LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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	2.252	19	28	35	rVB	687607	926135	15.64%	1.892%
2	4.028	325	330	337	rVB	72676	97529	1.65%	0.199%
3	5.134	512	518	525	rVB	221236	279657	4.72%	0.571%
4	5.528	579	585	588	rBV	5108102	5152545	87.03%	10.523%
5	6.528	748	755	759	rBV	5070703	5767127	97.41%	11.779%
6	6.669	774	779	782	rBV	5749865	5386637	90.98%	11.001%
7	6.898	814	818	821	rBV	1468708	1259496	21.27%	2.572%
8	7.057	840	845	848	rBV	4680508	4272599	72.17%	8.726%
9	7.457	907	913	916	rBV	3366998	3479550	58.77%	7.106%
10	8.175	1031	1035	1039	rBV	1843028	1573206	26.57%	3.213%
11	9.251	1213	1218	1221	rBV	6193648	5920528	100.00%	12.092%
12	9.639	1281	1284	1287	rBV	406195	294276	4.97%	0.601%
13	9.933	1329	1334	1337	rVB	1805447	1698465	28.69%	3.469%
14	10.716	1462	1467	1470	rBV	3584912	3071466	51.88%	6.273%
15	11.416	1582	1586	1589	rBV	1514548	1423201	24.04%	2.907%
16	11.939	1671	1675	1687	rBV	343946	325885	5.50%	0.666%
17	12.457	1759	1763	1768	rBV2	73293	77824	1.31%	0.159%
18	12.722	1805	1808	1812	rBV	97044	94432	1.59%	0.193%
19	12.998	1850	1855	1858	rBV	4803285	4300761	72.64%	8.784%
20	13.892	2003	2007	2011	rBV	511918	525297	8.87%	1.073%
21	14.045	2029	2033	2037	rBV	1539784	1360080	22.97%	2.778%
22	14.521	2112	2114	2118	rBV2	80922	76638	1.29%	0.157%
23	15.521	2279	2284	2289	rVB	933425	1158773	19.57%	2.367%
24	16.057	2372	2375	2381	rBV	65746	81204	1.37%	0.166%
25	17.762	2660	2665	2673	rVB4	165471	359638	6.07%	0.735%

