LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

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-BF031518.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	2.293	30	35	44	rVB	322777	405192	11.30%	1.848%
2	5.199	526	529	541	rVB	220045	216248	6.03%	0.987%
3	5.593	592	596	607	rBV	1235853	1119837	31.23%	5.109%
4	6.587	762	765	768	rBV	752869	704478	19.65%	3.214%
5	6.616	768	770	779	rVB	136859	128316	3.58%	0.585%
6	6.745	787	792	795	rBV	2085266	1993952	55.61%	9.096%
7	6.975	827	831	834	rBV	928063	710927	19.83%	3.243%
8	7.134	854	858	861	rBV	3089937	2672462	74.53%	12.192%
9	7.540	922	927	930	rBV	2144191	2020121	56.34%	9.216%
10	8.257	1045	1049	1054	rBV	1103831	885228	24.69%	4.038%
11	9.334	1227	1232	1235	rBV	3857903	3585896	100.00%	16.359%
12	9.722	1293	1298	1305	rBV	83881	89855	2.51%	0.410%
13	9.928	1330	1333	1336	rBV	96401	70676	1.97%	0.322%
14	10.016	1345	1348	1356	rVB2	992885	864358	24.10%	3.943%
15	10.428	1416	1418	1421	rVB	99607	80098	2.23%	0.365%
16	10.810	1479	1483	1491	rBV	1332285	1256574	35.04%	5.733%
17	10.904	1496	1499	1505	rVB	82313	77603	2.16%	0.354%
18	11.510	1598	1602	1610	rBV	899651	751703	20.96%	3.429%
19	13.098	1867	1872	1875	rBV	3089358	2770998	77.27%	12.641%
20	13.980	2018	2022	2027	rBV	134110	143393	4.00%	0.654%
21	14.163	2049	2053	2057	rBV	824588	714476	19.92%	3.259%
22	15.016	2195	2198	2203	rBV	90596	86069	2.40%	0.393%
23	15.704	2310	2315	2326	rVB	410390	571691	15.94%	2.608%

