

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
 Data File : BF091293.D
 Acq On : 23 Nov 2016 23:43
 Operator : UM/SJ
 Sample : H5740-09
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04(5-6)

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-BF112316.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	1.755	3	6	9	rBV	4477514	5207186	88.65%	8.336%
2	1.904	17	19	41	rVB	2881520	5586226	95.10%	8.943%
3	2.178	41	43	49	rVB	60035	120868	2.06%	0.193%
4	5.070	293	296	302	rBV	1267806	1986697	33.82%	3.180%
5	5.481	329	332	335	rBV	3723640	5461360	92.97%	8.743%
6	6.510	418	422	424	rBV	4913252	5874150	100.00%	9.404%
7	6.647	431	434	436	rBV	5320462	5129056	87.32%	8.211%
8	6.876	452	454	457	rBV	1413633	1272275	21.66%	2.037%
9	7.036	465	468	470	rBV	4361760	3813351	64.92%	6.105%
10	7.436	500	503	506	rBV	2333248	3422498	58.26%	5.479%
11	8.167	564	567	569	rBV	1595189	1764926	30.05%	2.825%
12	8.876	627	629	631	rBV	116767	95511	1.63%	0.153%
13	9.242	658	661	664	rBV	5519146	5157867	87.81%	8.257%
14	9.345	666	670	671	rBV	48624	67162	1.14%	0.108%
15	9.505	682	684	687	rBV2	46644	65912	1.12%	0.106%
16	9.573	688	690	692	rBV	58776	73848	1.26%	0.118%
17	9.630	694	695	698	rVB	341831	333106	5.67%	0.533%
18	9.916	718	720	722	rBV	1943919	1783330	30.36%	2.855%
19	9.950	722	723	725	rVB	161985	121673	2.07%	0.195%
20	10.122	736	738	740	rBV	179376	144269	2.46%	0.231%
