LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

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-BF110316.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	1.755	4	6	68	rVB	3396320	9207894	100.00%	18.330%
2	4.807	270	273	285	rBV	711141	1133357	12.31%	2.256%
3	5.253	310	312	315	rBV	3321794	4543743	49.35%	9.045%
4	6.316	402	405	408	rBV	3617376	4638191	50.37%	9.233%
5	6.430	413	415	418	rBV	4415398	4482825	48.68%	8.924%
6	6.659	433	435	441	rBV	1075128	1042542	11.32%	2.075%
7	6.819	446	449	451	rBV	3850677	3763939	40.88%	7.493%
8	7.230	482	485	495	rBV	2726451	2905229	31.55%	5.784%
9	7.950	545	548	550	rBV	1306413	1327601	14.42%	2.643%
10	9.025	639	642	645	rBV	4737980	4498342	48.85%	8.955%
11	9.425	674	677	679	rBV	739653	622704	6.76%	1.240%
12	9.699	698	701	703	rBV	1427086	1480496	16.08%	2.947%
13	10.488	767	770	772	rBV	2431174	2600862	28.25%	5.178%
14	10.613	779	781	785	rVB	121944	154350	1.68%	0.307%
15	11.059	818	820	821	rBV	113402	98398	1.07%	0.196%
16	11.174	828	830	834	rBV	1451773	1260644	13.69%	2.510%
17	12.762	966	969	971	rBV	3754159	3563452	38.70%	7.094%
18	13.665	1045	1048	1058	rBV	93026	145974	1.59%	0.291%
19	13.802	1058	1060	1063	rBV	990251	911463	9.90%	1.814%
20	14.568	1124	1127	1129	rBV	663599	844806	9.17%	1.682%
21	14.648	1132	1134	1137	rVB	166563	164062	1.78%	0.327%
22	15.174	1178	1180	1183	rBV	584754	842175	9.15%	1.677%

Sum of corrected areas: 50233049

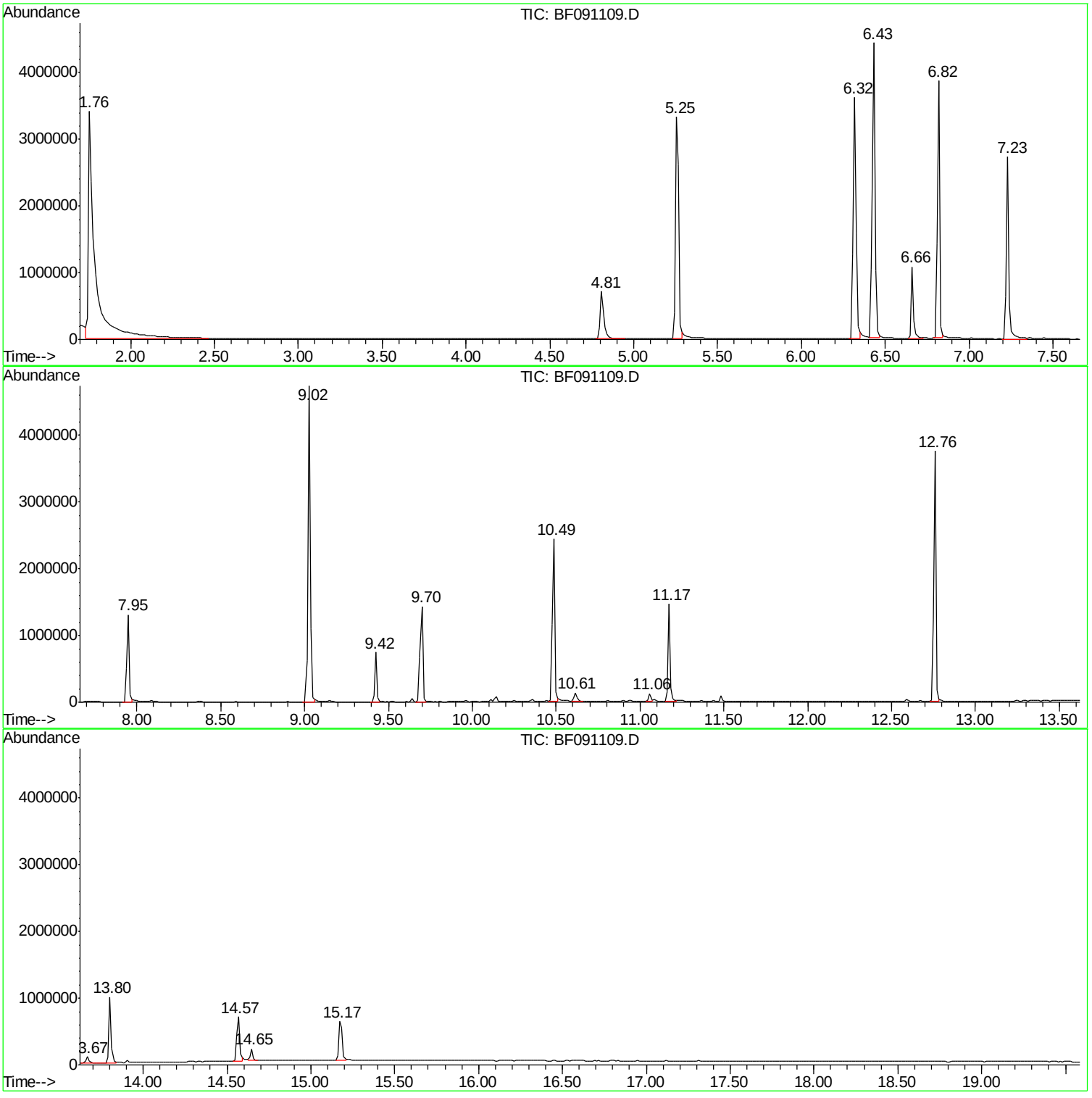
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

