

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
 Data File : BF084360.D
 Acq On : 10 Jan 2016 13:03
 Operator : SJ/UM
 Sample : H1043-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4S(0-10)

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-BF123115.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	5.047	257	259	268	rVB	1423657	2083717	26.18%	2.768%
2	5.481	294	297	299	rBV	5192951	7469424	93.85%	9.923%
3	6.510	383	387	389	rBV	6798845	7958562	100.00%	10.573%
4	6.624	395	397	400	rBV	5220524	7482032	94.01%	9.940%
5	6.853	415	417	419	rBV	2174755	1777982	22.34%	2.362%
6	7.013	428	431	433	rBV	6301281	5745118	72.19%	7.632%
7	7.424	464	467	469	rBV	4897853	5145225	64.65%	6.835%
8	7.539	474	477	482	rVB	170780	244193	3.07%	0.324%
9	8.145	527	530	532	rBV	2294952	2342556	29.43%	3.112%
10	9.219	621	624	627	rBV	7251482	7169828	90.09%	9.525%
11	9.345	633	635	636	rVB	62161	80045	1.01%	0.106%
12	9.619	656	659	661	rBV	1860870	1880224	23.63%	2.498%
13	9.836	676	678	681	rBV2	129121	195871	2.46%	0.260%
14	9.893	681	683	686	rVB	2663474	2436082	30.61%	3.236%
15	10.328	718	721	723	rBV2	364880	420750	5.29%	0.559%
16	10.545	737	740	744	rBV	102269	203251	2.55%	0.270%
17	10.682	749	752	755	rVV2	3743649	4949435	62.19%	6.575%
