

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
 Data File : BF091597.D
 Acq On : 14 Dec 2016 21:13
 Operator : UM/SJ
 Sample : H6006-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-13-10-15

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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	3.104	87	89	101	rBV5	21822	86133	1.04%	0.115%
2	4.967	249	252	260	rBV	1930523	2794269	33.65%	3.721%
3	5.401	287	290	292	rBV	7013969	7252847	87.34%	9.658%
4	6.442	377	381	383	rVB	6551404	8303946	100.00%	11.057%
5	6.567	389	392	394	rBV	7100445	7918894	95.36%	10.544%
6	6.796	409	412	414	rBV	1883060	1839246	22.15%	2.449%
7	6.944	423	425	428	rBV	4077771	5459661	65.75%	7.270%
8	7.356	458	461	464	rBV	4080951	4340526	52.27%	5.780%
9	8.076	522	524	527	rBV	2631997	2396514	28.86%	3.191%
10	9.162	616	619	621	rBV	7129851	7485284	90.14%	9.967%
11	9.276	628	629	632	rVB	94037	112386	1.35%	0.150%
12	9.550	651	653	656	rBV	1639619	1454663	17.52%	1.937%
13	9.836	675	678	680	rBV	2465504	2715035	32.70%	3.615%
14	10.625	744	747	749	rBV	3634522	4736854	57.04%	6.307%
15	10.739	756	757	763	rBV	76702	130033	1.57%	0.173%
16	11.196	795	797	798	rBV	89165	99201	1.19%	0.132%
17	11.311	805	807	811	rVB	2608036	2482827	29.90%	3.306%
18	11.551	825	828	830	rBV	797217	795253	9.58%	1.059%