Sum of corrected areas: 48962949

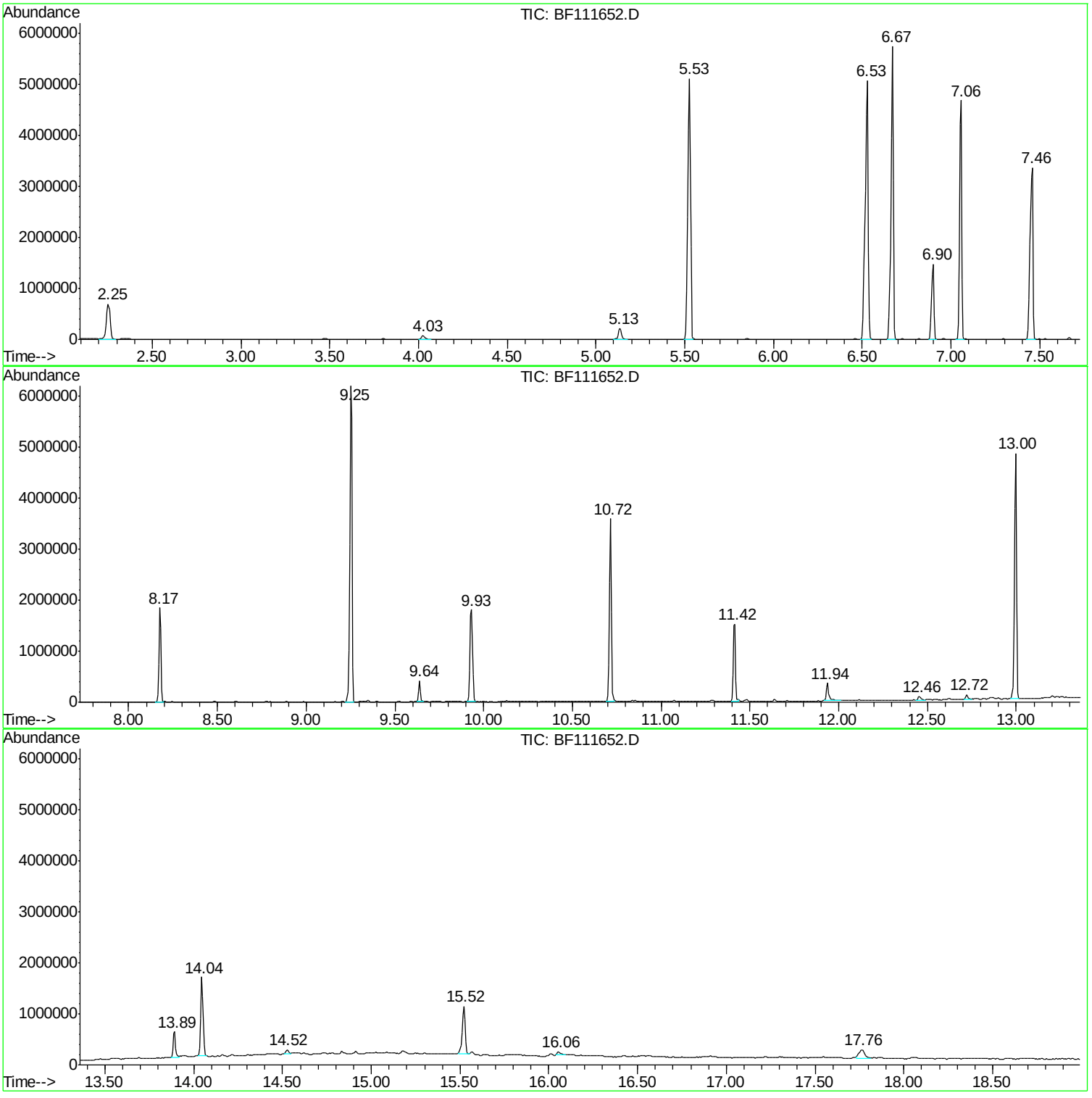
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