21	10.362	752	759	760	rBV2	75518	100069	1.70%	0.160%
22	10.465	766	768	770	rVB	145641	124037	2.11%	0.199%
23	10.705	786	789	792	rBV	3630036	3504088	59.65%	5.609%
24	10.831	798	800	805	rVB	103976	118845	2.02%	0.190%
25	11.196	831	832	835	rVB	56604	77154	1.31%	0.124%
26	11.402	847	850	851	rBV	1984495	1765602	30.06%	2.826%
27	11.471	854	856	858	rVB	144460	137807	2.35%	0.221%
28	11.939	895	897	899	rVV	286066	447110	7.61%	0.716%
29	12.008	902	903	908	rVB2	43434	74233	1.26%	0.119%
30	12.191	917	919	923	rVB2	36099	59554	1.01%	0.095%
31	12.614	953	956	957	rBV	161917	219007	3.73%	0.351%
32	12.716	963	965	972	rBV	153235	199072	3.39%	0.319%
33	12.831	972	975	977	rVB2	122693	178655	3.04%	0.286%
34	12.991	986	989	991	rVB	3718640	3844644	65.45%	6.155%

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Integration Parameters: rteint.p
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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-BF112316.M
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35	13.882	1065	1067	1072	rBV	115699	143460	2.44%	0.230%
36	14.031	1077	1080	1085	rBV	1481893	1403207	23.89%	2.246%
37	14.797	1145	1147	1154	rBV	527850	645842	10.99%	1.034%
38	14.899	1154	1156	1158	rVB	260178	262201	4.46%	0.420%
39	15.060	1167	1170	1176	rVB	30540	67512	1.15%	0.108%
40	15.471	1203	1206	1209	rBV	971895	1252145	21.32%	2.004%
41	19.037	1509	1518	1530	rVB6	52703	361825	6.16%	0.579%

