LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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	181	184	190	rBV	222706	297560	5.74%	0.597%
2	4.887	241	245	253	rBV	2406120	4041926	78.03%	8.109%
3	5.321	280	283	286	rBV	4300391	4626016	89.31%	9.281%
4	5.721	316	318	321	rBV	249656	236820	4.57%	0.475%
5	5.984	339	341	343	rVB	350004	293681	5.67%	0.589%
6	6.373	372	375	377	rBV	4646094	4968747	95.92%	9.969%
7	6.487	383	385	388	rBV	3649790	5179831	100.00%	10.392%
8	6.727	403	406	408	rBV	782356	1075144	20.76%	2.157%
9	6.876	417	419	422	rVB	3546004	3329179	64.27%	6.679%
10	7.287	452	455	458	rBV	2577731	2982528	57.58%	5.984%
11	8.007	516	518	520	rBV	1742810	1507802	29.11%	3.025%
12	8.042	520	521	523	rVB	88089	62287	1.20%	0.125%
13	8.750	582	583	586	rBV	56687	73997	1.43%	0.148%
14	9.093	610	613	615	rBV	4526604	5146642	99.36%	10.326%
15	9.482	645	647	649	rBV	545520	510780	9.86%	1.025%
16	9.699	664	666	669	rBV	72721	90934	1.76%	0.182%
17	9.756	669	671	673	rBV	1597206	1549292	29.91%	3.108%
18	10.202	708	710	712	rVB	165930	135393	2.61%	0.272%
19	10.419	727	729	732	rBV	49613	79094	1.53%	0.159%
20	10.545	737	740	743	rVV	3356698	3481815	67.22%	6.986%
21	10.671	750	751	756	rBV	148290	172646	3.33%	0.346%
22	11.116	789	790	795	rVB	48376	68921	1.33%	0.138%
23	11.242	798	801	802	rBV	1461111	1592900	30.75%	3.196%
24	11.791	846	849	850	rBV2	128561	163874	3.16%	0.329%
25	12.031	868	870	876	rBV2	50209	69669	1.35%	0.140%
26	12.442	904	906	908	rBV	92103	85780	1.66%	0.172%
27	12.659	923	925	928	rBV2	274396	291970	5.64%	0.586%
28	12.831	937	940	942	rBV	3476010	4233637	81.73%	8.494%
29	13.368	985	987	988	rBV	104874	138069	2.67%	0.277%
30	13.757	1018	1021	1028	rBV	251375	714734	13.80%	1.434%
31	13.871	1028	1031	1033	rBV	1120065	1295383	25.01%	2.599%
32	14.625	1095	1097	1103	rBV2	74734	142902	2.76%	0.287%
33	14.717	1103	1105	1107	rVB	142079	136682	2.64%	0.274%
34	15.254	1149	1152	1161	rVB	751053	1000133	19.31%	2.007%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

35	16.260	1238	1240	1244	rVB3	37095	65785	1.27%	0.132%

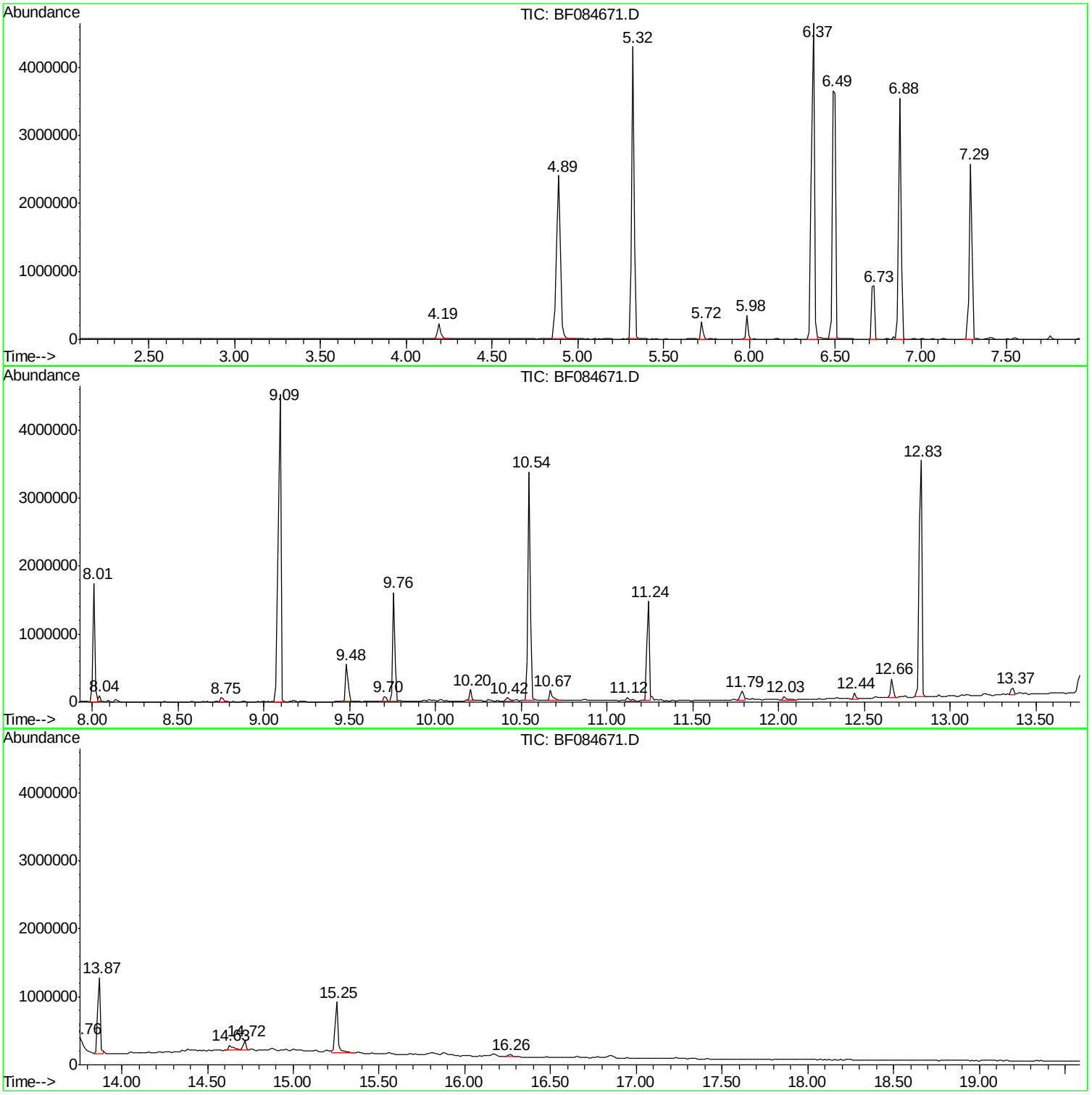
Sum of corrected areas: 49842553

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B011(25-27)

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
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Sample : H1273-10
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ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

