

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
 Data File : BF094736.D
 Acq On : 1 May 2017 2:25
 Operator : SJ/MA
 Sample : I2902-01
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1B

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-BF041717.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	1.990	6	9	14	rVB4	23748	37655	1.10%	0.152%
2	3.413	244	251	260	rBV	208369	240621	7.01%	0.974%
3	3.913	333	336	342	rBV	100677	102593	2.99%	0.415%
4	4.266	392	396	402	rBV	31547	41748	1.22%	0.169%
5	4.325	402	406	419	rVV	1127379	1218543	35.50%	4.934%
6	4.637	457	459	467	rVB	129551	120911	3.52%	0.490%
7	5.395	584	588	593	rBV	702747	810862	23.63%	3.283%
8	5.519	605	609	616	rBV	2427745	2285071	66.58%	9.252%
9	5.760	647	650	654	rVB	676271	611035	17.80%	2.474%
10	5.942	676	681	684	rBV	2388966	2171152	63.26%	8.791%
11	6.413	757	761	764	rBV	1595726	1734739	50.55%	7.024%
12	6.437	764	765	777	rVB2	40082	54305	1.58%	0.220%
13	7.148	883	886	895	rBV3	27585	46255	1.35%	0.187%
14	7.254	900	904	913	rVB	926872	858438	25.01%	3.476%
15	7.448	933	937	943	rBV3	30204	51265	1.49%	0.208%
16	7.636	966	969	976	rBV	82275	81950	2.39%	0.332%
17	7.813	987	999	1002	rBV	681960	1770004	51.57%	7.167%
18	8.013	1029	1033	1038	rBV	91416	92845	2.71%	0.376%
19	8.189	1060	1063	1073	rBV2	251845	283964	8.27%	1.150%
20	8.354	1088	1091	1094	rBV	42913	42024	1.22%	0.170%
21	8.413	1098	1101	1112	rVB	66687	92128	2.68%	0.373%
22	8.501	1112	1116	1118	rBV	41372	40037	1.17%	0.162%
23	8.578	1124	1129	1133	rBV	3207593	3432059	100.00%	13.897%
24	8.607	1133	1134	1141	rVB	69336	61702	1.80%	0.250%
25	8.866	1175	1178	1190	rBV3	34733	55890	1.63%	0.226%
26	9.083	1212	1215	1222	rVB	87027	88151	2.57%	0.357%
27	9.389	1263	1267	1277	rVB2	982273	948973	27.65%	3.842%
28	9.730	1321	1325	1332	rBV3	27160	35452	1.03%	0.144%
29	10.372	1429	1434	1446	rBV	1626049	1679445	48.93%	6.800%
30	10.566	1464	1467	1473	rBV	28853	39074	1.14%	0.158%
31	11.213	1573	1577	1581	rBV	905395	882149	25.70%	3.572%
32	11.948	1698	1702	1712	rBV3	105457	139774	4.07%	0.566%
33	12.583	1806	1810	1816	rVB5	25471	42028	1.22%	0.170%
34	12.818	1847	1850	1861	rVB	92089	128568	3.75%	0.521%

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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

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35	12.918	1863	1867	1873	rBV2	51188	62135	1.81%	0.252%
36	13.189	1908	1913	1917	rBV	2153127	2498128	72.79%	10.115%
37	13.530	1967	1971	1975	rVB3	29047	39248	1.14%	0.159%
38	14.283	2092	2099	2103	rBV6	27575	52127	1.52%	0.211%
39	14.360	2107	2112	2118	rVV3	47746	82884	2.41%	0.336%
40	14.465	2126	2130	2135	rBV	580989	626912	18.27%	2.538%
41	14.512	2135	2138	2141	rVB2	36103	35391	1.03%	0.143%
42	14.842	2192	2194	2206	rVB6	34966	77599	2.26%	0.314%
43	15.571	2314	2318	2322	rBV2	26717	35234	1.03%	0.143%
44	16.095	2402	2407	2421	rVB	485981	622994	18.15%	2.523%
45	17.012	2560	2563	2568	rVB7	21956	35305	1.03%	0.143%
46	18.083	2739	2745	2755	rBV5	68295	207876	6.06%	0.842%

