

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
 Data File : BF088132.D
 Acq On : 18 Jun 2016 14:16
 Operator : UM/SJ
 Sample : H3501-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS5-0-6

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-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	15	rVB	91002	151770	7.04%	0.696%
2	1.781	15	17	23	rVV	809091	1158958	53.78%	5.315%
3	1.861	23	24	39	rVB	88895	204139	9.47%	0.936%
4	2.056	39	41	53	rVB2	11793	40894	1.90%	0.188%
5	2.250	56	58	62	rVB	20013	25989	1.21%	0.119%
6	2.913	115	116	127	rBV	13911	36328	1.69%	0.167%
7	4.856	284	286	291	rBV	89268	147043	6.82%	0.674%
8	5.290	322	324	327	rBV	1634538	1907846	88.53%	8.749%
9	6.353	414	417	419	rBV	1745101	2005017	93.04%	9.195%
10	6.467	424	427	429	rBV	1704348	2155107	100.00%	9.883%
11	6.685	444	446	449	rBV	683260	574443	26.65%	2.634%
12	6.845	457	460	462	rBV	1976003	1812711	84.11%	8.313%
13	7.256	493	496	498	rBV	1144594	1111755	51.59%	5.098%
14	7.382	505	507	510	rVB2	17459	28029	1.30%	0.129%
15	7.736	535	538	545	rBV2	20754	34500	1.60%	0.158%
16	7.976	556	559	561	rBV	699593	724221	33.60%	3.321%
17	8.753	625	627	632	rVB	20497	37513	1.74%	0.172%
18	8.982	644	647	648	rBV	35055	32234	1.50%	0.148%
19	9.050	650	653	656	rVB	2146269	2145070	99.53%	9.837%
20	9.451	684	688	690	rBV	451471	397525	18.45%	1.823%
21	9.542	693	696	699	rVV2	48363	80096	3.72%	0.367%
22	9.725	709	712	714	rVB	759388	724848	33.63%	3.324%
23	10.056	736	741	745	rBV4	12568	34130	1.58%	0.157%
24	10.136	745	748	749	rBV	59079	59937	2.78%	0.275%
25	10.159	749	750	754	rVB	39269	38390	1.78%	0.176%
26	10.376	767	769	772	rBV	13880	22381	1.04%	0.103%