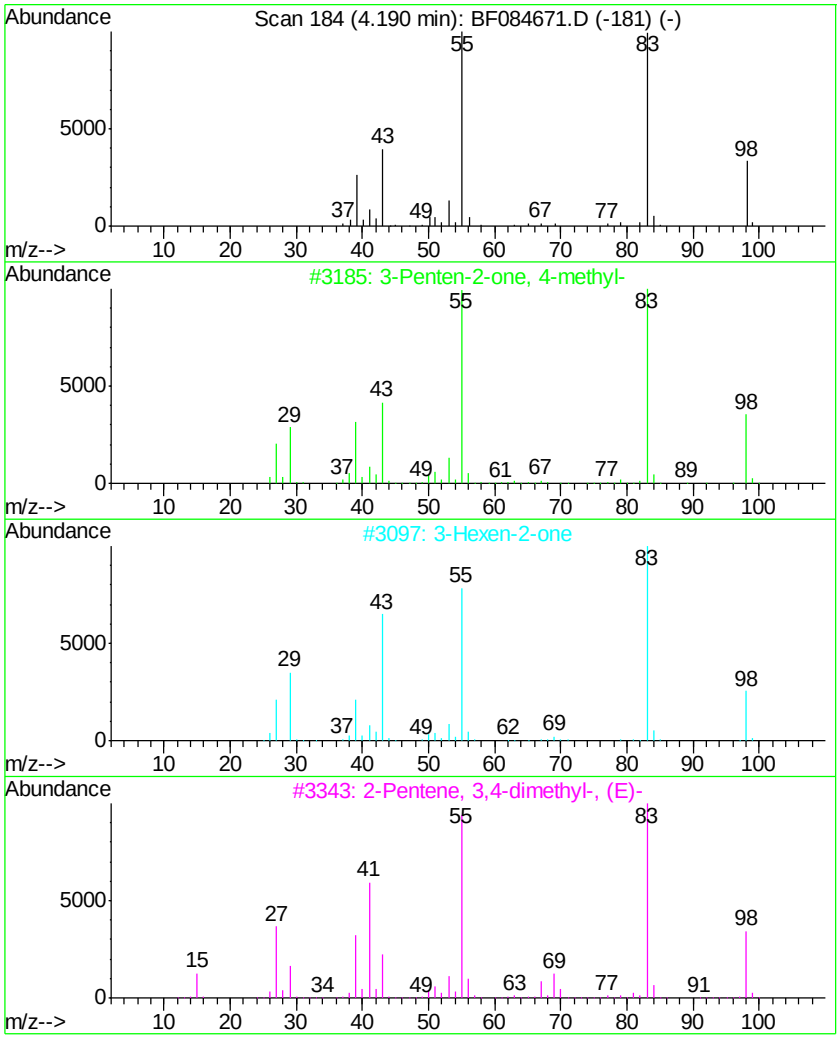
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

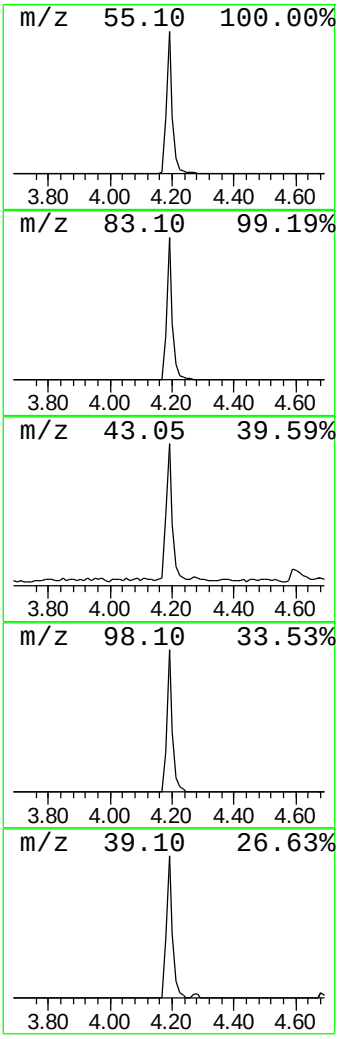
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	5.54 ng	297560	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	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

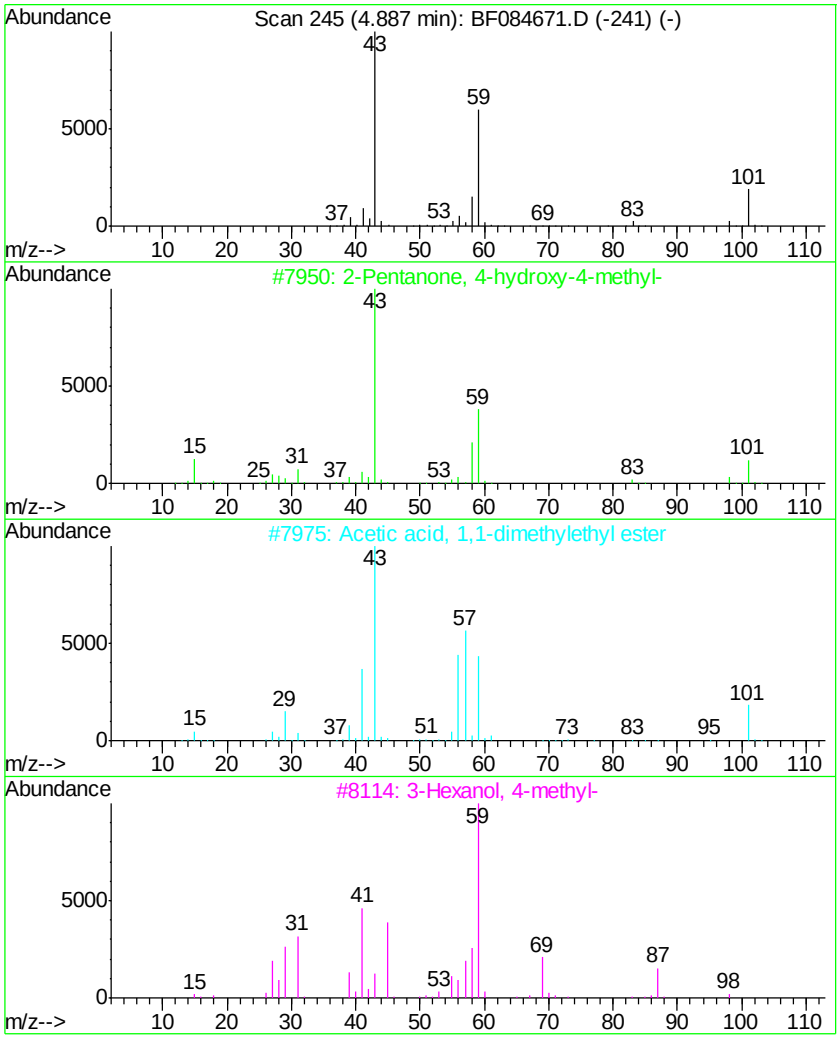
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

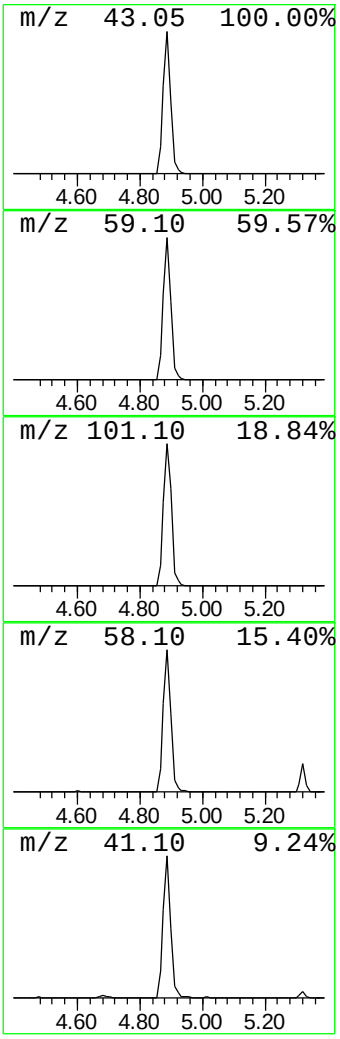
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	75.19 ng	4041930	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

