

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041615\
 Data File : BF078567.D
 Acq On : 16 Apr 2015 15:59
 Operator : TP/IZ
 Sample : G1890-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-COMP

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-BF040115.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	1.450	21	23	29	rBV	39017	62132	7.88%	0.786%
2	1.530	29	30	56	rVB	327250	744467	94.41%	9.423%
3	4.284	269	271	277	rBV	37307	64867	8.23%	0.821%
4	4.913	323	326	338	rVB	372211	468579	59.42%	5.931%
5	6.296	445	447	453	rBV	505622	503860	63.89%	6.377%
6	6.399	453	456	459	rVB	550717	527482	66.89%	6.676%
7	6.684	479	481	484	rBV	164045	165488	20.99%	2.095%
8	6.867	495	497	500	rBV	328481	382934	48.56%	4.847%
9	7.393	540	543	546	rBV	352678	311447	39.49%	3.942%
10	7.816	578	580	584	rVB	7381	10651	1.35%	0.135%
11	8.273	617	620	622	rBV	210891	248738	31.54%	3.148%
12	8.410	629	632	634	rBV	9467	12520	1.59%	0.158%
13	8.536	641	643	645	rBV	8326	10521	1.33%	0.133%
14	8.628	645	651	653	rVB4	4966	13234	1.68%	0.168%
15	8.856	670	671	673	rVB	11063	10443	1.32%	0.132%
16	9.622	735	738	740	rVB	574415	641757	81.38%	8.123%
17	9.771	749	751	754	rVB2	6225	9111	1.16%	0.115%
18	10.068	774	777	778	rVB	11817	14869	1.89%	0.188%
19	10.136	781	783	784	rVV	49798	50493	6.40%	0.639%
20	10.159	784	785	787	rVV	9980	10314	1.31%	0.131%
21	10.251	790	793	795	rBV	11223	14295	1.81%	0.181%
22	10.308	795	798	801	rVB3	8629	16073	2.04%	0.203%
23	10.376	801	804	805	rBV3	4741	8594	1.09%	0.109%
24	10.422	805	808	811	rVB	324229	304371	38.60%	3.852%
25	10.731	830	835	838	rBV2	3979	10048	1.27%	0.127%
26	10.822	838	843	847	rVB5	3388	9397	1.19%	0.119%
27	11.039	860	862	865	rBV	9242	10387	1.32%	0.131%
28	11.325	881	887	891	rBV3	5616	10336	1.31%	0.131%
29	11.394	891	893	896	rBV	394932	406459	51.54%	5.145%
30	11.622	911	913	917	rVB2	8739	16116	2.04%	0.204%
31	12.182	960	962	964	rBV	10896	14062	1.78%	0.178%
32	12.239	964	967	969	rVV	322999	308629	39.14%	3.906%
