LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF040618.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	5.028	496	500	511	rVB	149323	208507	5.60%	0.665%
2	5.428	563	568	571	rBV	3322093	3545104	95.22%	11.309%
3	6.451	736	742	746	rBV	3016185	3723205	100.00%	11.877%
4	6.581	759	764	767	rBV	3547000	3598439	96.65%	11.479%
5	6.634	770	773	785	rVB	35963	41906	1.13%	0.134%
6	6.804	798	802	805	rBV	1037975	813542	21.85%	2.595%
7	6.963	824	829	832	rBV	3121445	2848859	76.52%	9.088%
8	7.375	893	899	902	rBV	2248607	2359387	63.37%	7.526%
9	8.087	1016	1020	1023	rBV	1319848	1055719	28.36%	3.368%
10	9.163	1198	1203	1206	rBV	3792337	3599453	96.68%	11.482%
11	9.557	1266	1270	1273	rBV	556298	447991	12.03%	1.429%
12	9.769	1302	1306	1310	rVB	96260	76247	2.05%	0.243%
13	9.845	1315	1319	1327	rVB	1140239	1118503	30.04%	3.568%
14	10.269	1388	1391	1394	rVB	126148	95408	2.56%	0.304%
15	10.639	1449	1454	1457	rBV	2071498	2093521	56.23%	6.678%
16	10.739	1468	1471	1476	rBV	107798	101061	2.71%	0.322%
17	11.333	1568	1572	1575	rBV	1017948	936726	25.16%	2.988%
18	11.851	1658	1660	1668	rBV2	130954	130812	3.51%	0.417%
19	12.922	1837	1842	1845	rBV	2903041	2722306	73.12%	8.684%
20	13.804	1989	1992	2002	rBV	251696	271563	7.29%	0.866%
21	13.974	2017	2021	2028	rVB	886730	831634	22.34%	2.653%
22	14.439	2097	2100	2104	rBV3	30622	40259	1.08%	0.128%
23	15.433	2264	2269	2280	rBV	473742	649967	17.46%	2.073%
24	15.927	2350	2353	2359	rVB8	21215	37630	1.01%	0.120%

