

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
 Data File : BF088581.D
 Acq On : 1 Jul 2016 18:16
 Operator : UM/SJ
 Sample : H3836-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C1.1-03

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	1.644	3	5	12	rVB	190013	291001	6.02%	0.937%
2	1.735	12	13	23	rVV	535784	835923	17.28%	2.693%
3	1.861	23	24	39	rVB	2097174	4836545	100.00%	15.581%
4	2.056	39	41	78	rVB	140271	736550	15.23%	2.373%
5	2.707	95	98	102	rVB	39304	63321	1.31%	0.204%
6	3.050	125	128	148	rVB	57978	161856	3.35%	0.521%
7	4.982	294	297	306	rVB	230282	313416	6.48%	1.010%
8	5.404	331	334	336	rBV	2450777	2419426	50.02%	7.794%
9	6.445	421	425	427	rBV	2472280	2937217	60.73%	9.462%
10	6.570	434	436	439	rBV	2101553	2605163	53.86%	8.393%
11	6.810	454	457	459	rBV	789032	711801	14.72%	2.293%
12	6.970	468	471	473	rVB	1640069	2135477	44.15%	6.879%
13	7.370	503	506	508	rBV	1693378	1624000	33.58%	5.232%
14	8.090	567	569	572	rBV	1060298	905155	18.71%	2.916%
15	9.176	661	664	666	rBV	2066541	2944506	60.88%	9.486%
16	9.565	696	698	700	rBV	174341	176115	3.64%	0.567%
17	9.839	720	722	725	rVB	933496	922536	19.07%	2.972%
18	10.628	788	791	793	rBV	1551015	1513635	31.30%	4.876%
19	11.199	839	841	843	rBV	69754	73349	1.52%	0.236%
20	11.314	849	851	854	rVB	632110	775176	16.03%	2.497%
21	11.851	896	898	901	rBV	40994	58198	1.20%	0.187%
22	12.902	987	990	993	rBV	2211280	2047172	42.33%	6.595%
23	13.805	1067	1069	1073	rBV	196718	227846	4.71%	0.734%
24	13.942	1079	1081	1084	rBV	753674	689455	14.26%	2.221%
25	14.445	1122	1125	1128	rBV	79309	118371	2.45%	0.381%
26	15.051	1175	1178	1182	rVB2	20695	50949	1.05%	0.164%
27	15.348	1201	1204	1206	rBV	438930	593484	12.27%	1.912%
28	15.805	1241	1244	1246	rBV	40923	58194	1.20%	0.187%
29	16.880	1335	1338	1343	rBV5	40411	82592	1.71%	0.266%
30	17.989	1433	1435	1445	rVB6	22334	67055	1.39%	0.216%
31	19.166	1534	1538	1544	rVB7	21191	66031	1.37%	0.213%

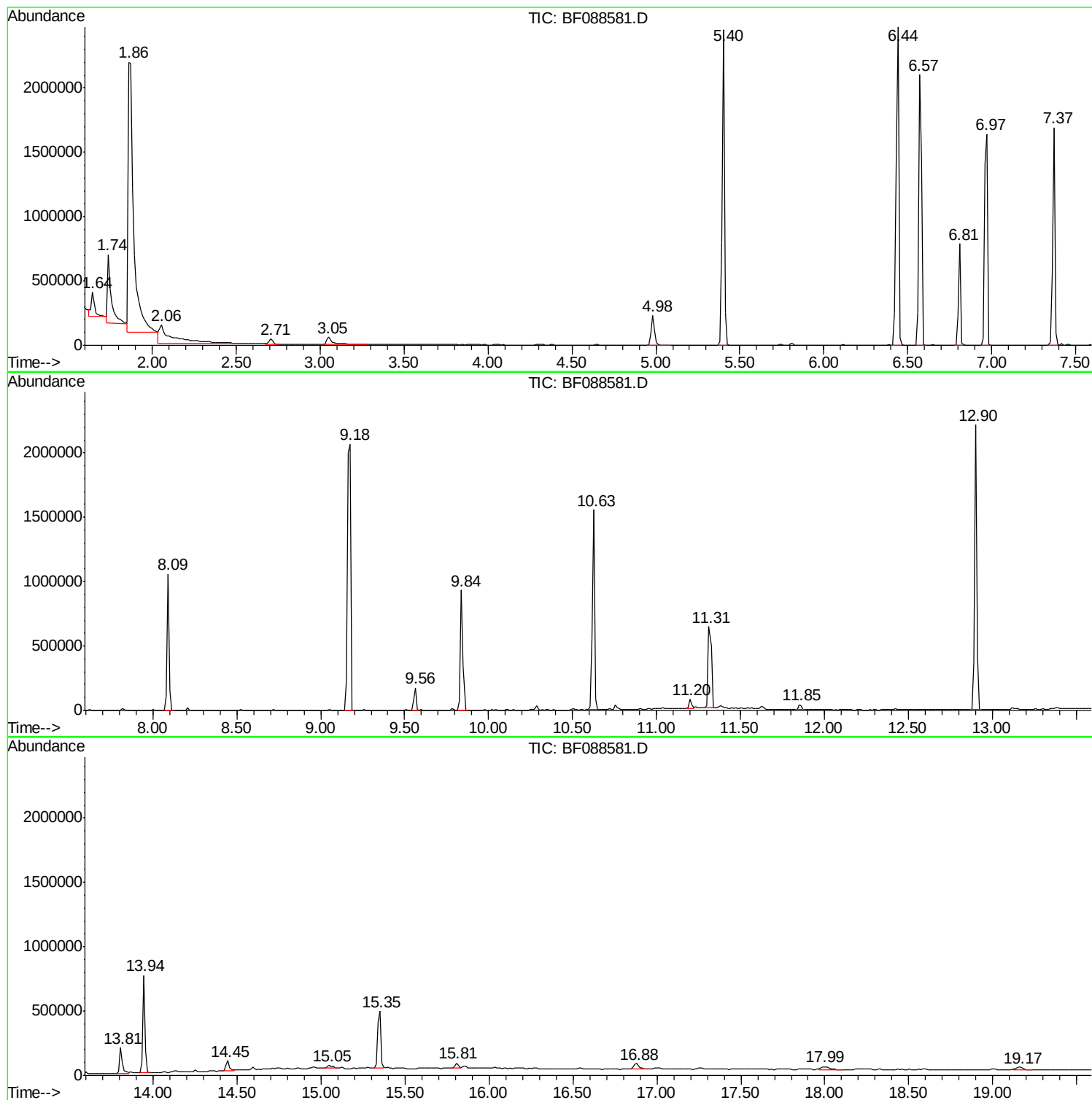
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Instrument :
BNA_F
ClientSampled :
C1.1-03

