

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
 Data File : BF084643.D
 Acq On : 29 Jan 2016 18:32
 Operator : SJ/IZ
 Sample : H1272-13
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B014(45-47)

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-BF012916.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	4.190	182	184	195	rVB	250232	316570	5.63%	0.622%
2	4.887	241	245	248	rBV	2198348	3947152	70.21%	7.753%
3	5.321	281	283	286	rBV	3949520	4674111	83.15%	9.181%
4	5.721	316	318	321	rVB	213987	226996	4.04%	0.446%
5	6.373	372	375	377	rBV	4726166	4888900	86.97%	9.603%
6	6.499	383	386	388	rBV	3724616	5048059	89.80%	9.916%
7	6.727	403	406	408	rBV	904874	1120624	19.93%	2.201%
8	6.876	417	419	422	rBV	3652993	3537083	62.92%	6.948%
9	7.287	452	455	458	rBV	2605349	2942404	52.34%	5.780%
10	8.007	516	518	520	rBV	1787000	1534348	27.29%	3.014%
11	9.093	610	613	615	rBV	4967864	5621536	100.00%	11.042%
12	9.482	645	647	649	rBV	616771	622270	11.07%	1.222%
13	9.699	664	666	669	rBV	64073	81577	1.45%	0.160%
14	9.756	669	671	674	rVV	1551079	1629317	28.98%	3.200%
15	10.202	708	710	712	rVB	175278	141816	2.52%	0.279%
16	10.419	726	729	732	rBV	49487	85211	1.52%	0.167%
17	10.545	738	740	743	rBV	3278095	3499694	62.26%	6.874%
18	10.670	750	751	758	rVB	163348	225839	4.02%	0.444%
19	11.116	789	790	792	rBV	66140	82635	1.47%	0.162%
20	11.242	798	801	803	rBV	1713536	1721298	30.62%	3.381%
21	12.031	868	870	873	rVB	56891	57930	1.03%	0.114%
22	12.831	937	940	942	rBV	5292098	5246298	93.32%	10.305%
23	13.756	1017	1021	1027	rBV2	81319	269118	4.79%	0.529%
24	13.871	1029	1031	1033	rVB	1900458	1738700	30.93%	3.415%
25	14.625	1095	1097	1103	rBV4	45894	75589	1.34%	0.148%
