LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

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-BF063016.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	1.735	11	13	15	rBV	424861	620188	13.40%	2.047%
2	1.770	15	16	23	rVB	415650	547328	11.82%	1.807%
3	1.873	23	25	39	rVB	2039822	4629238	100.00%	15.283%
4	2.055	39	41	49	rVB	75439	147336	3.18%	0.486%
5	2.707	95	98	102	rVB	108345	172555	3.73%	0.570%
6	3.061	126	129	143	rBV	105129	247571	5.35%	0.817%
7	4.981	294	297	303	rBV	259675	345247	7.46%	1.140%
8	5.404	331	334	336	rBV	2463950	2430665	52.51%	8.024%
9	6.444	421	425	427	rBV	2218174	2894353	62.52%	9.555%
10	6.570	433	436	439	rBV	2192396	2487585	53.74%	8.212%
11	6.810	454	457	459	rBV	841836	795363	17.18%	2.626%
12	6.959	468	470	473	rVB	1513134	2048408	44.25%	6.763%
13	7.370	503	506	508	rBV	1769246	1675890	36.20%	5.533%
14	8.090	567	569	572	rVB	1149696	995802	21.51%	3.287%
15	9.165	661	663	666	rVB	1923562	2830240	61.14%	9.344%
16	9.565	696	698	700	rBV	245937	237101	5.12%	0.783%
17	9.839	720	722	725	rVB2	992883	992080	21.43%	3.275%
18	10.628	788	791	793	rBV	1472941	1440729	31.12%	4.756%
19	10.753	801	802	806	rVB	40415	55448	1.20%	0.183%
20	11.199	839	841	843	rBV	83652	89448	1.93%	0.295%
21	11.313	849	851	854	rVV	624692	850657	18.38%	2.808%
22	11.382	854	857	861	rVB2	25001	54637	1.18%	0.180%
23	11.633	877	879	882	rVB	42251	59973	1.30%	0.198%
24	12.902	987	990	993	rBV	2071663	1953048	42.19%	6.448%
25	13.805	1067	1069	1073	rBV	125342	176528	3.81%	0.583%
26	13.942	1079	1081	1084	rBV	792502	740327	15.99%	2.444%
27	14.445	1122	1125	1128	rBV	60955	96905	2.09%	0.320%
28	15.348	1201	1204	1206	rBV	449253	605679	13.08%	2.000%
29	16.880	1335	1338	1343	rVB2	35611	70259	1.52%	0.232%

Sum of corrected areas: 30290588

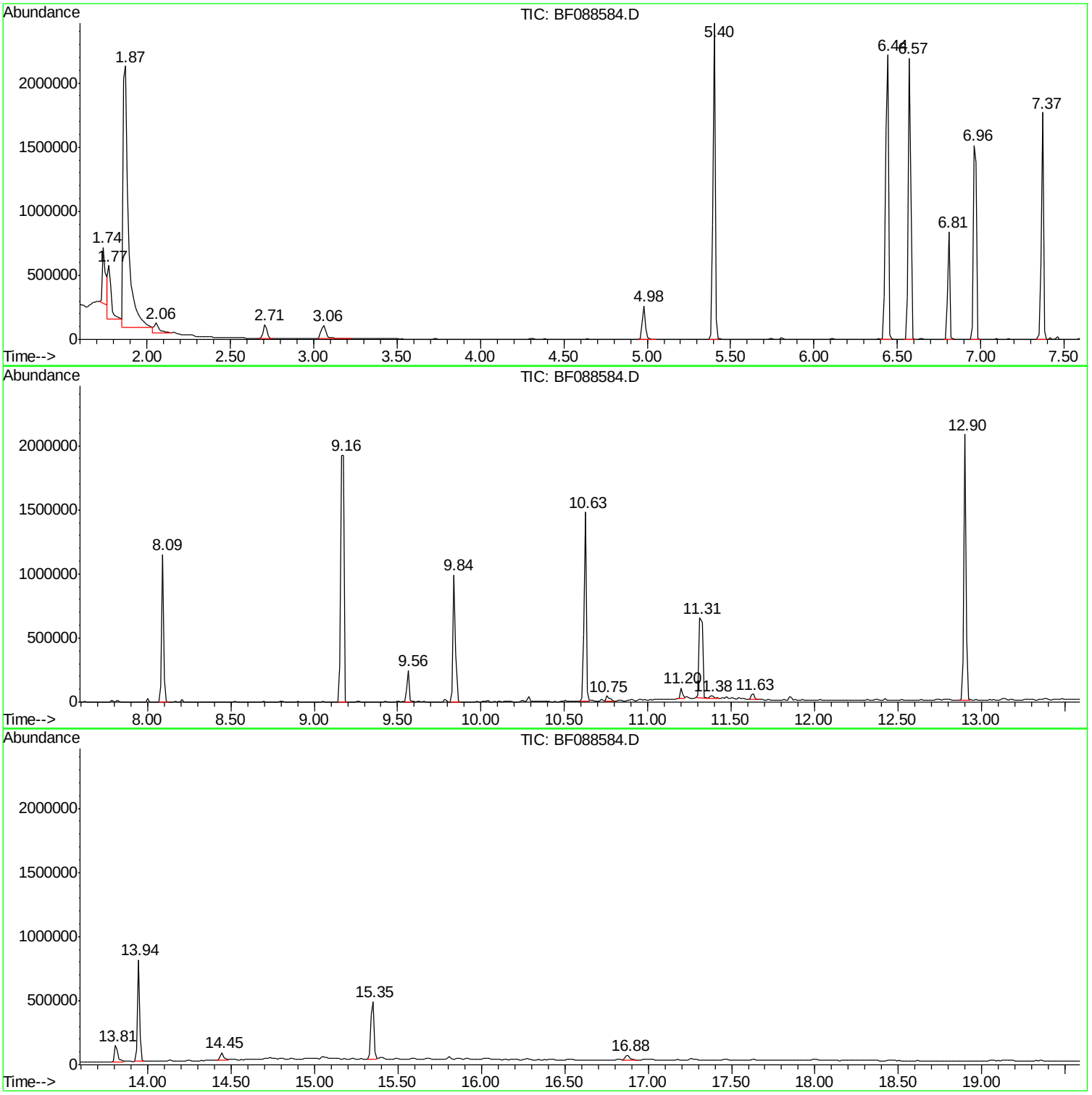
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