Sum of corrected areas: 21920151

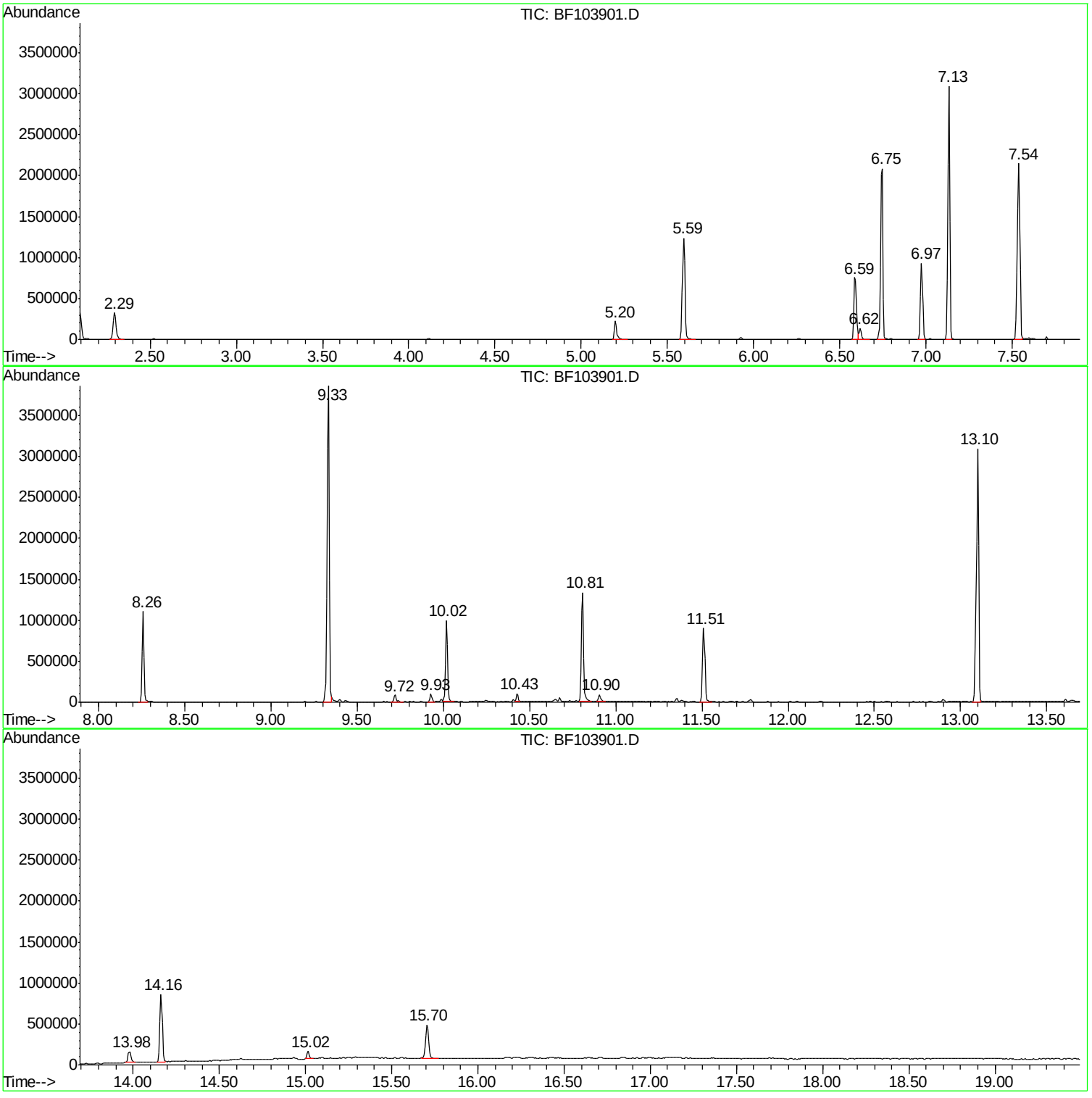
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

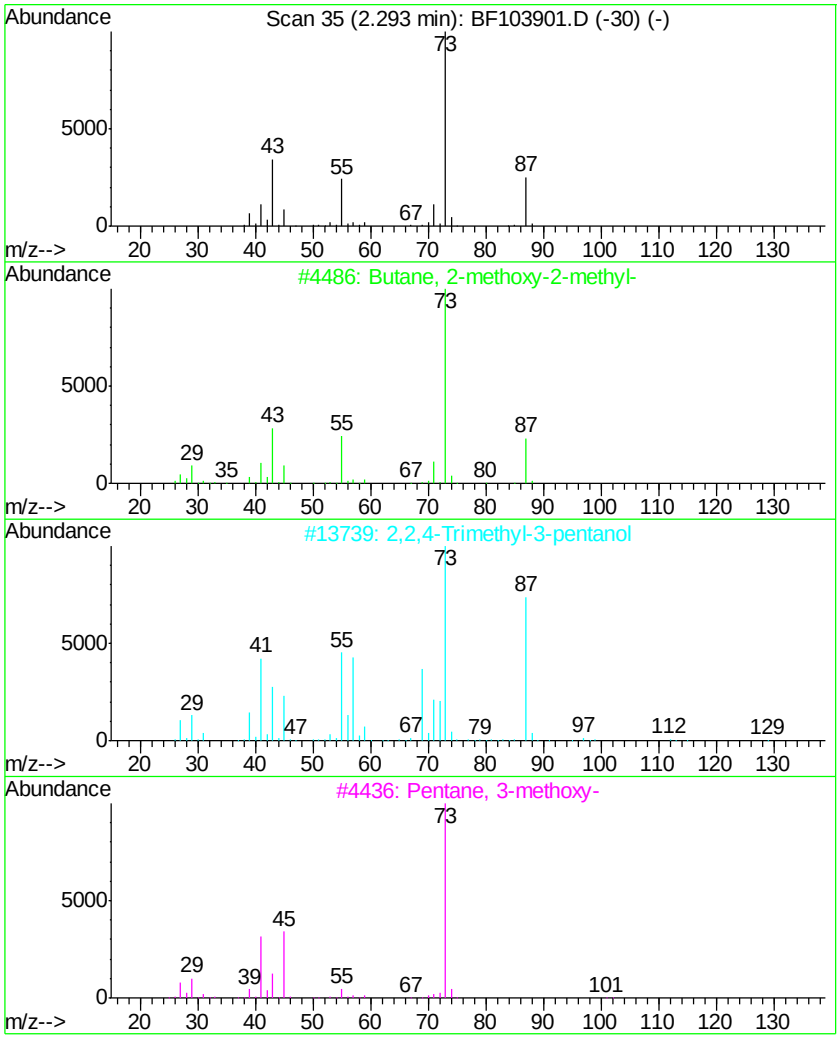
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