19	11.619	832	834	836	rVB	126687	109599	1.32%	0.146%
20	11.848	852	854	856	rBV2	211294	285550	3.44%	0.380%
21	12.019	867	869	872	rBV	93027	127805	1.54%	0.170%
22	12.099	874	876	880	rVB4	49562	89661	1.08%	0.119%
23	12.362	897	899	902	rBV	1679997	1792544	21.59%	2.387%
24	12.419	902	904	908	rVV2	65625	126792	1.53%	0.169%
25	12.522	911	913	915	rBV	148634	152512	1.84%	0.203%
26	12.728	929	931	934	rBV2	132827	238601	2.87%	0.318%
27	12.785	934	936	941	rVB2	68856	93752	1.13%	0.125%
28	12.899	943	946	949	rVV	5647618	5613988	67.61%	7.475%
29	13.357	983	986	987	rBV	164758	187636	2.26%	0.250%
30	13.379	987	988	992	rVB2	92476	134376	1.62%	0.179%
31	13.802	1023	1025	1032	rVB2	340173	427598	5.15%	0.569%
32	13.939	1035	1037	1040	rBV	1612587	1931333	23.26%	2.572%
33	14.431	1076	1080	1086	rBV6	50883	130526	1.57%	0.174%
34	14.797	1109	1112	1116	rBV	220165	278532	3.35%	0.371%

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Integration Parameters: rteint.p
Integrator: RTE
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Start Thrs: 0.2 Max Peaks: 100
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.957	1124	1126	1131	rVB	49617	101474	1.22%	0.135%
36	15.231	1147	1150	1153	rVB2	97166	138568	1.67%	0.185%
37	15.357	1158	1161	1164	rBV	1387665	1691430	20.37%	2.252%
38	15.700	1188	1191	1194	rVB	102864	194973	2.35%	0.260%