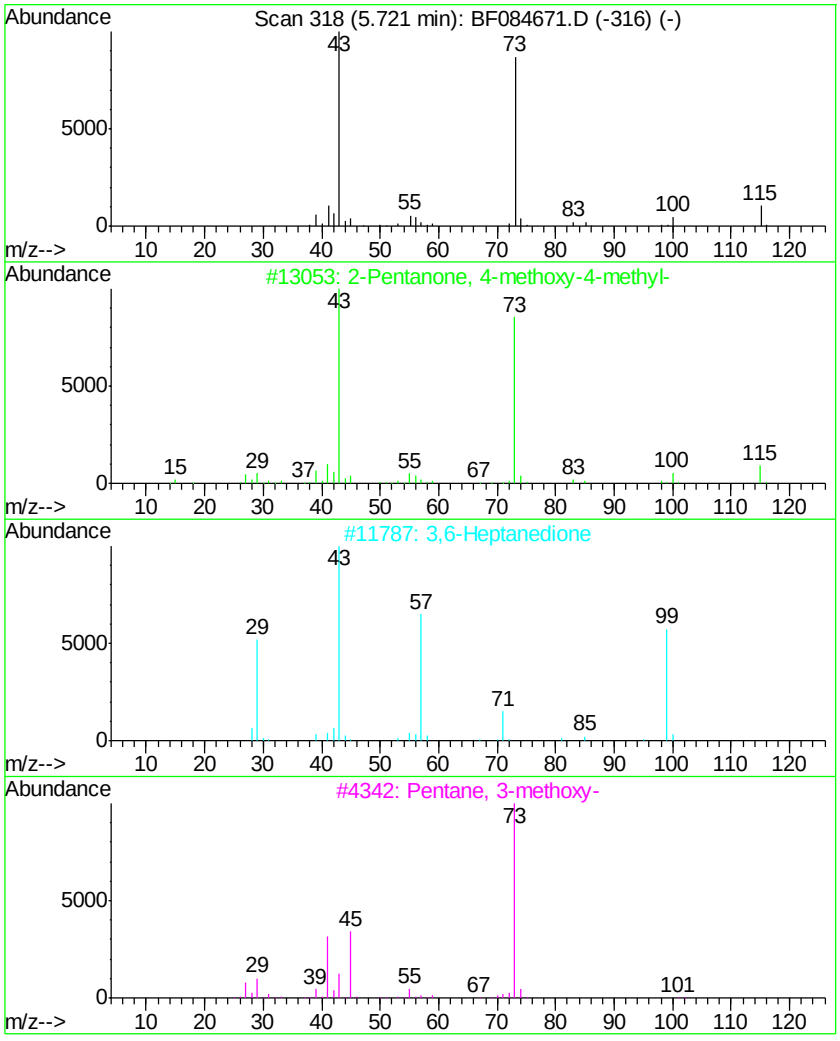
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

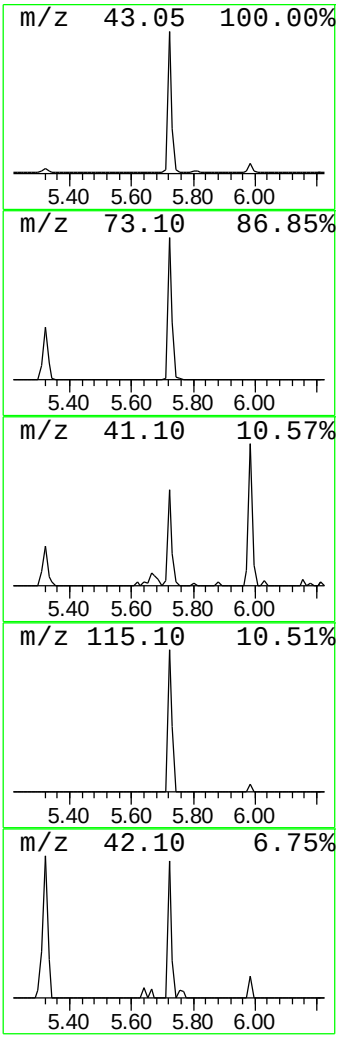
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	4.41 ng	236820	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2	3,6-Heptanedione	128	C7H12O2	001703-51-1	23
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

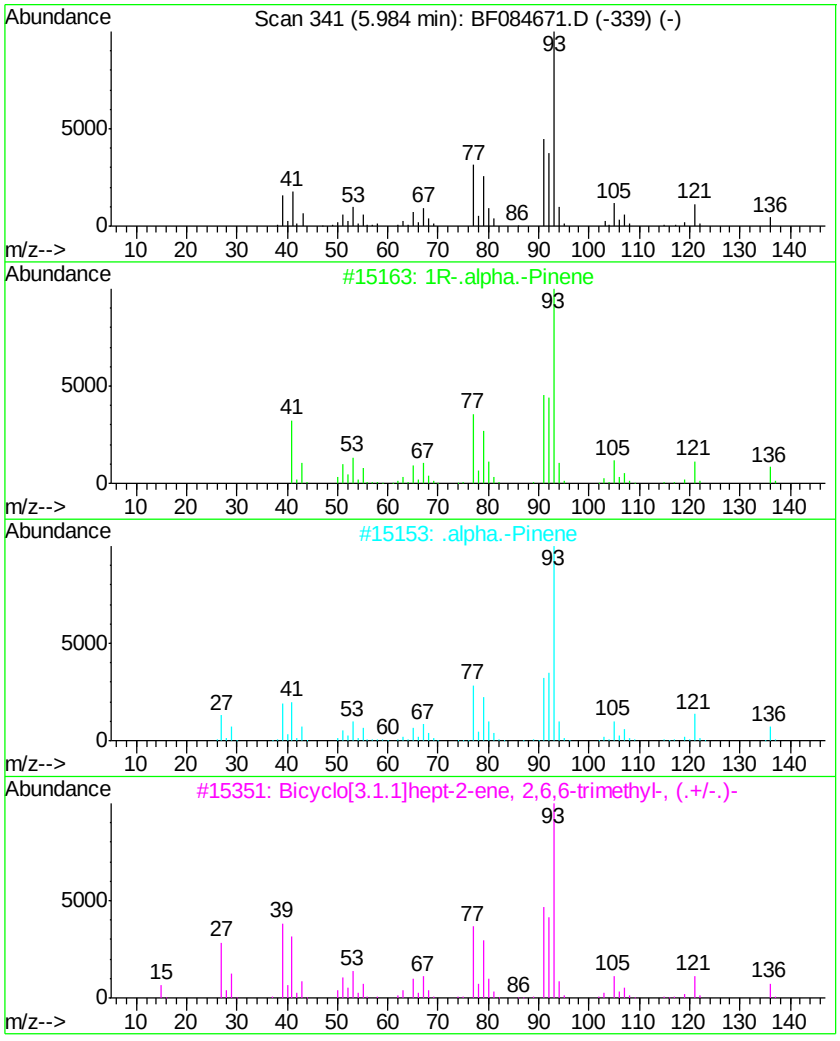
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

