LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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	189	rBV	139751	194473	5.34%	0.537%
2	4.887	241	245	247	rBV	1682337	2739819	75.28%	7.565%
3	5.321	280	283	285	rBV	3538323	3611928	99.25%	9.973%
4	5.721	316	318	321	rBV	170534	152966	4.20%	0.422%
5	6.362	372	374	377	rBV	2533919	3318493	91.18%	9.163%
6	6.487	383	385	388	rBV	3420972	3260395	89.59%	9.002%
7	6.716	403	405	408	rBV	769112	1023733	28.13%	2.827%
8	6.876	417	419	422	rVB	2773583	2389423	65.65%	6.598%
9	7.287	452	455	457	rBV	2346989	2113779	58.08%	5.836%
10	8.007	516	518	520	rBV	1752371	1446020	39.73%	3.993%
11	9.093	610	613	615	rBV	2750504	3639405	100.00%	10.049%
12	9.482	645	647	649	rBV	435203	391720	10.76%	1.082%
13	9.699	665	666	669	rBV	63347	79543	2.19%	0.220%
14	9.756	669	671	674	rVB	1572978	1524850	41.90%	4.210%
15	9.939	684	687	690	rBV2	19104	42204	1.16%	0.117%
16	10.202	708	710	712	rVB	167085	128785	3.54%	0.356%
17	10.419	726	729	732	rBV	40888	70441	1.94%	0.194%
18	10.545	738	740	743	rBV	2691051	2525601	69.40%	6.974%
19	10.671	749	751	756	rVB	127227	161414	4.44%	0.446%
20	11.116	789	790	792	rBV	36505	40373	1.11%	0.111%
21	11.242	798	801	803	rVB	1378647	1550966	42.62%	4.282%
22	12.831	937	940	942	rBV	2343473	3011276	82.74%	8.315%
23	13.768	1018	1022	1029	rBV2	36985	154743	4.25%	0.427%
24	13.871	1029	1031	1033	rVV	1300470	1260545	34.64%	3.481%
25	14.625	1095	1097	1103	rBV2	52881	77868	2.14%	0.215%
26	14.717	1103	1105	1108	rVV	127201	122275	3.36%	0.338%
27	15.254	1149	1152	1155	rBV	1056040	1183947	32.53%	3.269%