39	16.248	1236	1239	1249	rVB3	121674	317270	3.82%	0.422%
40	16.911	1293	1297	1303	rVB	113763	302306	3.64%	0.403%
41	17.723	1364	1368	1375	rVB2	70531	229815	2.77%	0.306%

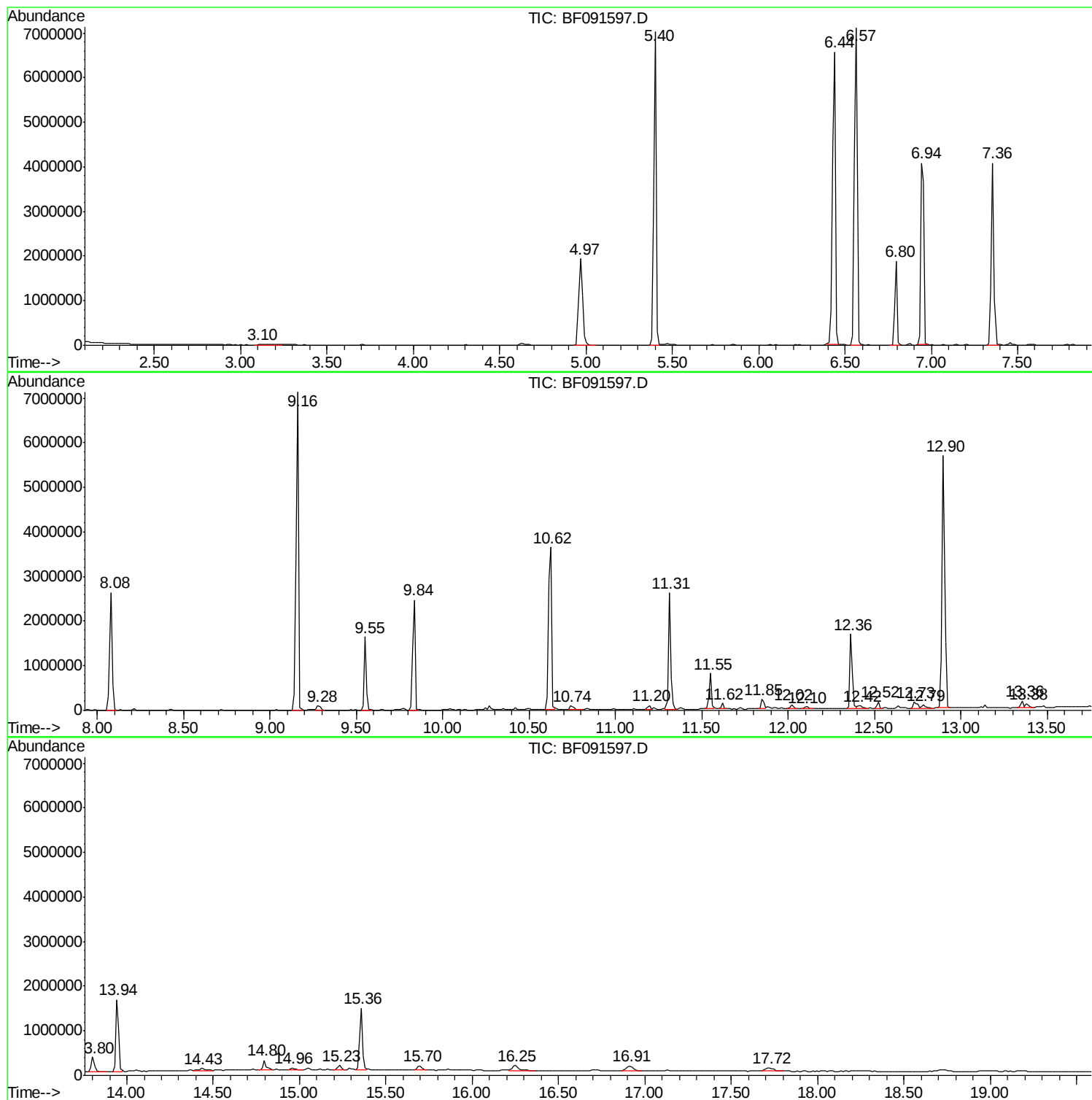
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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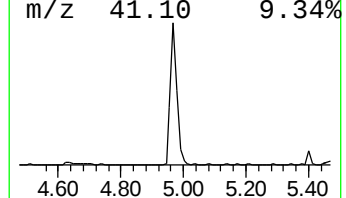
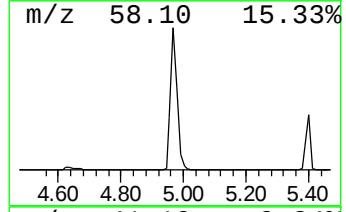
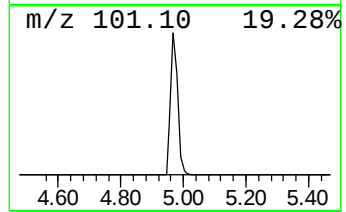
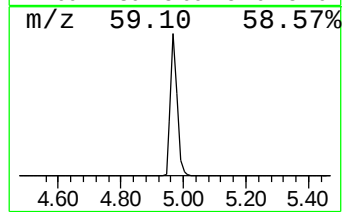
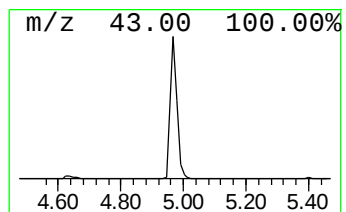
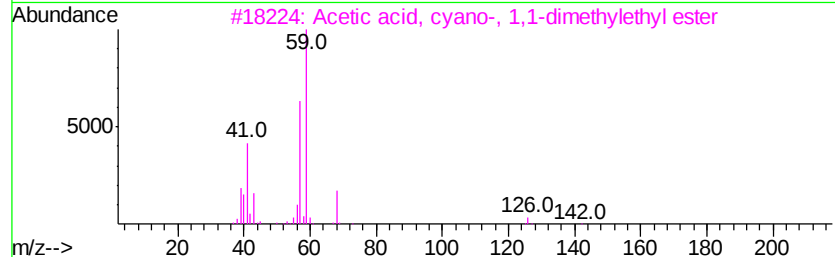
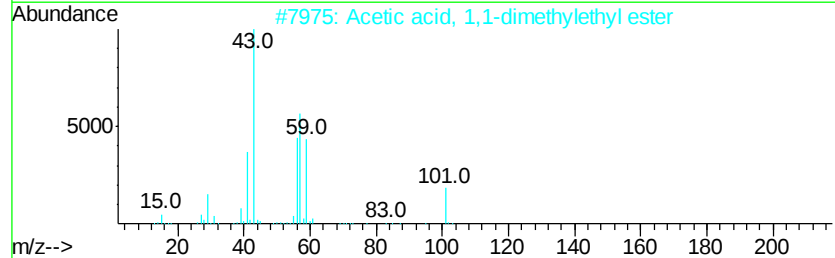
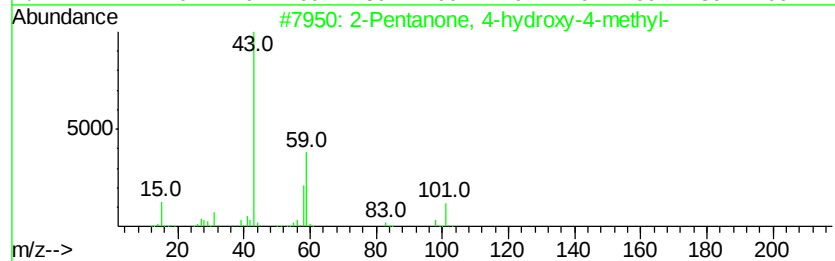
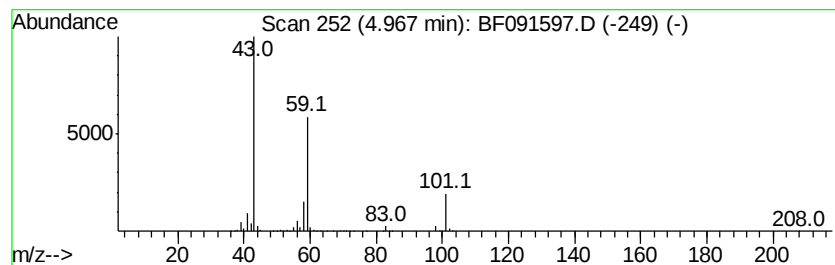
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	30.38 ng	2794270	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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ClientSampled :
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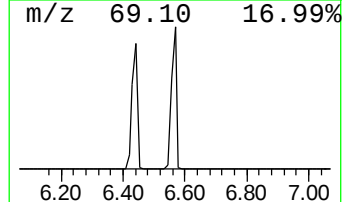
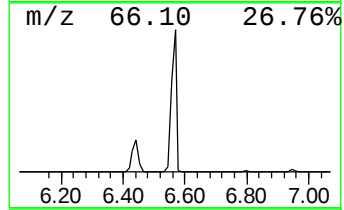
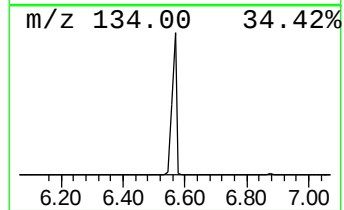
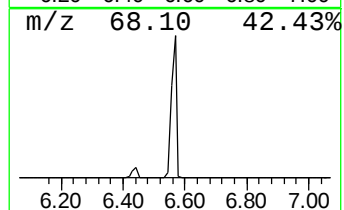
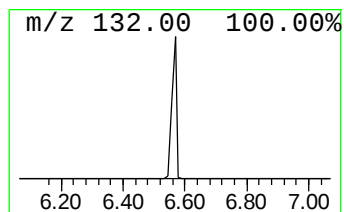
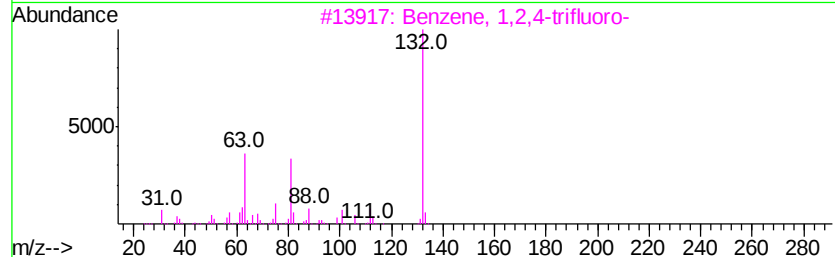
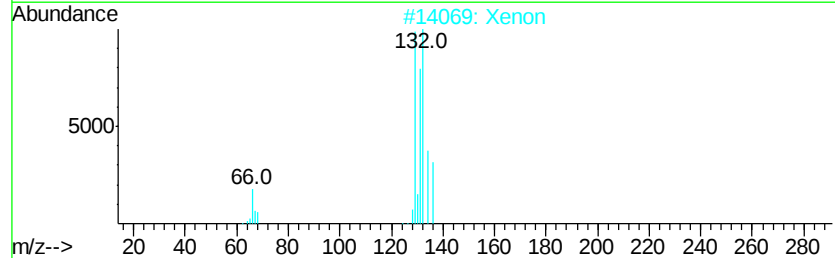
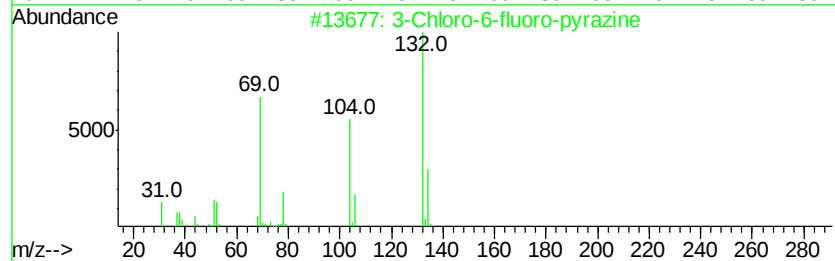
