

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
 Data File : BF088970.D
 Acq On : 13 Jul 2016 21:08
 Operator : UM/SJ
 Sample : H3988-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C4.2-6

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-BF063016.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	155231	240250	10.14%	1.140%
2	1.781	16	17	26	rVV	1335706	2153548	90.85%	10.222%
3	1.895	26	27	63	rVB	74439	352059	14.85%	1.671%
4	4.856	283	286	292	rVB	119544	198664	8.38%	0.943%
5	5.290	321	324	327	rBV	1540237	1783106	75.22%	8.464%
6	6.353	413	417	419	rVB	1383400	2194262	92.57%	10.416%
7	6.467	424	427	429	rBV	2048053	2117355	89.32%	10.051%
8	6.696	445	447	449	rBV	439063	442689	18.67%	2.101%
9	6.856	458	461	463	rBV	1261414	1639075	69.14%	7.780%
10	7.267	493	497	499	rBB	975036	1391523	58.70%	6.605%
11	7.382	503	507	511	rBB	34215	47407	2.00%	0.225%
12	7.976	557	559	562	rBB	620146	538800	22.73%	2.558%
13	9.062	651	654	656	rBV	2456018	2370494	100.00%	11.252%
14	9.450	686	688	691	rBV	385070	415310	17.52%	1.971%
15	9.725	710	712	715	rBB	575664	548659	23.15%	2.604%
16	10.513	778	781	784	rBV	1234623	1260580	53.18%	5.984%
17	10.651	791	793	797	rBV	24983	47331	2.00%	0.225%
18	11.096	829	832	833	rBV	27407	33818	1.43%	0.161%
19	11.199	839	841	844	rVB	478588	479745	20.24%	2.277%