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



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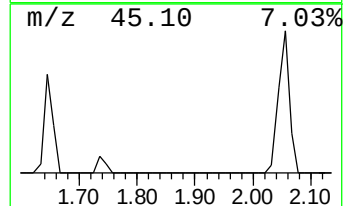
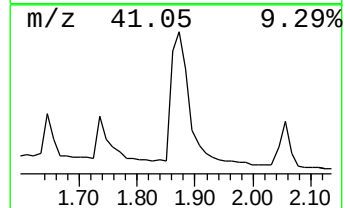
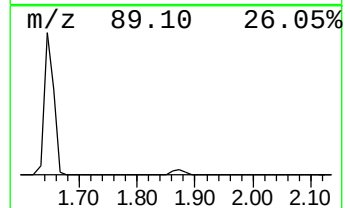
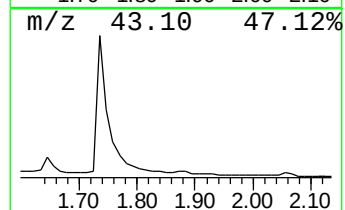
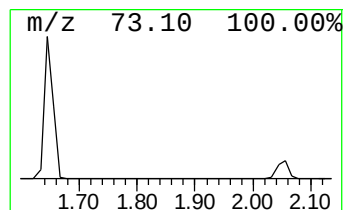
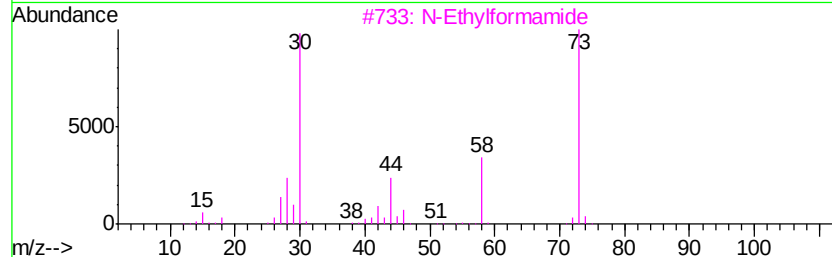
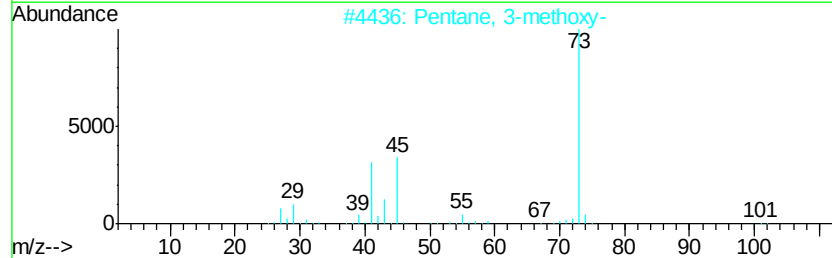
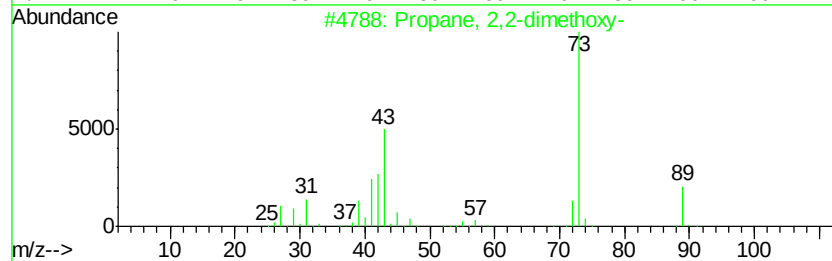
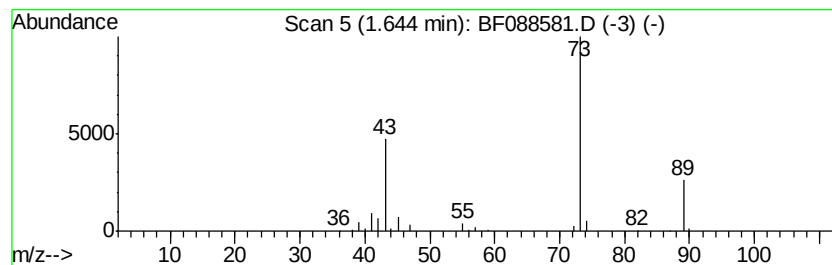
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	8.18 ng	291001	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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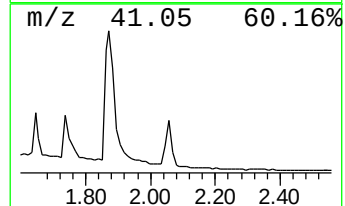
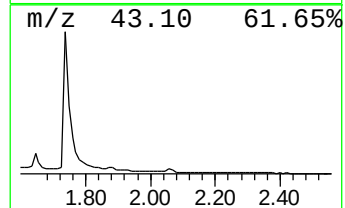
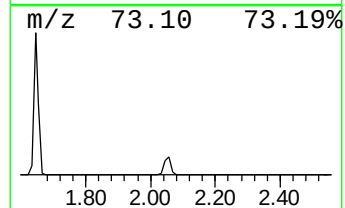
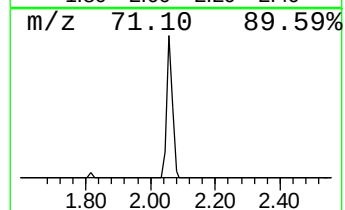
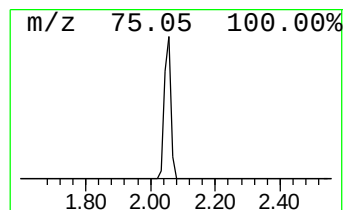
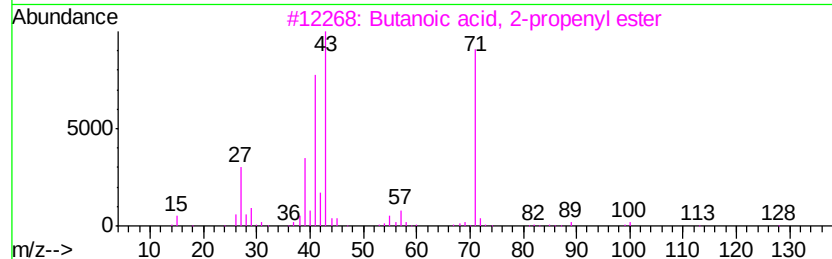
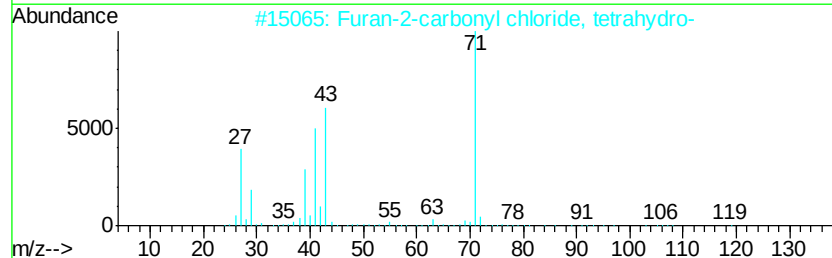
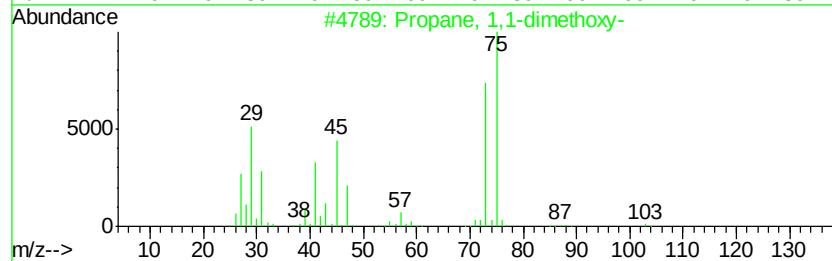
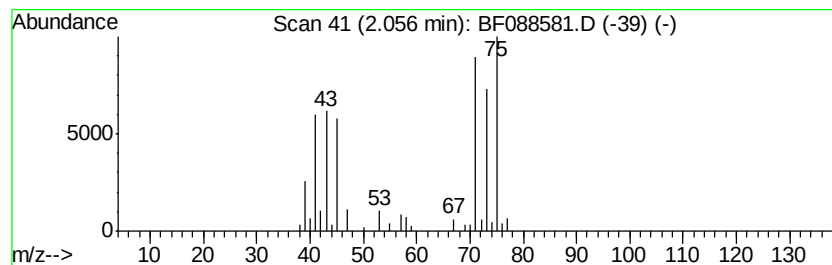
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Peak Number 4 unknown2.06 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	20.70 ng	736550	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	37
2		Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	22
3		Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	22
4		Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	17
5		Acrolein,dimethyl acetal	102	C5H10O2	006044-68-4	16



