LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092751.D
Acq On : 2 Feb 2017 22:37
Operator : SJ/MA
Sample : I1650-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-43-COMP

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-BF013017.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	2.247	13	14	21	rVB	106841	195247	3.71%	0.495%
2	2.407	24	28	31	rVB	52476	94506	1.79%	0.240%
3	5.116	262	265	274	rBV	1600419	2535842	48.12%	6.433%
4	5.550	300	303	305	rBV	4270776	5269415	100.00%	13.368%
5	6.579	390	393	396	rBV	3587783	4376526	83.06%	11.103%
6	6.704	401	404	407	rBV	3802662	4056283	76.98%	10.290%
7	6.933	422	424	426	rBV	1091557	874575	16.60%	2.219%
8	7.093	435	438	440	rBV	3646189	3311681	62.85%	8.401%
9	7.504	471	474	476	rBV	2768014	2753094	52.25%	6.984%
10	8.225	534	537	539	rBV	1304101	1148349	21.79%	2.913%
11	9.299	628	631	634	rBV	4418111	4349402	82.54%	11.034%
12	9.688	663	665	668	rBV	282215	259688	4.93%	0.659%
13	9.973	688	690	693	rBV	1281383	1162738	22.07%	2.950%
14	10.396	726	727	729	rVB	51095	60640	1.15%	0.154%
15	10.762	757	759	762	rBV2	1834604	2281356	43.29%	5.787%
16	10.876	767	769	773	rVB2	109831	158716	3.01%	0.403%
17	11.322	806	808	809	rBV	81549	71254	1.35%	0.181%
18	11.459	818	820	822	rBV	1252626	1086442	20.62%	2.756%
19	13.048	956	959	961	rBV	3505565	3430484	65.10%	8.703%
20	13.939	1035	1037	1044	rBV	85153	145955	2.77%	0.370%
21	14.099	1048	1051	1053	rVB	741552	814064	15.45%	2.065%
22	14.934	1122	1124	1127	rBV	80896	113899	2.16%	0.289%
23	15.562	1176	1179	1185	rBV	624971	868712	16.49%	2.204%

Sum of corrected areas: 39418868

