LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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	2.304	31	37	43	rVB	401893	518235	12.60%	1.926%
2	5.204	527	530	537	rBV	52993	59505	1.45%	0.221%
3	5.598	592	597	600	rBV	1651494	1548368	37.64%	5.754%
4	5.922	649	652	664	rVB	38336	41342	1.01%	0.154%
5	6.592	762	766	779	rBV	1110894	996781	24.23%	3.704%
6	6.745	787	792	795	rBV	3149105	2877365	69.95%	10.692%
7	6.975	827	831	834	rBV	954947	766250	18.63%	2.847%
8	7.134	853	858	861	rBV	3359476	2971874	72.25%	11.043%
9	7.539	921	927	930	rBV	2374307	2346440	57.05%	8.719%
10	8.257	1045	1049	1052	rBV	1231787	1001957	24.36%	3.723%
11	9.333	1227	1232	1235	rBV	4201500	4113250	100.00%	15.285%
12	9.716	1292	1297	1303	rBV	77551	83213	2.02%	0.309%
13	9.928	1330	1333	1336	rBV	64710	48941	1.19%	0.182%
14	10.016	1344	1348	1360	rVB	1256503	1110207	26.99%	4.125%
15	10.427	1416	1418	1421	rVB	83887	60872	1.48%	0.226%
16	10.810	1478	1483	1486	rBV	2273633	2139599	52.02%	7.951%
17	10.904	1496	1499	1508	rVB2	60652	79493	1.93%	0.295%
18	11.510	1598	1602	1610	rBV	1130942	964563	23.45%	3.584%
19	13.098	1867	1872	1875	rBV	3288662	3189470	77.54%	11.852%
20	13.974	2017	2021	2032	rBV	174319	192351	4.68%	0.715%
21	14.163	2049	2053	2062	rBV	803504	734194	17.85%	2.728%
22	15.015	2195	2198	2207	rVB	52781	55681	1.35%	0.207%
23	15.710	2310	2316	2324	rBV	506494	698190	16.97%	2.594%
24	17.456	2607	2613	2626	rVB4	93154	214347	5.21%	0.796%
25	17.892	2681	2687	2697	rVB10	40438	98633	2.40%	0.367%