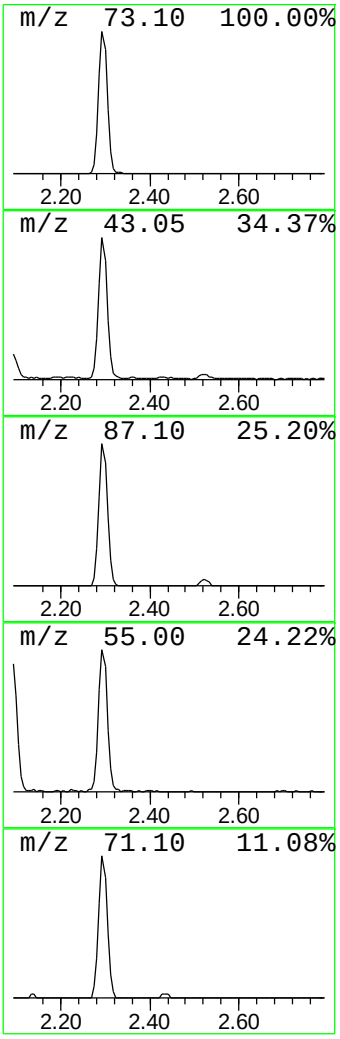
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	11.40 ng	405192	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

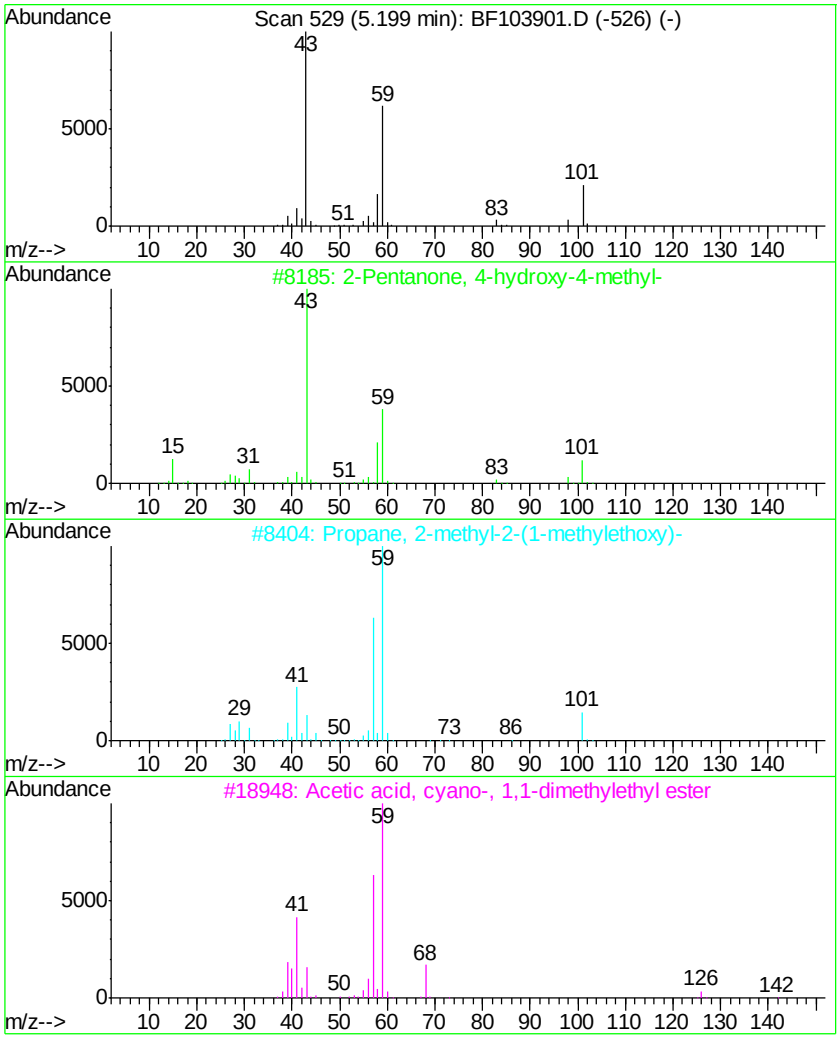
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

