LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

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-BF020318.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	2.187	10	17	26	rVB	521134	698521	13.45%	1.499%
2	5.116	512	515	523	rVB	140484	182605	3.51%	0.392%
3	5.498	575	580	583	rBV	4699497	5155191	99.23%	11.065%
4	6.504	745	751	762	rBV	4307734	5195189	100.00%	11.151%
5	6.651	771	776	779	rBV	5093183	4975145	95.76%	10.679%
6	6.881	811	815	818	rBV	1806508	1410555	27.15%	3.028%
7	7.039	837	842	845	rVB	4257524	3865343	74.40%	8.297%
8	7.445	905	911	914	rBV	3280017	3259636	62.74%	6.997%
9	8.163	1029	1033	1036	rBV	2326329	1876879	36.13%	4.029%
10	8.716	1123	1127	1131	rVB	79690	62943	1.21%	0.135%
11	9.239	1210	1216	1219	rBV	5483343	5042211	97.06%	10.823%
12	9.627	1278	1282	1285	rBV	948933	722882	13.91%	1.552%
13	9.822	1311	1315	1317	rBV	47065	66751	1.28%	0.143%
14	9.922	1327	1332	1335	rVB	2107976	1924867	37.05%	4.132%
15	10.633	1448	1453	1455	rBV	164264	151580	2.92%	0.325%
16	10.710	1460	1466	1469	rBV	2725370	2816917	54.22%	6.046%
17	11.404	1580	1584	1587	rBV	1925069	1655045	31.86%	3.552%
18	11.927	1669	1673	1686	rBV	523905	590992	11.38%	1.269%
19	12.616	1787	1790	1798	rBV	76652	114166	2.20%	0.245%
20	12.710	1802	1806	1814	rBV	144807	162521	3.13%	0.349%
21	12.992	1849	1854	1857	rBV	3633062	3535883	68.06%	7.590%
22	13.463	1930	1934	1939	rVB3	64241	73194	1.41%	0.157%
23	13.874	2001	2004	2013	rBV	663796	611981	11.78%	1.314%
24	14.045	2028	2033	2036	rBV	1190255	1160387	22.34%	2.491%
25	15.521	2279	2284	2292	rBV	882444	1178678	22.69%	2.530%
26	16.039	2369	2372	2378	rVB4	68496	98847	1.90%	0.212%