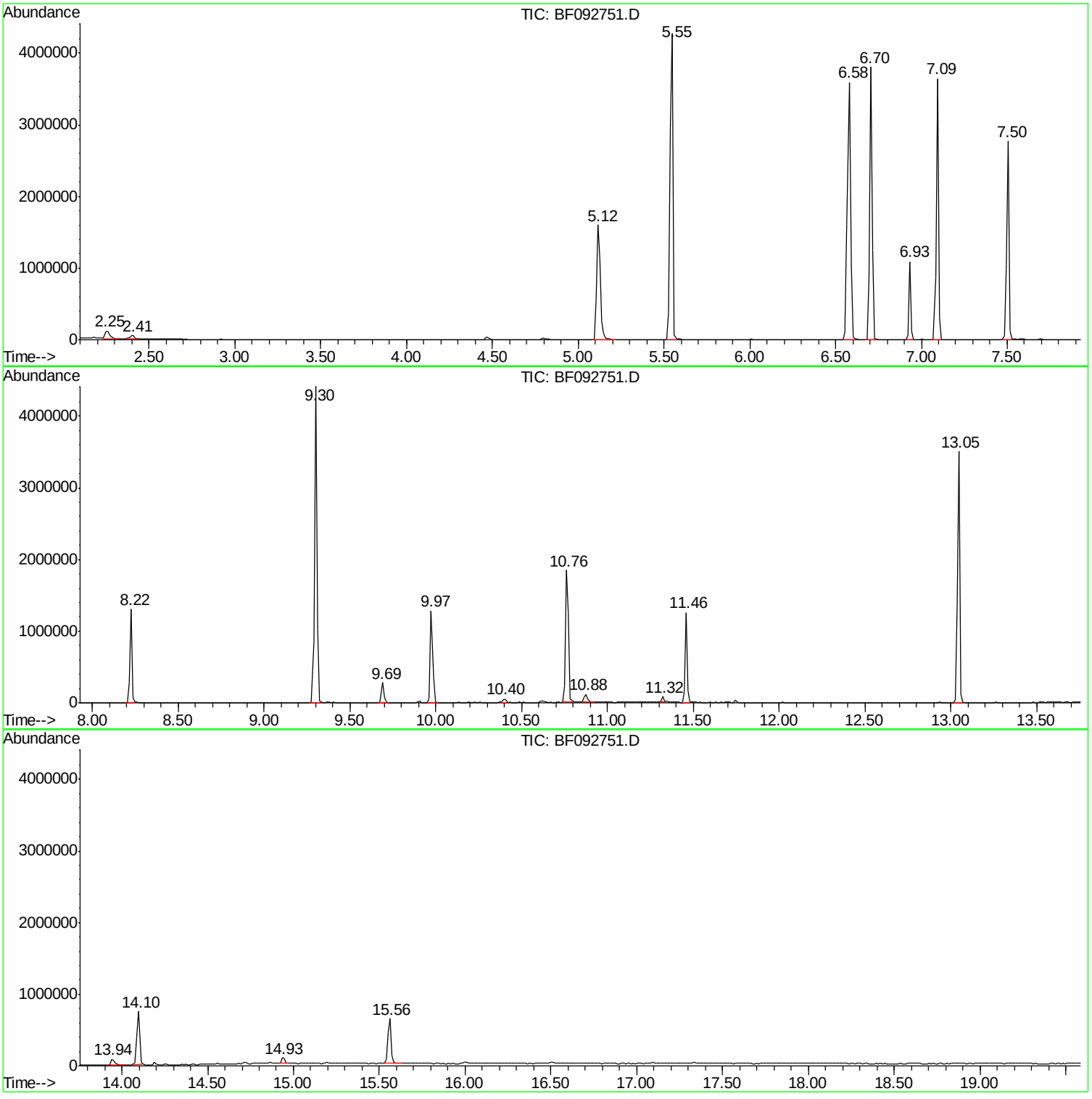
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092751.D
Acq On : 2 Feb 2017 22:37
Operator : SJ/MA
Sample : I1650-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-43-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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\BF020217\
Data File : BF092751.D
Acq On : 2 Feb 2017 22:37
Operator : SJ/MA
Sample : I1650-08
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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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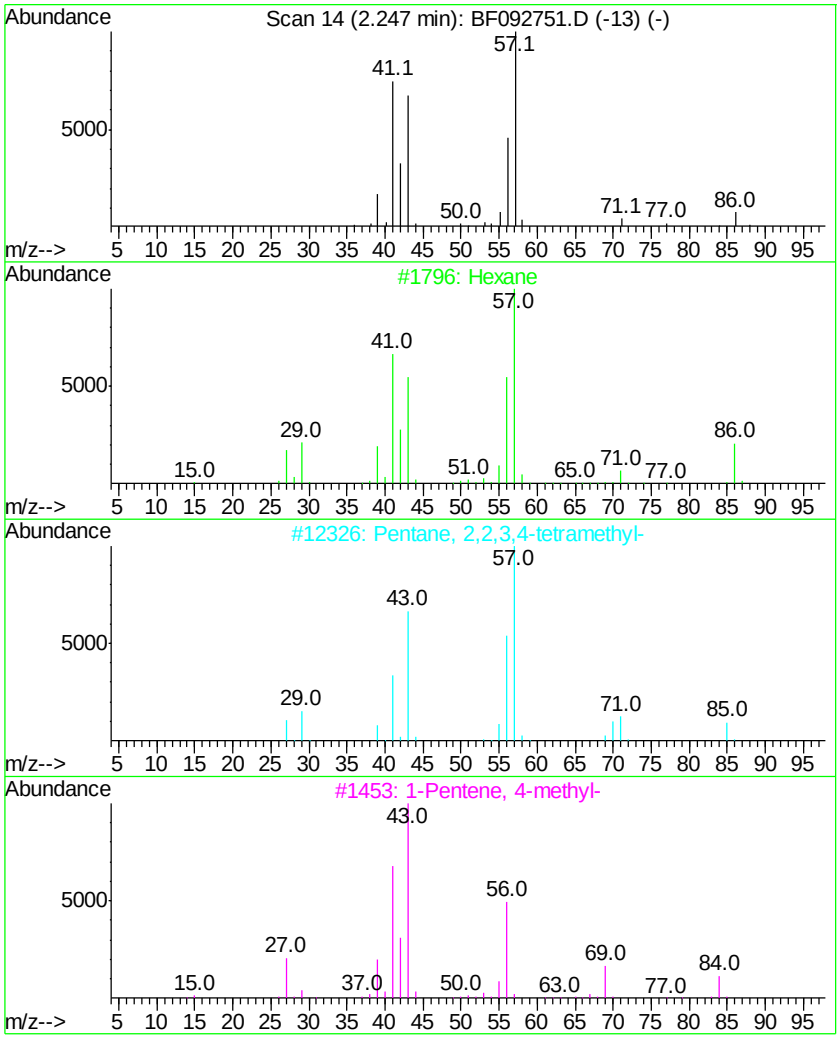
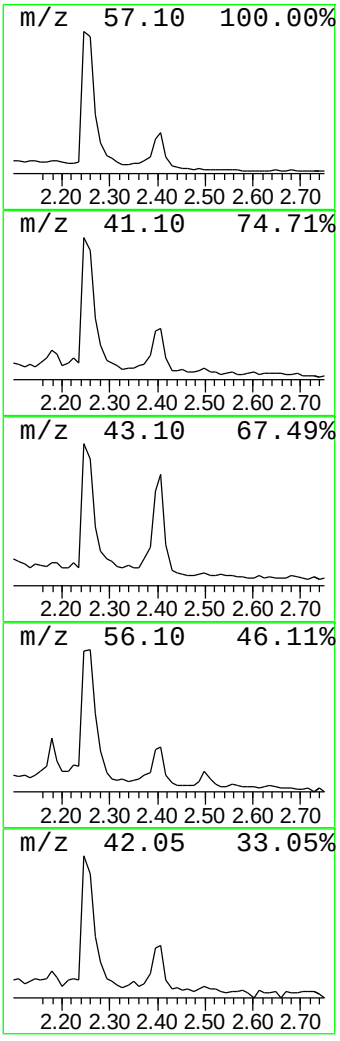
Peak Number 1 Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	4.46 ng	195247	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane	86	C6H14	000110-54-3	74
