

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
 Data File : BF088680.D
 Acq On : 4 Jul 2016 7:46
 Operator : UM/SJ
 Sample : H3856-02
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EPHC-B4(11-13)

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	1.850	22	23	34	rVB	75471	103047	4.37%	0.485%
2	2.981	120	122	141	rBV2	22308	86422	3.67%	0.407%
3	4.947	291	294	300	rVB	128874	163353	6.93%	0.769%
4	5.382	329	332	334	rBV	2027754	2293400	97.30%	10.798%
5	6.422	420	423	425	rBV	2250076	2356928	100.00%	11.097%
6	6.547	432	434	437	rBV	1929820	2113022	89.65%	9.949%
7	6.787	453	455	457	rBV	655756	643245	27.29%	3.029%
8	6.856	459	461	466	rBV	20646	28029	1.19%	0.132%
9	6.936	466	468	471	rVB	1356526	1718379	72.91%	8.091%
10	7.347	501	504	506	rBV	1570502	1425462	60.48%	6.712%
11	7.450	510	513	517	rBB	18769	23740	1.01%	0.112%
12	8.068	565	567	569	rBV	1071281	855416	36.29%	4.028%
13	9.142	659	661	664	rBV	2228348	2333956	99.03%	10.989%
14	9.428	684	686	688	rBV	21576	28402	1.21%	0.134%
15	9.542	694	696	698	rBV	470730	457130	19.40%	2.152%
16	9.816	718	720	723	rVB	1065214	883463	37.48%	4.160%
17	10.262	757	759	760	rVB	36949	29452	1.25%	0.139%
18	10.605	786	789	791	rBV	1115712	1304508	55.35%	6.142%
19	10.731	799	800	804	rVB	45323	43574	1.85%	0.205%
20	11.176	837	839	841	rBV	109628	99259	4.21%	0.467%
21	11.291	847	849	852	rVV	844695	727071	30.85%	3.423%
22	11.359	852	855	859	rVB2	25321	57021	2.42%	0.268%
23	11.599	875	876	879	rVB	72529	69063	2.93%	0.325%
24	11.828	895	896	898	rBV	36274	33336	1.41%	0.157%
25	12.708	971	973	977	rBV2	54325	72479	3.08%	0.341%
26	12.879	985	988	990	rBV	1841614	1851956	78.57%	8.720%
27	13.417	1033	1035	1037	rBV	33095	32325	1.37%	0.152%
