

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
 Data File : BF088633.D
 Acq On : 2 Jul 2016 22:59
 Operator : UM/SJ
 Sample : H3837-18
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C1.2-03

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	1.861	20	24	35	rVB	49232	88688	3.15%	0.360%
2	2.010	35	37	41	rVB2	49074	60220	2.14%	0.244%
3	3.016	123	125	138	rBV	10451	35262	1.25%	0.143%
4	4.959	292	295	300	rBB	208963	292426	10.38%	1.186%
5	5.393	330	333	335	rBV	2449860	2687378	95.35%	10.897%
6	6.433	421	424	426	rVB	2564110	2780922	98.67%	11.277%
7	6.559	432	435	437	rBV	2373318	2441980	86.64%	9.902%
8	6.719	448	449	452	rBV	36230	39700	1.41%	0.161%
9	6.799	453	456	457	rBV	572617	703194	24.95%	2.851%
10	6.947	467	469	472	rVB	1832712	1959539	69.53%	7.946%
11	7.359	502	505	507	rBV	1875444	1792044	63.58%	7.267%
12	8.079	566	568	570	rBV	1209448	991454	35.18%	4.020%
13	8.708	622	623	625	rVB	44740	33915	1.20%	0.138%
14	9.153	660	662	665	rBV	2266970	2818410	100.00%	11.429%
15	9.553	695	697	699	rVB	525455	471416	16.73%	1.912%
16	9.828	719	721	724	rVB	1001944	922885	32.74%	3.742%
17	10.251	753	758	759	rBV	36250	35077	1.24%	0.142%
18	10.616	787	790	792	rBV	1544893	1453177	51.56%	5.893%
19	10.742	800	801	806	rBV	40995	53449	1.90%	0.217%
20	11.302	848	850	853	rVB	589161	744598	26.42%	3.019%
21	11.851	895	898	899	rBV	29144	40842	1.45%	0.166%
22	12.365	941	943	946	rBV2	30645	41856	1.49%	0.170%
23	12.731	973	975	977	rBV	23853	34089	1.21%	0.138%
24	12.891	987	989	992	rBV	1996213	1862170	66.07%	7.551%
25	13.428	1034	1036	1038	rBV2	18405	28246	1.00%	0.115%
26	13.794	1066	1068	1073	rBV	173866	199717	7.09%	0.810%
27	13.931	1078	1080	1083	rBV	724849	745107	26.44%	3.021%
28	14.434	1121	1124	1127	rBV2	58765	116133	4.12%	0.471%
29	14.697	1145	1147	1148	rBV	34974	40497	1.44%	0.164%