18	10.796	759	762	769	rVV2	327639	665025	8.36%	0.883%
19	10.990	777	779	784	rBV	51262	110994	1.39%	0.147%
20	11.253	799	802	803	rBV	242051	219085	2.75%	0.291%
21	11.379	811	813	815	rBV	2813158	2532032	31.82%	3.364%
22	11.448	816	819	822	rVB2	82036	145124	1.82%	0.193%
23	11.608	830	833	837	rBV2	431741	532053	6.69%	0.707%
24	11.676	837	839	841	rVB	137862	115665	1.45%	0.154%
25	12.431	903	905	907	rBV	216225	253055	3.18%	0.336%
26	12.591	916	919	921	rBV	284818	294810	3.70%	0.392%
27	12.819	934	939	940	rBV2	261224	523402	6.58%	0.695%
28	12.854	940	942	947	rVV	555695	746363	9.38%	0.992%
29	12.968	949	952	955	rVB	6347686	6373927	80.09%	8.468%
30	13.208	969	973	975	rBV3	38852	106159	1.33%	0.141%
31	13.494	997	998	1000	rBV	85661	88868	1.12%	0.118%
32	13.539	1000	1002	1007	rVB4	33886	83138	1.04%	0.110%
33	13.871	1028	1031	1039	rBV	480752	797594	10.02%	1.060%
34	14.019	1041	1044	1046	rBV	1309411	1959388	24.62%	2.603%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.488	1084	1085	1091	rVB3	46711	128420	1.61%	0.171%
36	14.865	1116	1118	1121	rBV	199682	204602	2.57%	0.272%
37	15.037	1130	1133	1137	rVB	68245	146515	1.84%	0.195%
38	15.380	1161	1163	1166	rBV	74171	99043	1.24%	0.132%