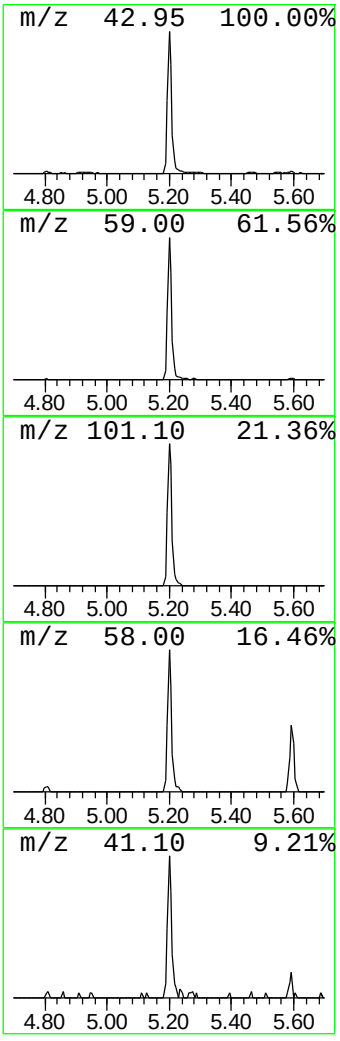
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	6.08 ng	216248	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

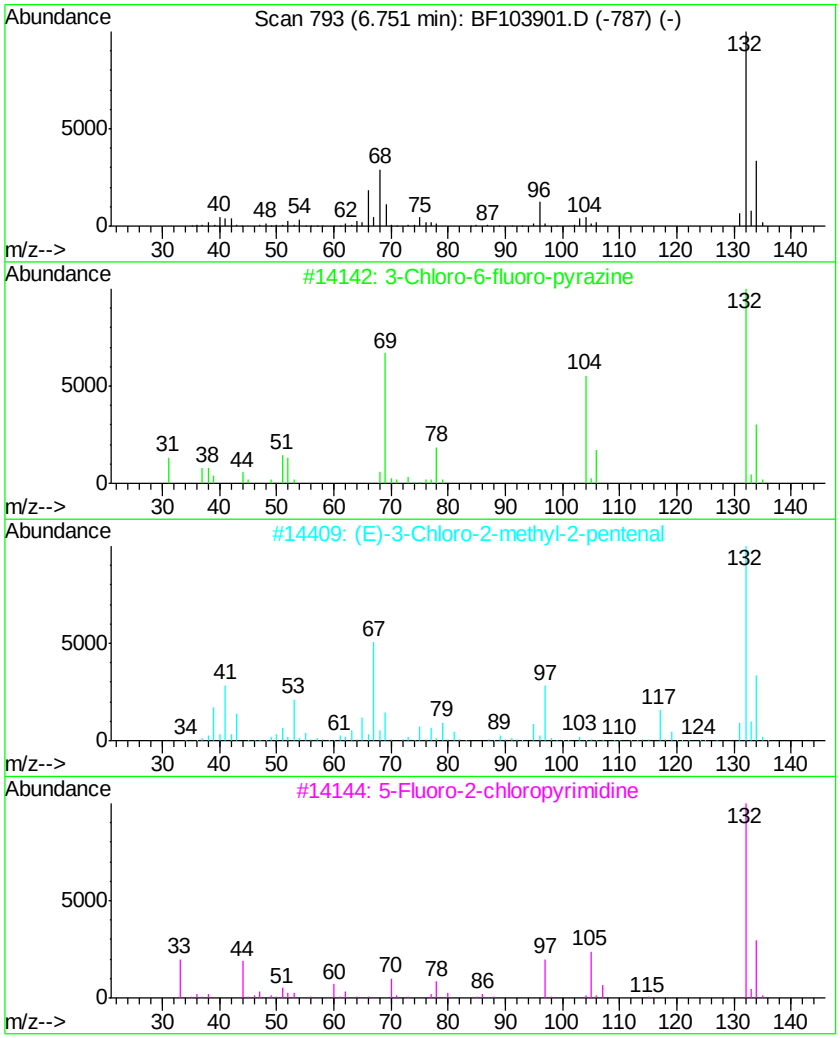
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