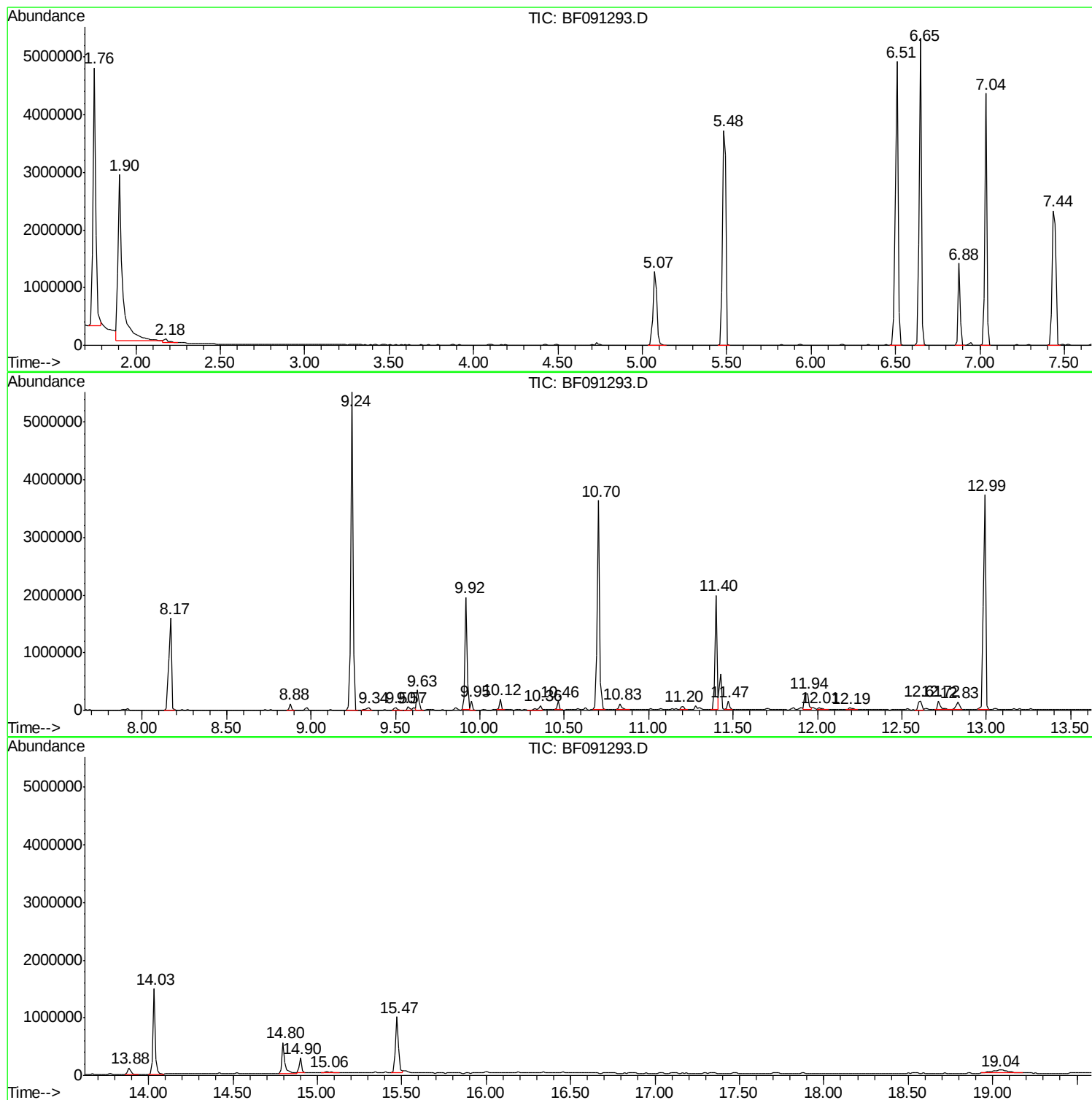
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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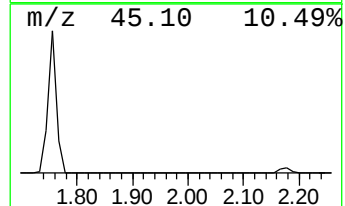
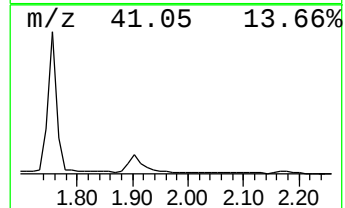
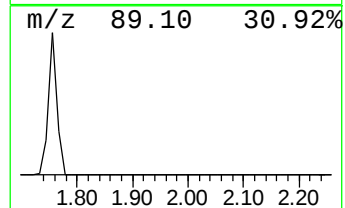
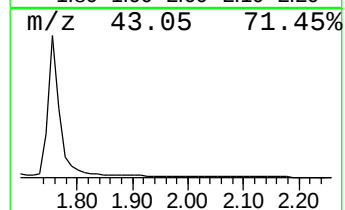
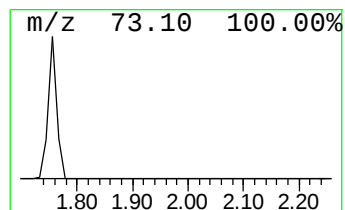
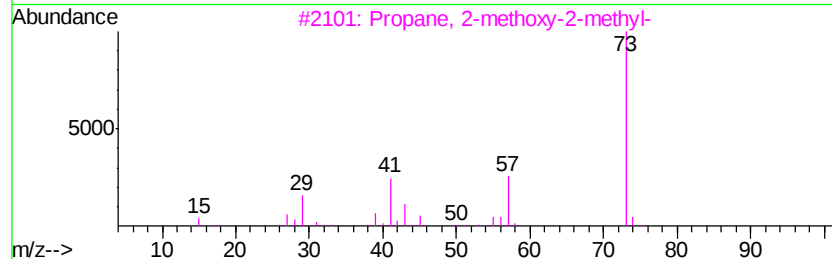
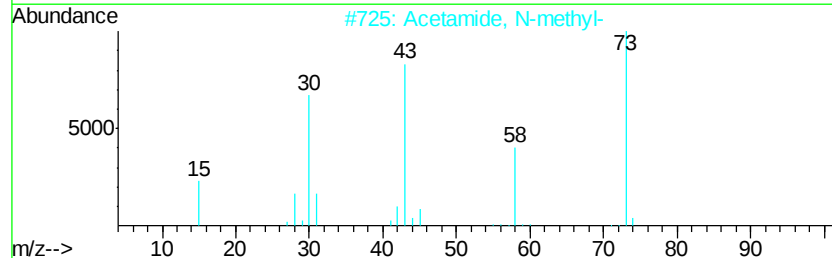
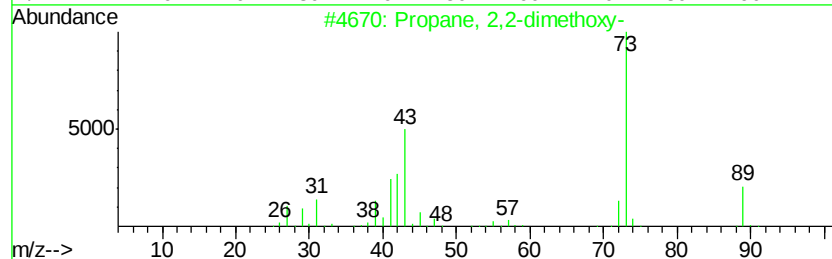
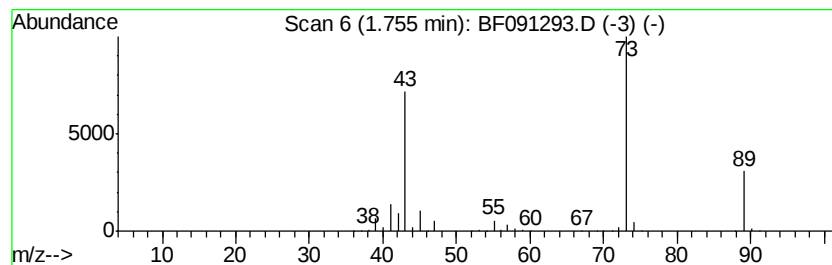
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.76 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	81.86 ng	5207190	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	23
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	17
5		Oxirane-2-carboxylic acid, ethyl...	116	C5H8O3	1000192-50-3	9



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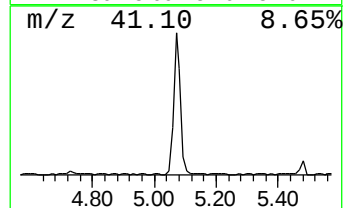
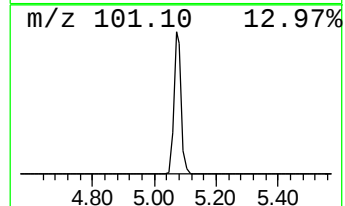
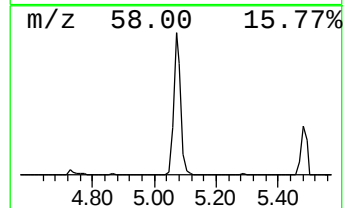
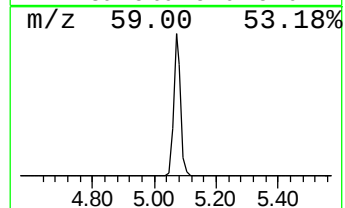
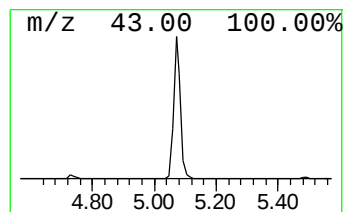
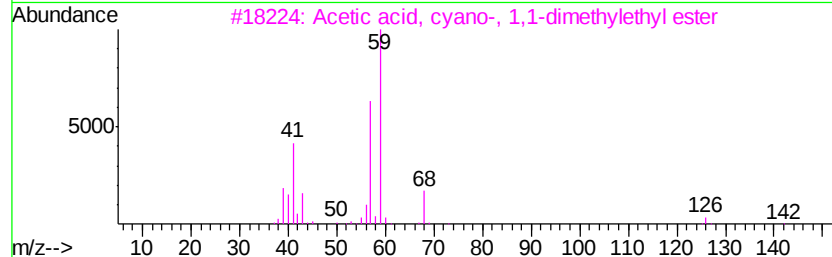
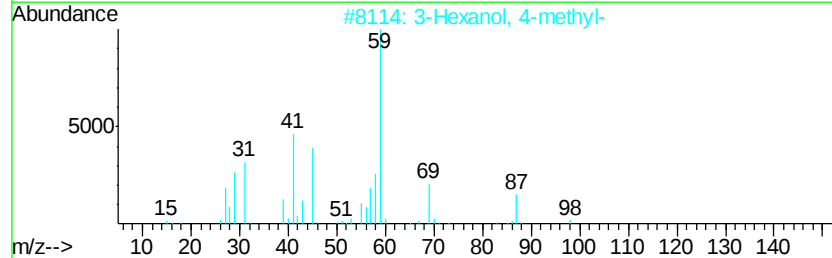
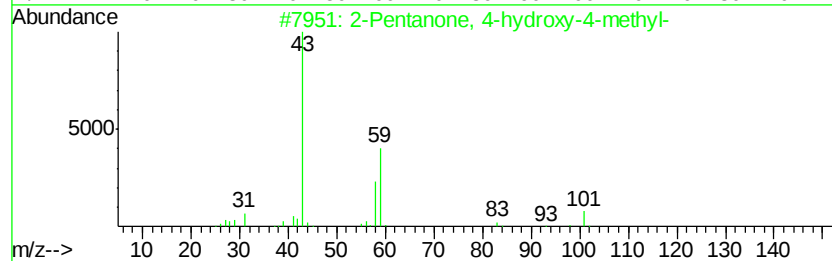
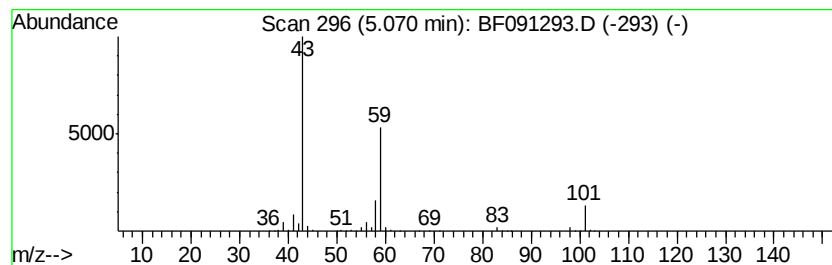
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	31.23 ng	1986700	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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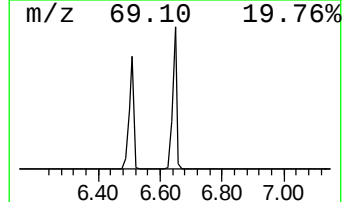