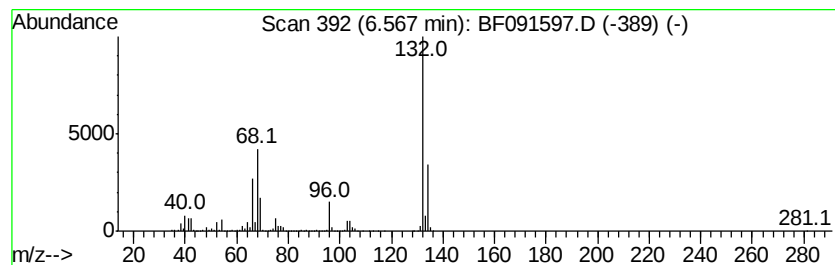
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	86.11 ng	7918890	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Xenon	132	Xe	007440-63-3	9
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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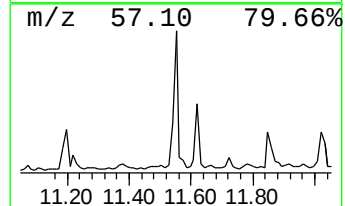
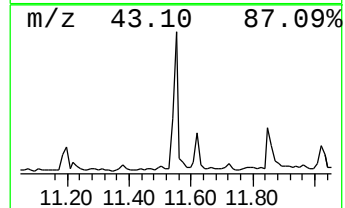
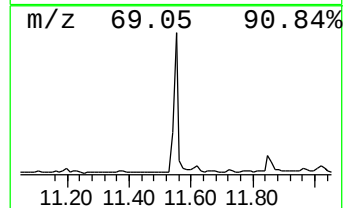
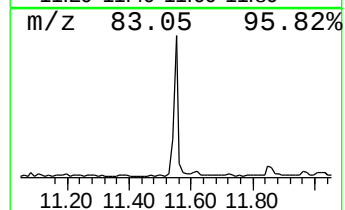
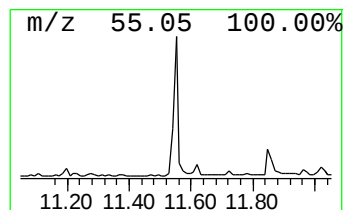
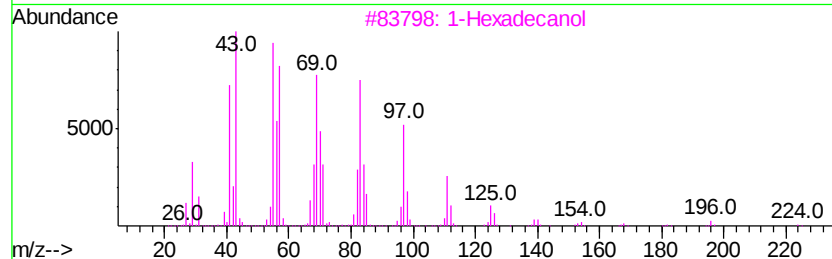
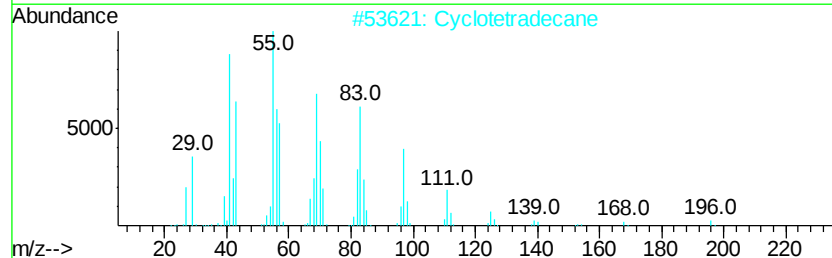
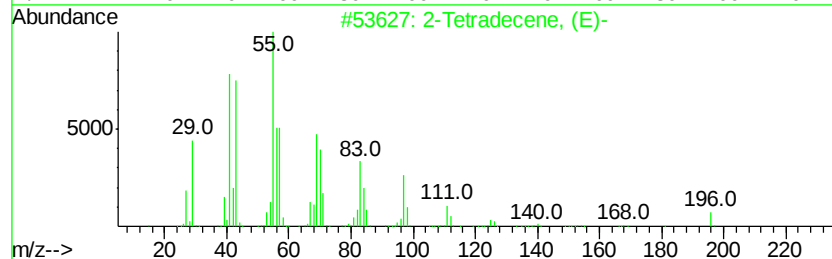
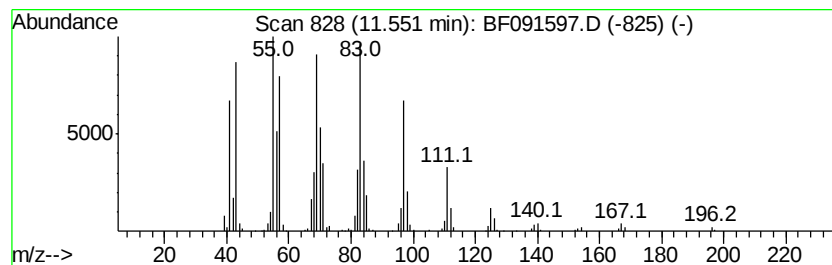
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Tetradecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.55	6.41 ng	795253	Phenanthrene-d10	11.31	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tetradecene, (E)-	196	C14H28	035953-53-8	97
2	Cyclotetradecane	196	C14H28	000295-17-0	96
3	1-Hexadecanol	242	C16H34O	036653-82-4	94
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	1-Pentadecanol	228	C15H32O	000629-76-5	91



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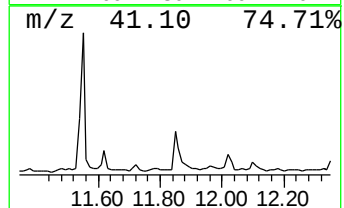
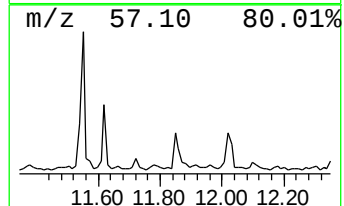
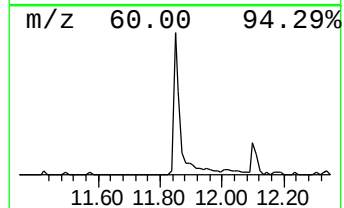
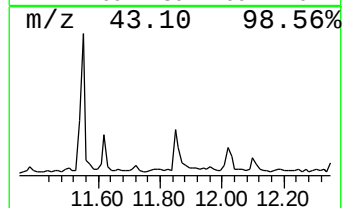