26	14.717	1103	1105	1108	rVV	209536	195591	3.48%	0.384%
27	15.254	1149	1152	1155	rBV	1210825	1378260	24.52%	2.707%

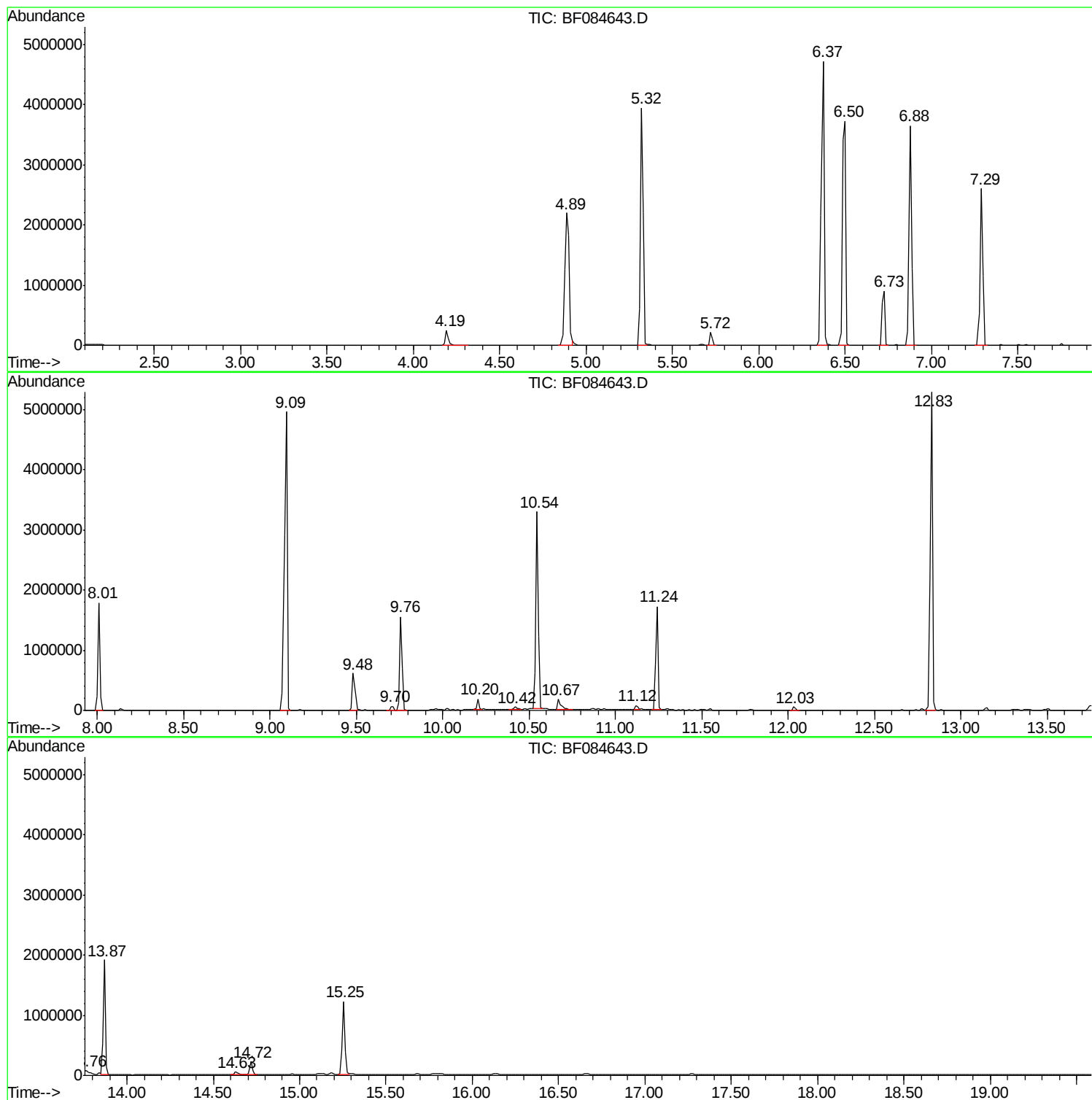
Sum of corrected areas: 50908926

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

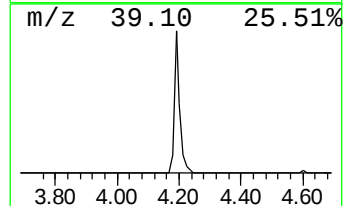
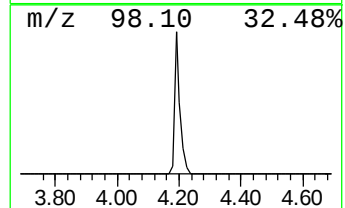
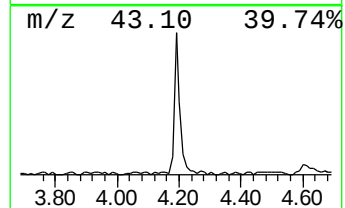
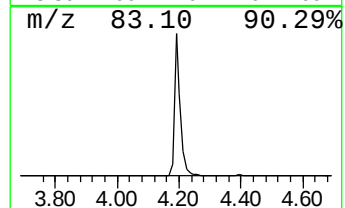
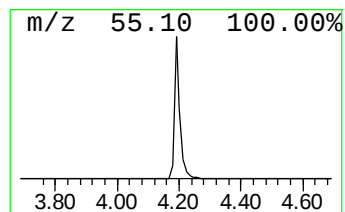
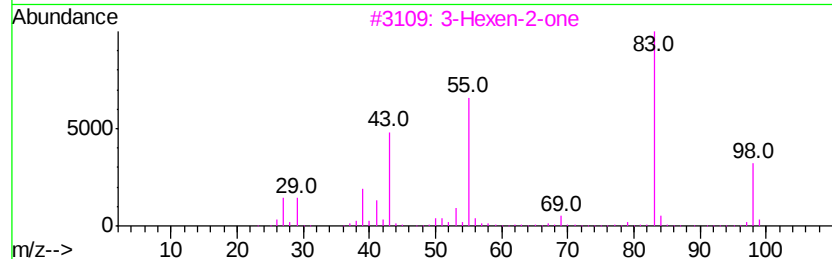
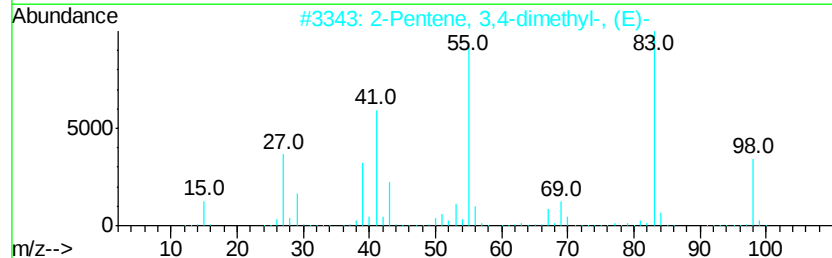
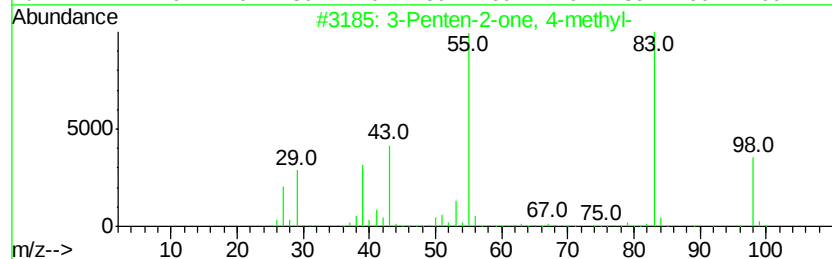
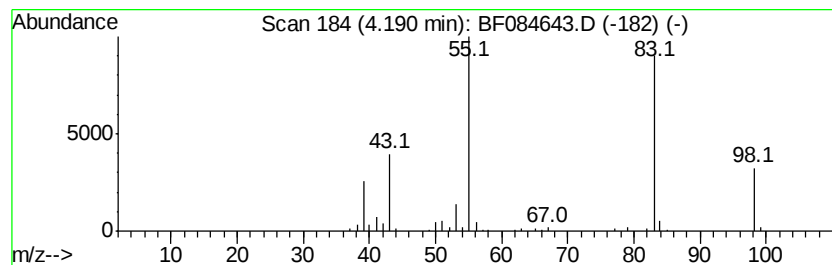
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	5.65 ng	316570	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3			3-Hexen-2-one	98	C6H10O	000763-93-9	87
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

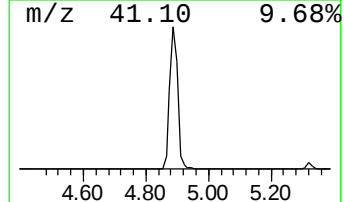