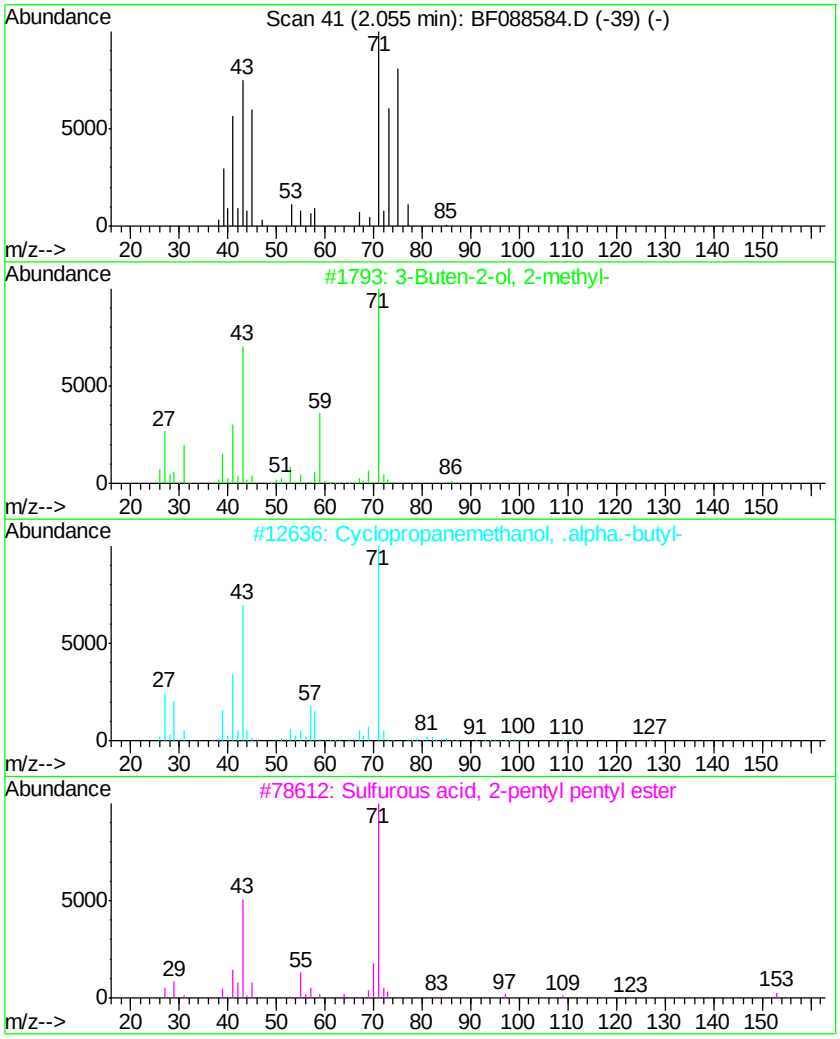
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

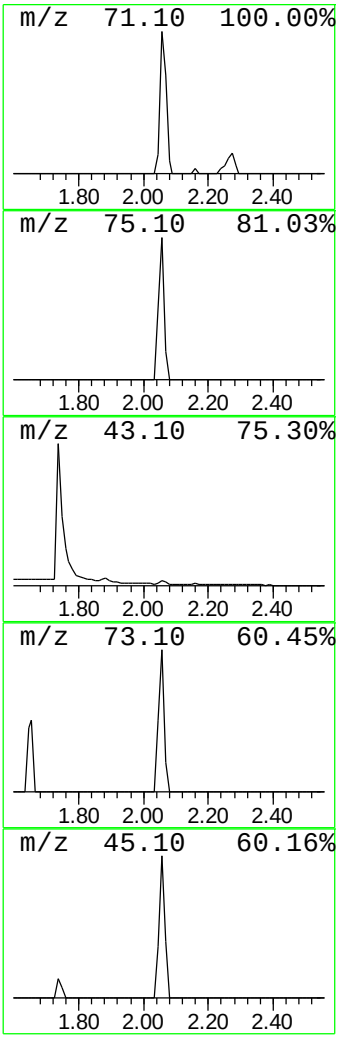
****

Peak Number 4 unknown2.06 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	3.70 ng	147336	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	25
2	Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	25
3	Sulfurous acid, 2-pentyl pentyl ...	222	C10H22O3S	1000309-15-4	17
4	1-Penten-3-ol, 3-methyl-	100	C6H12O	000918-85-4	17
5	Pantolactone	130	C6H10O3	000599-04-2	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