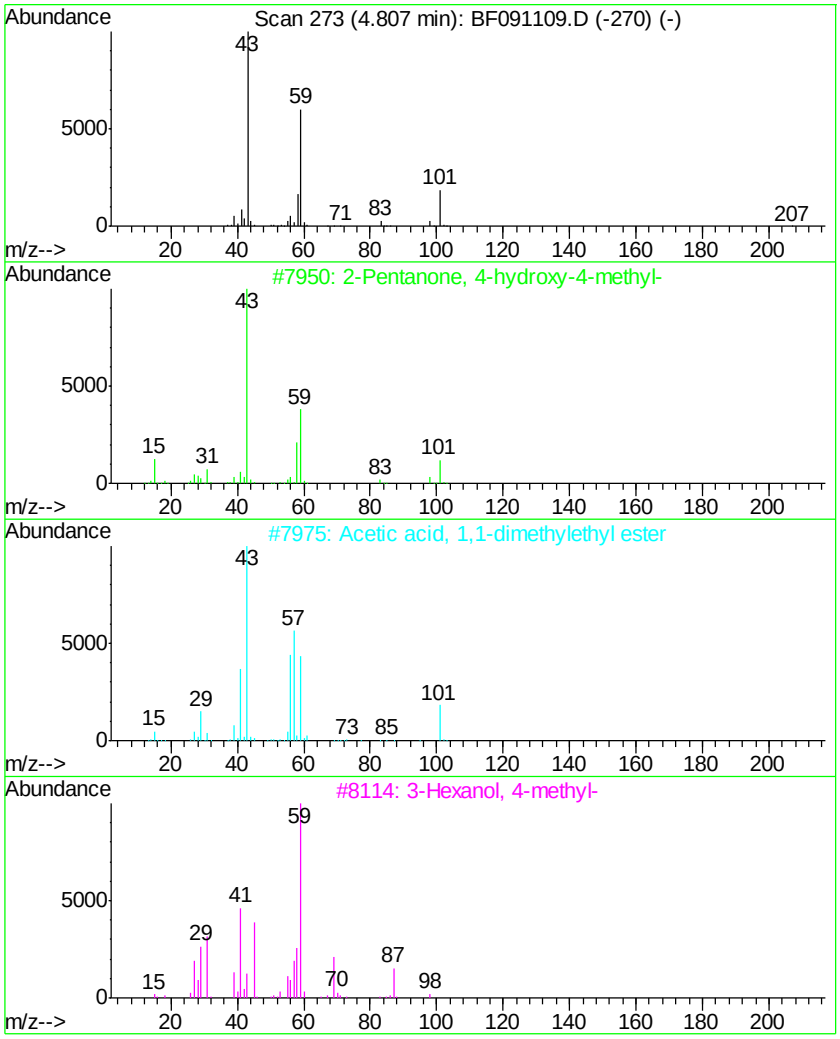
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