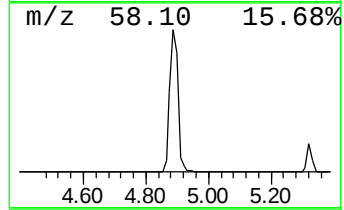
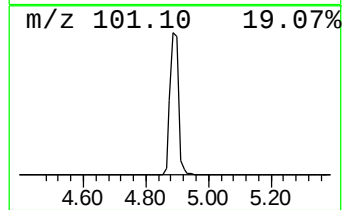
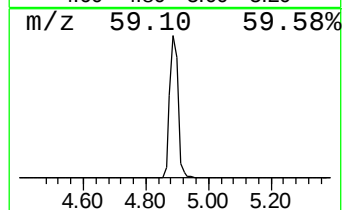
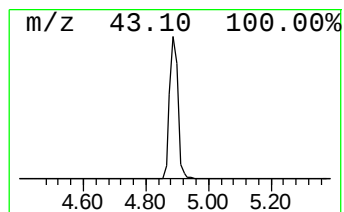
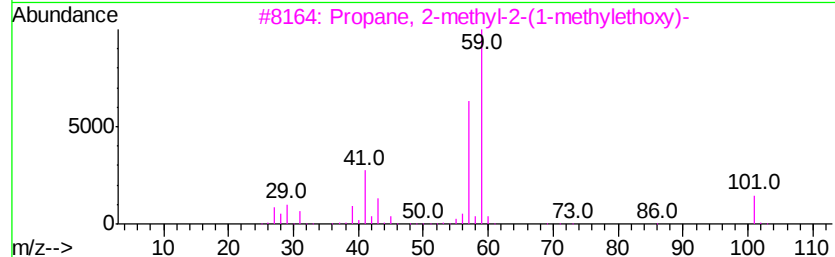
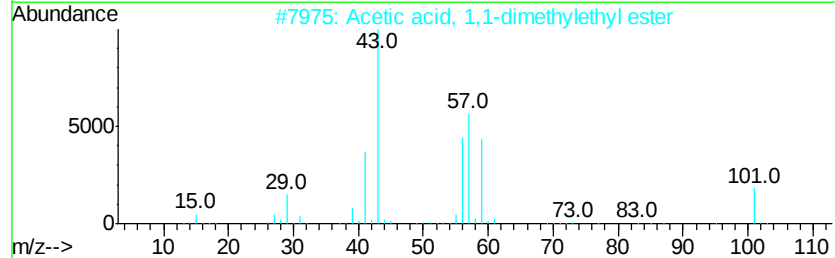
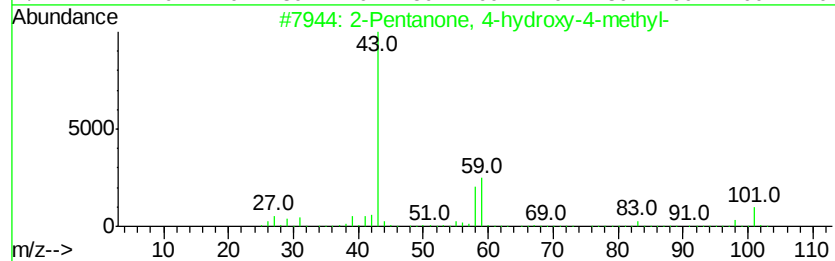
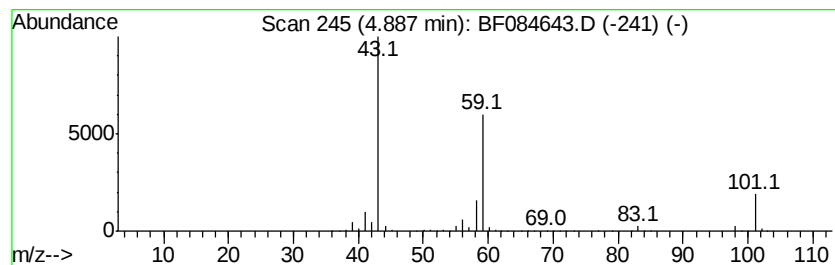
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	70.45 ng	3947150	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

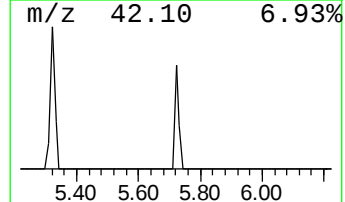
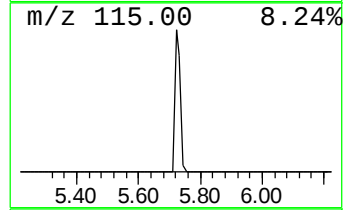
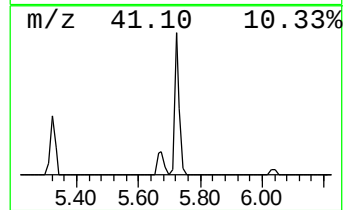
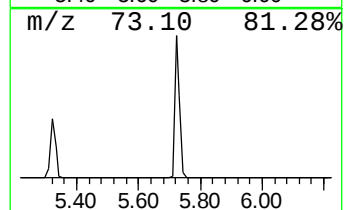
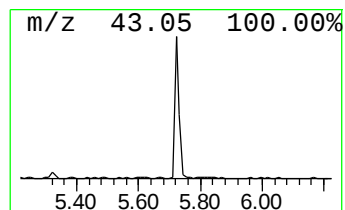
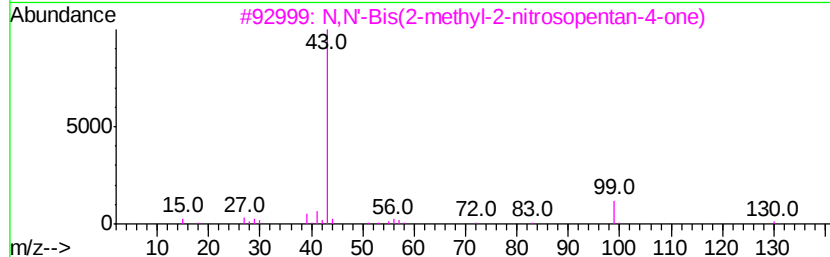
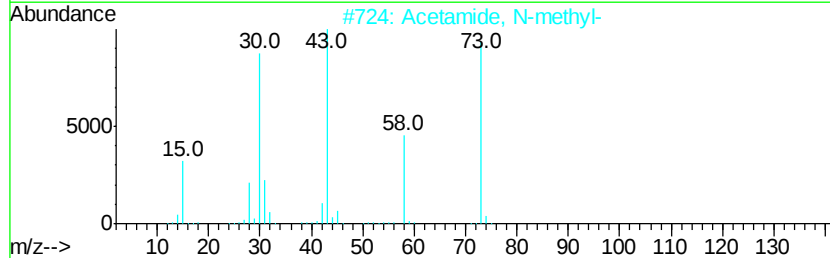
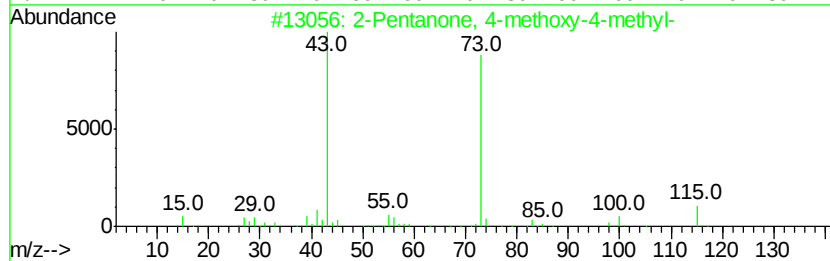
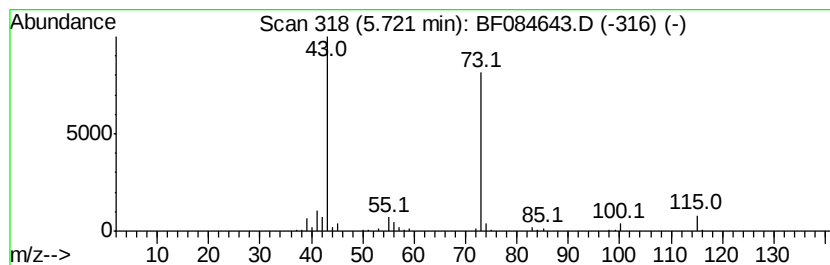