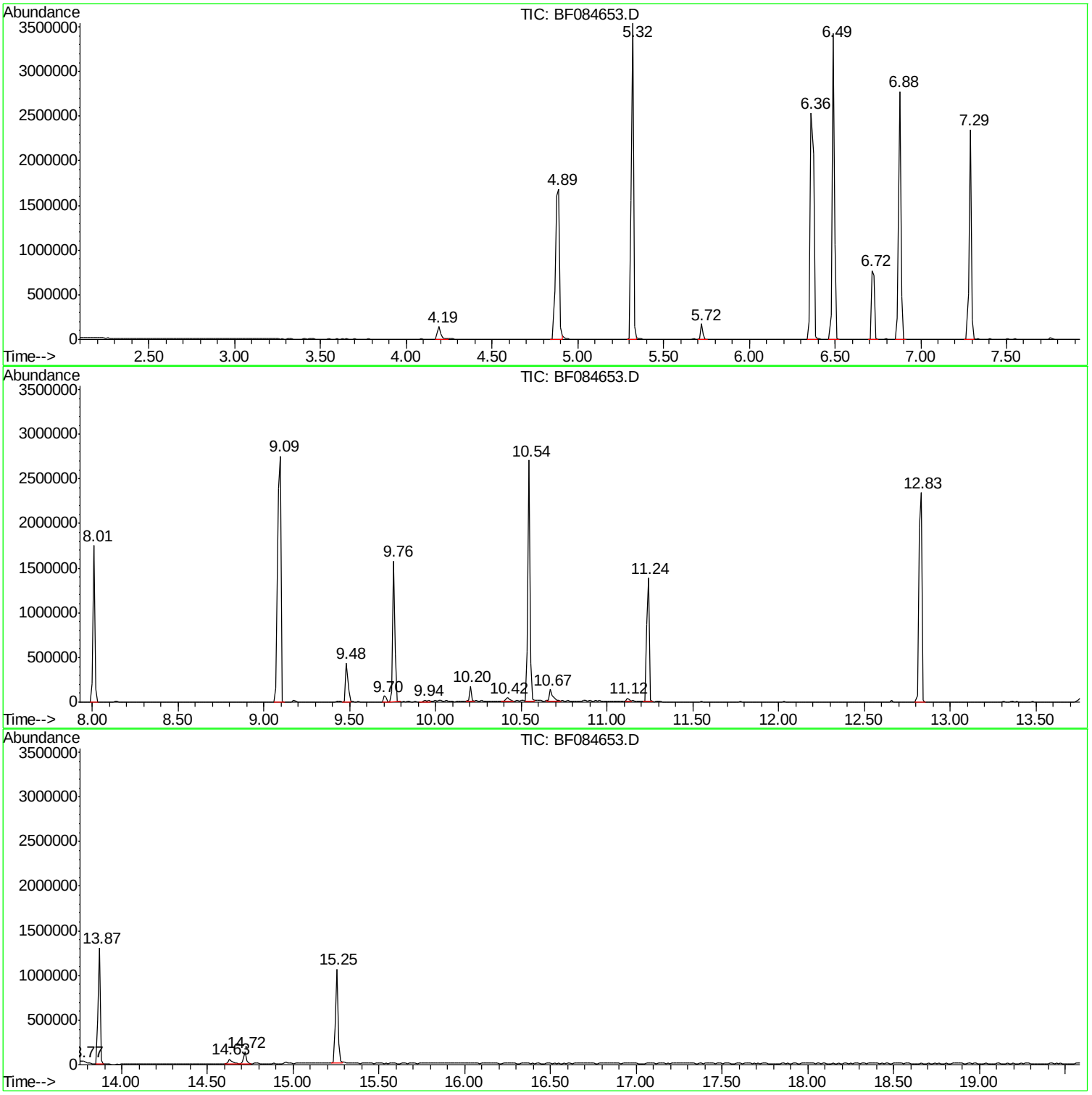
Sum of corrected areas: 36216985

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B011(40-42)

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\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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

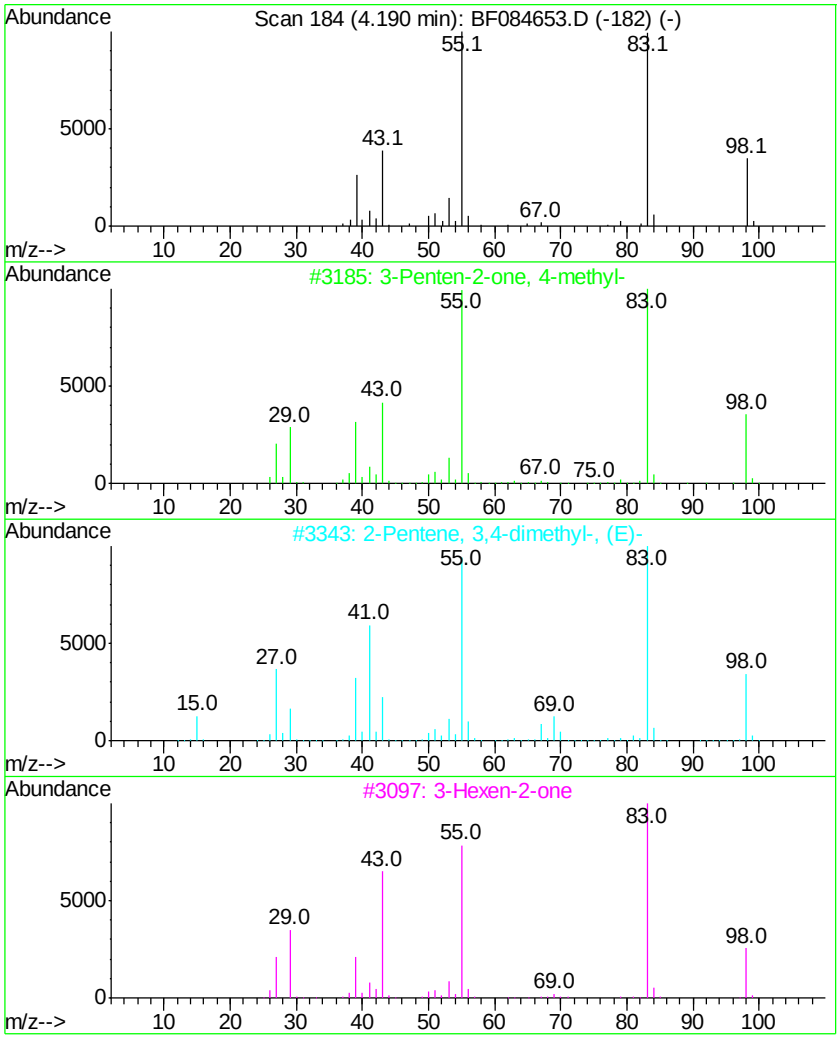
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