Sum of corrected areas: 46588909

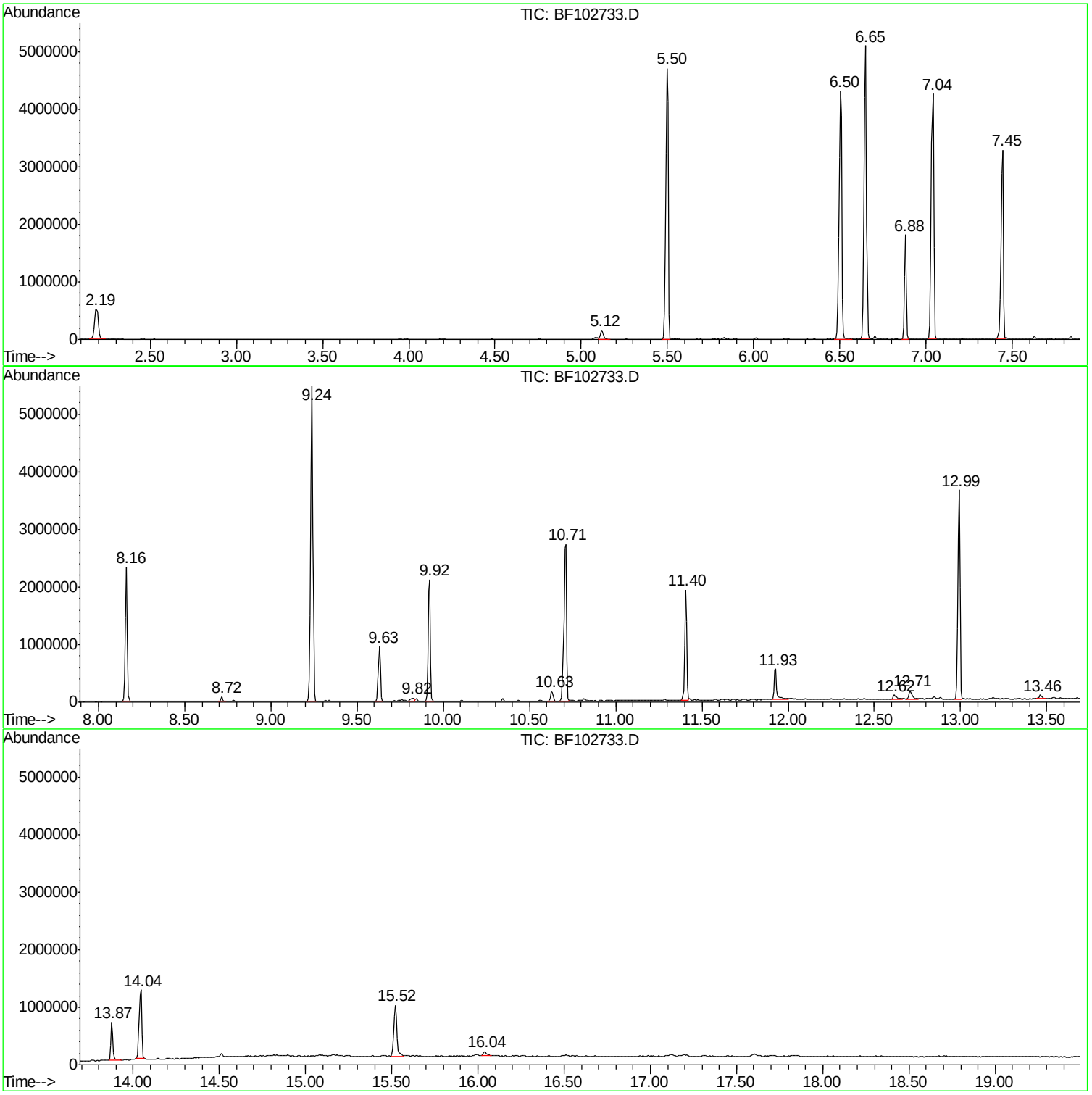
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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 : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

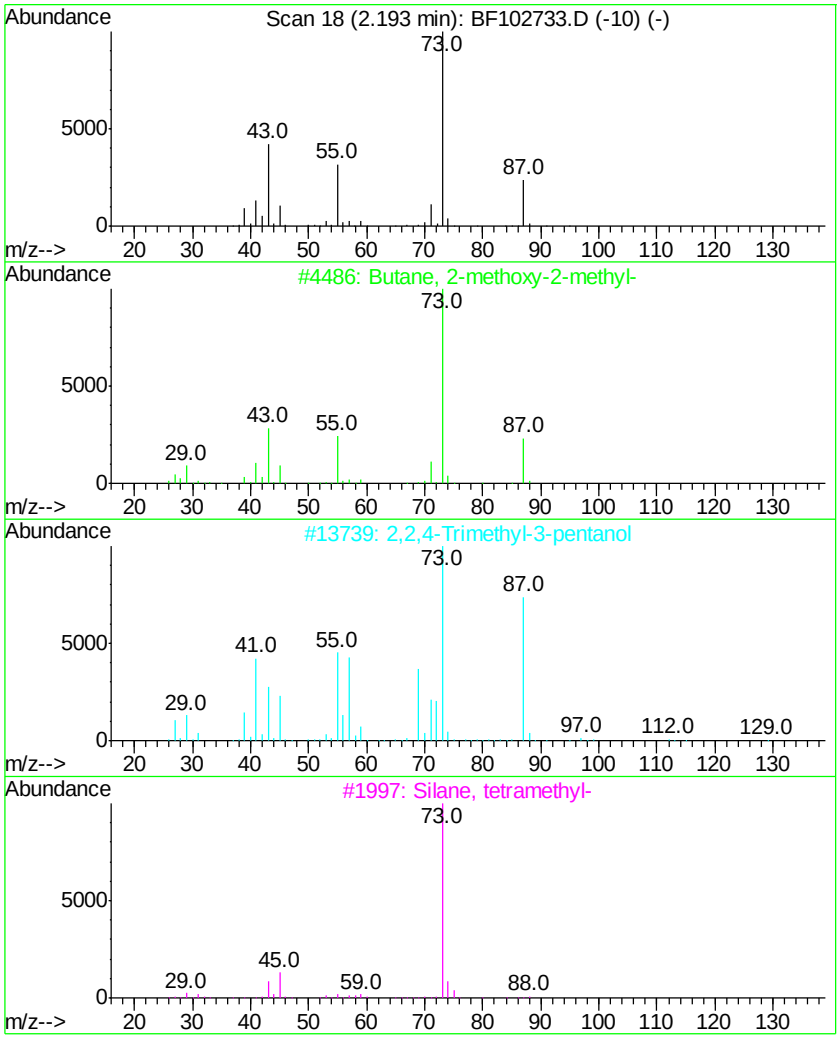
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

