

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071316\
 Data File : BF088979.D
 Acq On : 14 Jul 2016 1:34
 Operator : UM/SJ
 Sample : H3946-11
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P7-B7(0-8)C

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	5	7	16	rVB	197755	337911	15.32%	1.654%
2	1.781	16	17	26	rVV	1279591	2100002	95.24%	10.279%
3	1.907	26	28	51	rVB2	70510	264474	11.99%	1.294%
4	4.856	283	286	293	rVB	263821	438424	19.88%	2.146%
5	5.302	321	325	327	rBV	1786043	2085761	94.59%	10.209%
6	5.690	357	359	363	rVB	33289	31722	1.44%	0.155%
7	6.353	413	417	419	rBV	1744924	2118556	96.08%	10.370%
8	6.467	424	427	429	rBV	2003260	1979695	89.78%	9.690%
9	6.696	445	447	449	rBB	463203	418373	18.97%	2.048%
10	6.856	458	461	463	rBB	1552051	1710806	77.59%	8.374%
11	7.267	493	497	499	rBV	1174855	1404145	63.68%	6.873%
12	7.976	557	559	562	rBB	495368	484342	21.97%	2.371%
13	9.062	651	654	656	rBV	2437998	2205013	100.00%	10.793%
14	9.450	686	688	691	rVB	263943	245389	11.13%	1.201%
15	9.725	710	712	714	rBV	455425	470947	21.36%	2.305%
16	10.513	779	781	784	rVB	1093252	1033800	46.88%	5.060%
17	10.651	790	793	799	rVB	17938	32420	1.47%	0.159%
18	11.096	829	832	833	rBV	19955	24564	1.11%	0.120%
19	11.199	839	841	844	rBV	360809	403046	18.28%	1.973%