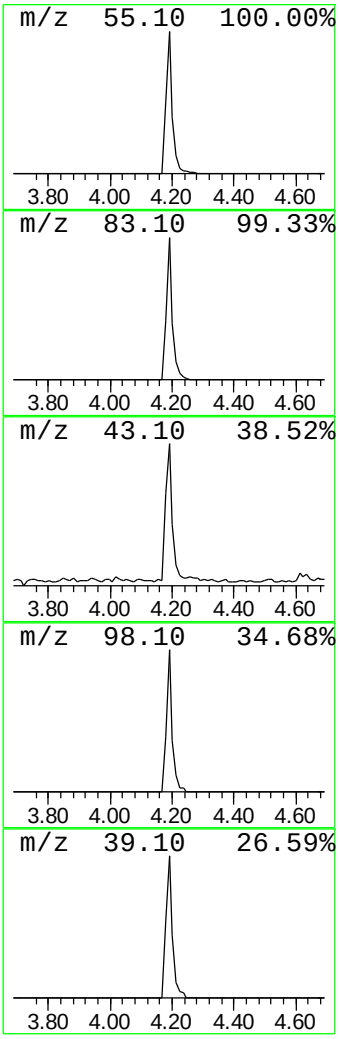
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	3.80 ng	194473	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	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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

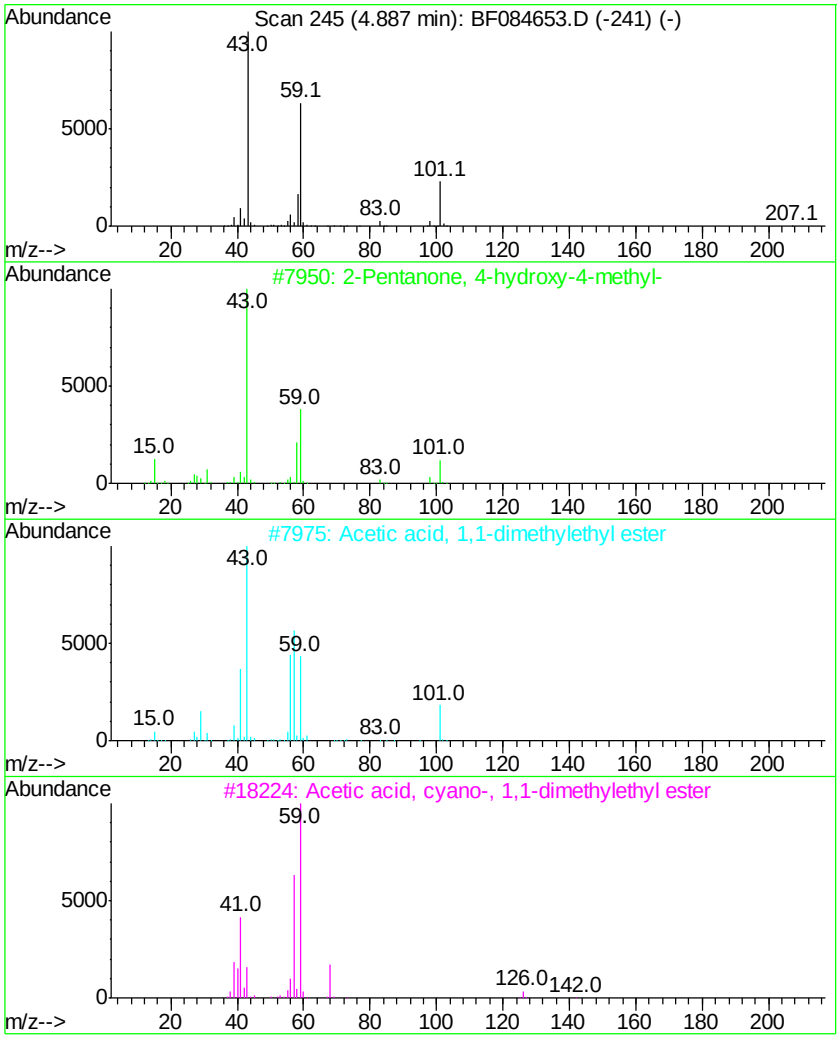
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