20	11.439	860	862	867	rVV	100686	143675	6.06%	0.682%
21	11.519	867	869	871	rVB	25134	24407	1.03%	0.116%
22	11.748	888	889	891	rBV	41850	32669	1.38%	0.155%
23	12.262	932	934	937	rBV	96925	100920	4.26%	0.479%
24	12.628	964	966	968	rBV	52267	48486	2.05%	0.230%
25	12.788	977	980	983	rBV	1481156	1352840	57.07%	6.422%
26	13.691	1057	1059	1064	rVB	145525	156209	6.59%	0.741%
27	13.828	1068	1071	1073	rBV	397187	377846	15.94%	1.794%
28	14.331	1112	1115	1122	rBV	51814	89411	3.77%	0.424%
29	14.914	1164	1166	1171	rBV2	15571	40694	1.72%	0.193%
30	15.200	1188	1191	1193	rBV	305788	358269	15.11%	1.701%
31	16.628	1313	1316	1324	rVB5	27240	62222	2.62%	0.295%
32	17.680	1404	1408	1412	rBV5	8661	24439	1.03%	0.116%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C4.2-6

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

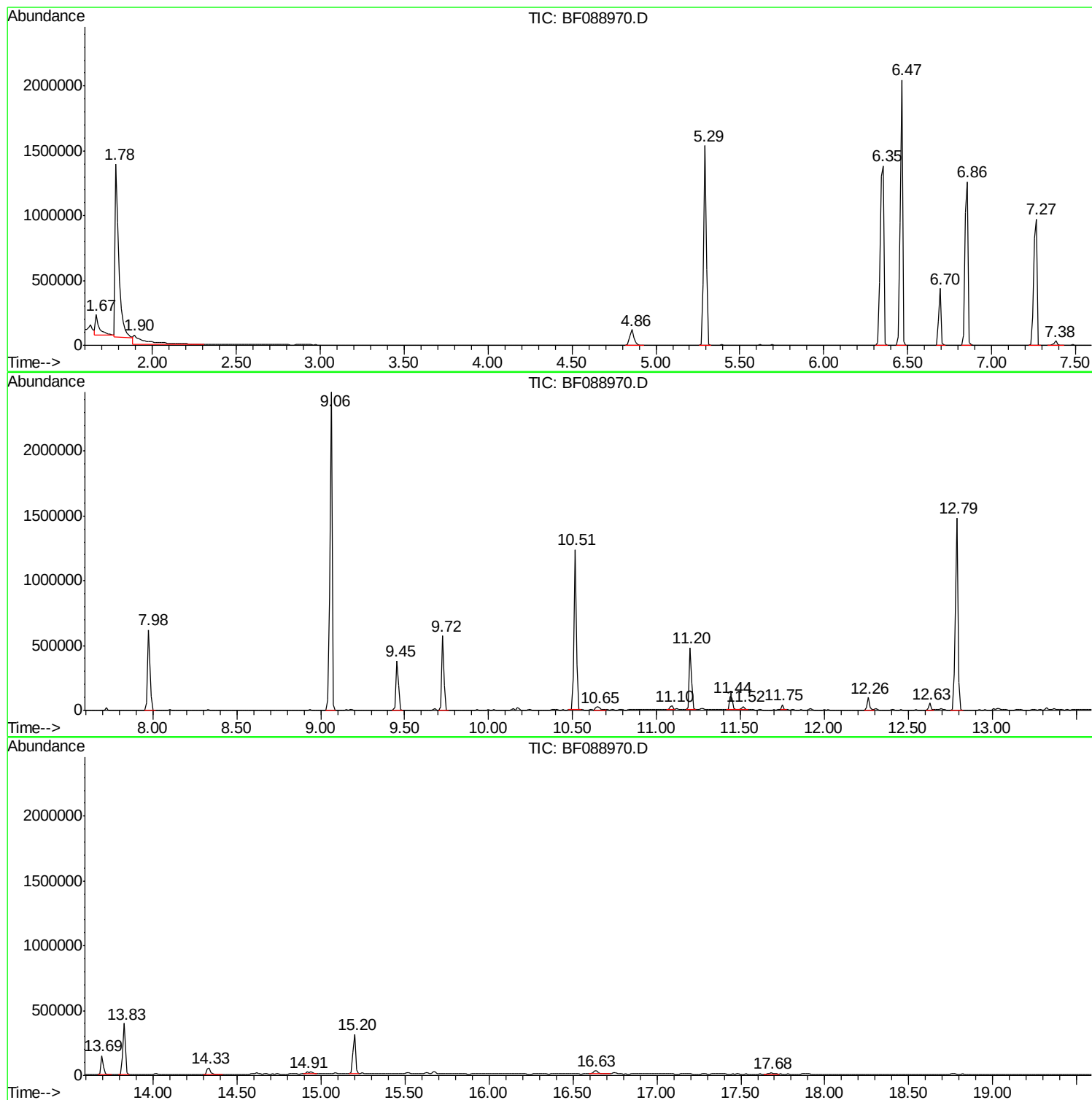
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Instrument :
BNA_F
ClientSampled :
C4.2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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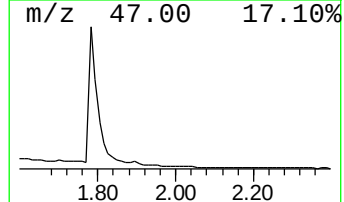
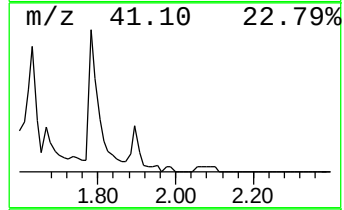
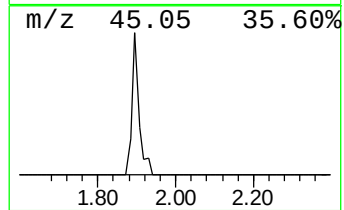
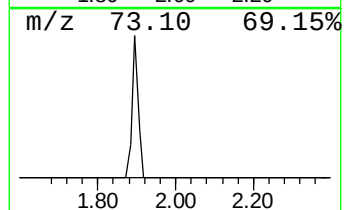
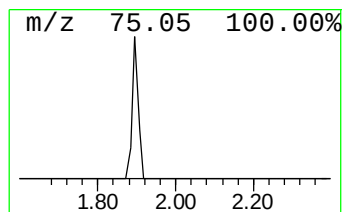
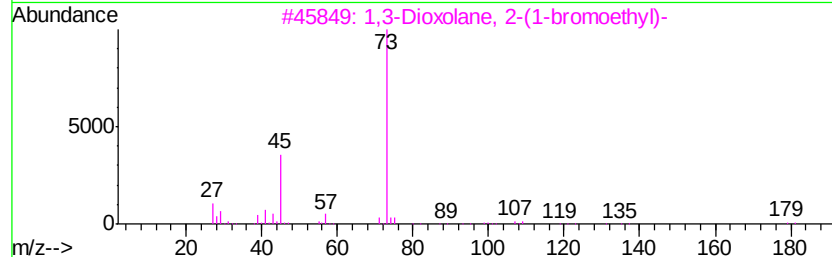