Sum of corrected areas: 26911121

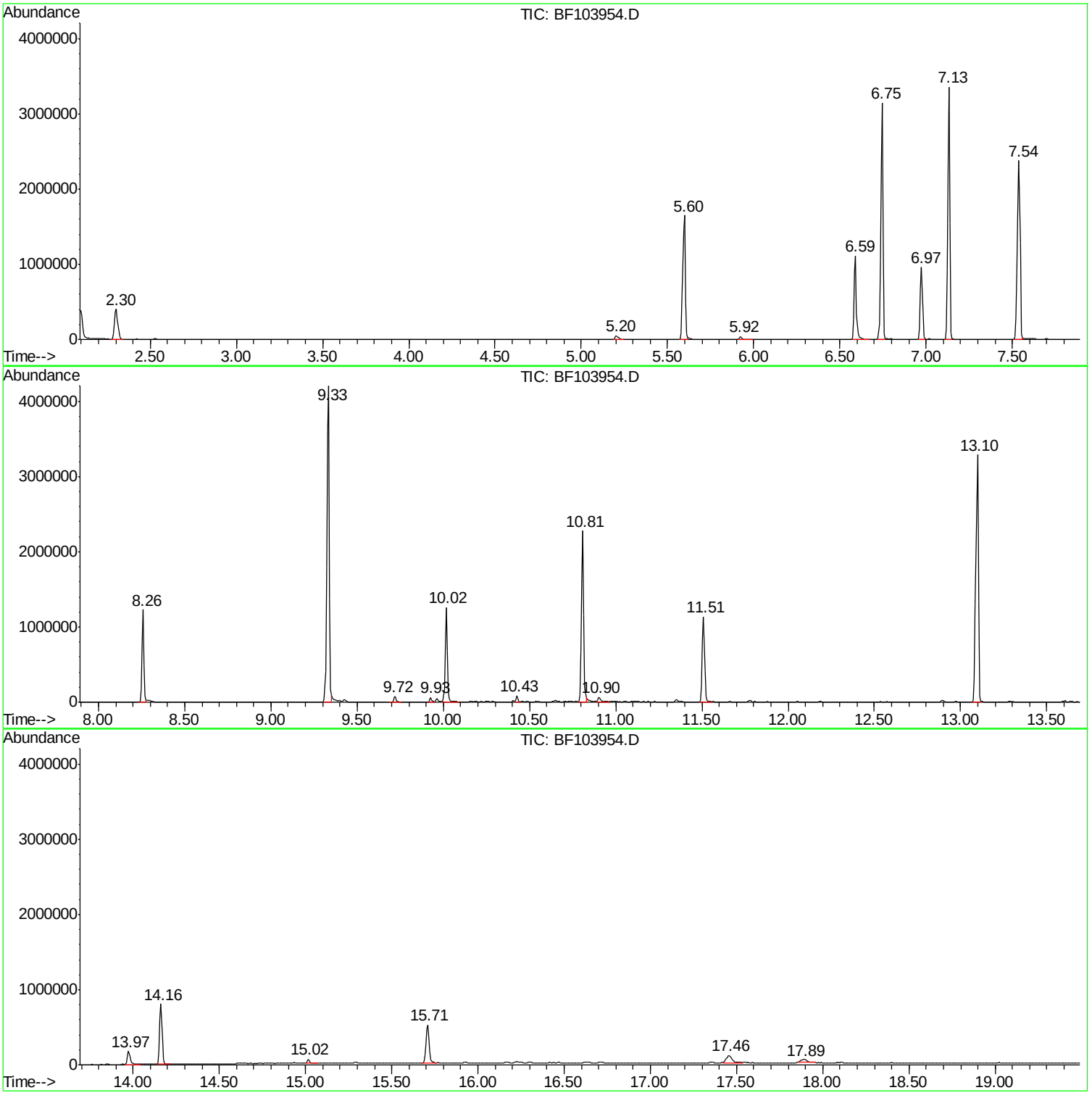
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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

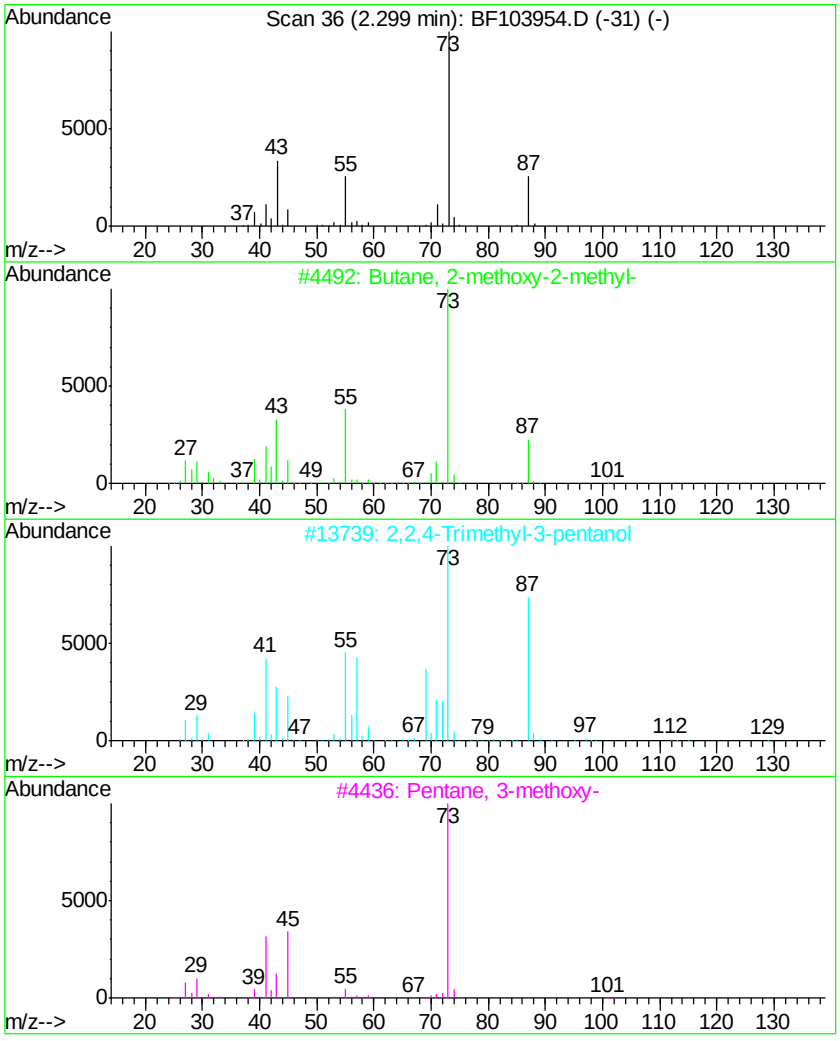
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