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	4.05 ng	226996	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12
4		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
5		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

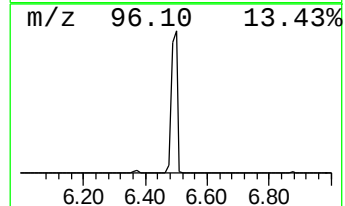
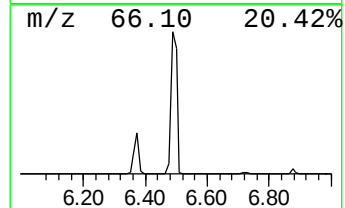
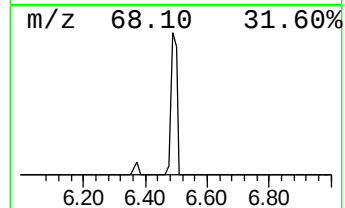
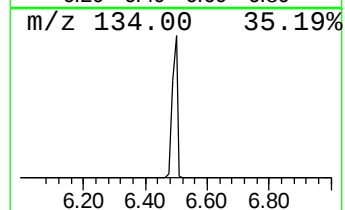
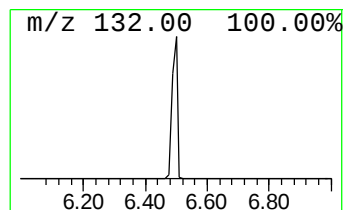
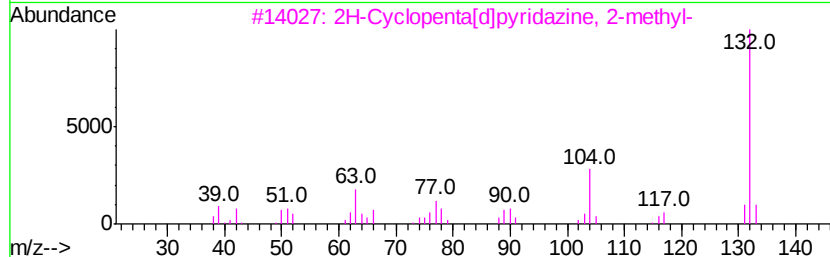
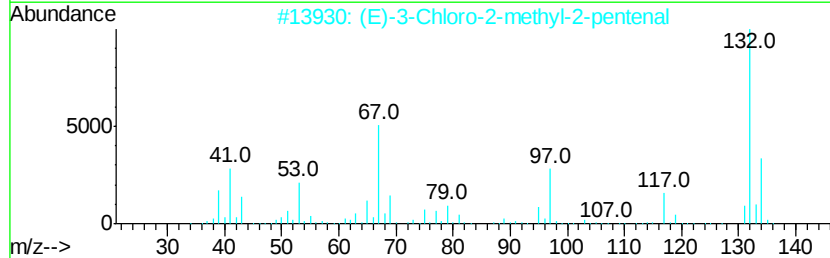
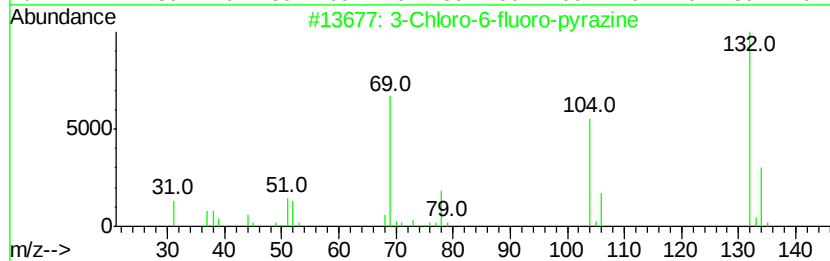
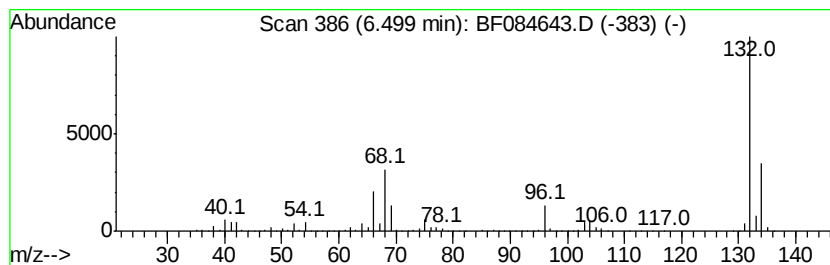
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	90.09 ng	5048060	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		Xenon	132	Xe	007440-63-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

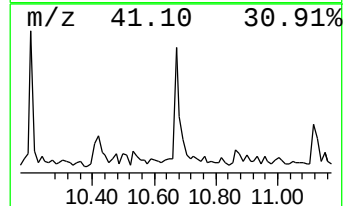