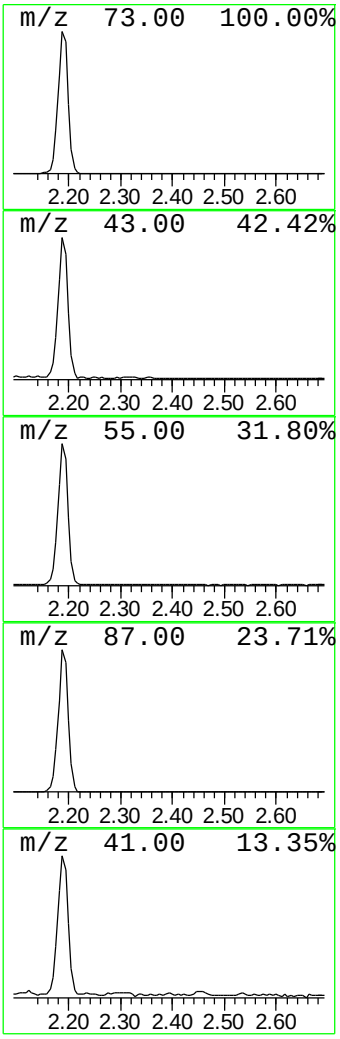
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	9.90 ng	698521	1,4-Dichlorobenzene-d4	6.88

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

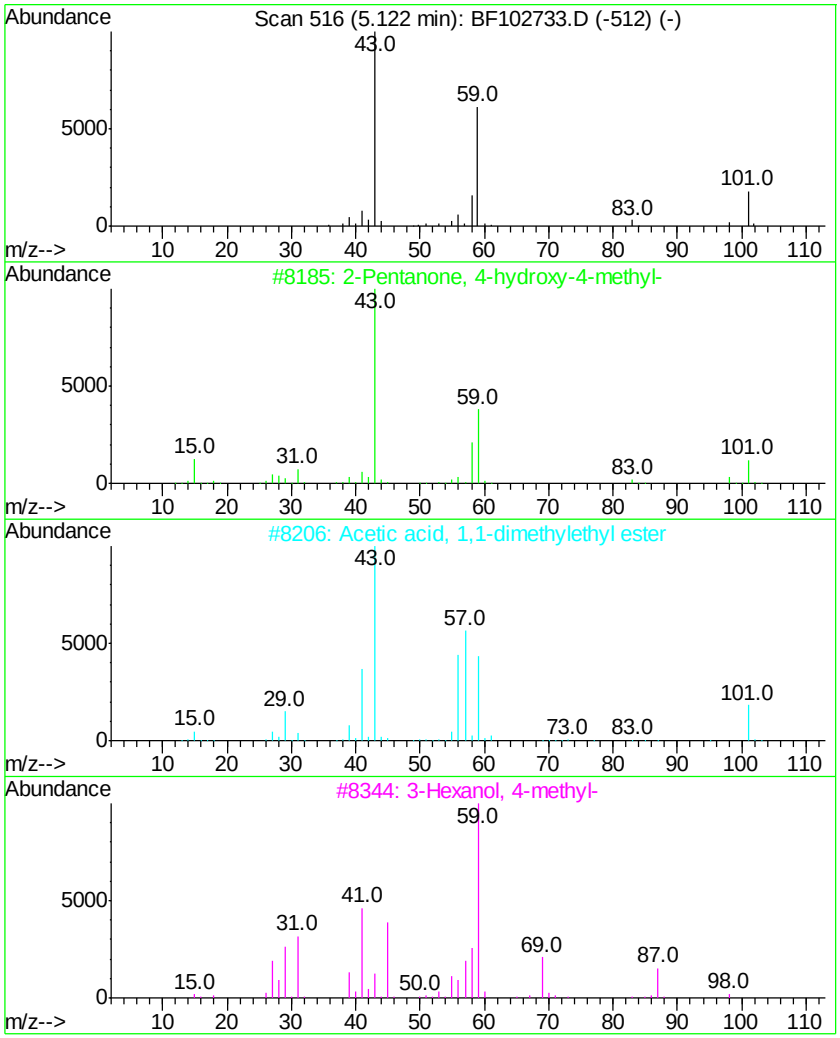
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