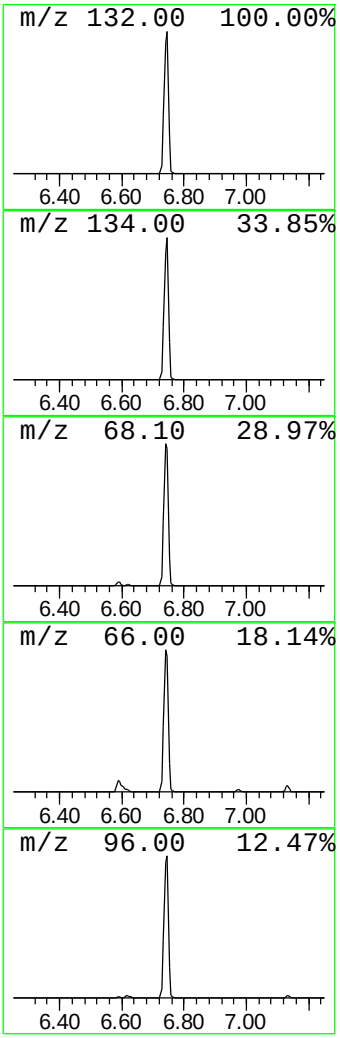
****

Peak Number 3 unknown6.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	56.09 ng	1993950	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