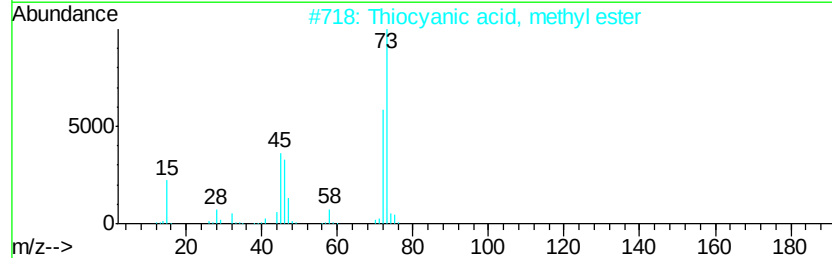
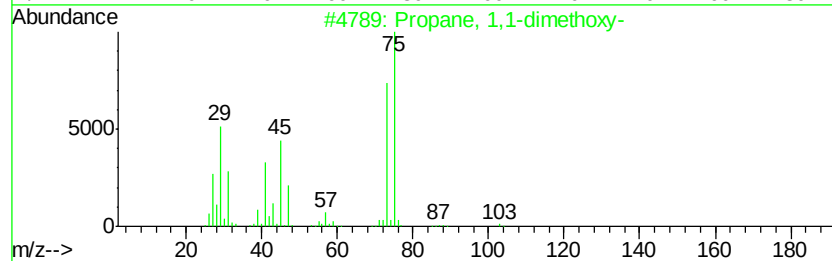
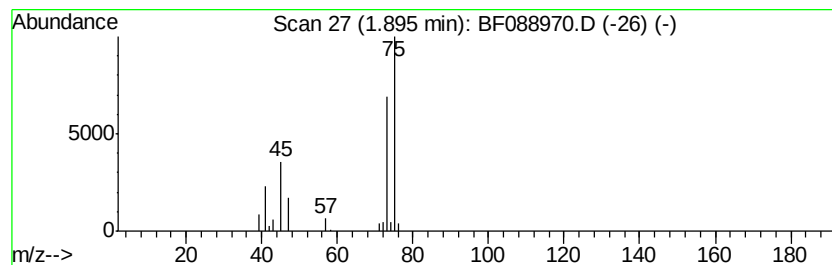
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.90	15.91 ng	352059	1,4-Dichlorobenzene-d4	6.70

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	9
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9



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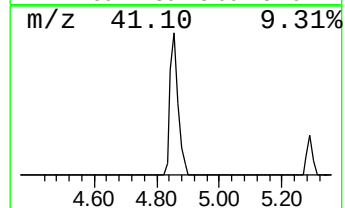
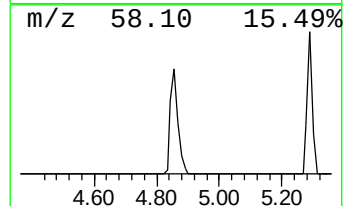
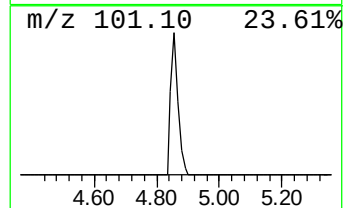
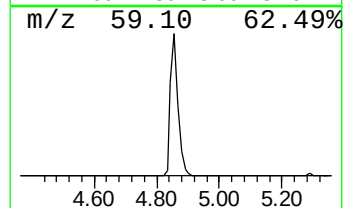
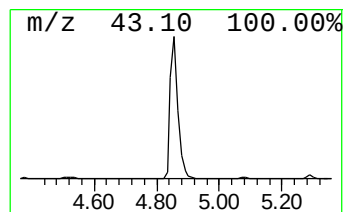
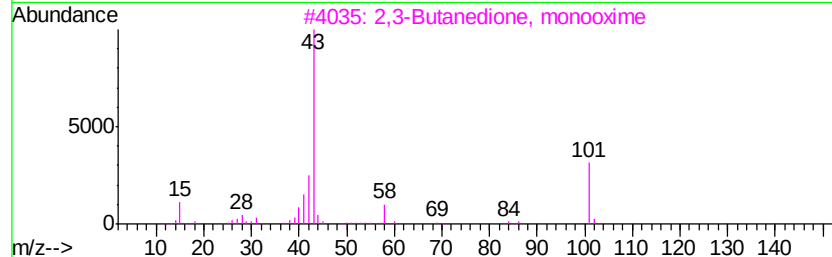
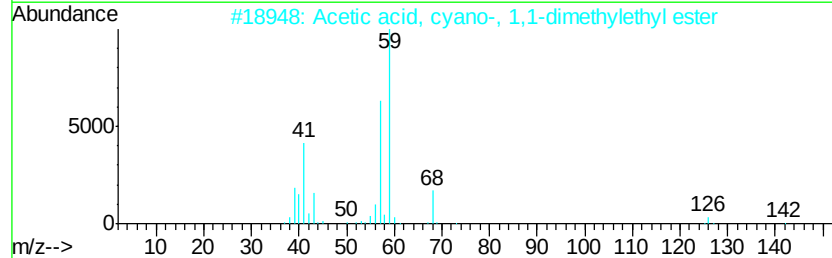
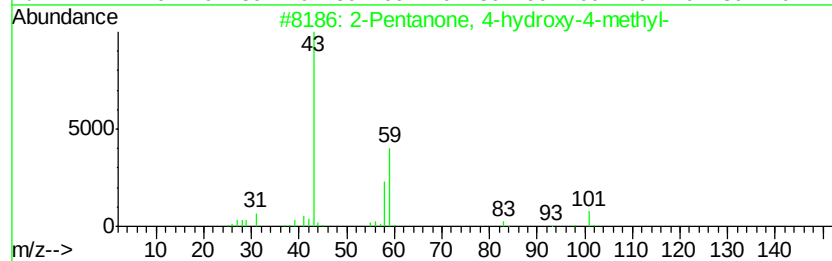
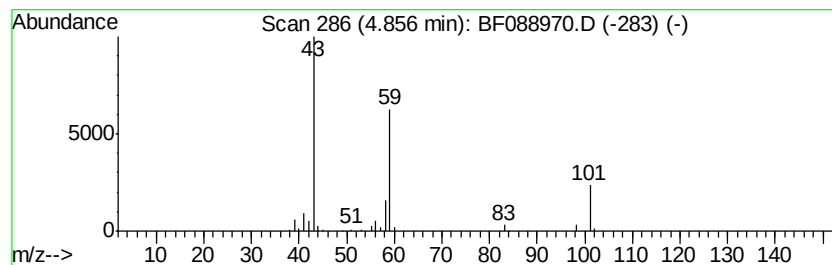
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	8.98 ng	198664	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		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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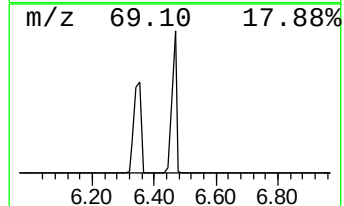
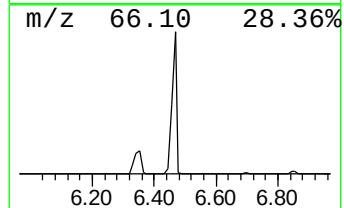
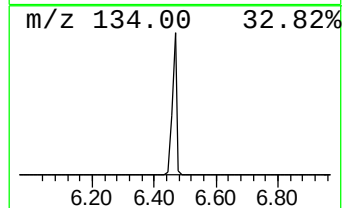
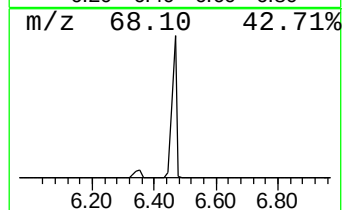
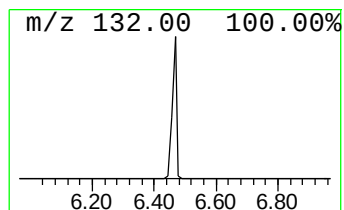
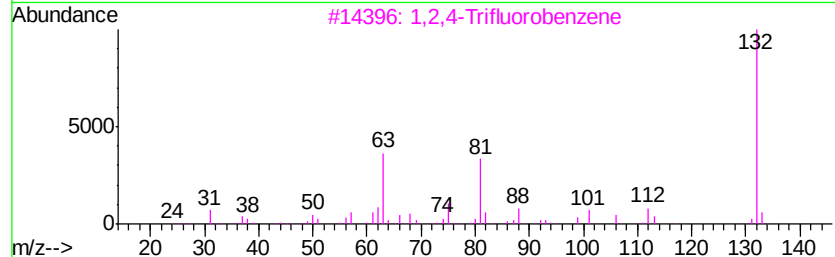
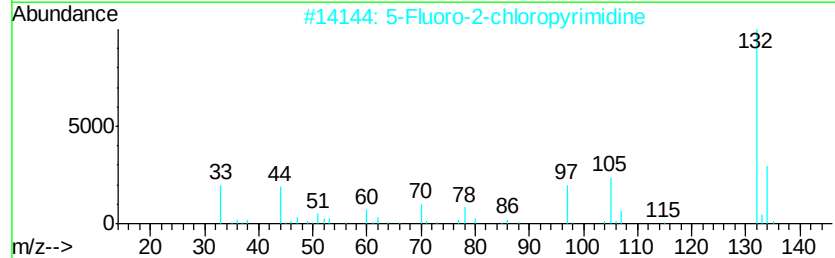
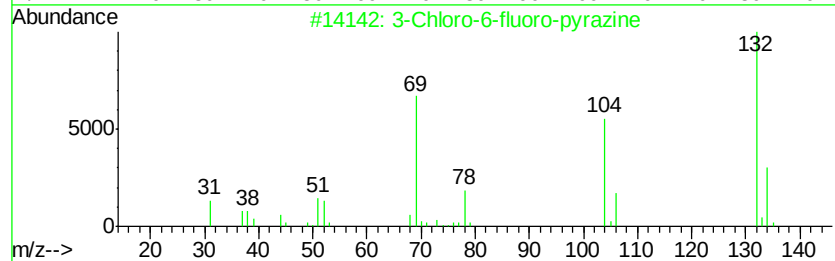