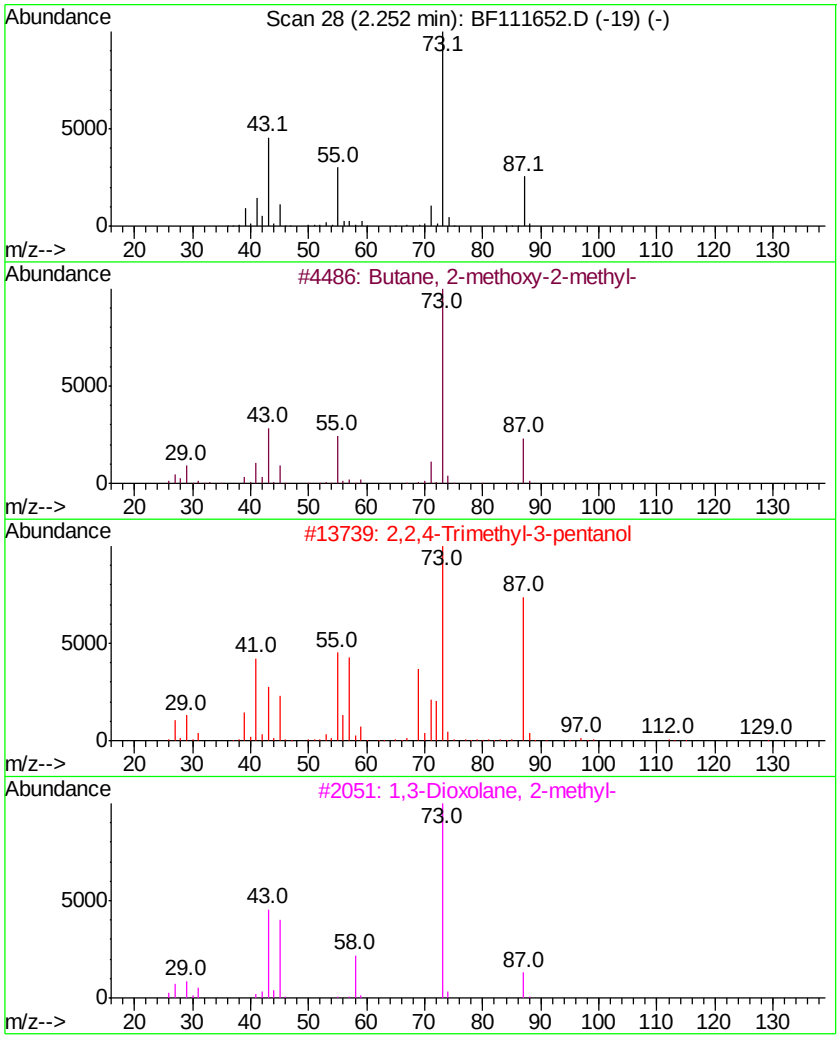
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