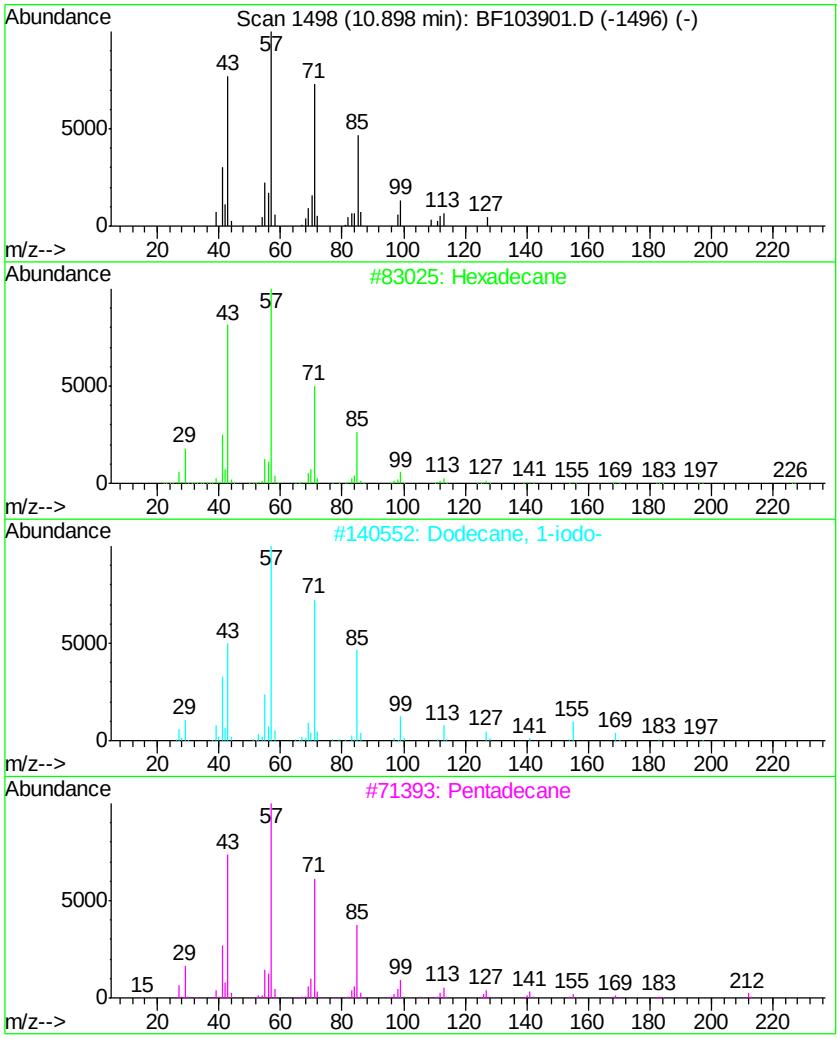
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

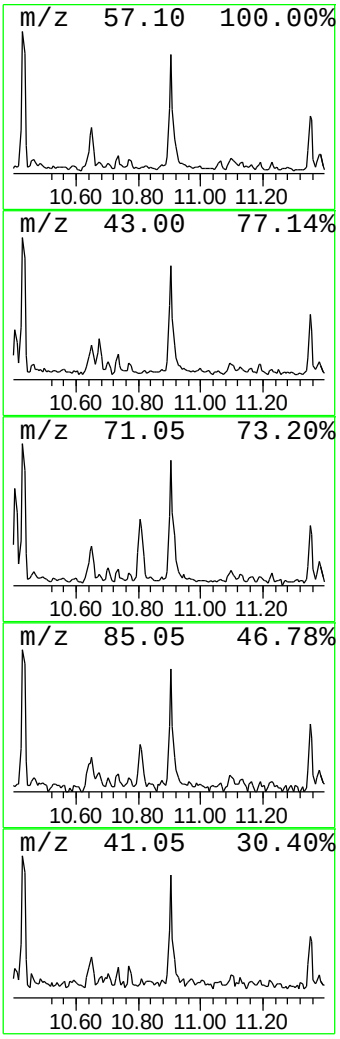
****

Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.06 ng	77603	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