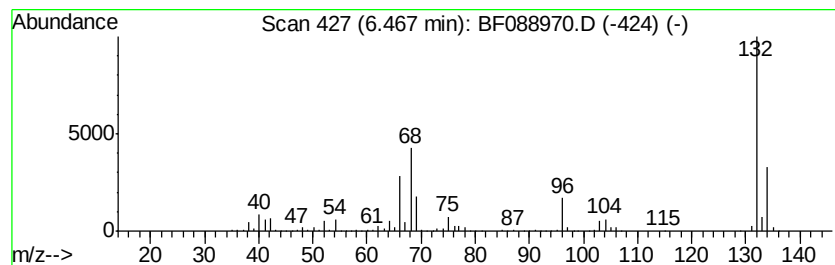
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	95.66 ng	2117360	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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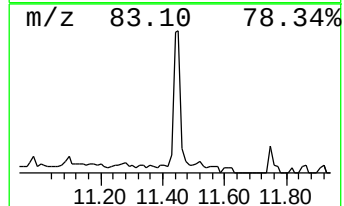
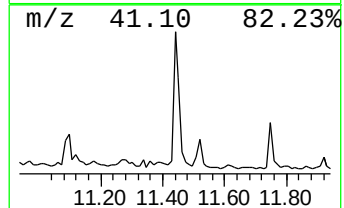
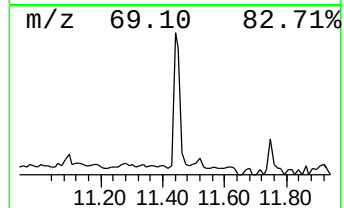
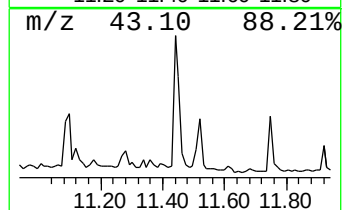
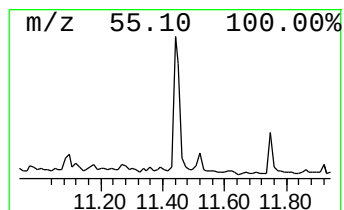
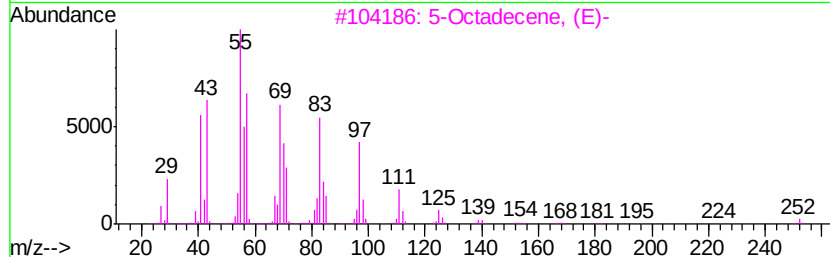
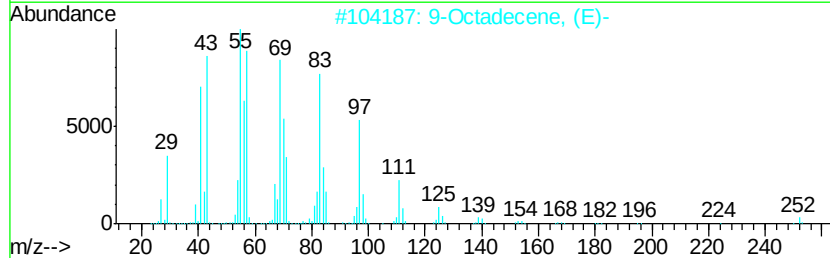
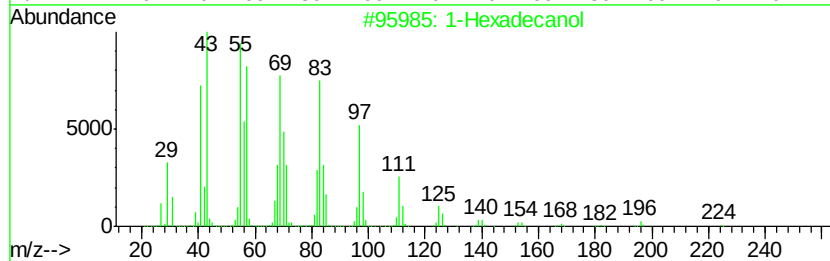
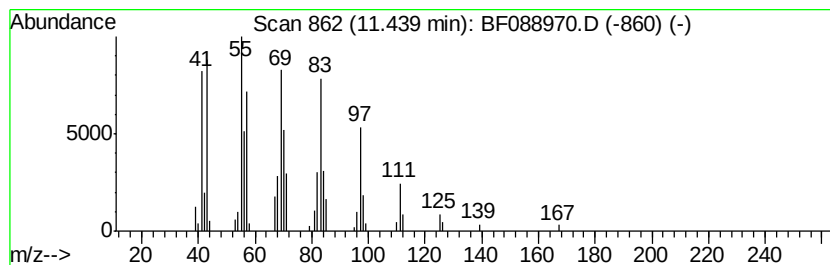
Instrument :
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ClientSampleId :
C4.2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.44	5.99 ng	143675	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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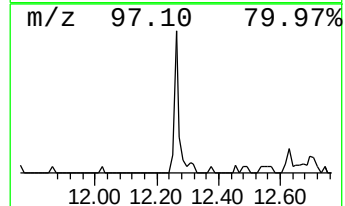
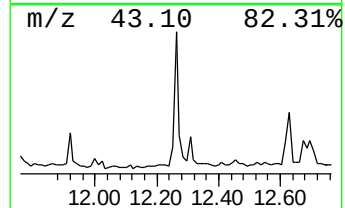
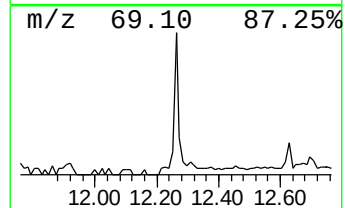
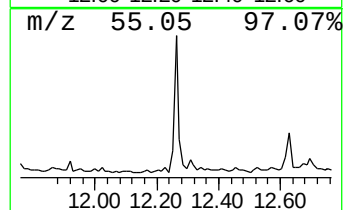
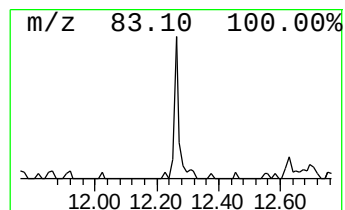
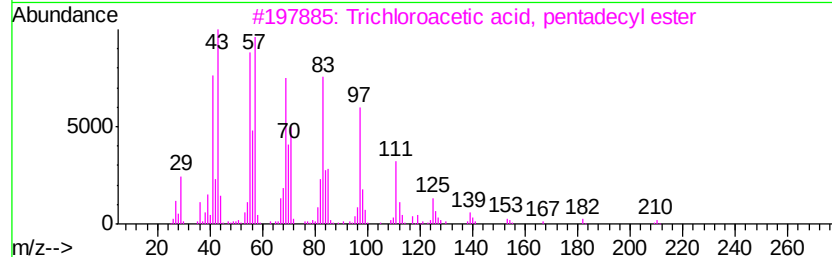
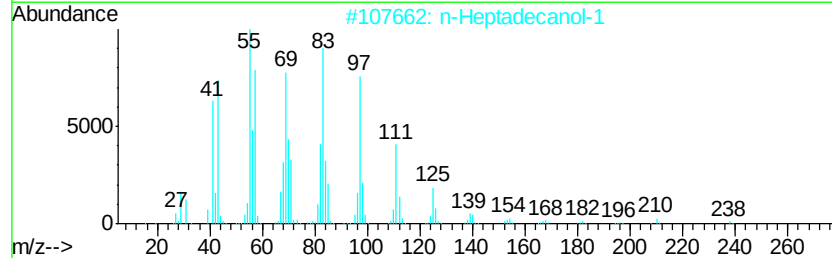
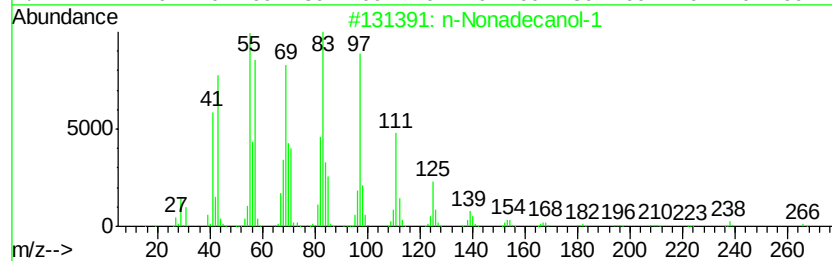
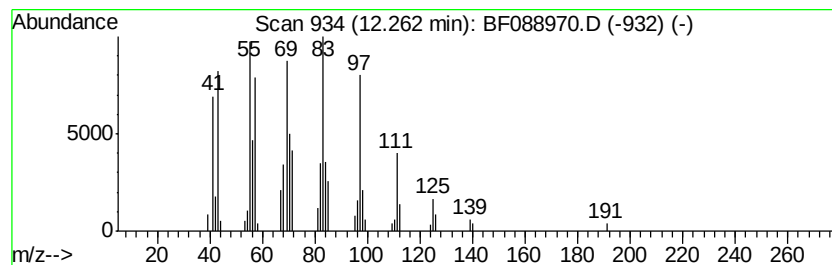
Instrument :
BNA_F
ClientSampled :