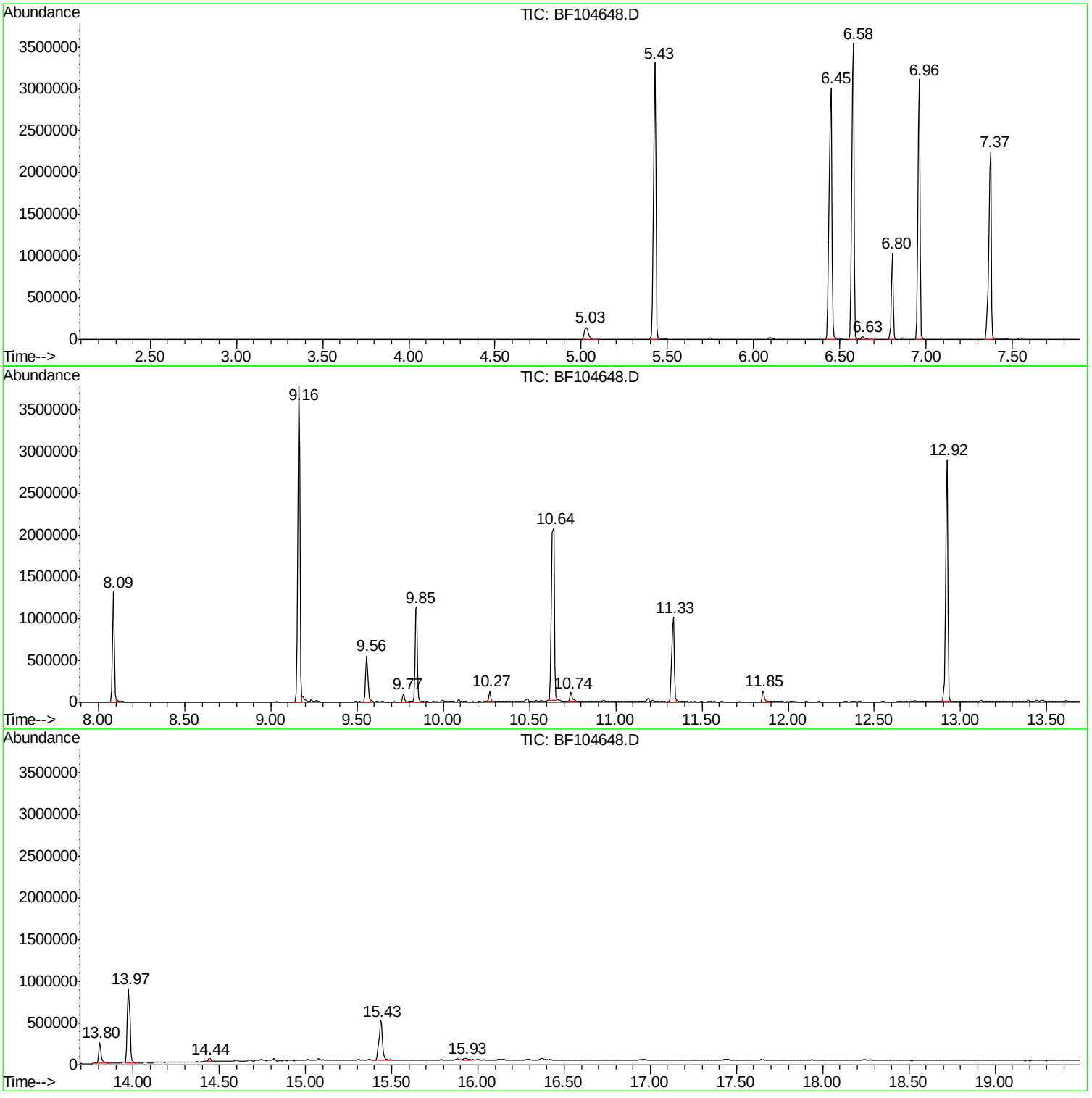
Sum of corrected areas: 31347749

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

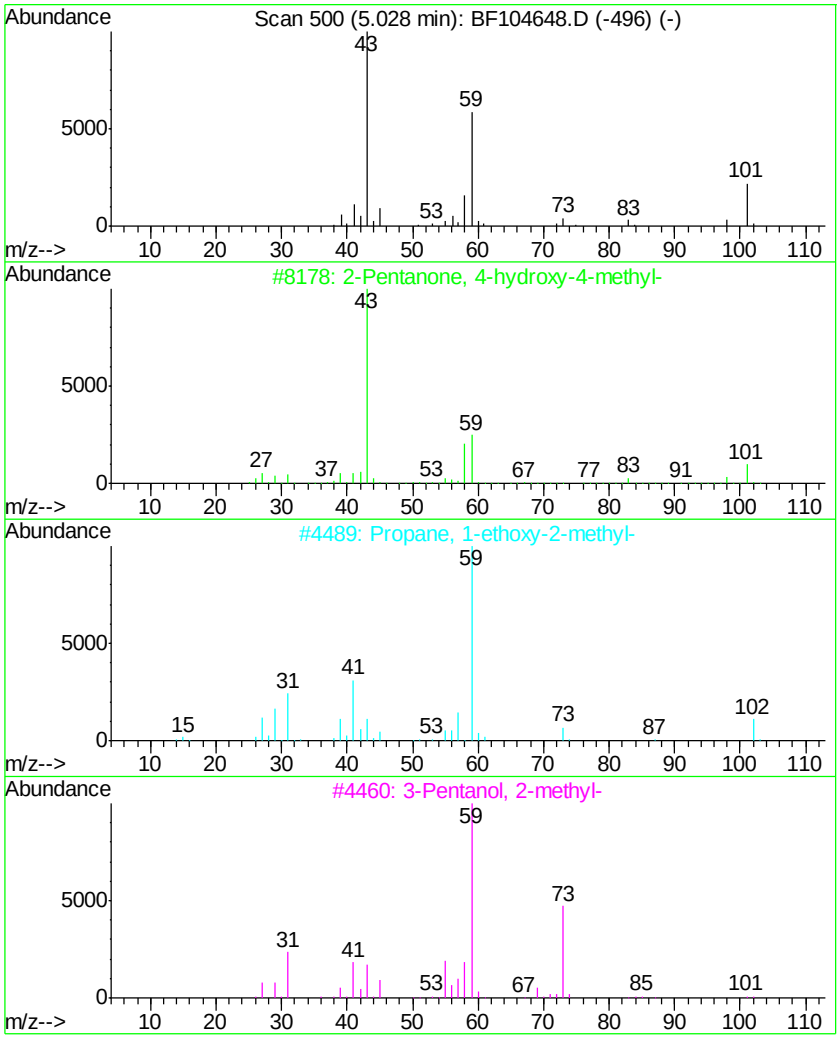
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