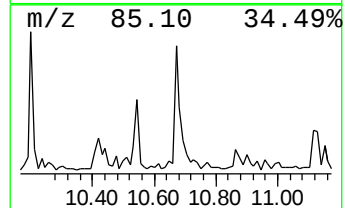
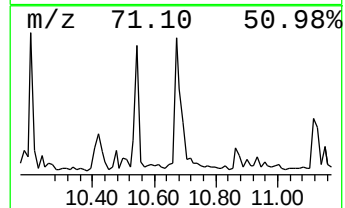
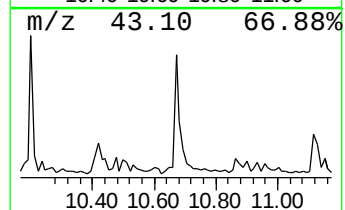
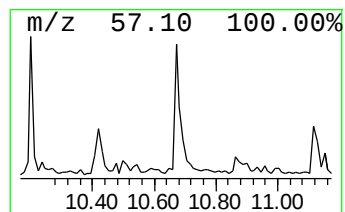
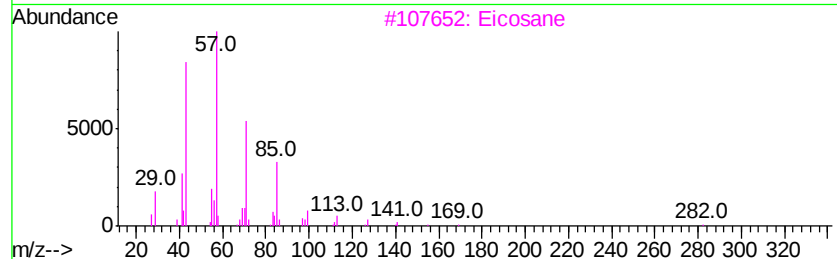
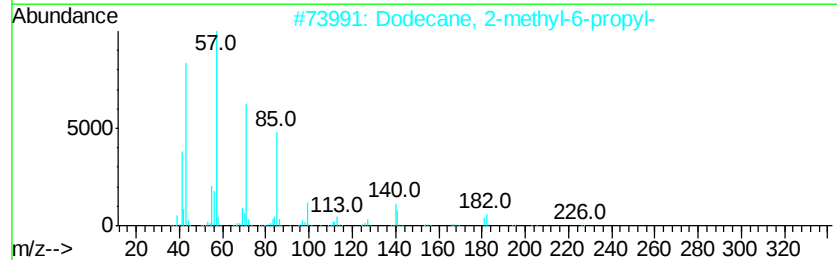
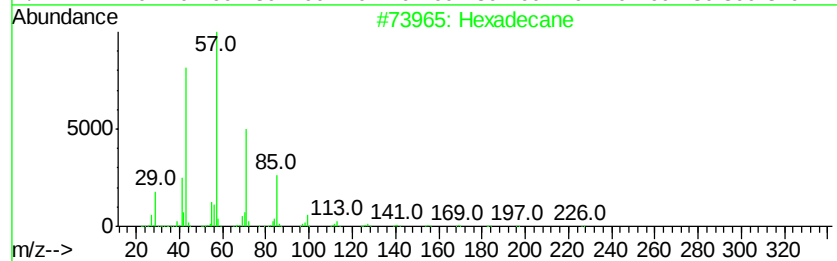
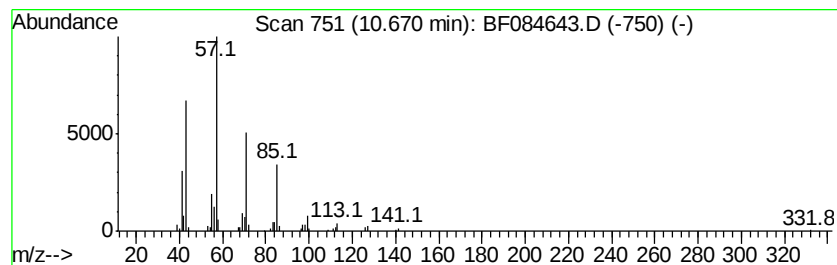
Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.67	2.62 ng	225839	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
3	Eicosane	282	C20H42	000112-95-8	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tridecane	184	C13H28	000629-50-5	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

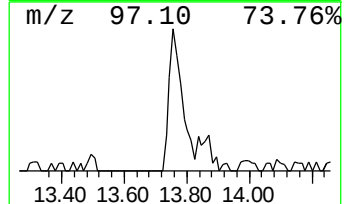
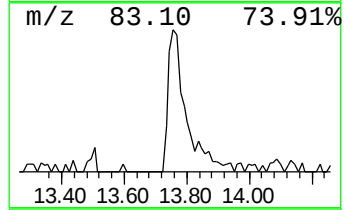
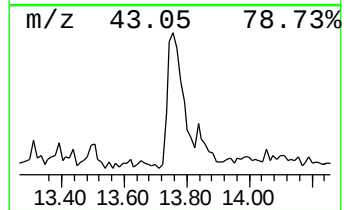
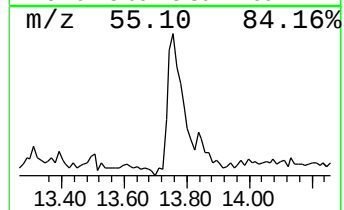
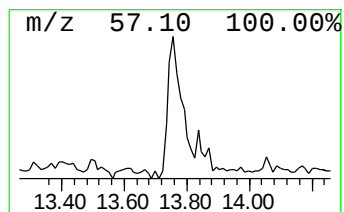