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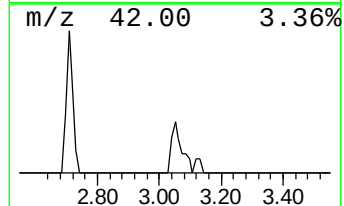
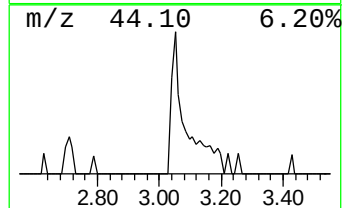
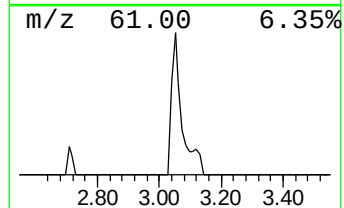
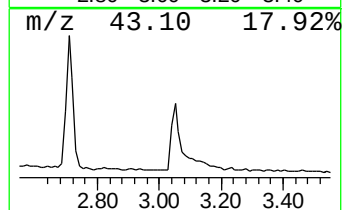
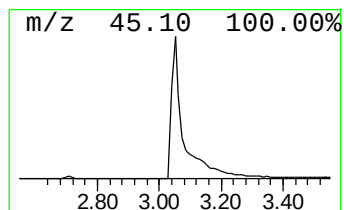
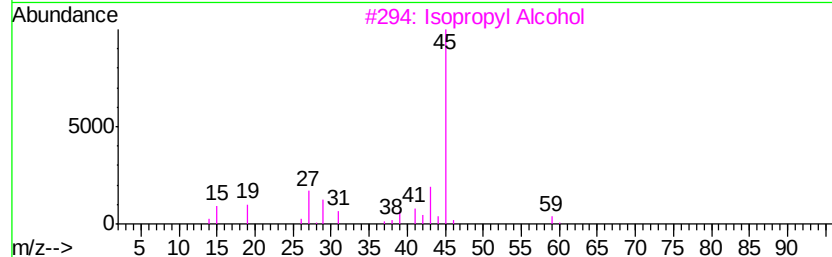
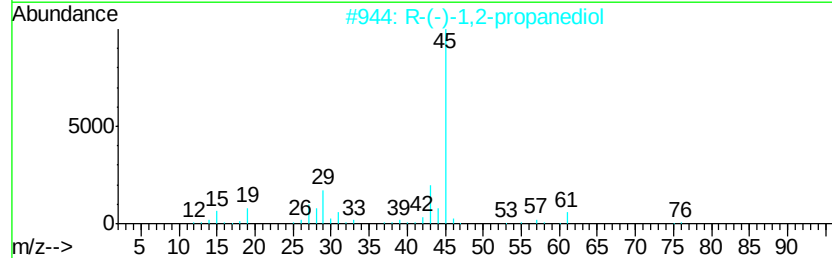
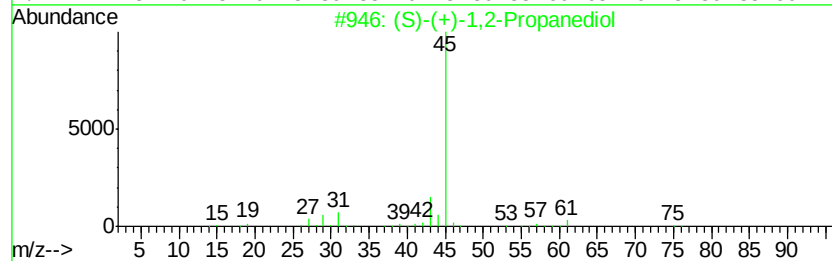
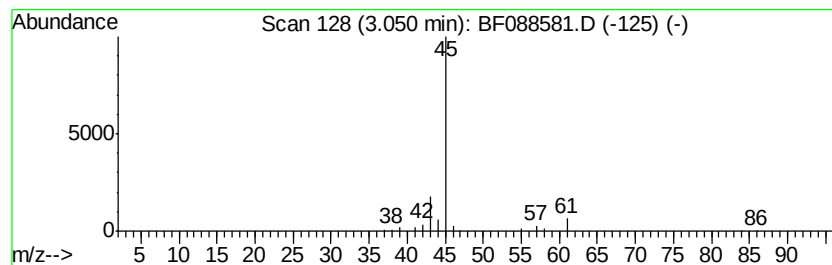
Instrument :
BNA_F
ClientSampleId :
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Peak Number 5 (S)-(+)-1,2-Propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.05	4.55 ng	161856	1,4-Dichlorobenzene-d4	6.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Formamide	45	CH3NO	000075-12-7	7