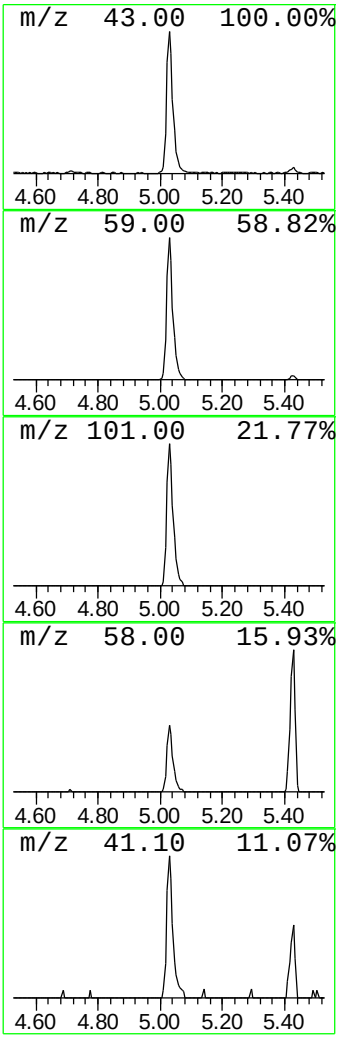
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	5.13 ng	208507	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

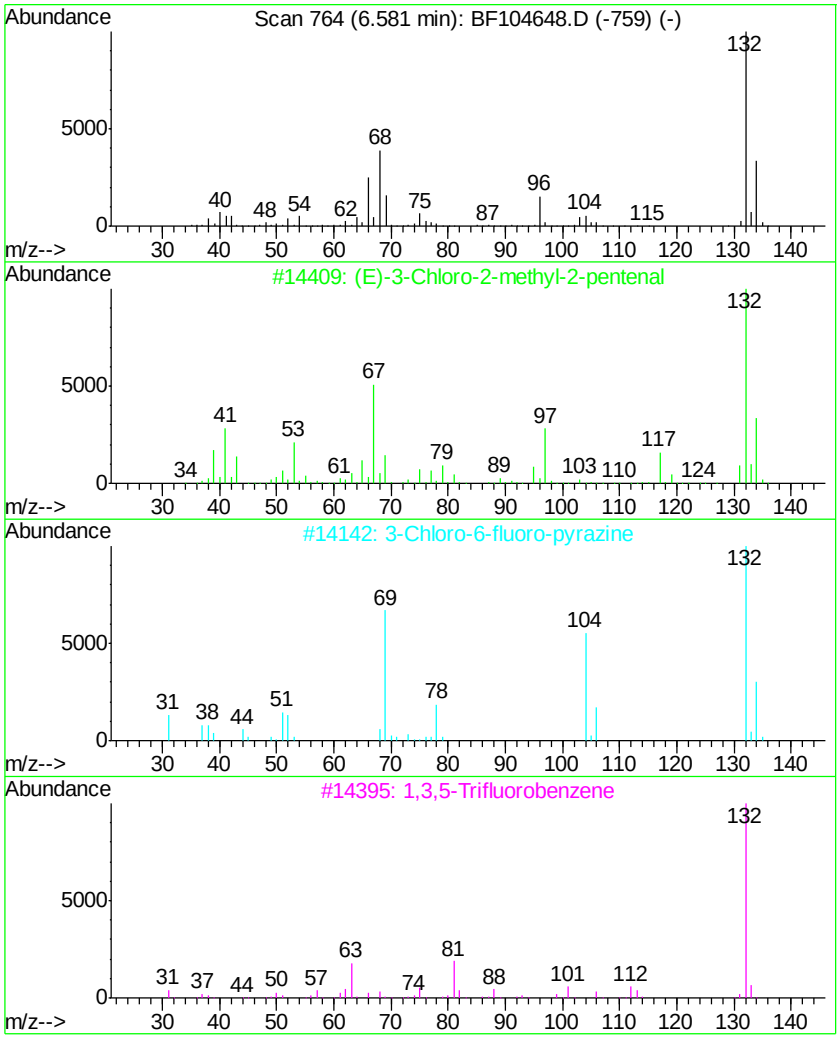
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