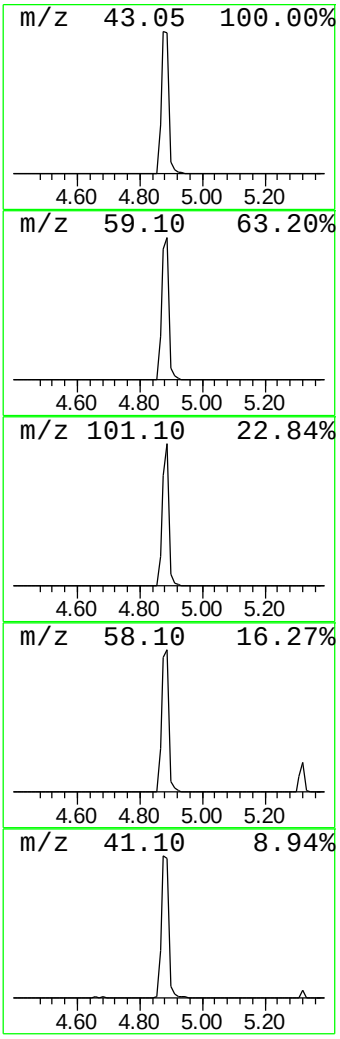
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	53.53 ng	2739820	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	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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

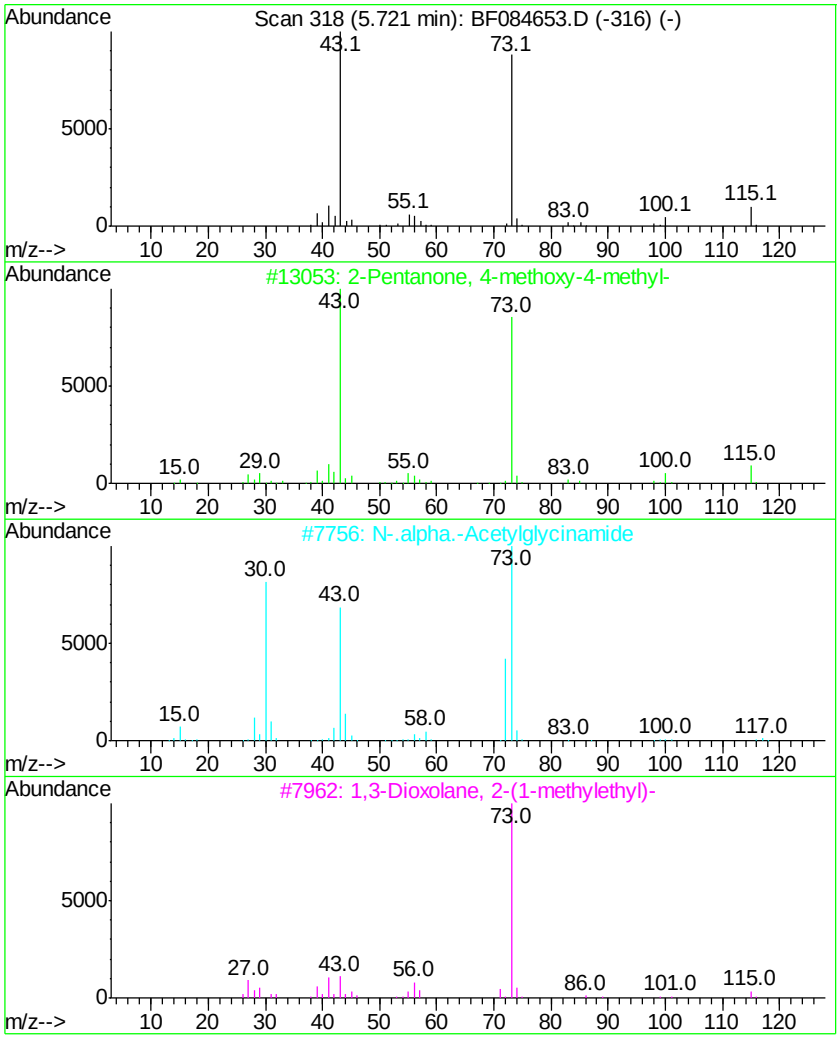
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

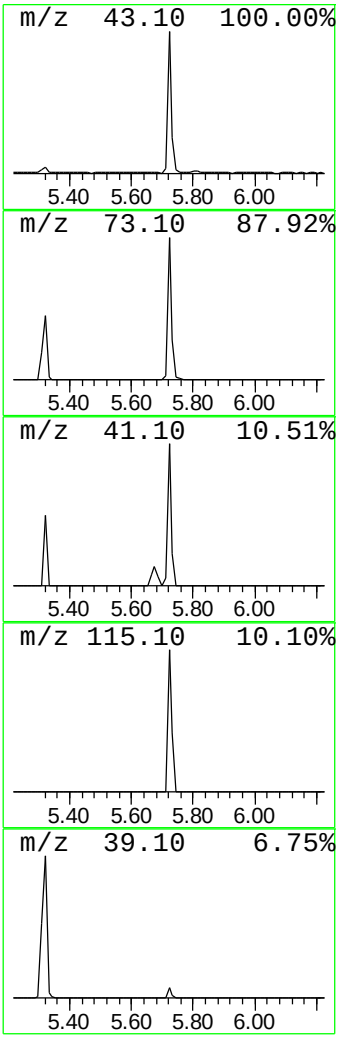
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.99 ng	152966	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	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	35
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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