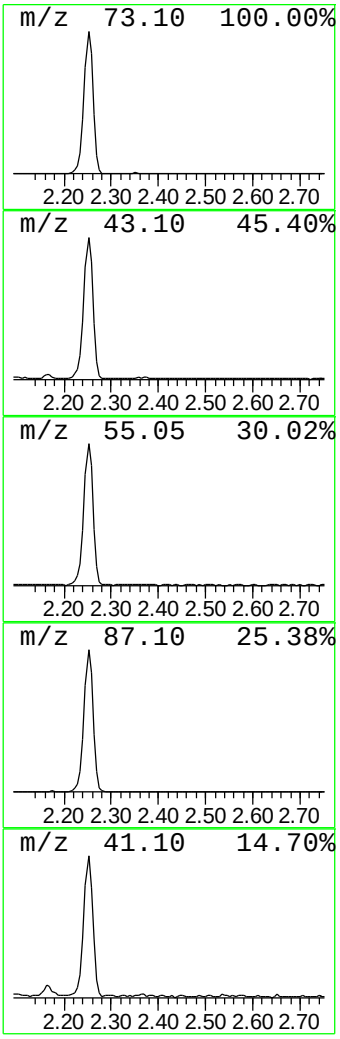
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	14.71 ng	926135	1,4-Dichlorobenzene-d4	6.90

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

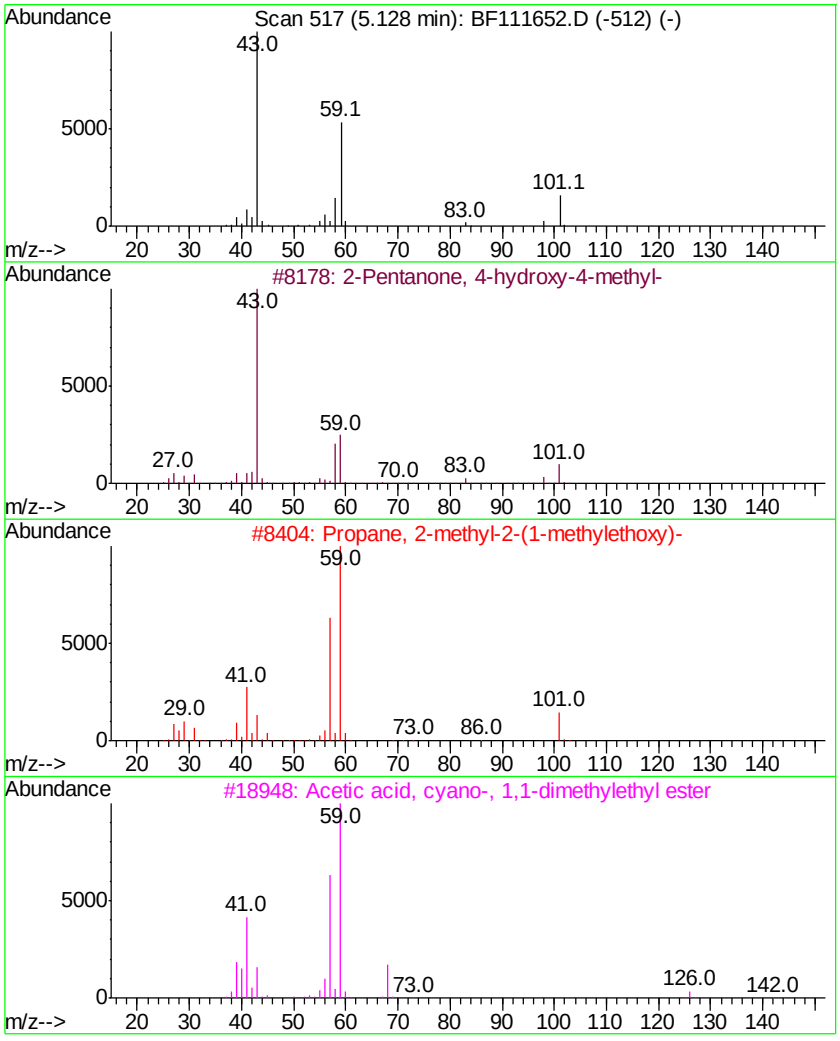
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