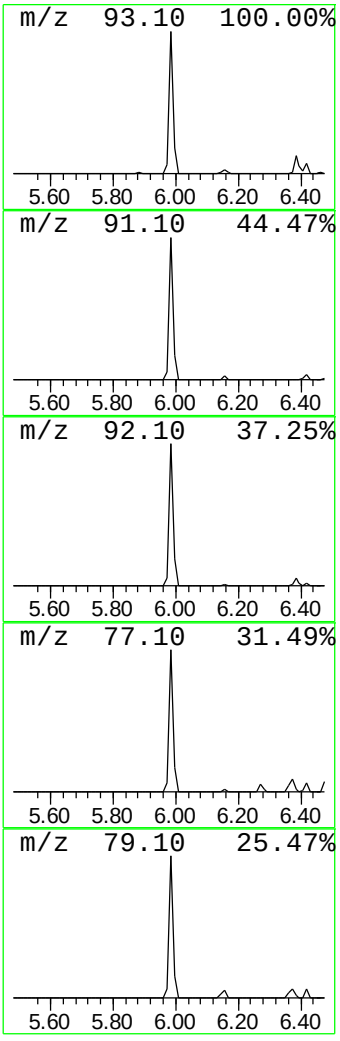
****

Peak Number 4 1R-.alpha.-Pinene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.98	5.46 ng	293681	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1R-.alpha.-Pinene	136	C10H16	007785-70-8	95
2	.alpha.-Pinene	136	C10H16	000080-56-8	95
3	Bicyclo[3.1.1]hept-2-ene, 2,6,6-...	136	C10H16	002437-95-8	94
4	Bicyclo[4.1.0]hept-3-ene, 3,7,7-...	136	C10H16	000498-15-7	91
5	3-Carene	136	C10H16	013466-78-9	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

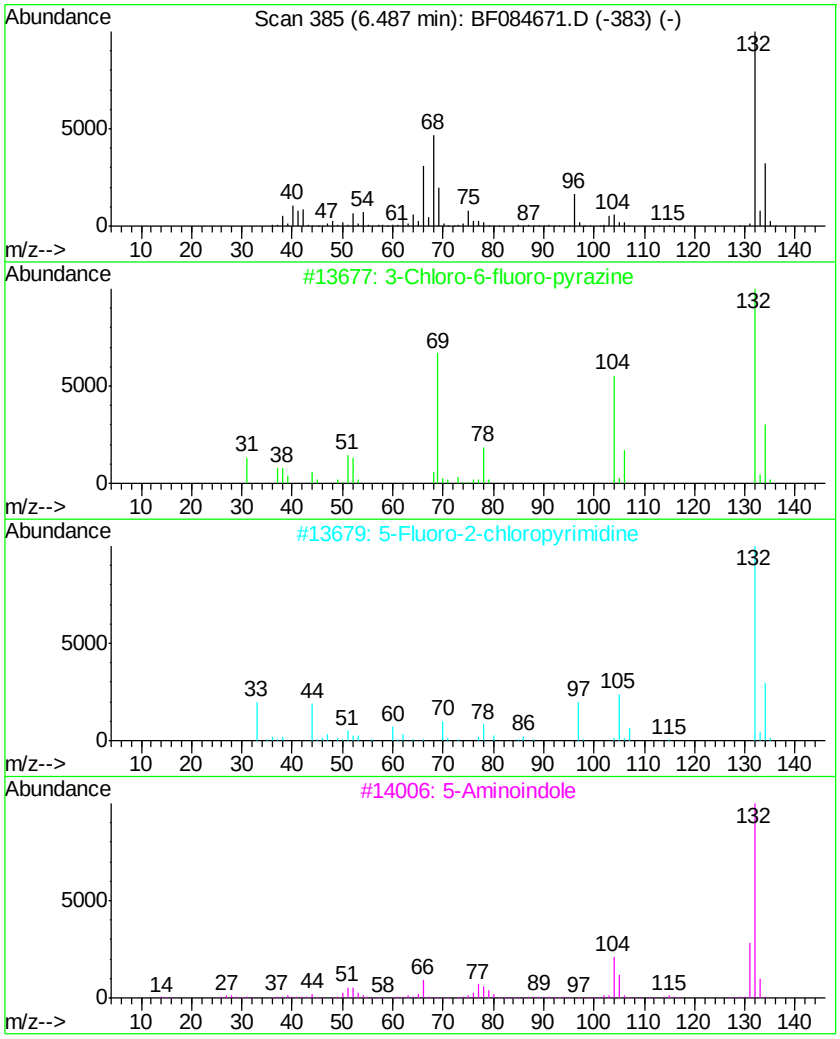
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