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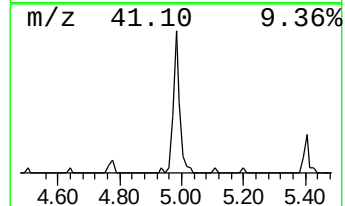
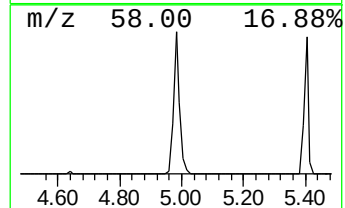
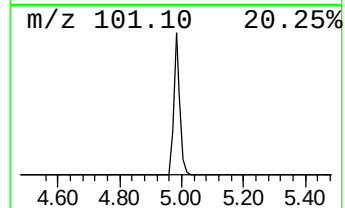
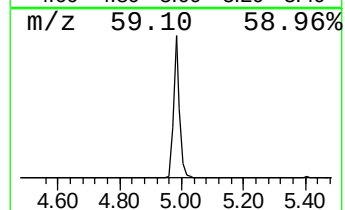
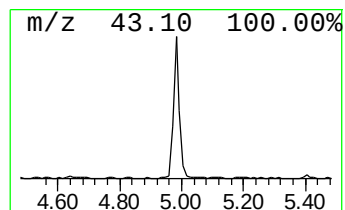
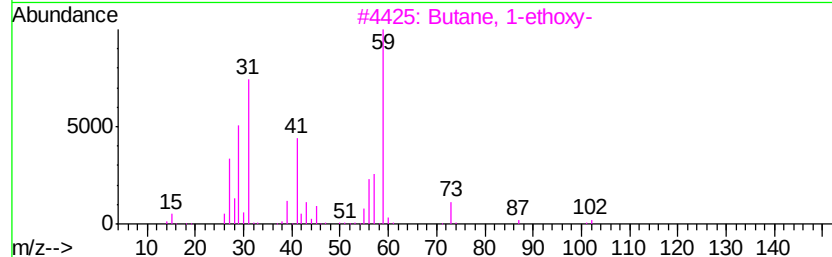
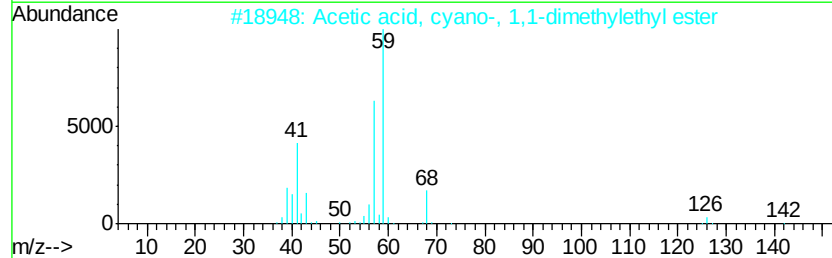
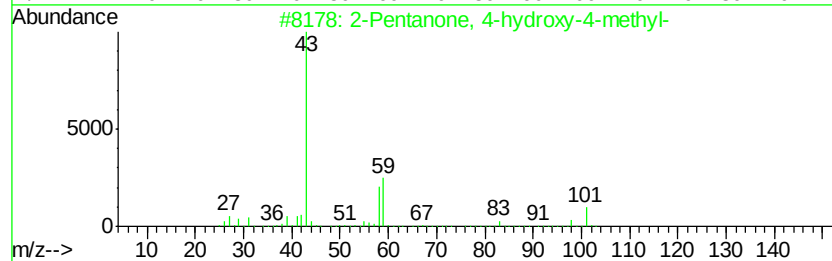
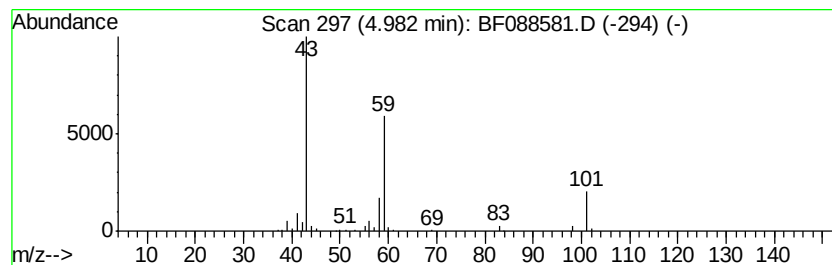
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	8.81 ng	313416	1,4-Dichlorobenzene-d4	6.81

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-dimethy...	141	C7H11NO2	001116-98-9	23
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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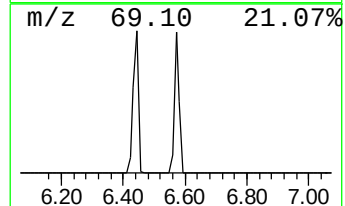
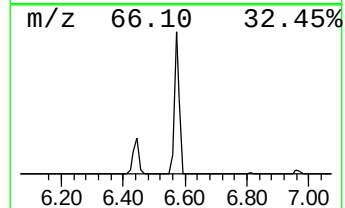
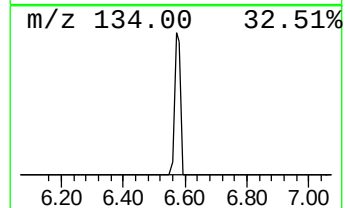
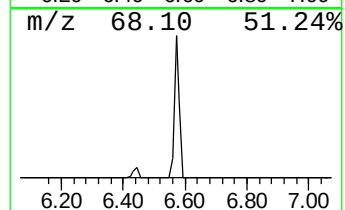
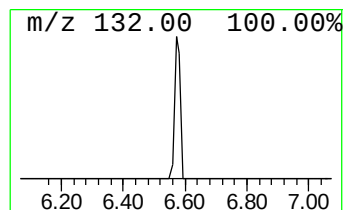
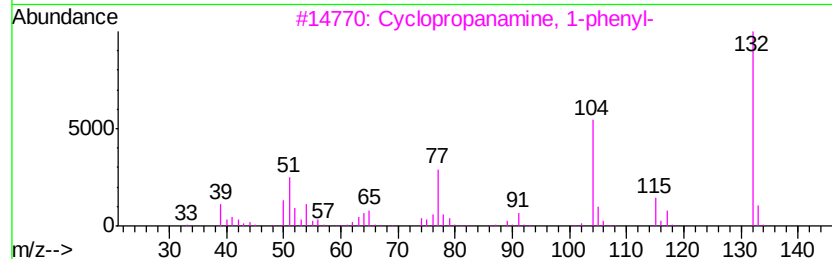
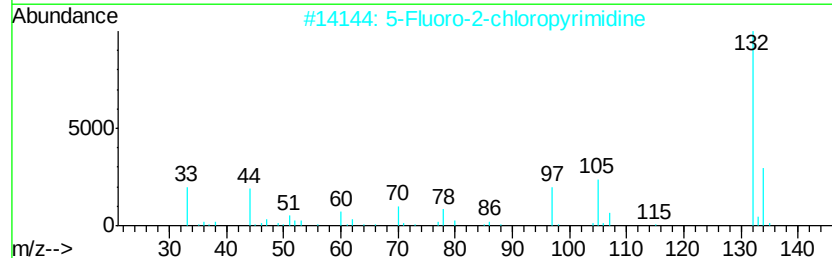
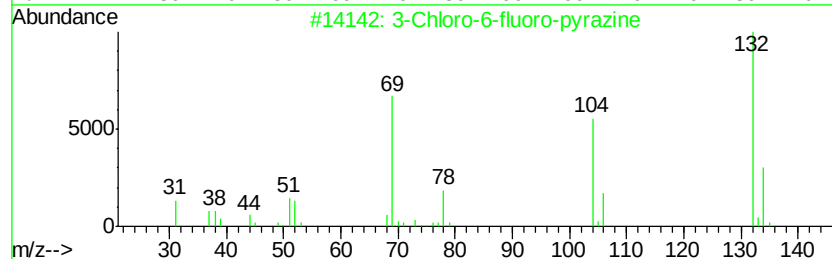
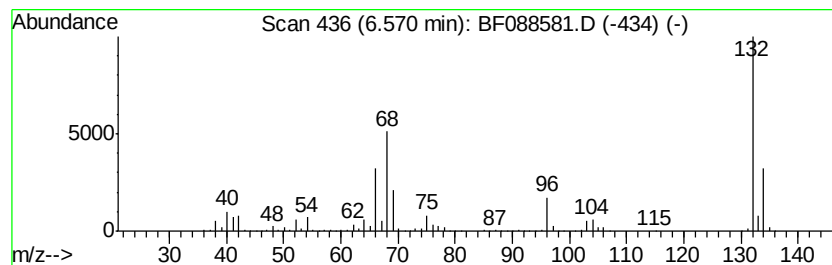
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	73.20 ng	2605160	1,4-Dichlorobenzene-d4	6.81