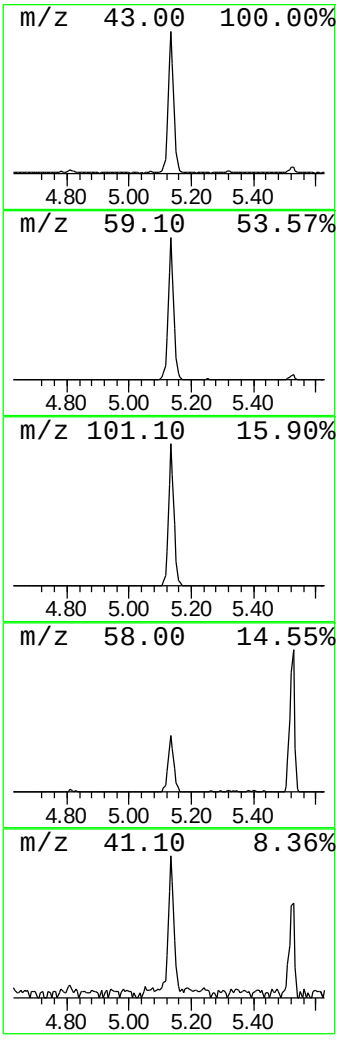
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.44 ng	279657	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

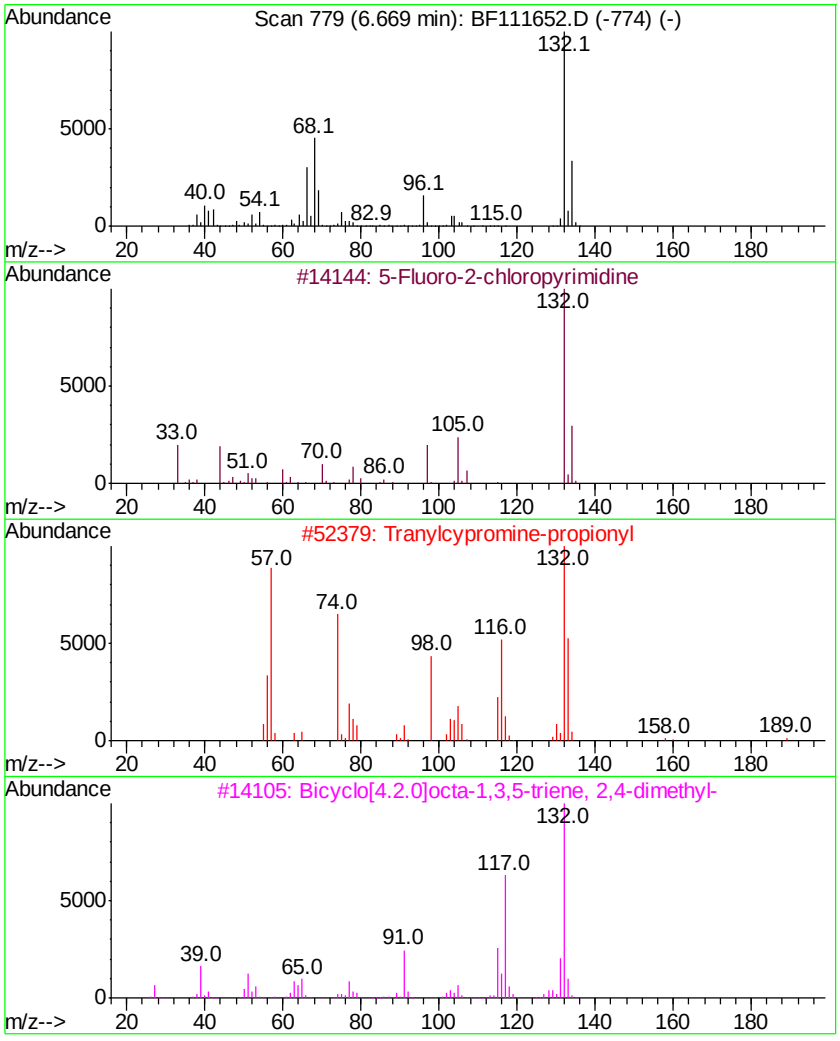
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