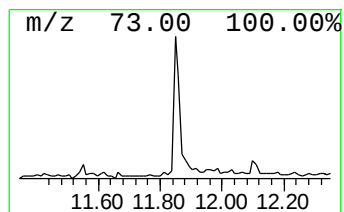
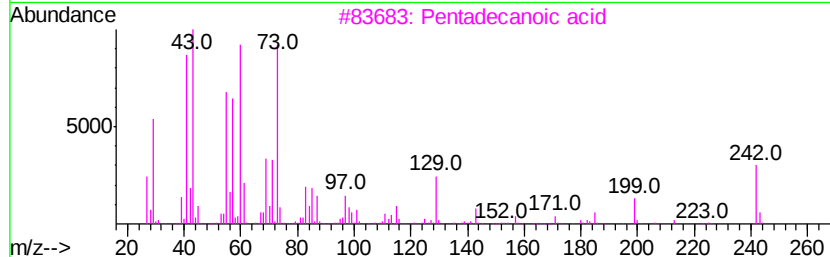
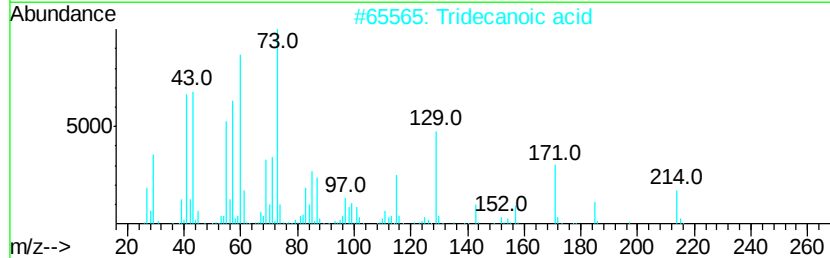
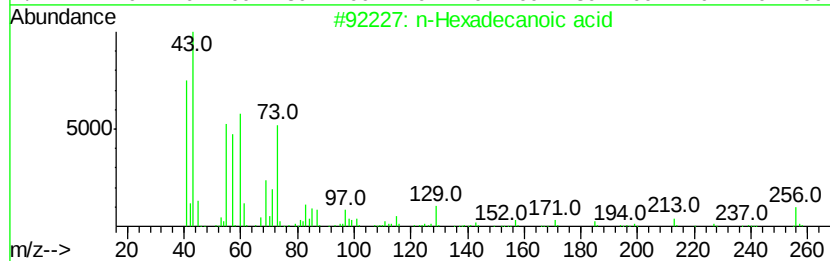
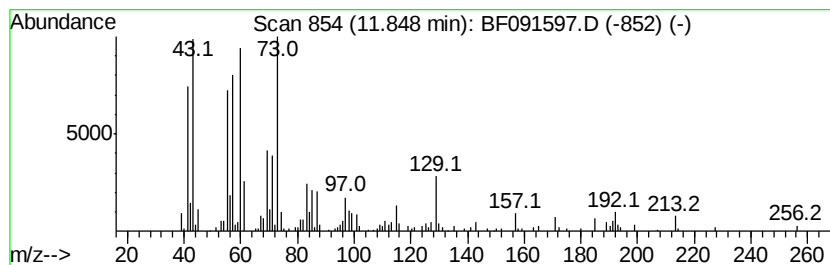
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	2.30 ng	285550	Phenanthrene-d10		11.31
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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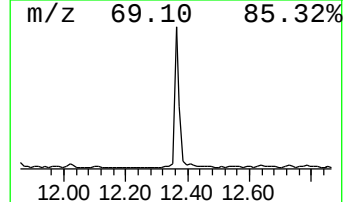
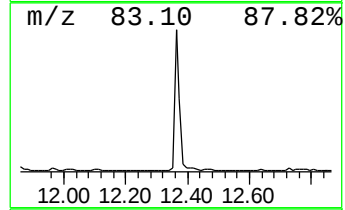
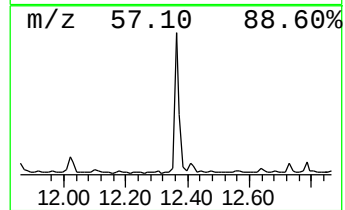
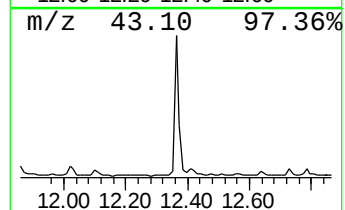
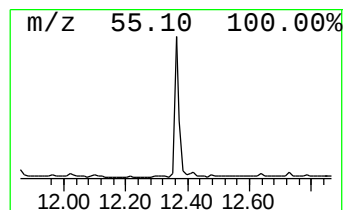
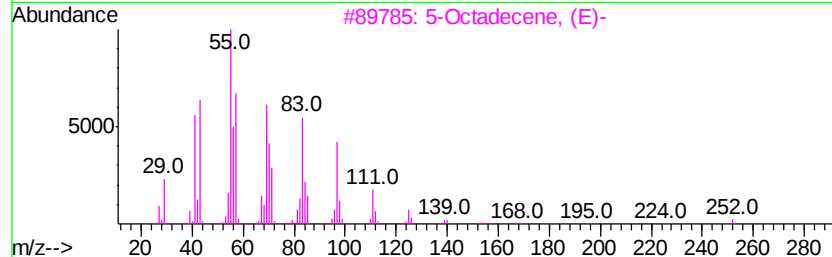
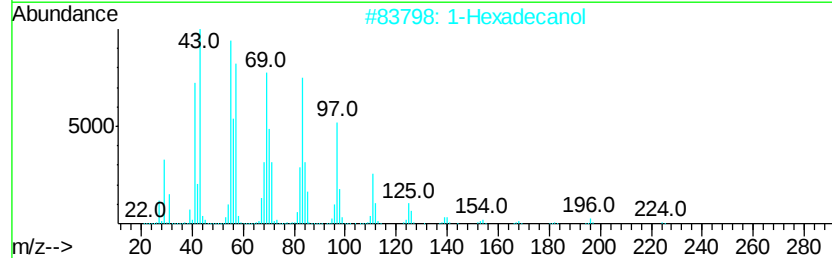
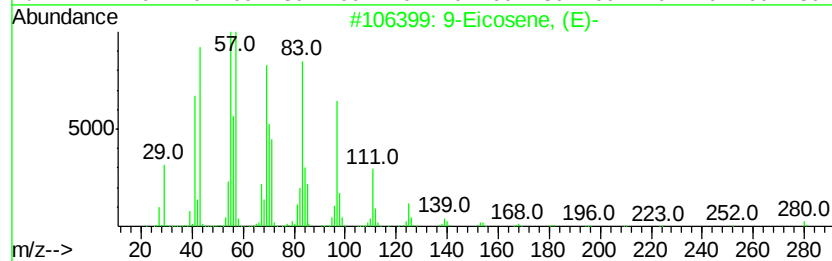
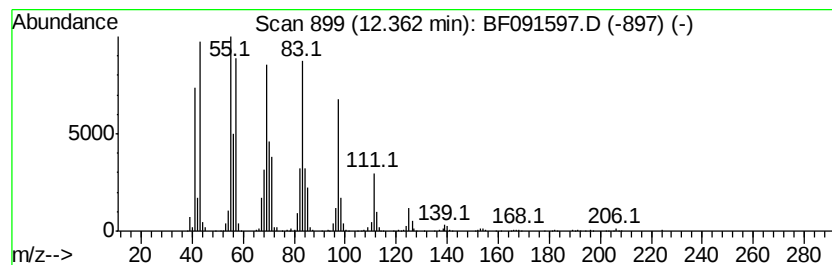
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TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	14.44 ng	1792540	Phenanthrene-d10	11.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Eicosene, (E)-	280	C20H40	074685-29-3	94
2		1-Hexadecanol	242	C16H34O	036653-82-4	94
3		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091597.D
Acq On : 14 Dec 2016 21:13
Operator : UM/SJ
Sample : H6006-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-13-10-15

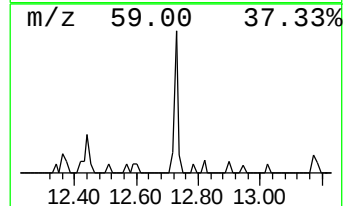