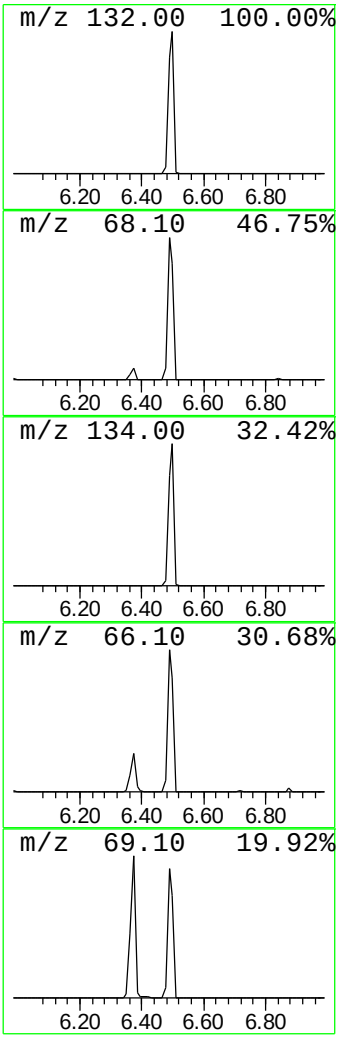
****

Peak Number 5 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	96.36 ng	5179830	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : H1273-10
Misc :
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Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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
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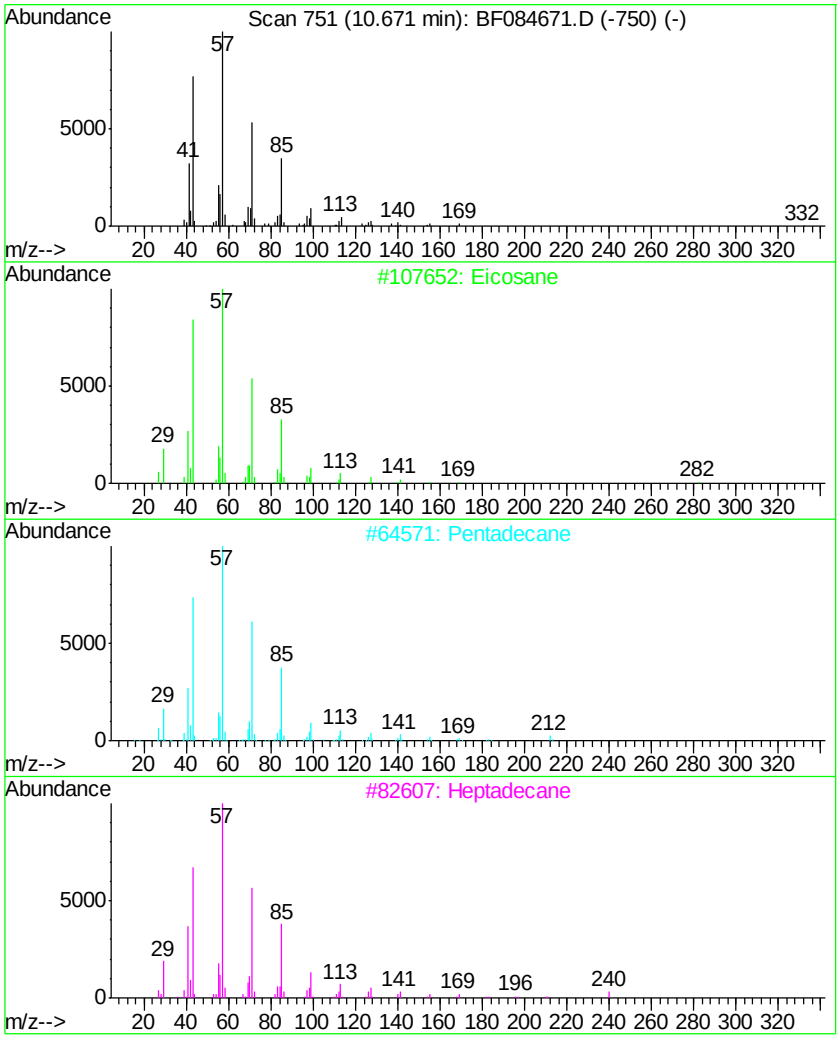
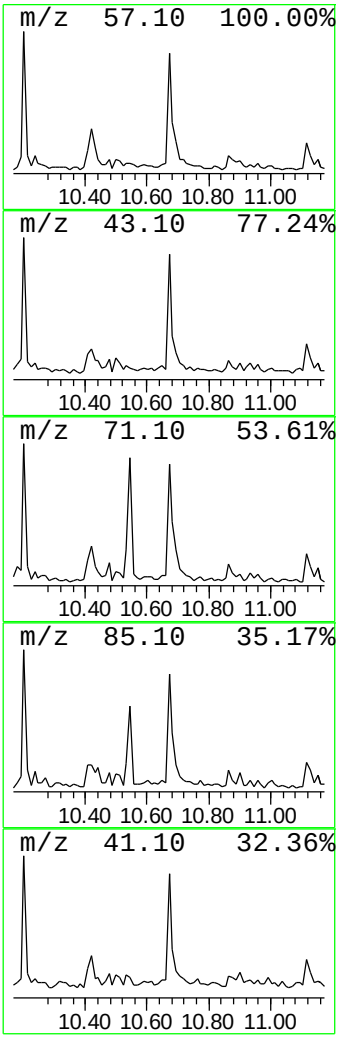
Peak Number 7 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.17 ng	172646	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Hexadecane	226	C16H34	000544-76-3	90





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Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

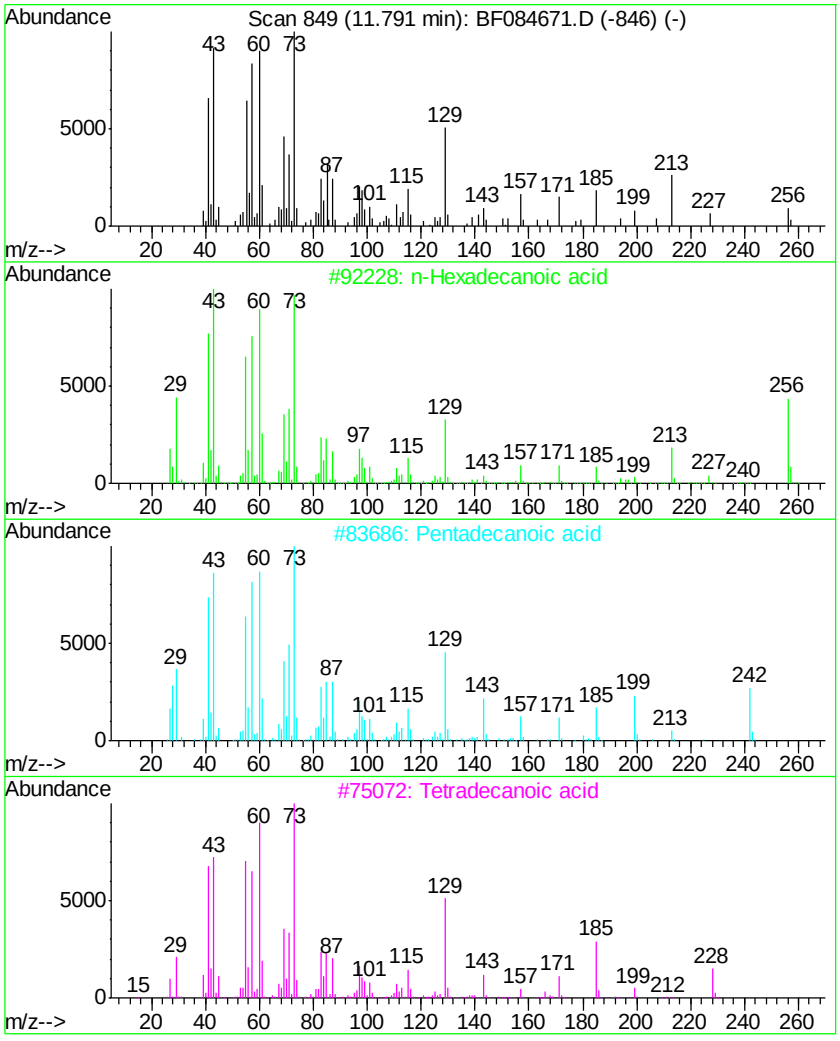
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

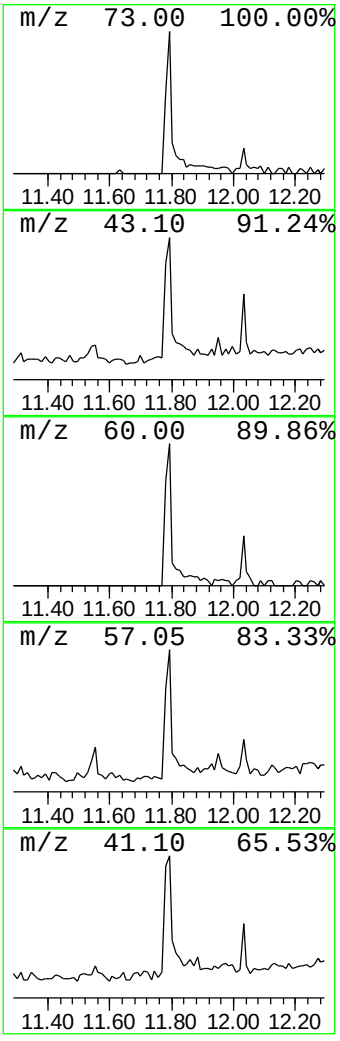
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	2.06 ng	163874	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Misc :
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ClientSampleId : SUP-B011(25-27)