2	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	42
3	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	40
4	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	38
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	37





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092751.D
Acq On : 2 Feb 2017 22:37
Operator : SJ/MA
Sample : I1650-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-43-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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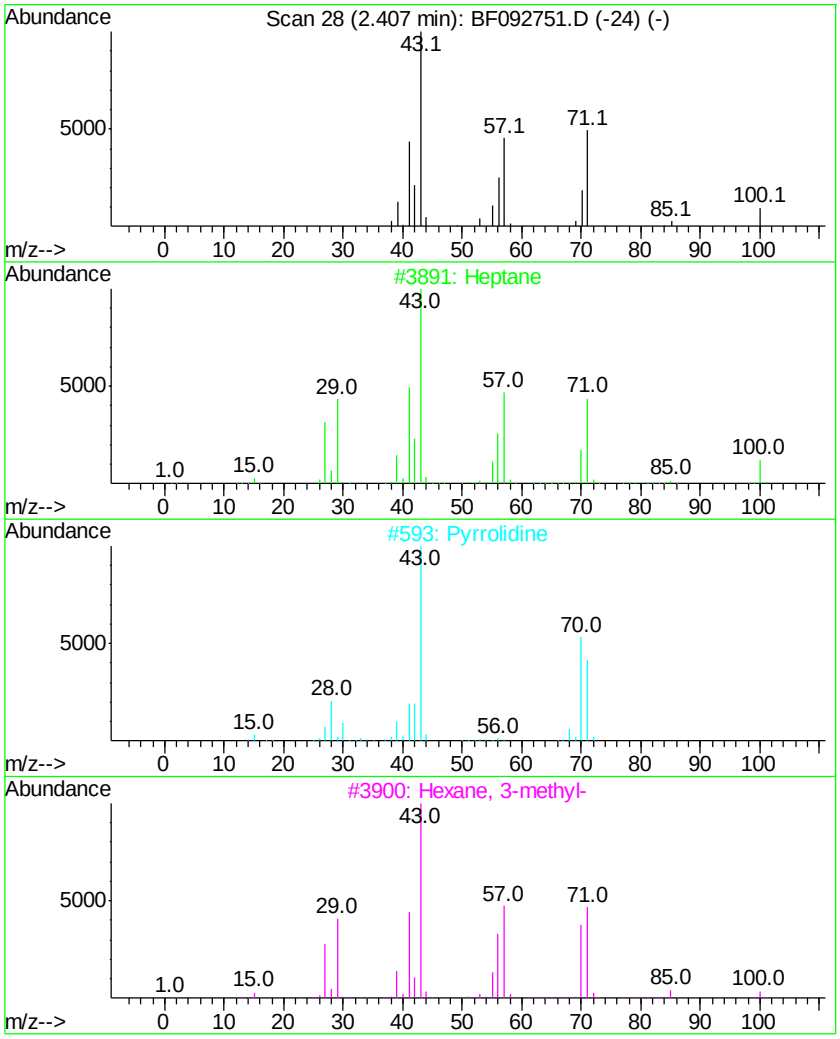
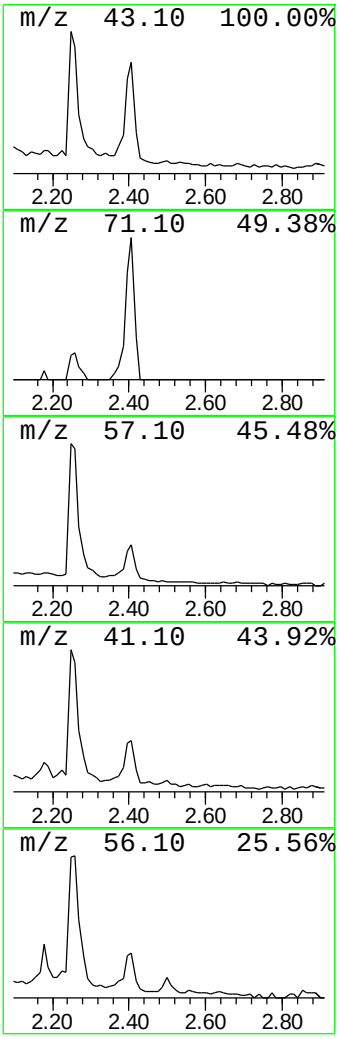
Peak Number 2 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.41	2.16 ng	94506	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Pyrrolidine	71	C4H9N	000123-75-1	43