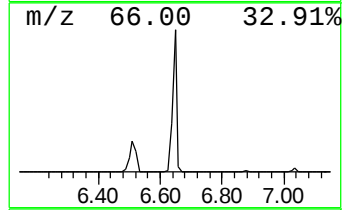
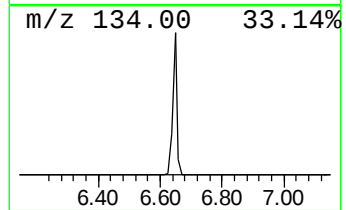
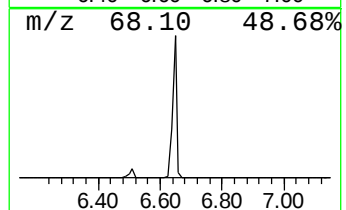
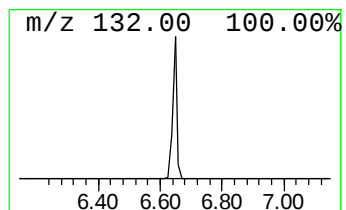
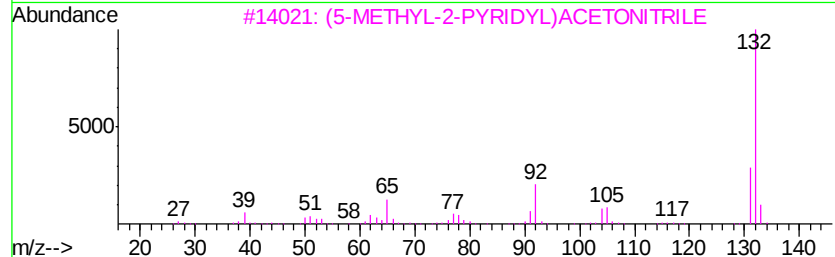
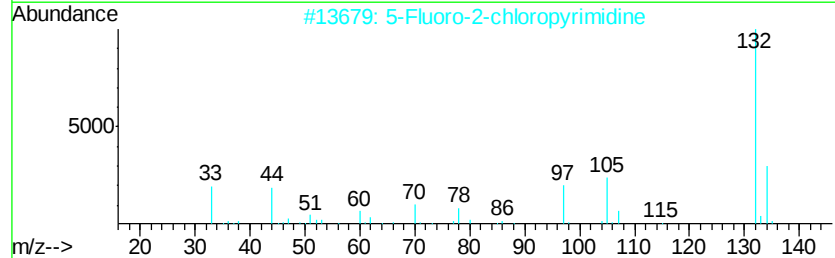
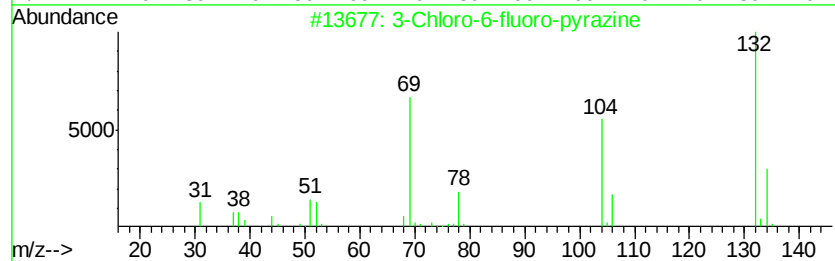
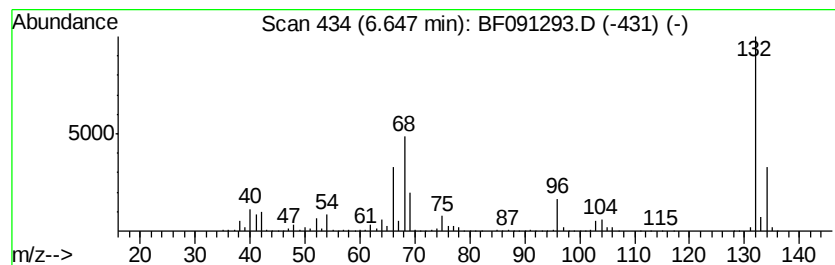
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	80.63 ng	5129060	1,4-Dichlorobenzene-d4	6.88

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	16
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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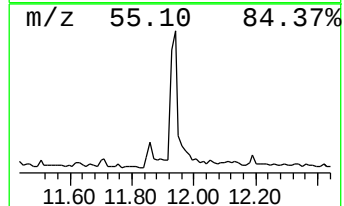
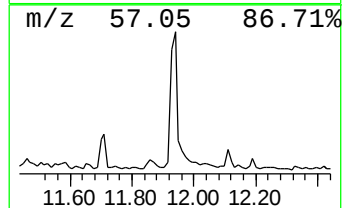
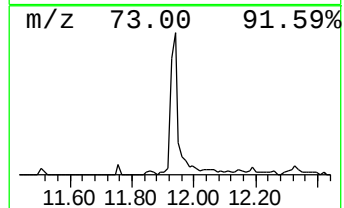
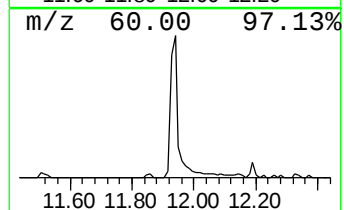
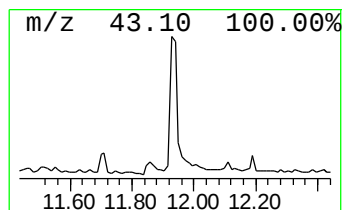
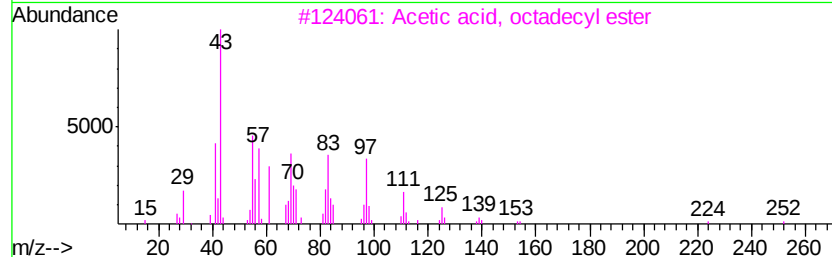
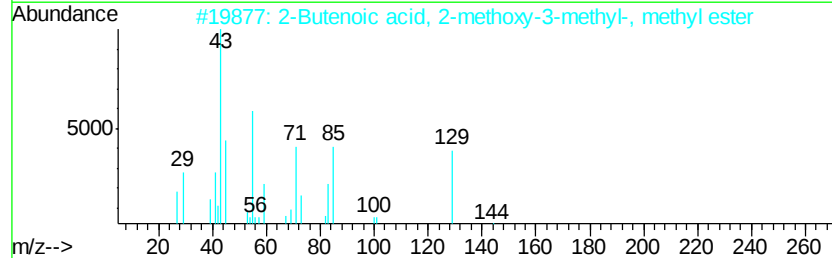
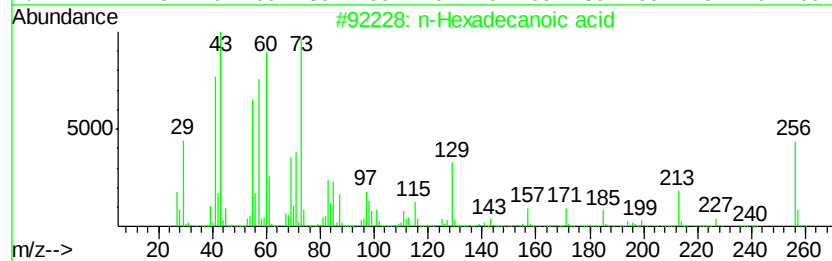
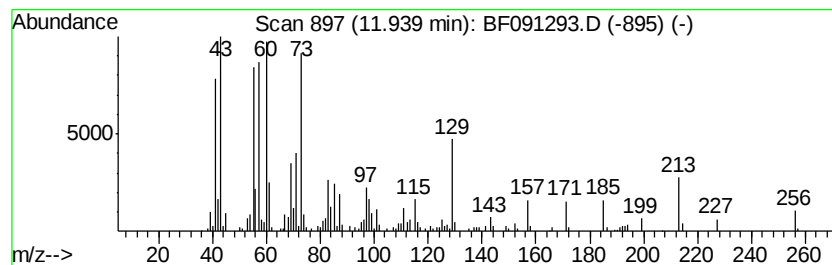
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.94	5.06 ng	447110	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18
3	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	15
4	Decane	142	C10H22	000124-18-5	11
5	Undecane	156	C11H24	001120-21-4	11



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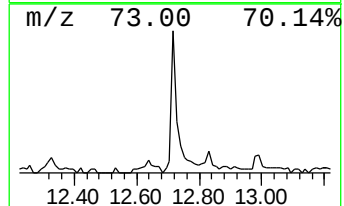