33	12.617	998	1000	1004	rBV2	19452	33364	4.23%	0.422%
34	12.708	1007	1008	1010	rVB	10629	10537	1.34%	0.133%

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Max Peaks: 100
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35	12.994	1031	1033	1035	rBV2	7377	12160	1.54%	0.154%
36	13.725	1095	1097	1099	rVB	41573	38875	4.93%	0.492%
37	13.771	1099	1101	1103	rBV	9892	9529	1.21%	0.121%
38	13.999	1119	1121	1123	rVB	52082	50067	6.35%	0.634%
39	14.228	1139	1141	1144	rBV	710112	788578	100.00%	9.981%
40	14.422	1152	1158	1162	rBV	16112	38583	4.89%	0.488%
41	14.502	1162	1165	1167	rBV	7922	14951	1.90%	0.189%
42	14.548	1167	1169	1173	rBV3	7348	19738	2.50%	0.250%
43	14.765	1186	1188	1190	rVB3	7249	9394	1.19%	0.119%
44	14.891	1197	1199	1202	rBV3	5159	11632	1.48%	0.147%
45	15.028	1209	1211	1215	rBV3	4648	8873	1.13%	0.112%
46	15.177	1222	1224	1227	rBV	8015	11264	1.43%	0.143%
47	15.314	1234	1236	1240	rBV5	7131	13446	1.71%	0.170%
48	15.428	1244	1246	1249	rBV	106397	156413	19.83%	1.980%