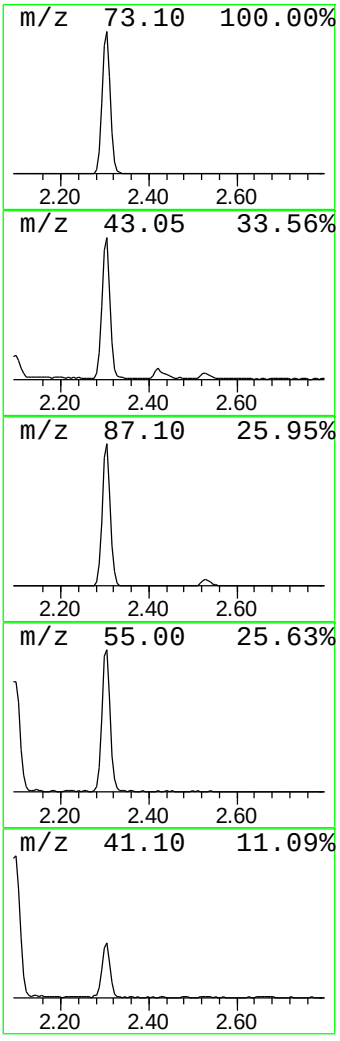
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	13.53 ng	518235	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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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

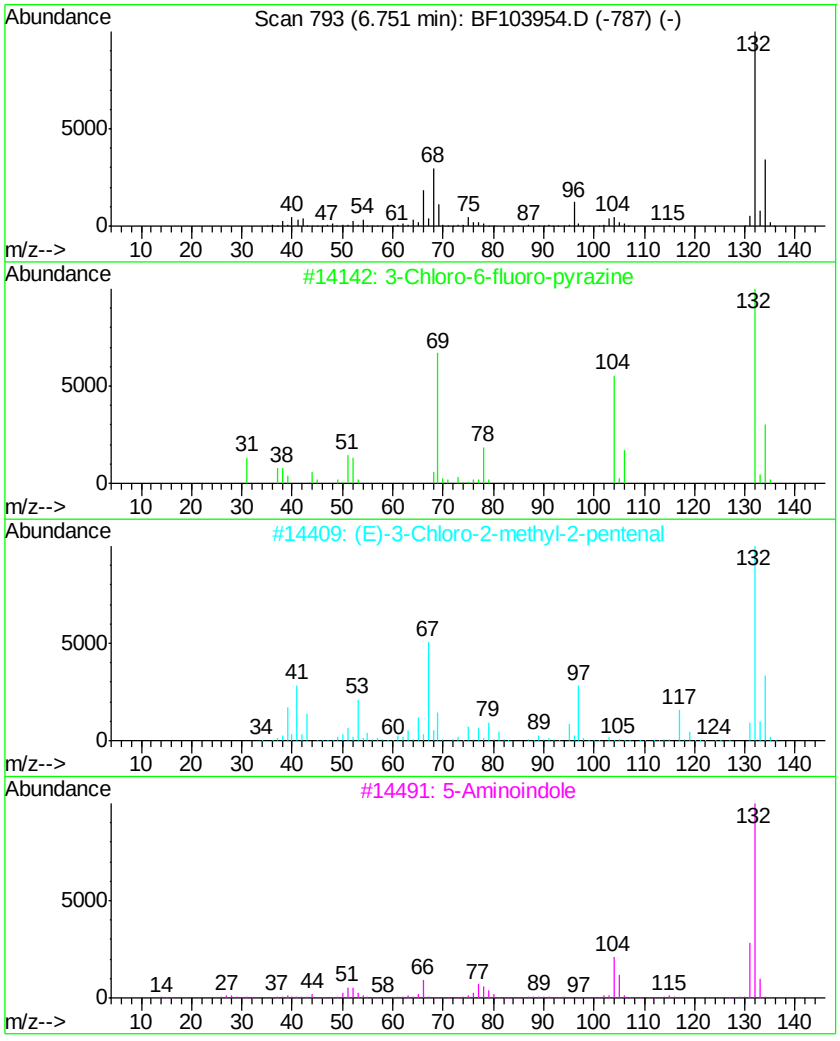
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