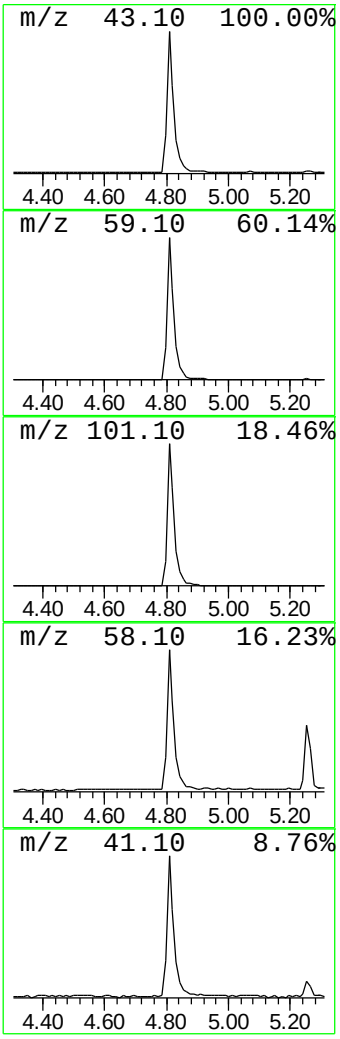
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	21.74 ng	1133360	1,4-Dichlorobenzene-d4	6.66

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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

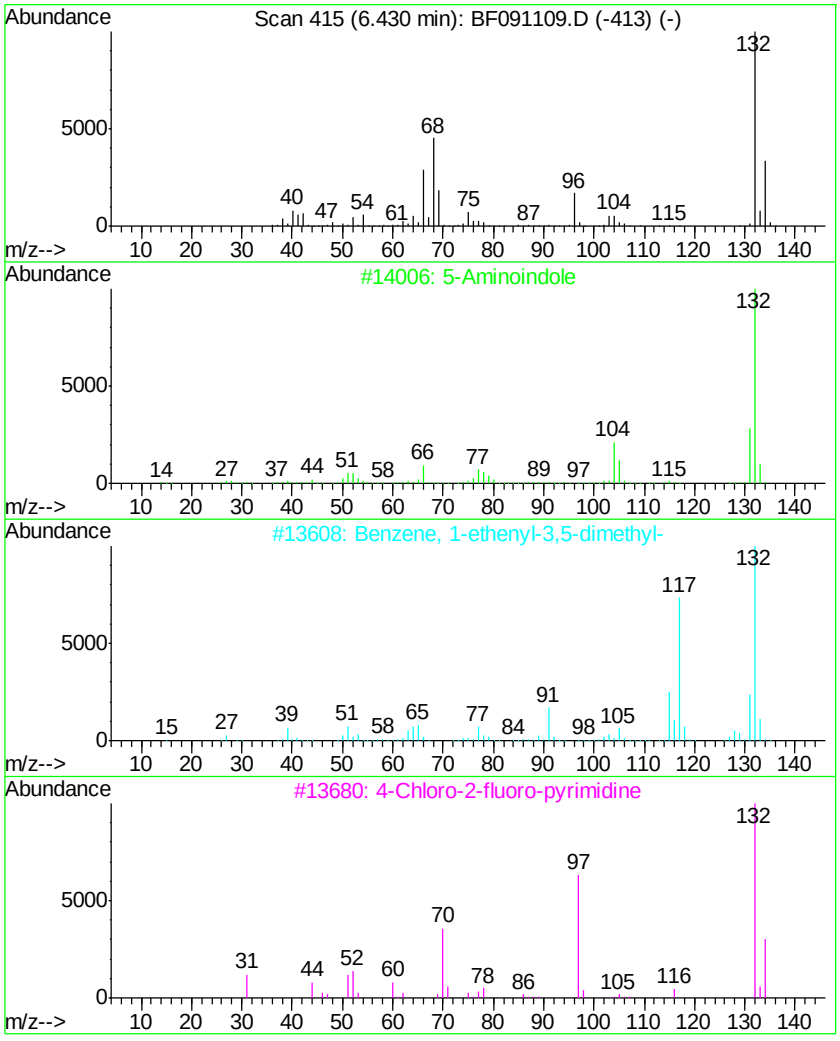
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

