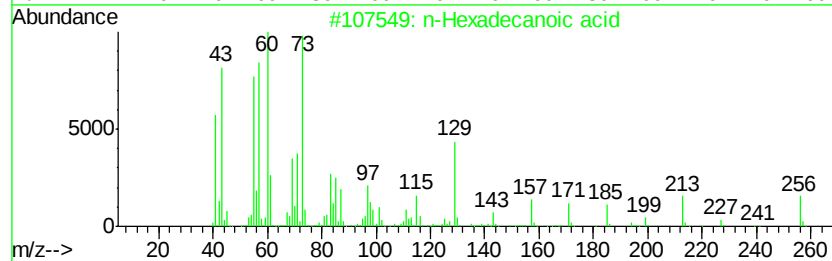
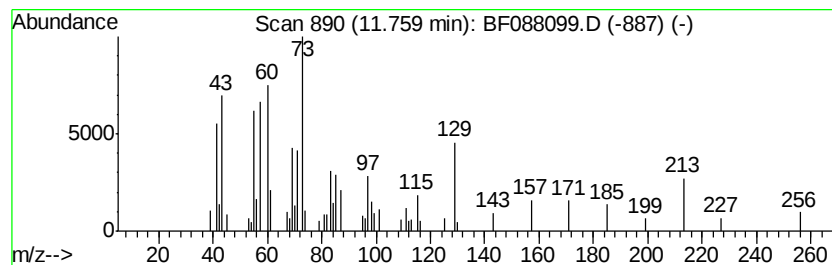
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.38 ng	118024	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061716\
Data File : BF088099.D
Acq On : 17 Jun 2016 18:08
Operator : UM/SJ
Sample : H3558-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-11

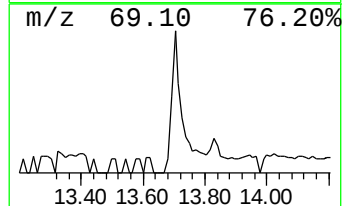
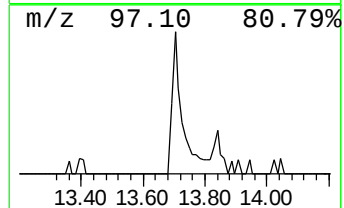
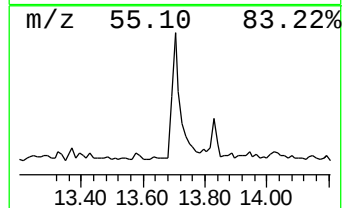
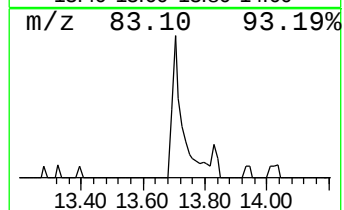
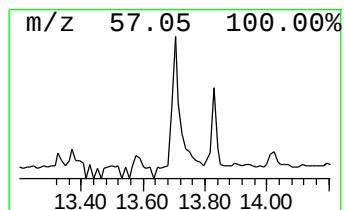
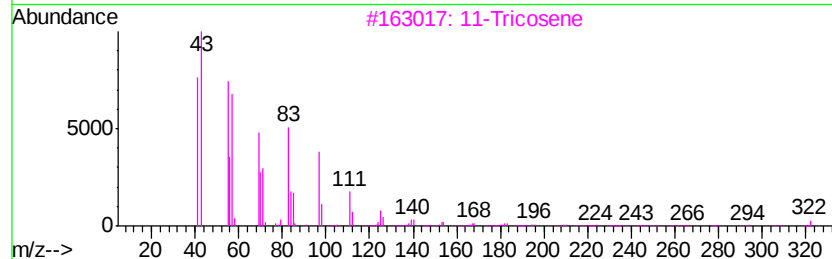
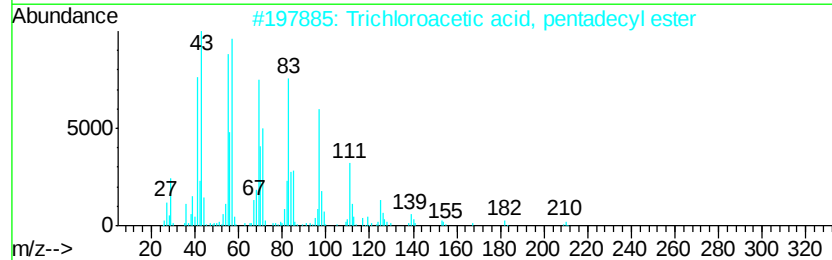
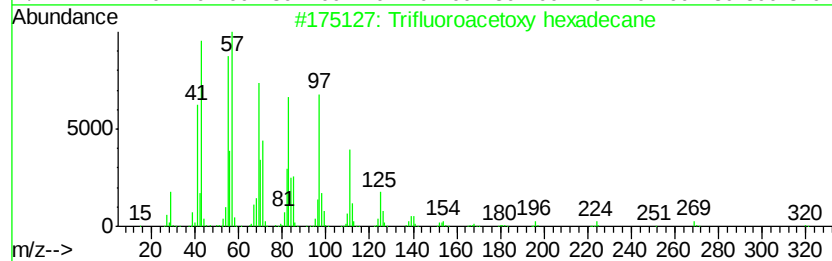
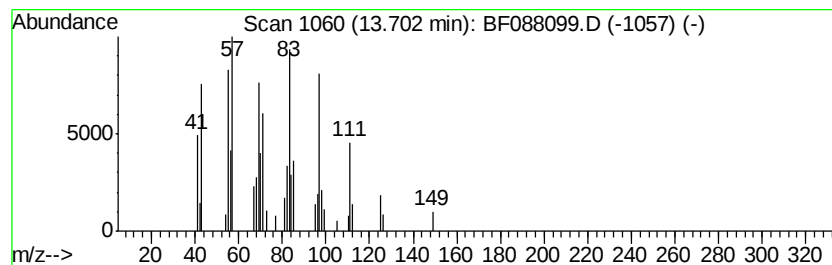
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.22 ng	90204	Chrysene-d12	13.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3			11-Tricosene	322	C23H46	052078-56-5	91