20	12.411	944	947	949	rBV	33992	33823	1.53%	0.166%
21	12.628	963	966	968	rBV	28744	36453	1.65%	0.178%
22	12.788	978	980	983	rBV	1445154	1350534	61.25%	6.610%
23	13.474	1035	1040	1042	rBV3	12806	27944	1.27%	0.137%
24	13.542	1045	1046	1048	rVV	20830	36583	1.66%	0.179%
25	13.588	1048	1050	1051	rVV	41009	47011	2.13%	0.230%
26	13.611	1051	1052	1054	rVB	34154	42823	1.94%	0.210%
27	13.657	1054	1056	1057	rBV	28665	24999	1.13%	0.122%
28	13.691	1057	1059	1063	rVV2	78613	105423	4.78%	0.516%
29	13.828	1068	1071	1073	rBV	432821	418043	18.96%	2.046%
30	14.331	1111	1115	1119	rBV4	15610	40312	1.83%	0.197%
31	14.411	1119	1122	1125	rBV2	16743	40675	1.84%	0.199%
32	14.674	1143	1145	1148	rBV2	30843	42130	1.91%	0.206%
33	14.822	1155	1158	1159	rBV	19617	30720	1.39%	0.150%
34	15.200	1188	1191	1194	rBV	267167	302377	13.71%	1.480%

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ClientSampleId :
P7-B7(0-8)C

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

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35	15.680	1230	1233	1236	rVB3	11681	28485	1.29%	0.139%
36	15.817	1243	1245	1252	rVB5	15216	32891	1.49%	0.161%

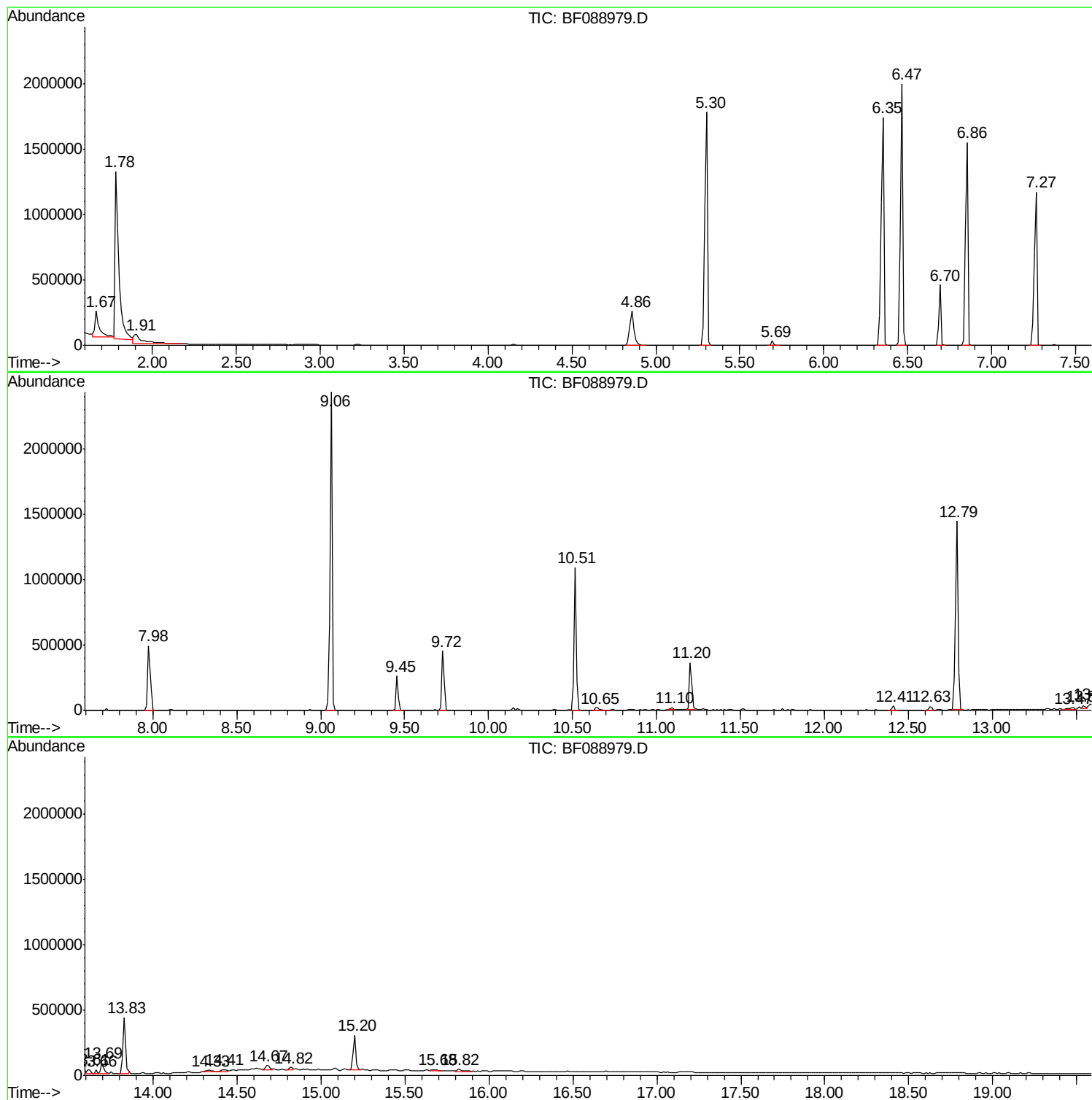