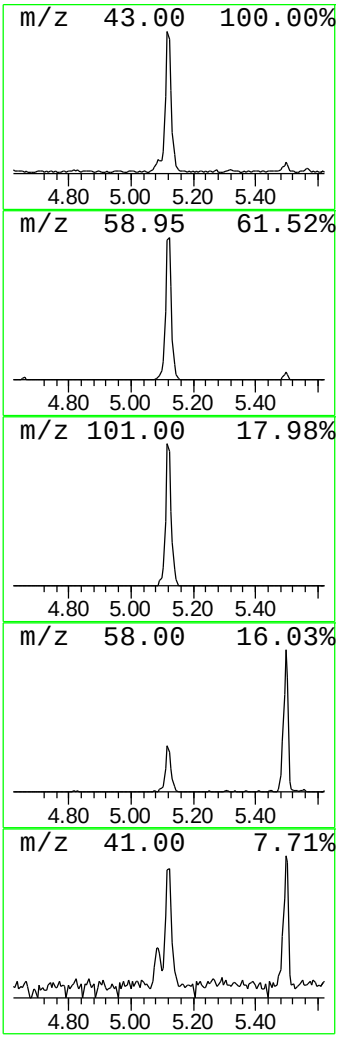
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.59 ng	182605	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

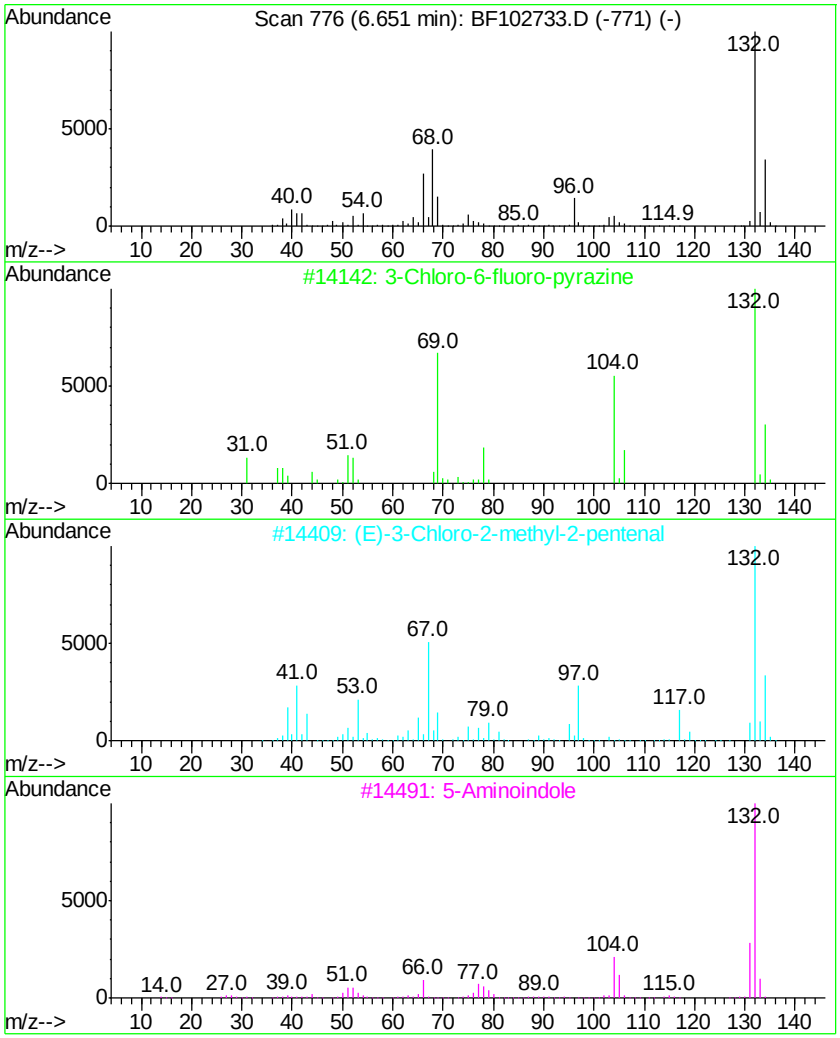
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

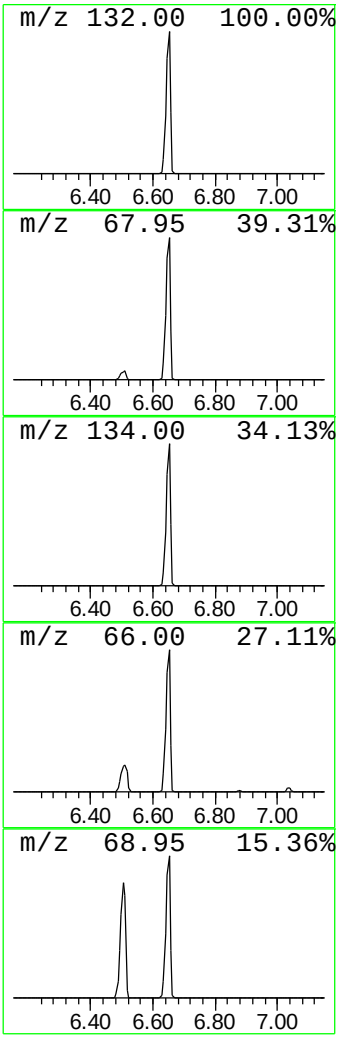
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	70.54 ng	4975150	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