49	15.497	1249	1252	1253	rVV	309466	460922	58.45%	5.834%
50	15.520	1253	1254	1257	rVB	37649	41119	5.21%	0.520%
51	16.240	1315	1317	1319	rVB3	14435	19488	2.47%	0.247%
52	16.765	1360	1363	1368	rBV	59351	138720	17.59%	1.756%
53	16.880	1371	1373	1376	rVV	16596	25407	3.22%	0.322%
54	17.074	1388	1390	1392	rBV	32284	44212	5.61%	0.560%
55	17.143	1393	1396	1398	rBV	42334	57351	7.27%	0.726%
56	17.200	1398	1401	1404	rBV	300207	412184	52.27%	5.217%
57	17.840	1454	1457	1460	rBV3	41940	81243	10.30%	1.028%

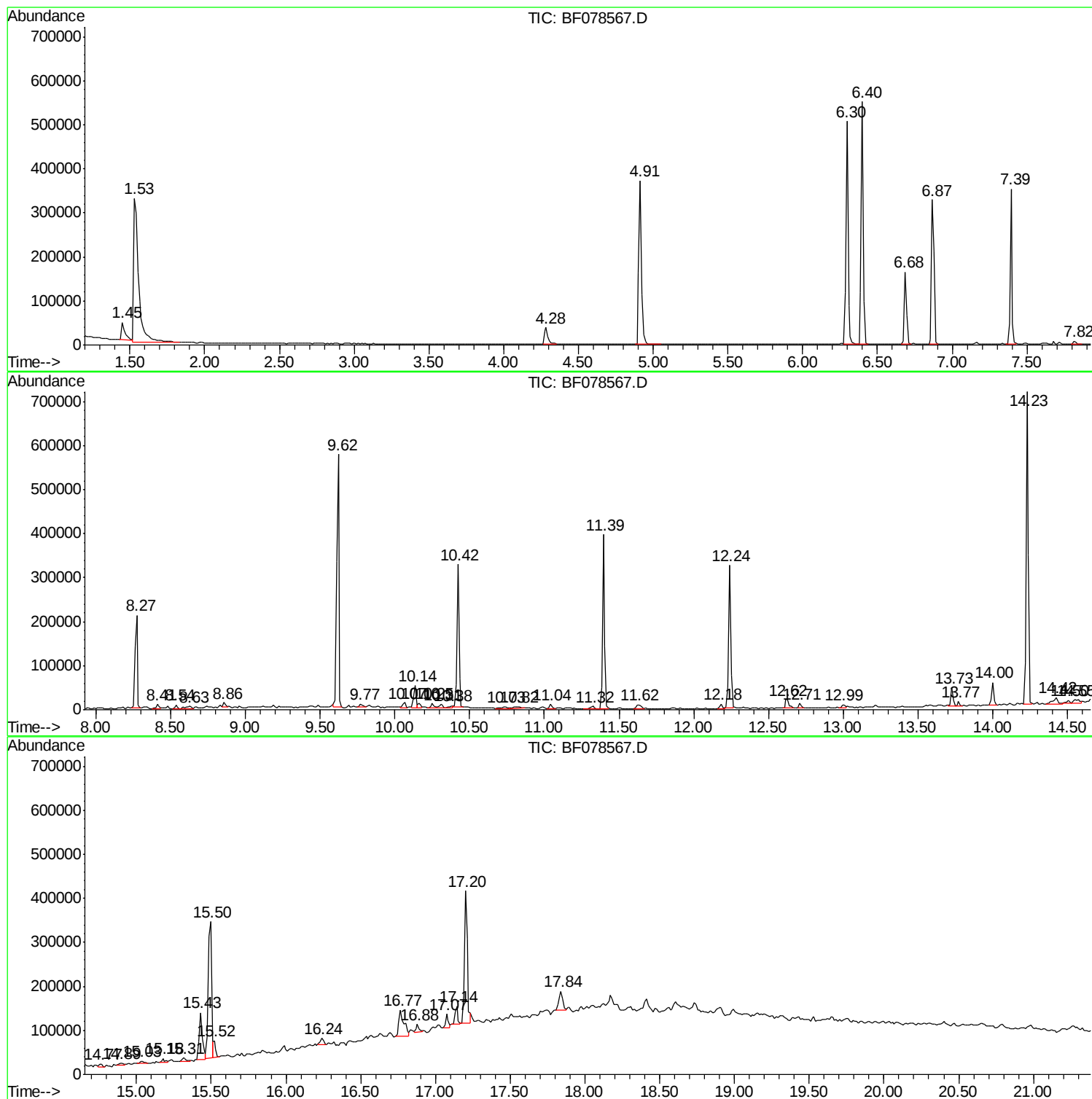
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
SB-03-COMP

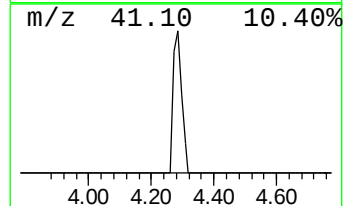
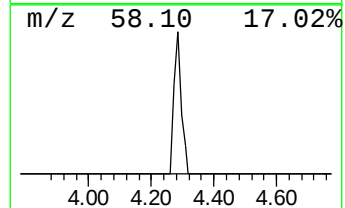
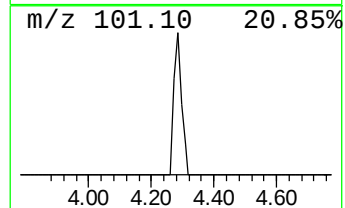
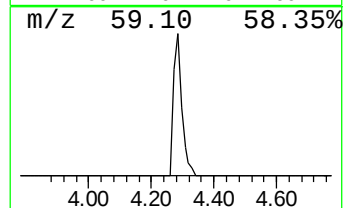
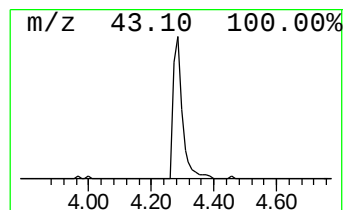
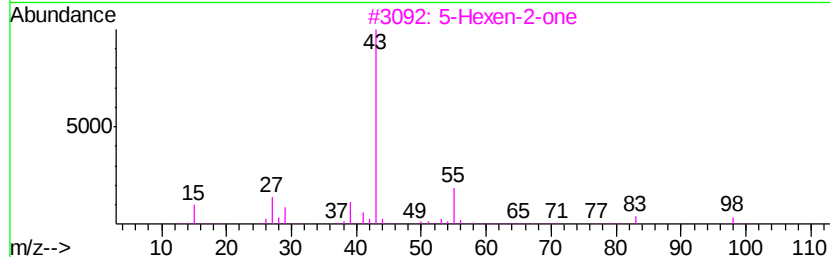
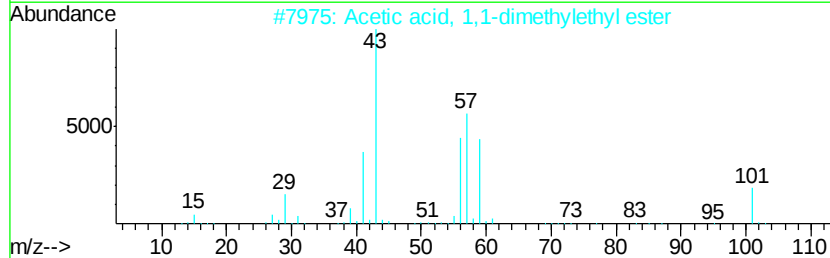
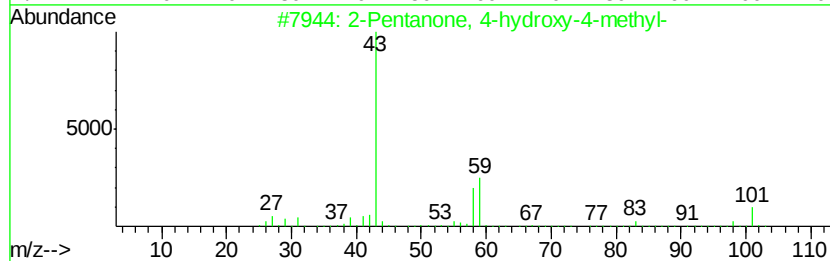