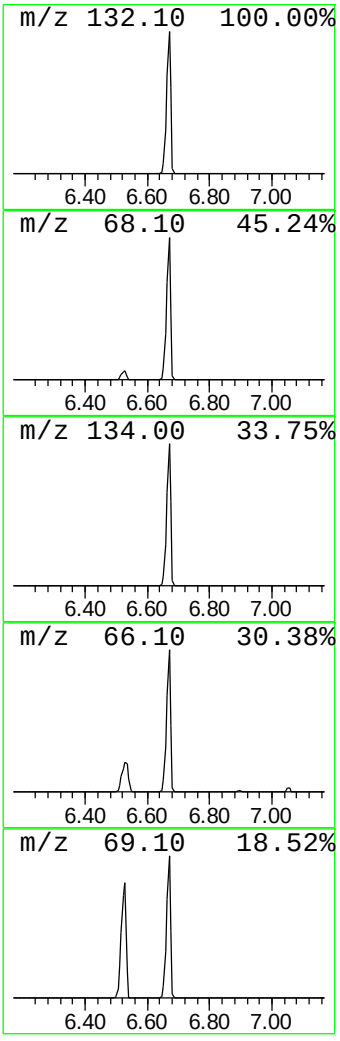
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	85.54 ng	5386640	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

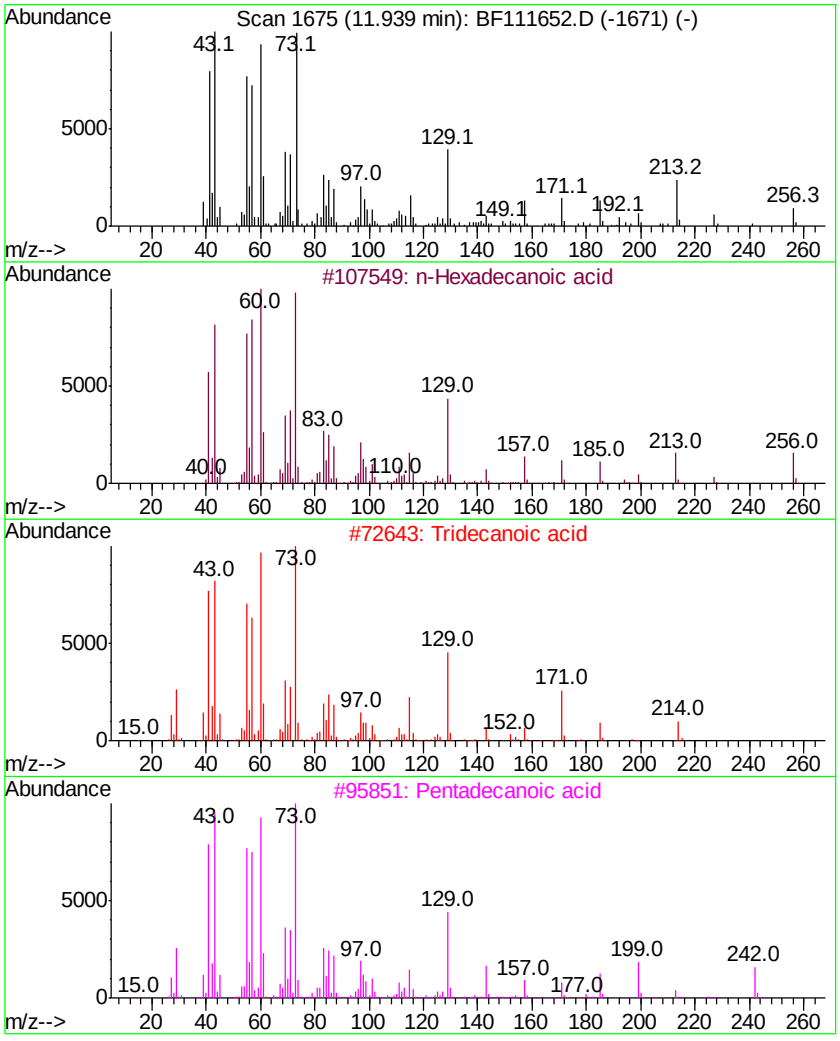
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