30	14.788	1153	1155	1157	rVB	42750	46673	1.66%	0.189%
31	15.211	1190	1192	1195	rVB	19753	31165	1.11%	0.126%
32	15.337	1200	1203	1205	rBV	424165	605695	21.49%	2.456%
33	15.840	1245	1247	1251	rVB4	17346	36674	1.30%	0.149%
34	16.857	1333	1336	1340	rVB	143357	261635	9.28%	1.061%

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

35	17.154	1360	1362	1365	rVB3	15762	31118	1.10%	0.126%
36	17.611	1399	1402	1408	rVB7	19635	48273	1.71%	0.196%
37	18.011	1434	1437	1440	rVB5	36579	85484	3.03%	0.347%

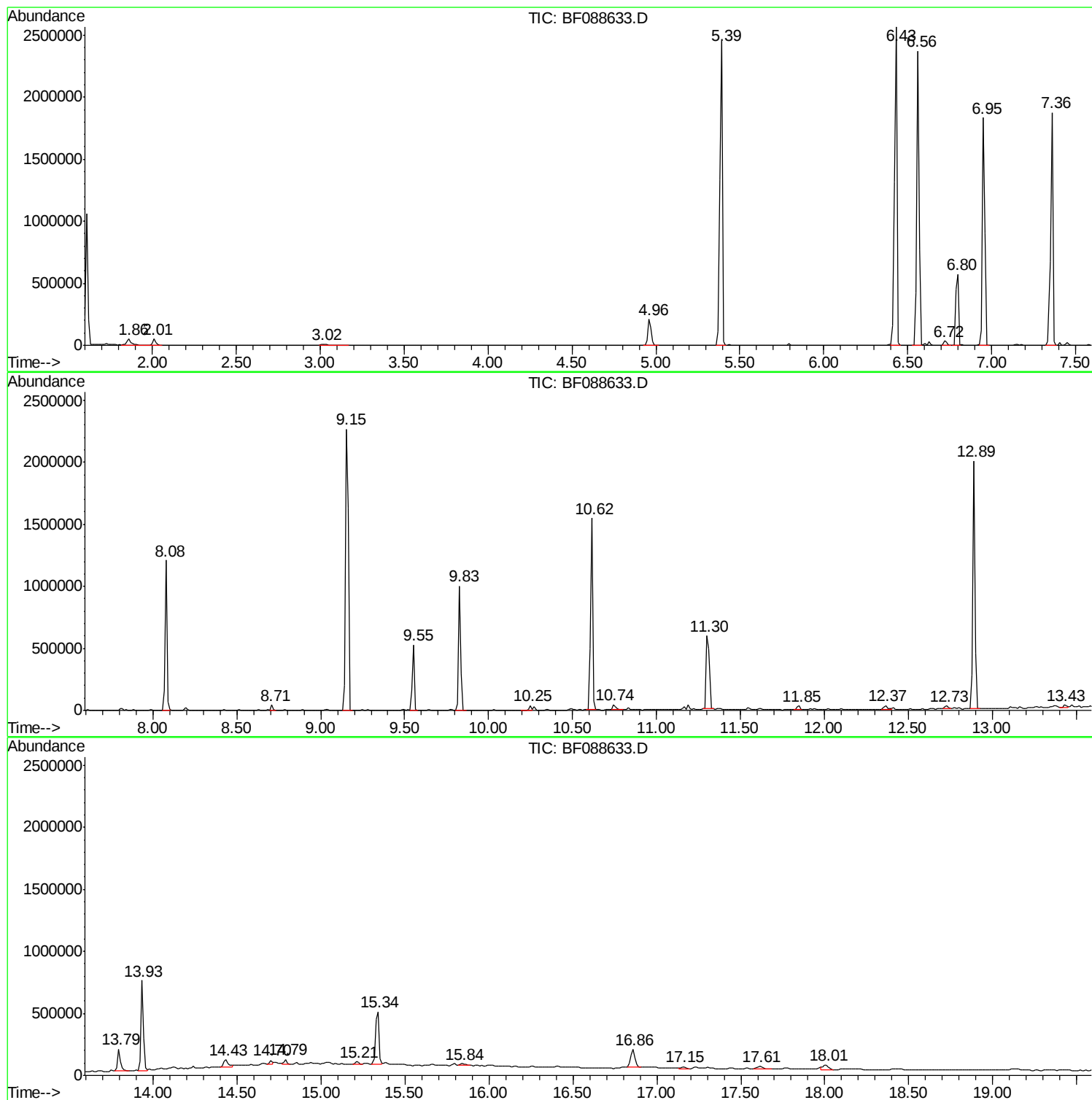
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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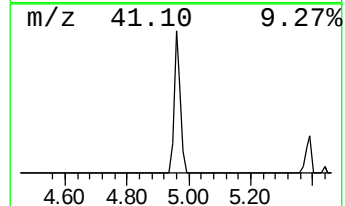
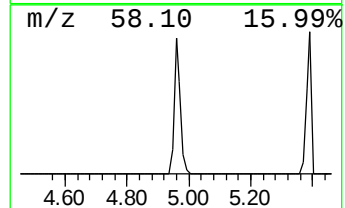
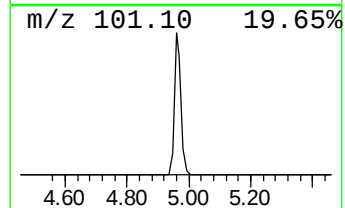
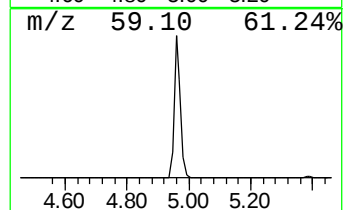
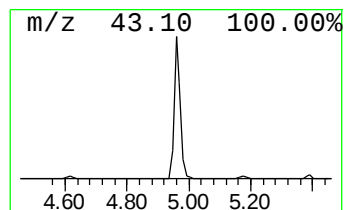
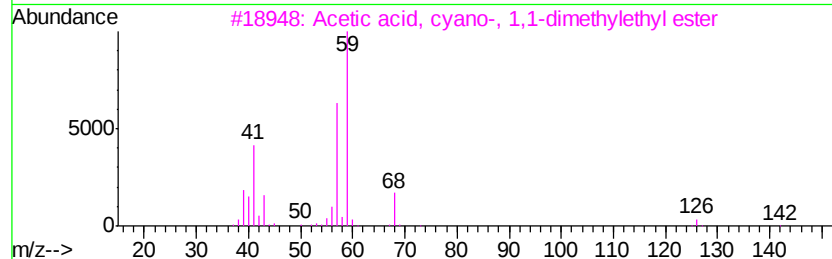