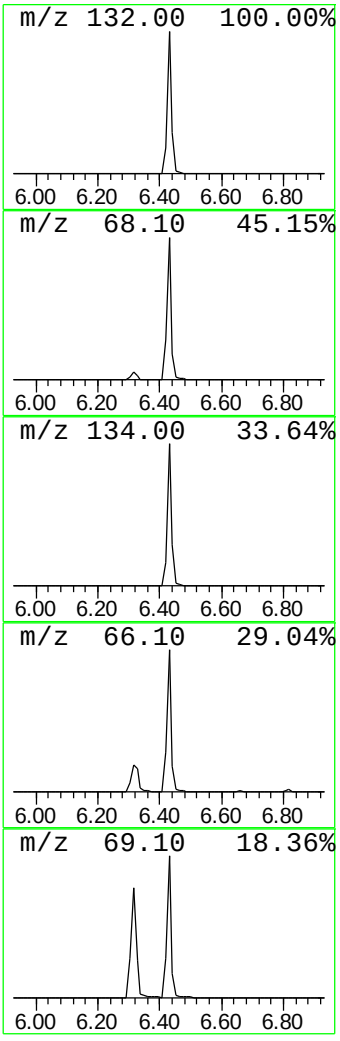
****

Peak Number 3 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	86.00 ng	4482830	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

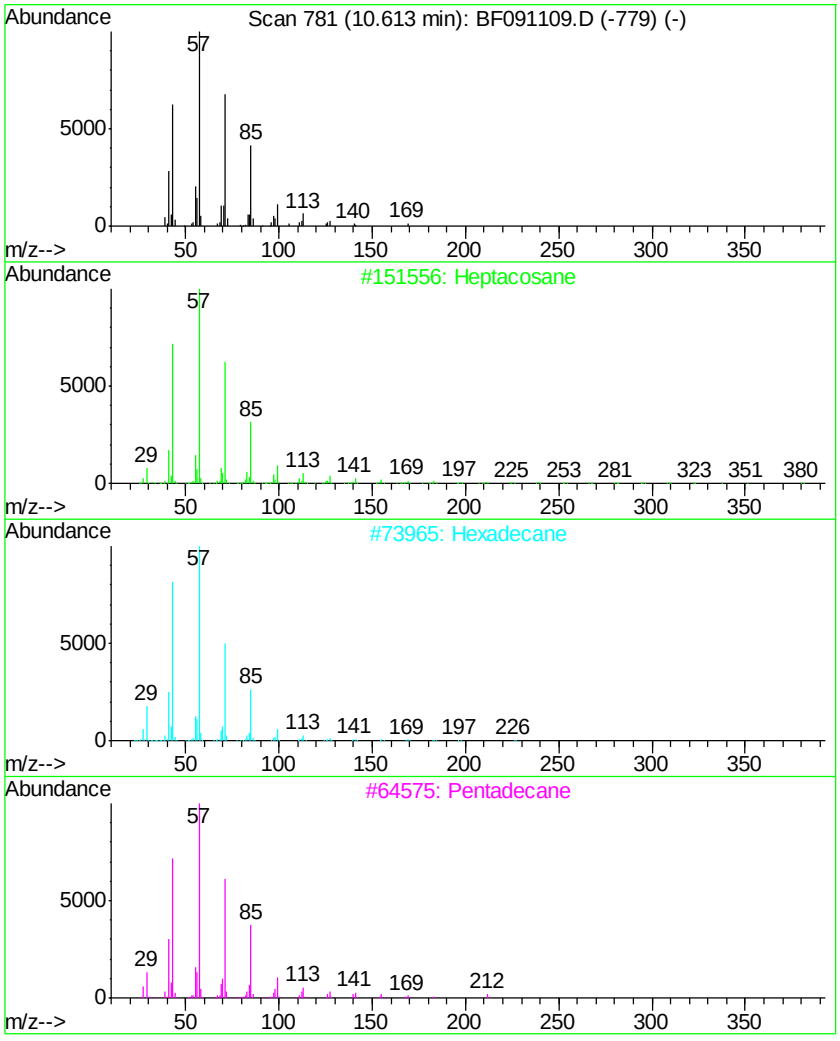
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