27	10.514	778	781	783	rBV	934048	1060256	49.20%	4.862%
28	10.639	790	792	796	rBV	47916	89750	4.16%	0.412%
29	10.834	805	809	810	rBV3	11084	24497	1.14%	0.112%
30	10.948	817	819	821	rVB	18857	26073	1.21%	0.120%
31	10.994	821	823	826	rVB3	19760	36304	1.68%	0.166%
32	11.085	829	831	832	rBV	49514	74470	3.46%	0.342%
33	11.199	839	841	845	rBV	718477	633739	29.41%	2.906%
34	11.268	845	847	850	rVB2	19418	33400	1.55%	0.153%

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35	11.439	859	862	865	rBV3	44535	81158	3.77%	0.372%
36	11.508	865	868	870	rVV	61574	68510	3.18%	0.314%
37	11.668	880	882	883	rBV	17576	24435	1.13%	0.112%
38	11.748	887	889	892	rVV2	77097	137742	6.39%	0.632%
39	11.794	892	893	898	rVB4	25818	54918	2.55%	0.252%
40	11.908	901	903	905	rBV	44225	42732	1.98%	0.196%
41	12.251	931	933	936	rBV2	25963	46565	2.16%	0.214%
42	12.297	936	937	939	rVB	34724	31703	1.47%	0.145%
43	12.411	944	947	948	rBV	71796	80952	3.76%	0.371%
44	12.639	965	967	968	rBV	44705	57389	2.66%	0.263%
45	12.674	968	970	972	rVV	334855	340491	15.80%	1.561%
46	12.788	977	980	982	rBV	1674542	1772662	82.25%	8.129%
47	13.691	1056	1059	1063	rBV2	93001	159376	7.40%	0.731%
48	13.828	1069	1071	1073	rBV	589282	629820	29.22%	2.888%
49	14.674	1143	1145	1147	rBV	159796	209237	9.71%	0.960%
50	15.211	1190	1192	1196	rVB	290207	399102	18.52%	1.830%

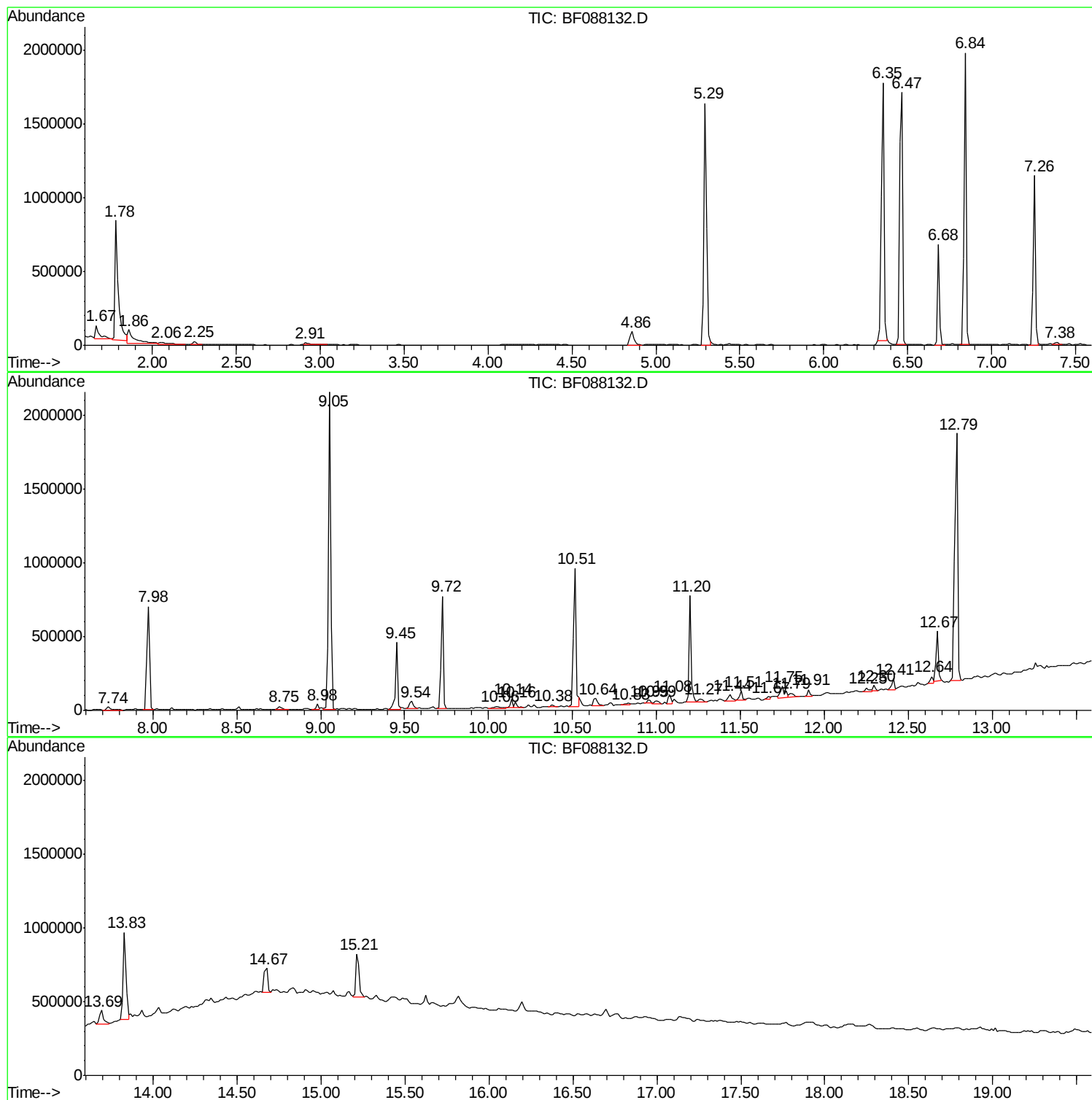
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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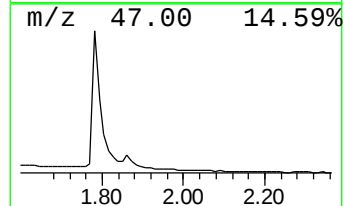
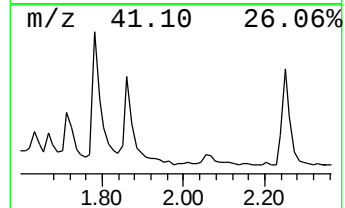
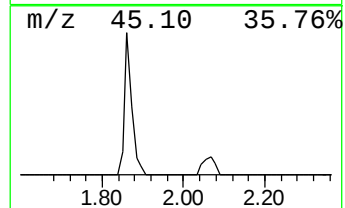
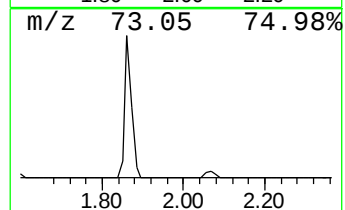
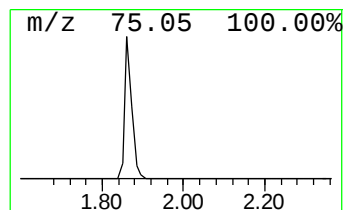