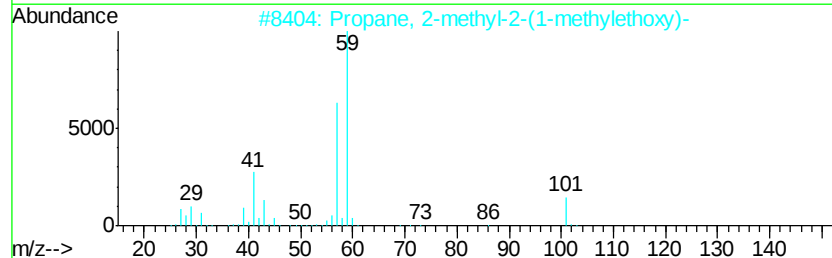
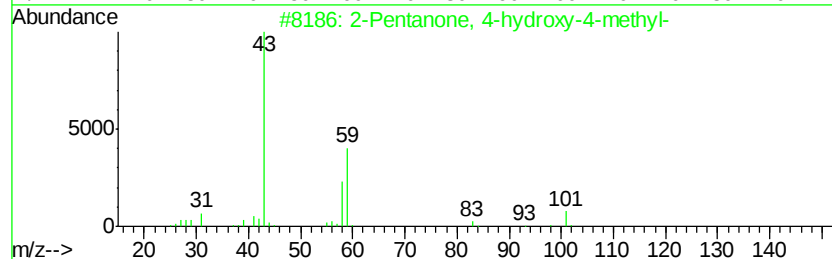
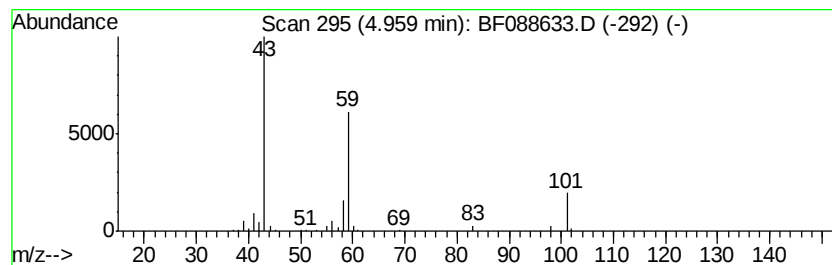
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	8.32 ng	292426	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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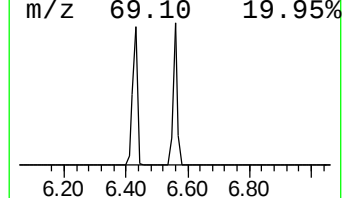
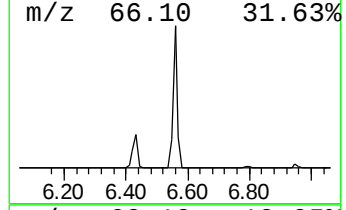
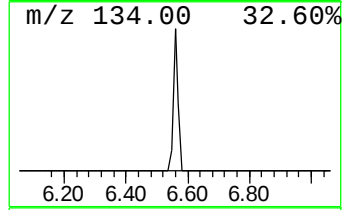
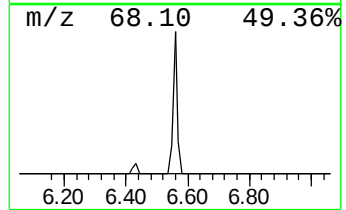
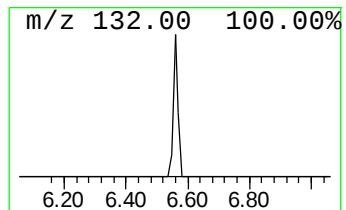
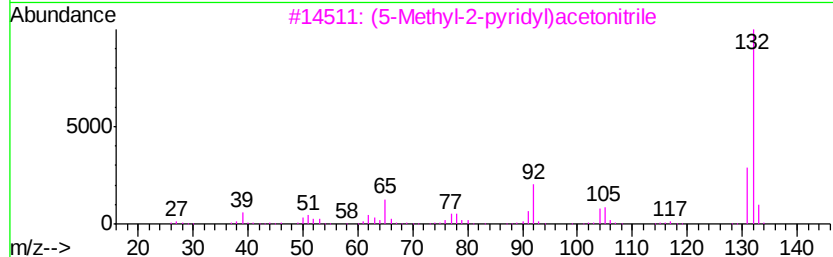
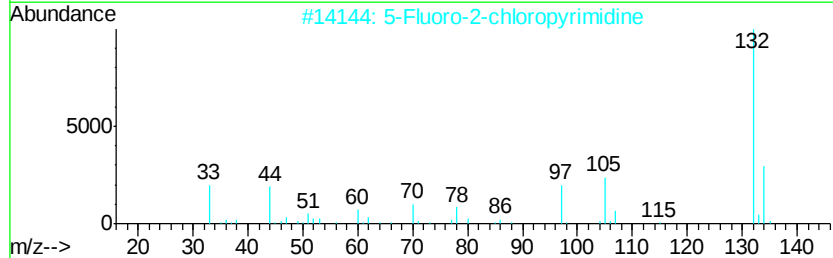
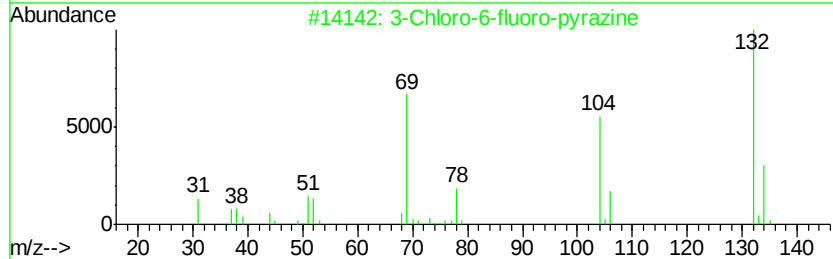
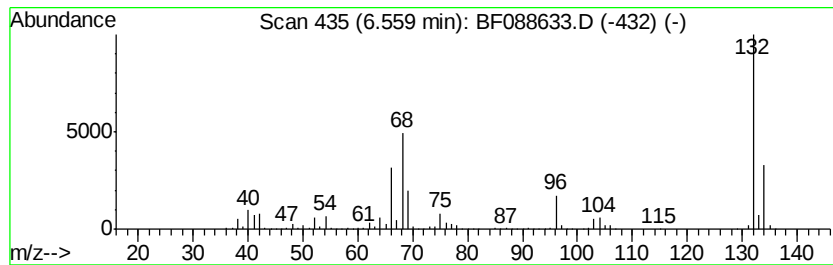
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	69.45 ng	2441980	1,4-Dichlorobenzene-d4	6.80

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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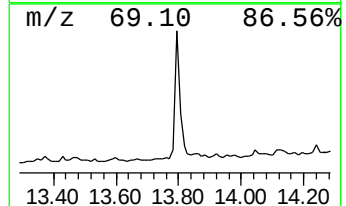