C4.2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Nonadecanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.26	4.21 ng	100920	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	91
5	1-Heptadecene	238	C17H34	006765-39-5	91



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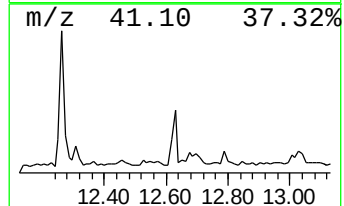
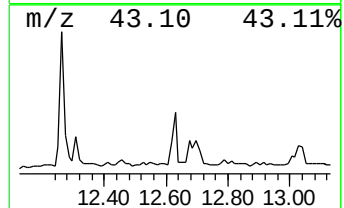
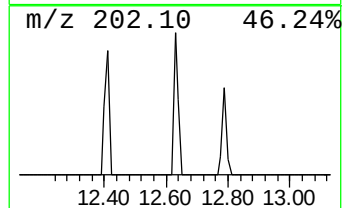
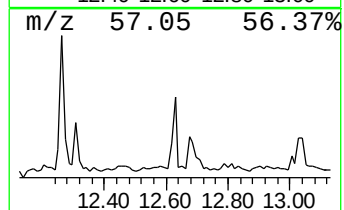
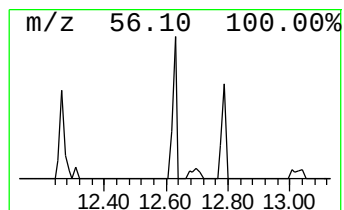
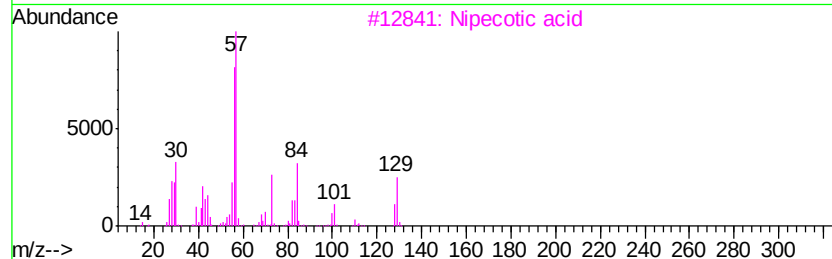
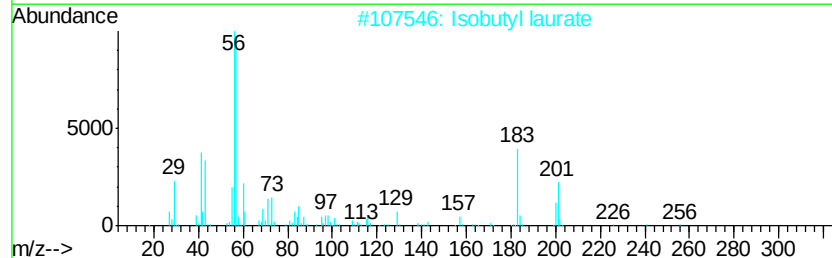
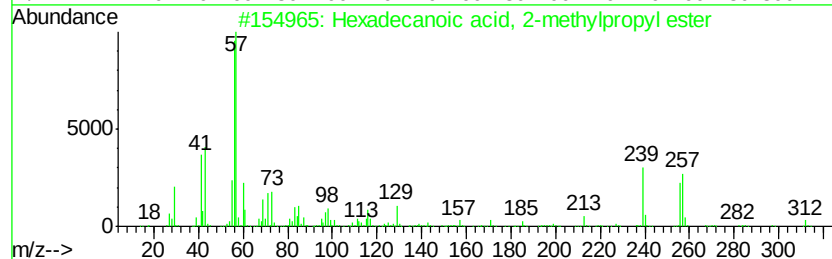
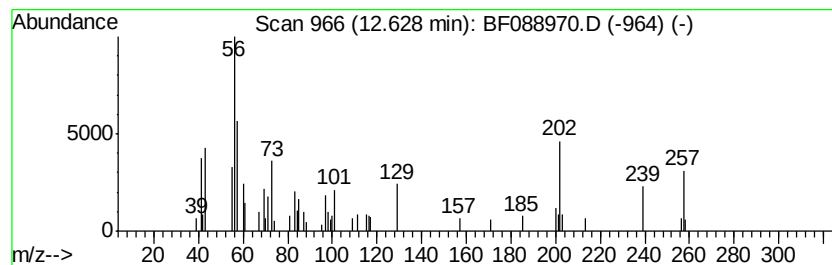
Instrument :
BNA_F
ClientSampleId :
C4.2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown12.63 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.63	2.57 ng	48486	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	46
2	Isobutyl laurate	256	C16H32O2	037811-72-6	38
3	Nipecotic acid	129	C6H11NO2	000498-95-3	37
4	n-Butyl laurate	256	C16H32O2	000106-18-3	37
5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	37



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088970.D
Acq On : 13 Jul 2016 21:08
Operator : UM/SJ
Sample : H3988-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

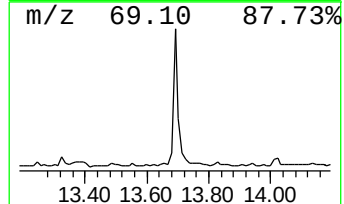
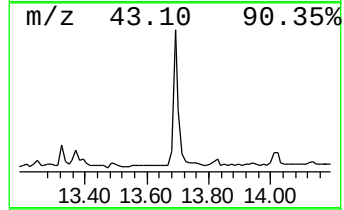