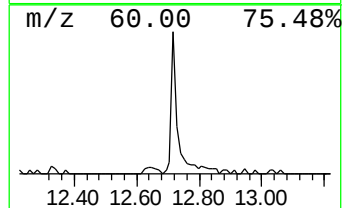
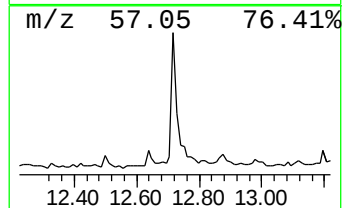
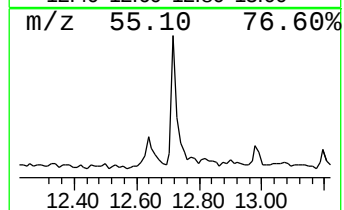
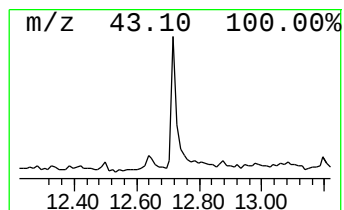
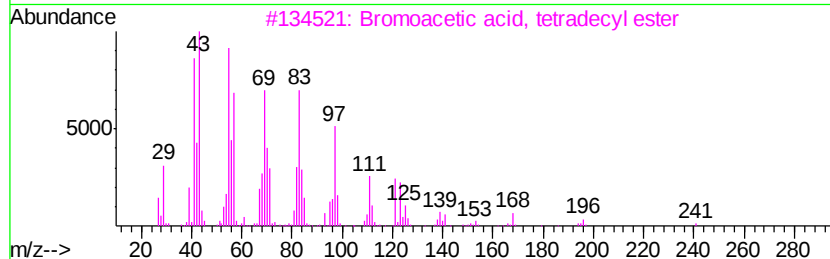
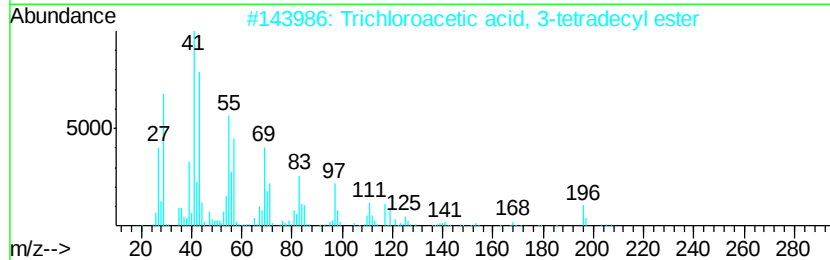
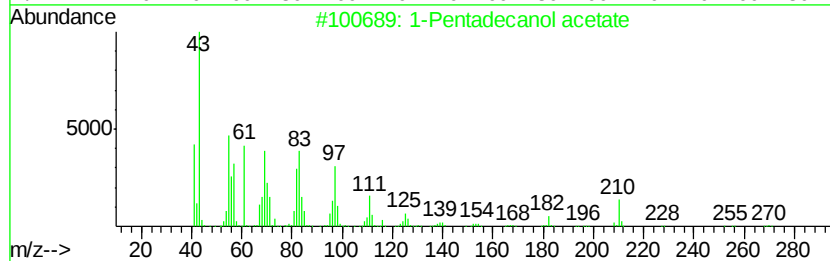
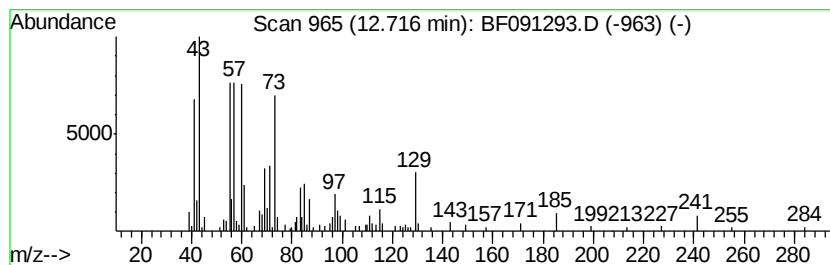
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown12.72 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.84 ng	199072	Chrysene-d12	14.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecanol acetate	270	C17H34O2	000629-58-3	15
2			Trichloroacetic acid, 3-tetradec...	358	C16H29Cl3O2	1000282-06-7	11
3			Bromoacetic acid, tetradecyl ester	334	C16H31BrO2	018992-01-3	11
4			Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	11
5			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091293.D
Acq On : 23 Nov 2016 23:43
Operator : UM/SJ
Sample : H5740-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

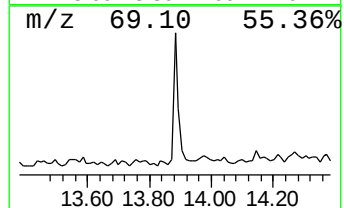
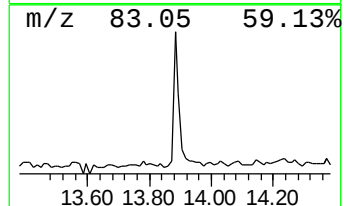
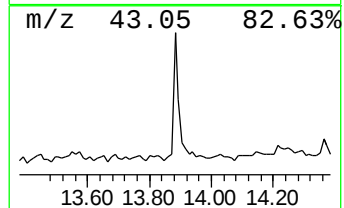
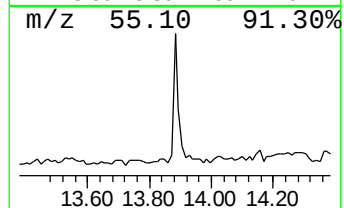
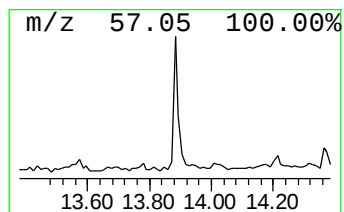
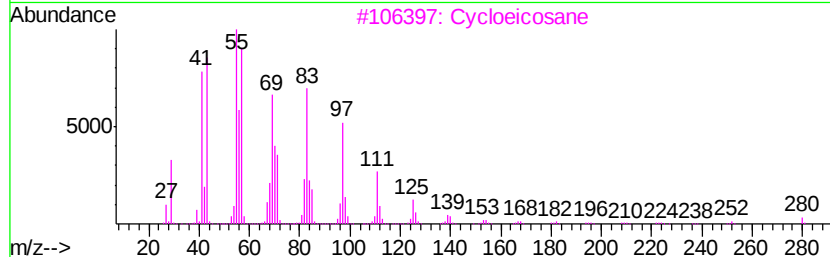
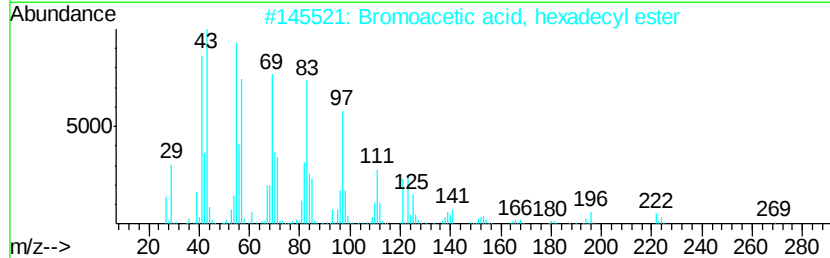
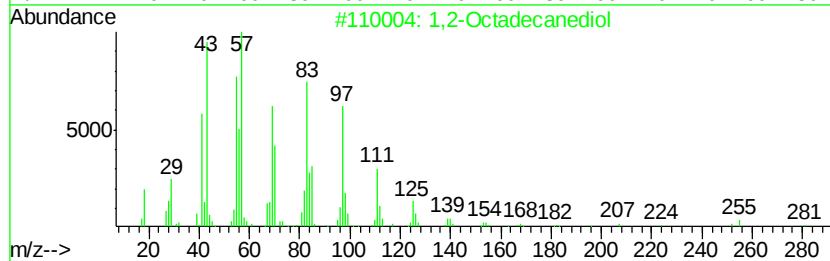
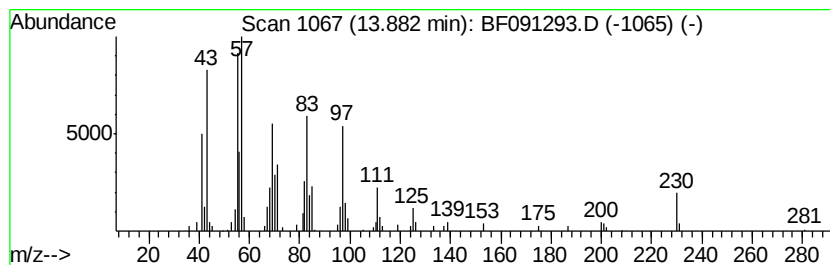
Instrument :
BNA_F
ClientSampleId :