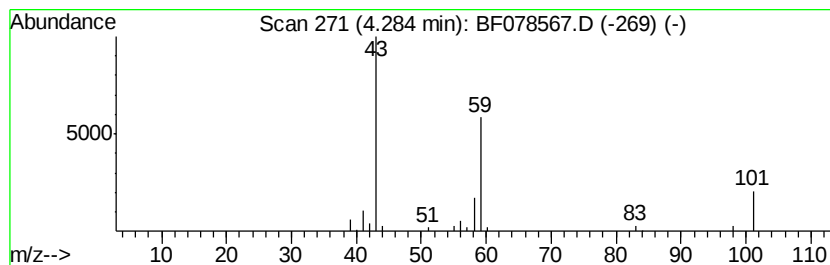
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	7.84 ng	64867	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	50	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9	
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9	



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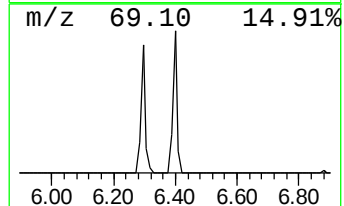
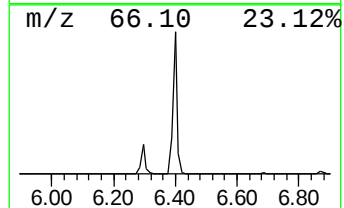
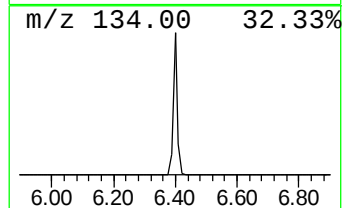
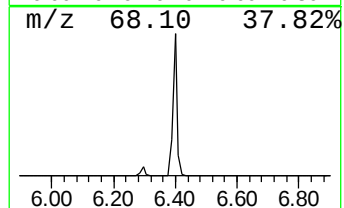
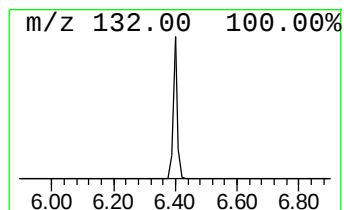
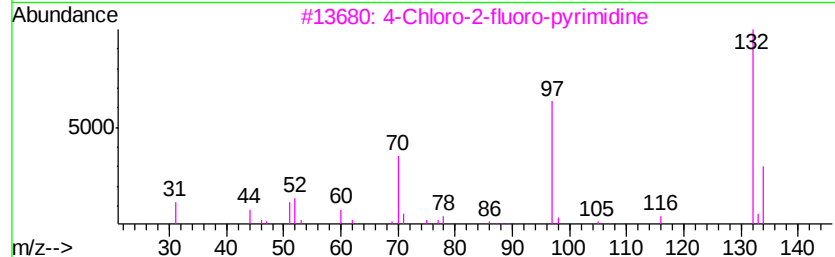
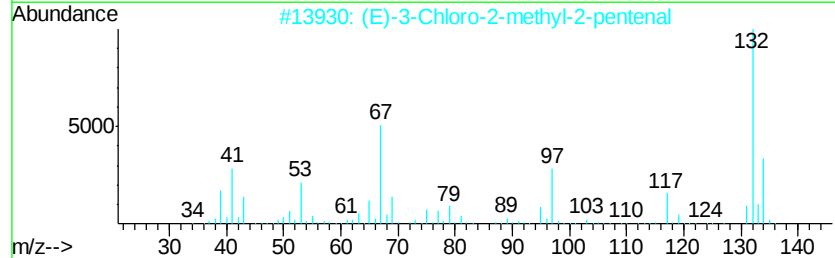
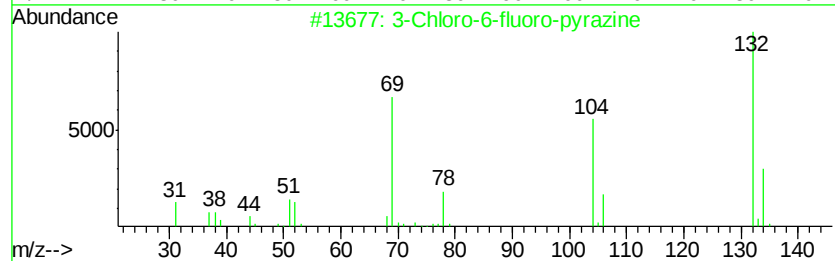
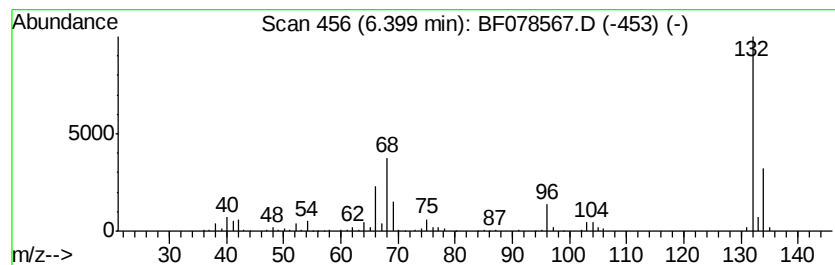
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	63.75 ng	527482	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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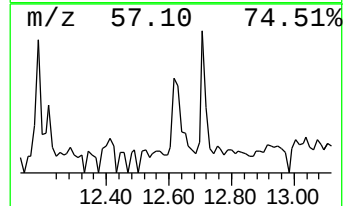
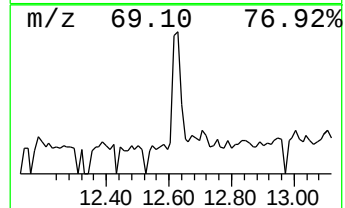
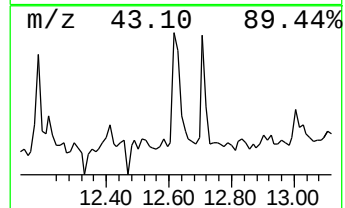