39	15.437	1166	1168	1171	rBV	896179	1319895	16.58%	1.753%
40	15.962	1211	1214	1219	rBV6	32046	116129	1.46%	0.154%
41	17.243	1324	1326	1334	rVB	37908	128606	1.62%	0.171%

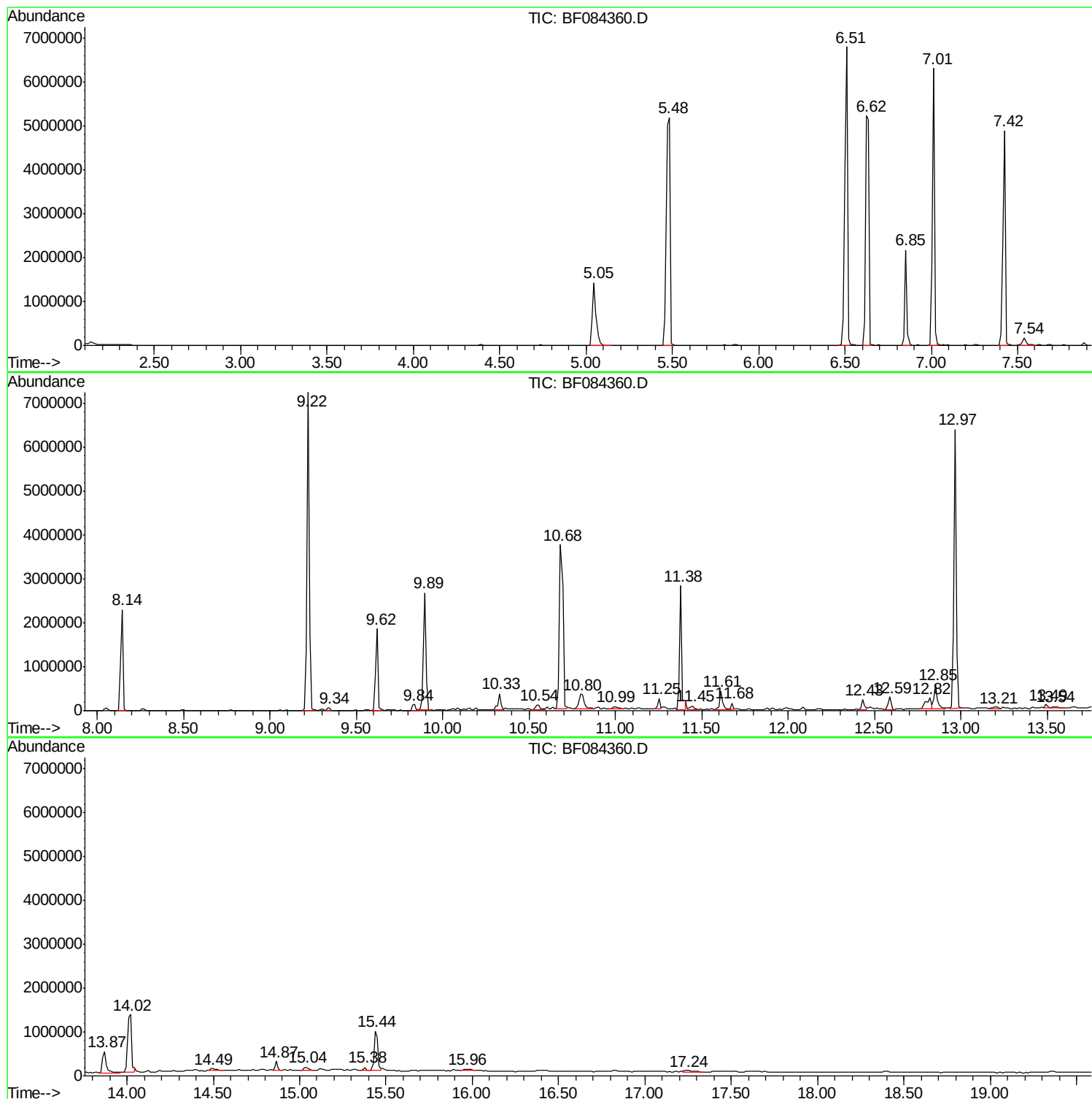
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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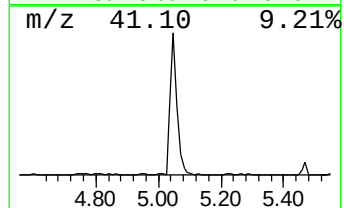
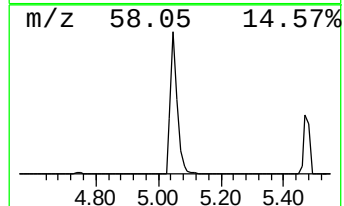
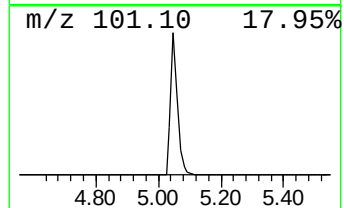
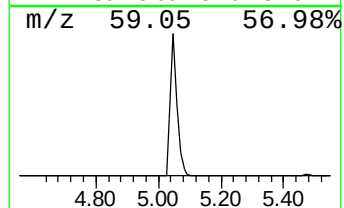
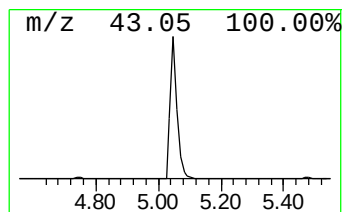
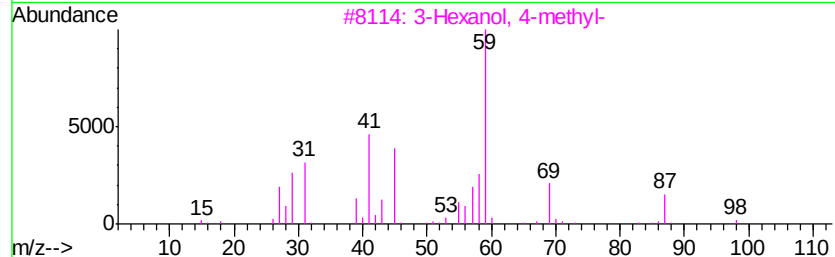
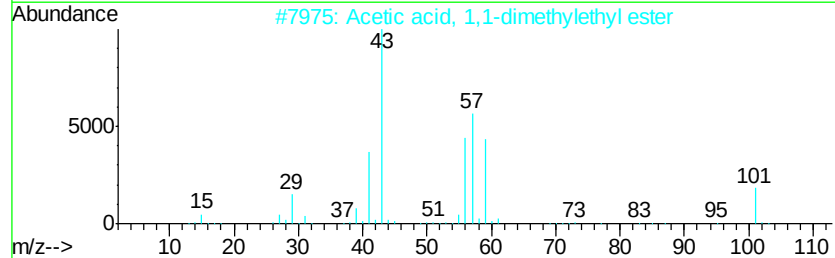
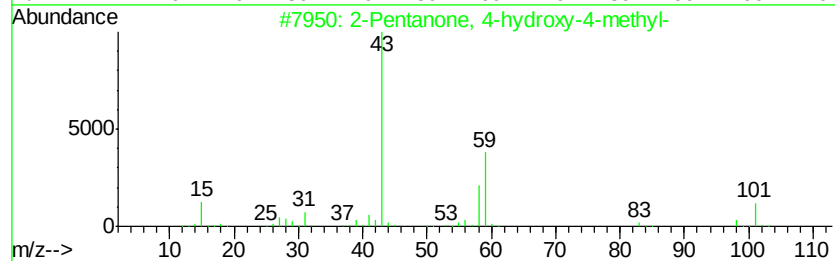
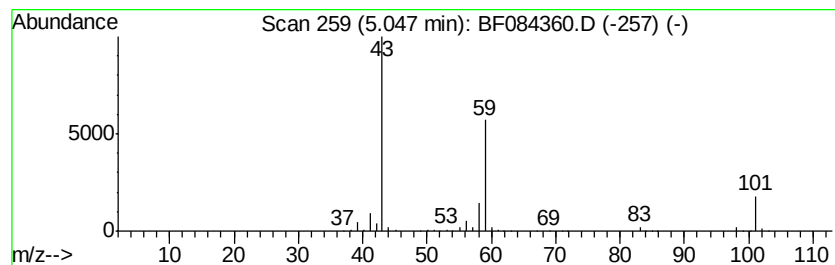
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	23.44 ng	2083720	1,4-Dichlorobenzene-d4	6.85

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		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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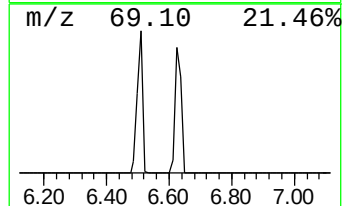
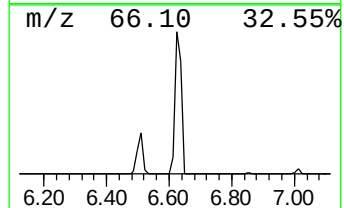
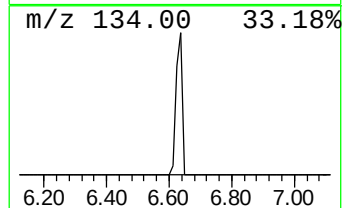
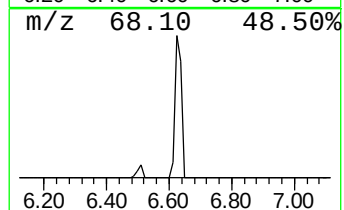
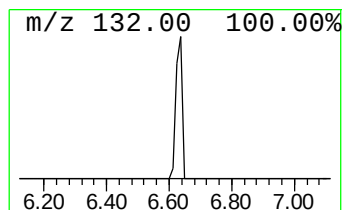
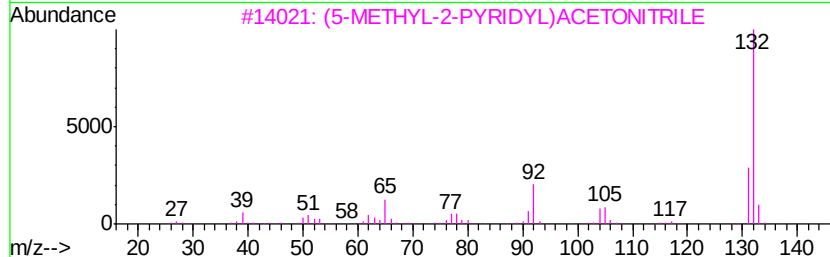
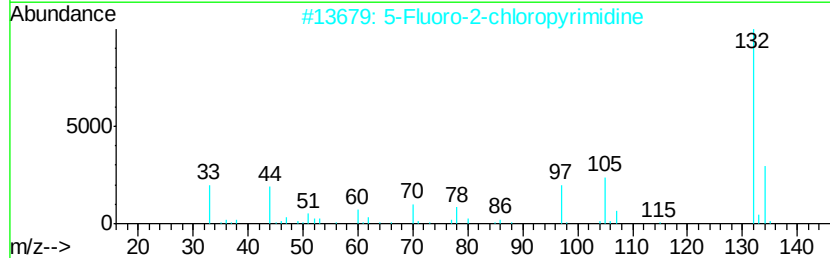