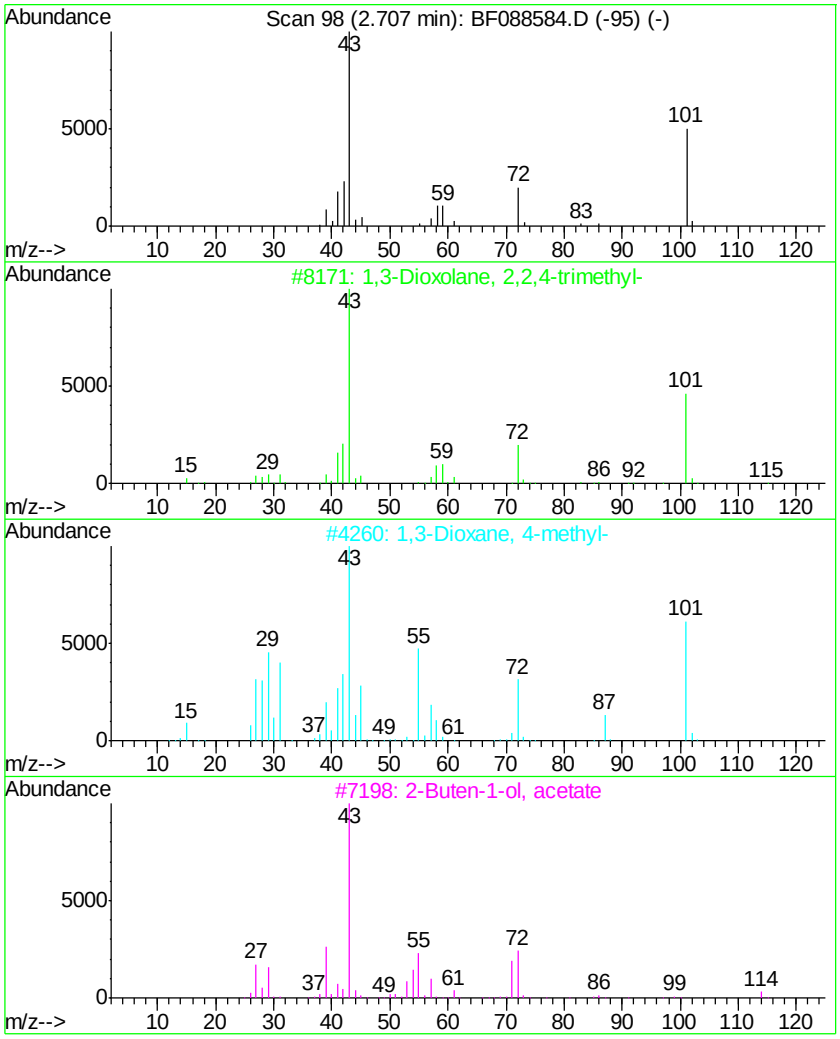
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

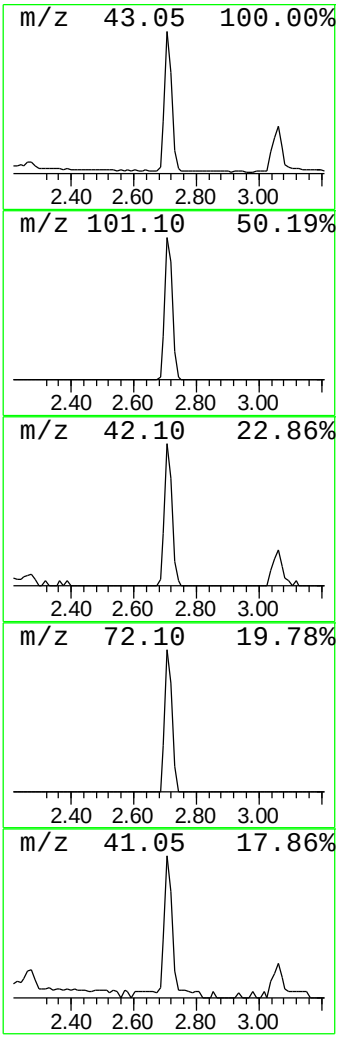
****

Peak Number 5 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.71	4.34 ng	172555	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
3	2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	12
4	1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	12
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