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		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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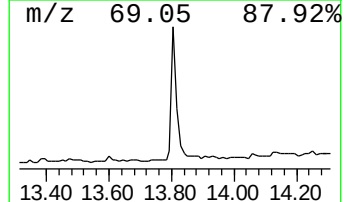
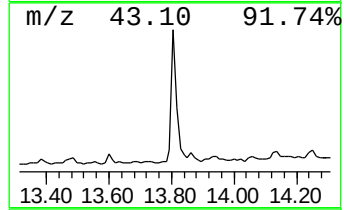
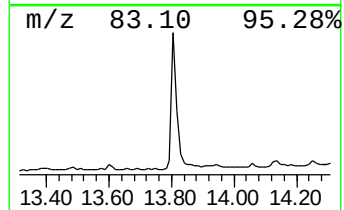
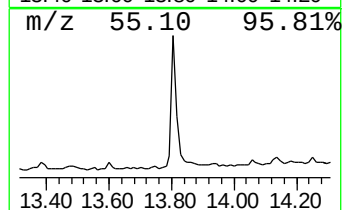
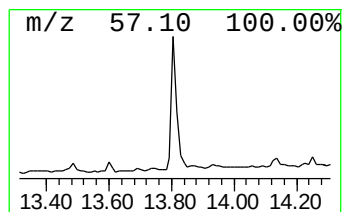
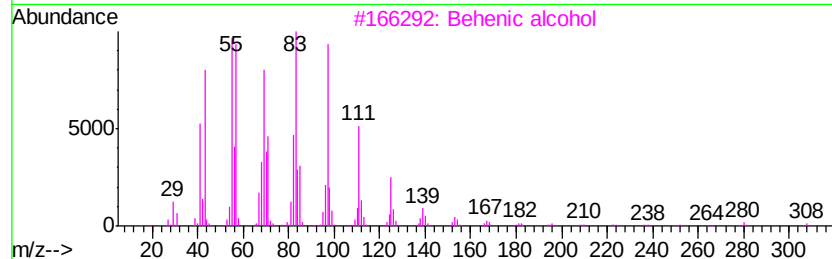
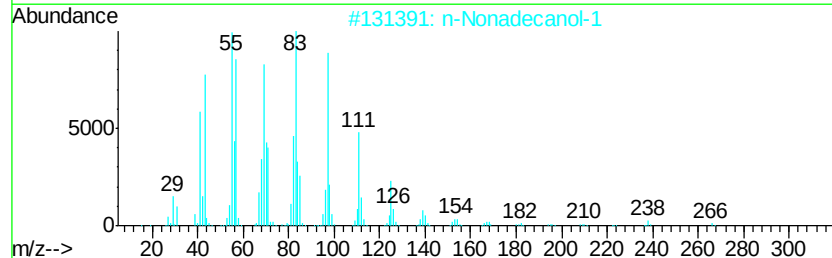
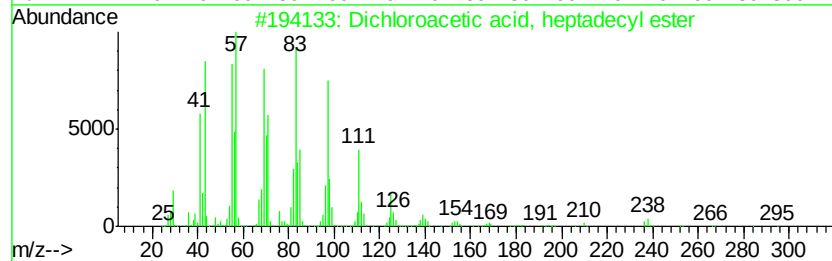
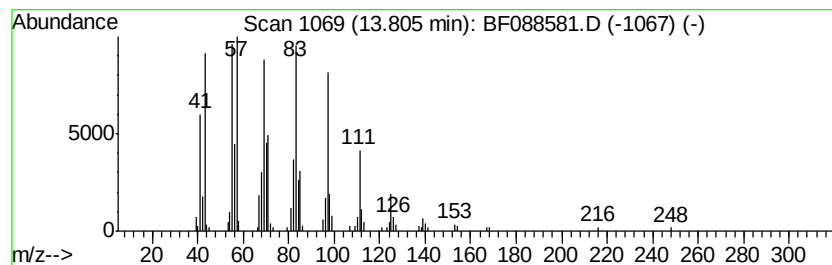
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	6.61 ng	227846	Chrysene-d12	13.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3			Behenic alcohol	326	C22H46O	000661-19-8	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\BF070116\
Data File : BF088581.D
Acq On : 1 Jul 2016 18:16
Operator : UM/SJ
Sample : H3836-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.1-03