28	13.680	1053	1058	1059	rBV5	9352	30170	1.28%	0.142%
29	13.805	1066	1069	1076	rBV	52477	123369	5.23%	0.581%
30	13.920	1076	1079	1081	rBV	644098	662514	28.11%	3.119%
31	14.400	1119	1121	1124	rBV2	29366	40307	1.71%	0.190%
32	15.314	1198	1201	1203	rBV	430981	549092	23.30%	2.585%

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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

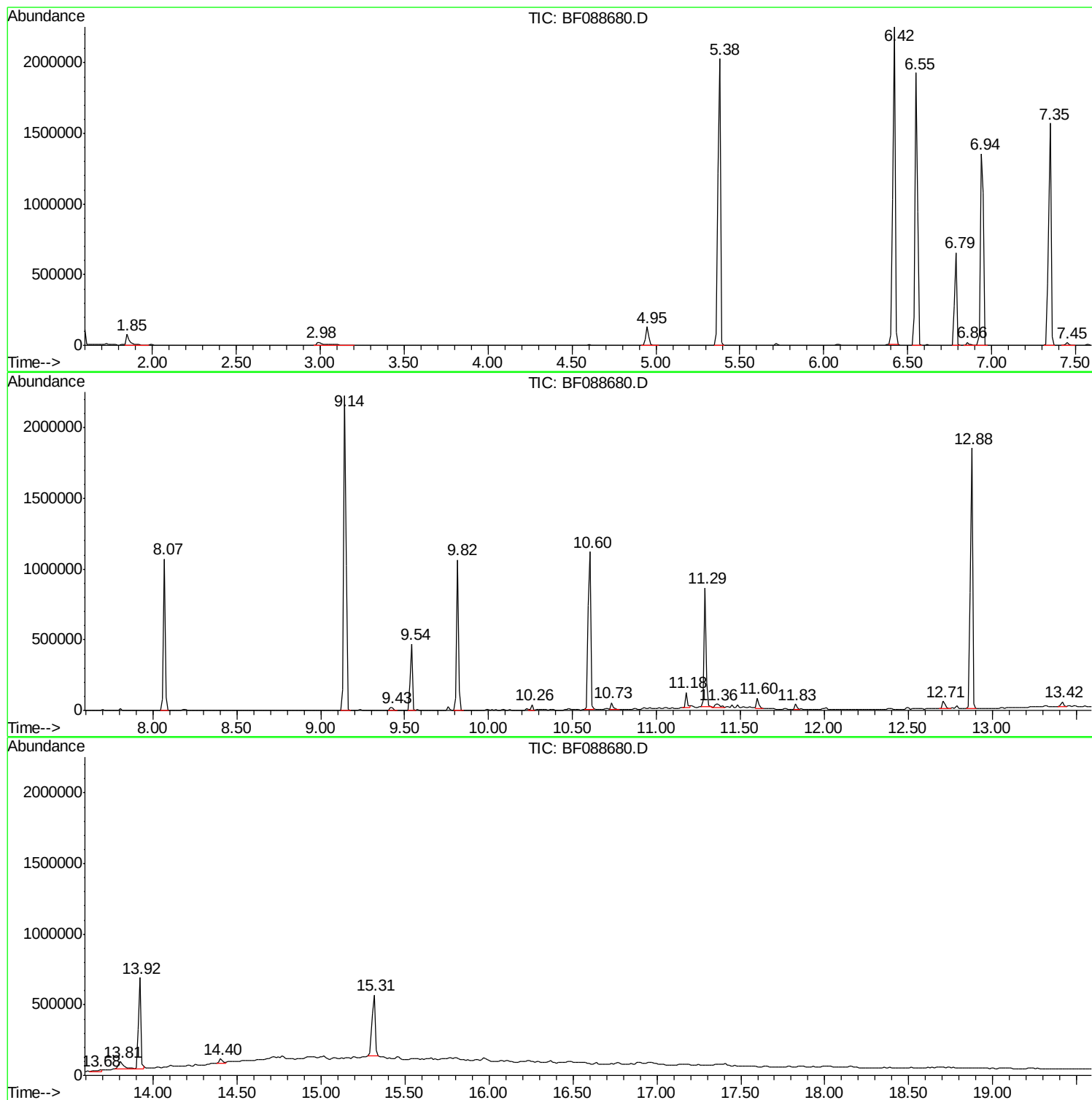
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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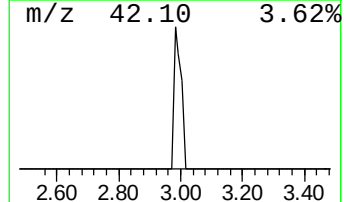
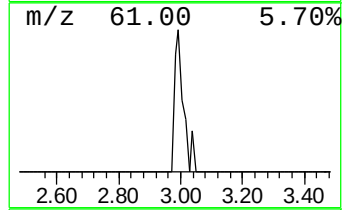
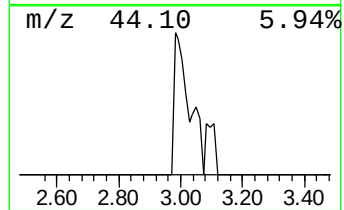
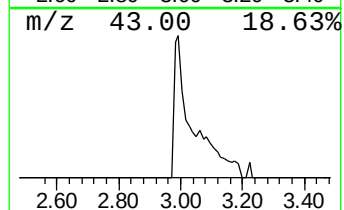
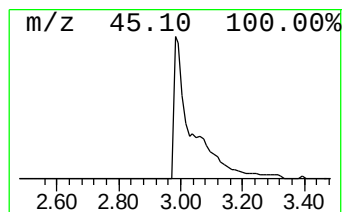
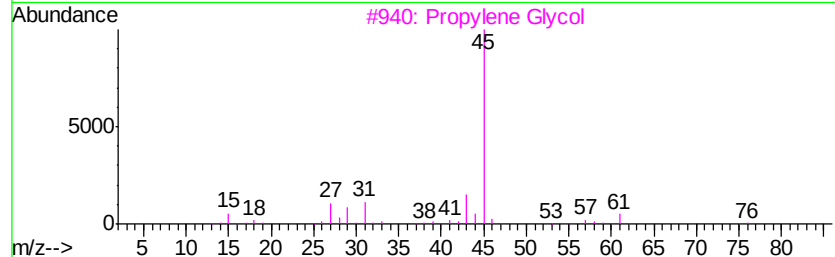
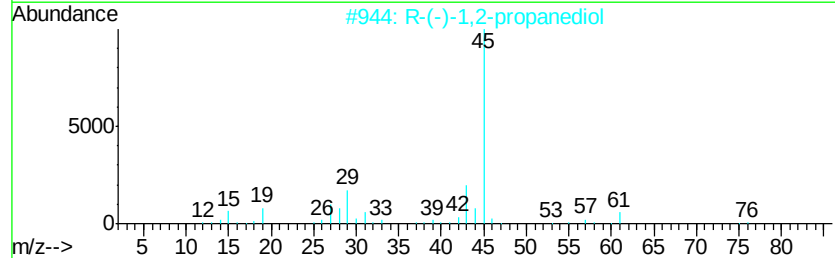