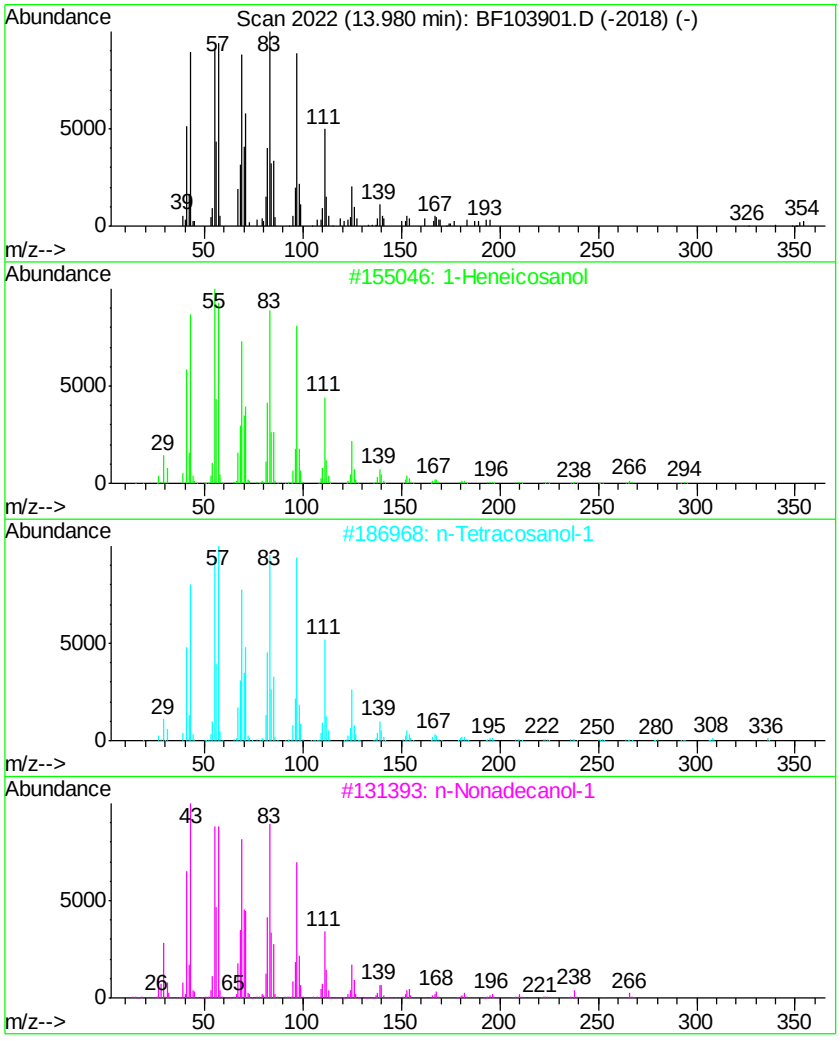
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

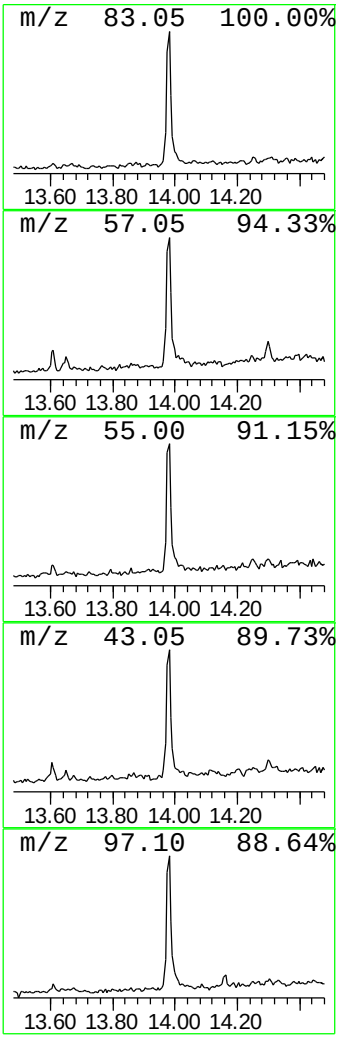
****

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	4.01 ng	143393	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