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	42
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	38
5	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092751.D
Acq On : 2 Feb 2017 22:37
Operator : SJ/MA
Sample : I1650-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-43-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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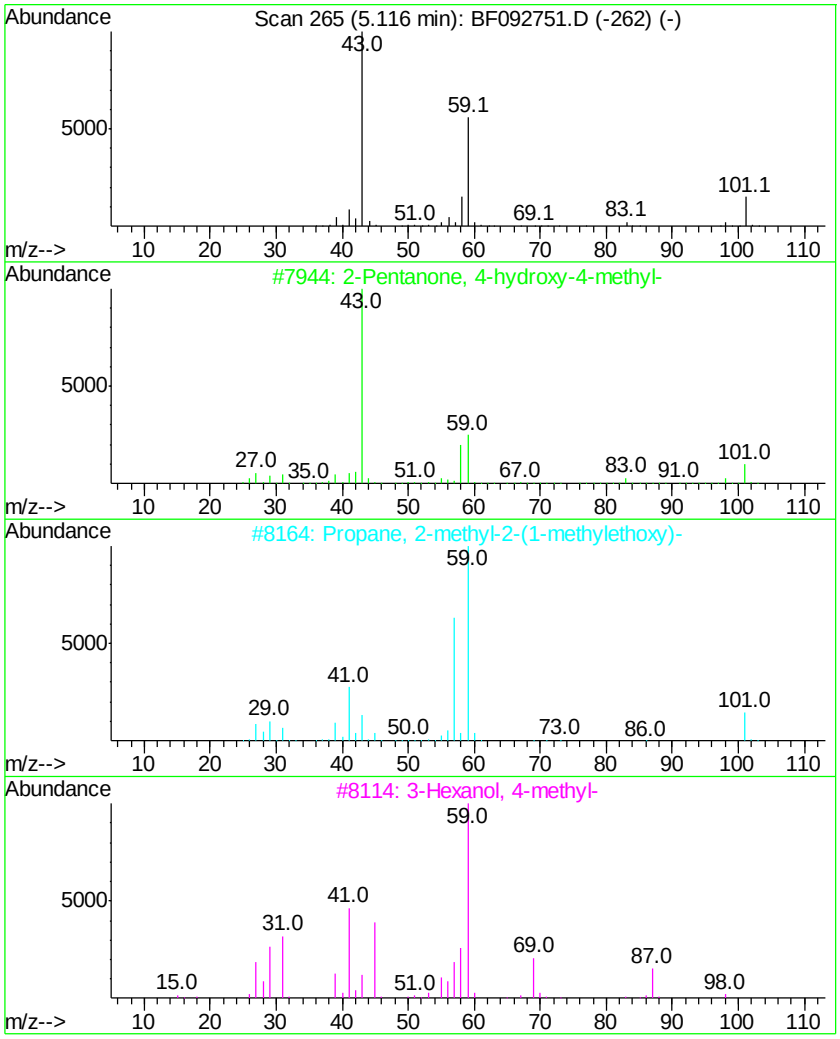
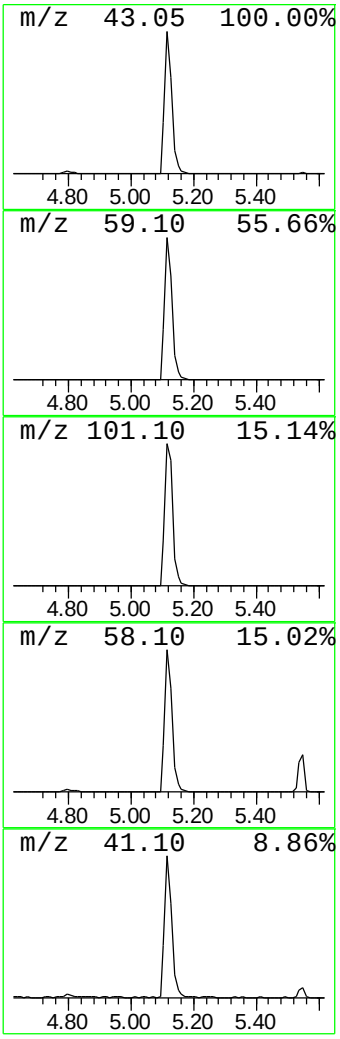
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	57.99 ng	2535840	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092751.D
Acq On : 2 Feb 2017 22:37
Operator : SJ/MA