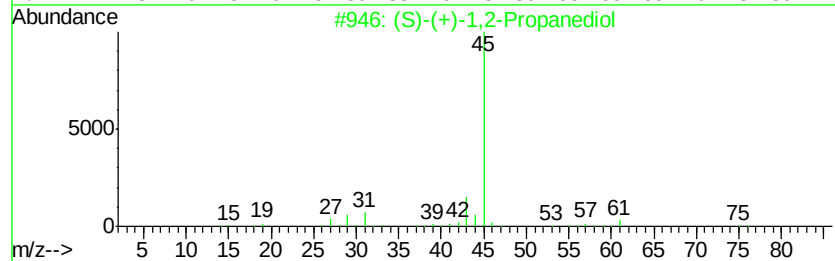
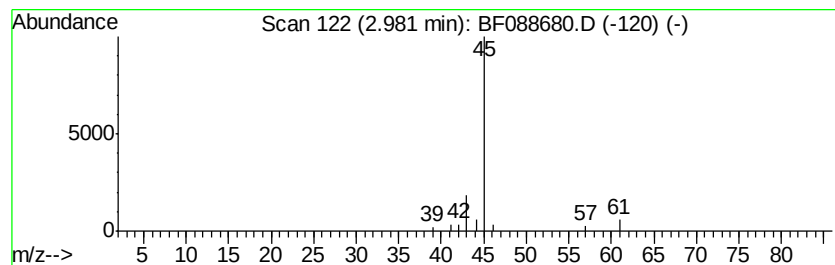
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	2.69 ng	86422	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3			Propylene Glycol	76	C3H8O2	000057-55-6	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Formamide	45	CH3NO	000075-12-7	7



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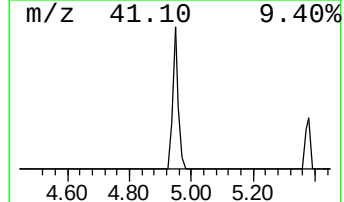
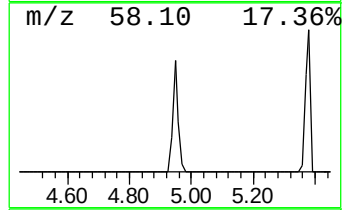
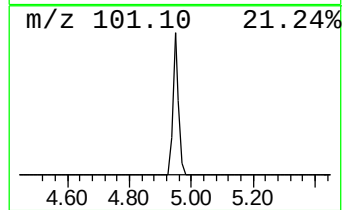
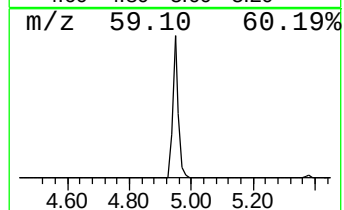
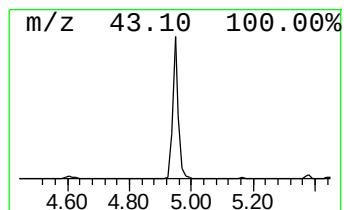
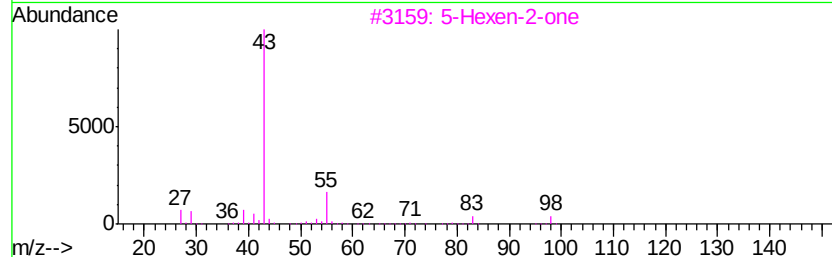
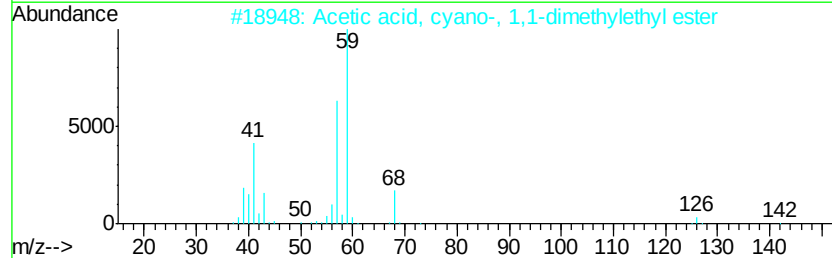
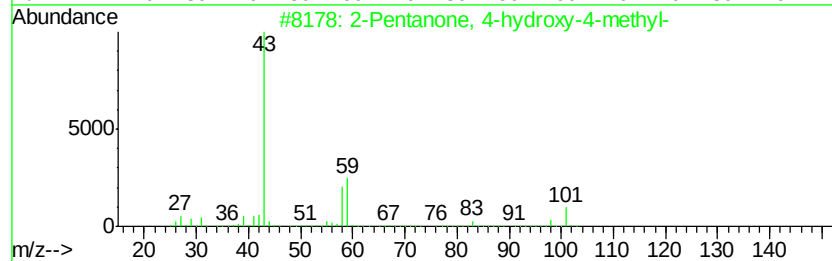
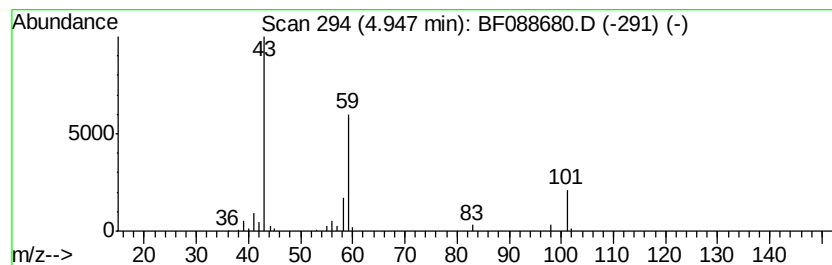