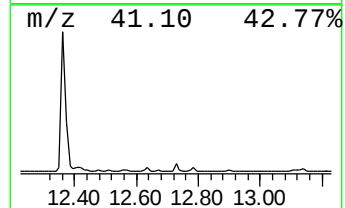
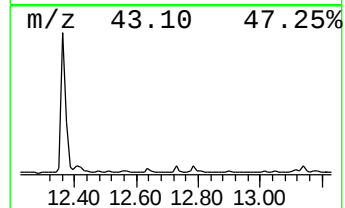
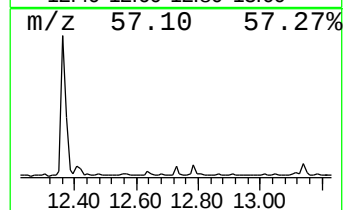
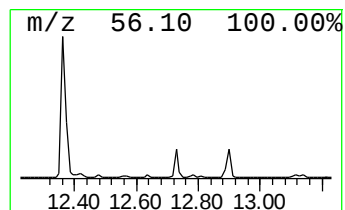
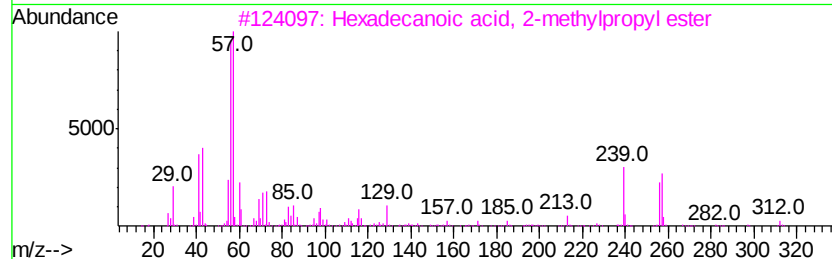
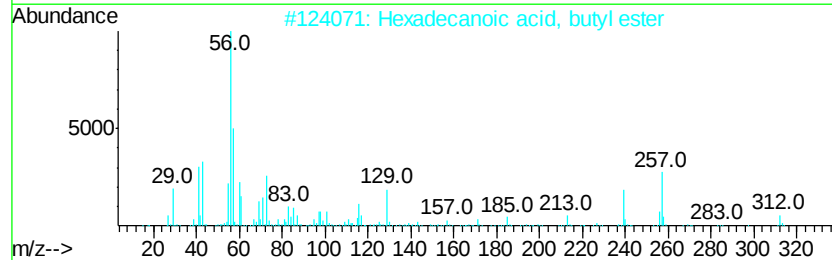
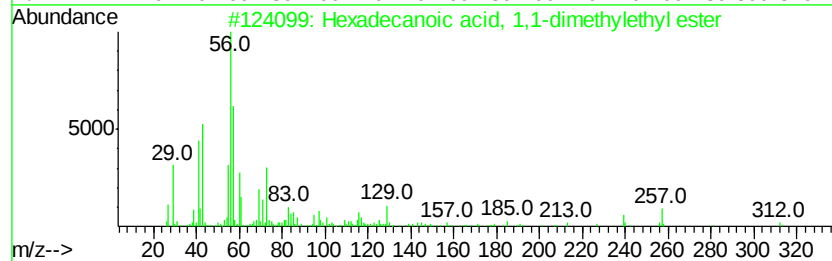
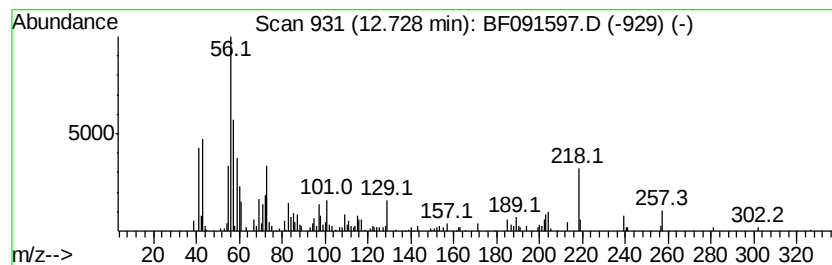
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.47 ng	238601	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	70
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	40
4		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
Data File : BF091597.D
Acq On : 14 Dec 2016 21:13
Operator : UM/SJ
Sample : H6006-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-13-10-15

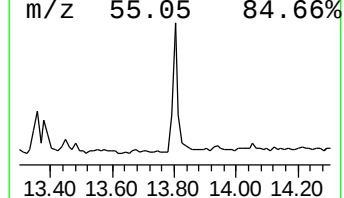
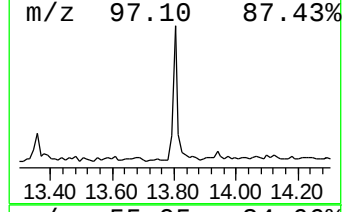
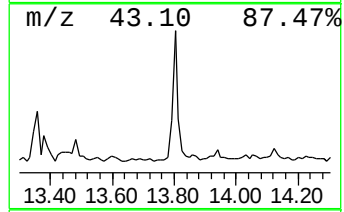
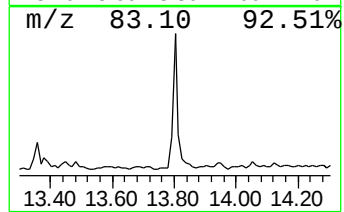
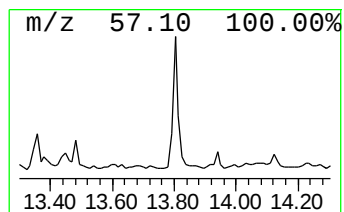
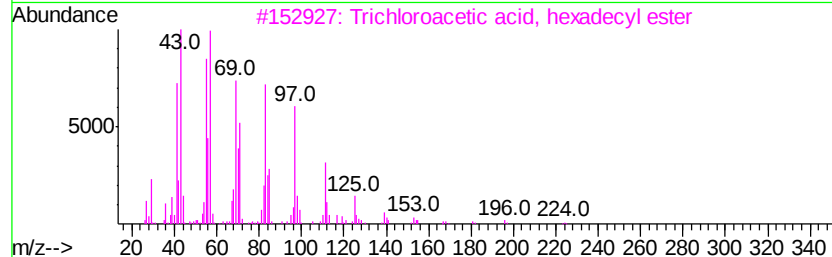
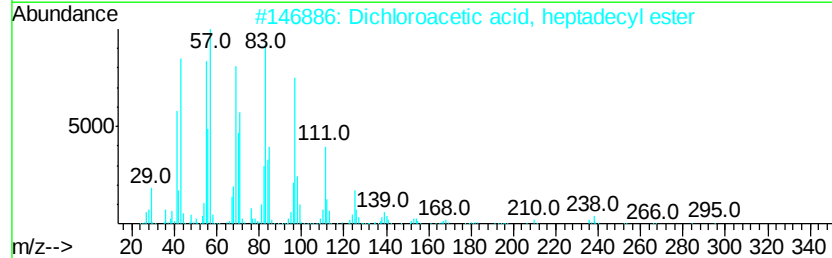
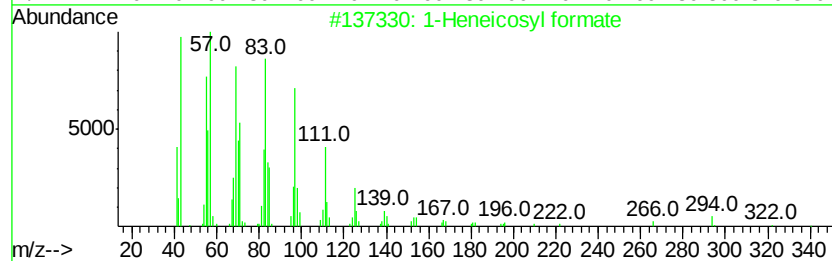
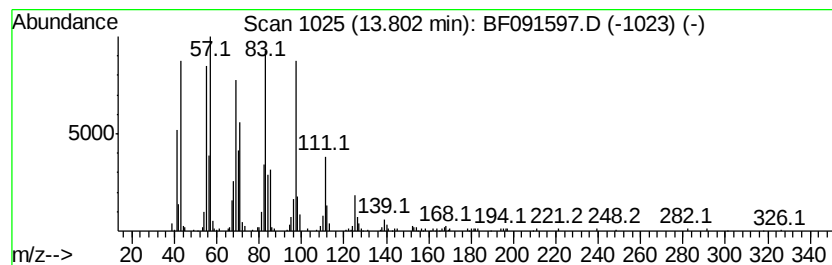
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	4.43 ng	427598	Chrysene-d12	13.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091597.D
Acq On : 14 Dec 2016 21:13
Operator : UM/SJ