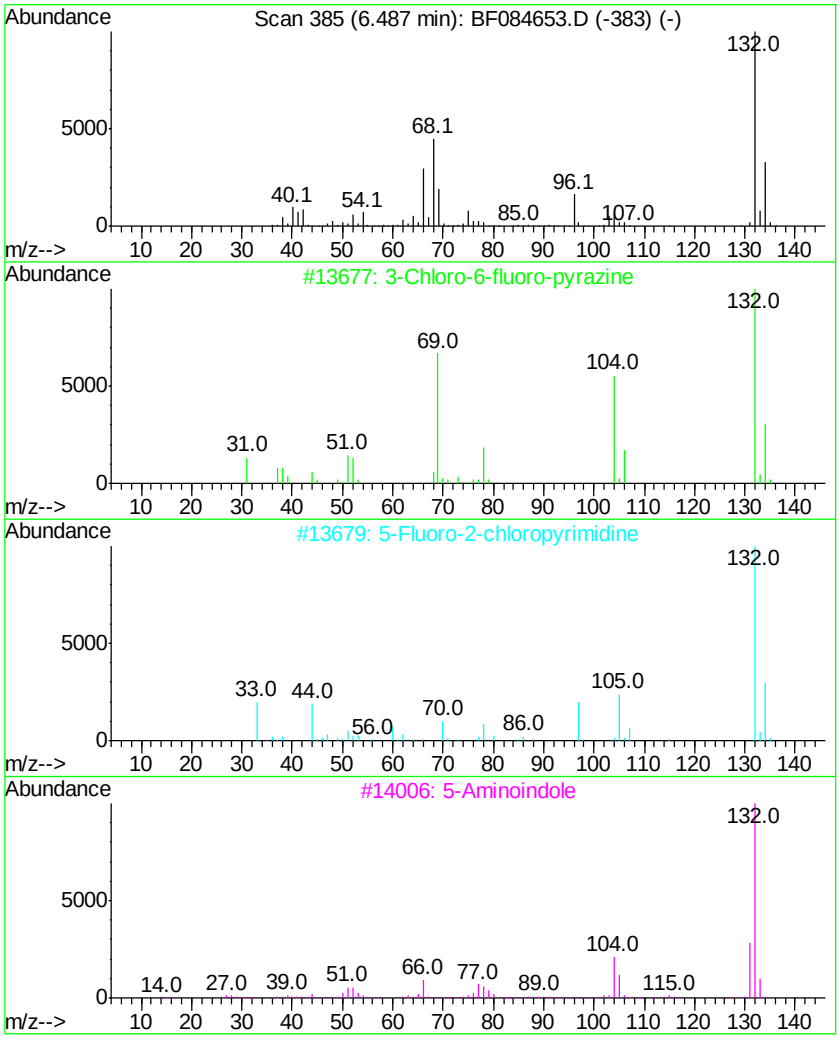
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

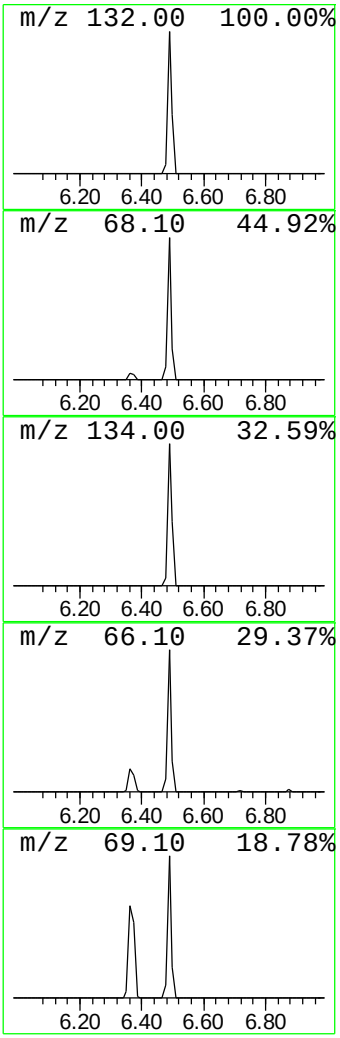
****

Peak Number 4 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	63.70 ng	3260400	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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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