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	5.08 ng	163353	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetone	58	C3H6O	000067-64-1	9



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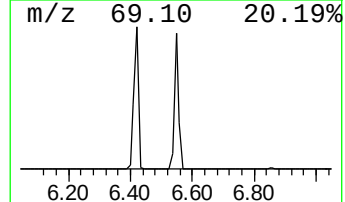
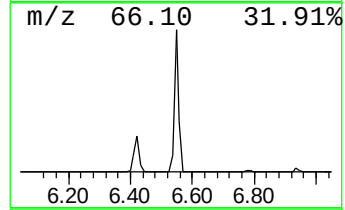
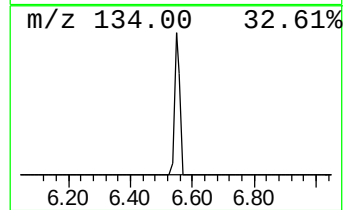
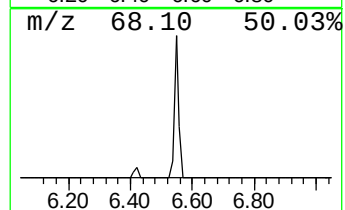
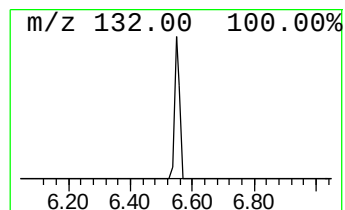
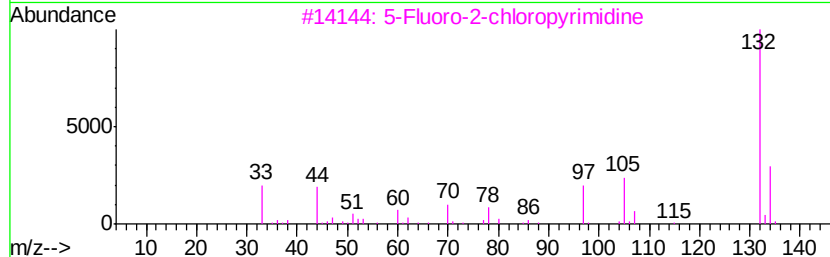
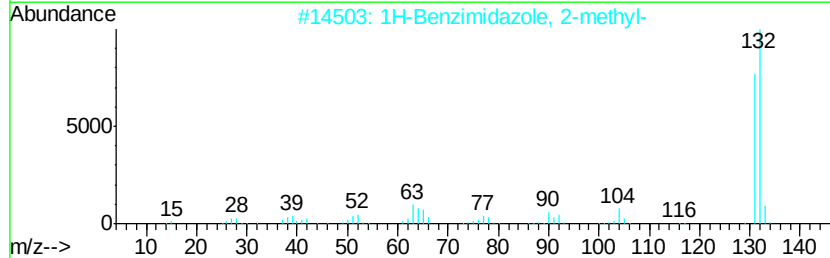
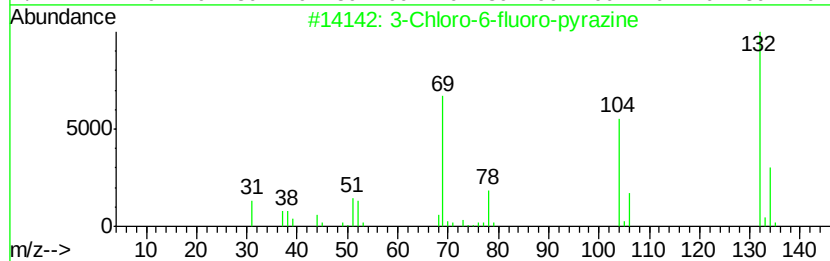
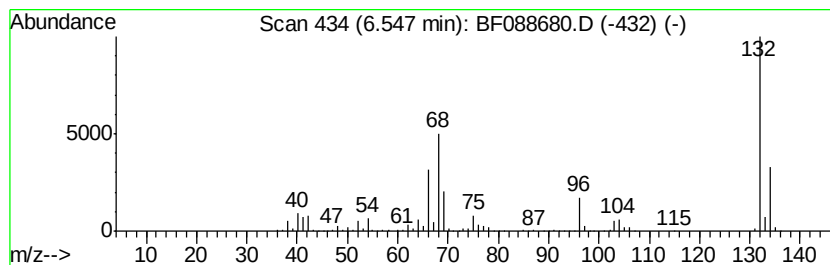
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	65.70 ng	2113020	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22	
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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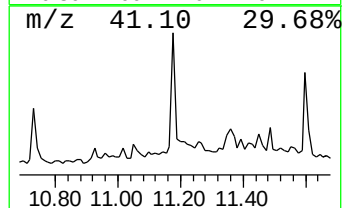
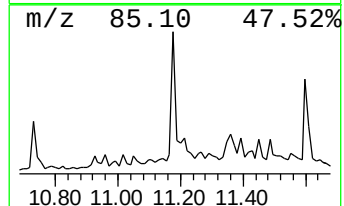