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

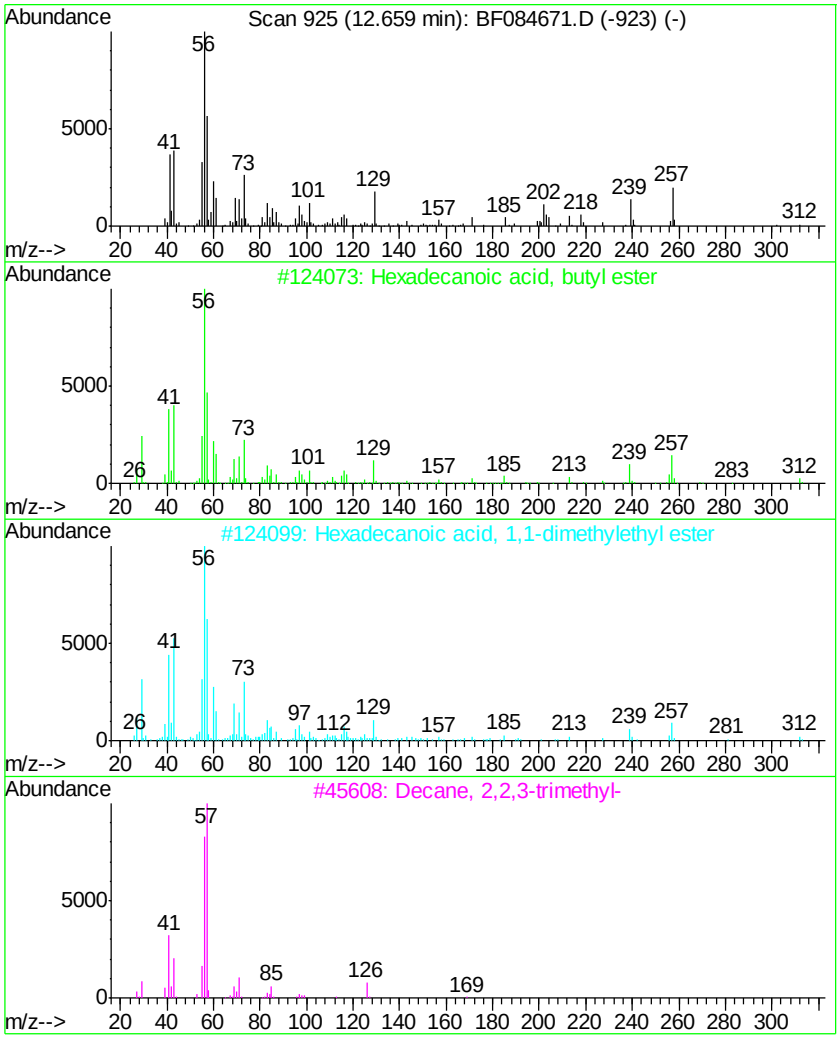
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

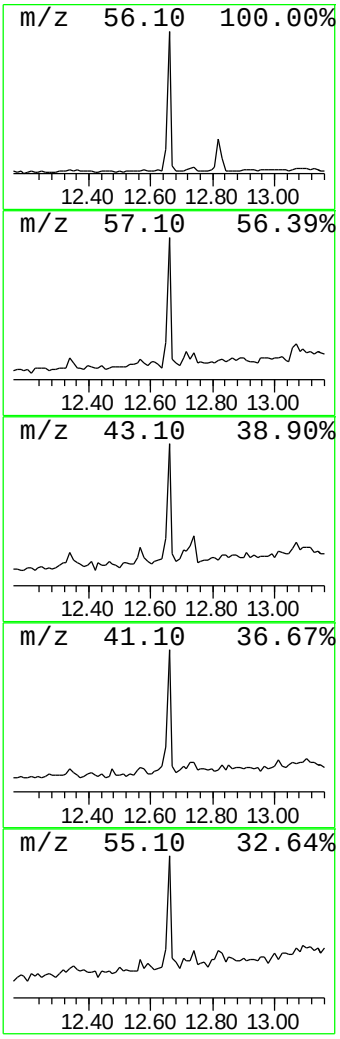
****

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	4.51 ng	291970	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	35
5	1-Decene, 9-methyl-	154	C11H22	061142-78-7	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

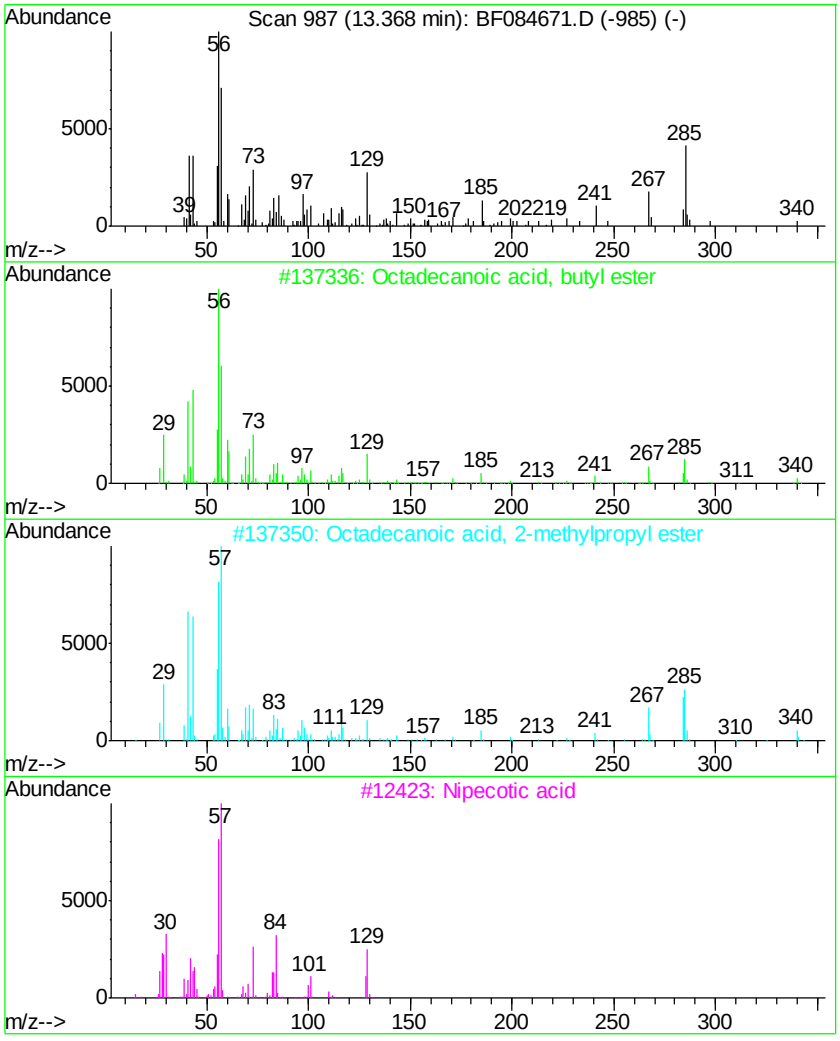
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

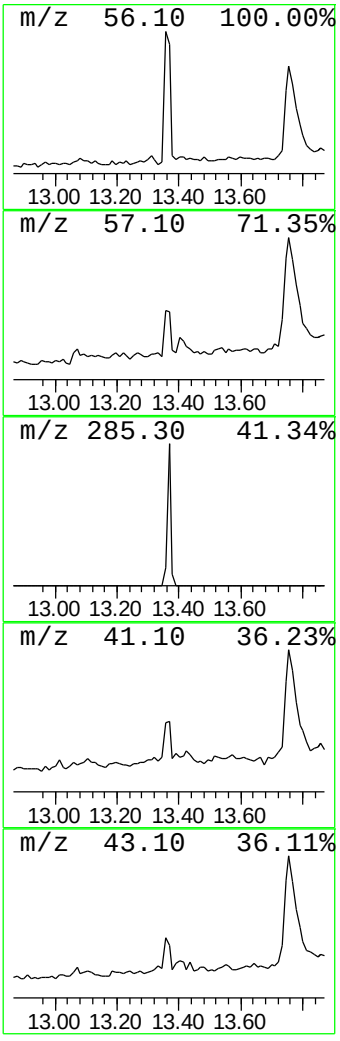
****

Peak Number 10 Octadecanoic acid, butyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	2.13 ng	138069	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	42
3	Nipecotic acid	129	C6H11NO2	000498-95-3	37
4	Cyclohexanecarboxylic acid, 2-am...	143	C7H13NO2	005691-19-0	30
5	6-[N-Aziridyl]hexadiene-1,3	123	C8H13N	1000255-07-7	27