Sample : H6006-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

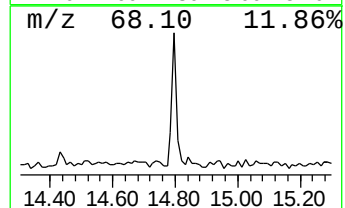
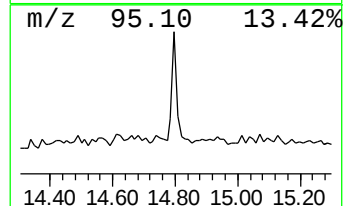
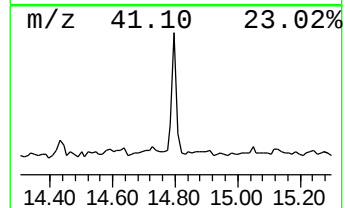
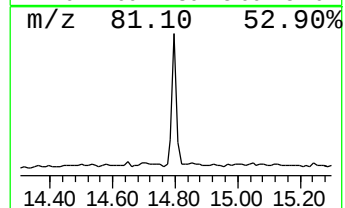
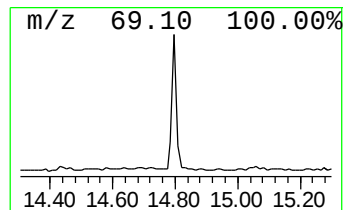
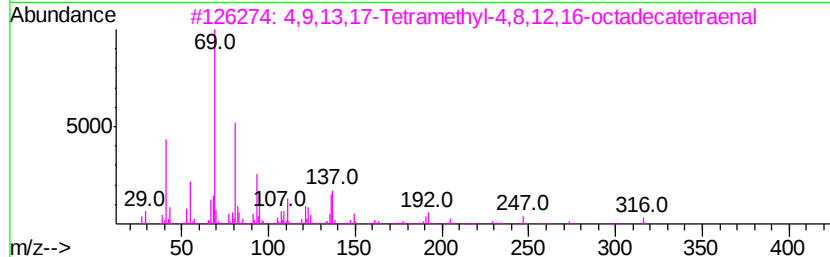
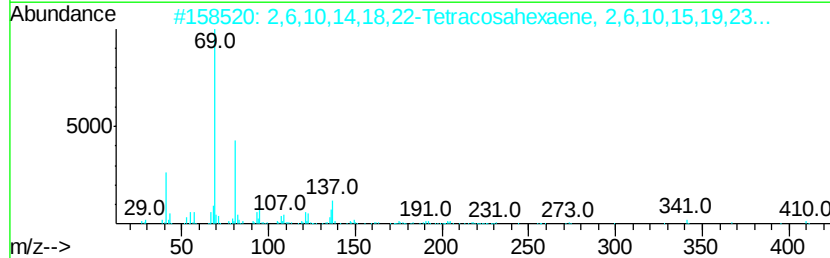
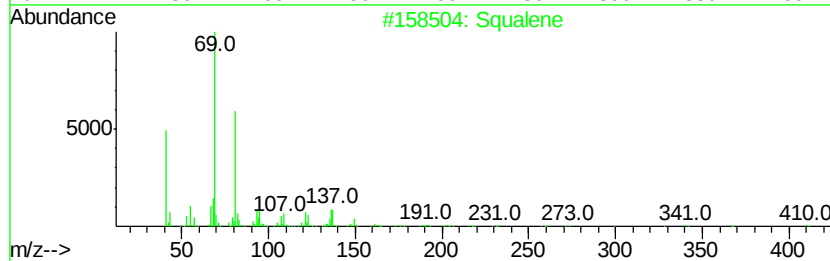
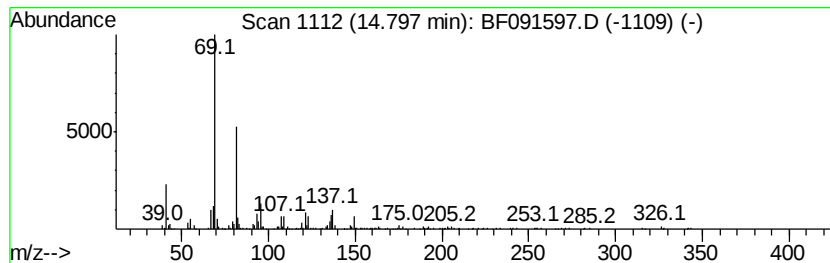
Instrument :
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ClientSampleId :
WC-13-10-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.29 ng	278532	Perylene-d12	15.36
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	4,9,13,17-Tetramethyl-4,8,12,16-...		316 C22H360	056882-09-8 83
4	1,5,9-Decatriene, 2,3,5,8-tetram...		192 C14H24	230646-72-7 72
5	2,6,10,14-Hexadecatetraenoic aci...		332 C22H3602	024035-35-6 64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091597.D
Acq On : 14 Dec 2016 21:13
Operator : UM/SJ
Sample : H6006-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC-13-10-15

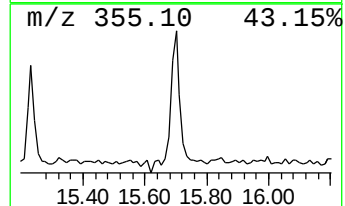
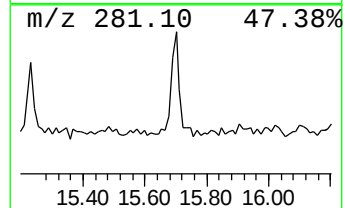
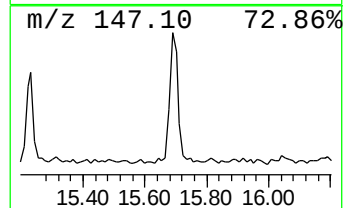
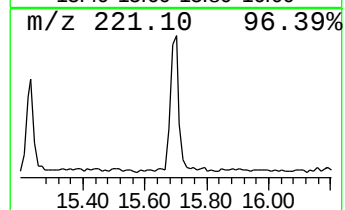
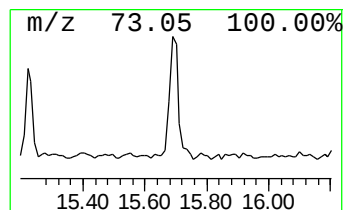
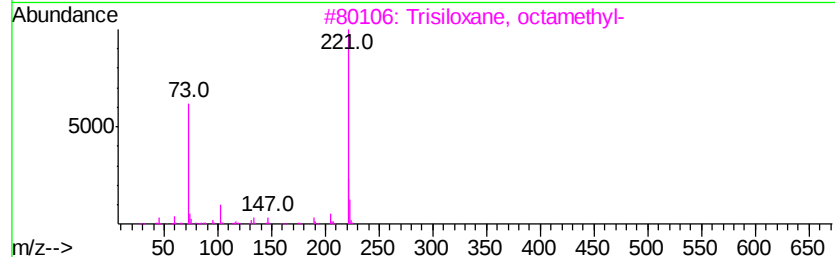