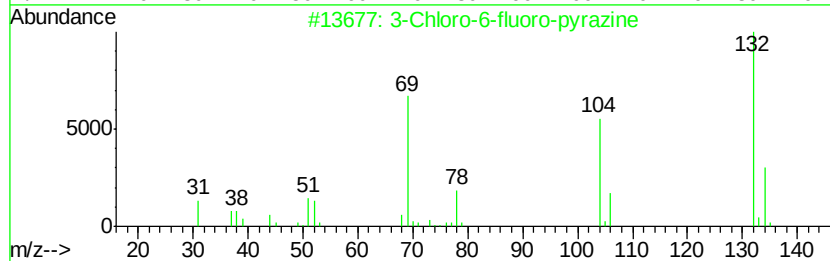
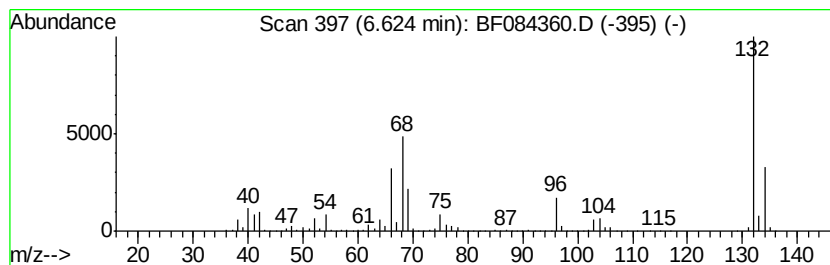
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	84.16 ng	7482030	1,4-Dichlorobenzene-d4	6.85

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	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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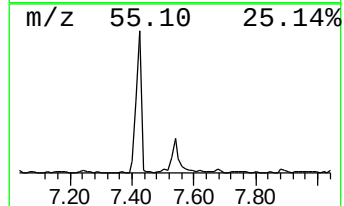
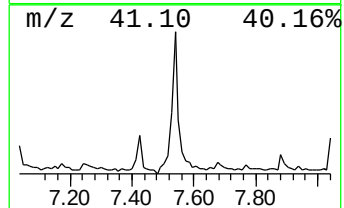
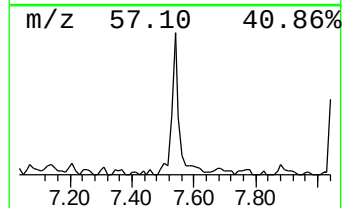
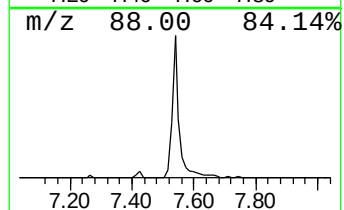
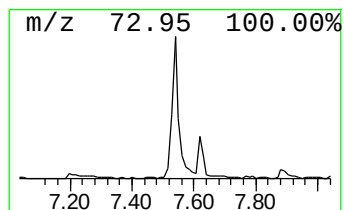
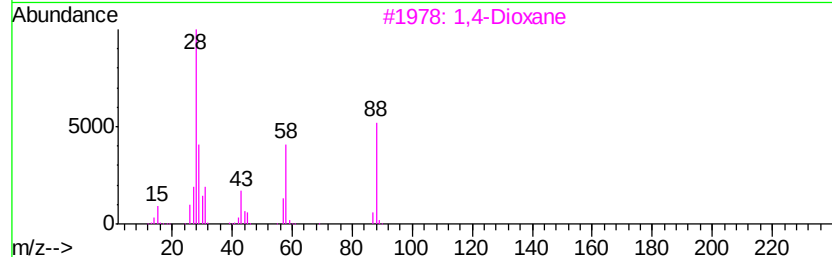
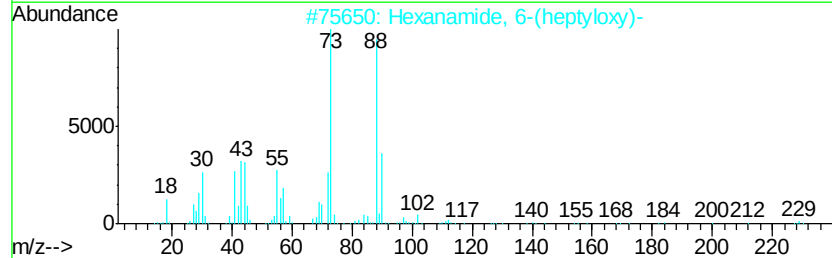
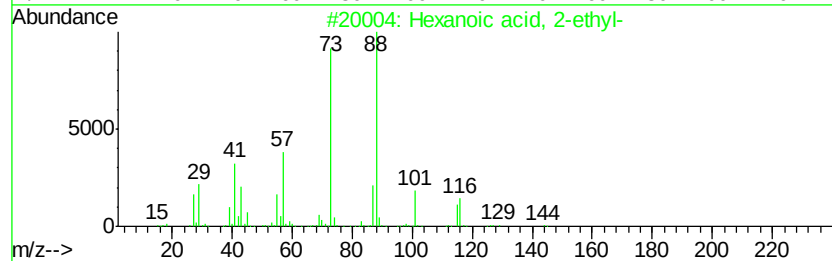
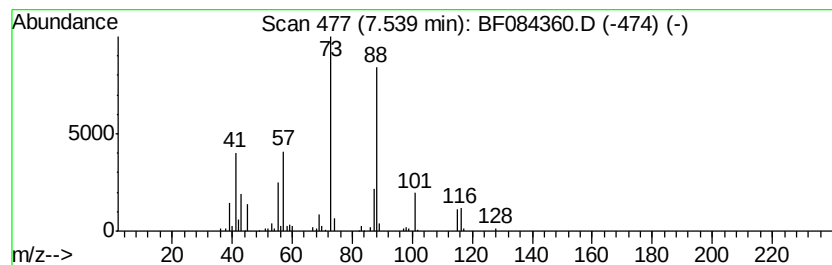
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	2.08 ng	244193	Naphthalene-d8	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2		Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	38
3		1,4-Dioxane	88	C4H8O2	000123-91-1	37
4		Acetic acid, diethyl-	116	C6H12O2	000088-09-5	37
5		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	33



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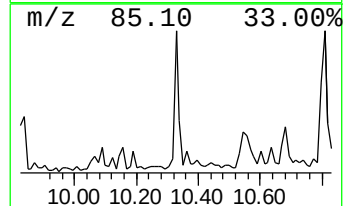
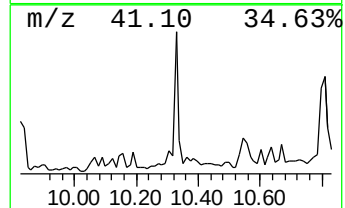