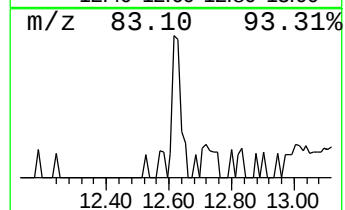
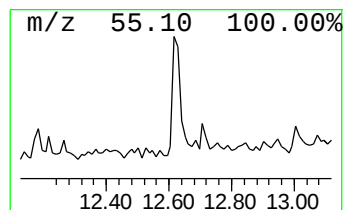
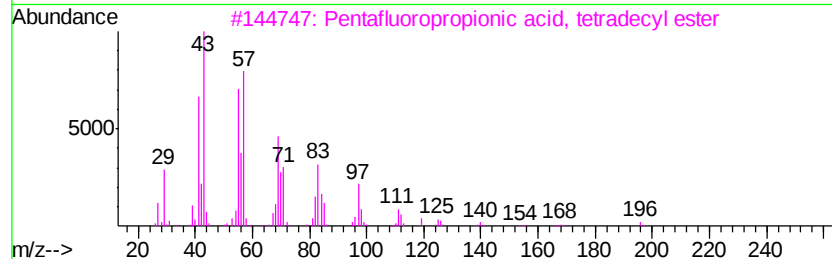
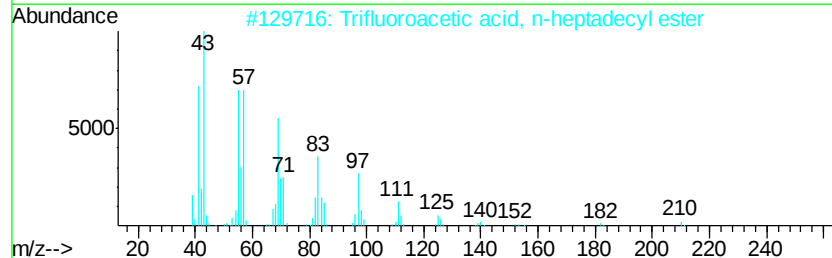
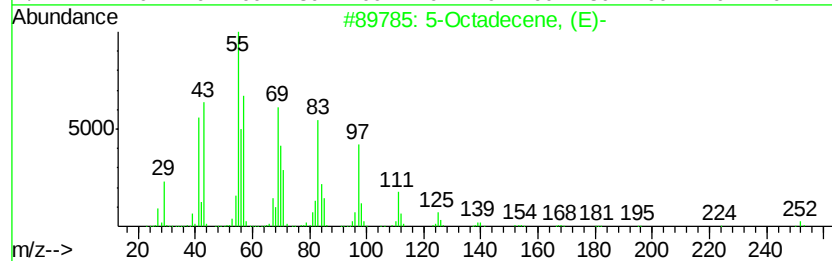
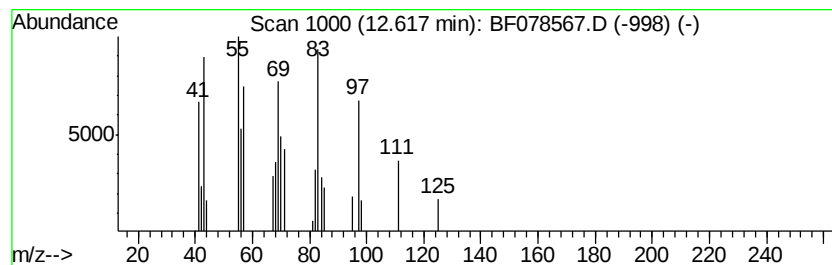
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Octadecene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.62	2.16 ng	33364	Phenanthrene-d10	12.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	90	
2	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	80	
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	72	
4	1-Hexacosanol	382	C26H54O	000506-52-5	72	
5	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	64	



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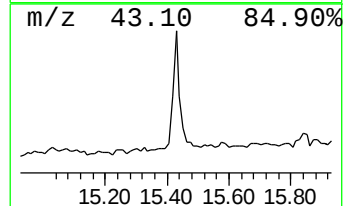
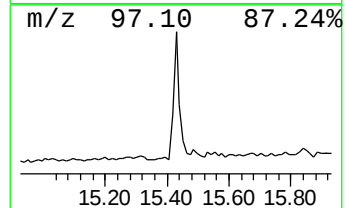
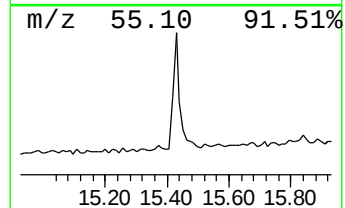
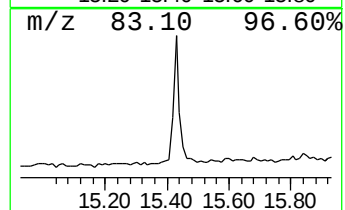
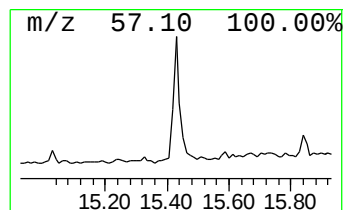