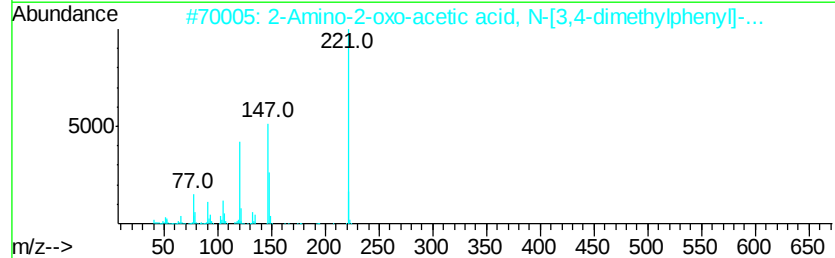
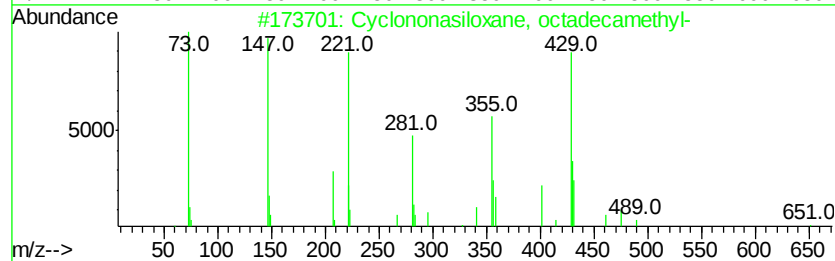
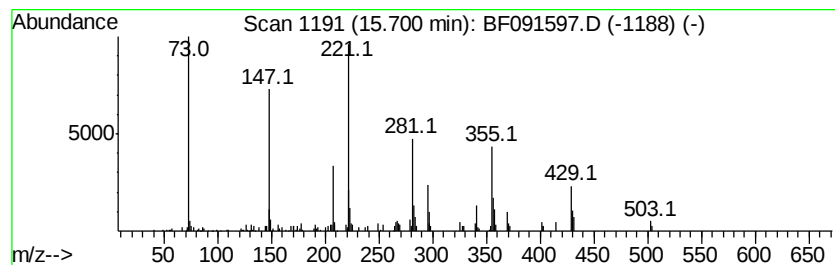
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.70 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.31 ng	194973	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	49
2		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15N03	024451-17-0	32
3		Trisiloxane, octamethyl-	236	C8H2402Si3	000107-51-7	27
4		Tris(trimethylsilyl)borate	278	C9H27B03Si3	004325-85-3	27
5		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091597.D
Acq On : 14 Dec 2016 21:13
Operator : UM/SJ
Sample : H6006-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-13-10-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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
2-Pentanone, 4-hy...	4.97	30.4	ng	2794270	1	6.80	1839250	20.0
unknown6.57	6.57	86.1	ng	7918890	1	6.80	1839250	20.0
2-Tetradecene, (E)-	11.55	6.4	ng	795253	4	11.31	2482830	20.0
n-Hexadecanoic acid	11.85	2.3	ng	285550	4	11.31	2482830	20.0
9-Eicosene, (E)-	12.36	14.4	ng	1792540	4	11.31	2482830	20.0
Hexadecanoic acid...	12.73	2.5	ng	238601	5	13.94	1931330	20.0
1-Heneicosyl formate	13.80	4.4	ng	427598	5	13.94	1931330	20.0
Squalene	14.80	3.3	ng	278532	6	15.36	1691430	20.0
unknown15.70	15.70	2.3	ng	194973	6	15.36	1691430	20.0