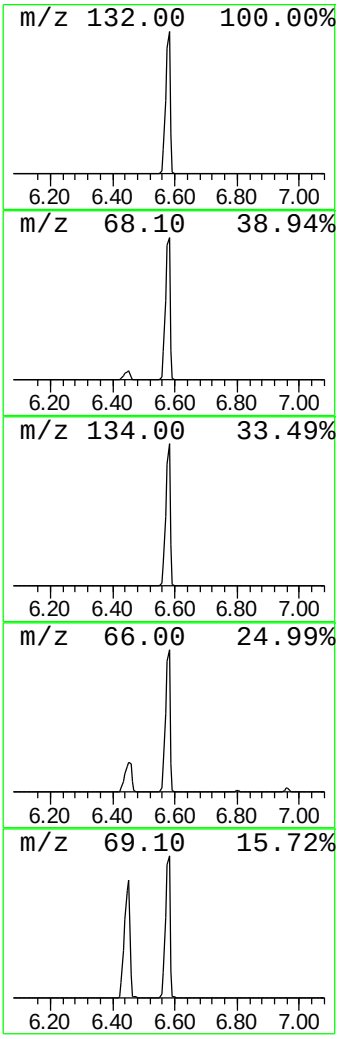
****

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	88.46 ng	3598440	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