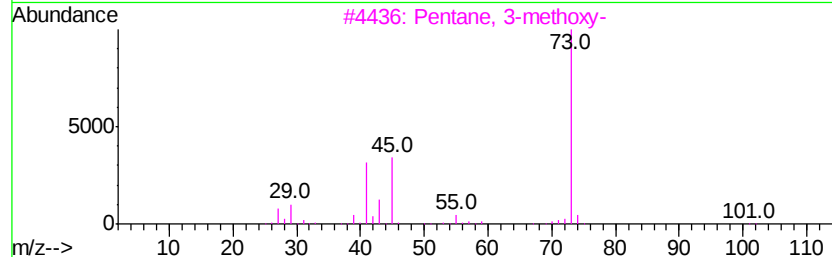
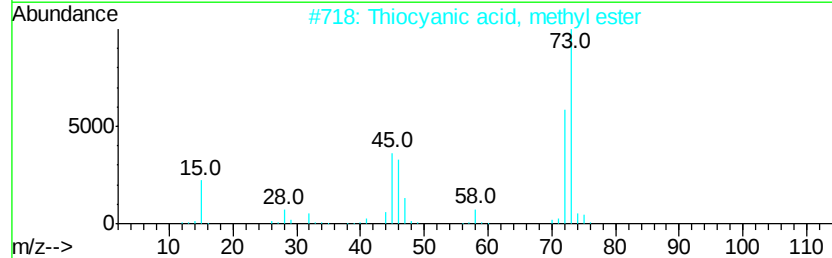
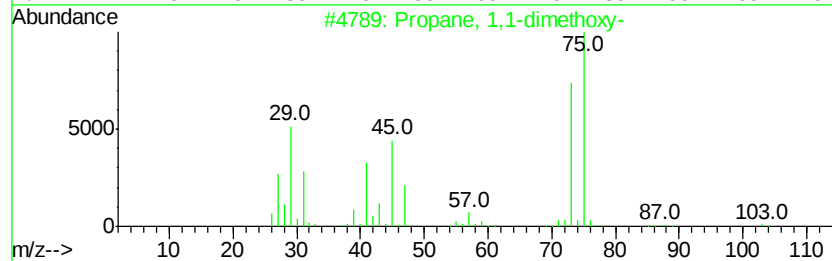
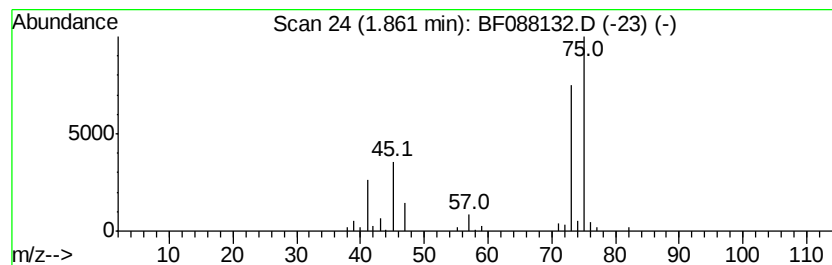
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.86	7.11 ng	204139	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	16
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
5		Glycine	75	C2H5NO2	000056-40-6	9



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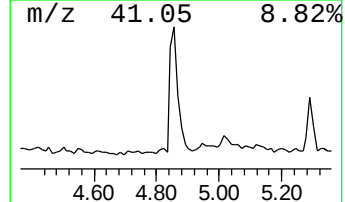
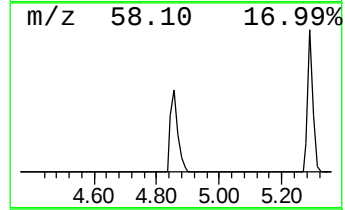
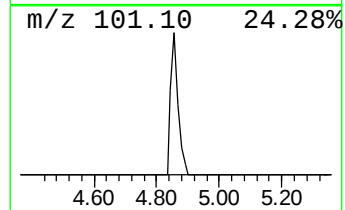
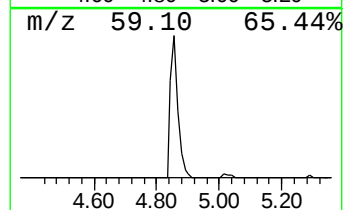
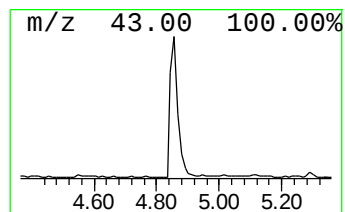
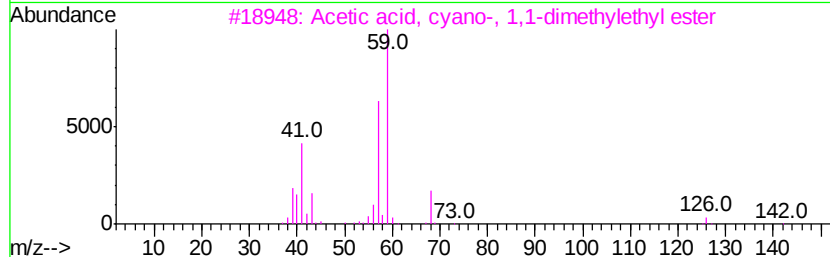
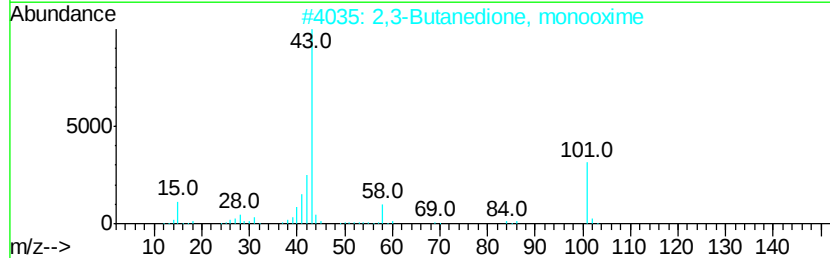
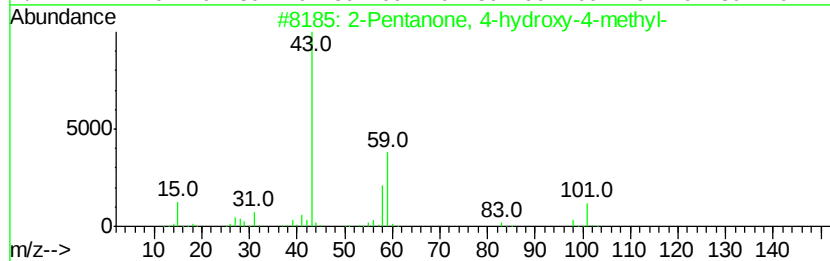
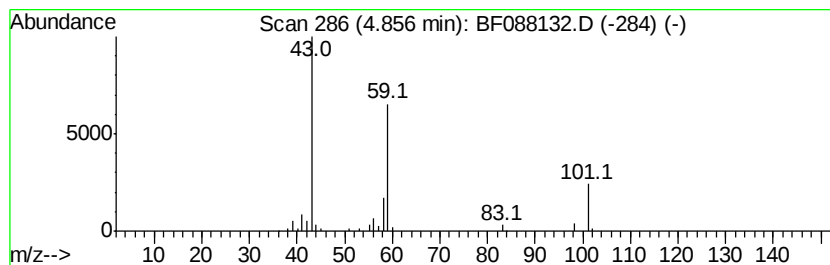
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	5.12 ng	147043	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17		
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17		
5	Acetone	58	C3H6O	000067-64-1	10		



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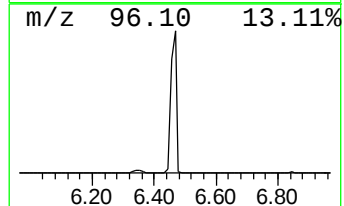
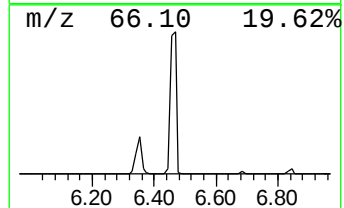
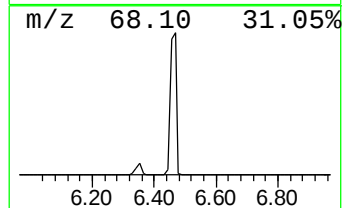
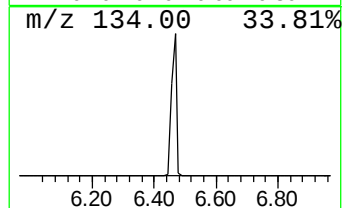
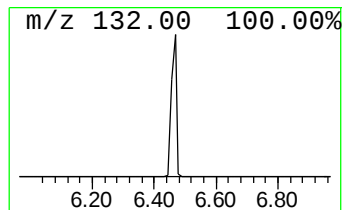
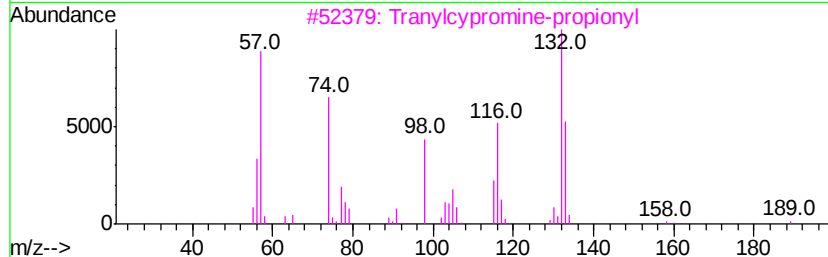
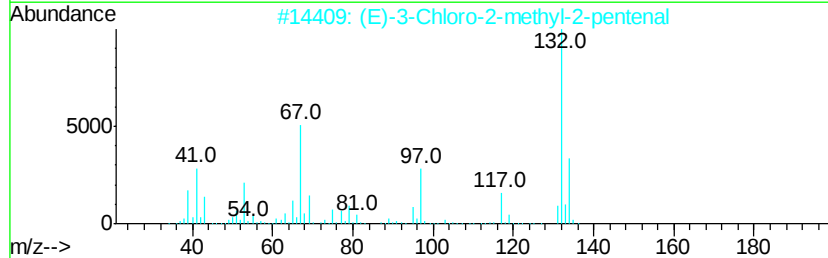
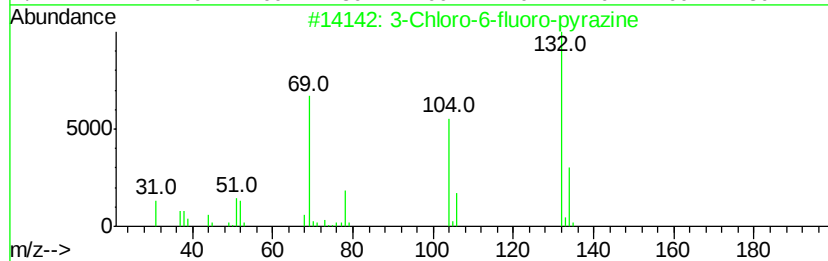
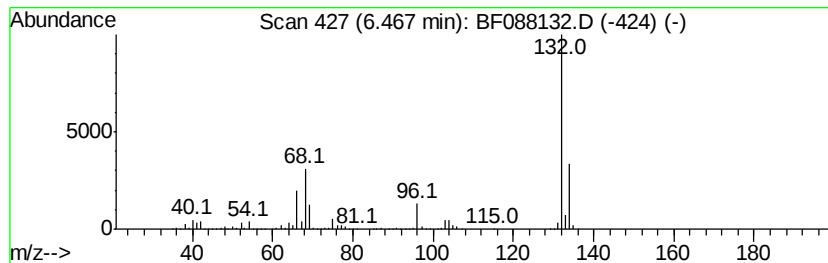
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	75.03 ng	2155110	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25	
3	Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	16	