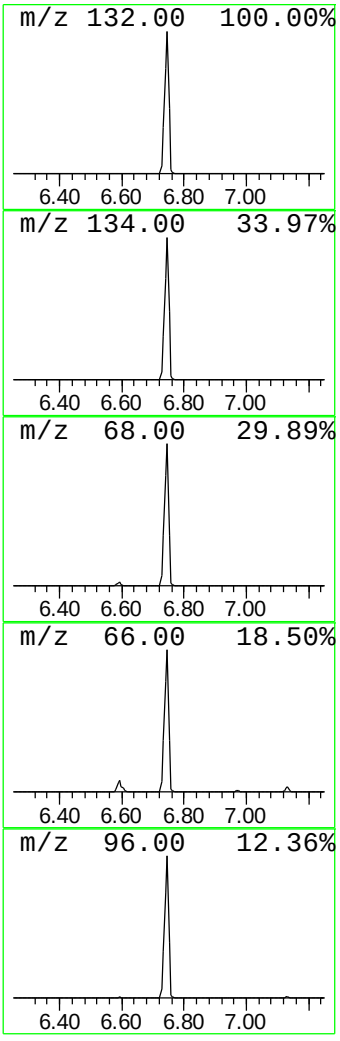
****

Peak Number 2 unknown6.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	75.10 ng	2877370	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	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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

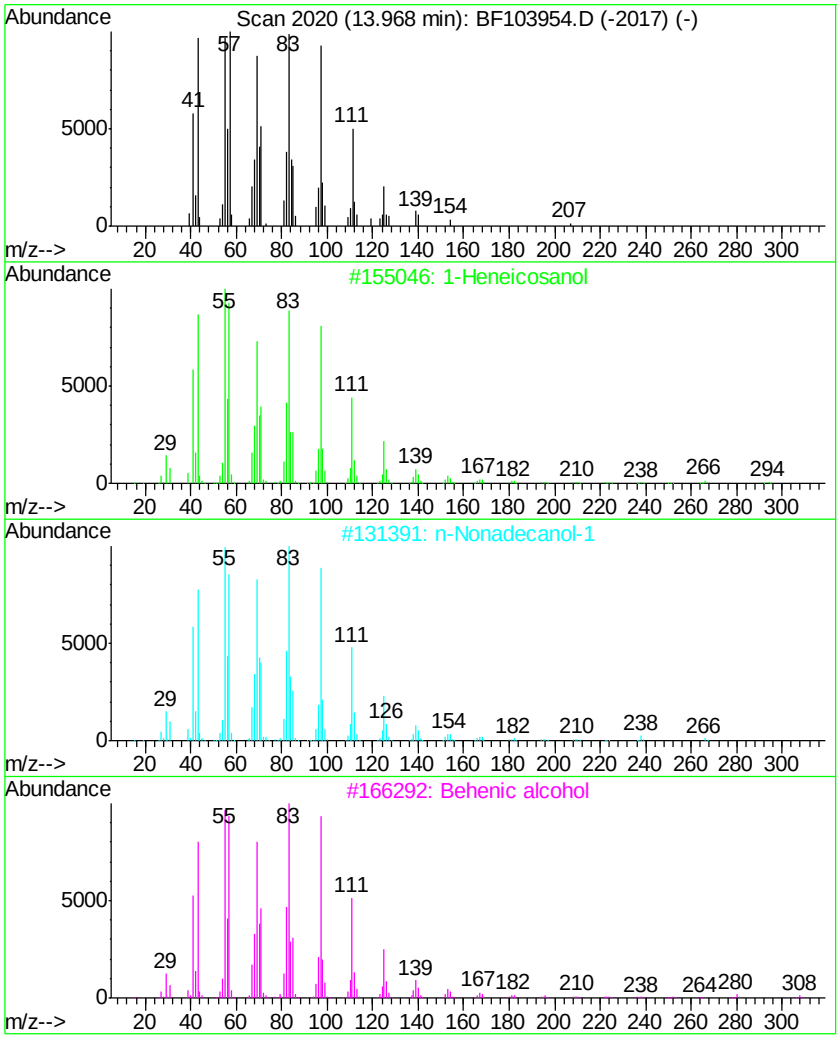
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