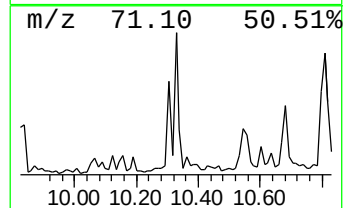
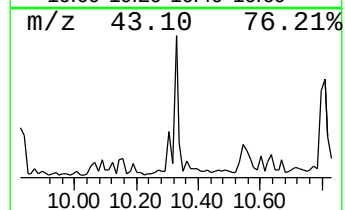
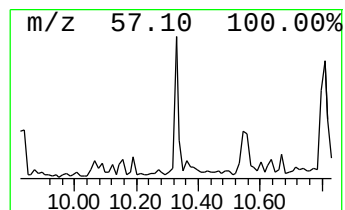
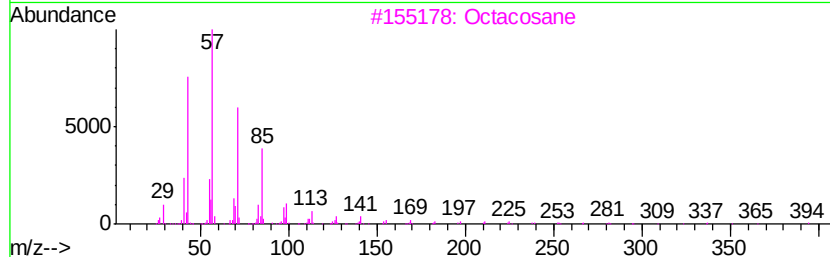
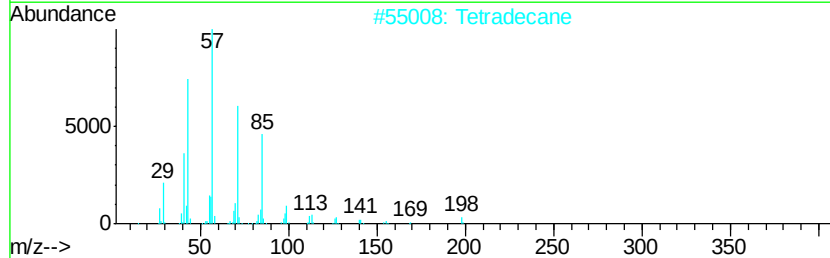
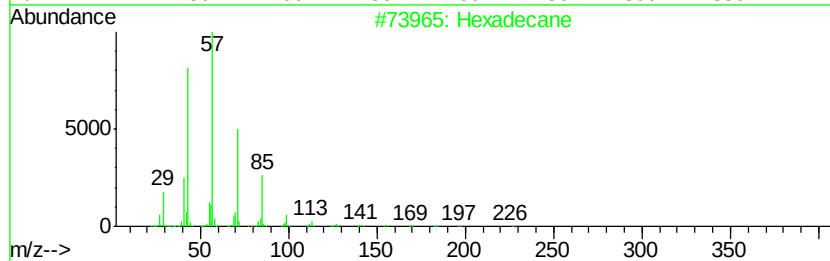
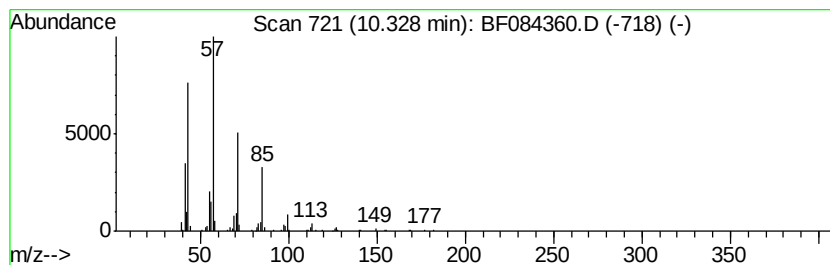
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.45 ng	420750	Acenaphthene-d10	9.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tetradecane		198	C14H30	000629-59-4	90
3	Octacosane		394	C28H58	000630-02-4	86
4	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	78
5	Pentadecane		212	C15H32	000629-62-9	78



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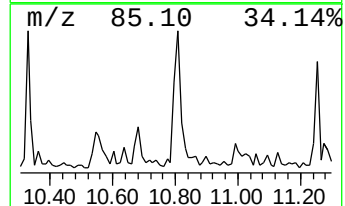
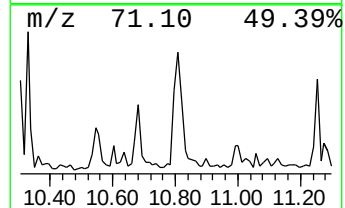
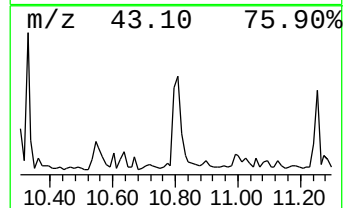
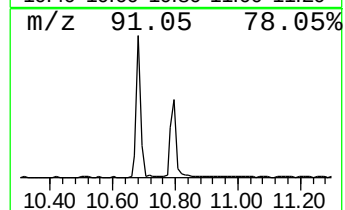
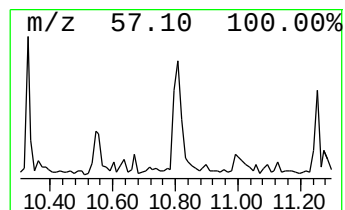
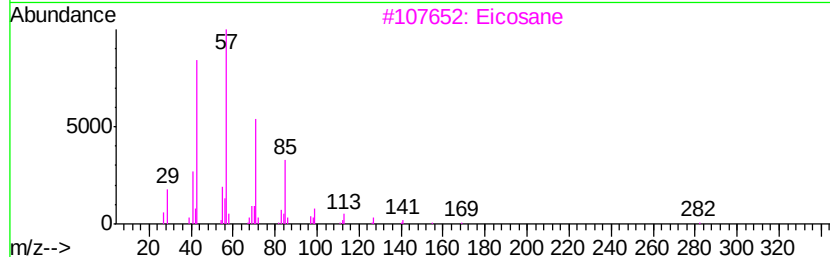
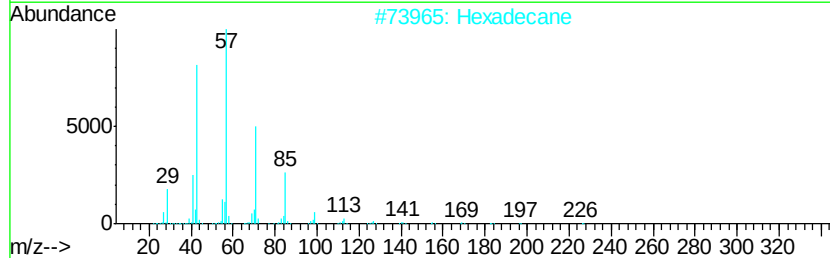
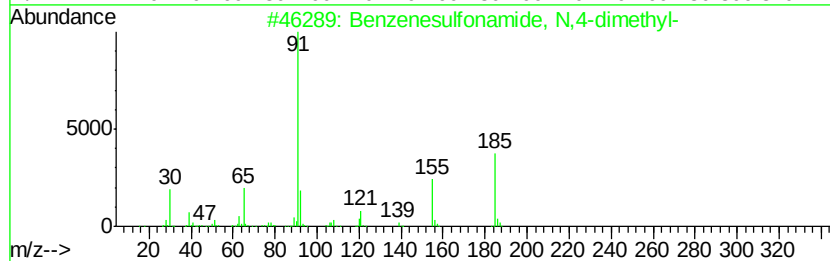
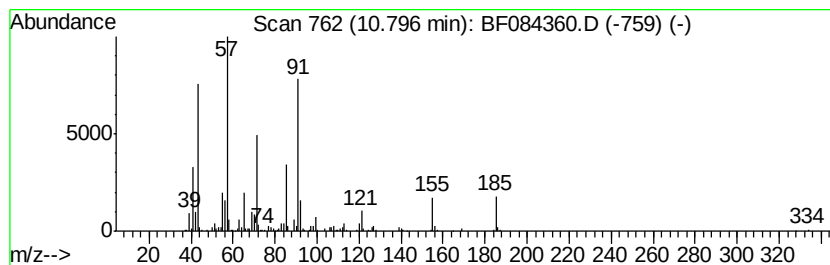
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	5.25 ng	665025	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	84
2		Hexadecane	226	C16H34	000544-76-3	45
3		Eicosane	282	C20H42	000112-95-8	43