4	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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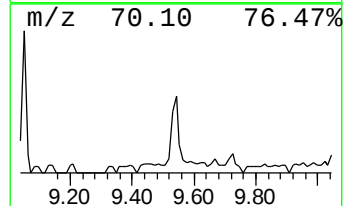
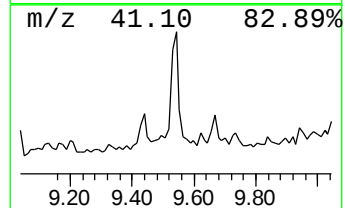
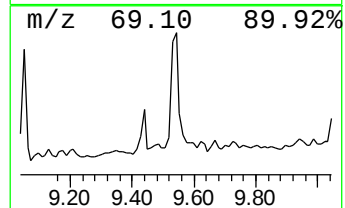
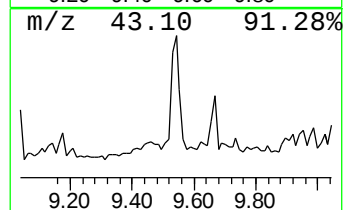
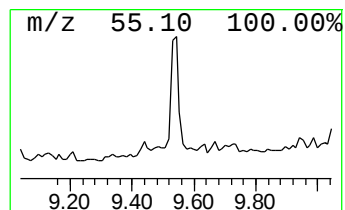
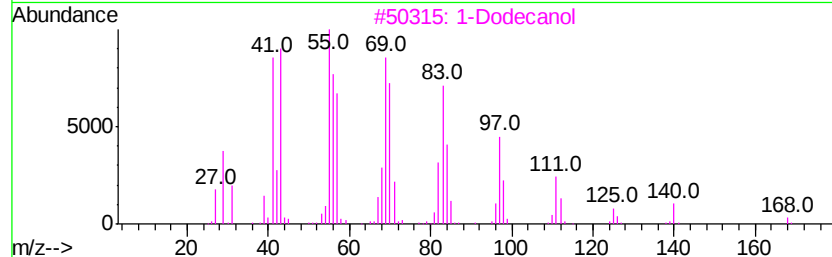
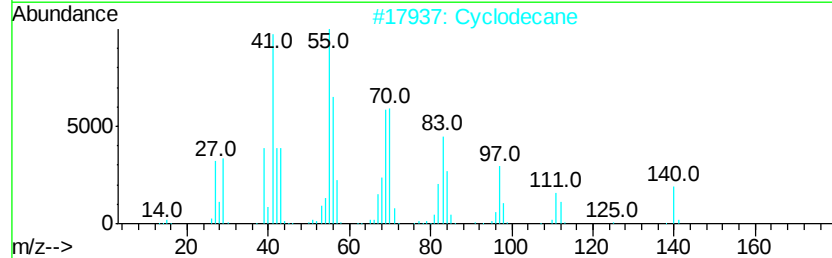
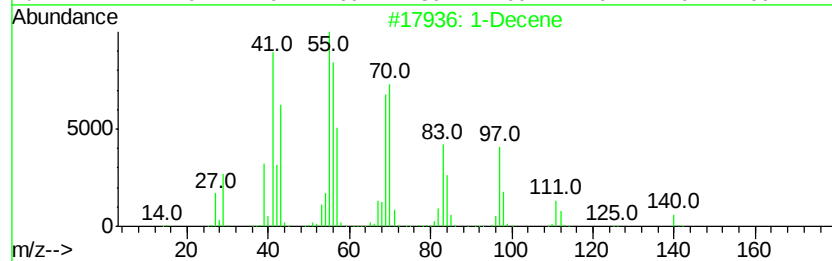
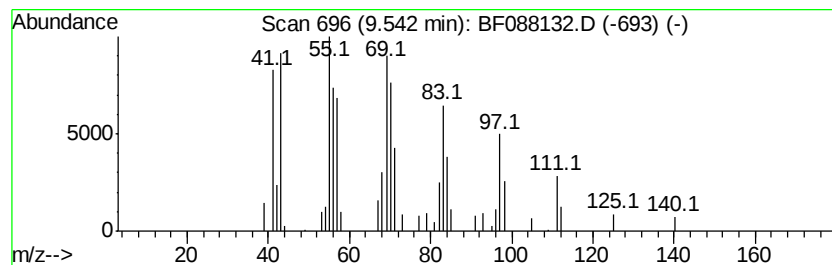
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Peak Number 7 1-Decene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	2.21 ng	80096	Acenaphthene-d10	9.72
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Decene		140 C10H20	000872-05-9 95
2	Cyclodecane		140 C10H20	000293-96-9 91
3	1-Dodecanol		186 C12H26O	000112-53-8 91
4	1-Undecanol		172 C11H24O	000112-42-5 83
5	Carbonochloridic acid, decyl ester		220 C11H21ClO2	055488-51-2 80



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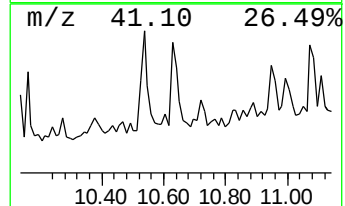
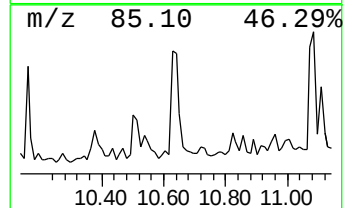
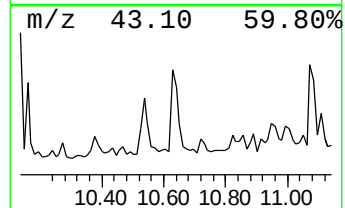
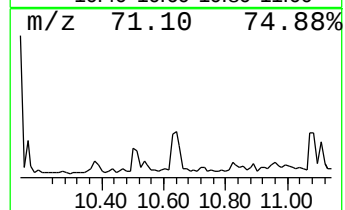
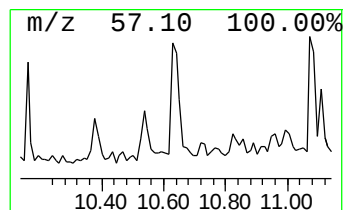
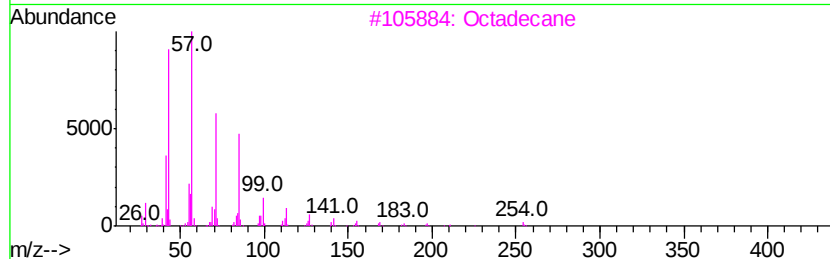
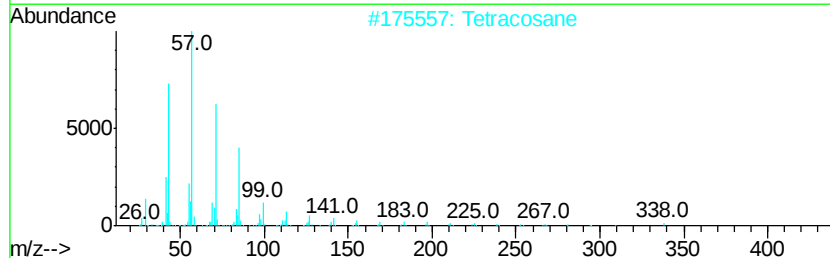
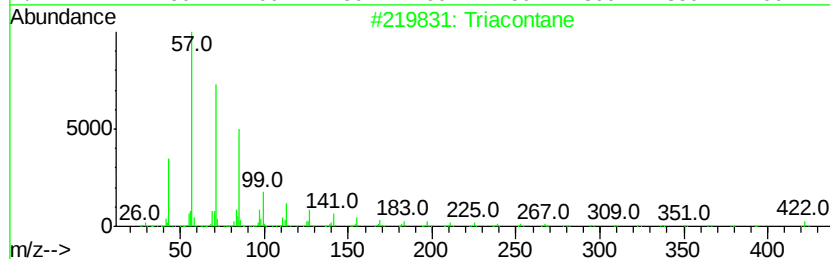
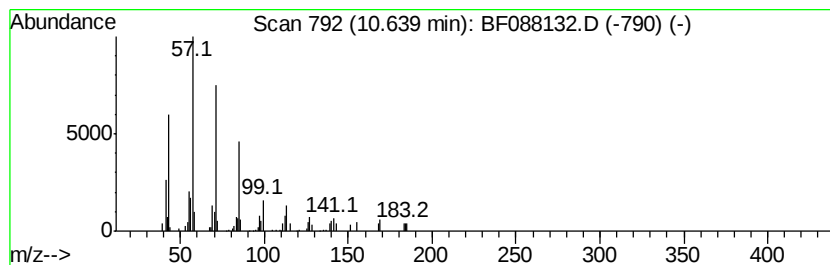
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ClientSampleId :
SS5-0-6

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 8 Triacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.64	2.83 ng	89750	Phenanthrene-d10		11.20
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	87