Sample : I1650-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-43-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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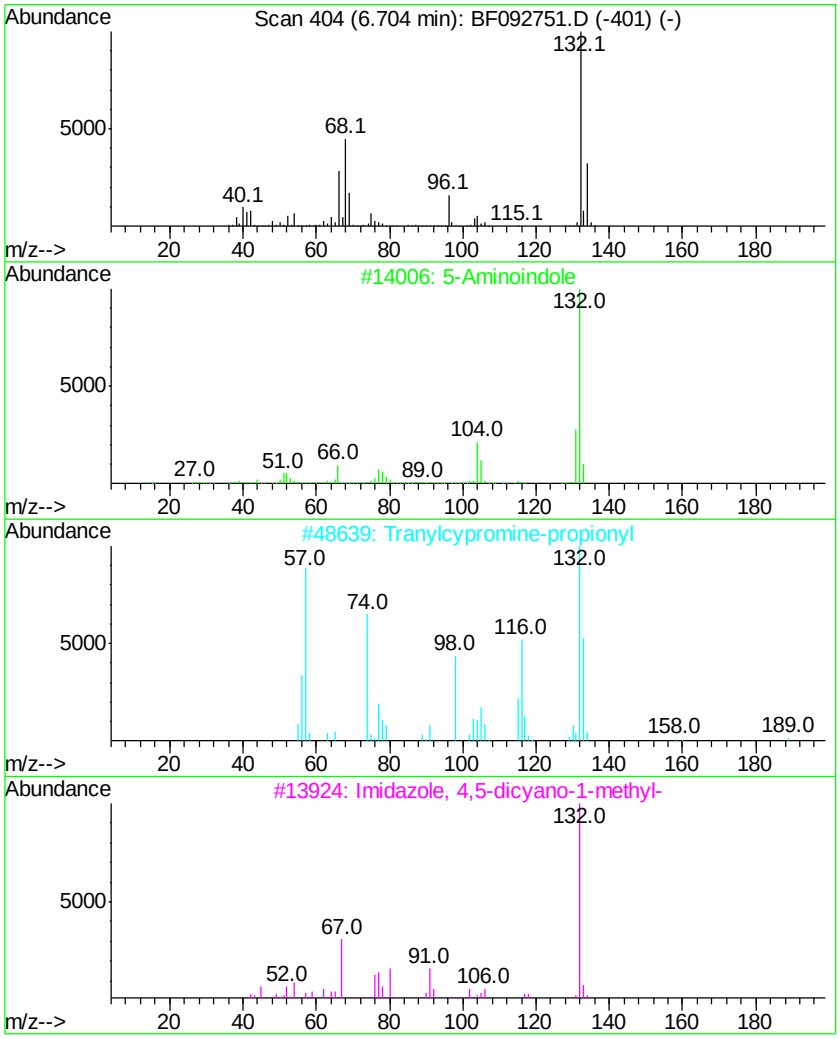
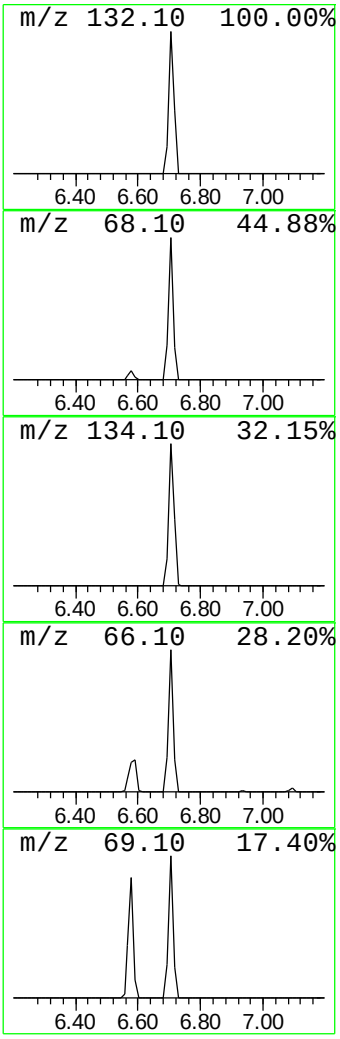
Peak Number 4 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	92.76 ng	4056280	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
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Operator : SJ/MA
Sample : I1650-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-43-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
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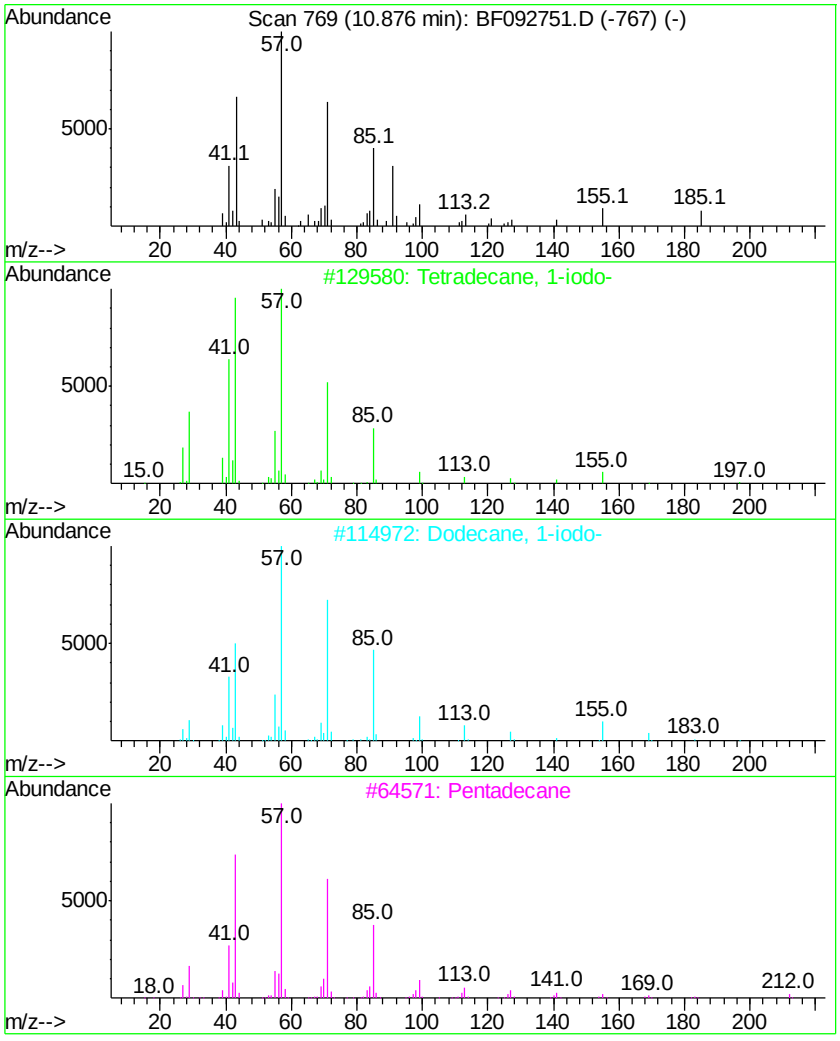
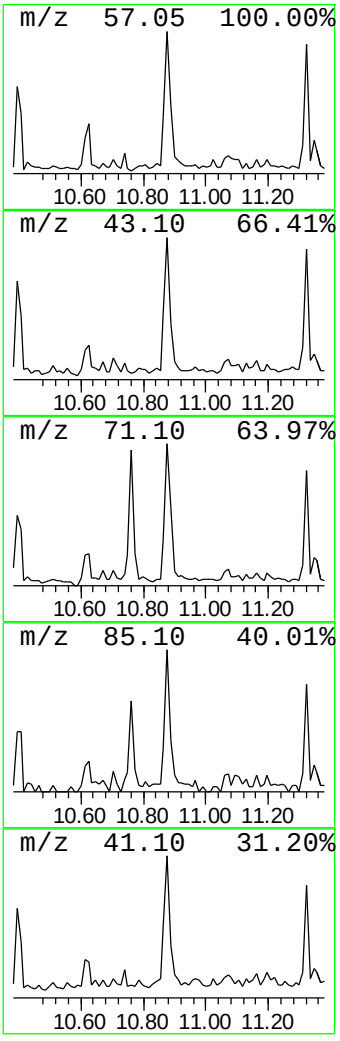
Peak Number 6 Tetradecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.92 ng	158716	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Pentadecane	212	C15H32	000629-62-9	80