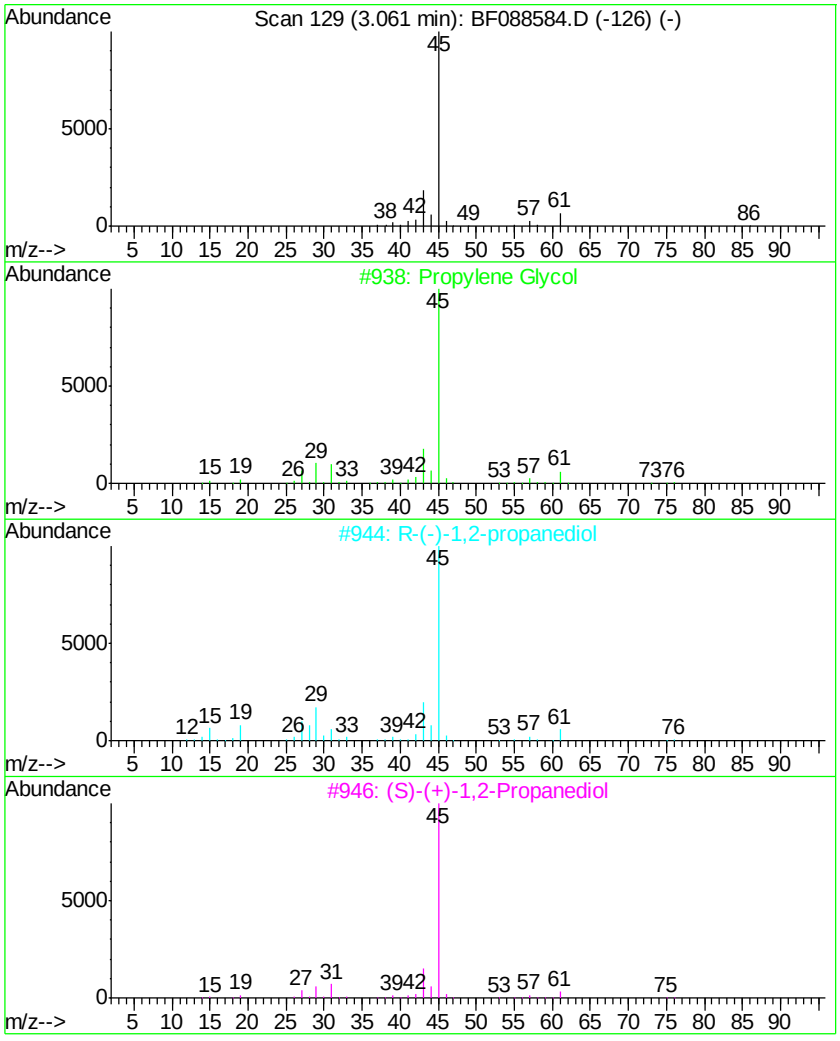
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

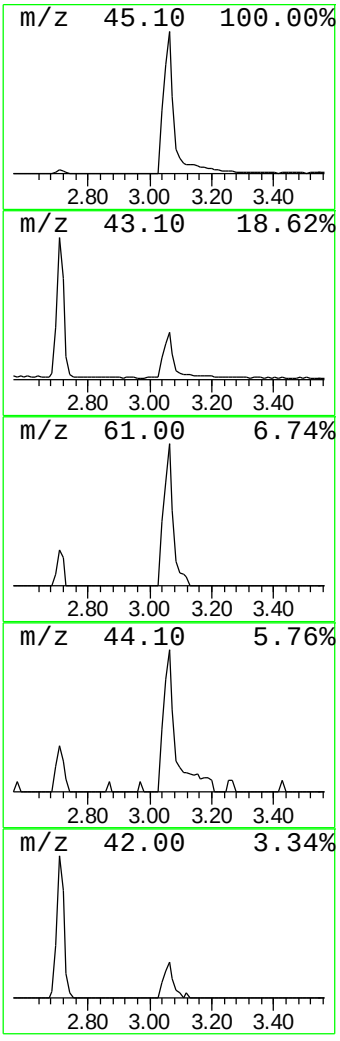
****

Peak Number 6 unknown3.06 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	6.23 ng	247571	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Butanol	74	C4H10O	000078-92-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