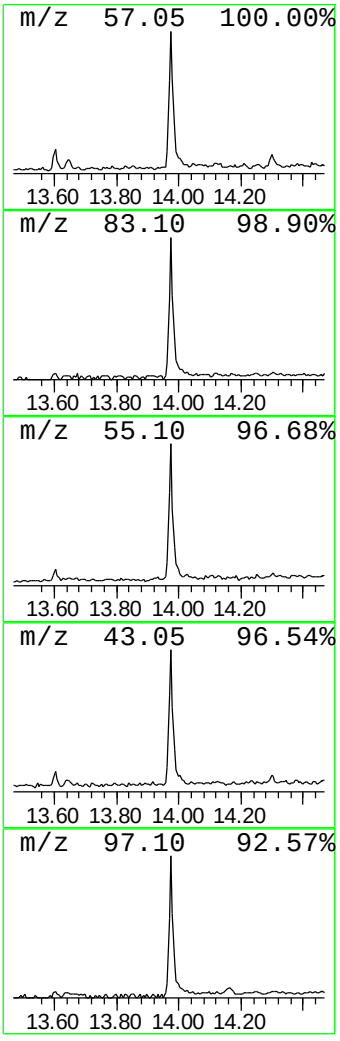
****

Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	5.24 ng	192351	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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

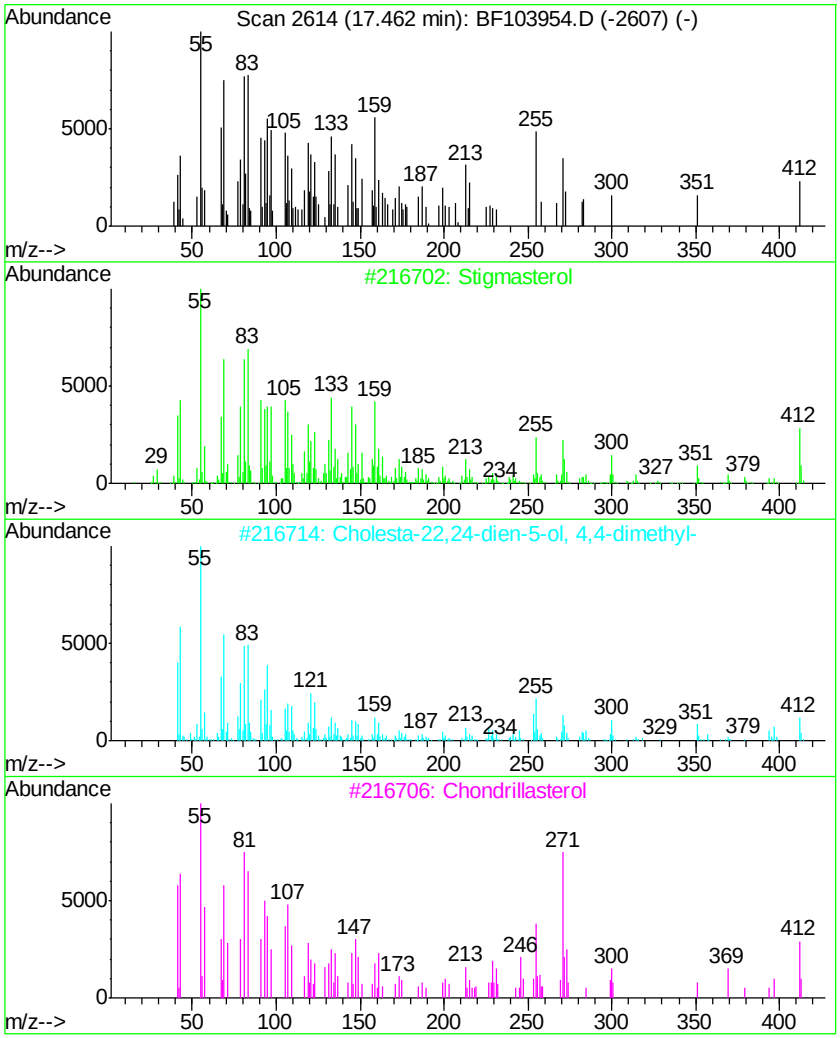
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