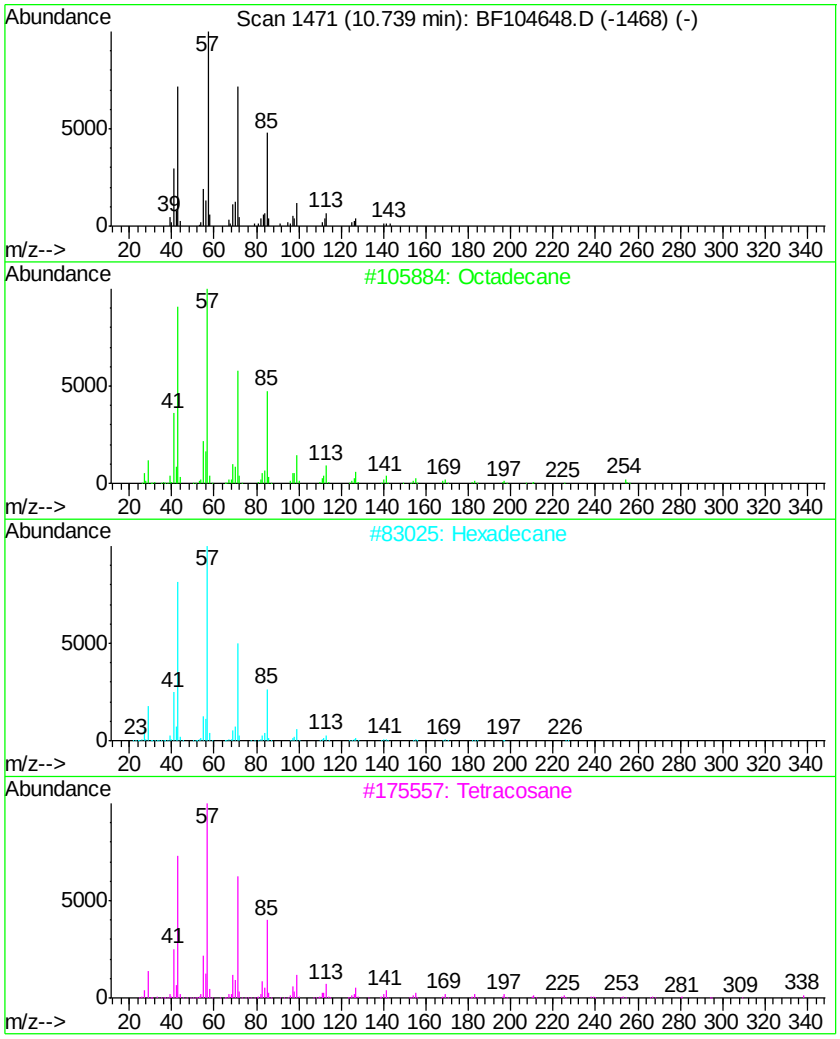
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

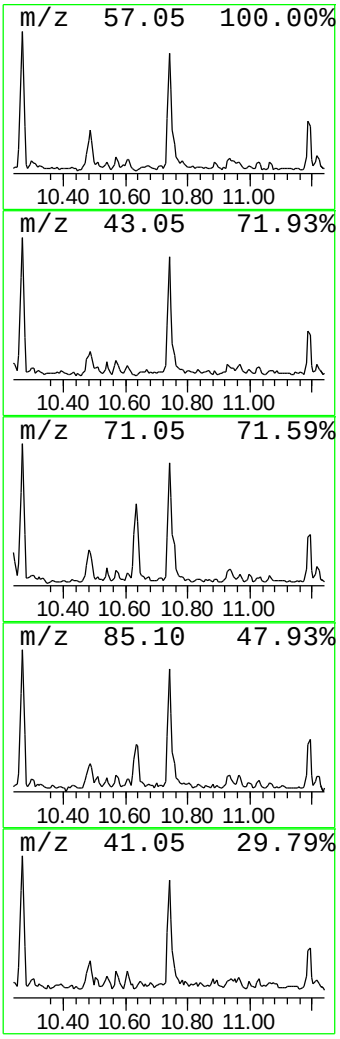
****

Peak Number 4 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.16 ng	101061	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	Eicosane	282	C20H42	000112-95-8	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