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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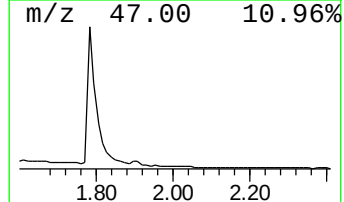
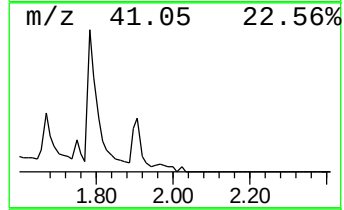
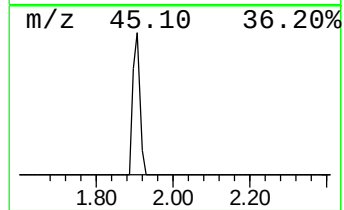
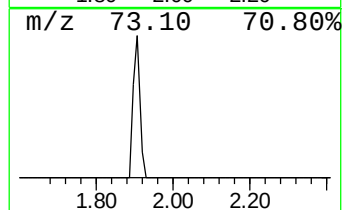
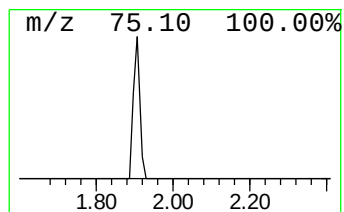
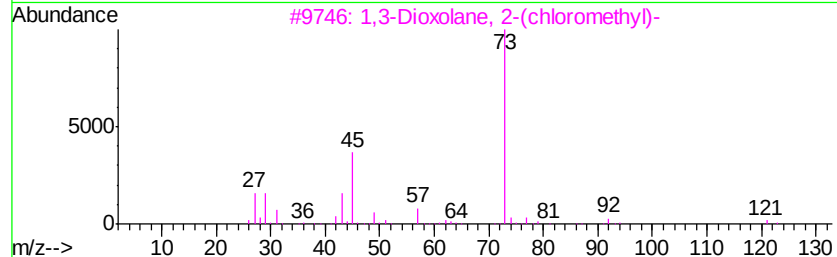
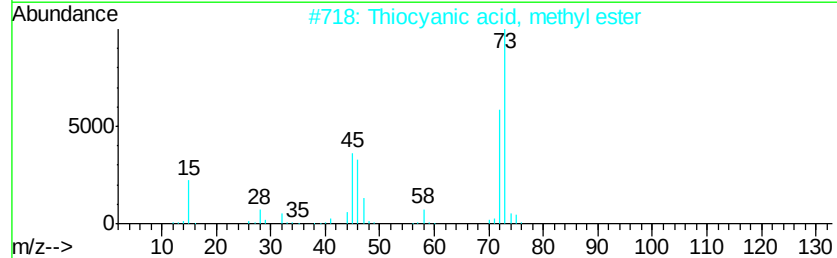
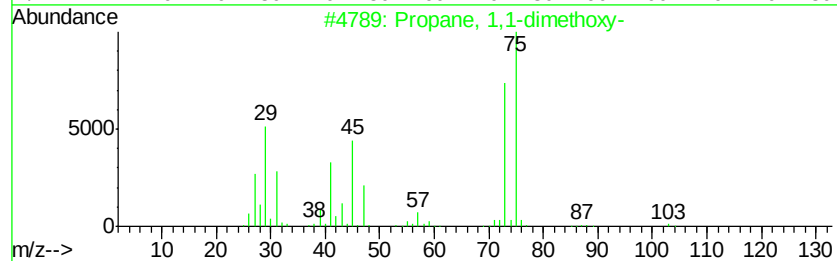
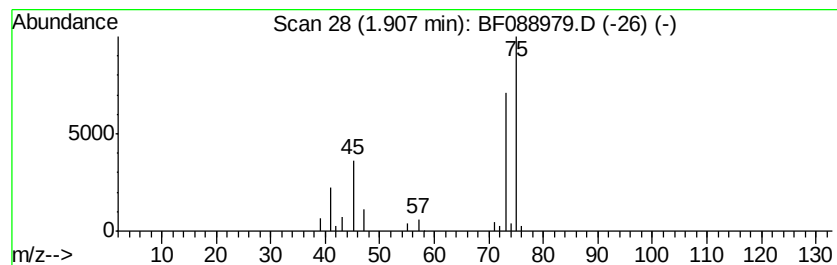
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.91	12.64 ng	264474	1,4-Dichlorobenzene-d4	6.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	12
3		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	8
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	8



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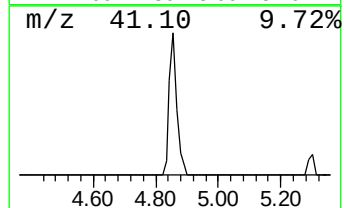
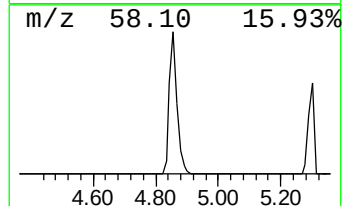
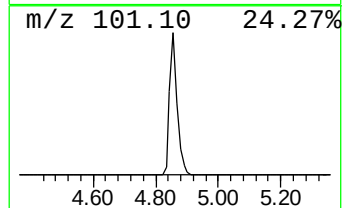
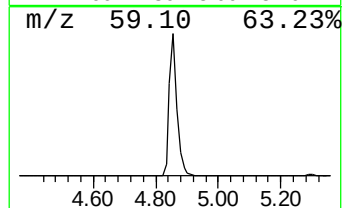
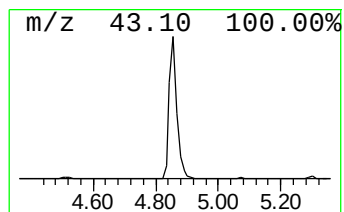
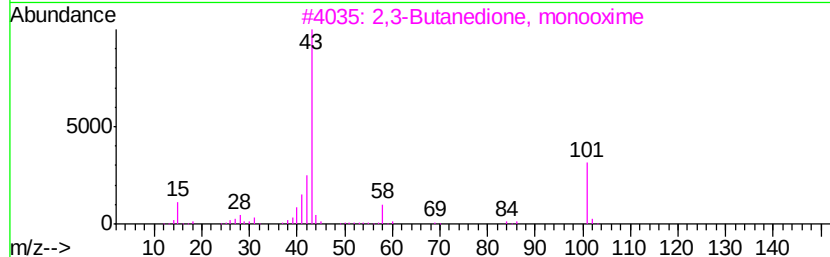
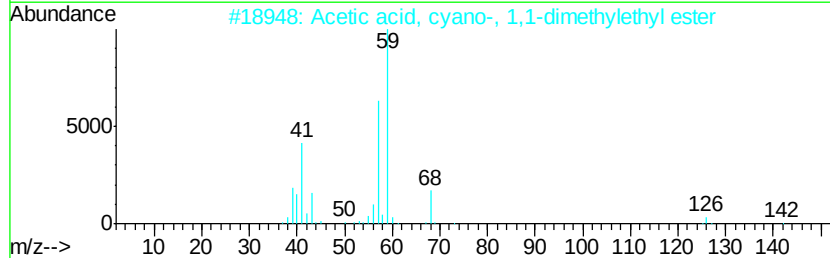
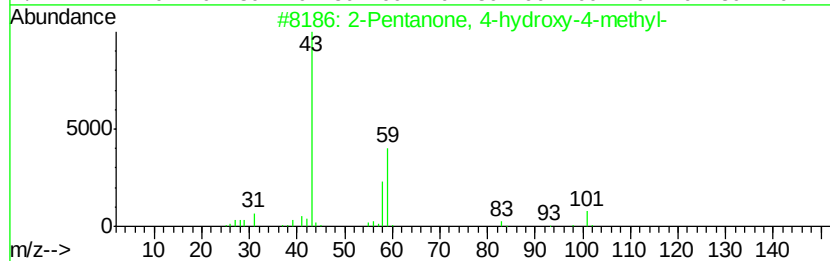
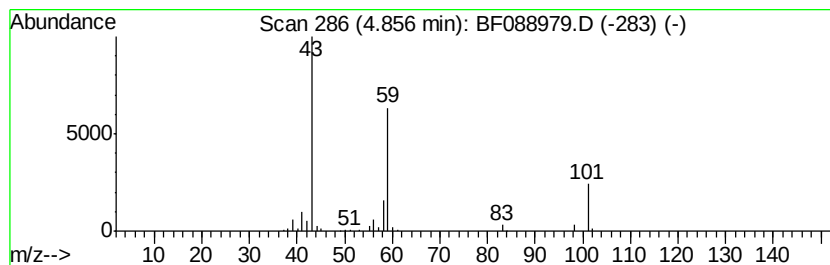
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	20.96 ng	438424	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	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetone	58	C3H6O	000067-64-1	10