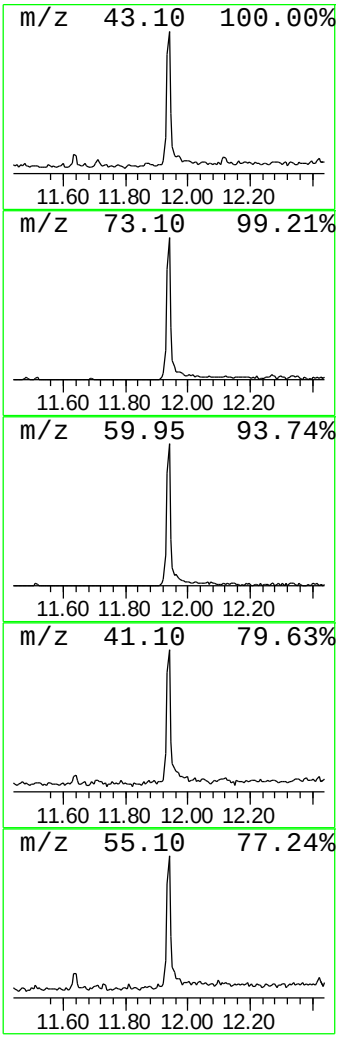
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	4.58 ng	325885	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

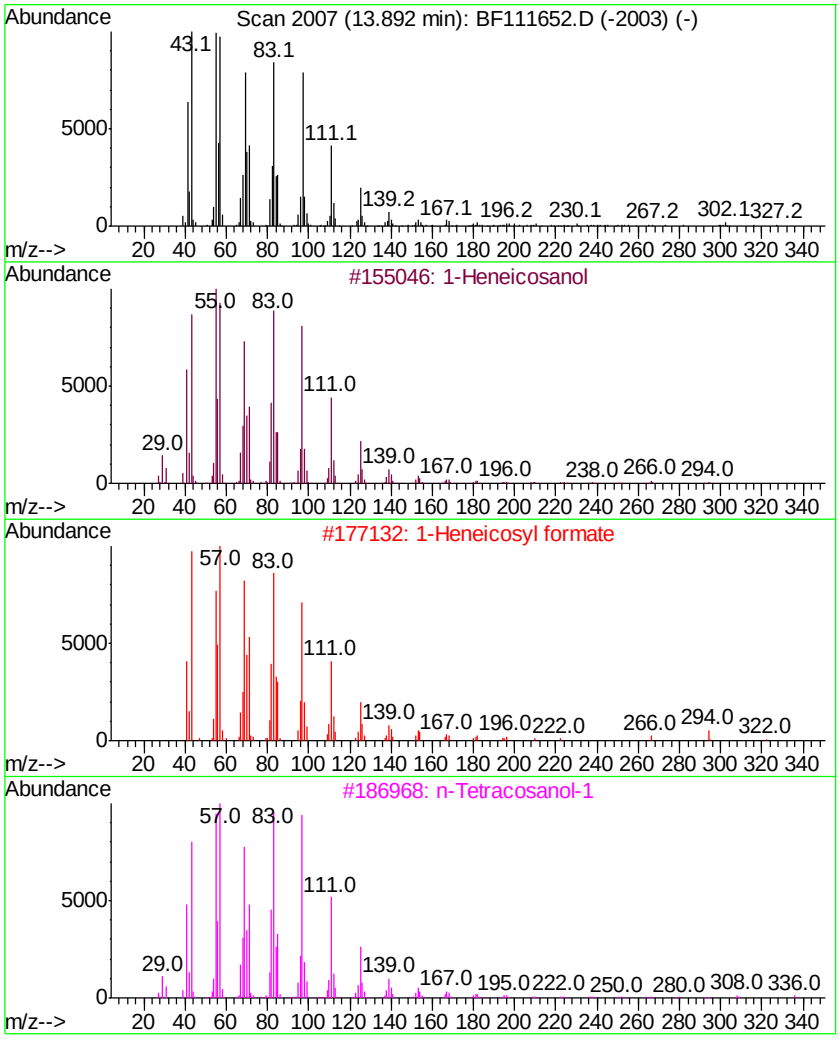
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

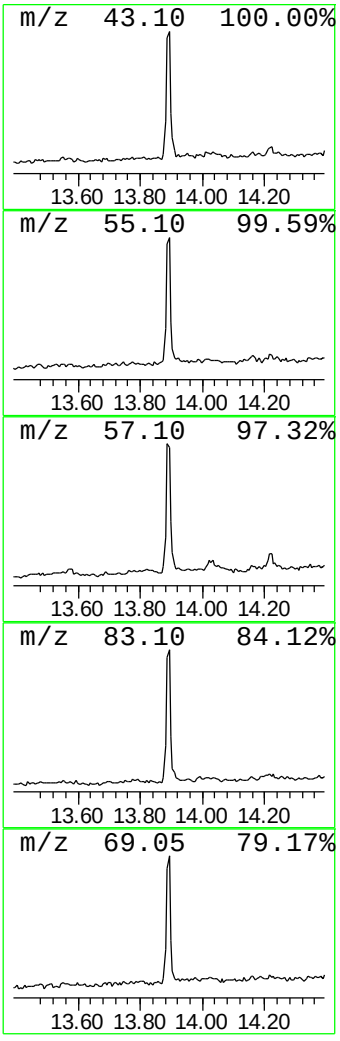
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	7.72 ng	525297	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