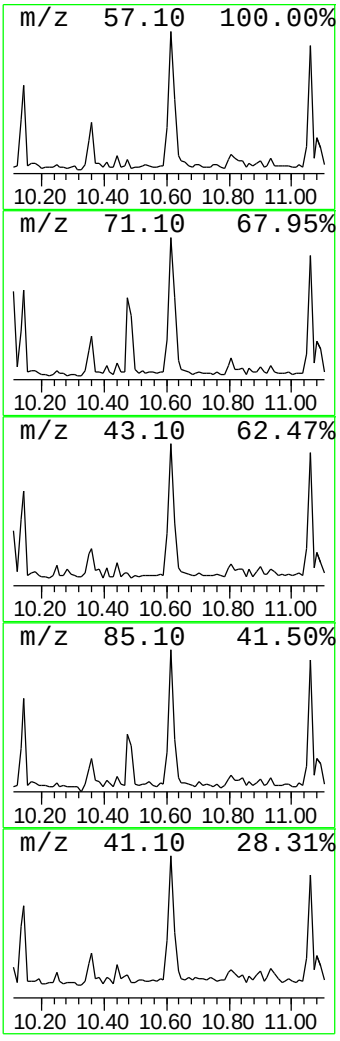
****

Peak Number 5 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	2.45 ng	154350	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tetracosane	338	C24H50	000646-31-1	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

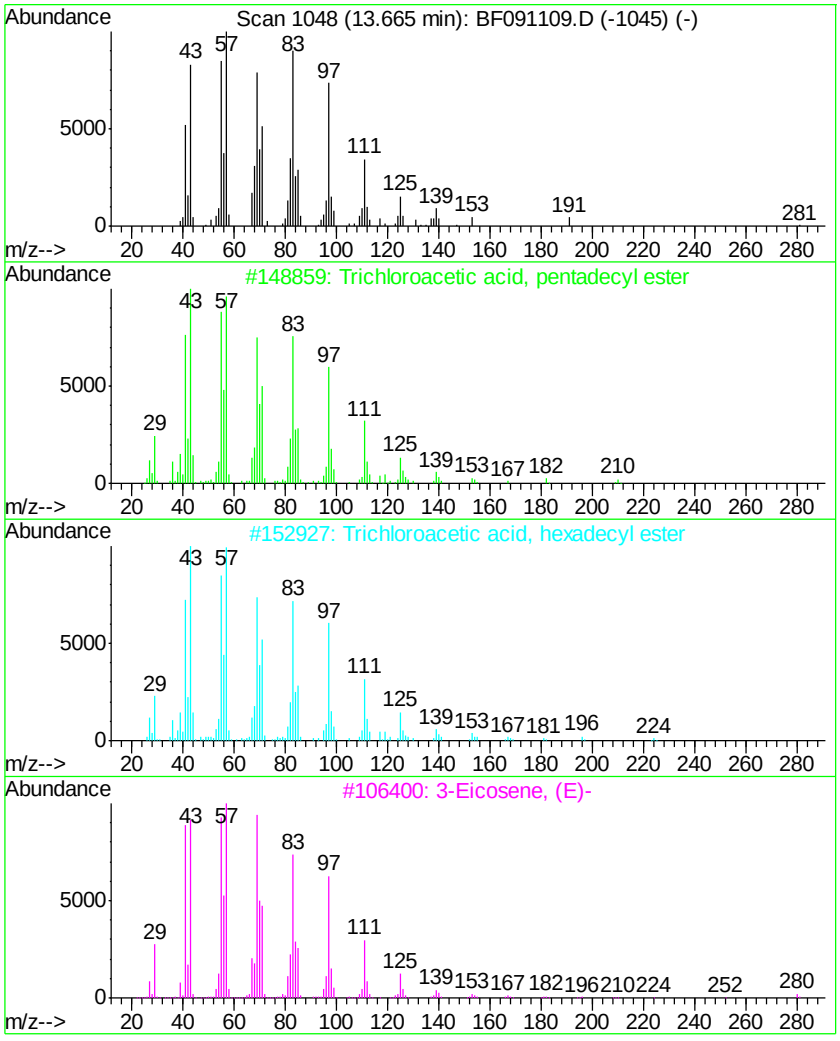
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