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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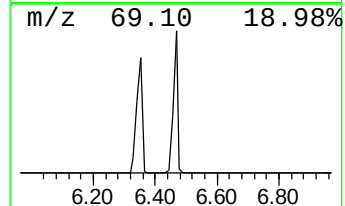
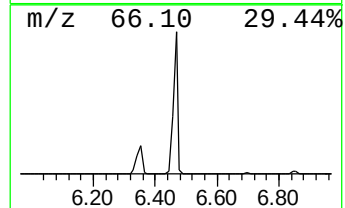
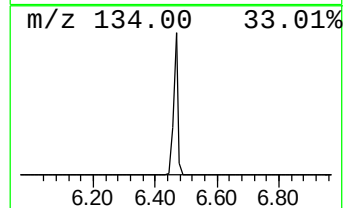
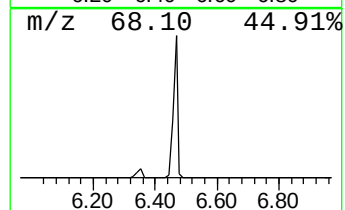
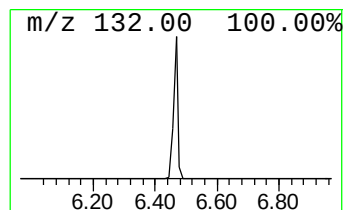
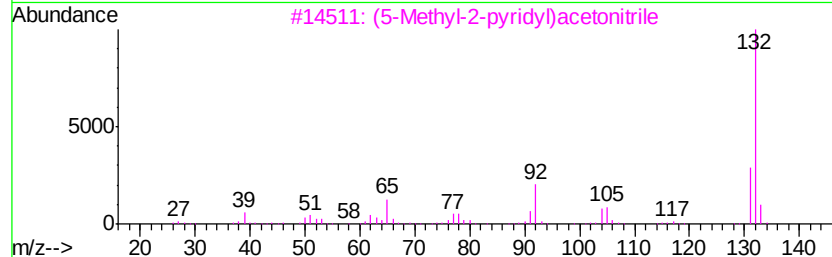
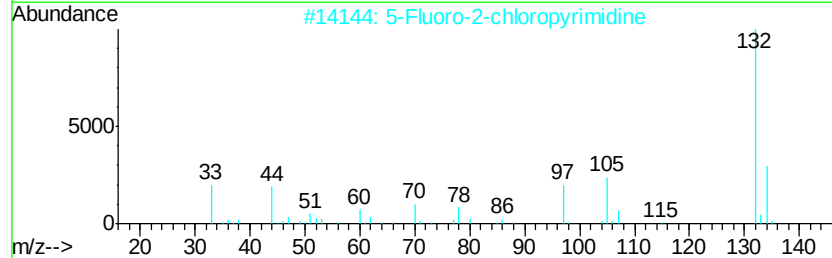
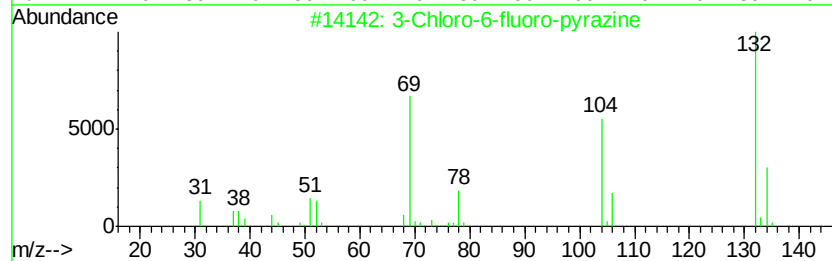
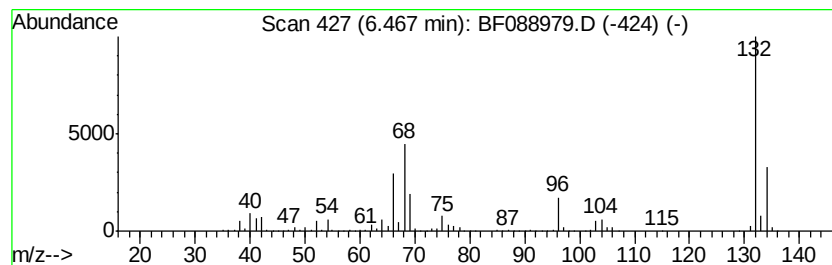
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	94.64 ng	1979700	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	(5-Methyl-2-pyridyl)acetonitrile			132	C8H8N2	1000241-93-9	10
4	Tranlylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
5	N-(-3,4-Methylenedioxyphenylisop...			267	C17H17NO2	1000378-96-6	10



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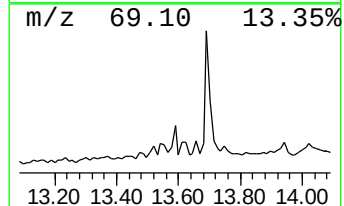
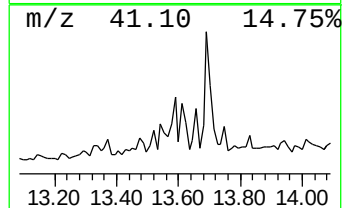
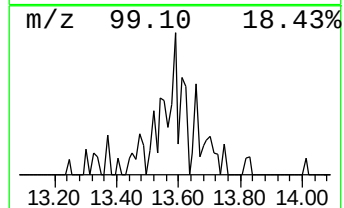
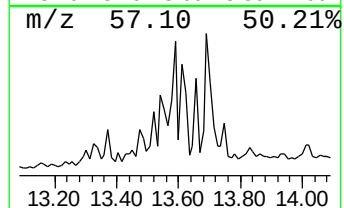
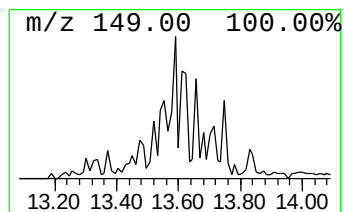
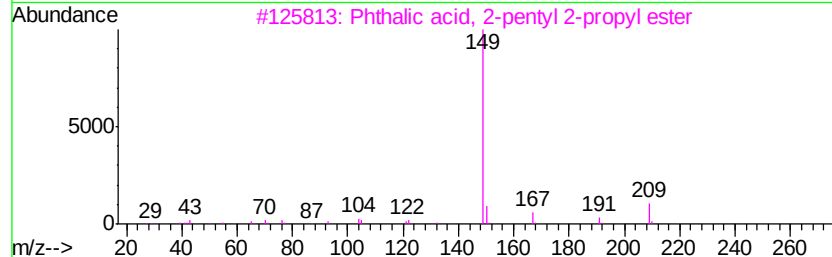
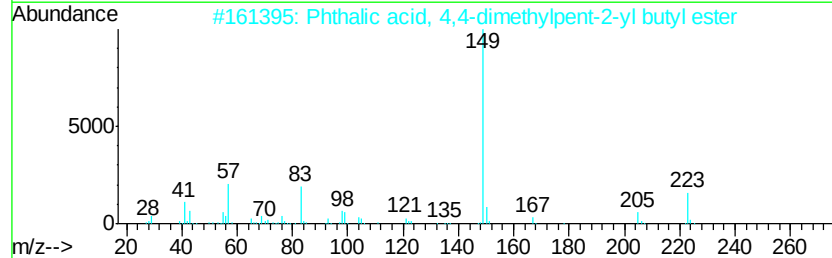
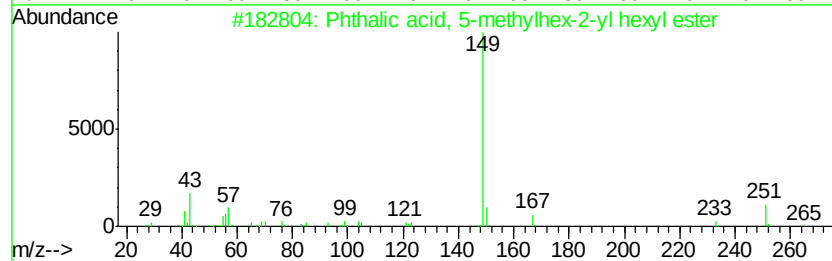