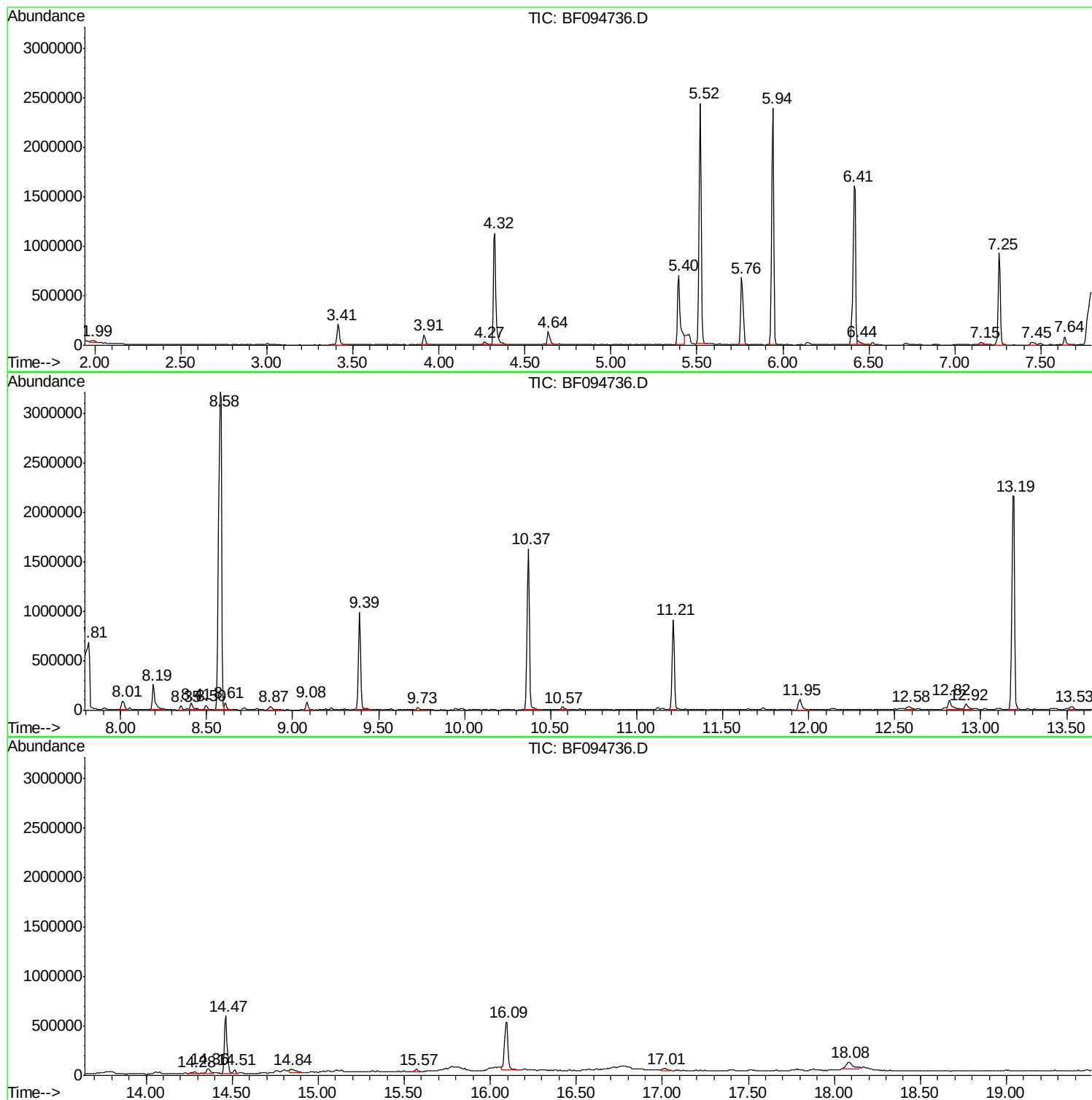
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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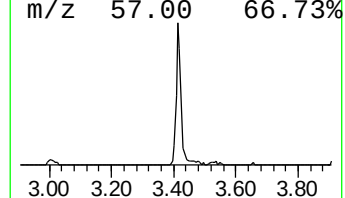
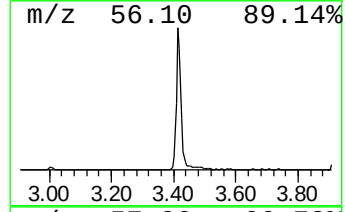
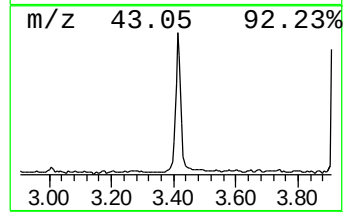
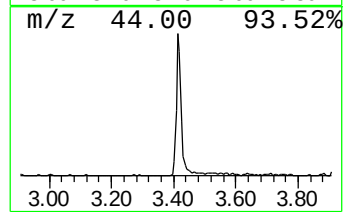
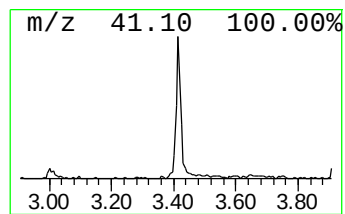
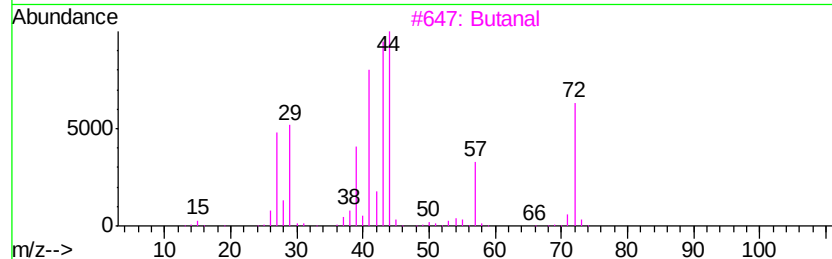
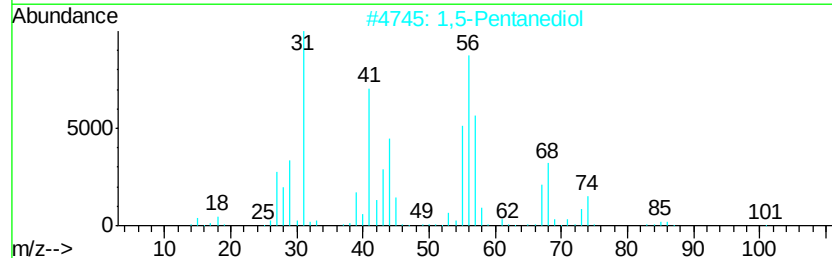
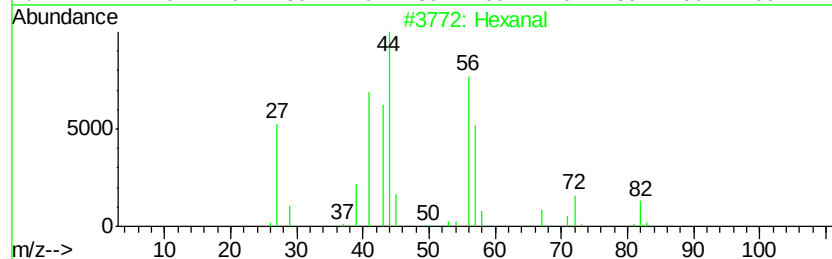
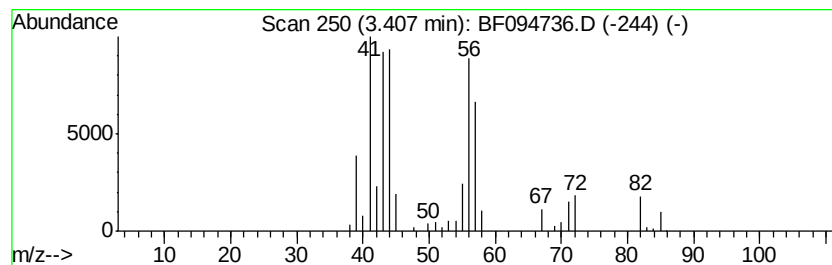
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.41	7.88 ng	240621	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	1,5-Pentanediol	104	C5H12O2	000111-29-5	33
3	Butanal	72	C4H8O	000123-72-8	27
4	Glutaraldehyde	100	C5H8O2	000111-30-8	25
5	O-Methylisourea	74	C2H6N2O	002440-60-0	12