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Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

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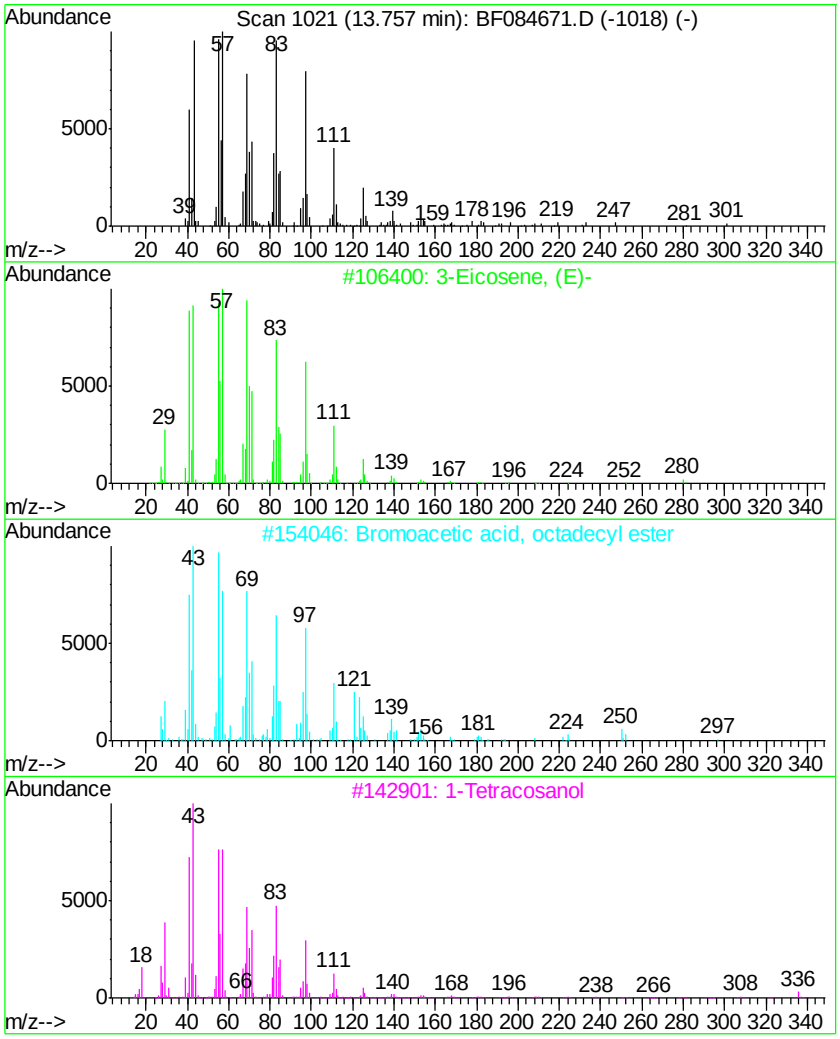
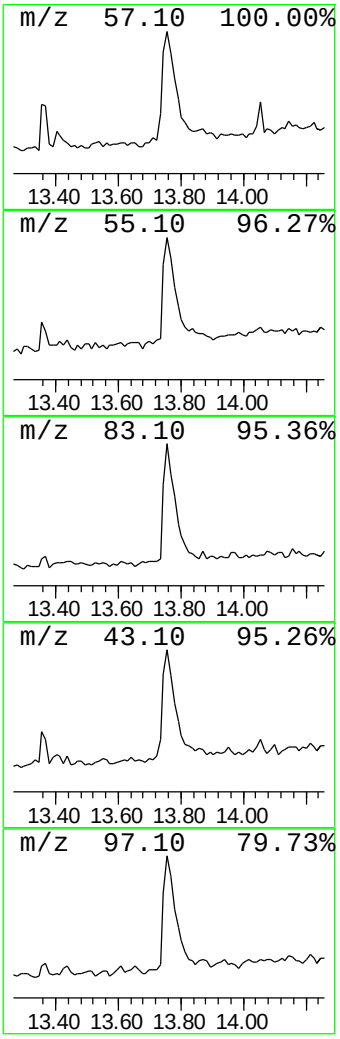
Peak Number 11 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	11.04 ng	714734	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
3	1-Tetracosanol	354	C24H50O	000506-51-4	87
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
5	1-Nonadecene	266	C19H38	018435-45-5	83





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Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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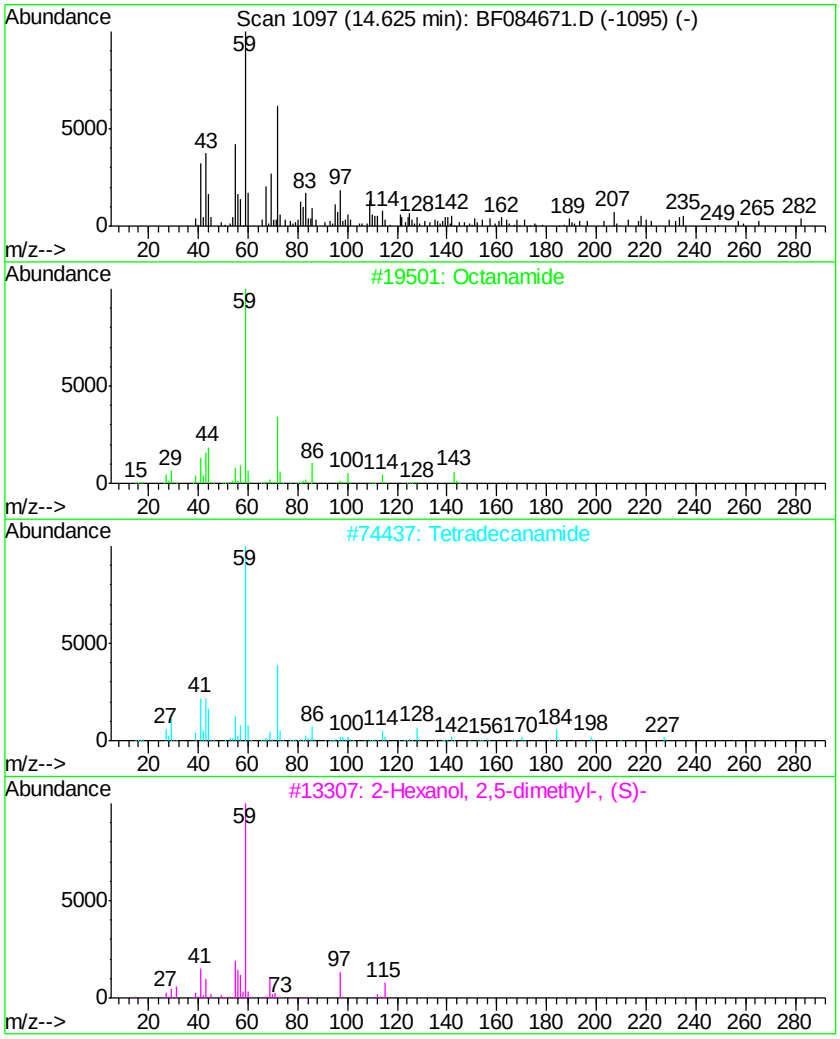
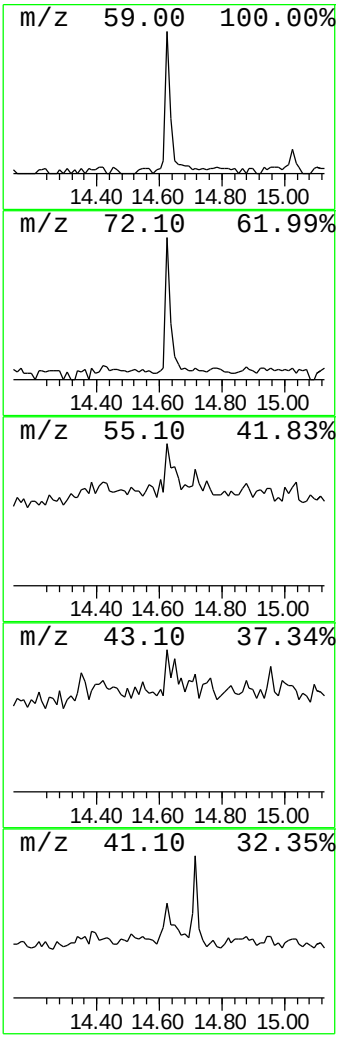
Peak Number 12 Octanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.86 ng	142902	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanamide	143	C8H17NO	000629-01-6	50
2	Tetradecanamide	227	C14H29NO	000638-58-4	50
3	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	38
4	Methyl N-chloroacetylcarbamate	151	C4H6ClNO3	013558-70-8	38
5	Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	37