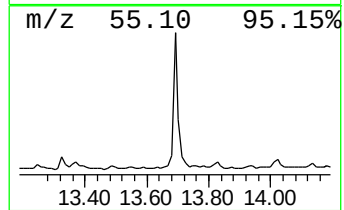
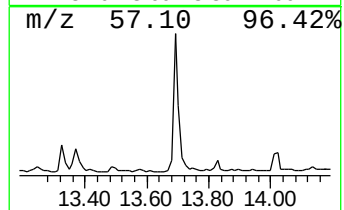
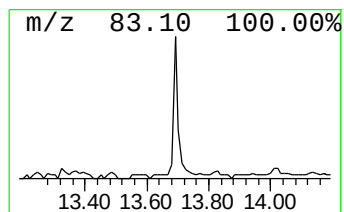
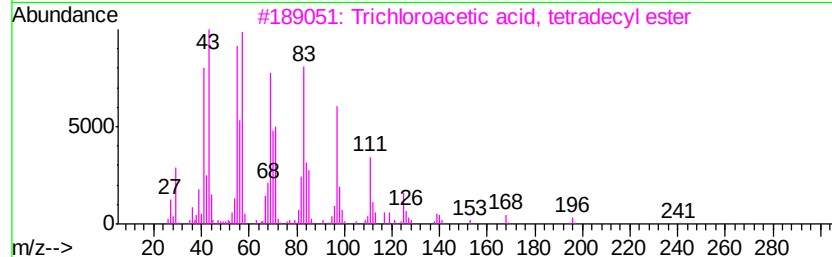
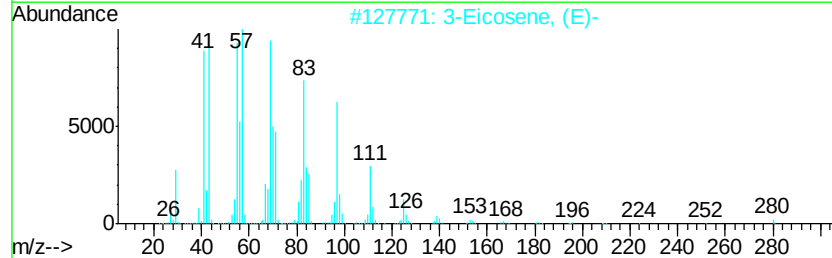
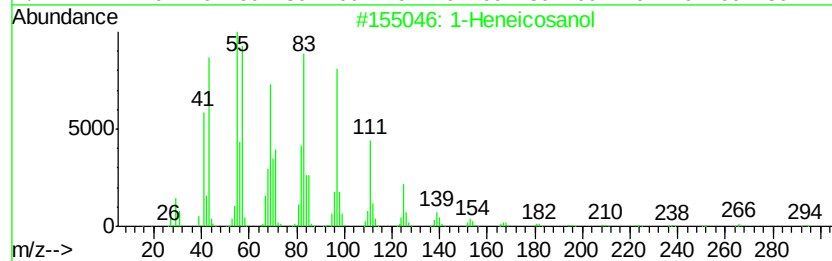
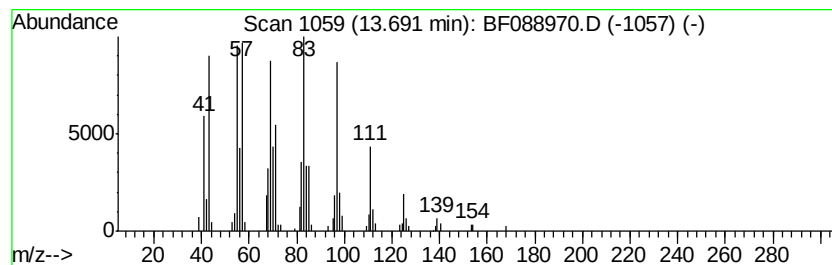
Instrument :
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ClientSampleId :
C4.2-6

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	8.27 ng	156209	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088970.D
Acq On : 13 Jul 2016 21:08
Operator : UM/SJ
Sample : H3988-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

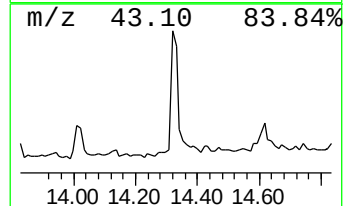
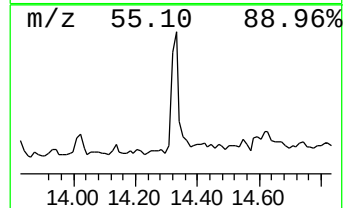
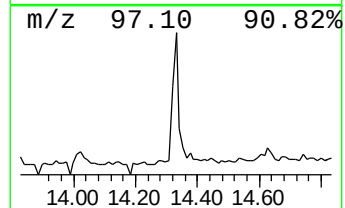
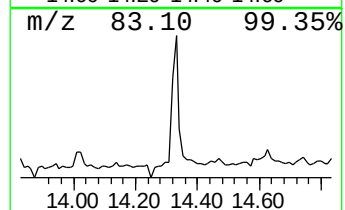
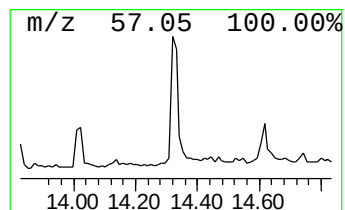
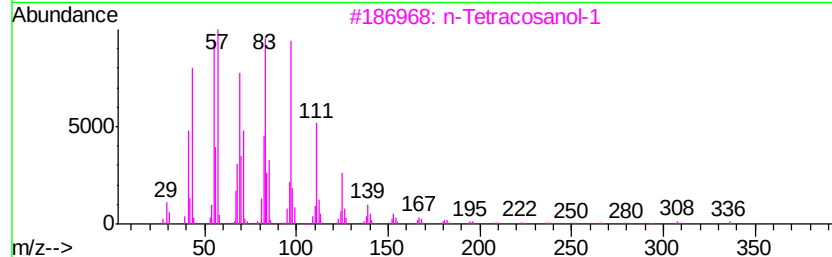
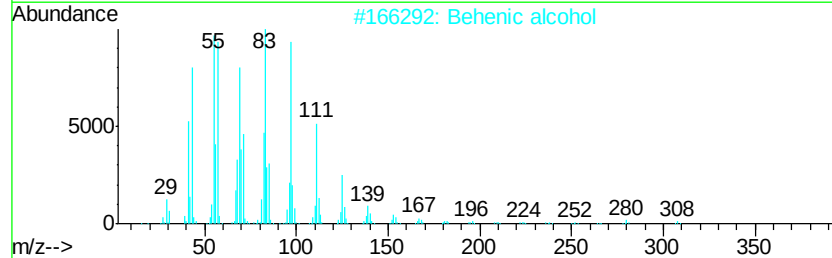
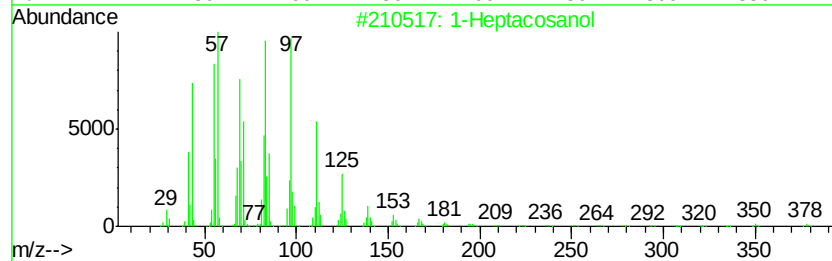
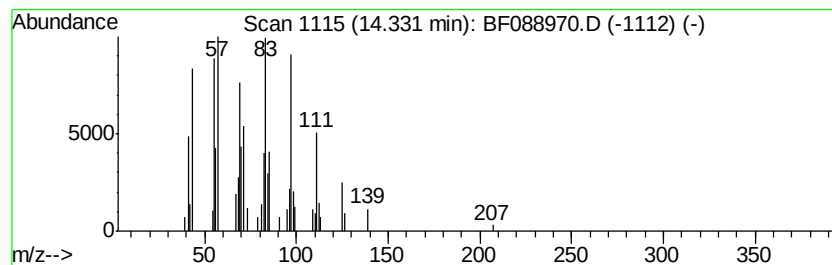
Instrument :
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ClientSampleId :
C4.2-6

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.33	4.73 ng	89411	Chrysene-d12		13.83
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Octacosanol	410	C28H58O	000557-61-9	93
5	1-Nonadecene	266	C19H38	018435-45-5	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071316\