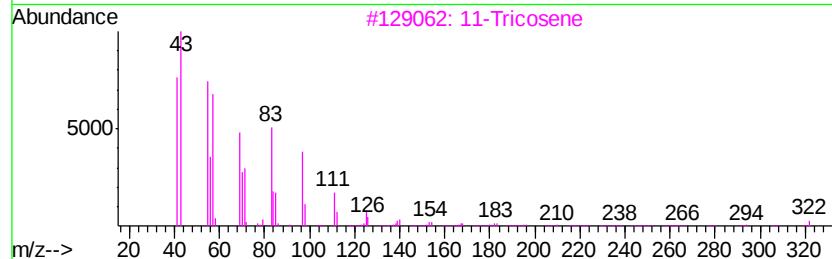
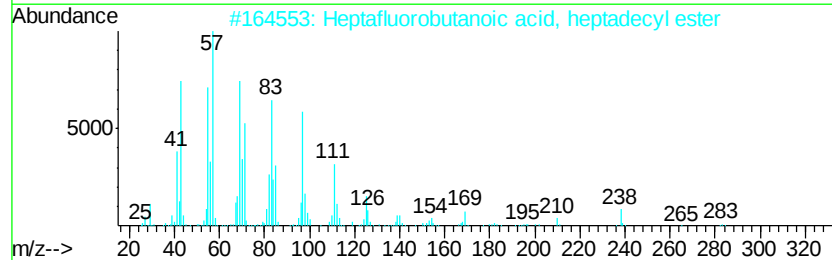
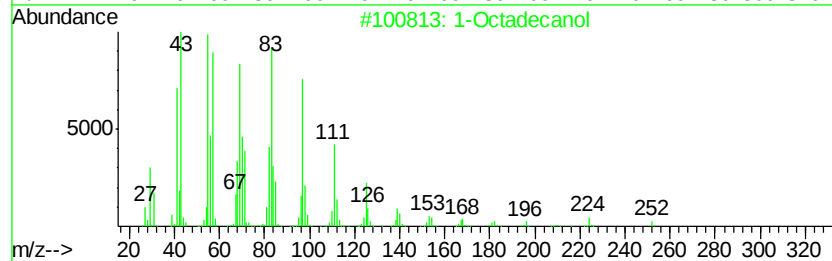
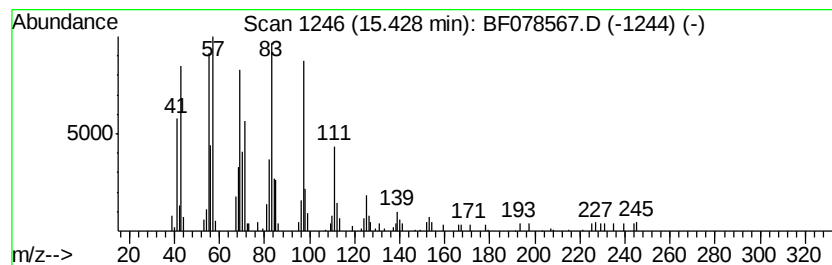
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Octadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.43	6.79 ng	156413	Chrysene-d12	15.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	95
2	Heptafluorobutanoic acid, heptadecanoic acid	452	C21H35F7O2	1000282-97-3	94
3	11-Tricosene	322	C23H46	052078-56-5	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	1-Nonadecene	266	C19H38	018435-45-5	91



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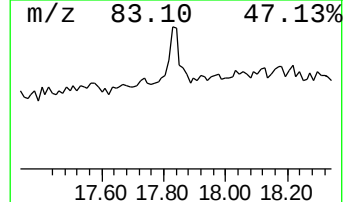
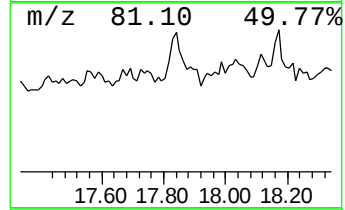
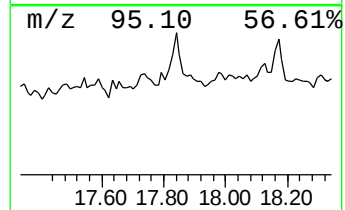
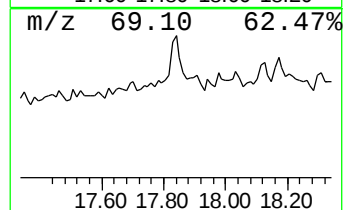
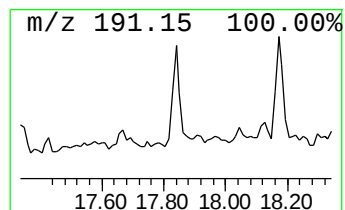
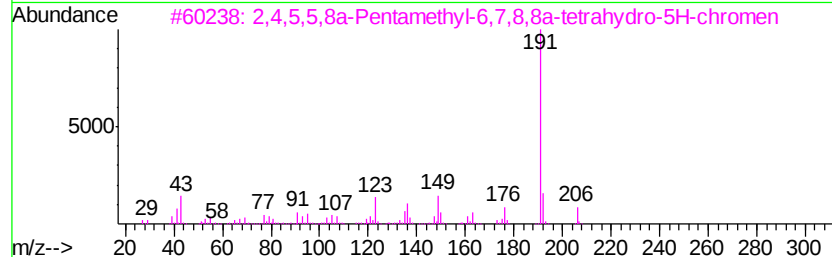
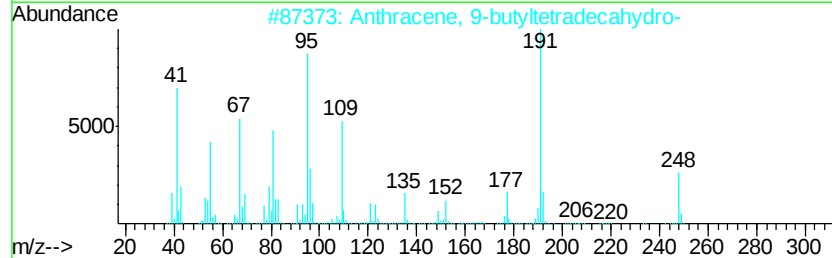
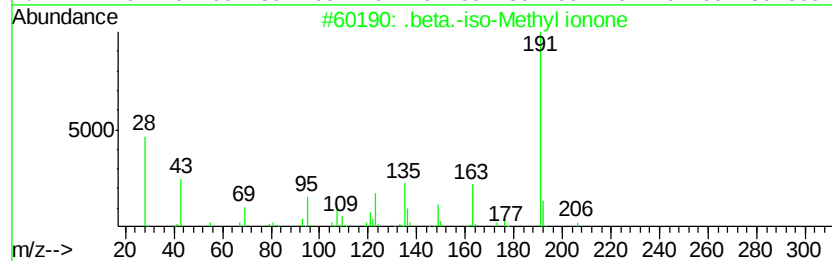
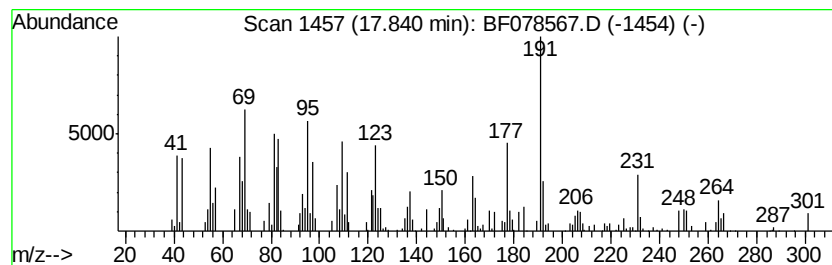
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.84 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	3.94 ng	81243	Perylene-d12	17.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
2		Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	38
3		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	22
4		1H-Inden-1-one, 2,3-dihydro-5,6-...	206	C12H14O3	004082-25-1	14
5		4-Methylimidazole-5-butyric acid...	250	C10H13F3N2O2	1000129-15-9	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041615\
Data File : BF078567.D
Acq On : 16 Apr 2015 15:59
Operator : TP/IZ
Sample : G1890-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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...	4.28	7.8	ng	64867	1	6.68	165488	20.0
unknown6.40	6.40	63.8	ng	527482	1	6.68	165488	20.0
5-Octadecene, (E)-	12.62	2.2	ng	33364	4	12.24	308629	20.0
1-Octadecanol	15.43	6.8	ng	156413	5	15.50	460922	20.0
unknown17.84	17.84	3.9	ng	81243	6	17.20	412184	20.0