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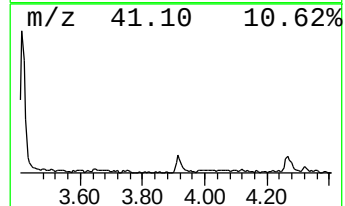
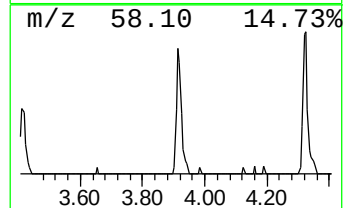
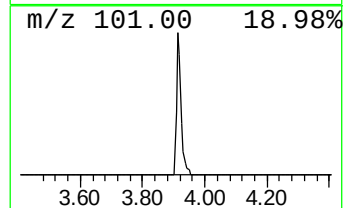
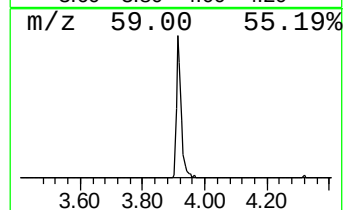
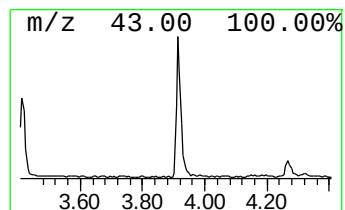
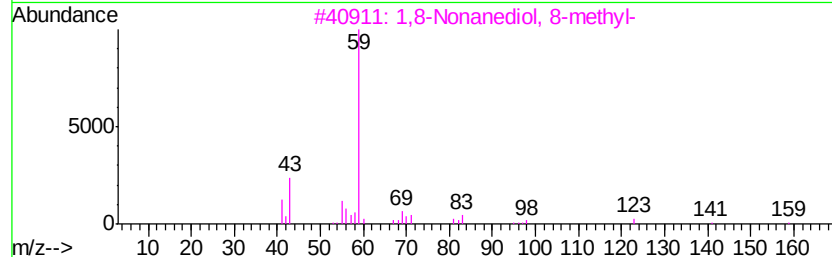
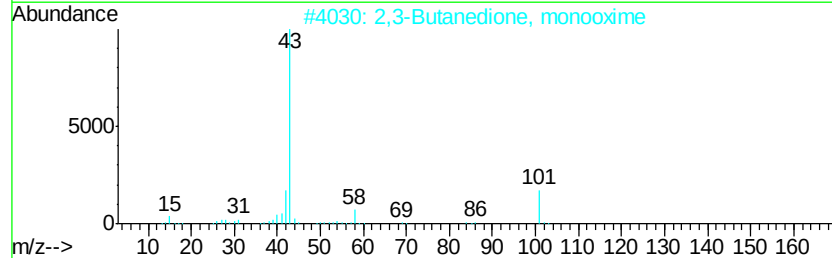
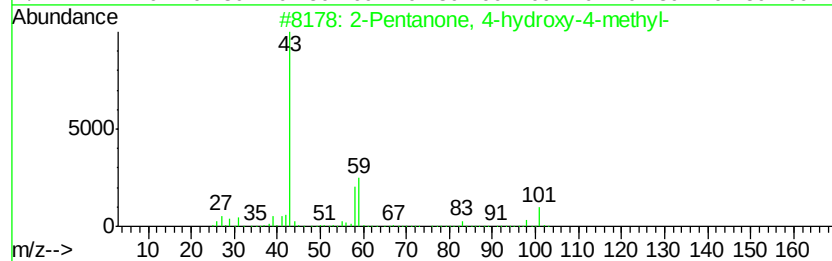
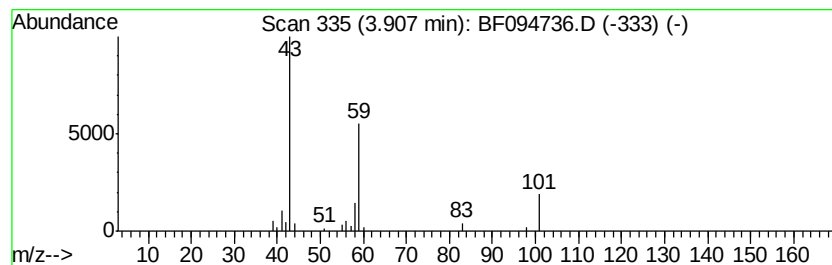
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.91	3.36 ng	102593	1,4-Dichlorobenzene-d4	5.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5			Butane	58	C4H10	000106-97-8	9



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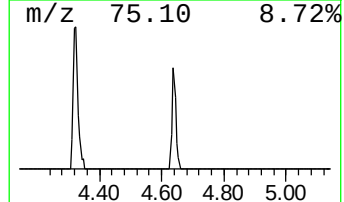
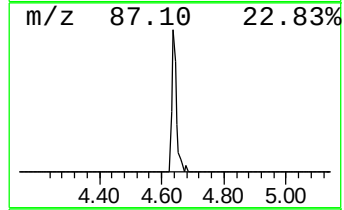
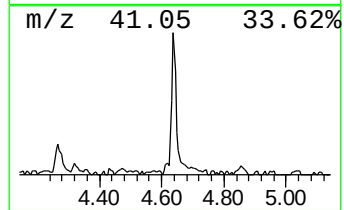
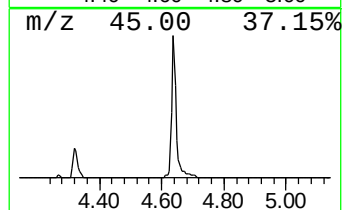
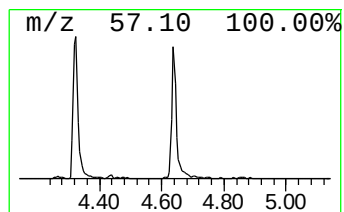
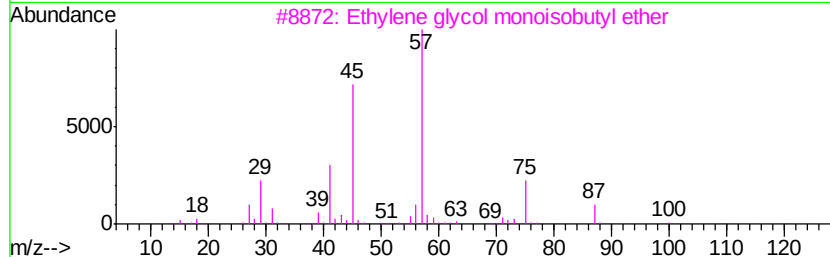
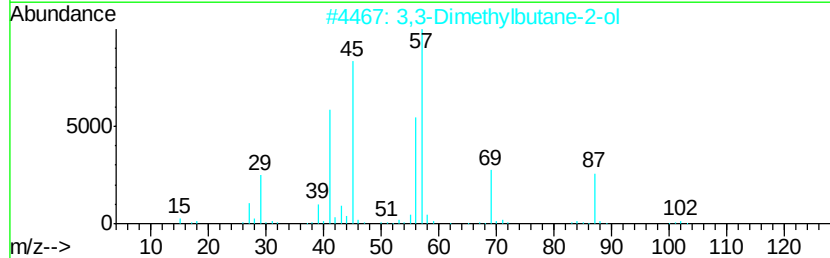
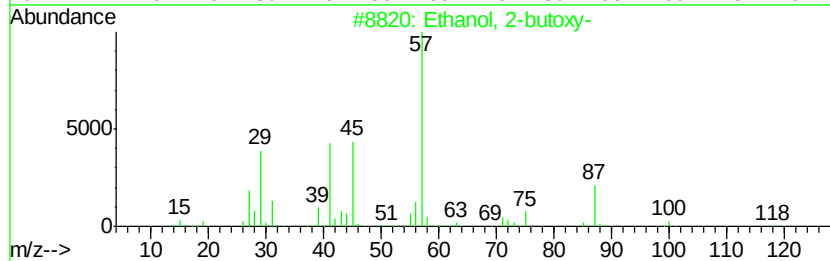
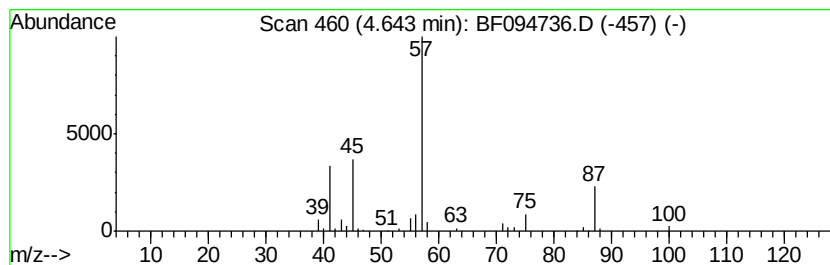
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	3.96 ng	120911	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
3		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
4		Propane, 1-(chloromethoxy)-2-met...	122	C5H11ClO	034180-11-5	27
5		n-Butyl ether	130	C8H18O	000142-96-1	25