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061716\
Data File : BF088099.D
Acq On : 17 Jun 2016 18:08
Operator : UM/SJ
Sample : H3558-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-11

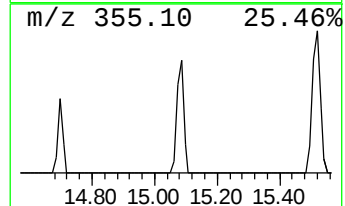
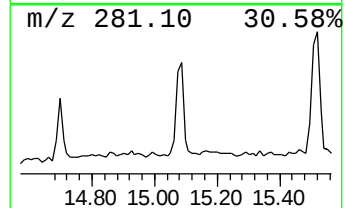
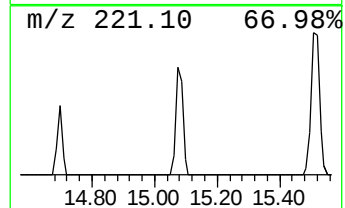
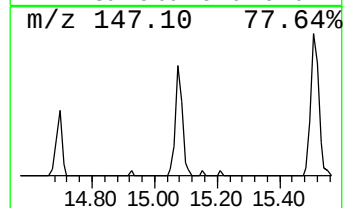
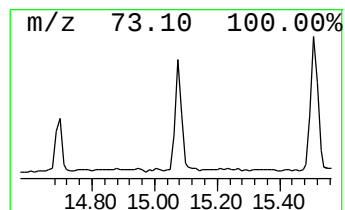
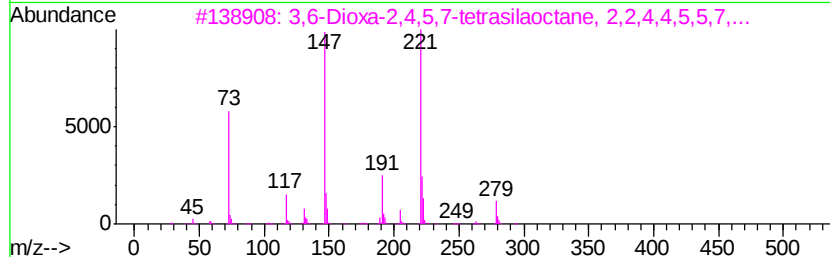
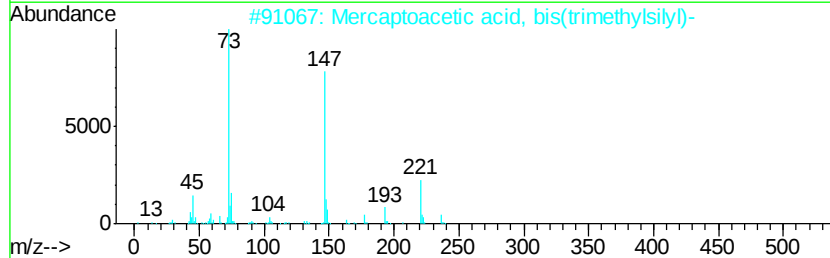
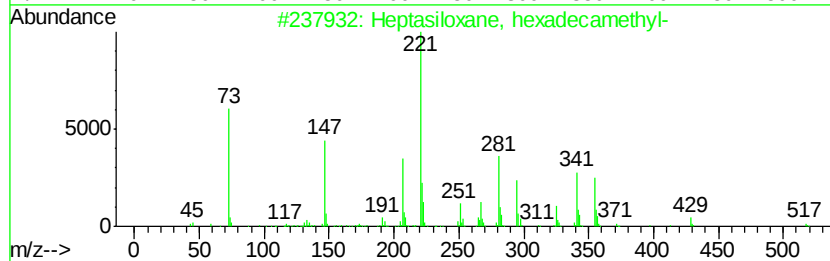
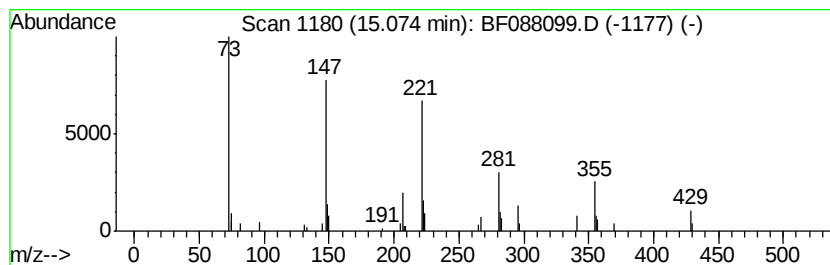
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.07 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.15 ng	64356	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	49
2		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	37
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	35
5		3-Oxa-6-thia-2,7-disilaoctane, 2...	222	C8H22OSSi2	078921-31-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061716\
Data File : BF088099.D
Acq On : 17 Jun 2016 18:08
Operator : UM/SJ
Sample : H3558-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.14	16.3	ng	485180	1	6.70	595755	20.0
2-Pentanone, 4-hy...	4.83	23.2	ng	690347	1	6.70	595755	20.0
2-Pentanone, 4-me...	5.69	3.2	ng	94897	1	6.70	595755	20.0
unknown6.46	6.46	35.6	ng	1061200	1	6.70	595755	20.0
Heptacosane	10.64	2.1	ng	102524	4	11.21	991326	20.0
n-Hexadecanoic acid	11.76	2.4	ng	118024	4	11.21	991326	20.0
Trifluoroacetoxy ...	13.70	2.2	ng	90204	5	13.84	811586	20.0
unknown15.07	15.07	2.1	ng	64356	6	15.22	597985	20.0