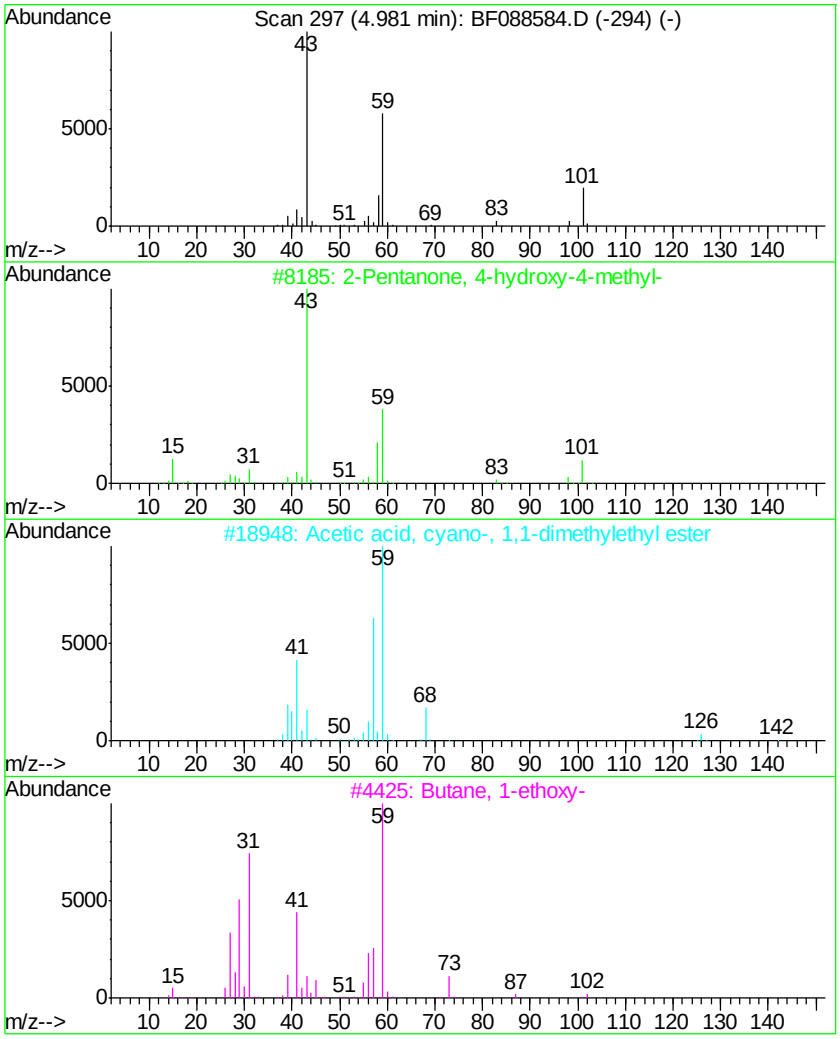
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

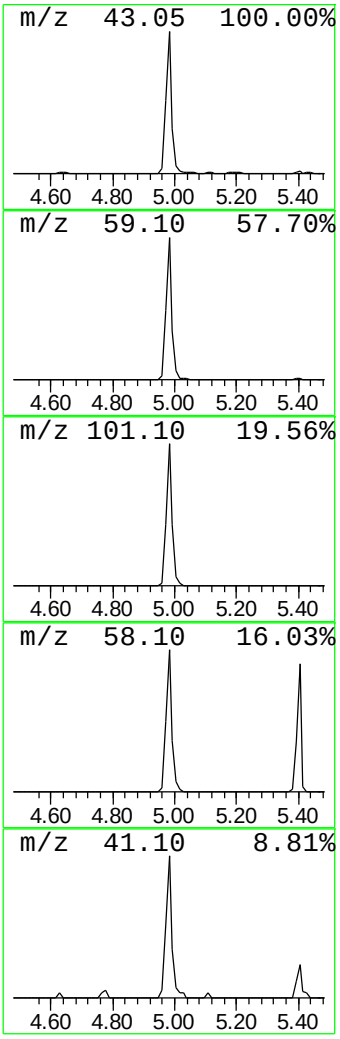
****

Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	8.68 ng	345247	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

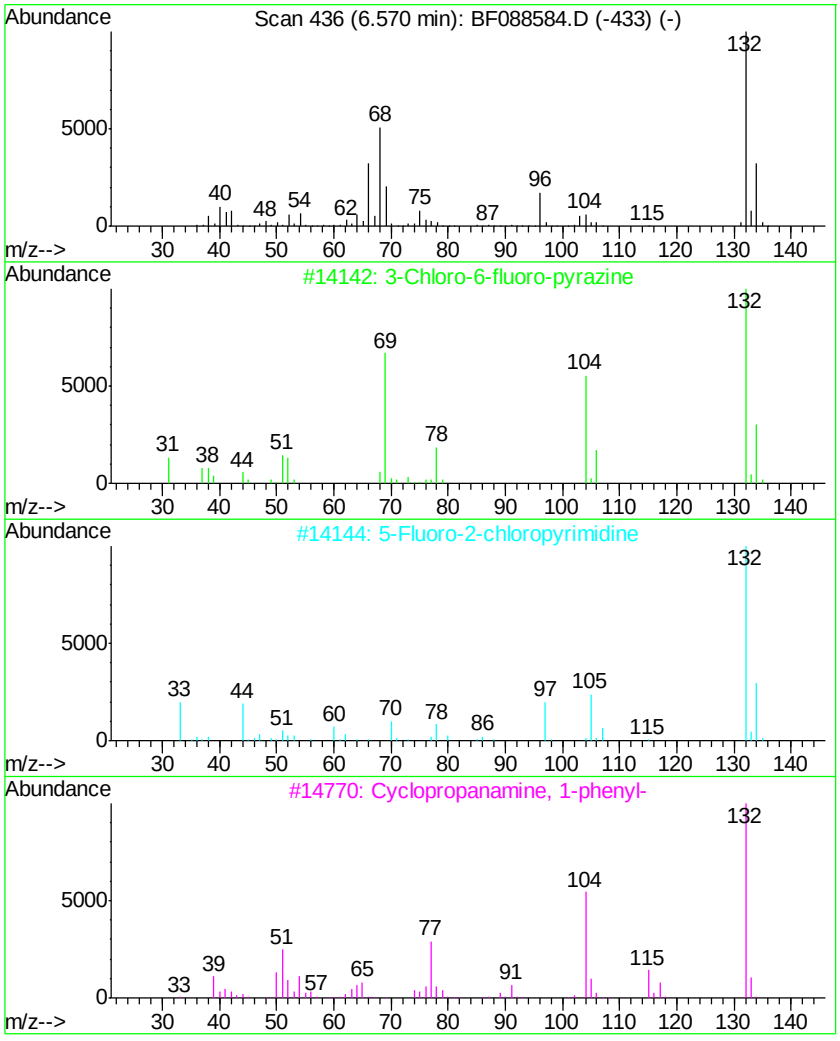
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