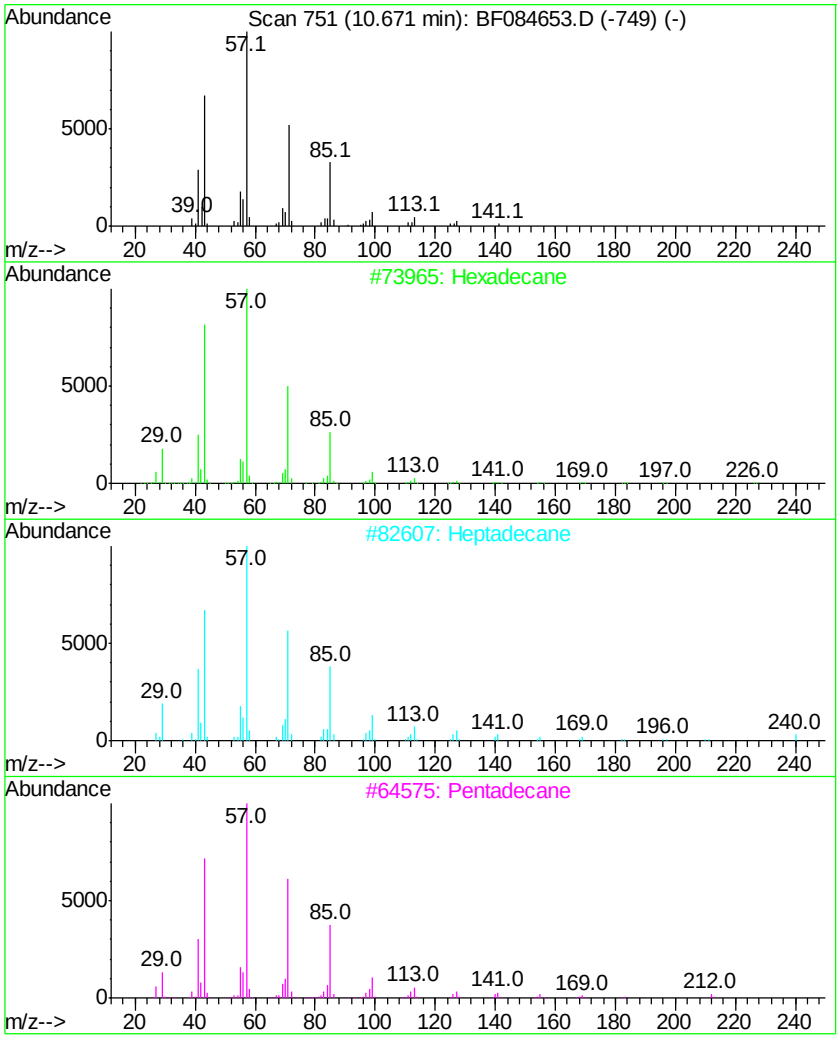
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

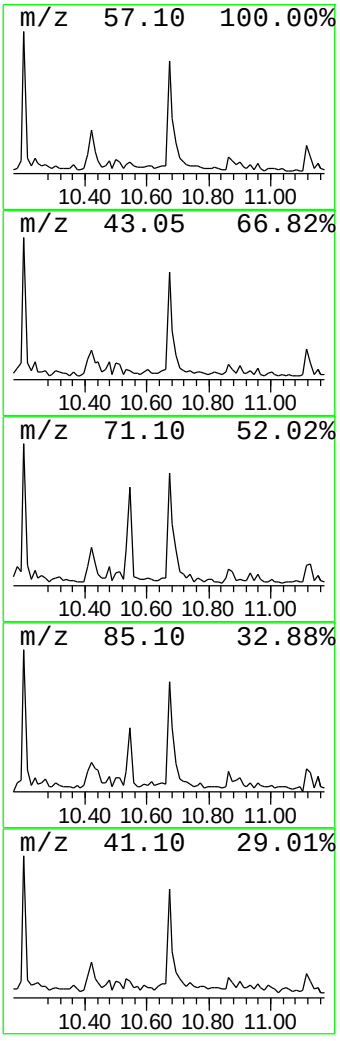
****

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.08 ng	161414	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Heptadecane	240	C17H36	000629-78-7	72
3	Pentadecane	212	C15H32	000629-62-9	72
4	Tridecane	184	C13H28	000629-50-5	64
5	Eicosane	282	C20H42	000112-95-8	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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