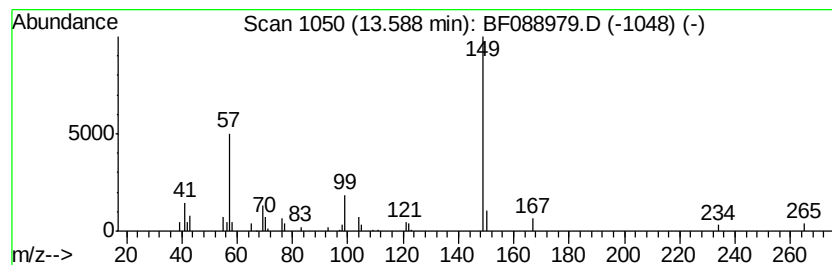
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Phthalic acid, 5-methylhex-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	2.25 ng	47011	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 5-methylhex-2-yl ...	348	C21H32O4	1000371-08-8	78
2		Phthalic acid, 4,4-dimethylpent-...	320	C19H28O4	1000371-14-1	78
3		Phthalic acid, 2-pentyl 2-propyl...	278	C16H22O4	1000315-56-2	72
4		Phthalic acid, isobutyl 4-methyl...	306	C18H26O4	1000356-87-2	64
5		Phthalic acid, ethyl tetradecyl ...	390	C24H38O4	1000309-00-5	64



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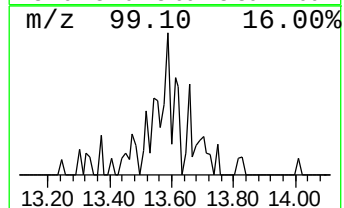
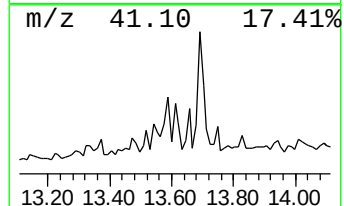
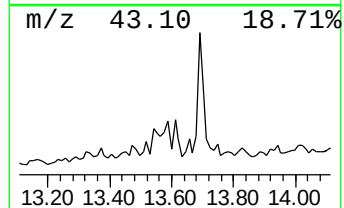
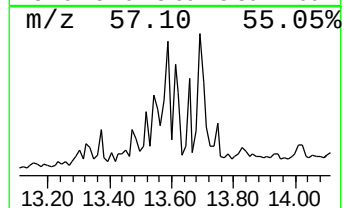
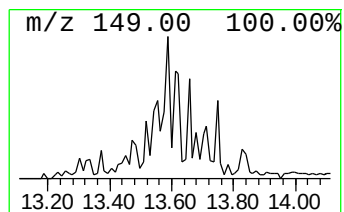
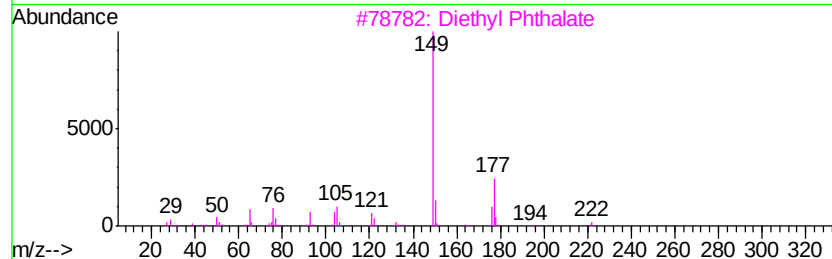
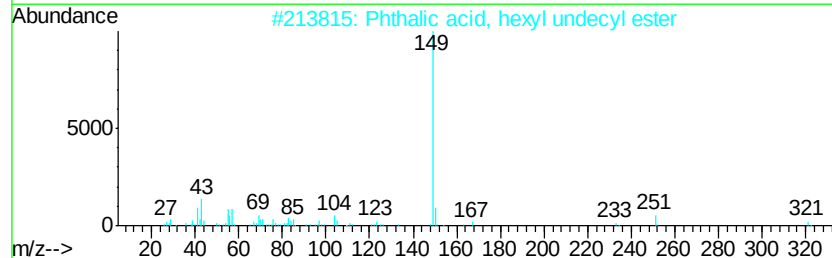
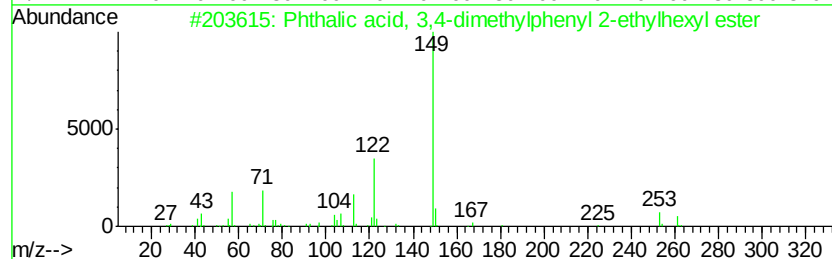
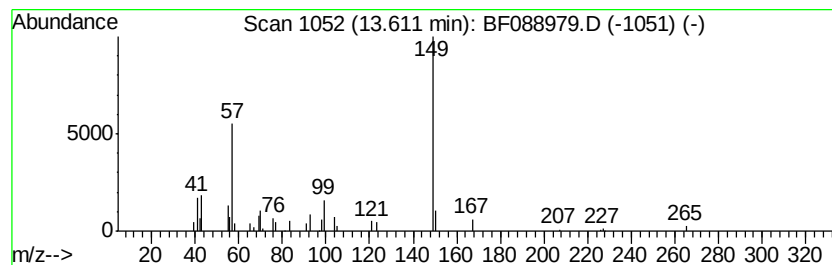
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Peak Number 8 Phthalic acid, 3,4-dimethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.05 ng	42823	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 3,4-dimethylphenyl...	382	C24H30O4	1000315-70-7	72