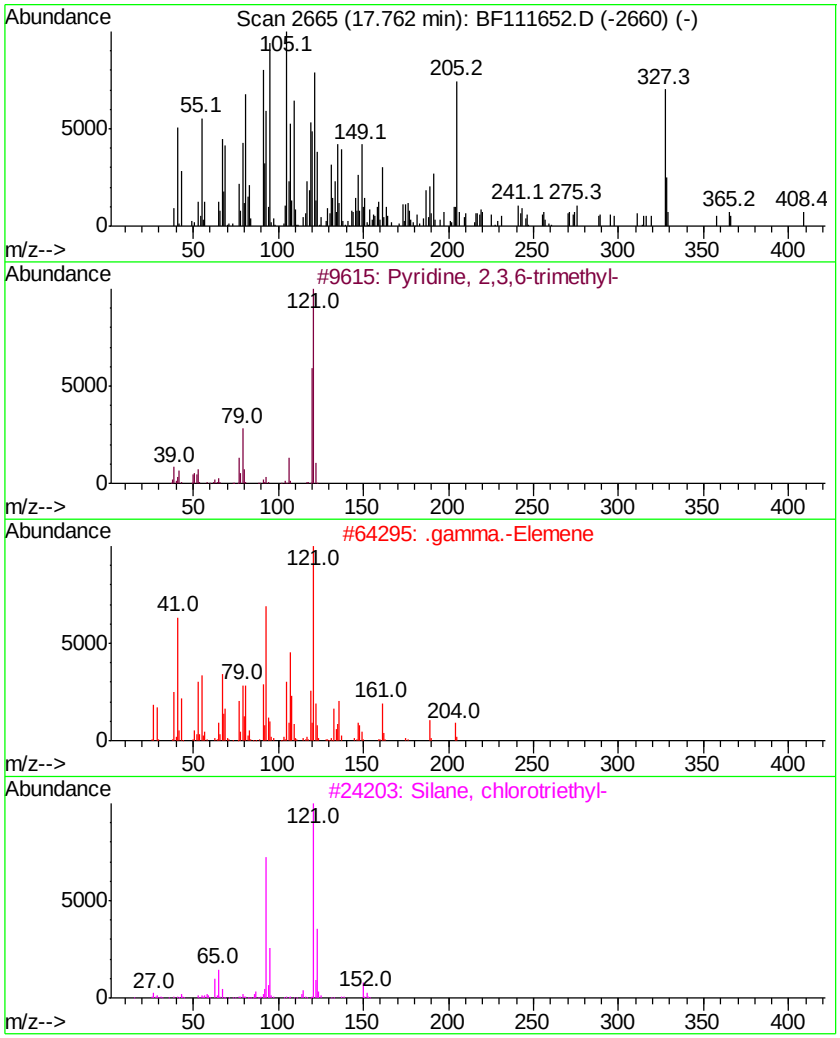
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

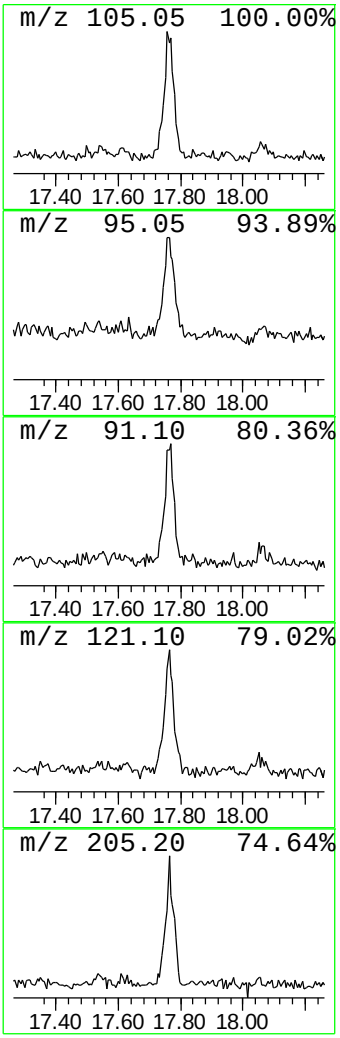
****

Peak Number 7 unknown17.76 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.76	6.21 ng	359638	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2,3,6-trimethyl-	121	C8H11N	001462-84-6	25
2	.gamma.-Elemene	204	C15H24	029873-99-2	25
3	Silane, chlorotriethyl-	150	C6H15ClSi	000994-30-9	15
4	2(5H)-Furanone, 4-methyl-3,5,5-t...	260	C17H24O2	089902-28-3	14
5	Fumaric acid, di(4-methoxyphenyl...	328	C18H16O6	1000344-75-2	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122018\
Data File : BF111652.D
Acq On : 20 Dec 2018 21:27
Operator : JU/SJ
Sample : J6357-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	2.25	14.7	ng	926135	1	6.90	1259500	20.0
2-Pentanone, 4-hy...	5.13	4.4	ng	279657	1	6.90	1259500	20.0
unknown6.67	6.67	85.5	ng	5386640	1	6.90	1259500	20.0
n-Hexadecanoic acid	11.94	4.6	ng	325885	4	11.42	1423200	20.0
1-Heneicosanol	13.89	7.7	ng	525297	5	14.05	1360080	20.0
unknown17.76	17.76	6.2	ng	359638	6	15.52	1158770	20.0