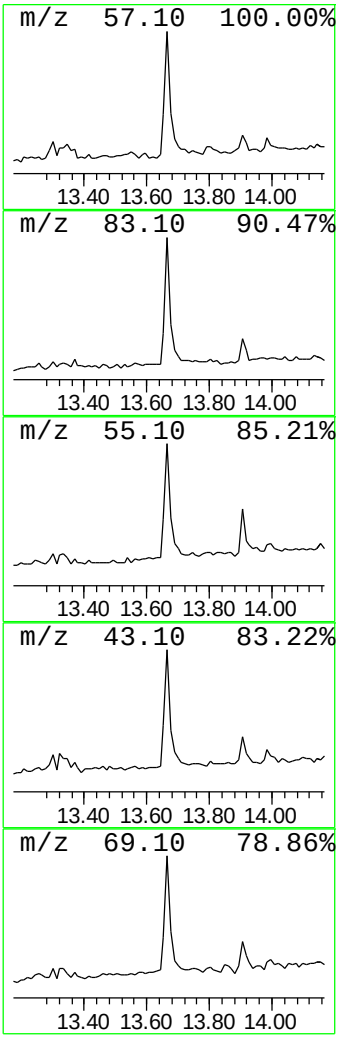
****

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	3.20 ng	145974	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