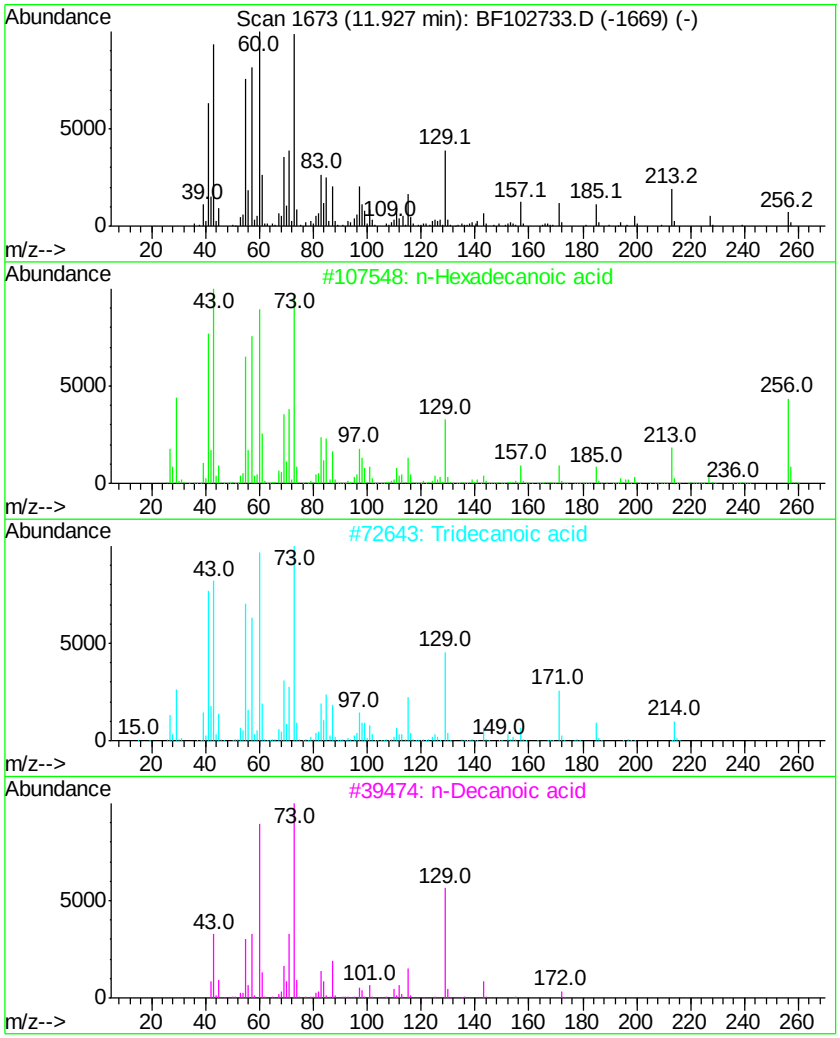
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

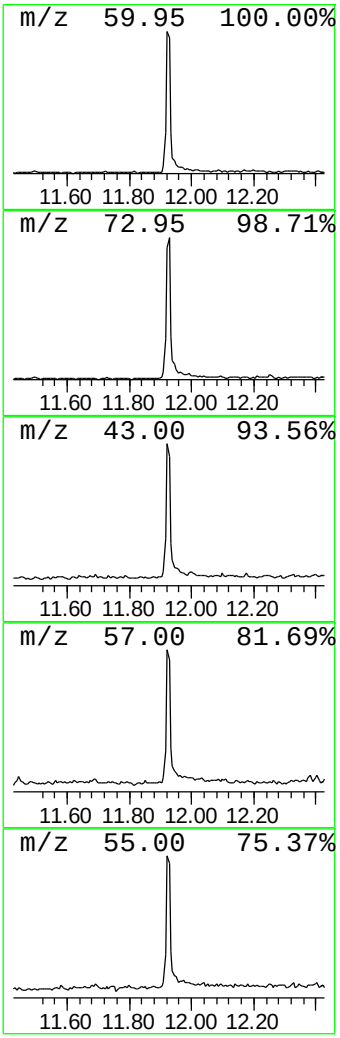
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	7.14 ng	590992	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	n-Decanoic acid	172	C10H20O2	000334-48-5	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	86





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

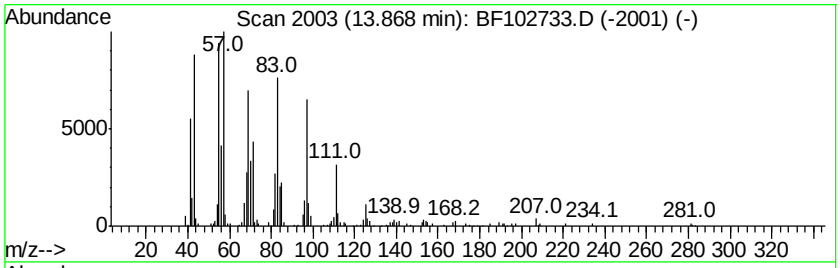
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