2	Tetracosane	338	C24H50	000646-31-1	87
3	Octadecane	254	C18H38	000593-45-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088132.D
Acq On : 18 Jun 2016 14:16
Operator : UM/SJ
Sample : H3501-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS5-0-6

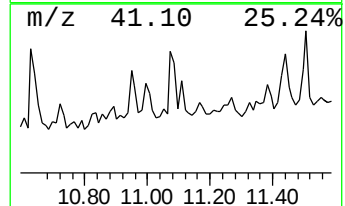
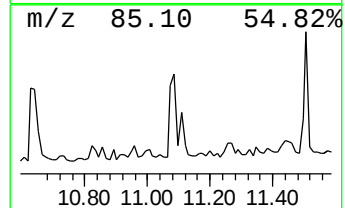
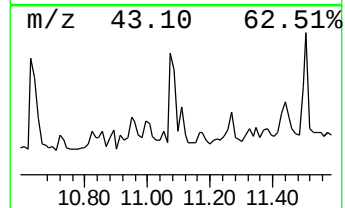
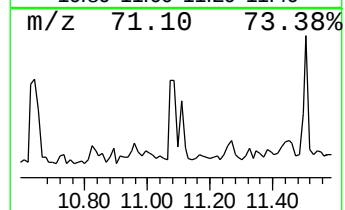
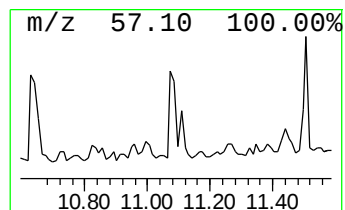
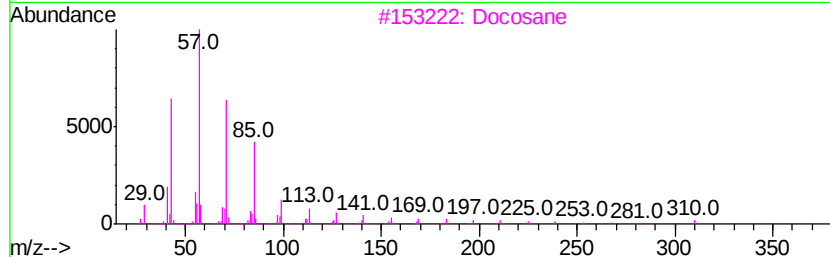
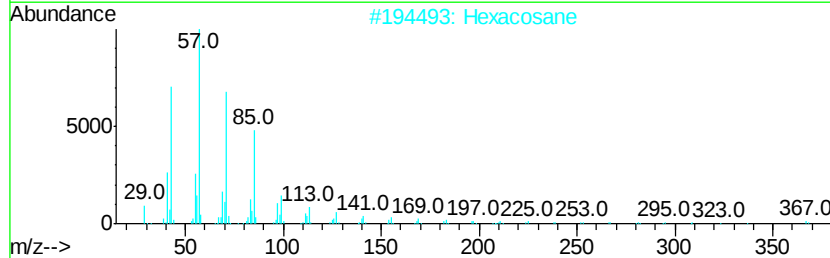
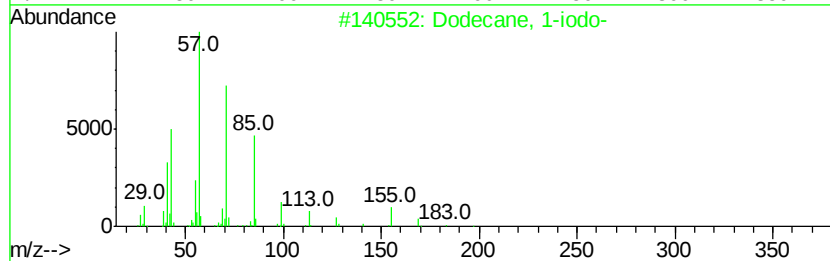
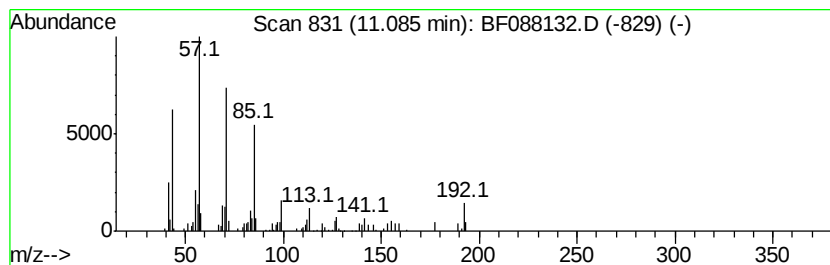
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dodecane, 1-iodo- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	2.35 ng	74470	Phenanthrene-d10	11.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
2			Hexacosane	366	C26H54	000630-01-3	83
3			Docosane	310	C22H46	000629-97-0	80
4			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088132.D
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Sample : H3501-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

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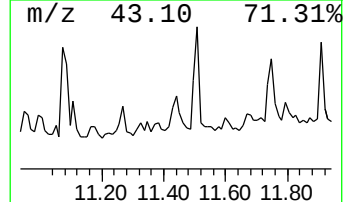
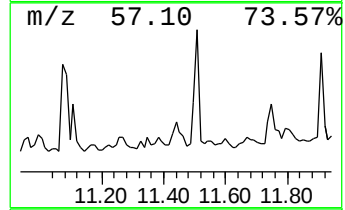
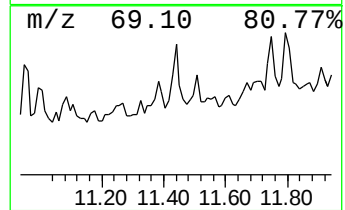
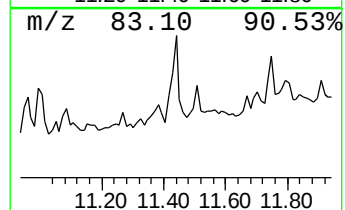
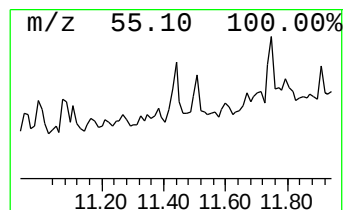
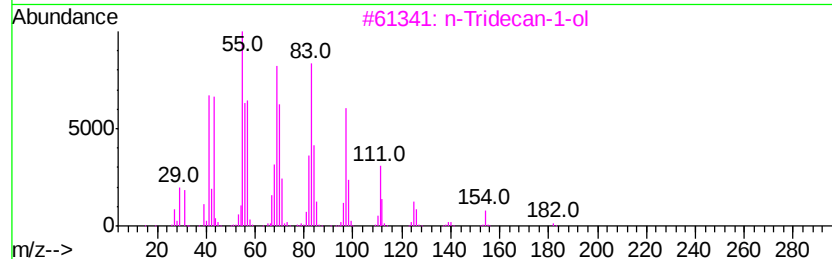
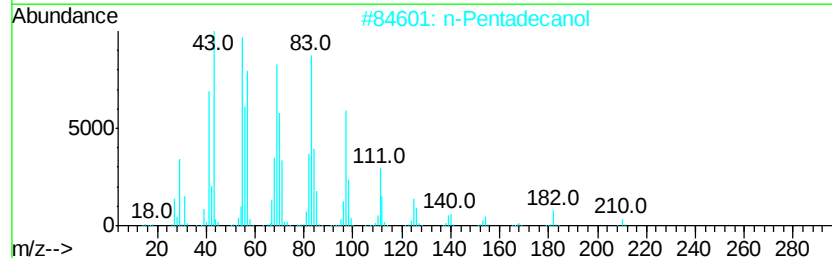
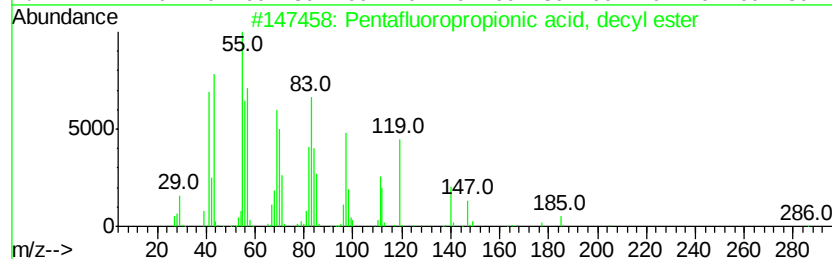
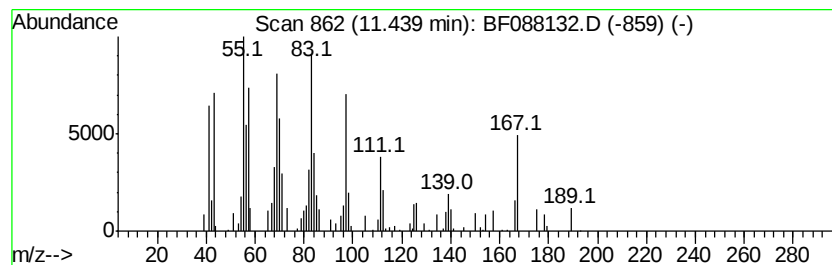
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	2.56 ng	81158	Phenanthrene-d10	11.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, decyl...	304	C13H21F5O2	959000-65-8	83