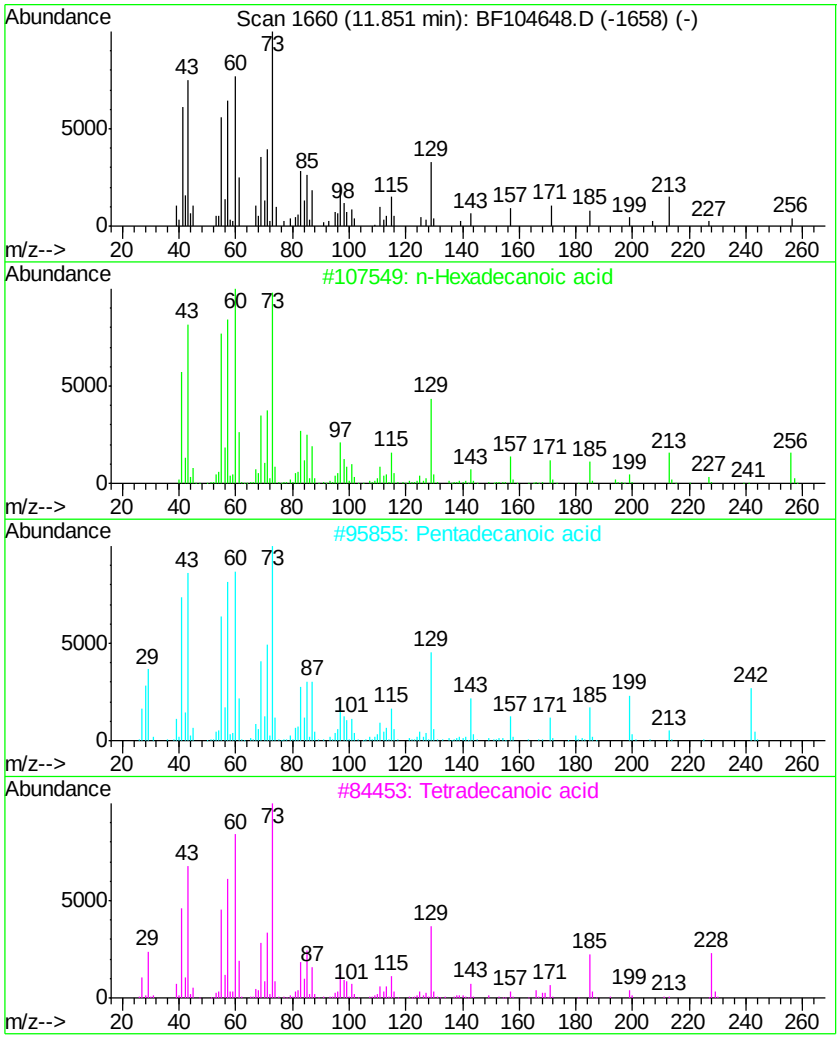
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

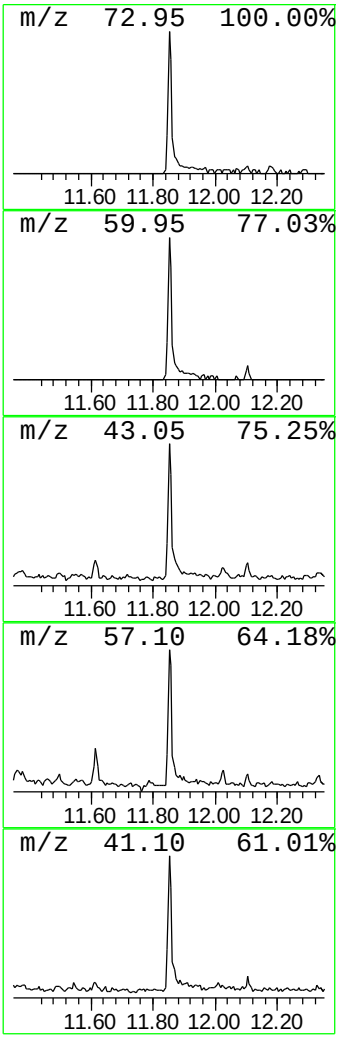
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.79 ng	130812	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	18
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