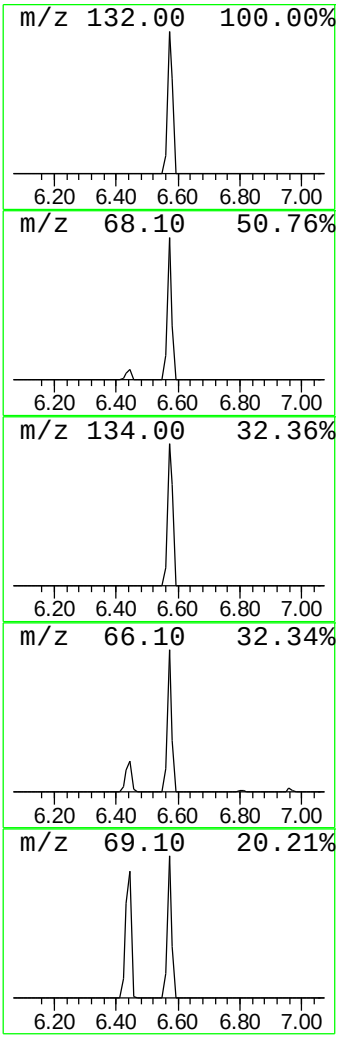
****

Peak Number 8 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	62.55 ng	2487590	1,4-Dichlorobenzene-d4	6.81

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	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

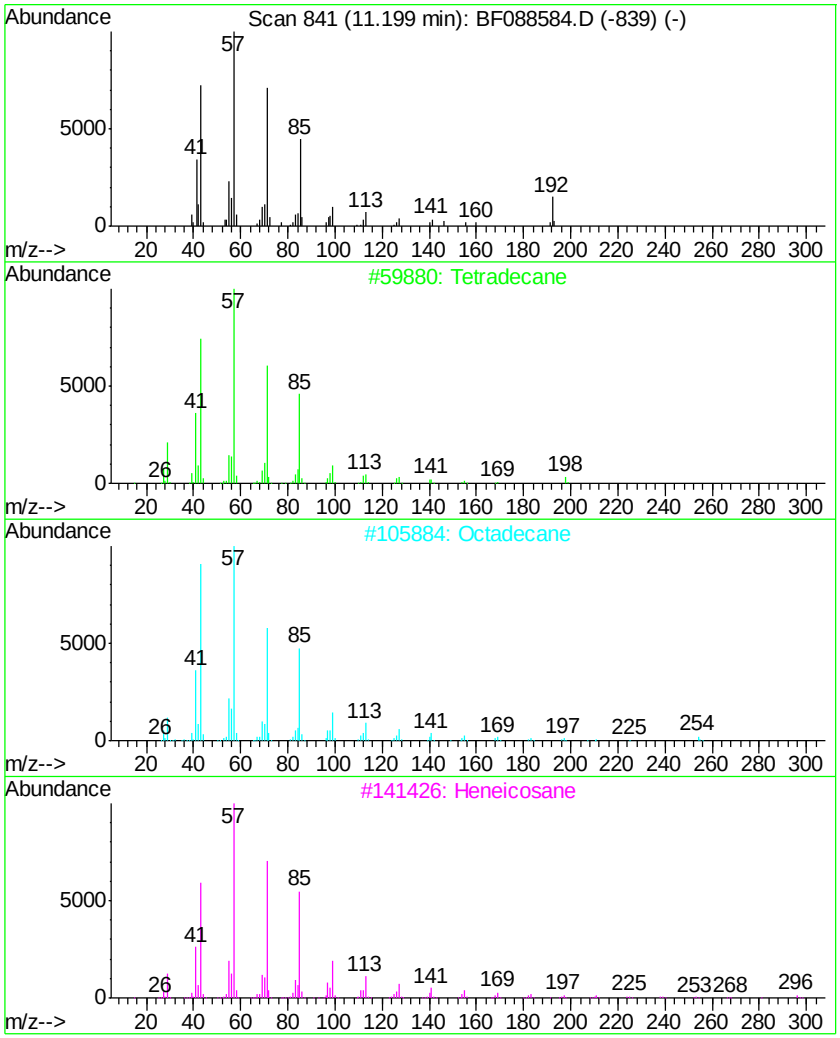
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