2			n-Pentadecanol	228	C15H32O	000629-76-5	81
3			n-Tridecan-1-ol	200	C13H28O	000112-70-9	81
4			1-Tetradecanol	214	C14H30O	000112-72-1	81
5			1-Hexadecanol	242	C16H34O	036653-82-4	81



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Data File : BF088132.D
Acq On : 18 Jun 2016 14:16
Operator : UM/SJ
Sample : H3501-05
Misc :
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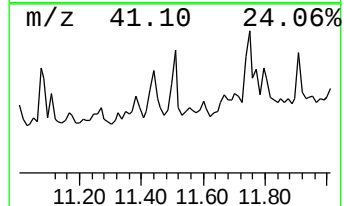
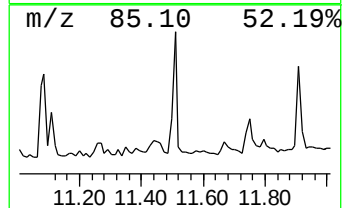
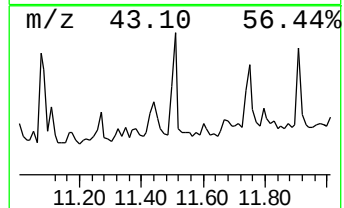
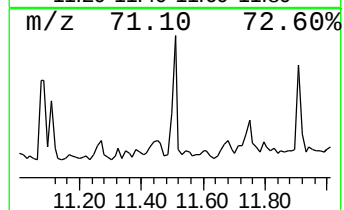
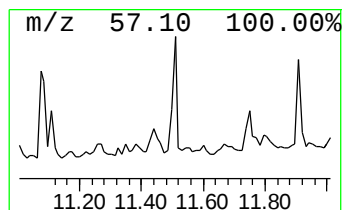
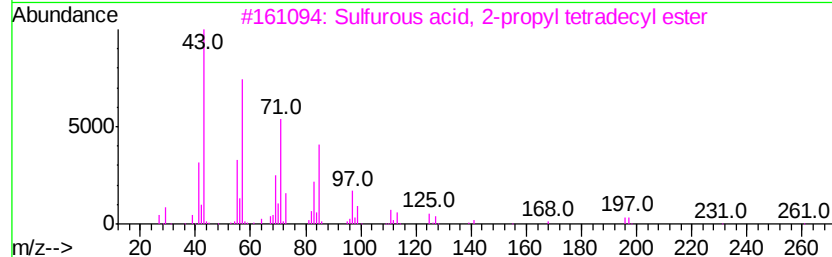
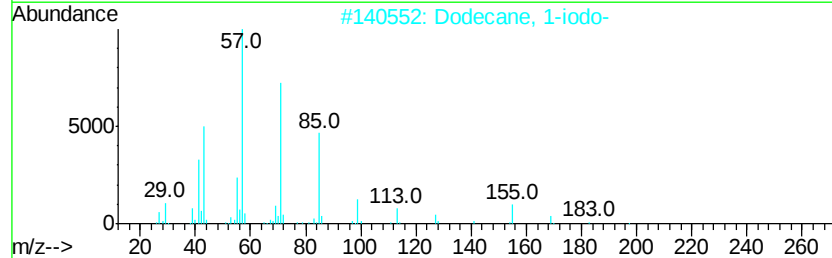
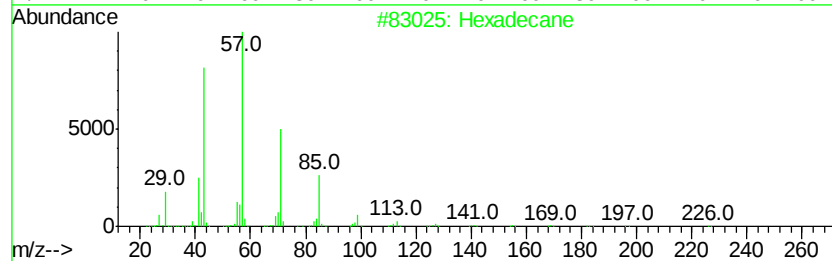
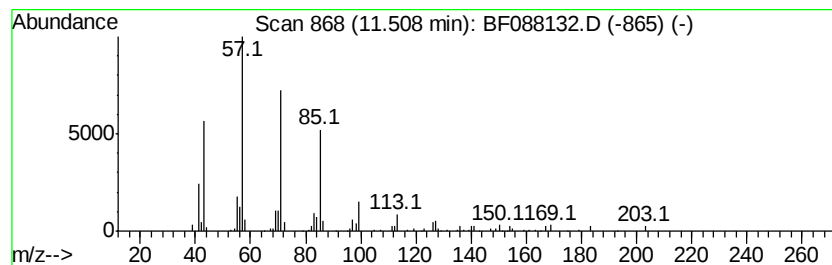
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.51	2.16 ng	68510	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Sulfurous acid, 2-propyl tetradecyl ester	320	C17H36O3S	1000309-12-5	86
4	Heneicosane	296	C21H44	000629-94-7	80
5	Sulfurous acid, pentadecyl 2-propyl ester	334	C18H38O3S	1000309-12-6	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088132.D
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Operator : UM/SJ
Sample : H3501-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

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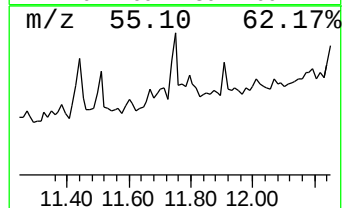
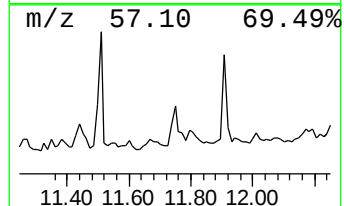
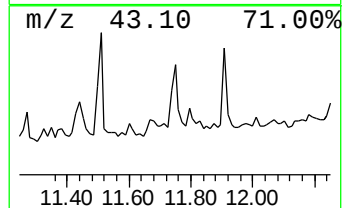
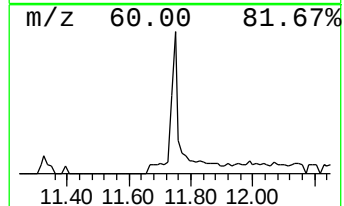
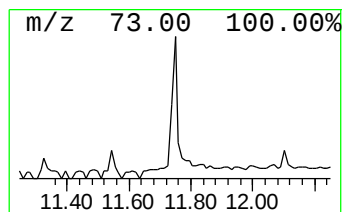
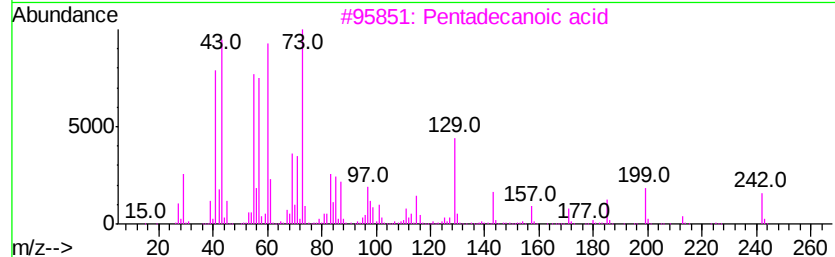