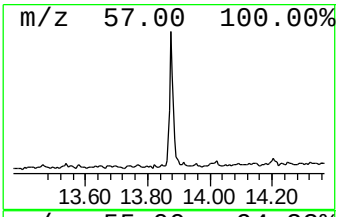
****

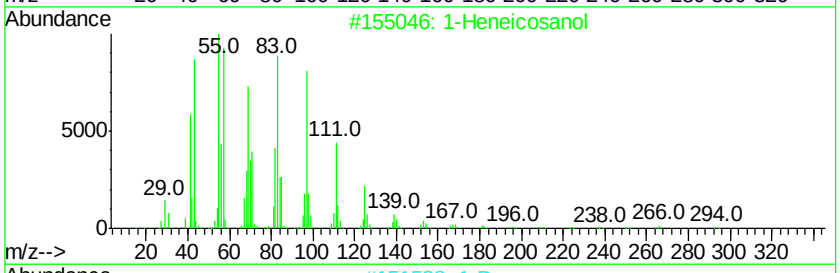
Peak Number 6 1-Heneicosanol Concentration Rank 3

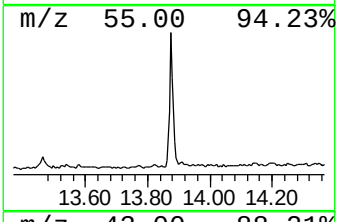
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	10.55 ng	611981	Chrysene-d12	14.04

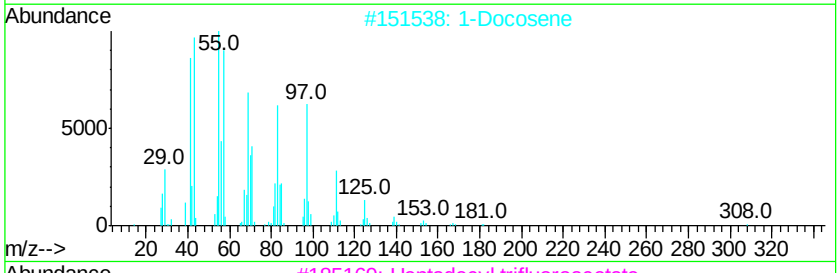
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91

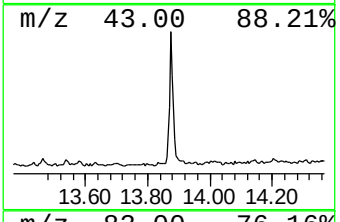


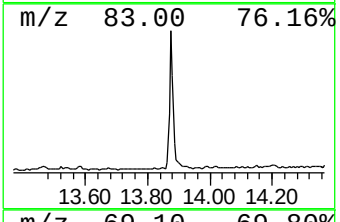


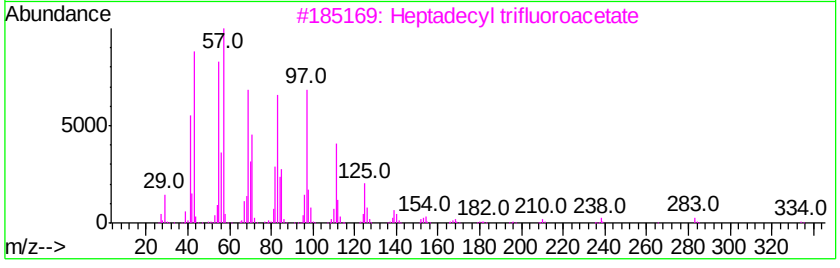


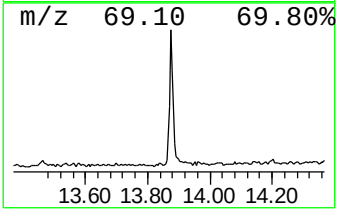












Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102733.D
Acq On : 5 Feb 2018 13:07
Operator : SJ/JU
Sample : J1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.19	9.9	ng	698521	1	6.88	1410560	20.0
2-Pentanone, 4-hy...	5.12	2.6	ng	182605	1	6.88	1410560	20.0
unknown6.65	6.65	70.5	ng	4975150	1	6.88	1410560	20.0
n-Hexadecanoic acid	11.93	7.1	ng	590992	4	11.40	1655050	20.0
1-Heneicosanol	13.87	10.6	ng	611981	5	14.04	1160390	20.0