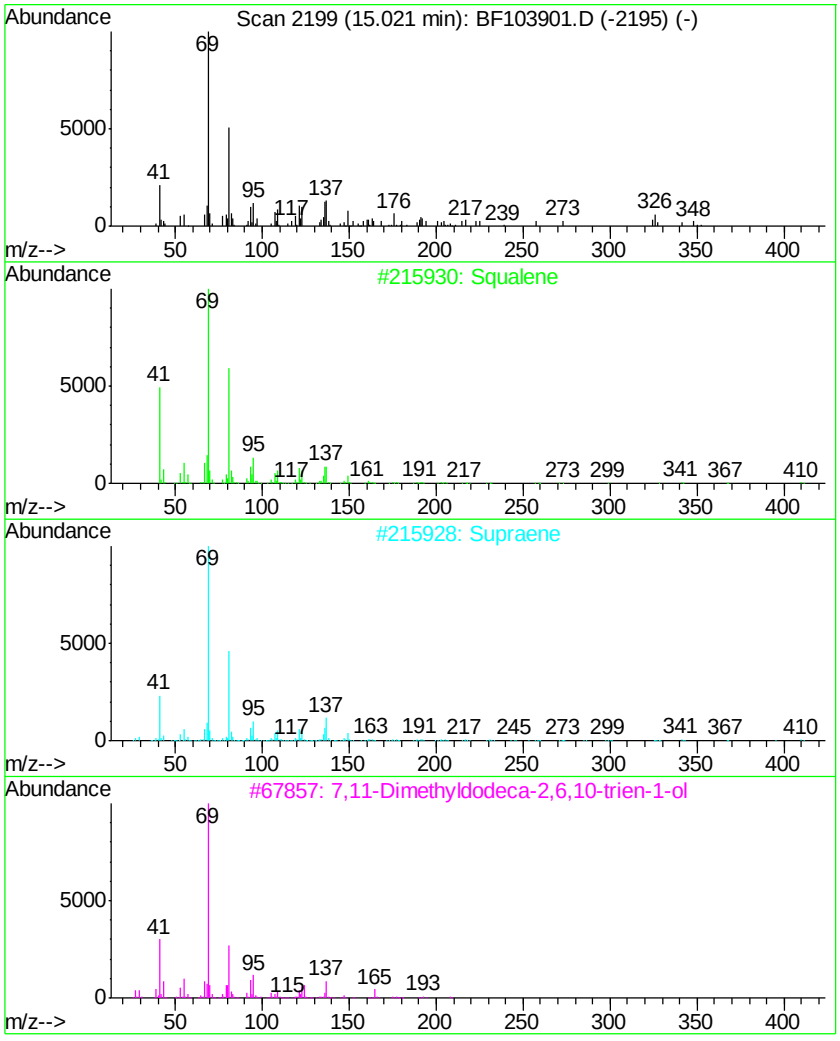
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

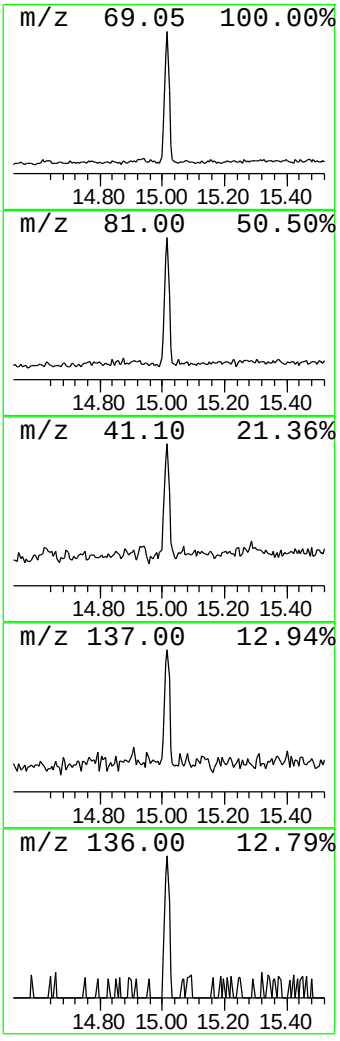
****

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.01 ng	86069	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	81
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
5	trans-Farnesol	222	C15H26O	000106-28-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032318\
Data File : BF103901.D
Acq On : 24 Mar 2018 1:22
Operator : JU/SJ
Sample : J2012-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 031918-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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
Butane, 2-methoxy...	2.29	11.4	ng	405192	1	6.97	710927	20.0
2-Pentanone, 4-hy...	5.20	6.1	ng	216248	1	6.97	710927	20.0
unknown6.75	6.75	56.1	ng	1993950	1	6.97	710927	20.0
Hexadecane	10.90	2.1	ng	77603	4	11.51	751703	20.0
1-Heneicosanol	13.98	4.0	ng	143393	5	14.16	714476	20.0
Squalene	15.02	3.0	ng	86069	6	15.70	571691	20.0