SB-04(5-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1,2-Octadecanediol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.88	2.04 ng	143460	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Octadecanediol	286	C18H38O2	020294-76-2	90
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
3	Cycloeicosane	280	C20H40	000296-56-0	87
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
5	1-Octadecanol	270	C18H38O	000112-92-5	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091293.D
Acq On : 23 Nov 2016 23:43
Operator : UM/SJ
Sample : H5740-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

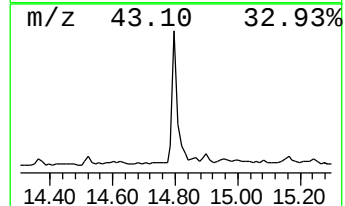
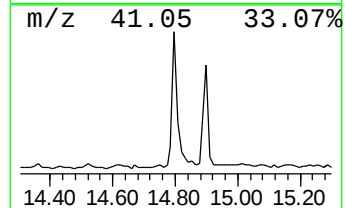
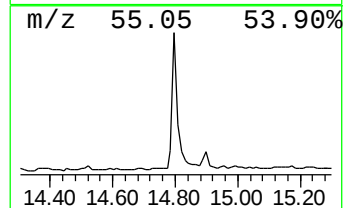
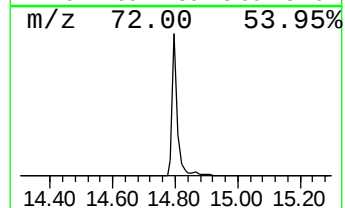
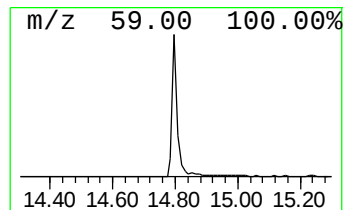
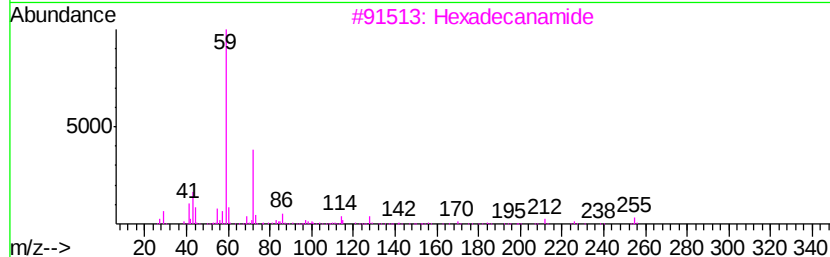
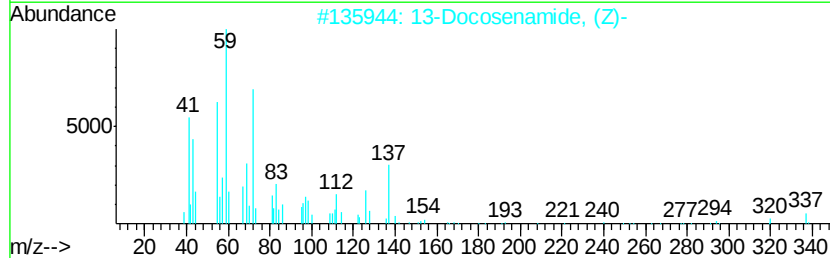
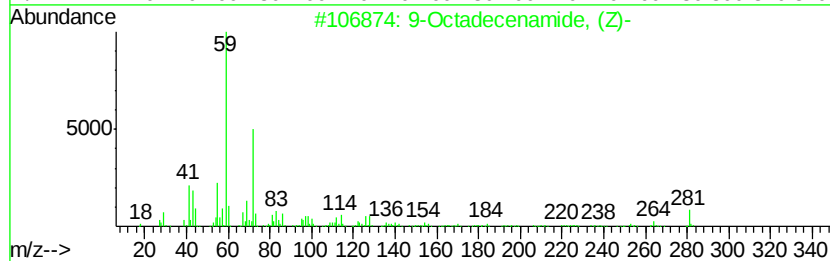
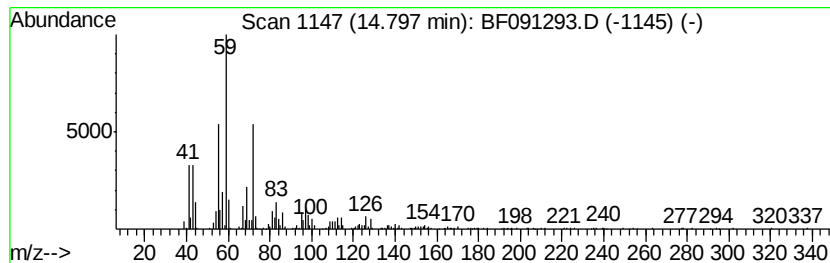
Instrument :
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ClientSampleId :
SB-04(5-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	10.32 ng	645842	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0 91
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5 78
3	Hexadecanamide	255	C16H33NO	000629-54-9 72
4	Tetradecanamide	227	C14H29NO	000638-58-4 72