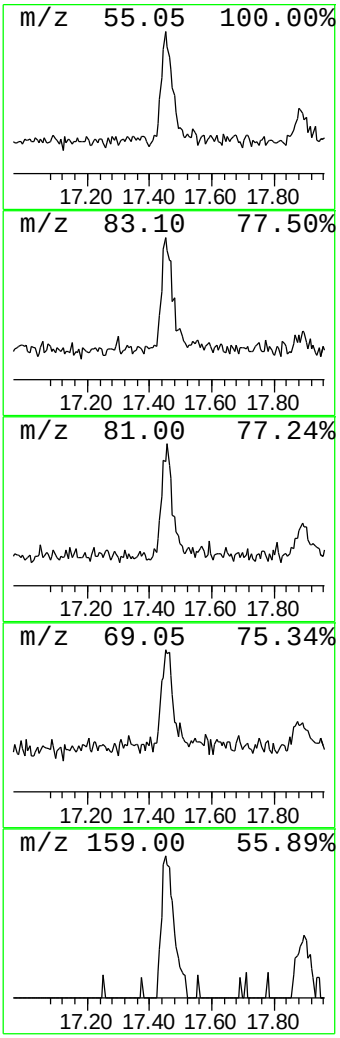
****

Peak Number 5 Stigmasterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.46	6.14 ng	214347	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	99
2	Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	41
3	Chondrillasterol	412	C29H48O	000481-17-4	22
4	Cycloprop[7,8]ergost-22-en-3-ol,...	412	C29H48O	053866-87-8	18
5	3,4-Difluorobenzoic acid, eicosy...	438	C27H44F2O2	1000338-87-6	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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