Data File : BF088970.D
Acq On : 13 Jul 2016 21:08
Operator : UM/SJ
Sample : H3988-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C4.2-6

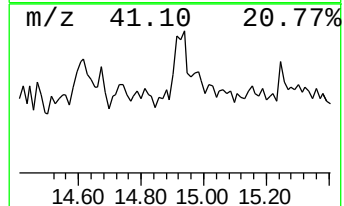
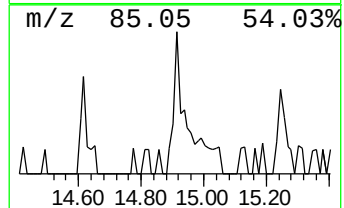
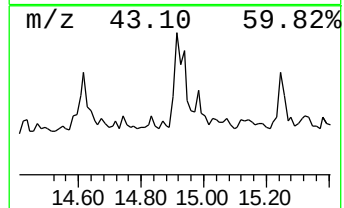
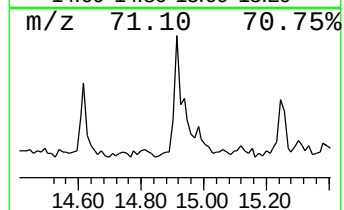
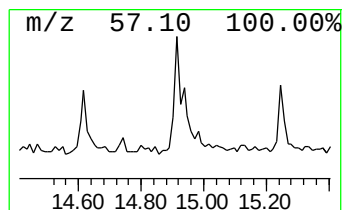
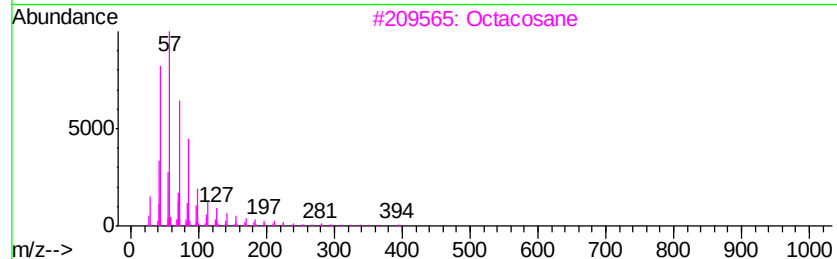
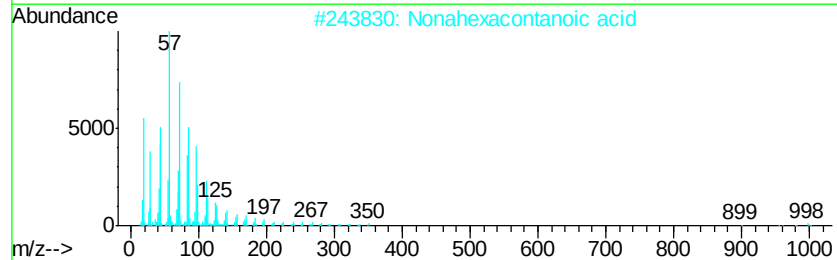
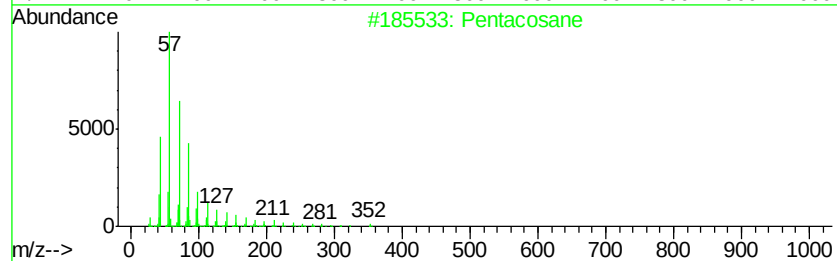
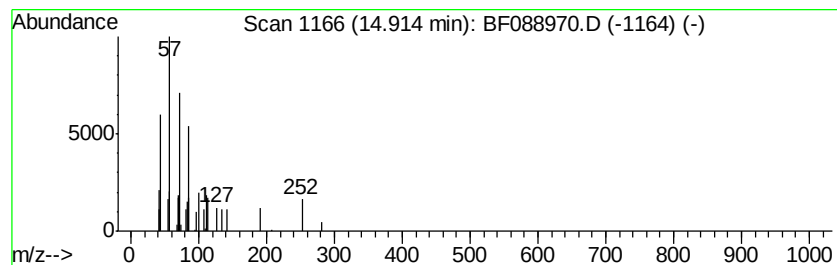
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	2.27 ng	40694	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	64
2		Nonahexacontanoic acid	999	C69H138O2	040710-32-5	64
3		Octacosane	394	C28H58	000630-02-4	64
4		Hexacosane	366	C26H54	000630-01-3	64
5		Eicosane, 2-methyl-	296	C21H44	001560-84-5	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088970.D
Acq On : 13 Jul 2016 21:08
Operator : UM/SJ
Sample : H3988-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C4.2-6

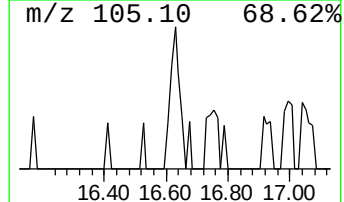
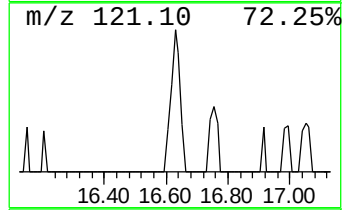
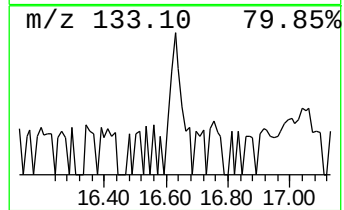
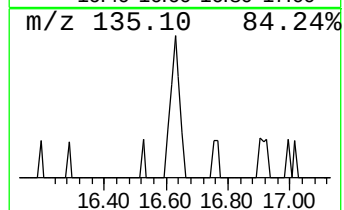
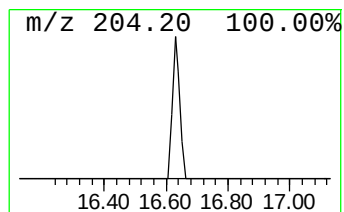
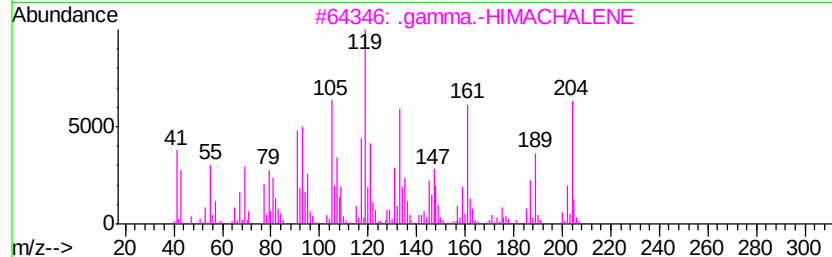
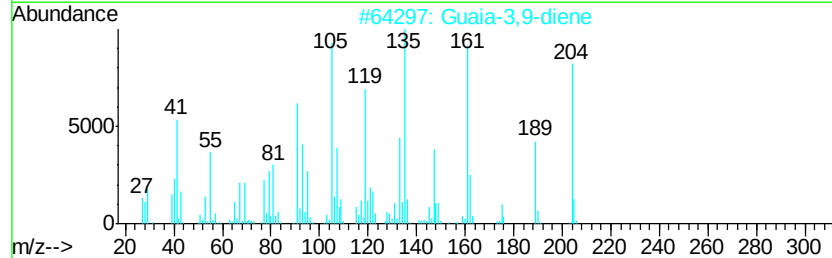