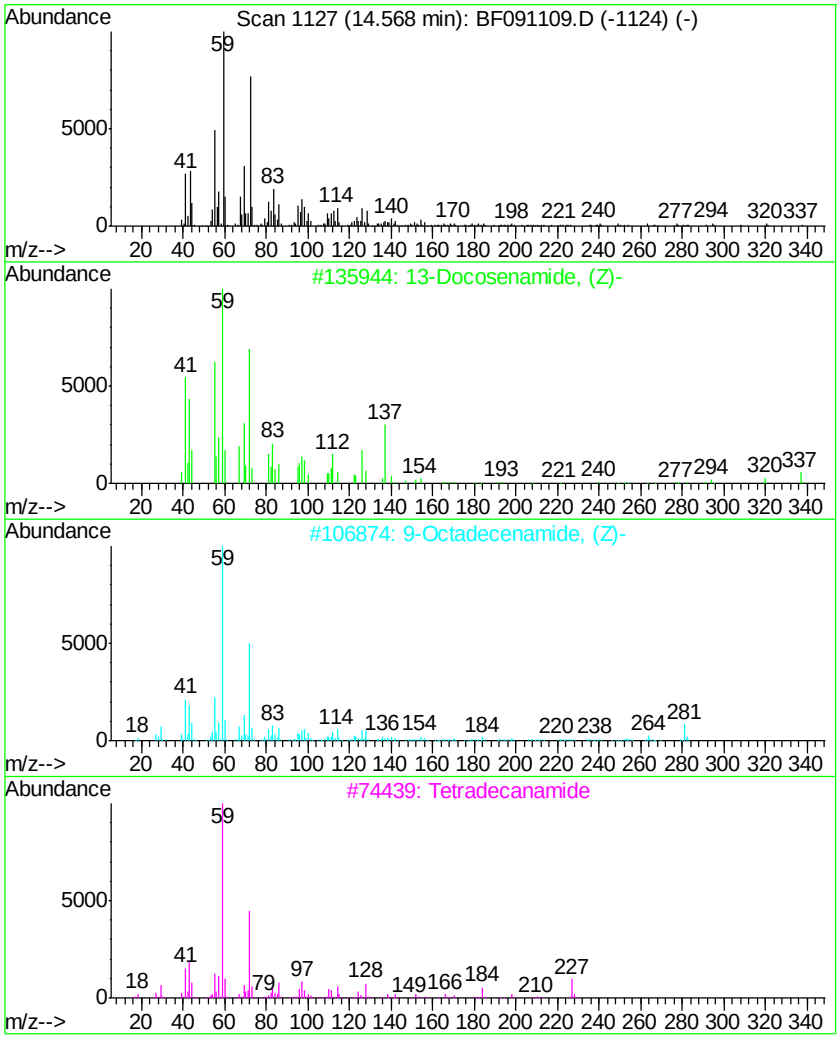
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

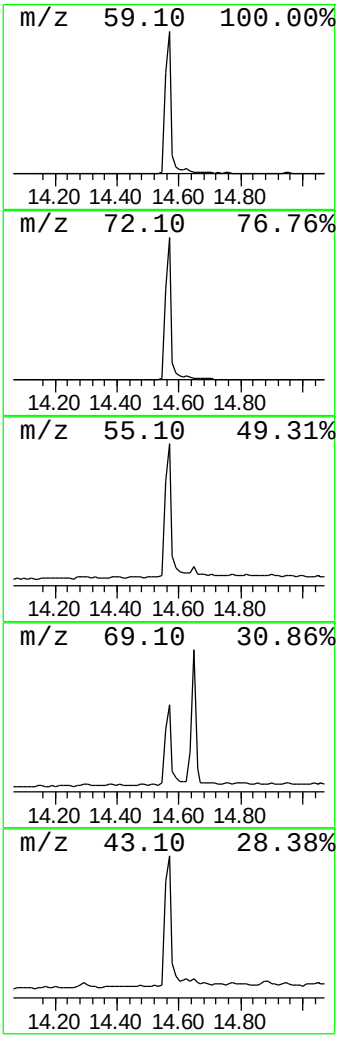
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	20.06 ng	844806	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	62
3	Tetradecanamide	227	C14H29NO	000638-58-4	50
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	43
5	Hexadecanamide	255	C16H33NO	000629-54-9	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