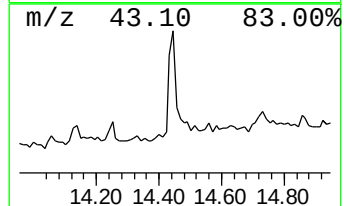
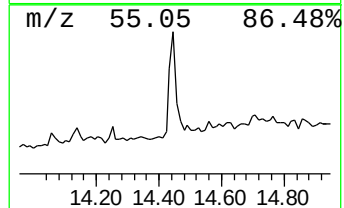
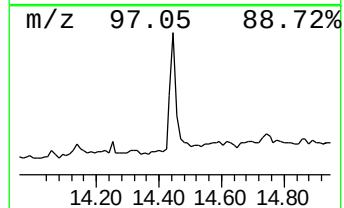
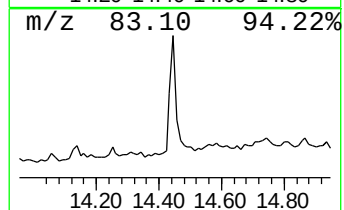
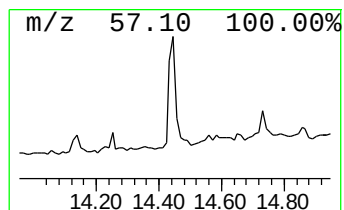
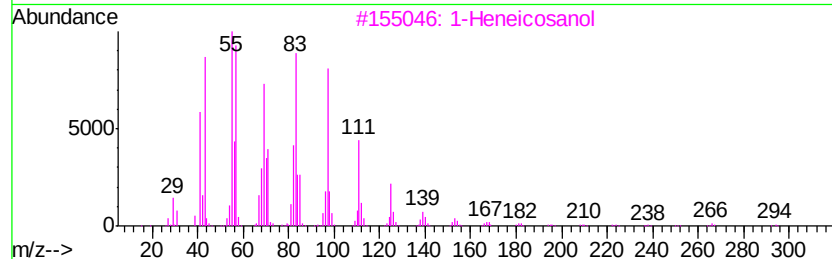
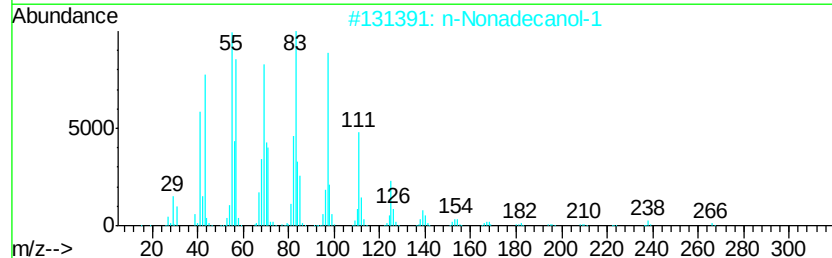
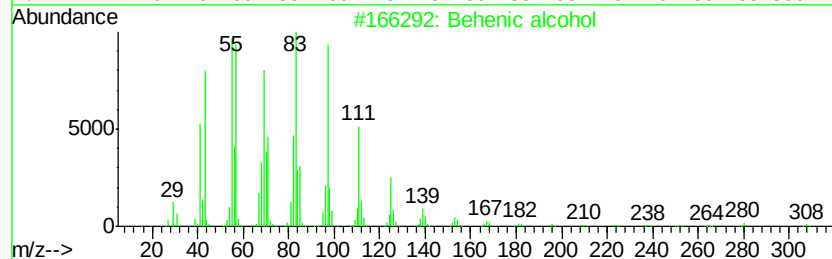
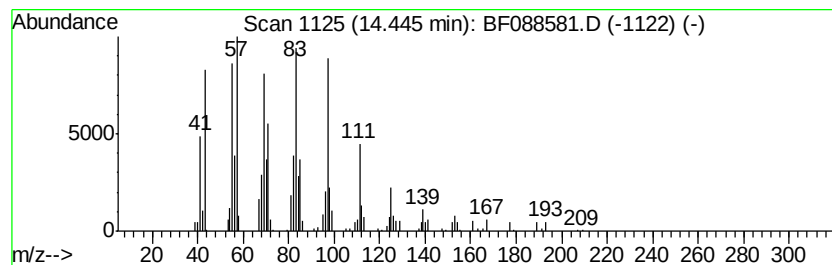
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Behenic alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.43 ng	118371	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		1-Heptacosanol	396	C27H56O	002004-39-9	94
5		Octacosanol	410	C28H58O	000557-61-9	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088581.D
Acq On : 1 Jul 2016 18:16
Operator : UM/SJ
Sample : H3836-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.1-03