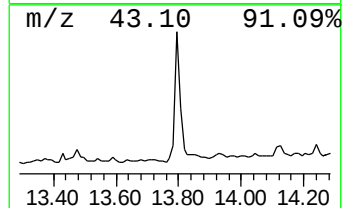
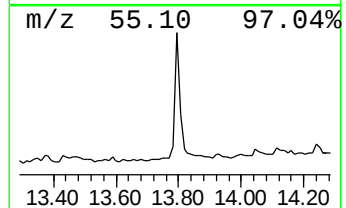
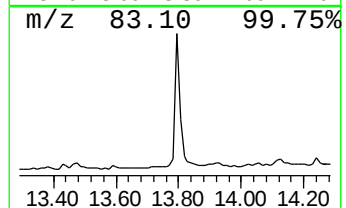
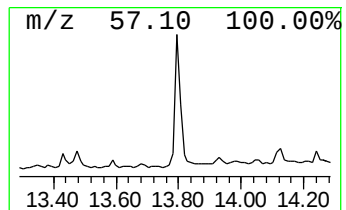
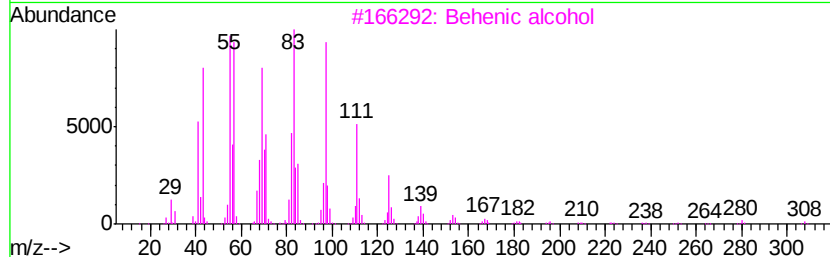
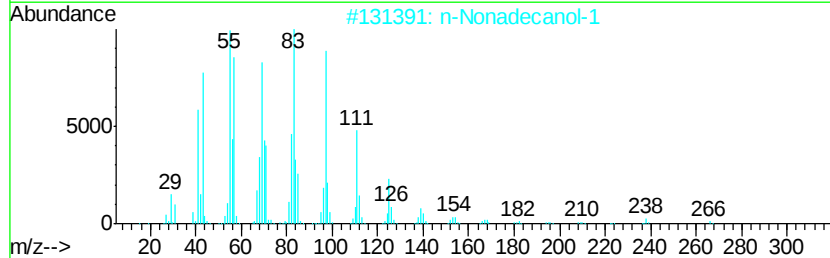
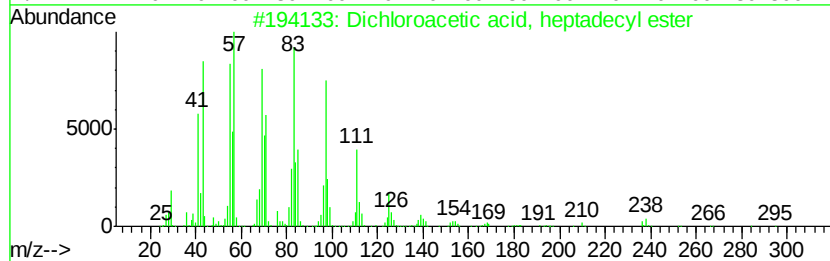
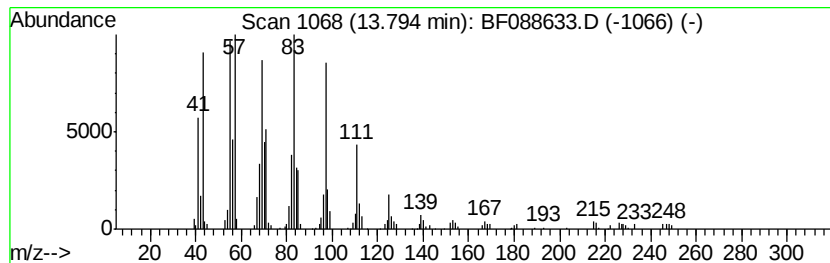
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	5.36 ng	199717	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94



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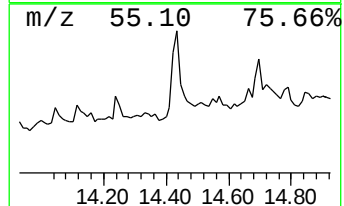
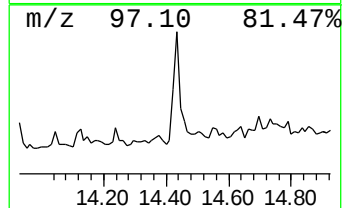
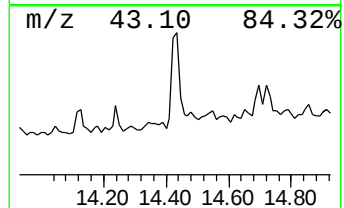
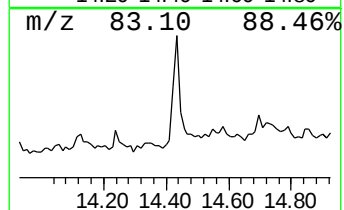
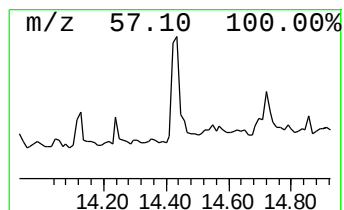
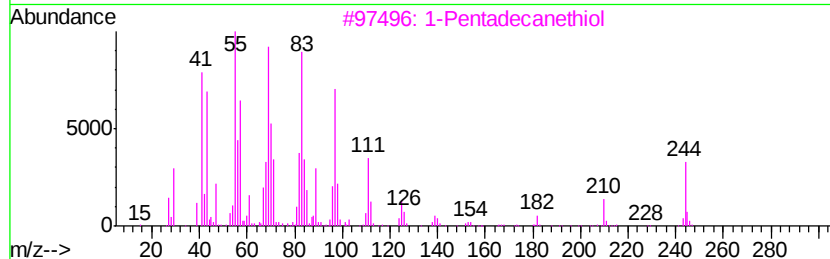
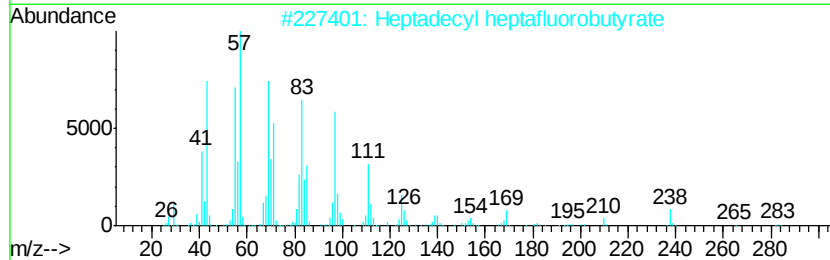
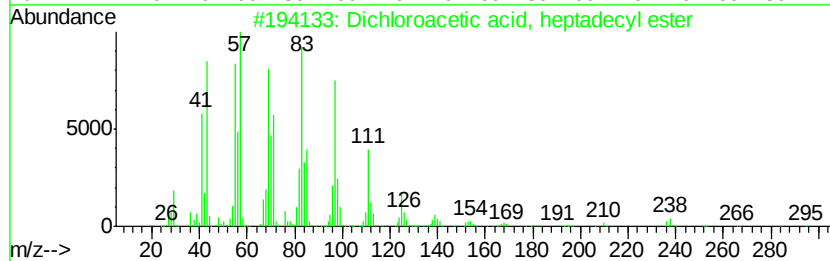
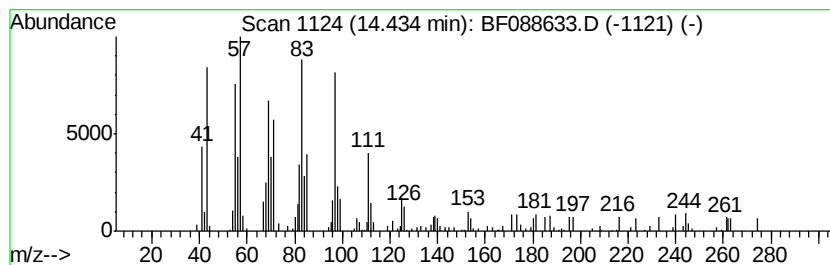