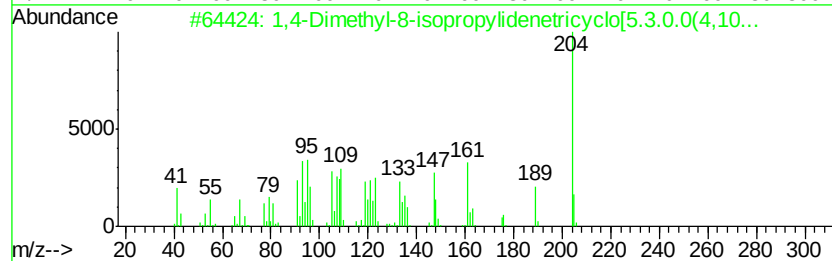
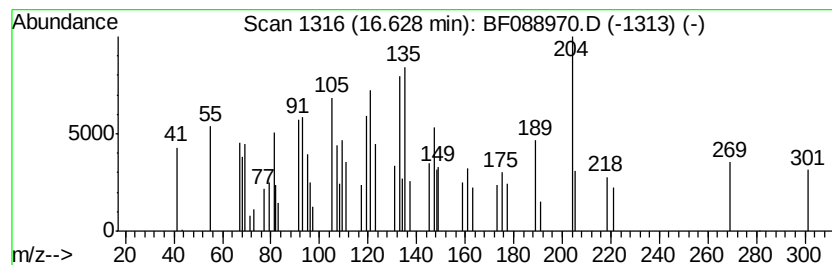
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,4-Dimethyl-8-isopropylide... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	3.47 ng	62222	Perylene-d12	15.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	83
2			Guaia-3,9-diene	204	C15H24	000489-83-8	53
3			.gamma.-HIMACHALENE	204	C15H24	1000140-08-0	53
4			2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	52
5			.alpha.-Guaiene	204	C15H24	003691-12-1	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071316\
Data File : BF088970.D
Acq On : 13 Jul 2016 21:08
Operator : UM/SJ
Sample : H3988-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C4.2-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	1.90	15.9	ng	352059	1	6.70	442689	20.0
2-Pentanone, 4-hy...	4.86	9.0	ng	198664	1	6.70	442689	20.0
unknown6.47	6.47	95.7	ng	2117360	1	6.70	442689	20.0
1-Hexadecanol	11.44	6.0	ng	143675	4	11.20	479745	20.0
n-Nonadecanol-1	12.26	4.2	ng	100920	4	11.20	479745	20.0
unknown12.63	12.63	2.6	ng	48486	5	13.83	377846	20.0
1-Heneicosanol	13.69	8.3	ng	156209	5	13.83	377846	20.0
1-Heptacosanol	14.33	4.7	ng	89411	5	13.83	377846	20.0
Pentacosane	14.91	2.3	ng	40694	6	15.20	358269	20.0
1,4-Dimethyl-8-is...	16.63	3.5	ng	62222	6	15.20	358269	20.0