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

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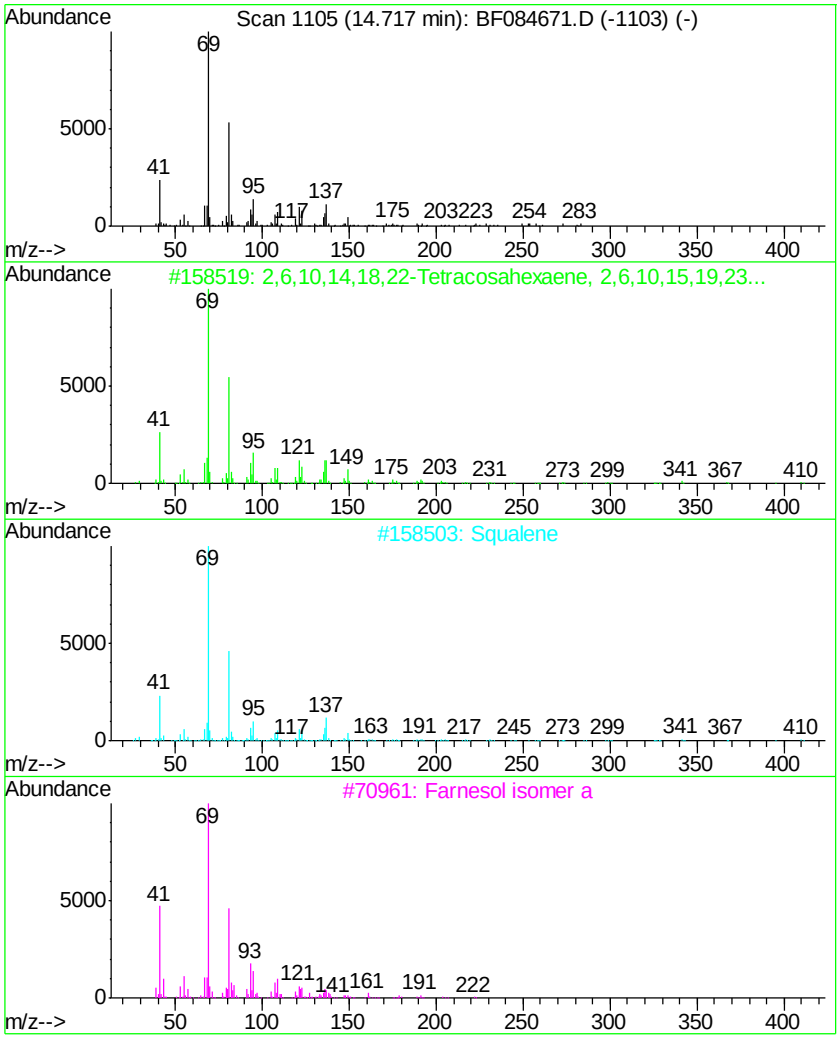
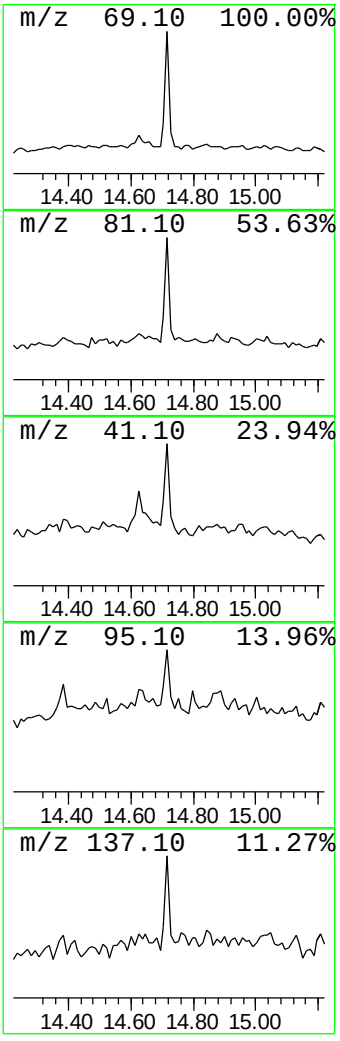
Peak Number 13 2,6,10,14,18,22-Tetracosahe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.73 ng	136682	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
2	Squalene	410	C30H50	007683-64-9	87
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013016\
Data File : BF084671.D
Acq On : 30 Jan 2016 8:23
Operator : SJ/IZ
Sample : H1273-10
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(25-27)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.19	5.5	ng	297560	1	6.73	1075140	20.0
2-Pentanone, 4-hy...	4.89	75.2	ng	4041930	1	6.73	1075140	20.0
2-Pentanone, 4-me...	5.72	4.4	ng	236820	1	6.73	1075140	20.0
1R-.alpha.-Pinene	5.98	5.5	ng	293681	1	6.73	1075140	20.0
unknown6.49	6.49	96.4	ng	5179830	1	6.73	1075140	20.0
Eicosane	10.67	2.2	ng	172646	4	11.24	1592900	20.0
n-Hexadecanoic acid	11.79	2.1	ng	163874	4	11.24	1592900	20.0
Hexadecanoic acid...	12.66	4.5	ng	291970	5	13.87	1295380	20.0
Octadecanoic acid...	13.37	2.1	ng	138069	5	13.87	1295380	20.0
3-Eicosene, (E)-	13.76	11.0	ng	714734	5	13.87	1295380	20.0
Octanamide	14.63	2.9	ng	142902	6	15.25	1000130	20.0
2,6,10,14,18,22-T...	14.72	2.7	ng	136682	6	15.25	1000130	20.0