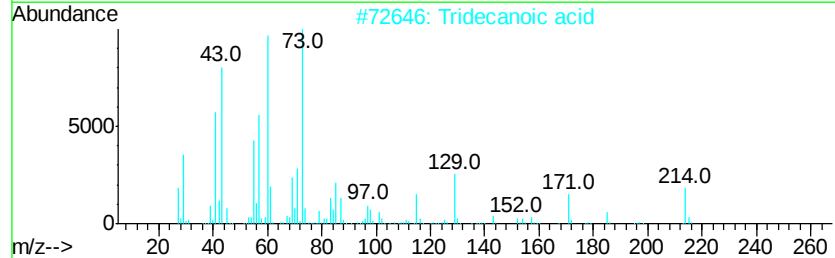
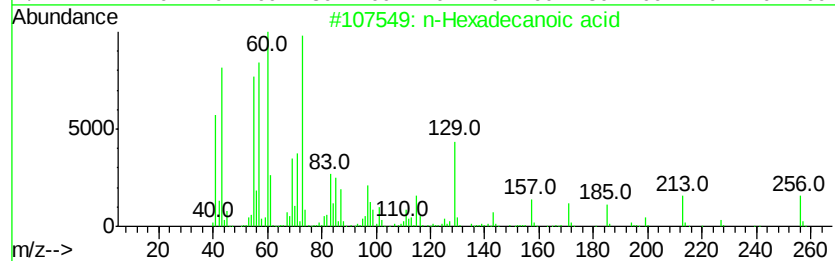
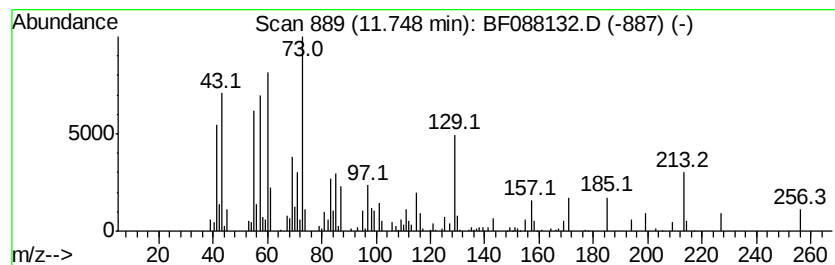
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	4.35 ng	137742	Phenanthrene-d10	11.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
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Misc :
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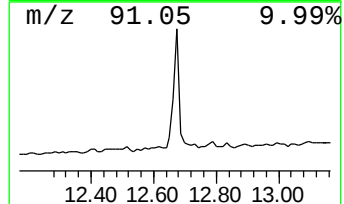
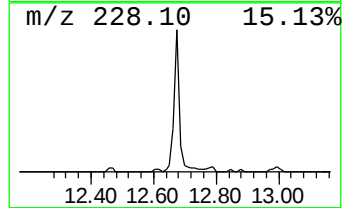
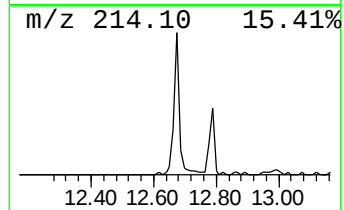
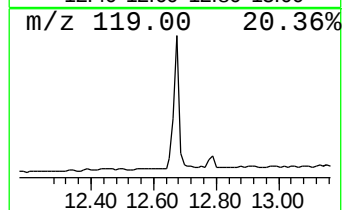
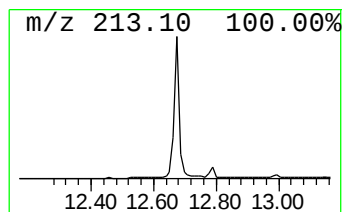
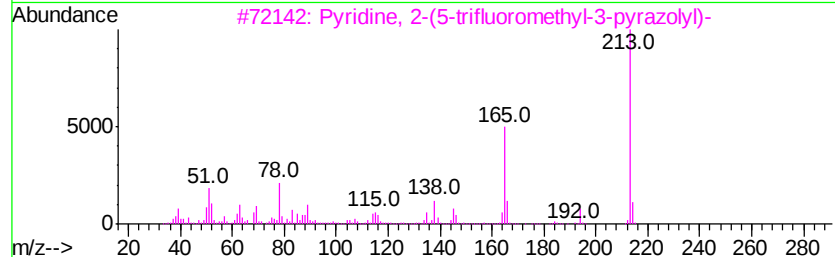
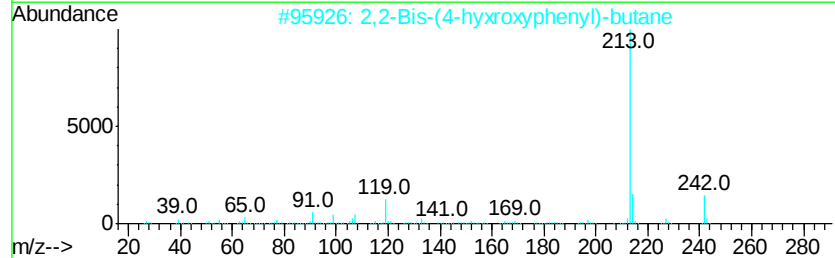
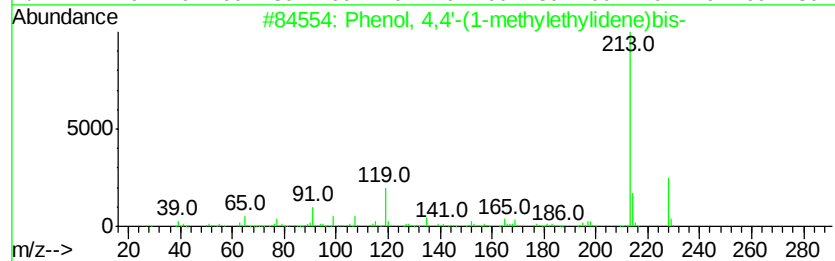
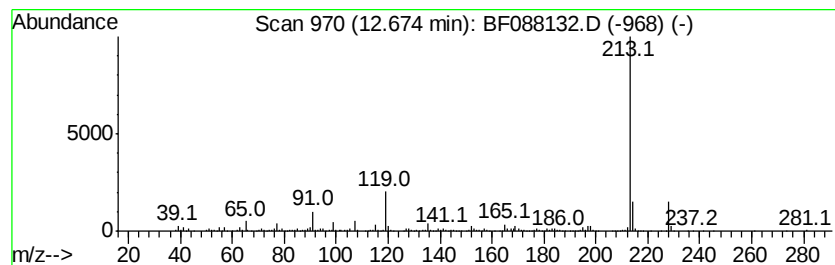
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	10.81 ng	340491	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	97
2		2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
3		Pyridine, 2-(5-trifluoromethyl-3-pyrazolyl)-	213	C9H6F3N3	003974-71-8	53
4		2-Bromo-7-(methylamino)tropone	213	C8H8BrNO	103539-25-9	53
5		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
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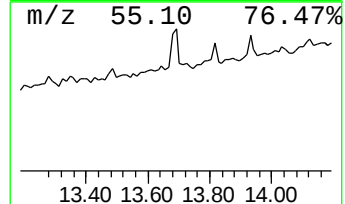
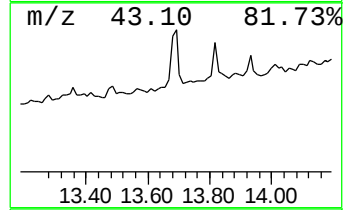
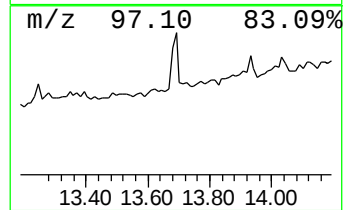
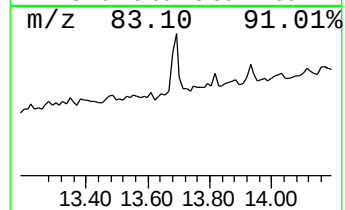
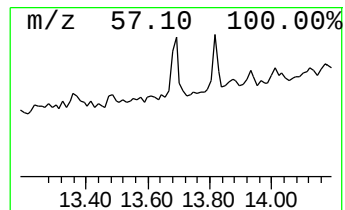
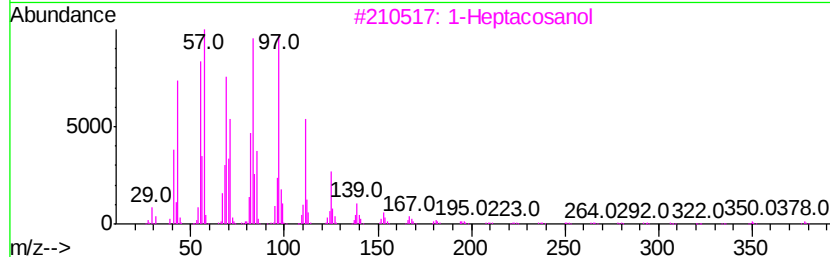
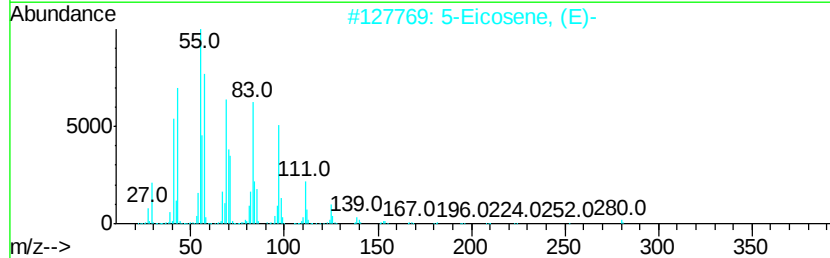
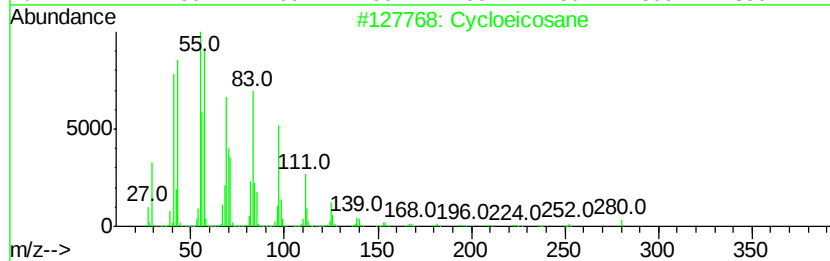
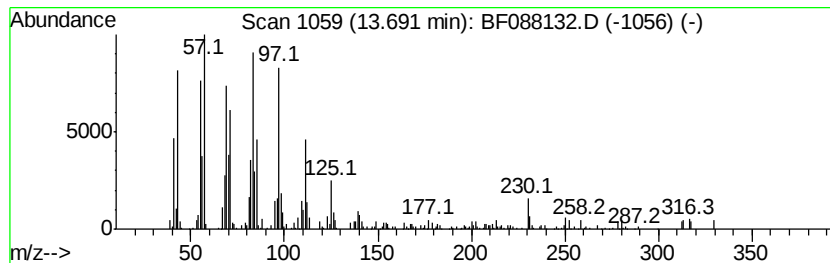
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Cycloeicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	5.06 ng	159376	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