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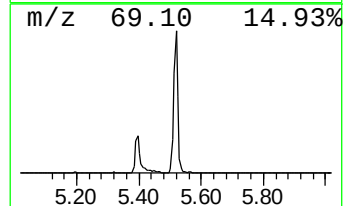
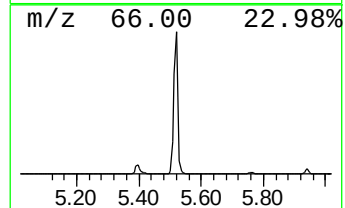
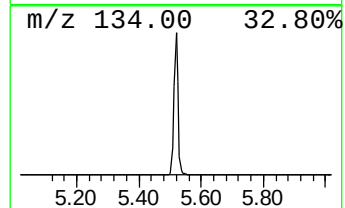
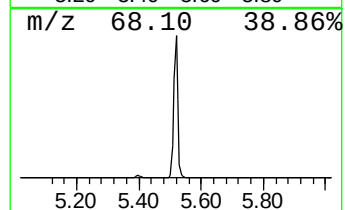
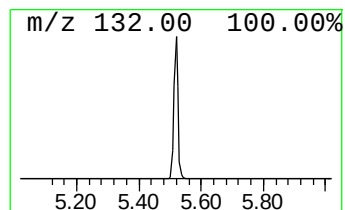
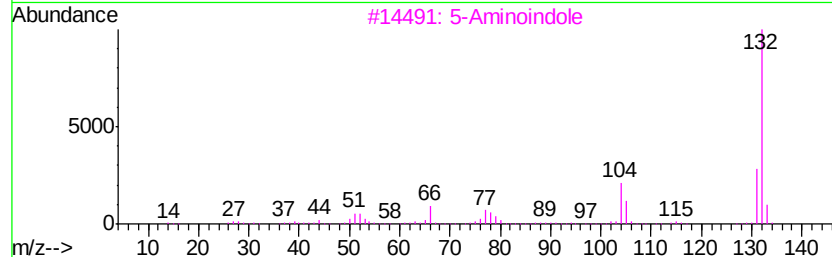
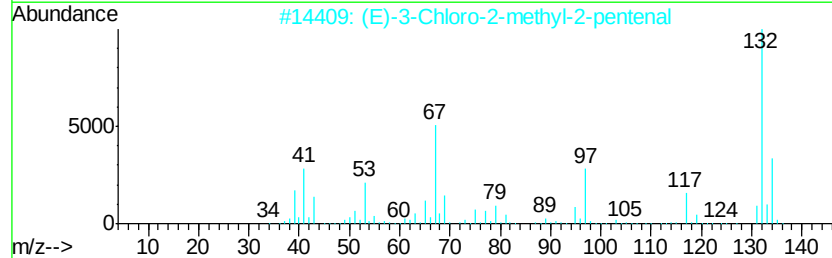
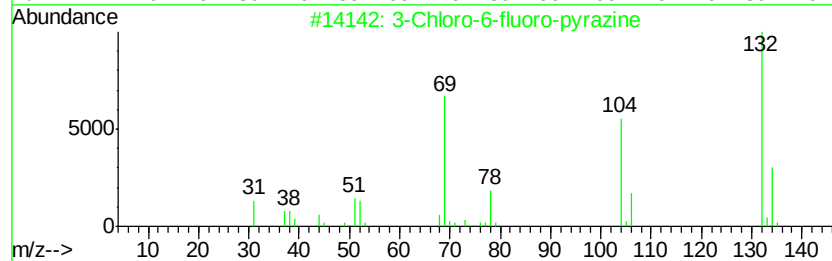
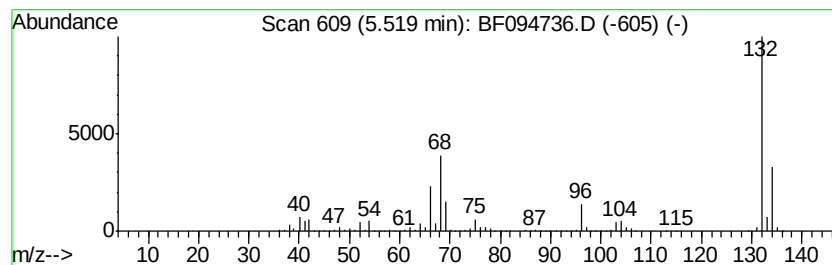
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	74.79 ng	2285070	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
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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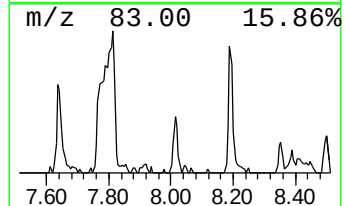
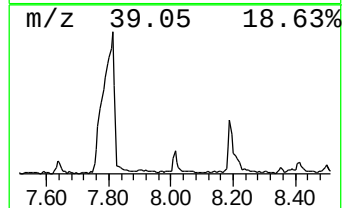
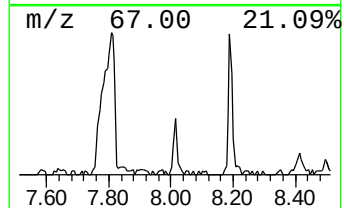
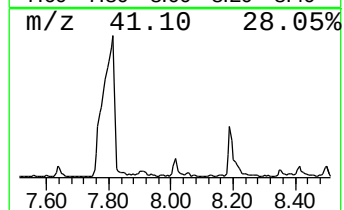
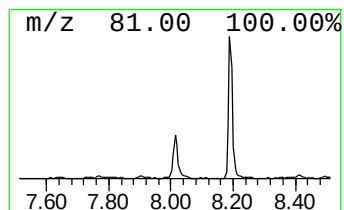
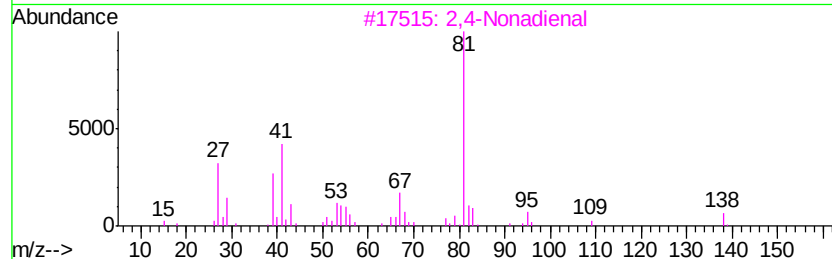
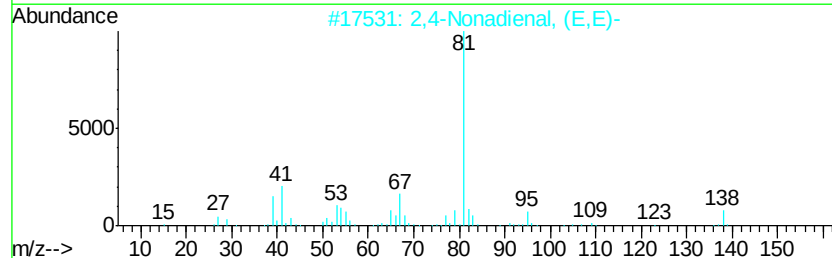
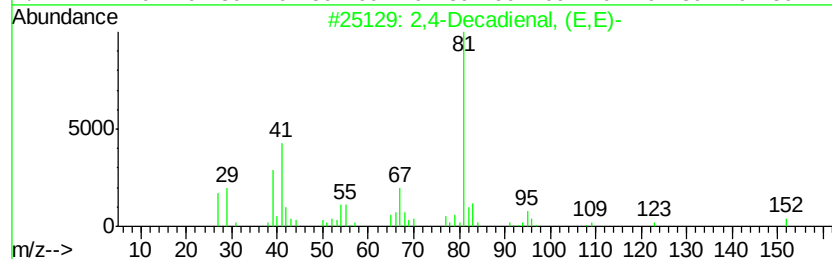
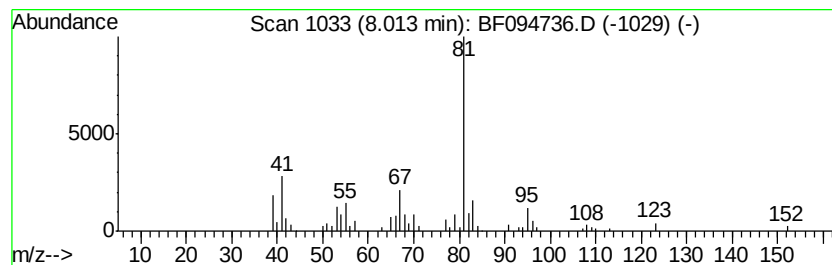
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 2,4-Decadienal, (E,E)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	2.16 ng	92845	Napthalene-d8	7.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	90
2		2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	78
3		2,4-Nonadienal	138	C9H14O	006750-03-4	72
4		2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	64
5		2,4-Heptadiene, (E,E)-	96	C7H12	002384-94-3	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094736.D
Acq On : 1 May 2017 2:25
Operator : SJ/MA
Sample : I2902-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