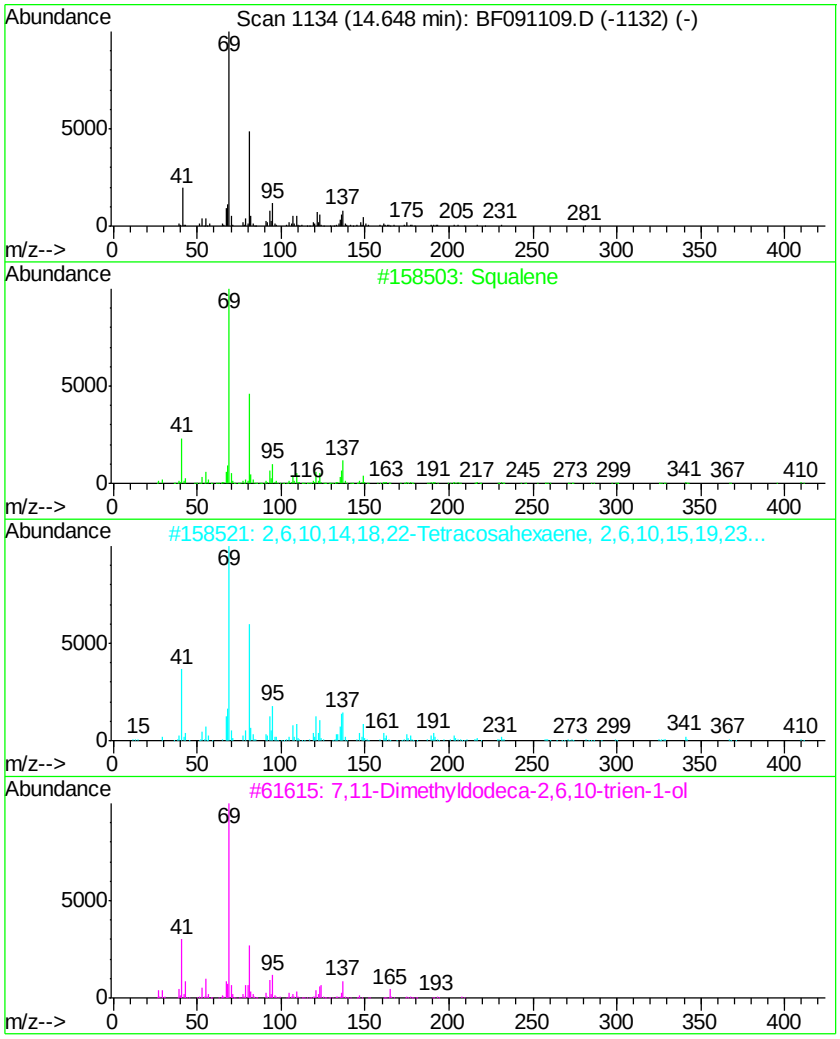
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

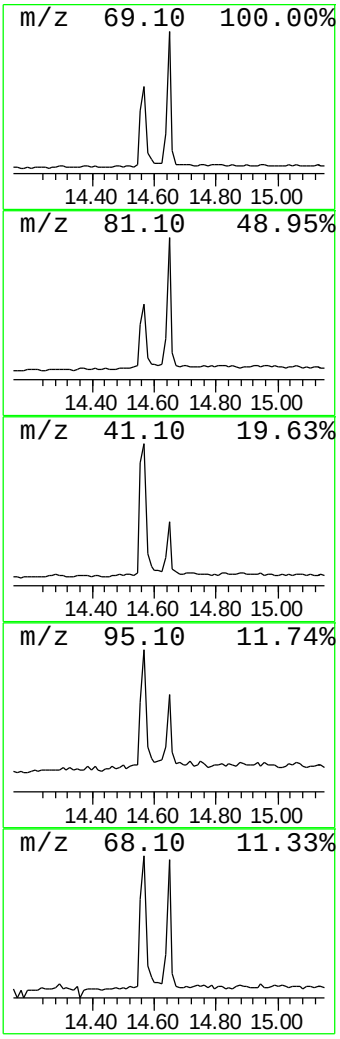
****

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	3.90 ng	164062	Perylene-d12	15.19

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	90
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
5	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110816\
Data File : BF091109.D
Acq On : 9 Nov 2016 4:38
Operator : UM/SJ
Sample : H5593-05
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-SIDEWALL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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
2-Pentanone, 4-hy...	4.81	21.7	ng	1133360	1	6.66	1042540	20.0
unknown6.43	6.43	86.0	ng	4482830	1	6.66	1042540	20.0
Heptacosane	10.61	2.5	ng	154350	4	11.17	1260640	20.0
Trichloroacetic a...	13.67	3.2	ng	145974	5	13.80	911463	20.0
13-Docosenamide, ...	14.57	20.1	ng	844806	6	15.19	842175	20.0
Squalene	14.65	3.9	ng	164062	6	15.19	842175	20.0