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5	Tetradecane	198	C14H30	000629-59-4	80





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Sample : I1650-08
Misc :
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Instrument : BNA_F
ClientSampleId : SB-43-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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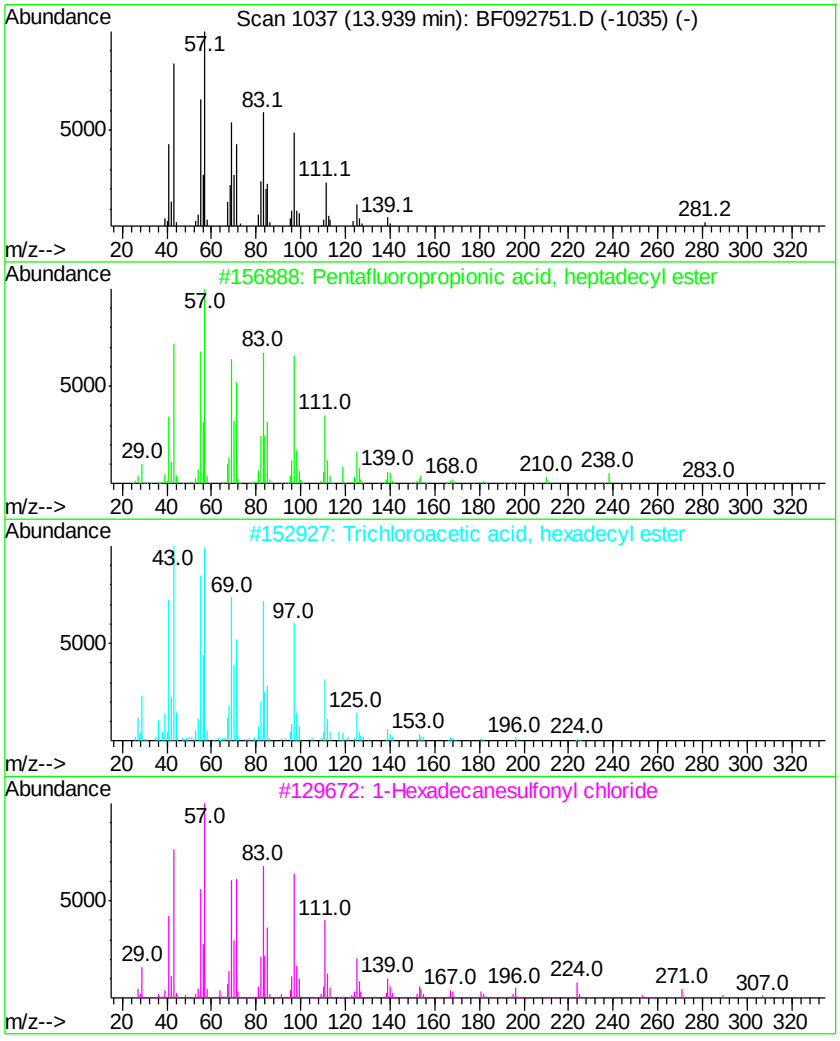
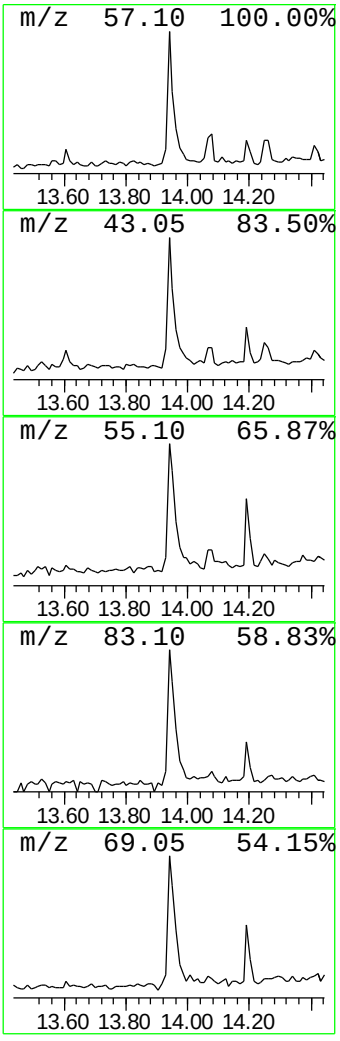
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.59 ng	145955	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	81





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

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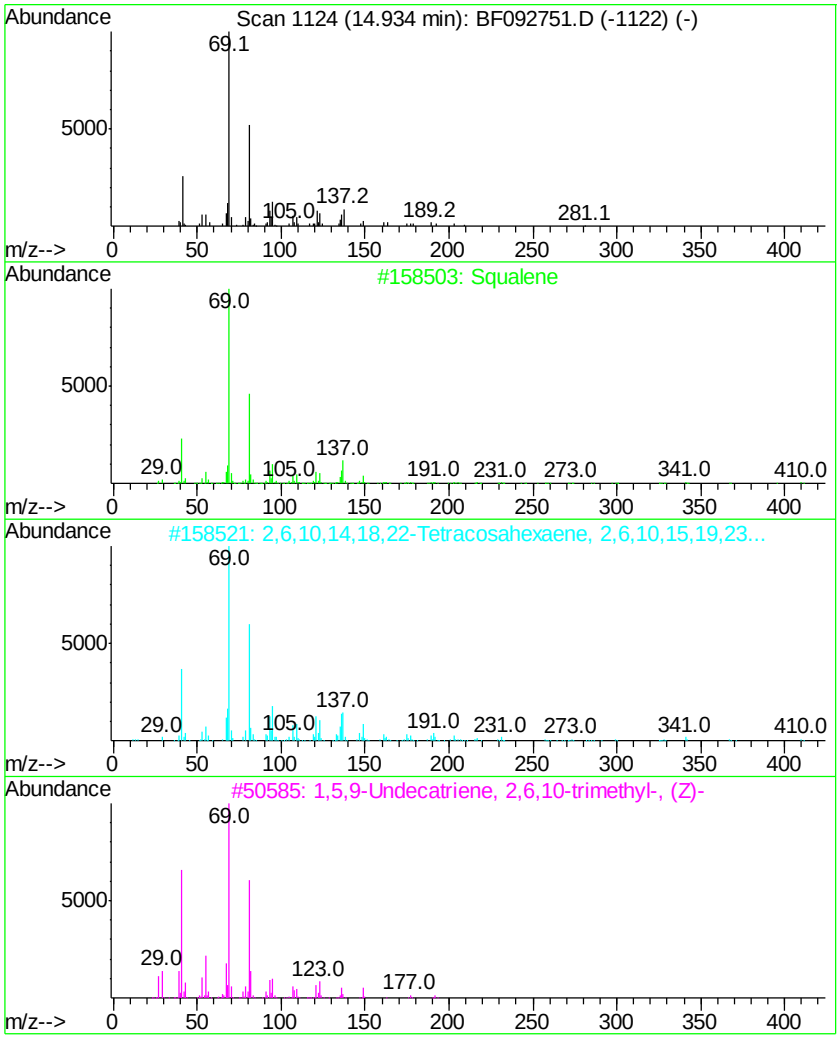