4		Undecane	156	C11H24	001120-21-4	43
5		Pentadecane	212	C15H32	000629-62-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
Data File : BF084360.D
Acq On : 10 Jan 2016 13:03
Operator : SJ/UM
Sample : H1043-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

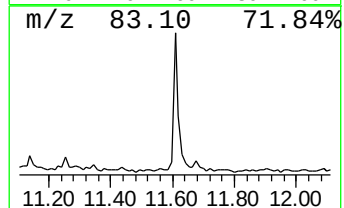
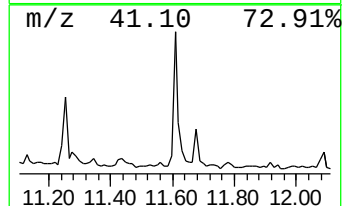
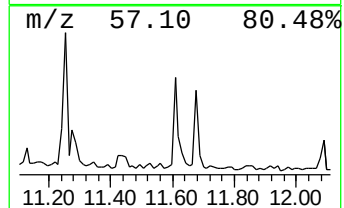
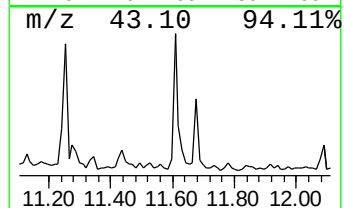
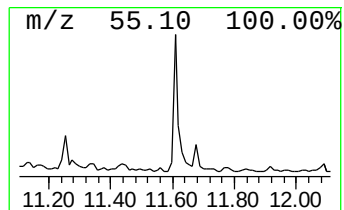
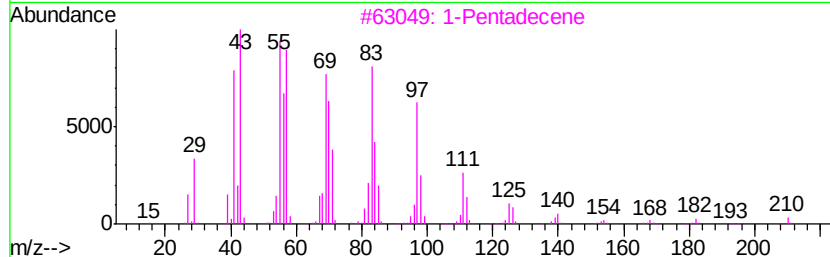
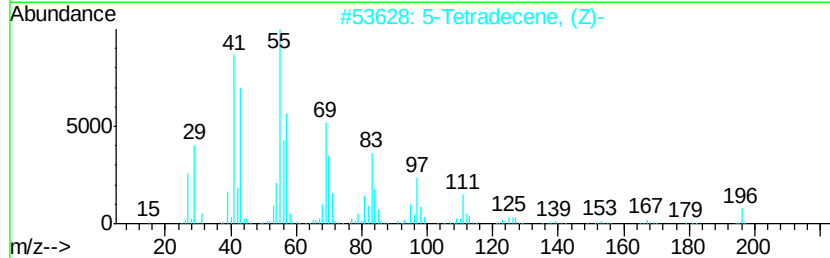
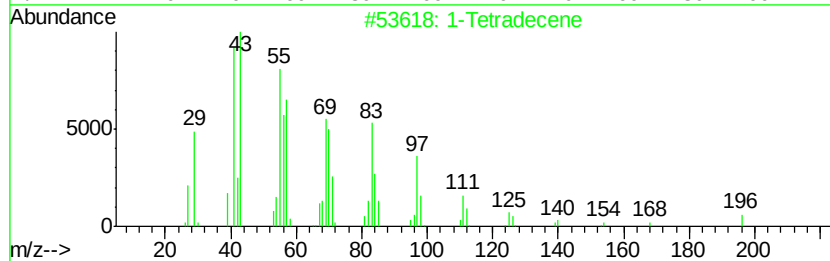
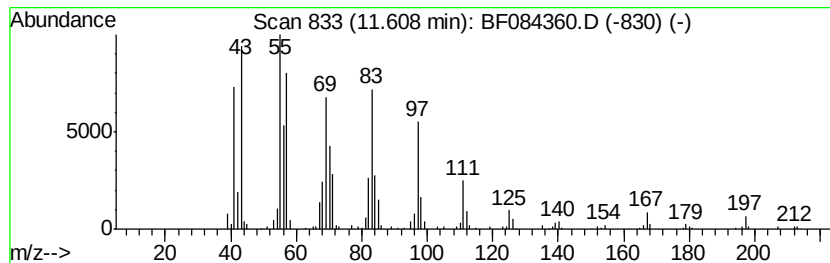
Instrument :
BNA_F
ClientSampleId :
SB-4S(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tetradecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.61	4.20 ng	532053	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	95
2	5-Tetradecene, (Z)-	196	C14H28	041446-62-2	94
3	1-Pentadecene	210	C15H30	013360-61-7	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084360.D
Acq On : 10 Jan 2016 13:03
Operator : SJ/UM
Sample : H1043-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4S(0-10)

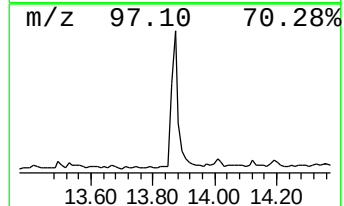