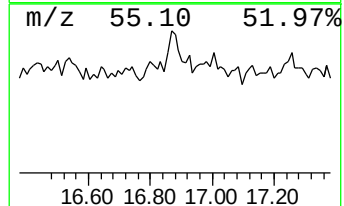
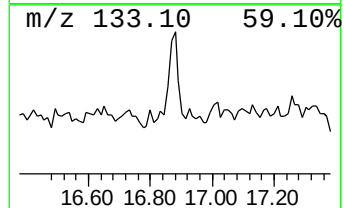
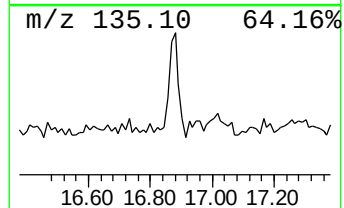
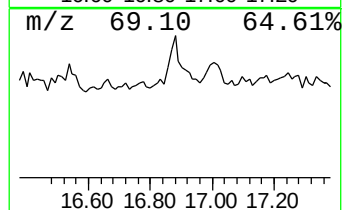
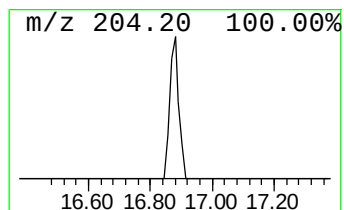
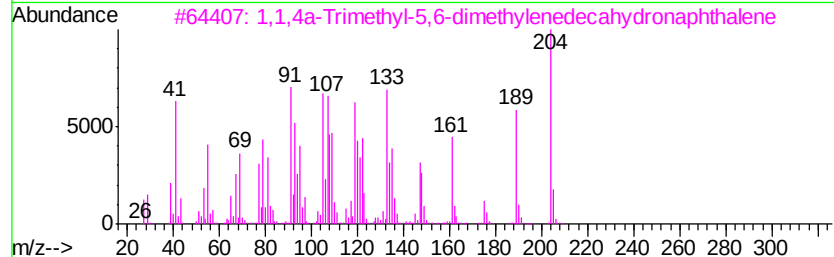
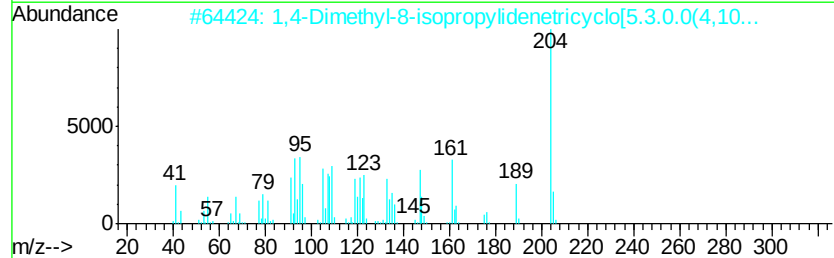
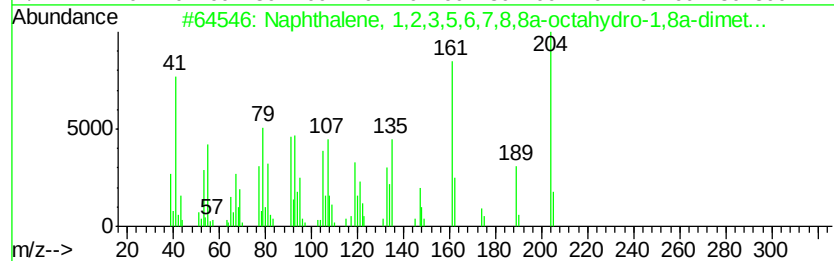
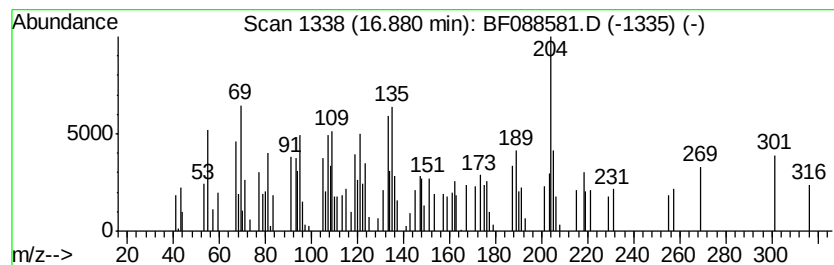
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	2.78 ng	82592	Perylene-d12	15.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	64
2			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	64
3			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	49
4			(-)-Tricyclo[6.2.1.0(4,11)]undec...	204	C15H24	1000154-06-7	47
5			1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088581.D
Acq On : 1 Jul 2016 18:16
Operator : UM/SJ
Sample : H3836-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

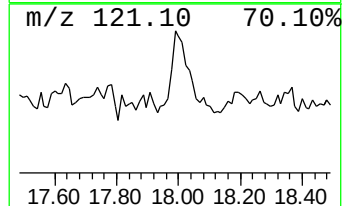
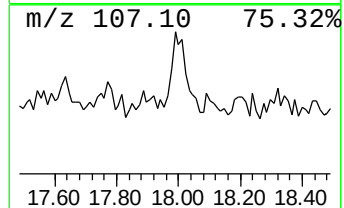
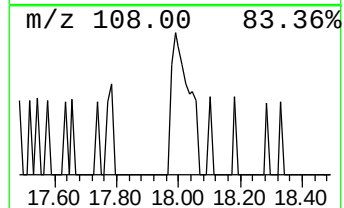
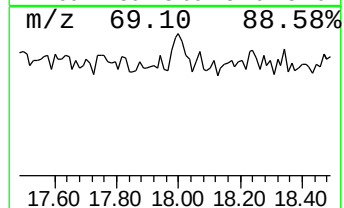
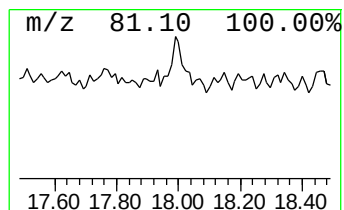
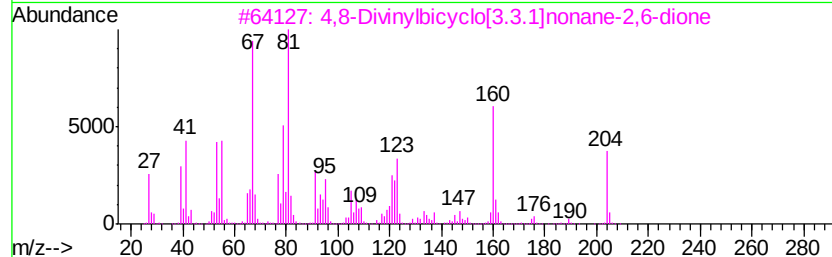
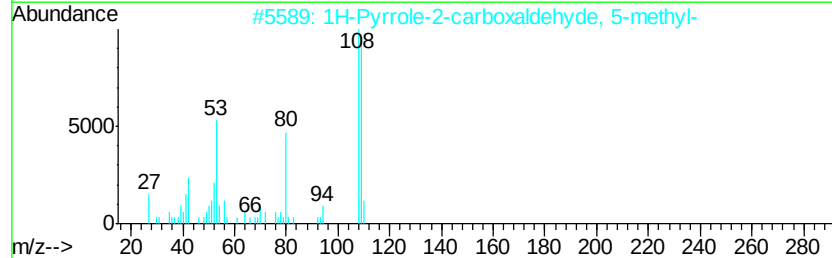
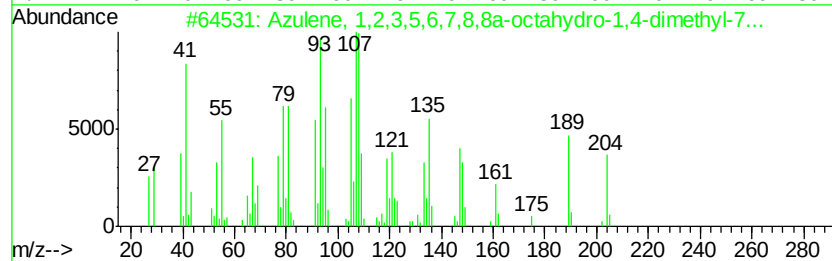
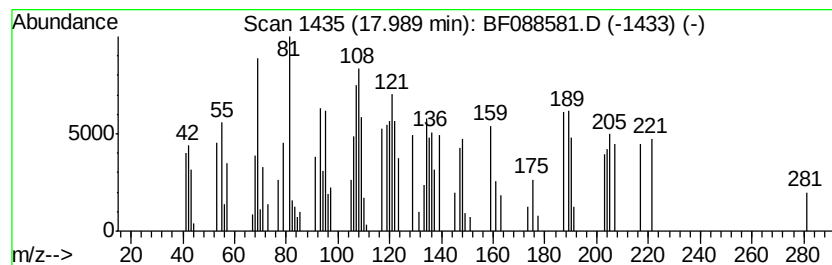
Instrument :
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ClientSampleId :
C1.1-03