2		Phthalic acid, hexyl undecyl ester	404	C25H40O4	1000308-91-6	64
3		Diethyl Phthalate	222	C12H14O4	000084-66-2	64
4		Phthalic acid, 2-ethylhexyl pent...	348	C21H32O4	1000309-01-3	64
5		Phthalic acid, but-3-yn-2-yl 2-p...	288	C17H20O4	1000315-75-5	64



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Misc :
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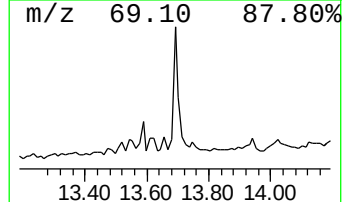
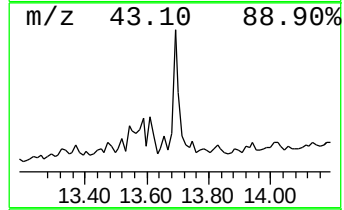
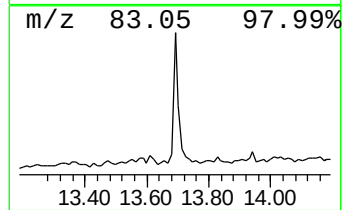
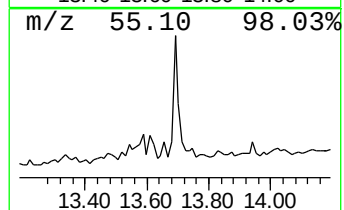
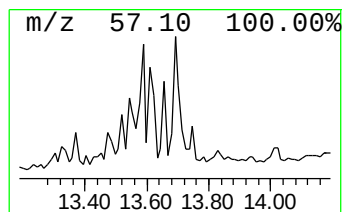
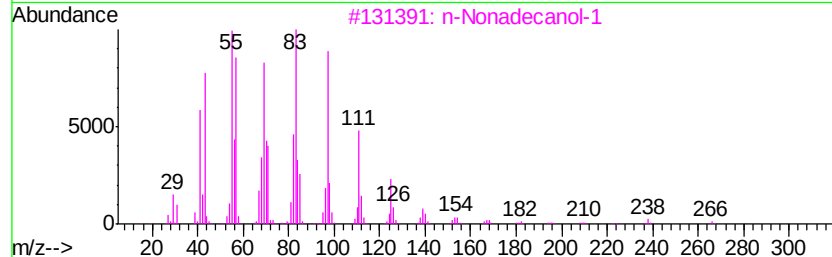
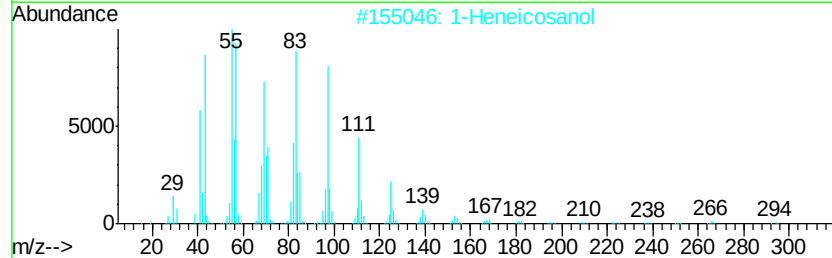
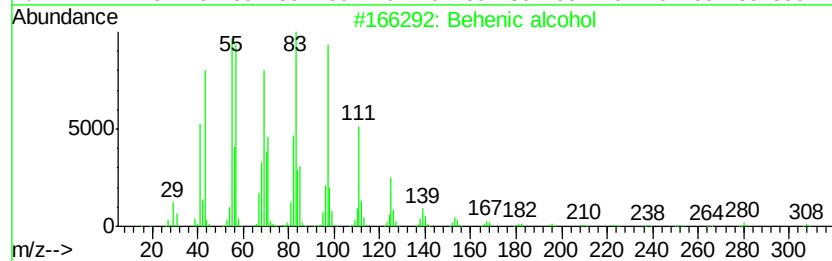
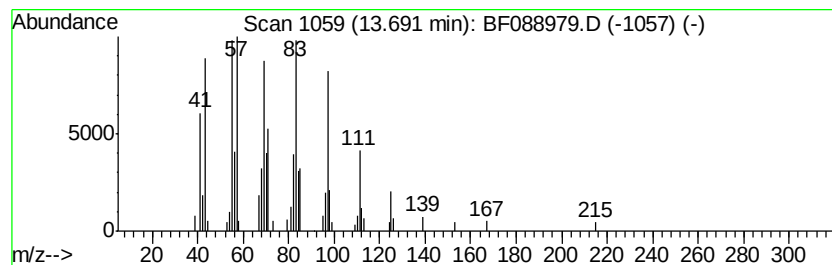
Instrument :
BNA_F
ClientSampleId :
P7-B7(0-8)C

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 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	5.04 ng	105423	Chrysene-d12	13.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 95
2		1-Heneicosanol	312 C21H44O	015594-90-8 95
3		n-Nonadecanol-1	284 C19H40O	001454-84-8 94
4		n-Tetracosanol-1	354 C24H50O	000506-51-4 94
5		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071316\
Data File : BF088979.D
Acq On : 14 Jul 2016 1:34
Operator : UM/SJ