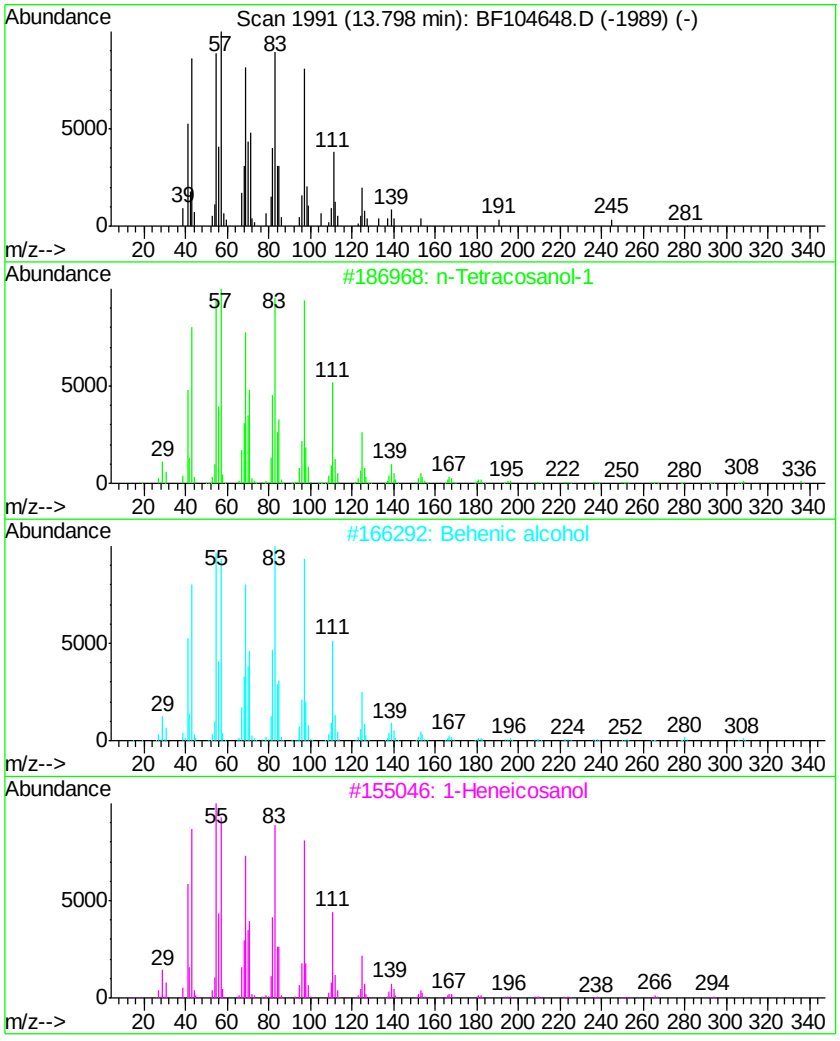
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

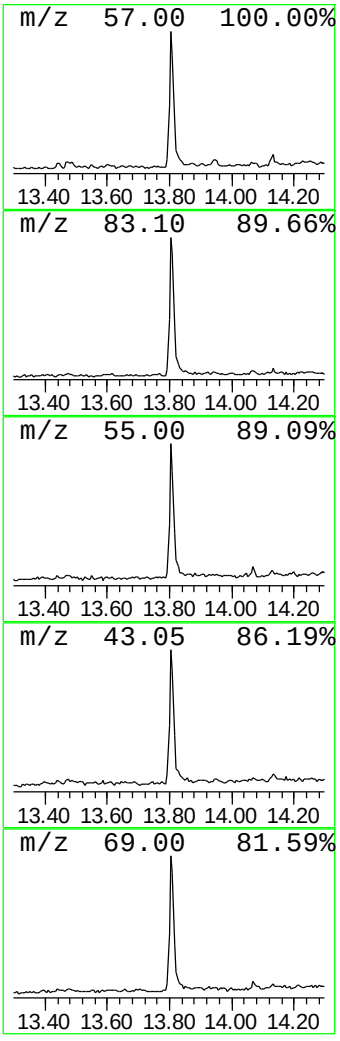
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	6.53 ng	271563	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	1-Heptacosanol	396	C27H56O	002004-39-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041918\
Data File : BF104648.D
Acq On : 20 Apr 2018 00:16
Operator : JU/SJ
Sample : J2455-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.03	5.1	ng	208507	1	6.80	813542	20.0
unknown6.58	6.58	88.5	ng	3598440	1	6.80	813542	20.0
Octadecane	10.74	2.2	ng	101061	4	11.33	936726	20.0
n-Hexadecanoic acid	11.85	2.8	ng	130812	4	11.33	936726	20.0
n-Tetracosanol-1	13.80	6.5	ng	271563	5	13.97	831634	20.0