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 12 unknown17.99 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.99	2.26 ng	67055	Perylene-d12	15.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	47
2	1H-Pyrrole-2-carboxaldehyde, 5-m...	109	C6H7NO	001192-79-6	27
3	4,8-Divinylbicyclo[3.3.1]nonane-...	204	C13H16O2	1000210-69-3	25
4	Cyclohexanecarboxamide, N-furfuryl-	207	C12H17NO2	006341-32-8	22
5	Isocaryophyllene	204	C15H24	1000140-07-2	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088581.D
Acq On : 1 Jul 2016 18:16
Operator : UM/SJ
Sample : H3836-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.1-03

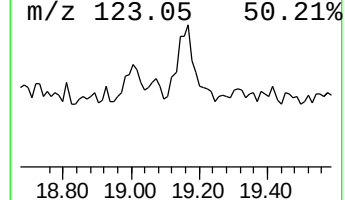
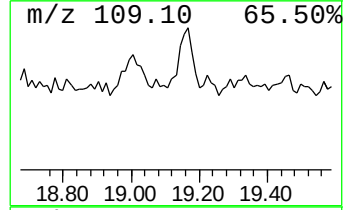
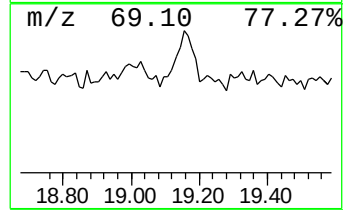
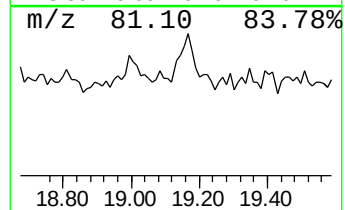
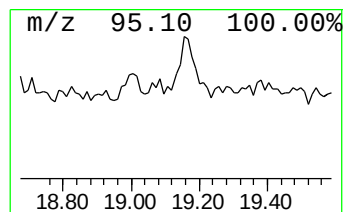
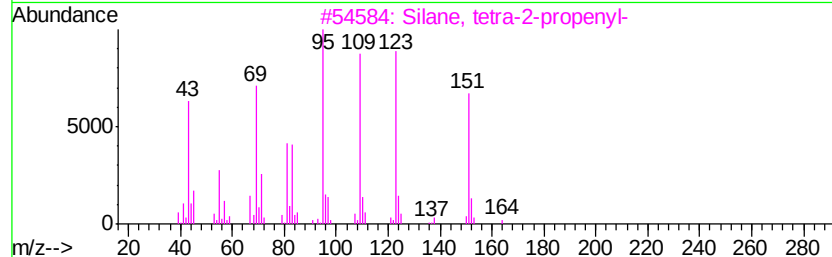
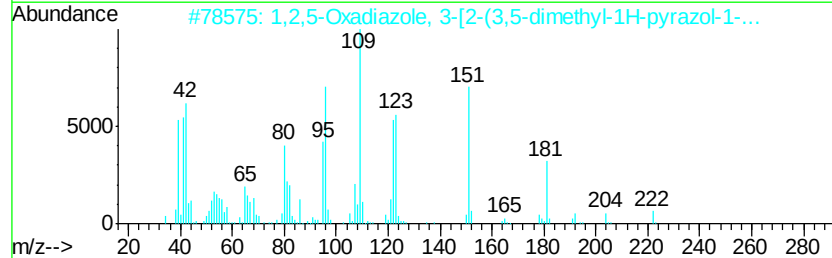
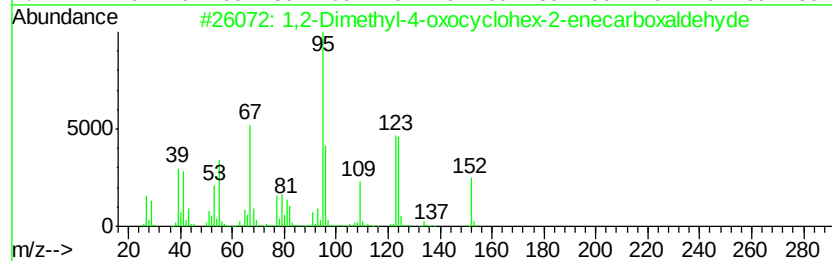
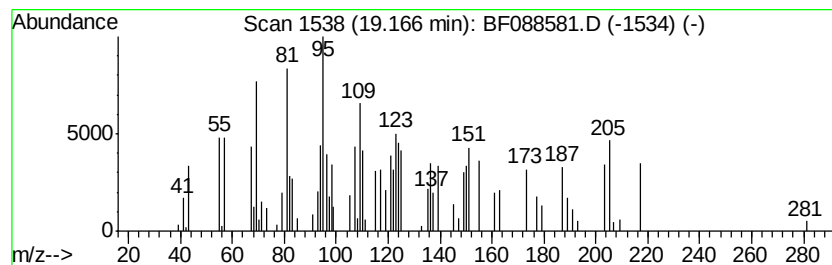
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown19.17 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.17	2.23 ng	66031	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Dimethyl-4-oxocyclohex-2-ene...	152	C9H12O2	1000187-01-2	38
2		1,2,5-Oxadiazole, 3-[2-(3,5-dime...	222	C10H14N4O2	324021-80-9	27
3		Silane, tetra-2-propenyl-	192	C12H20Si	001112-66-9	27
4		7,9-Dimethyl-8-nitrobicyclo[4.3....	225	C12H19NO3	129967-66-4	27
5		1H-Pyrazole, 1-methyl-4-methylam...	125	C6H11N3	1000294-10-8	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088581.D
Acq On : 1 Jul 2016 18:16
Operator : UM/SJ
Sample : H3836-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.1-03

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
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unknown2.06	2.06	20.7	ng	736550	1	6.81	711801	20.0
(S)-(+)-1,2-Propa...	3.05	4.5	ng	161856	1	6.81	711801	20.0
2-Pentanone, 4-hy...	4.98	8.8	ng	313416	1	6.81	711801	20.0
unknown6.57	6.57	73.2	ng	2605160	1	6.81	711801	20.0
Dichloroacetic ac...	13.81	6.6	ng	227846	5	13.94	689455	20.0
Behenic alcohol	14.45	3.4	ng	118371	5	13.94	689455	20.0
Naphthalene, 1,2,...	16.88	2.8	ng	82592	6	15.35	593484	20.0
unknown17.99	17.99	2.3	ng	67055	6	15.35	593484	20.0
unknown19.17	19.17	2.2	ng	66031	6	15.35	593484	20.0