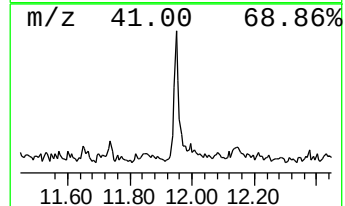
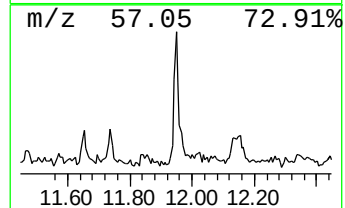
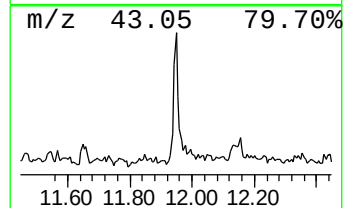
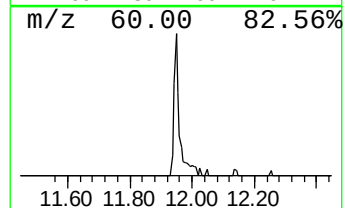
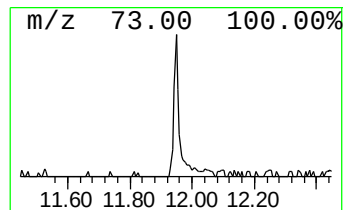
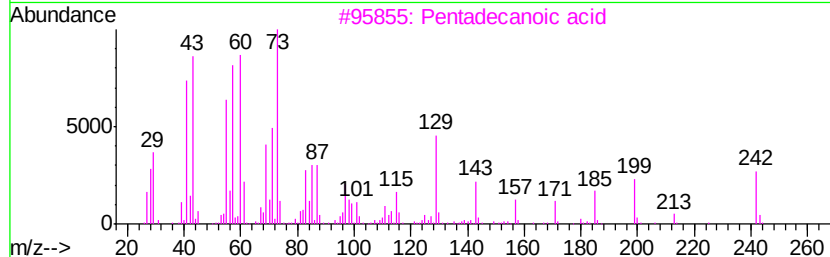
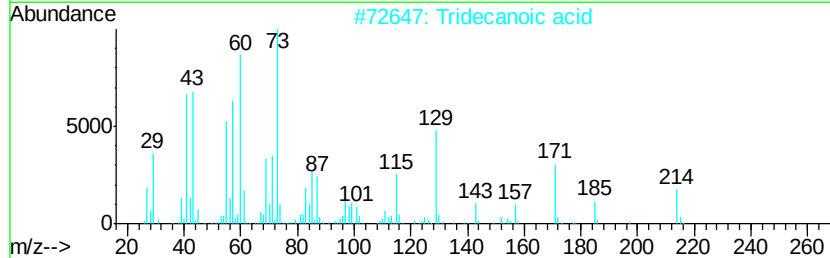
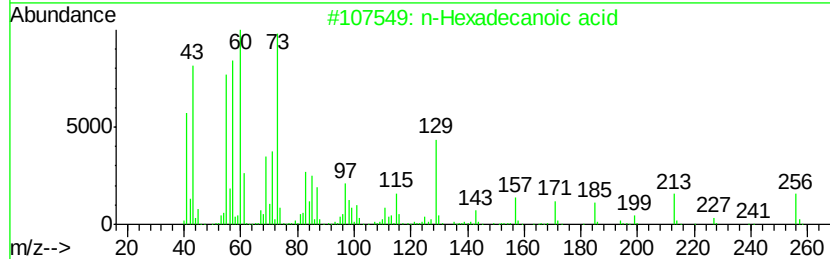
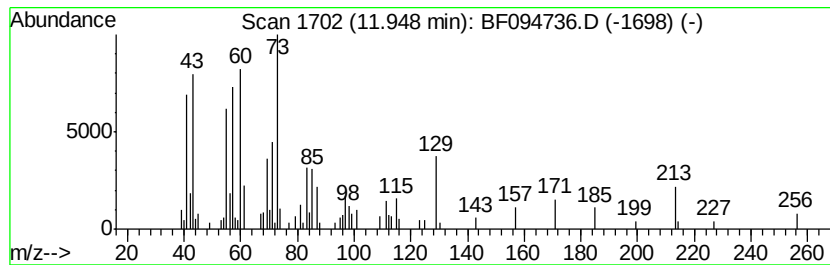
Instrument :
BNA_F
ClientSampleId :
MW-1B