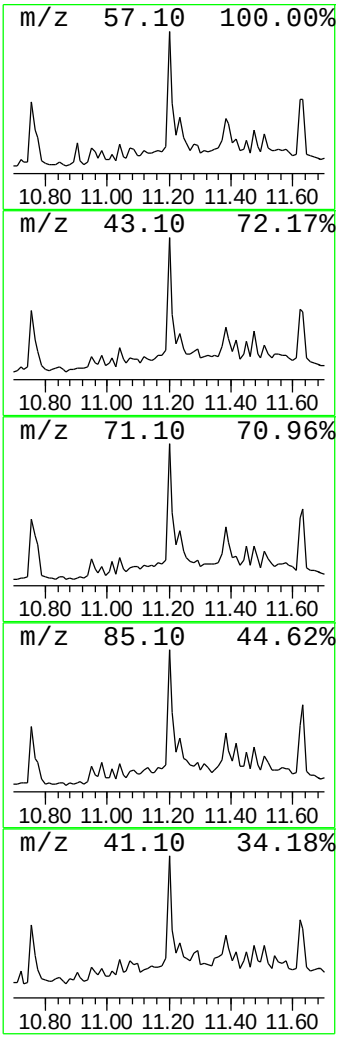
****

Peak Number 10 Tetradecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	2.10 ng	89448	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	87
2	Octadecane	254	C18H38	000593-45-3	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Tetracosane	338	C24H50	000646-31-1	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

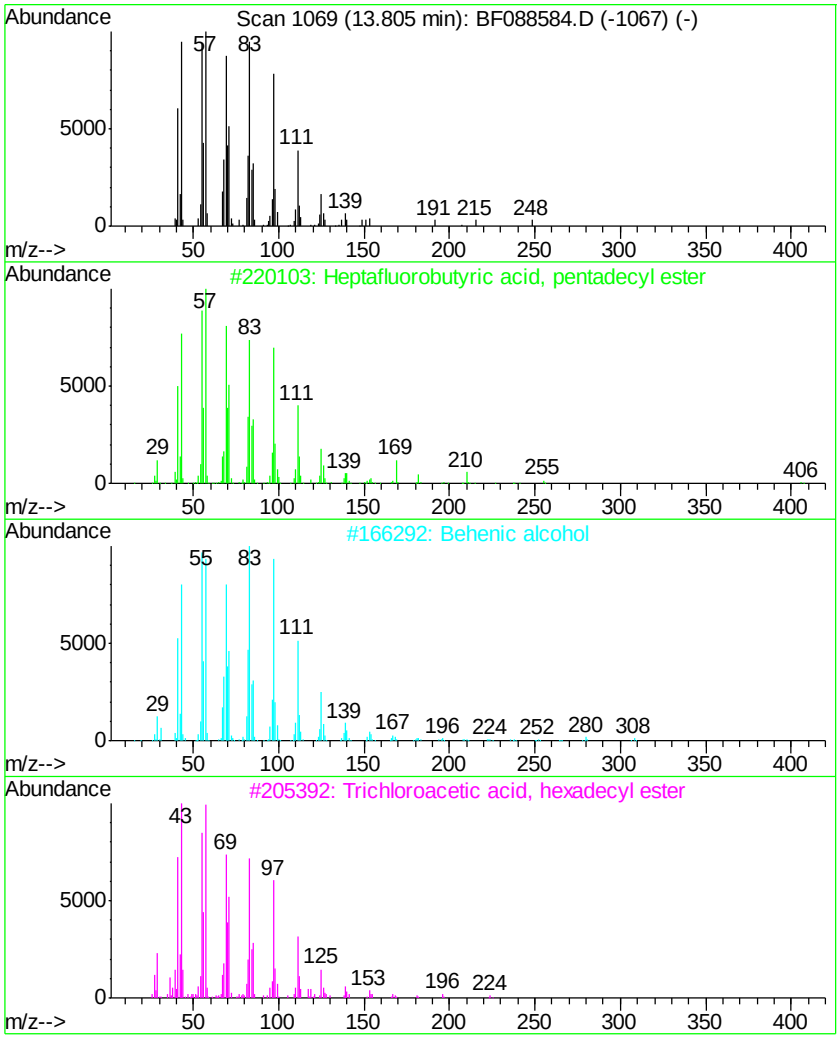
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

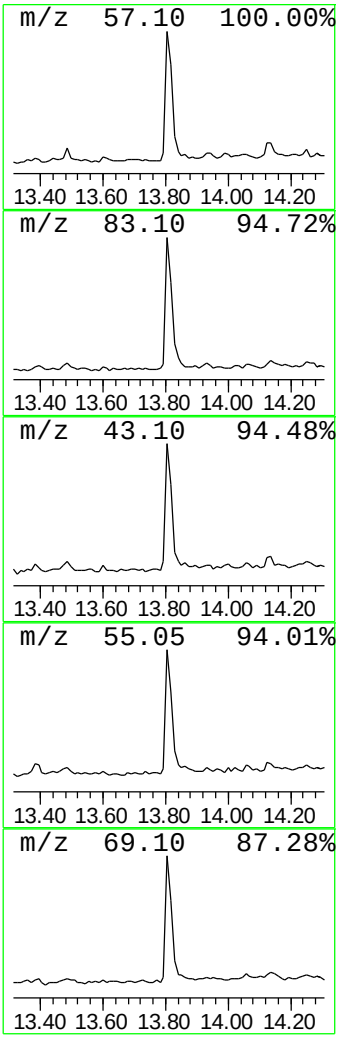
****

Peak Number 11 Heptafluorobutyric acid, pe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.77 ng	176528	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