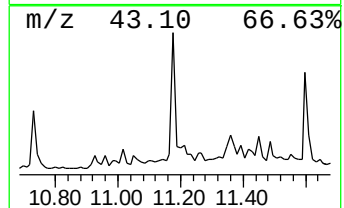
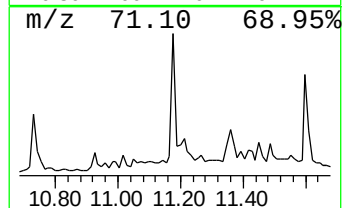
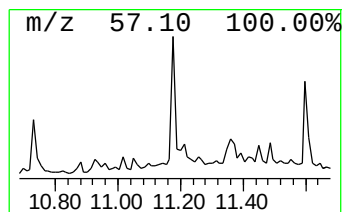
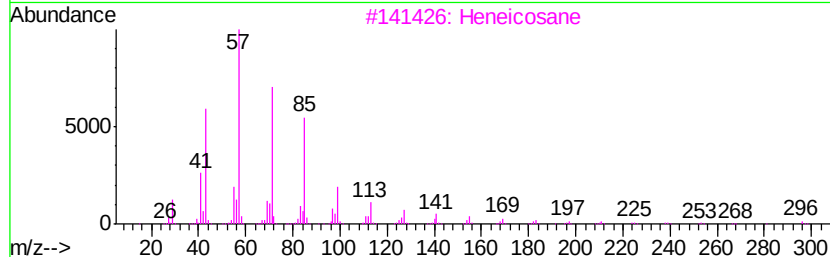
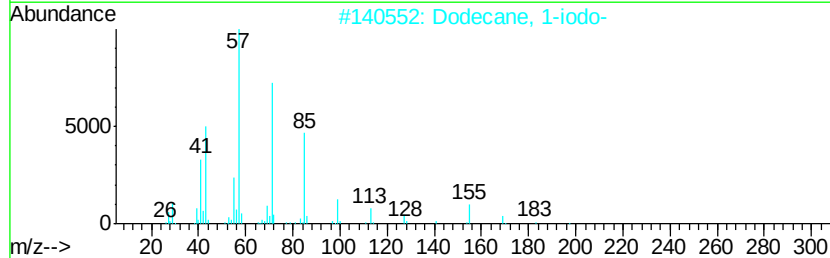
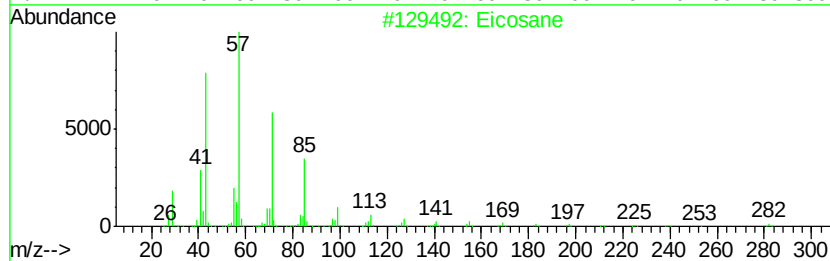
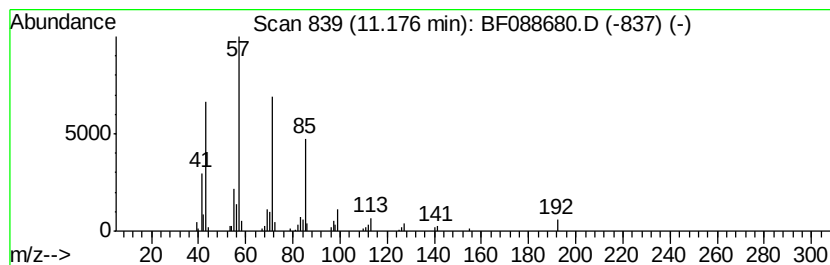
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.18	2.73 ng	99259	Phenanthrene-d10		11.29	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	86
2	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
3	Heneicosane		296	C21H44	000629-94-7	86
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	86
5	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	86



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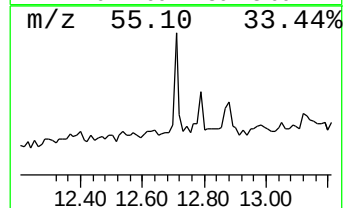
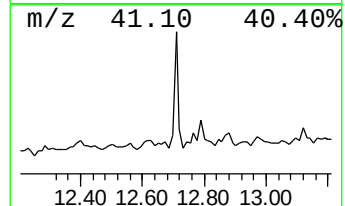
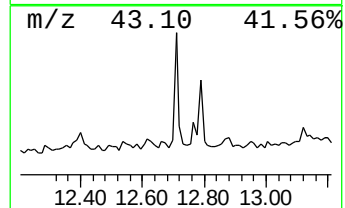