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ALS Vial : 8 Sample Multiplier: 1

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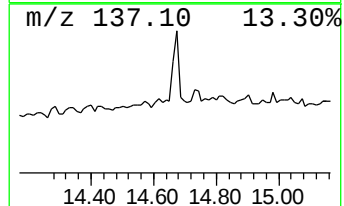
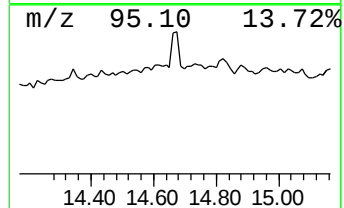
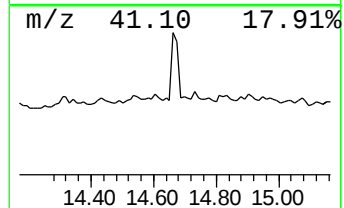
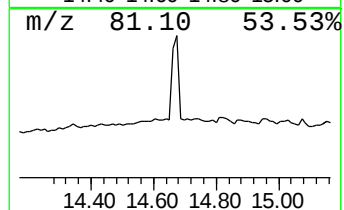
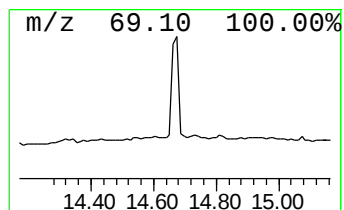
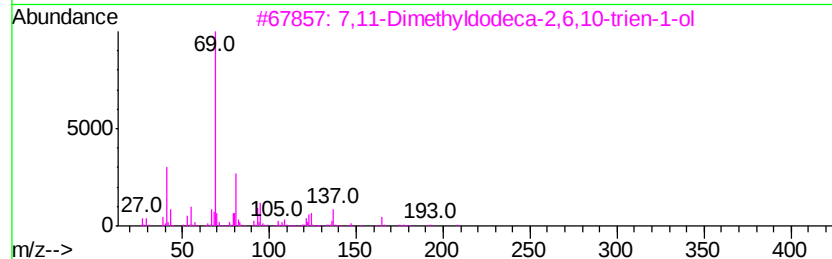
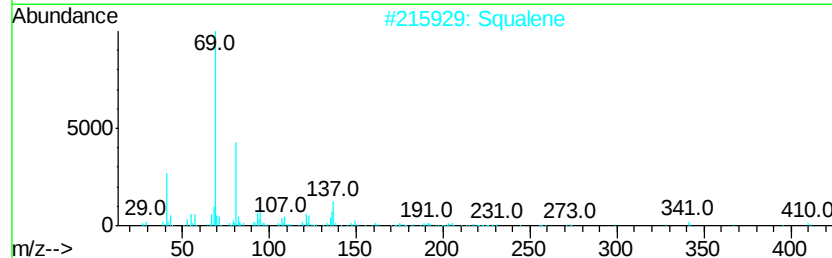
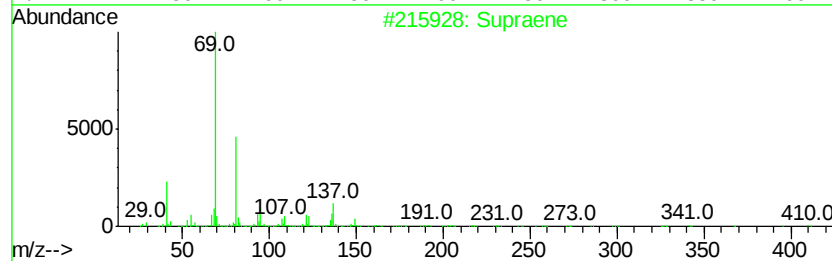
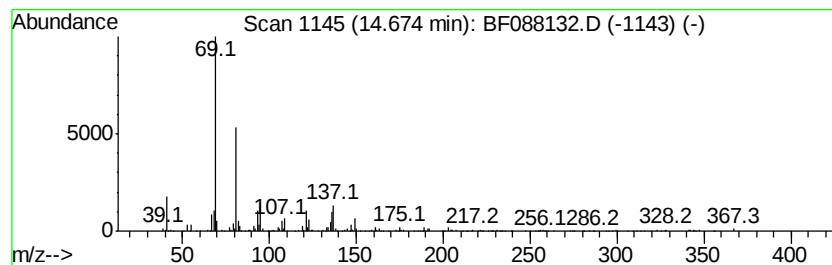
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	10.49 ng	209237	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24	125529-10-4	64
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
 Data File : BF088132.D
 Acq On : 18 Jun 2016 14:16
 Operator : UM/SJ
 Sample : H3501-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS5-0-6

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
Propane, 1,1-dime...	1.86	7.1 ng		204139	1	6.68	574443	20.0
2-Pentanone, 4-hy...	4.86	5.1 ng		147043	1	6.68	574443	20.0
unknown6.47	6.47	75.0 ng		2155110	1	6.68	574443	20.0
1-Decene	9.54	2.2 ng		80096	3	9.72	724848	20.0
triacontane	10.64	2.8 ng		89750	4	11.20	633739	20.0
Dodecane, 1-iodo-	11.09	2.4 ng		74470	4	11.20	633739	20.0
Pentafluoropropio...	11.44	2.6 ng		81158	4	11.20	633739	20.0
Hexadecane	11.51	2.2 ng		68510	4	11.20	633739	20.0
n-Hexadecanoic acid	11.75	4.3 ng		137742	4	11.20	633739	20.0
Phenol, 4,4'-(1-m...	12.67	10.8 ng		340491	5	13.83	629820	20.0
Cycloeicosane	13.69	5.1 ng		159376	5	13.83	629820	20.0
Supraene	14.67	10.5 ng		209237	6	15.21	399102	20.0