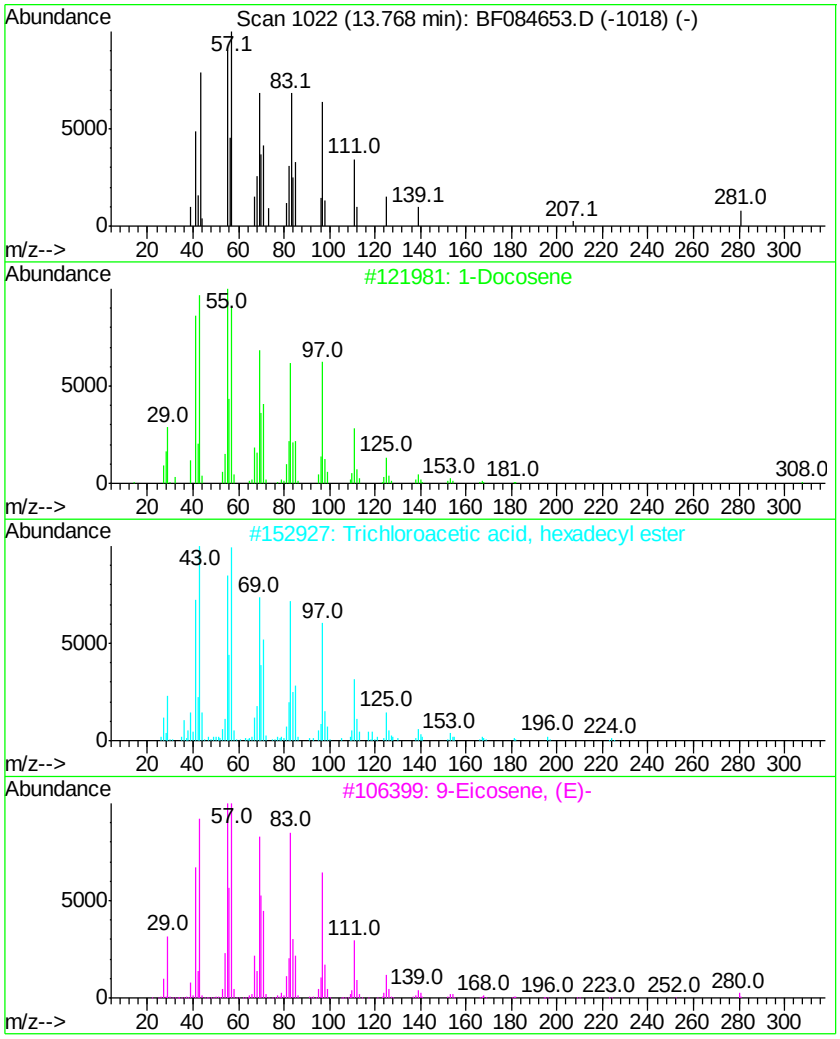
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

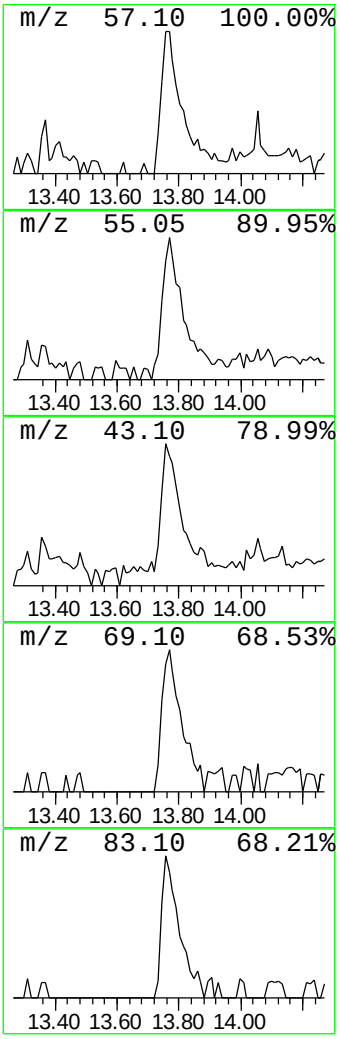
****

Peak Number 7 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.46 ng	154743	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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