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.95	3.17 ng	139774	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Heptanoic acid	130	C7H14O2	000111-14-8	25
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094736.D
Acq On : 1 May 2017 2:25
Operator : SJ/MA
Sample : I2902-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

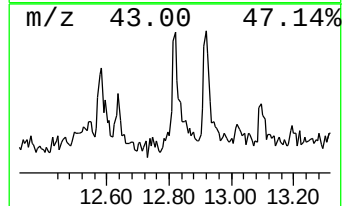
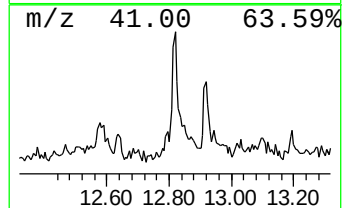
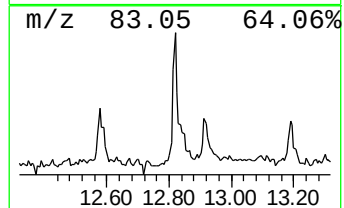
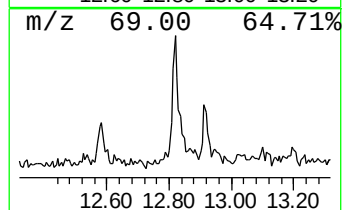
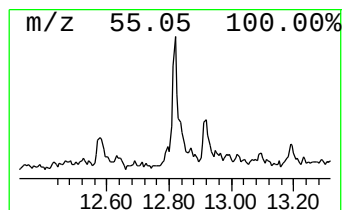
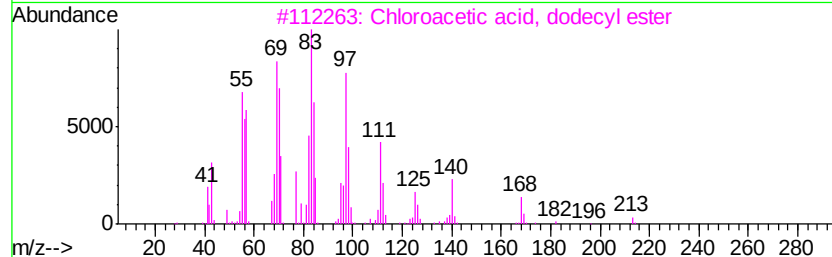
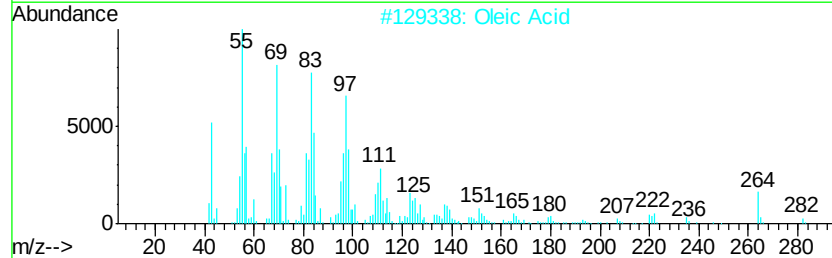
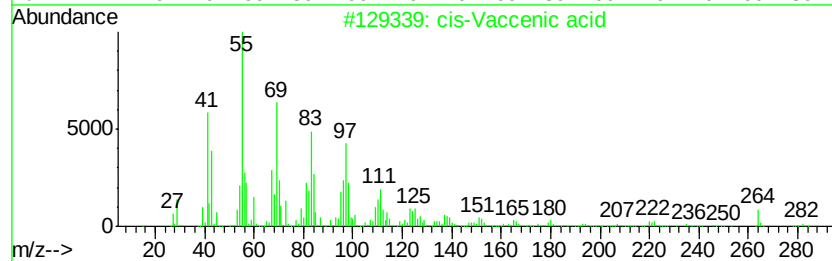
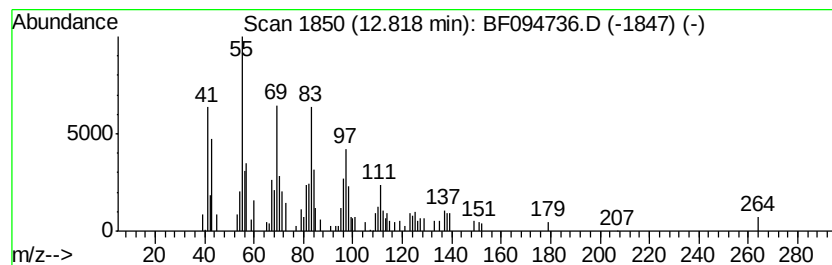
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 cis-Vaccenic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.82	2.91 ng	128568	Phenanthrene-d10		11.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	90
2	Oleic Acid	282	C18H34O2	000112-80-1	83
3	Chloroacetic acid, dodecyl ester	262	C14H27ClO2	006316-04-7	68
4	1-Dodecanol	186	C12H26O	000112-53-8	64
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094736.D
Acq On : 1 May 2017 2:25
Operator : SJ/MA
Sample : I2902-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