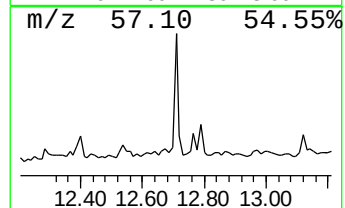
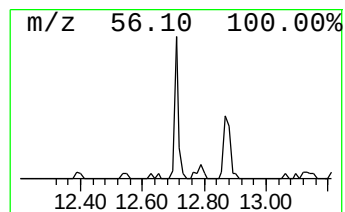
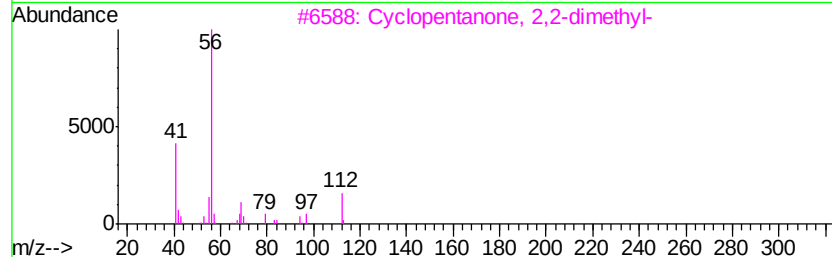
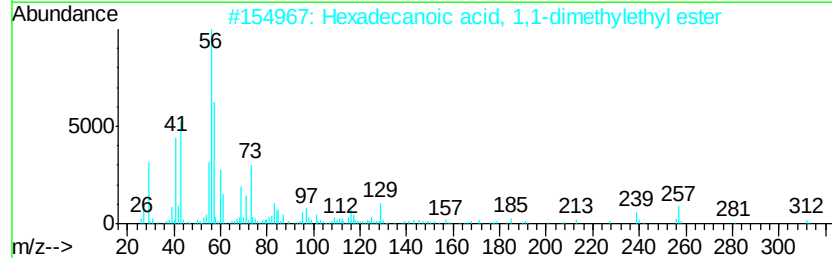
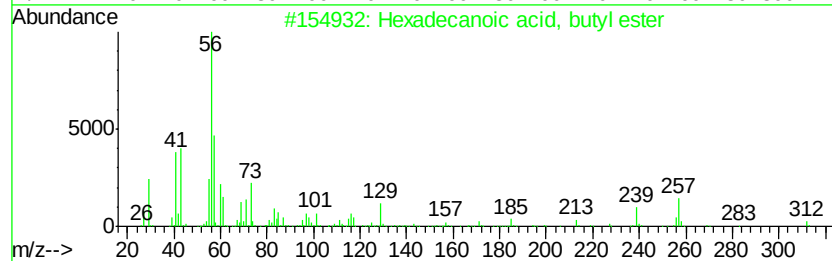
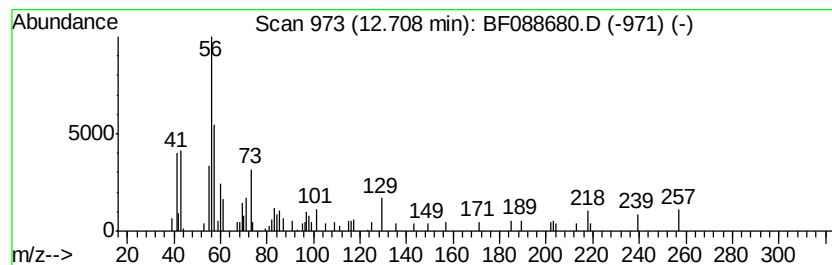
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.19 ng	72479	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	35
4		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27



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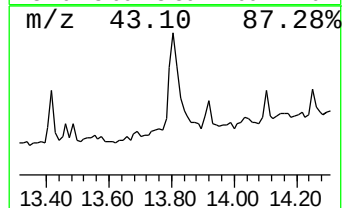
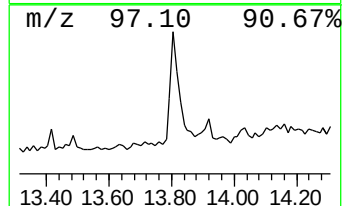
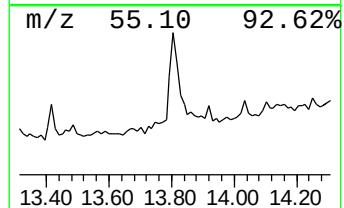
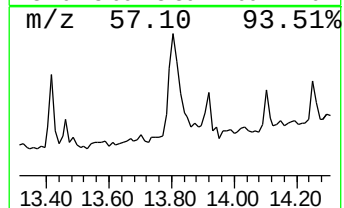
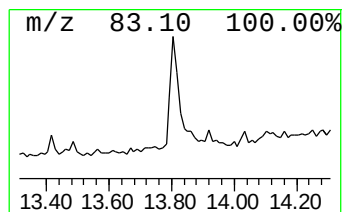
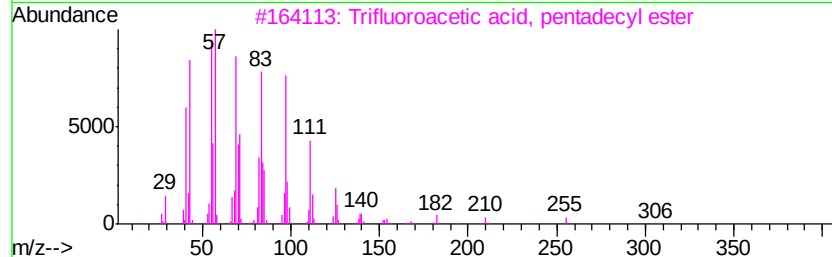
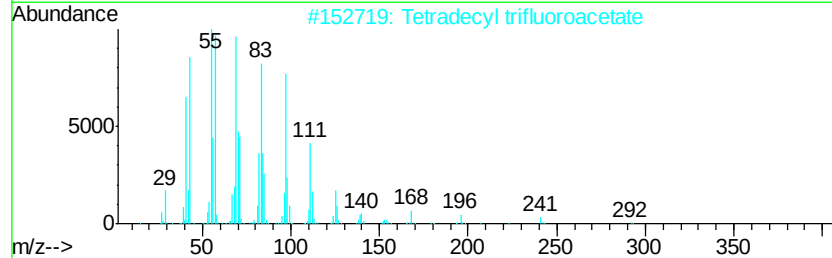
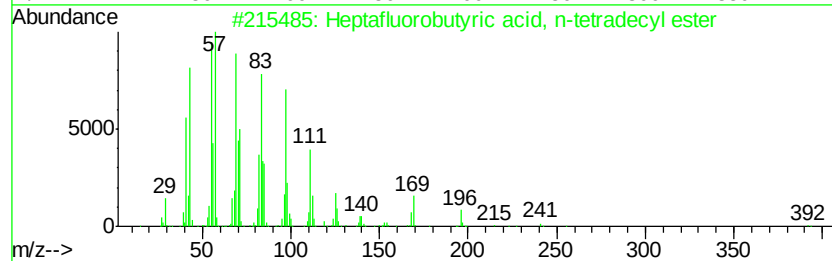
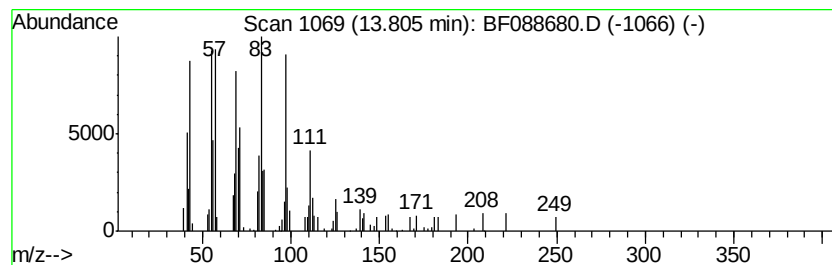
Instrument :
BNA_F
ClientSampleId :
EPHC-B4(11-13)

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 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.81	3.72 ng	123369	Chrysene-d12	13.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	95
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088680.D
Acq On : 4 Jul 2016 7:46
Operator : UM/SJ
Sample : H3856-02
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EPHC-B4(11-13)

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
(S)-(+)-1,2-Propa...	2.98	2.7	ng	86422	1	6.79	643245	20.0
2-Pentanone, 4-hy...	4.95	5.1	ng	163353	1	6.79	643245	20.0
unknown6.55	6.55	65.7	ng	2113020	1	6.79	643245	20.0
Eicosane	11.18	2.7	ng	99259	4	11.29	727071	20.0
Hexadecanoic acid...	12.71	2.2	ng	72479	5	13.92	662514	20.0
Heptafluorobutyri...	13.81	3.7	ng	123369	5	13.92	662514	20.0