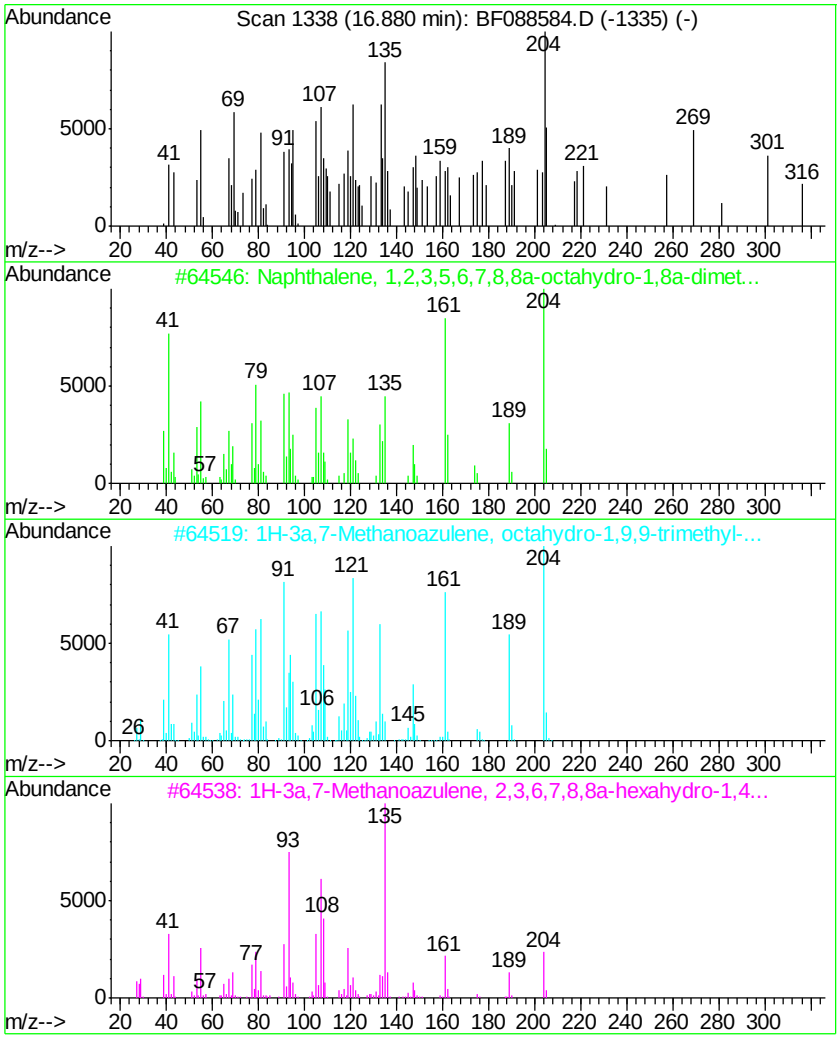
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

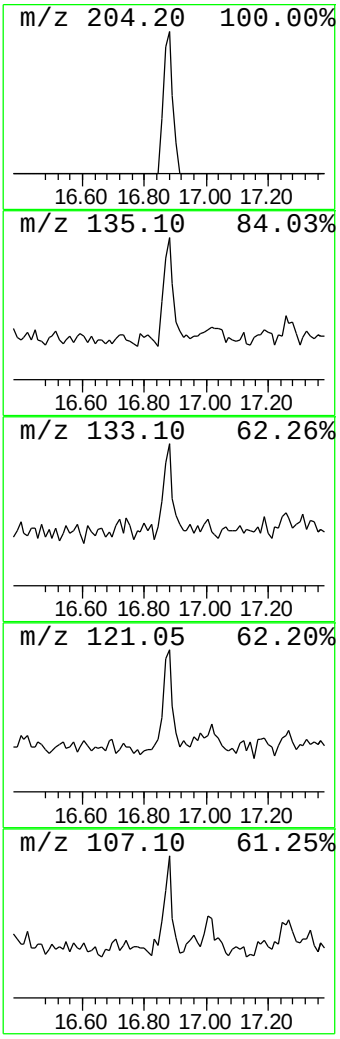
****

Peak Number 13 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	2.32 ng	70259	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	60
2	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	55
3	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	49
4	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	49
5	.alpha.-Bulnesene	204	C15H24	1000374-19-9	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088584.D
Acq On : 1 Jul 2016 19:44
Operator : UM/SJ
Sample : H3836-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.1-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.06	2.06	3.7	ng	147336	1	6.81	795363	20.0
1,3-Dioxolane, 2,...	2.71	4.3	ng	172555	1	6.81	795363	20.0
unknown3.06	3.06	6.2	ng	247571	1	6.81	795363	20.0
2-Pentanone, 4-hy...	4.98	8.7	ng	345247	1	6.81	795363	20.0
unknown6.57	6.57	62.5	ng	2487590	1	6.81	795363	20.0
Tetradecane	11.20	2.1	ng	89448	4	11.32	850657	20.0
Heptafluorobutyri...	13.81	4.8	ng	176528	5	13.94	740327	20.0
Naphthalene, 1,2,...	16.88	2.3	ng	70259	6	15.35	605679	20.0