Sample : H3946-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P7-B7(0-8)C

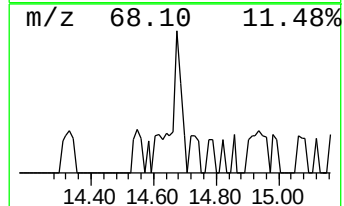
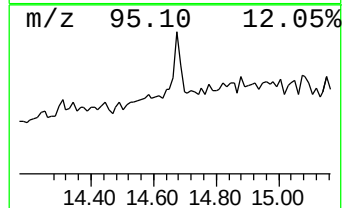
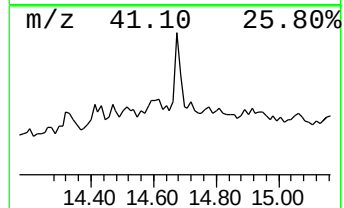
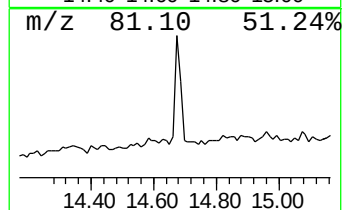
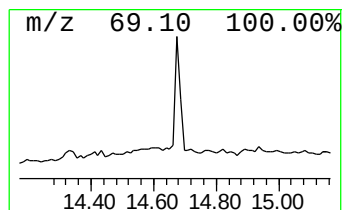
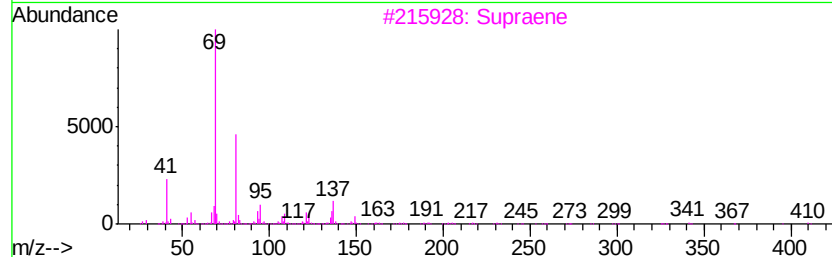
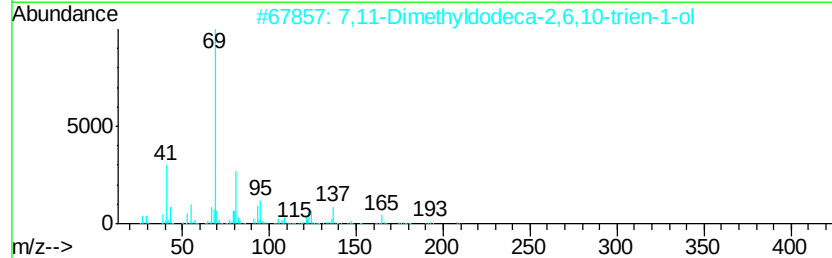
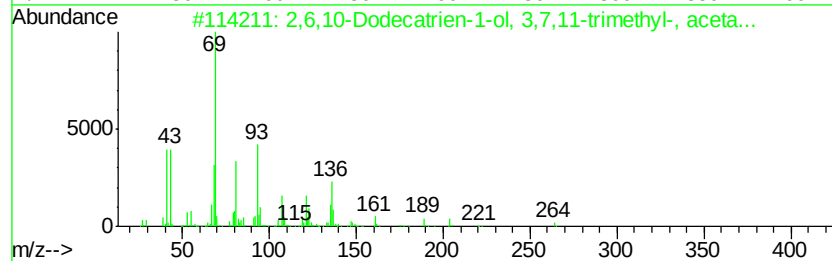
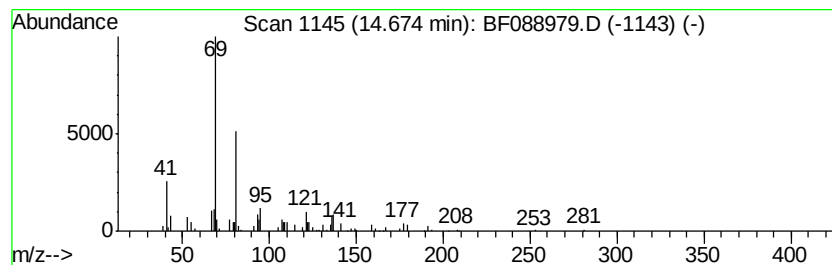
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.79 ng	42130	Perylene-d12	15.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64		
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64		
3	Supraene	410	C30H50	007683-64-9	64		
4	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	62		
5	Propanoic acid, 2,2-dimethyl-, [...]	306	C20H34O2	1000164-38-8	59		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088979.D
Acq On : 14 Jul 2016 1:34
Operator : UM/SJ
Sample : H3946-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P7-B7(0-8)C

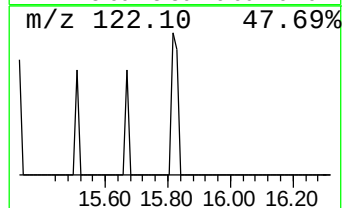
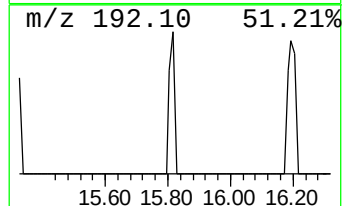
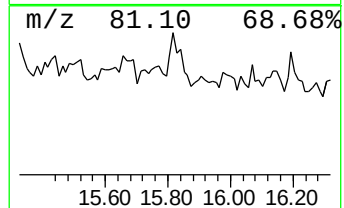
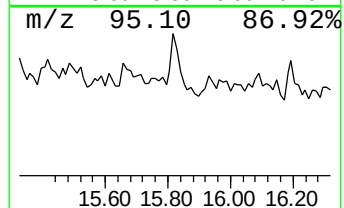
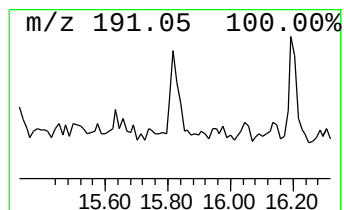
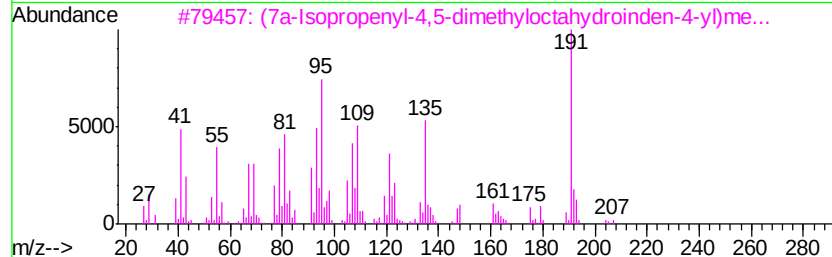