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1 59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091293.D
Acq On : 23 Nov 2016 23:43
Operator : UM/SJ
Sample : H5740-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

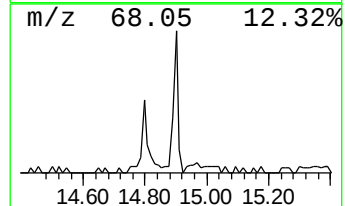
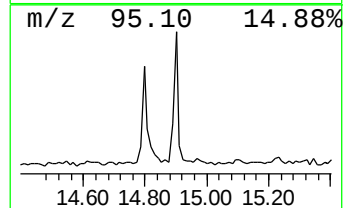
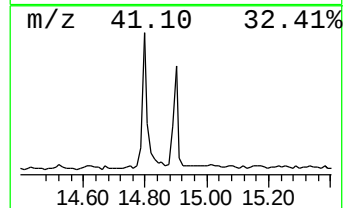
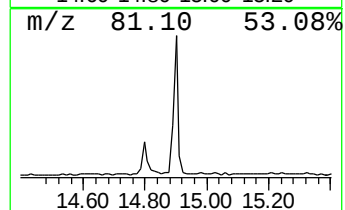
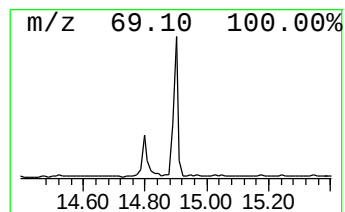
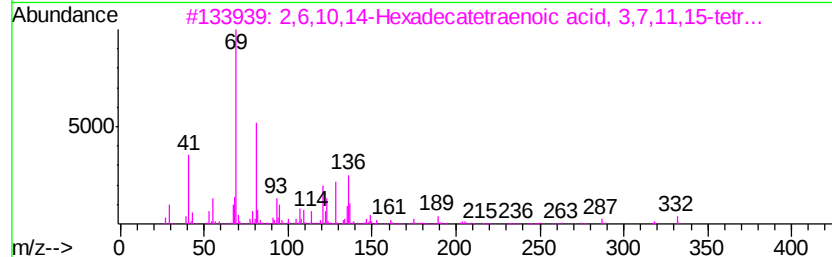
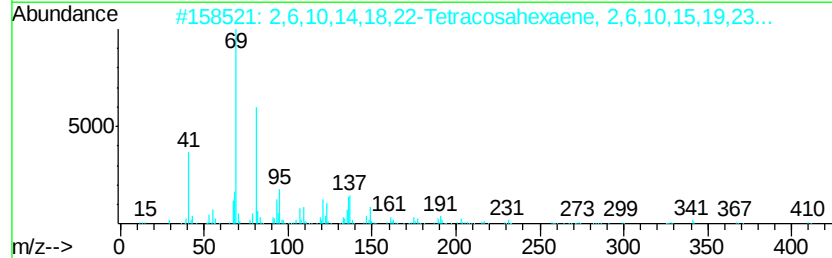
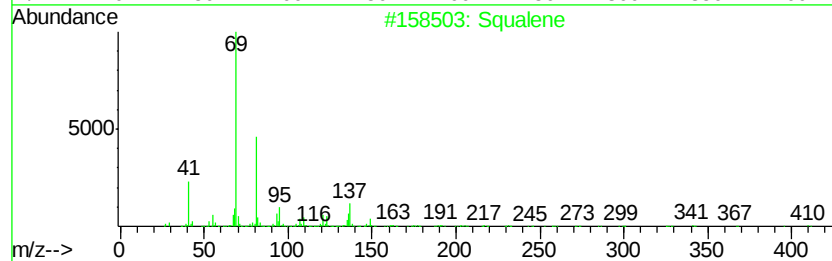
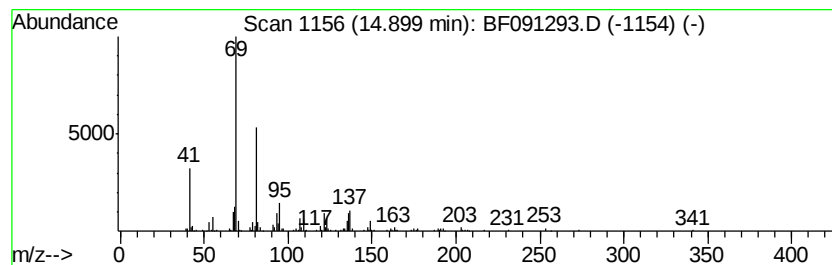
Instrument :
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ClientSampleId :
SB-04(5-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	4.19 ng	262201	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 91
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 91
3	2,6,10,14-Hexadecatetraenoic aci...		332 C22H36O2	024035-35-6 72
4	2,6-Octadiene, 2,6-dimethyl-		138 C10H18	002792-39-4 50
5	1,5-Heptadiene, 2,6-dimethyl-		124 C9H16	006709-39-3 49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091293.D
Acq On : 23 Nov 2016 23:43
Operator : UM/SJ
Sample : H5740-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(5-6)

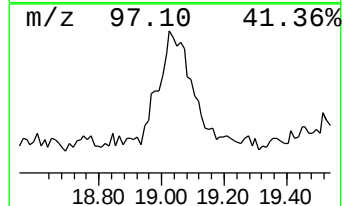
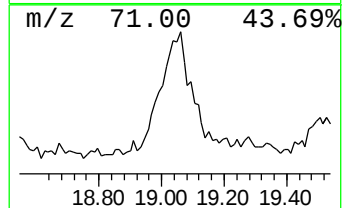
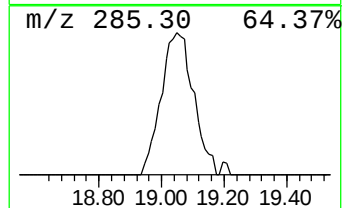
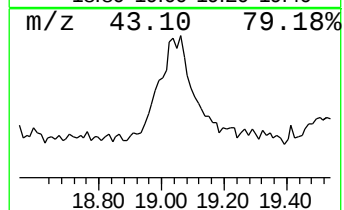