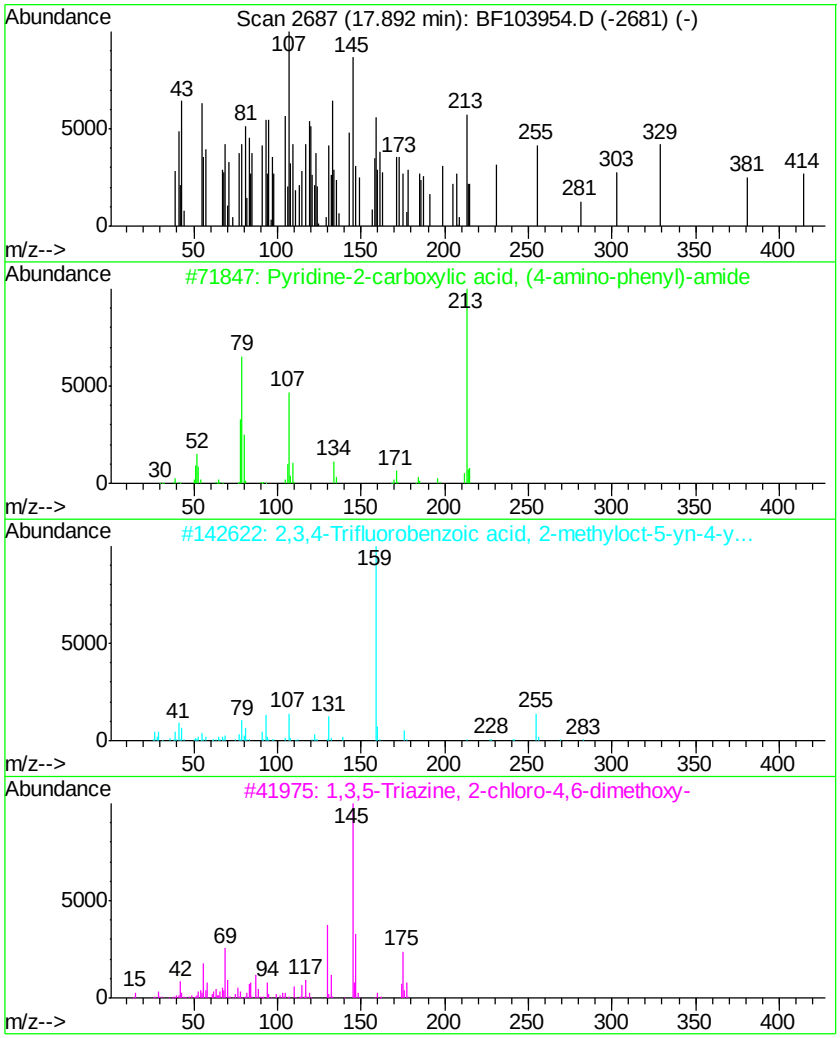
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

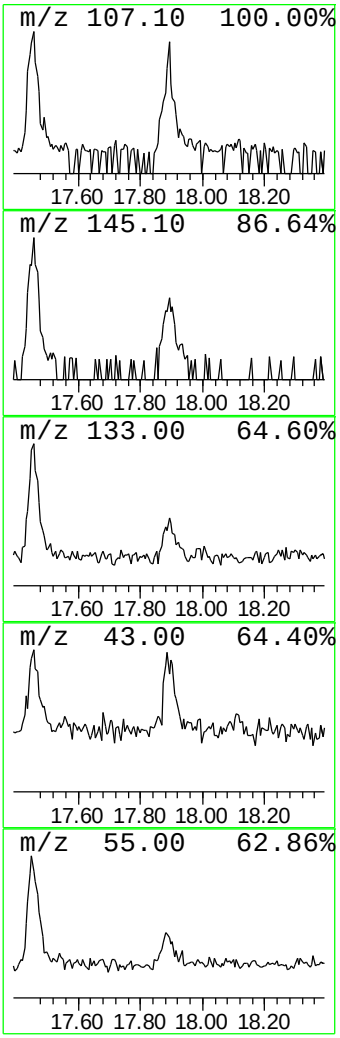
****

Peak Number 6 unknown17.89 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	2.83 ng	98633	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-2-carboxylic acid, (4-a...	213	C12H11N3O	1000317-78-7	14
2	2,3,4-Trifluorobenzoic acid, 2-m...	298	C16H17F3O2	1000292-55-6	14
3	1,3,5-Triazine, 2-chloro-4,6-dim...	175	C5H6ClN3O2	003140-73-6	11
4	1-(4-Pyridin-2-yl-piperazin-1-yl...	205	C11H15N3O	1000368-48-3	10
5	N-(6-Chloro-5-hydroxy-4-pyridazi...	187	C6H6ClN3O2	098142-22-4	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032618\
Data File : BF103954.D
Acq On : 27 Mar 2018 4:12
Operator : JU/SJ
Sample : J2046-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-02

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...	2.30	13.5	ng	518235	1	6.97	766250	20.0
unknown6.75	6.75	75.1	ng	2877370	1	6.97	766250	20.0
1-Heneicosanol	13.97	5.2	ng	192351	5	14.16	734194	20.0
Stigmasterol	17.46	6.1	ng	214347	6	15.71	698190	20.0
unknown17.89	17.89	2.8	ng	98633	6	15.71	698190	20.0