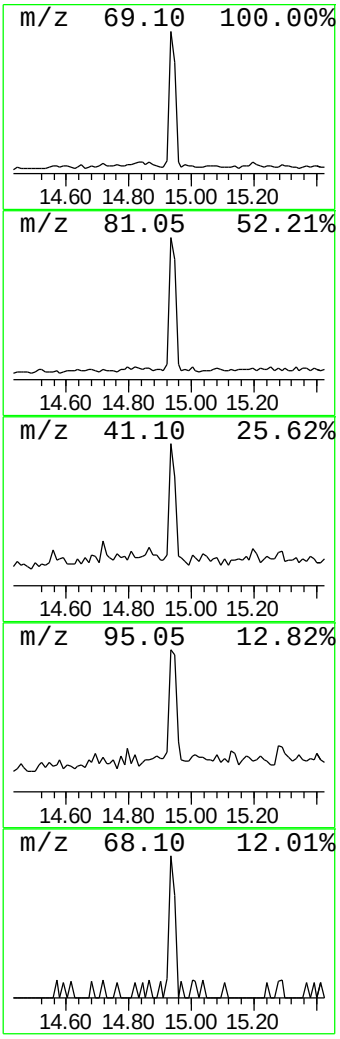
Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.62 ng	113899	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5	.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O6	1000154-77-2	78





Tentatively Identified Compound (LSC) summary

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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
Hexane	2.25	4.5	ng	195247	1	6.93	874575	20.0
Heptane	2.41	2.2	ng	94506	1	6.93	874575	20.0
2-Pentanone, 4-hy...	5.12	58.0	ng	2535840	1	6.93	874575	20.0
unknown6.70	6.70	92.8	ng	4056280	1	6.93	874575	20.0
Tetradecane, 1-iodo-	10.88	2.9	ng	158716	4	11.46	1086440	20.0
Pentafluoropropio...	13.94	3.6	ng	145955	5	14.10	814064	20.0
Squalene	14.93	2.6	ng	113899	6	15.56	868712	20.0