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	3.12 ng	116133	Chrysene-d12	13.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		1-Pentadecanethiol	244	C15H32S	025276-70-4	93
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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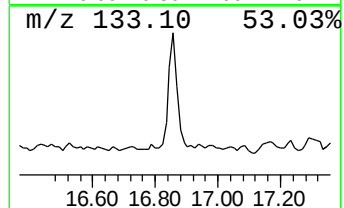
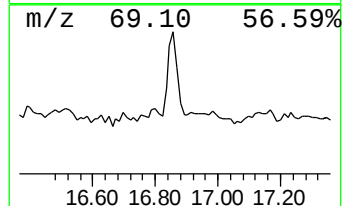
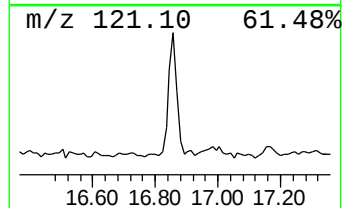
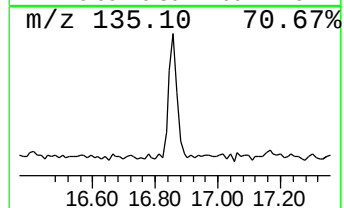
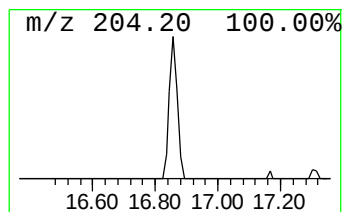
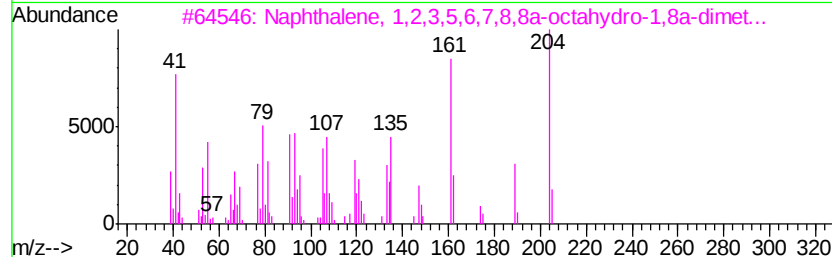
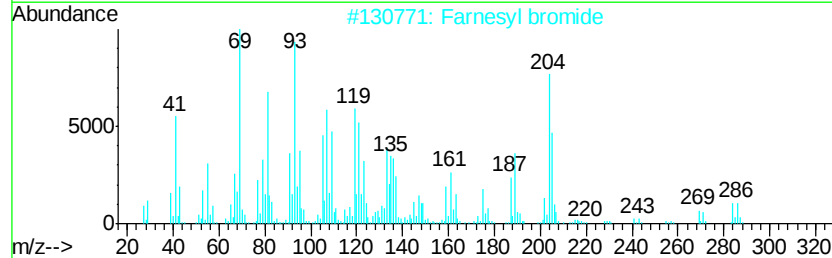
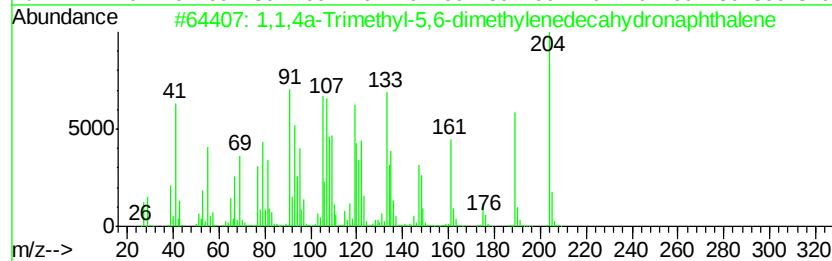
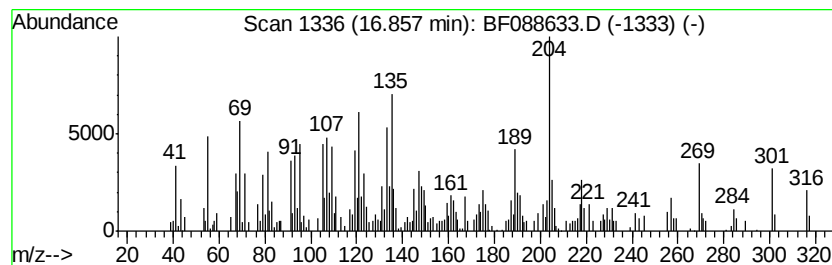
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Peak Number 7 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	8.64 ng	261635	Perylene-d12	15.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	72		