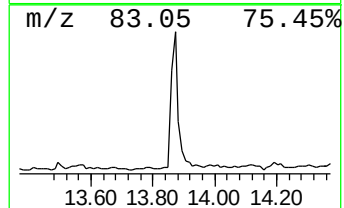
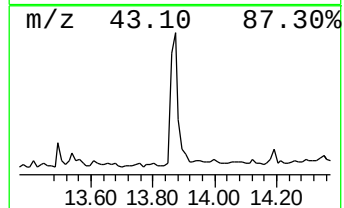
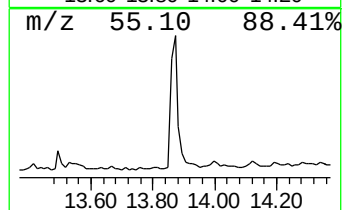
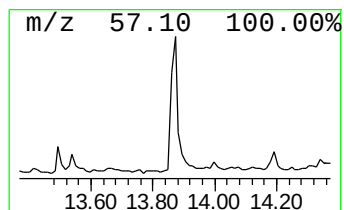
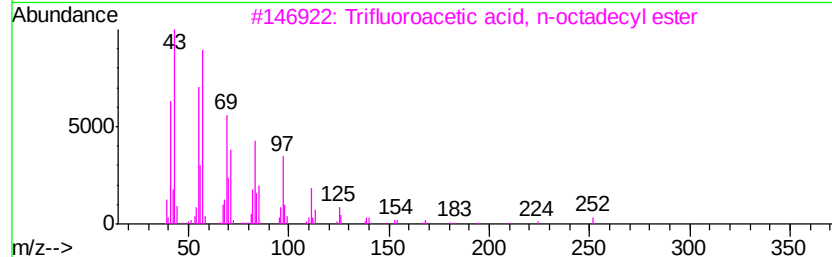
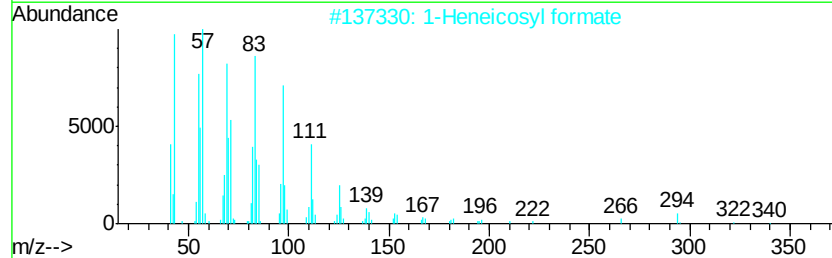
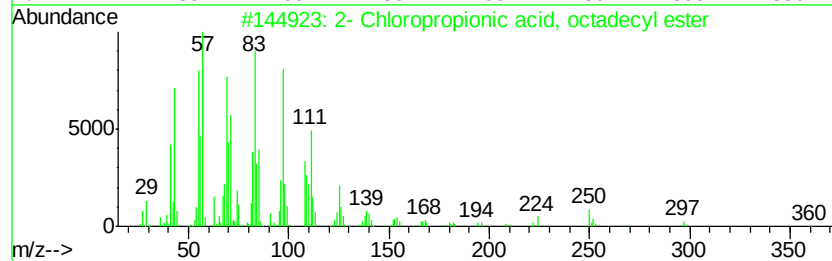
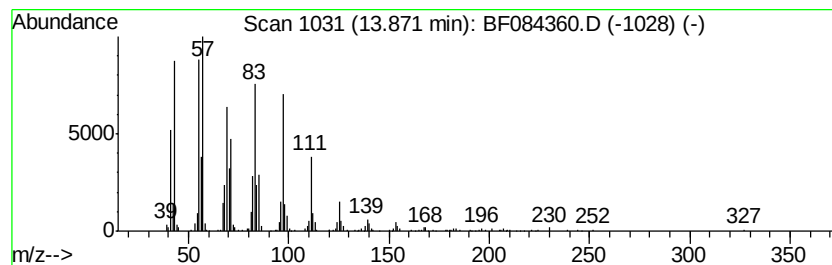
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2- Chloropropionic acid, oc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.14 ng	797594	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3		Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
4		1-Docosene	308	C22H44	001599-67-3	90
5		10-Heneicosene (c,t)	294	C21H42	095008-11-0	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
 Data File : BF084360.D
 Acq On : 10 Jan 2016 13:03
 Operator : SJ/UM
 Sample : H1043-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

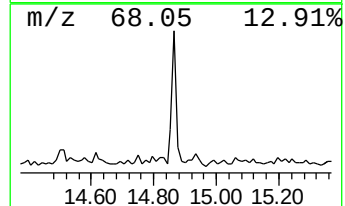
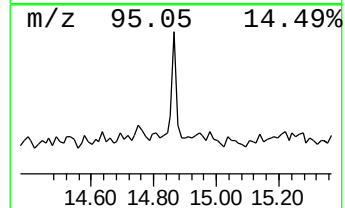
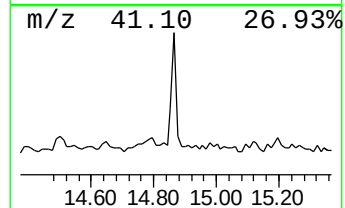
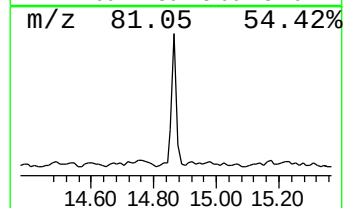
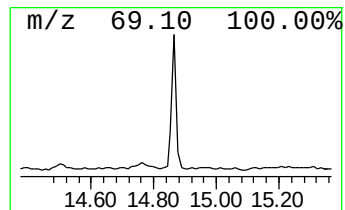
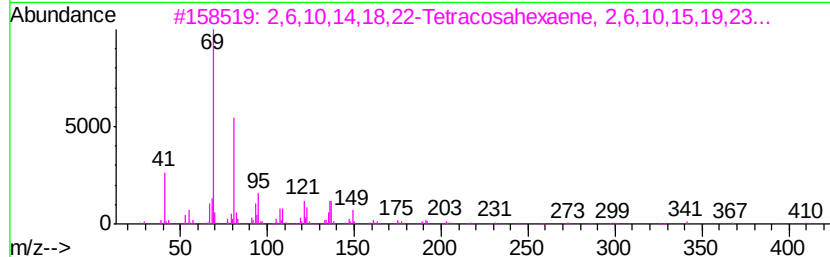
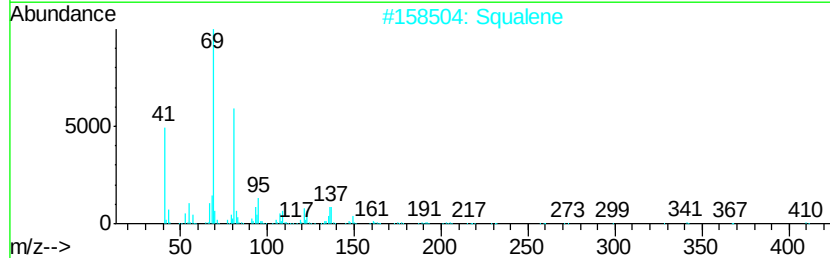
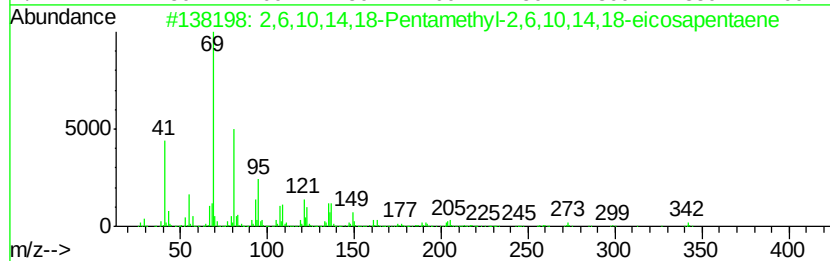
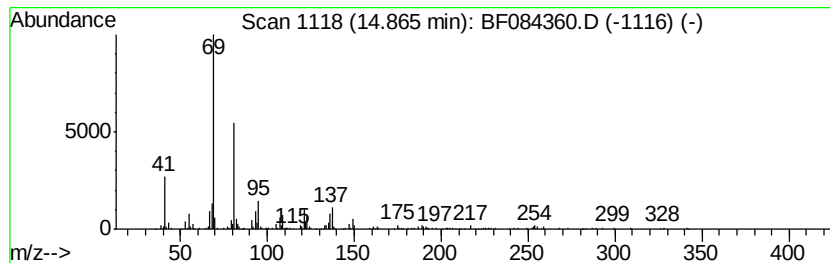
Instrument :
 BNA_F
 ClientSampleId :
 SB-4S(0-10)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.10 ng	204602	Perylene-d12	15.44
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342 C25H42	075581-03-2	93
2	Squalene	410 C30H50	007683-64-9	91
3	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
4	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H240	125529-10-4	72
5	2,6,10,14-Hexadecatetraenoic aci...	332 C22H3602	024035-35-6	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
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Operator : SJ/UM
Sample : H1043-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4S(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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
2-Pentanone, 4-hy...	5.05	23.4	ng	2083720	1	6.85	1777980	20.0
unknown6.62	6.62	84.2	ng	7482030	1	6.85	1777980	20.0
Hexanoic acid, 2-...	7.54	2.1	ng	244193	2	8.14	2342560	20.0
Hexadecane	10.33	3.5	ng	420750	3	9.89	2436080	20.0
Benzenesulfonamid...	10.80	5.3	ng	665025	4	11.38	2532030	20.0
1-Tetradecene	11.61	4.2	ng	532053	4	11.38	2532030	20.0
2-Chloropropioni...	13.87	8.1	ng	797594	5	14.02	1959390	20.0
2,6,10,14,18-Pent...	14.87	3.1	ng	204602	6	15.44	1319900	20.0