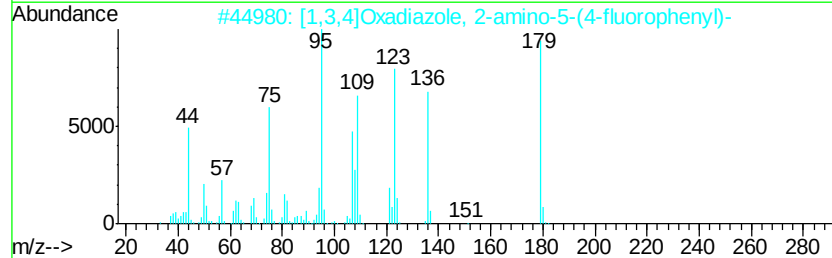
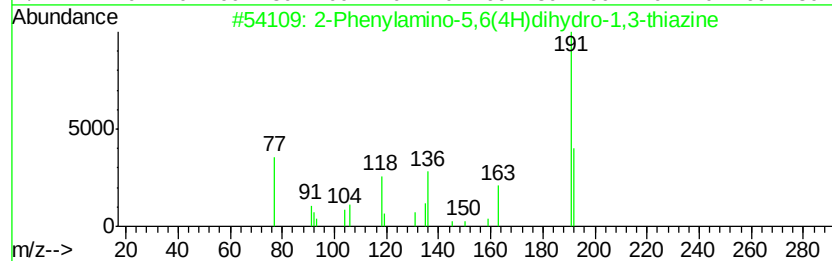
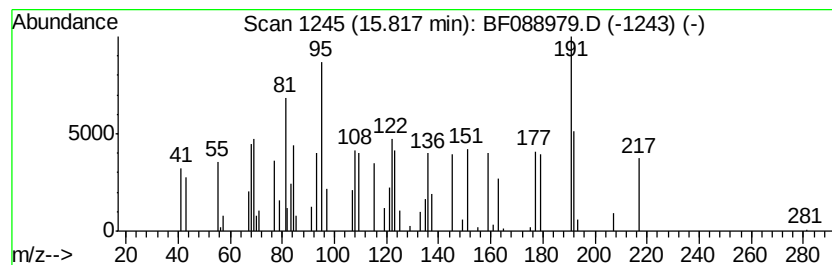
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.82 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	2.18 ng	32891	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	38
2		[1,3,4]Oxadiazole, 2-amino-5-(4-...	179	C8H6FN3O	1000316-48-2	18
3		(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	16
4		N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	14
5		Bicyclo[3.3.1]nonan-9-one, 1,2,4...	225	C12H19NO3	129967-65-3	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071316\
Data File : BF088979.D
Acq On : 14 Jul 2016 1:34
Operator : UM/SJ
Sample : H3946-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P7-B7(0-8)C

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...	1.91	12.6	ng	264474	1	6.70	418373	20.0
2-Pentanone, 4-hy...	4.86	21.0	ng	438424	1	6.70	418373	20.0
unknown6.47	6.47	94.6	ng	1979700	1	6.70	418373	20.0
Phthalic acid, 5-...	13.59	2.3	ng	47011	5	13.83	418043	20.0
Phthalic acid, 3,...	13.61	2.0	ng	42823	5	13.83	418043	20.0
Behenic alcohol	13.69	5.0	ng	105423	5	13.83	418043	20.0
2,6,10-Dodecatric...	14.67	2.8	ng	42130	6	15.20	302377	20.0
unknown15.82	15.82	2.2	ng	32891	6	15.20	302377	20.0