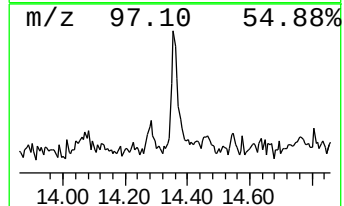
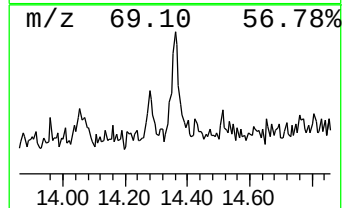
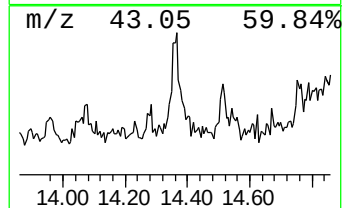
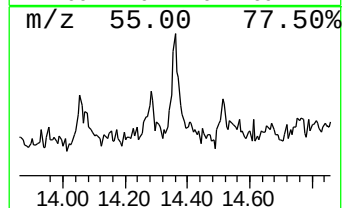
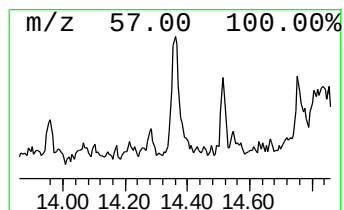
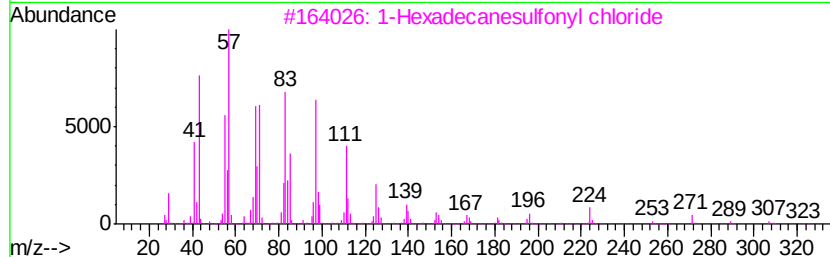
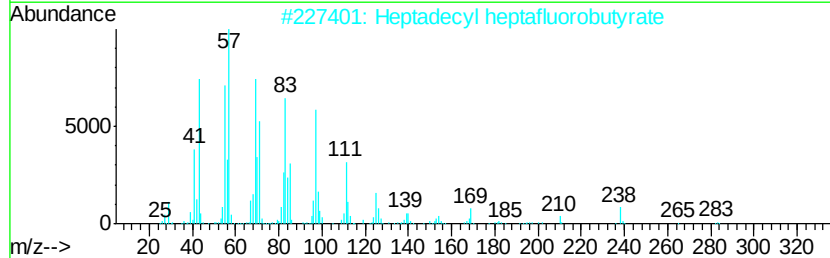
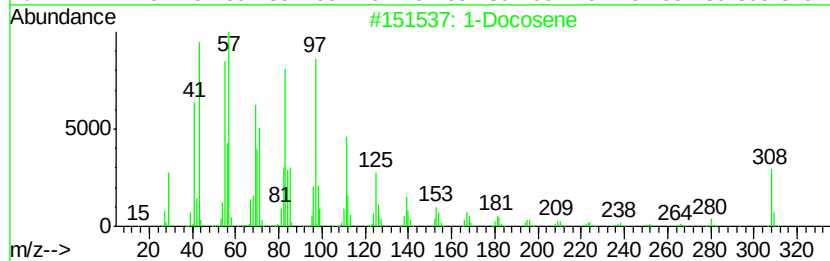
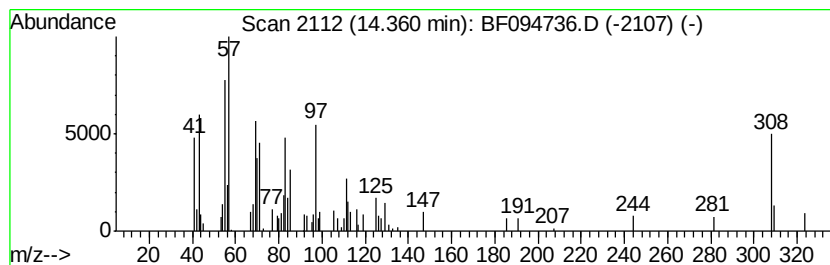
Instrument :
BNA_F
ClientSampleId :
MW-1B

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.64 ng	82884	Chrysene-d12	14.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 87
2	Heptadecyl heptafluorobutyrate		452 C21H35F7O2	959085-66-6 70
3	1-Hexadecanesulfonyl chloride		324 C16H33ClO2S	038775-38-1 62
4	Heptafluorobutyric acid, n-octad...		466 C22H37F7O2	000400-57-7 58
5	Carbonic acid, heptadecyl isobut...		356 C22H44O3	1000314-61-4 58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043017\
Data File : BF094736.D
Acq On : 1 May 2017 2:25
Operator : SJ/MA
Sample : I2902-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1B

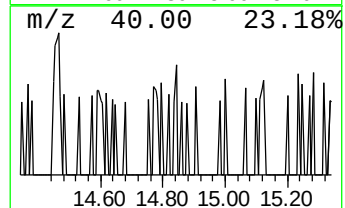
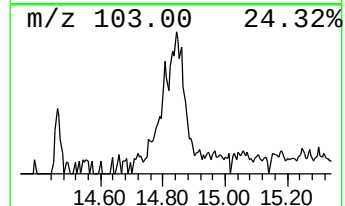
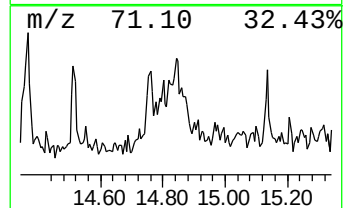
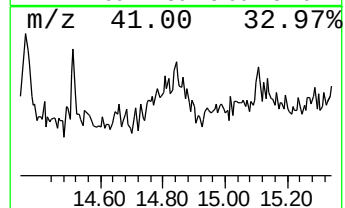
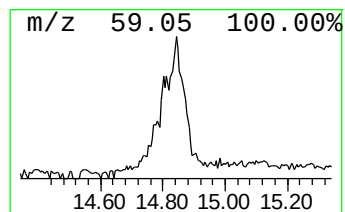
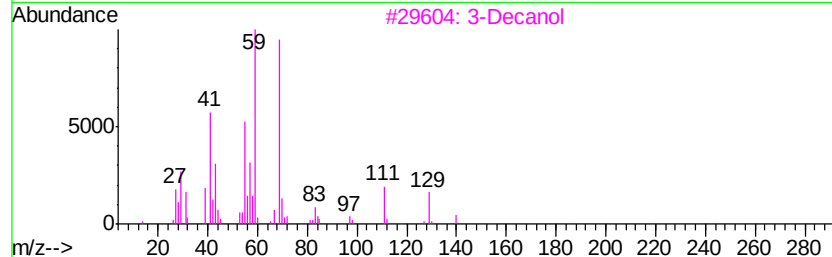
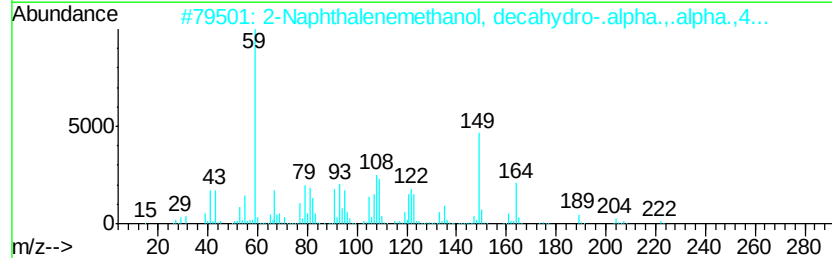
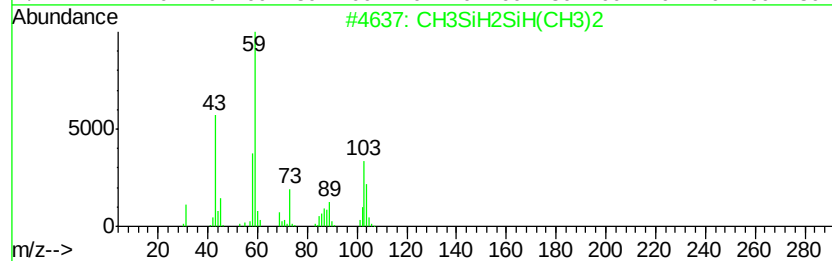
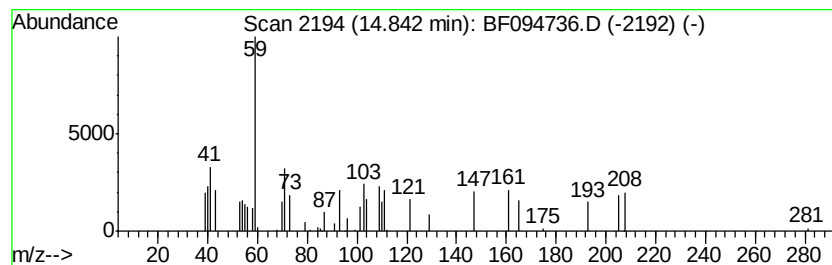
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.84 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.48 ng	77599	Chrysene-d12	14.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			CH3SiH2SiH(CH3)2	104	C3H12Si2	000814-74-4	27
2			2-Naphthalenemethanol, decahydro...	222	C15H26O	000473-15-4	17
3			3-Decanol	158	C10H22O	001565-81-7	12
4			tert-Butyl-[2-[2-[2-[2-[2-[2-...	542	C25H54O10Si	1000352-09-9	12
5			Octane, 1-(1-methoxyethoxy)-	188	C11H24O2	054789-26-3	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094736.D
Acq On : 1 May 2017 2:25
Operator : SJ/MA
Sample : I2902-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1B