2	Farnesyl bromide	284	C15H25Br	006874-67-5	70		
3	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	58		
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	58		
5	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	50		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088633.D
Acq On : 2 Jul 2016 22:59
Operator : UM/SJ
Sample : H3837-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

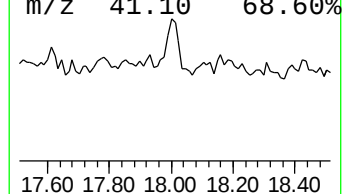
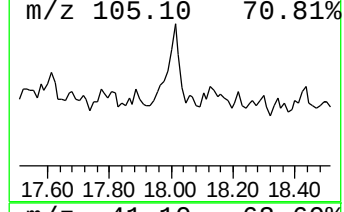
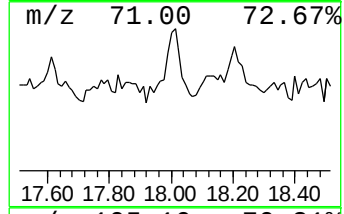
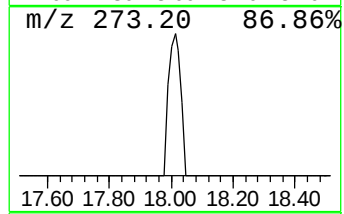
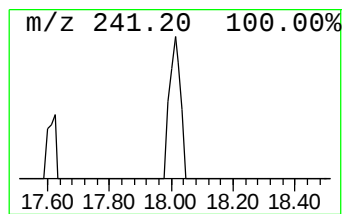
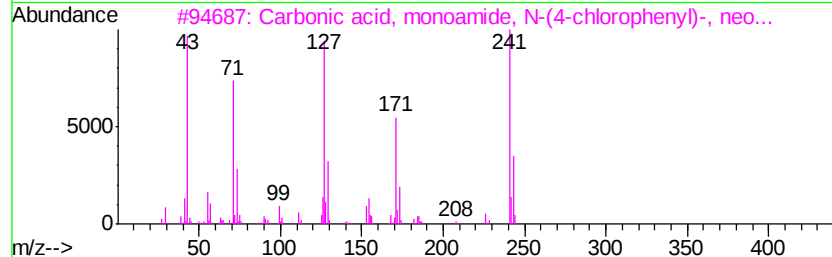
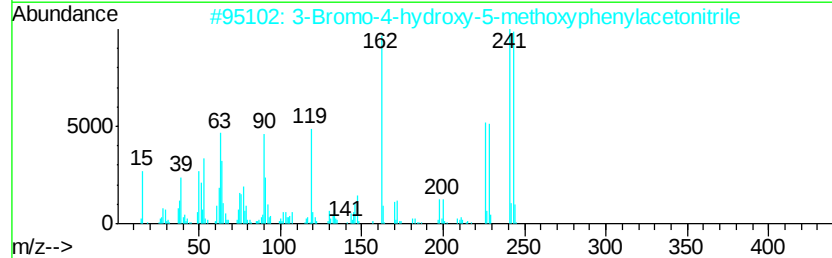
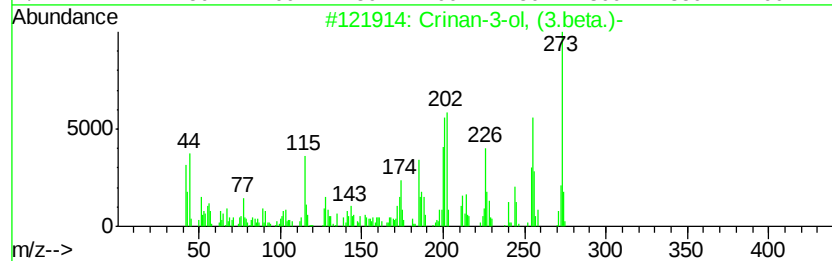
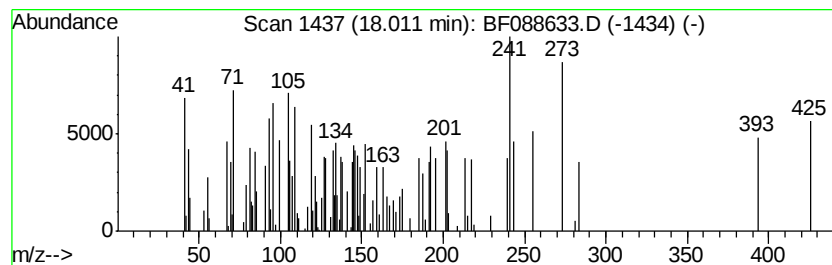
Instrument :
BNA_F
ClientSampleId :
C1.2-03

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 unknown18.01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.01	2.82 ng	85484	Perylene-d12	15.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Crinan-3-ol, (3.beta.)-	273	C16H19NO3	010279-81-9	27
2	3-Bromo-4-hydroxy-5-methoxypheny...	241	C9H8BrNO2	081038-44-0	25
3	Carbonic acid, monoamide, N-(4-c...	241	C12H16ClNO2	1000339-99-7	10
4	1-(6-Methyl-3-pyridyl)-3-(2-naph...	273	C19H15NO	010040-71-8	9
5	2-(4-Chloro-phenyl)-8-methyl-ind...	241	C15H12ClN	1000337-21-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-03

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
2-Pentanone, 4-hy...	4.96	8.3	ng	292426	1	6.80	703194	20.0
unknown6.56	6.56	69.5	ng	2441980	1	6.80	703194	20.0
Dichloroacetic ac...	13.79	5.4	ng	199717	5	13.93	745107	20.0
Heptadecyl hepta...	14.43	3.1	ng	116133	5	13.93	745107	20.0
1,1,4a-Trimethyl-...	16.86	8.6	ng	261635	6	15.34	605695	20.0
unknown18.01	18.01	2.8	ng	85484	6	15.34	605695	20.0