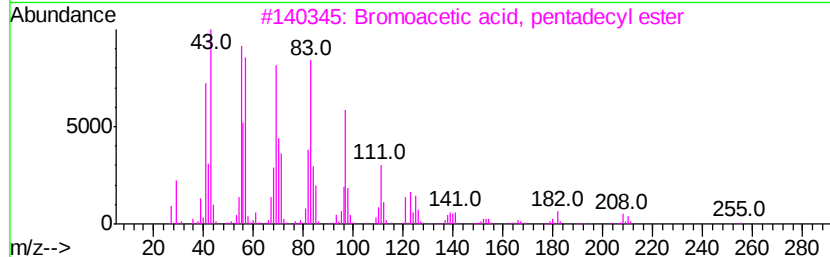
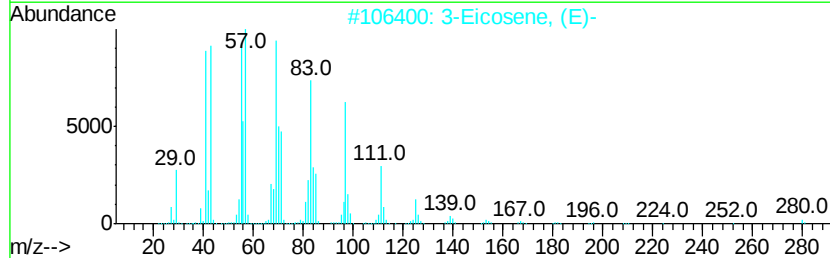
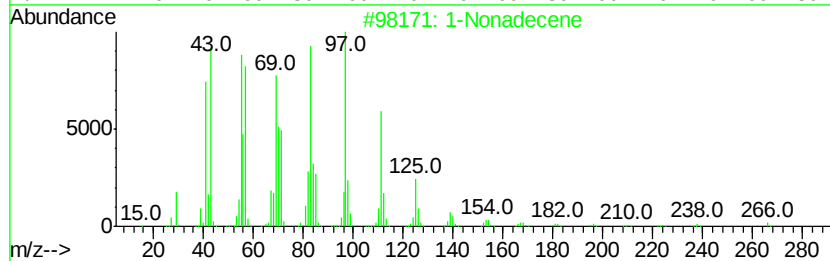
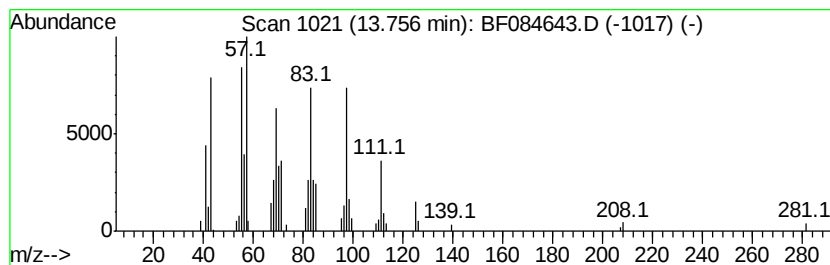
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	3.10 ng	269118	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonadecene	266	C19H38	018435-45-5	87
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	81
3		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	81
4		1-Octadecanol	270	C18H38O	000112-92-5	81
5		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

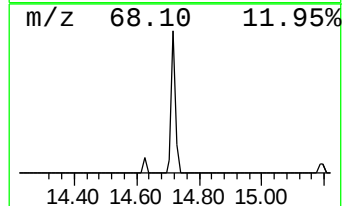
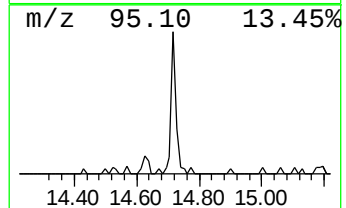
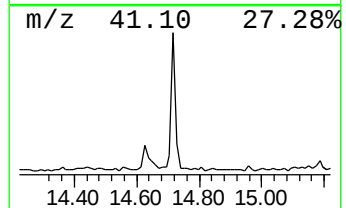
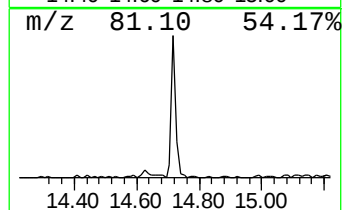
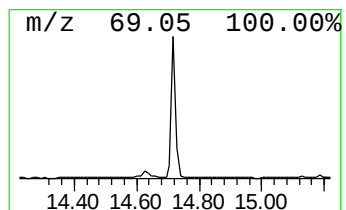
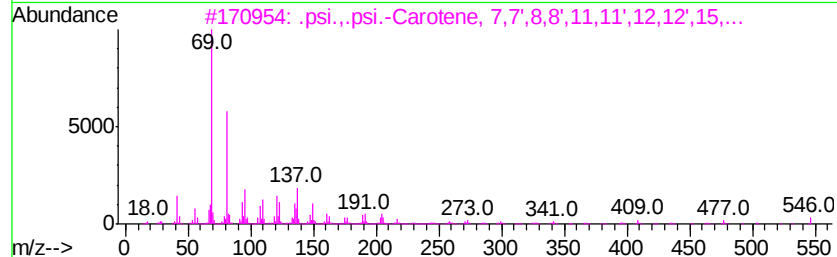
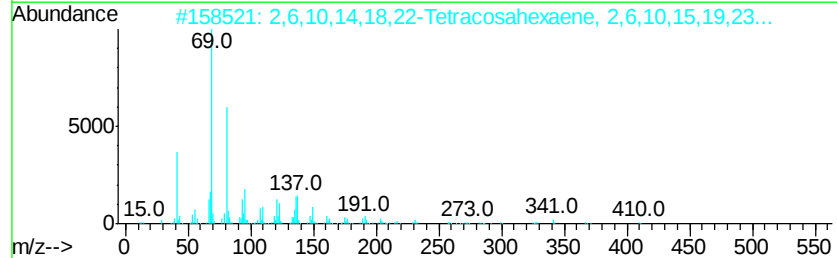
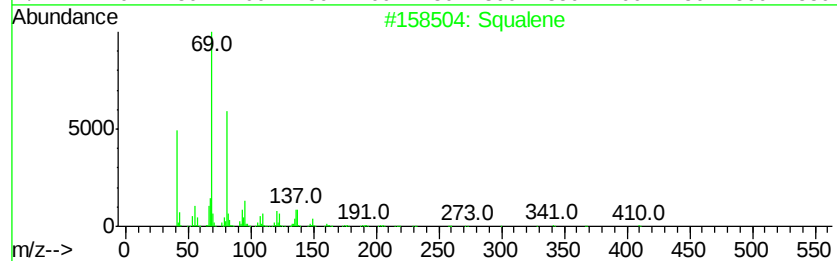