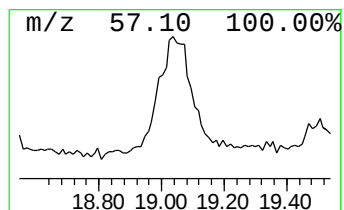
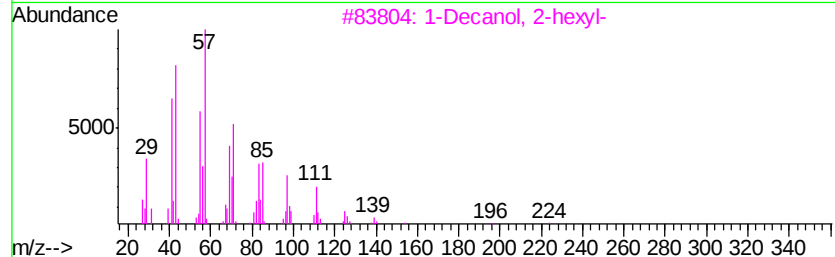
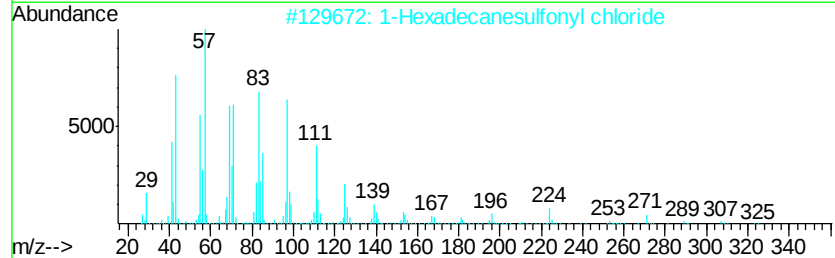
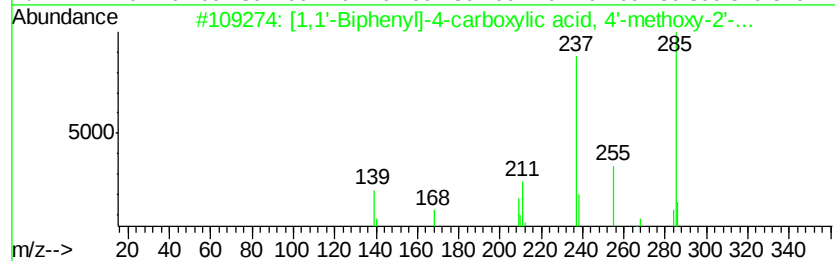
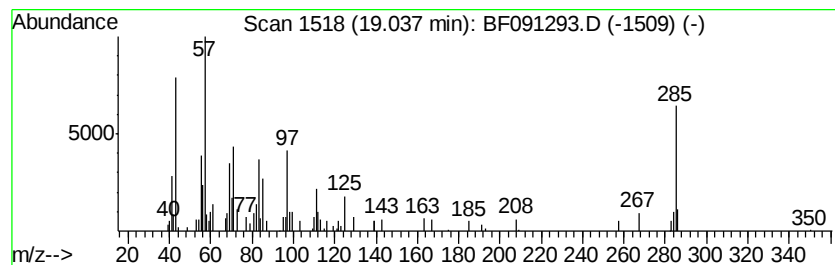
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 [1,1'-Biphenyl]-4-carboxyli... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	5.78 ng	361825	Perylene-d12	15.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,1'-Biphenyl]-4-carboxylic aci...	285	C16H15N04	053366-26-0	64
2			1-Hexadecanesulfonyl chloride	324	C16H33Cl02S	038775-38-1	53
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	43
4			1-Octadecanethiol	286	C18H38S	002885-00-9	38
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091293.D
Acq On : 23 Nov 2016 23:43
Operator : UM/SJ
Sample : H5740-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(5-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.76	1.76	81.9	ng	5207190	1	6.88	1272280	20.0
2-Pentanone, 4-hy...	5.07	31.2	ng	1986700	1	6.88	1272280	20.0
unknown6.65	6.65	80.6	ng	5129060	1	6.88	1272280	20.0
n-Hexadecanoic acid	11.94	5.1	ng	447110	4	11.40	1765600	20.0
unknown12.72	12.72	2.8	ng	199072	5	14.03	1403210	20.0
1,2-Octadecanediol	13.88	2.0	ng	143460	5	14.03	1403210	20.0
9-Octadecenamide, ...	14.80	10.3	ng	645842	6	15.47	1252150	20.0
Squalene	14.90	4.2	ng	262201	6	15.47	1252150	20.0
[1,1'-Biphenyl]-4...	19.04	5.8	ng	361825	6	15.47	1252150	20.0