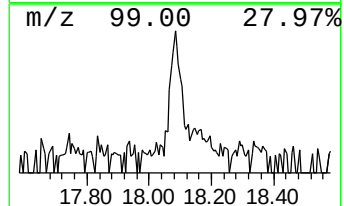
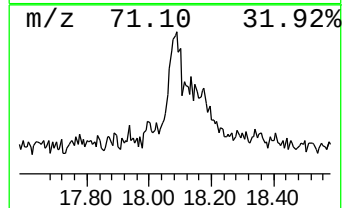
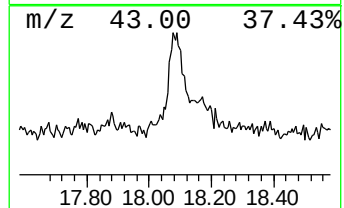
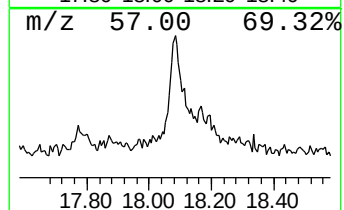
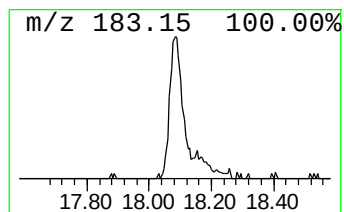
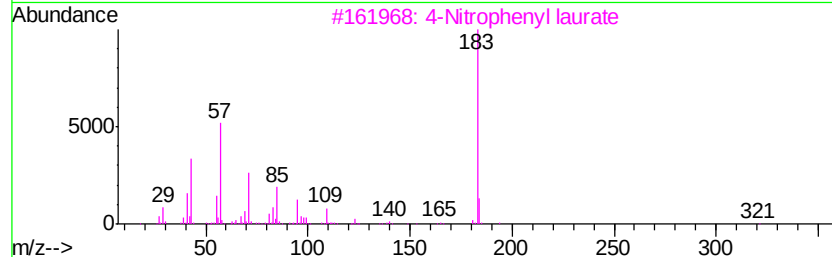
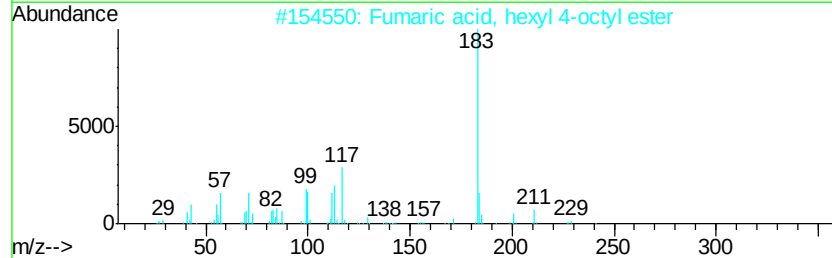
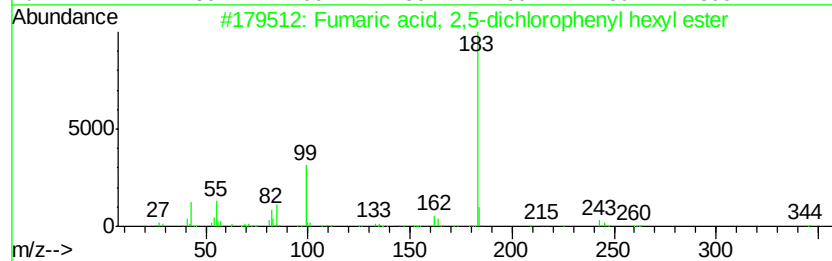
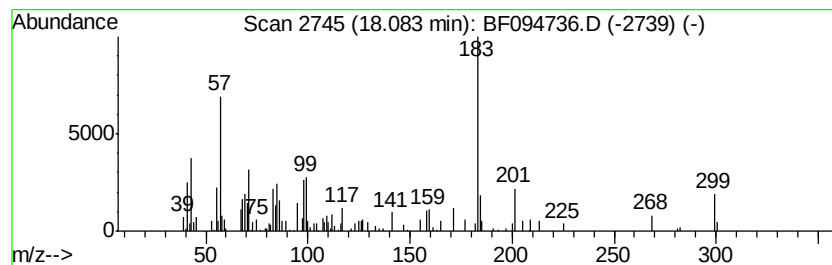
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown18.08 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	6.67 ng	207876	Perylene-d12	16.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, 2,5-dichlorophenyl...	344	C16H18Cl2O4	1000345-32-0	43
2		Fumaric acid, hexyl 4-octyl ester	312	C18H32O4	1000339-21-7	43
3		4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	43
4		Lauric acid, 3,4-dichlorophenyl ...	344	C18H26Cl2O2	1000357-92-7	43
5		Fumaric acid, 4-heptyl hexyl ester	298	C17H30O4	1000348-51-5	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043017\
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ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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
Hexanal	3.41	7.9	ng	240621	1	5.76	611035	20.0
2-Pentanone, 4-hy...	3.91	3.4	ng	102593	1	5.76	611035	20.0
Ethanol, 2-butoxy-	4.64	4.0	ng	120911	1	5.76	611035	20.0
unknown5.52	5.52	74.8	ng	2285070	1	5.76	611035	20.0
2,4-Decadienal, (...)	8.01	2.2	ng	92845	2	7.25	858438	20.0
n-Hexadecanoic acid	11.95	3.2	ng	139774	4	11.21	882149	20.0
cis-Vaccenic acid	12.82	2.9	ng	128568	4	11.21	882149	20.0
1-Docosene	14.36	2.6	ng	82884	5	14.47	626912	20.0
unknown14.84	14.84	2.5	ng	77599	5	14.47	626912	20.0
unknown18.08	18.08	6.7	ng	207876	6	16.09	622994	20.0