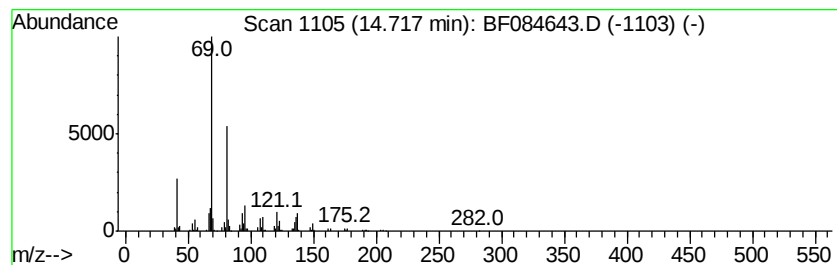
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.84 ng	195591	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	78
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084643.D
Acq On : 29 Jan 2016 18:32
Operator : SJ/IZ
Sample : H1272-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B014(45-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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
3-Penten-2-one, 4...	4.19	5.7	ng	316570	1	6.73	1120620	20.0
2-Pentanone, 4-hy...	4.89	70.5	ng	3947150	1	6.73	1120620	20.0
2-Pentanone, 4-me...	5.72	4.0	ng	226996	1	6.73	1120620	20.0
unknown6.50	6.50	90.1	ng	5048060	1	6.73	1120620	20.0
Hexadecane	10.67	2.6	ng	225839	4	11.24	1721300	20.0
1-Nonadecene	13.76	3.1	ng	269118	5	13.87	1738700	20.0
Squalene	14.72	2.8	ng	195591	6	15.25	1378260	20.0