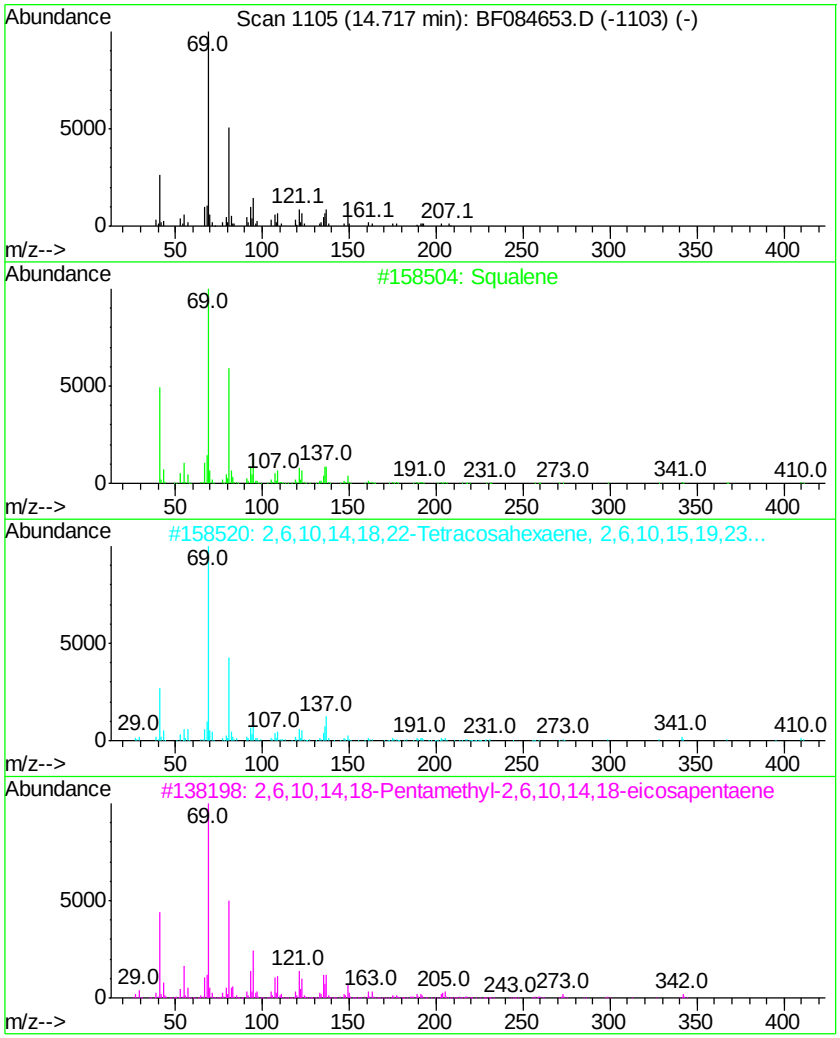
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

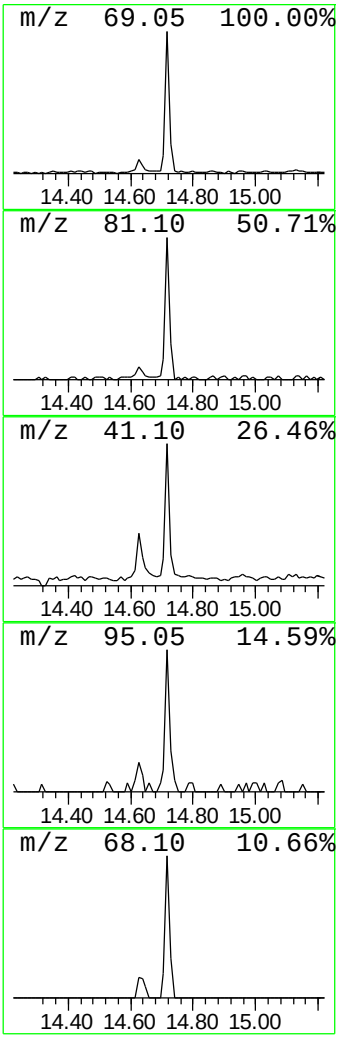
****

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.07 ng	122275	Perylene-d12	15.25

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	86
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084653.D
Acq On : 29 Jan 2016 23:37
Operator : SJ/IZ
Sample : H1273-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B011(40-42)

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	3.8	ng	194473	1	6.73	1023730	20.0
2-Pentanone, 4-hy...	4.89	53.5	ng	2739820	1	6.73	1023730	20.0
2-Pentanone, 4-me...	5.72	3.0	ng	152966	1	6.73	1023730	20.0
unknown6.49	6.49	63.7	ng	3260400	1	6.73	1023730	20.0
Hexadecane	10.67	2.1	ng	161414	4	11.24	1550970	20.0
1-Docosene	13.77	2.5	ng	154743	5	13.87	1260550	20.0
Squalene	14.72	2.1	ng	122275	6	15.25	1183950	20.0