LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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-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	5.022	495	499	505	rVB	99397	126011	4.20%	0.476%
2	5.422	562	567	570	rBV	2577185	2578900	85.88%	9.747%
3	6.440	735	740	745	rBV	2403456	2741460	91.30%	10.362%
4	6.575	759	763	767	rBV	2583477	2676858	89.14%	10.117%
5	6.804	799	802	806	rBV	883388	796733	26.53%	3.011%
6	6.963	825	829	832	rBV	2434706	2088152	69.54%	7.892%
7	7.369	893	898	901	rBV	1589903	1678861	55.91%	6.345%
8	7.451	908	912	914	rBV	32962	33656	1.12%	0.127%
9	8.092	1017	1021	1024	rBV	1176103	1032937	34.40%	3.904%
10	9.169	1199	1204	1207	rBV	3328068	3002846	100.00%	11.350%
11	9.557	1265	1270	1273	rBV	217161	182304	6.07%	0.689%
12	9.775	1299	1307	1310	rBV	80991	75148	2.50%	0.284%
13	9.845	1315	1319	1323	rBV2	1189281	1055100	35.14%	3.988%
14	10.275	1389	1392	1395	rVB	116617	86513	2.88%	0.327%
15	10.492	1425	1429	1432	rBV	39951	43692	1.46%	0.165%
16	10.639	1448	1454	1457	rBV	1706607	1712444	57.03%	6.472%
17	10.751	1469	1473	1477	rBV	183015	203290	6.77%	0.768%
18	11.198	1546	1549	1551	rBV	80388	61860	2.06%	0.234%
19	11.227	1551	1554	1558	rVB	54186	50209	1.67%	0.190%
20	11.275	1560	1562	1566	rBV2	50783	51892	1.73%	0.196%
21	11.333	1566	1572	1575	rBV	1077088	934118	31.11%	3.531%
22	11.557	1606	1610	1612	rBV3	45513	56512	1.88%	0.214%
23	11.822	1653	1655	1658	rBV2	38019	36270	1.21%	0.137%
24	11.863	1658	1662	1666	rBV	455203	440065	14.65%	1.663%
25	12.033	1688	1691	1694	rBV4	47591	50520	1.68%	0.191%
26	12.380	1747	1750	1753	rBV3	33890	35507	1.18%	0.134%
27	12.651	1793	1796	1798	rBV	77689	87636	2.92%	0.331%
28	12.927	1838	1843	1846	rBV	2541852	2415778	80.45%	9.131%
29	13.816	1992	1994	1998	rVB	172413	171757	5.72%	0.649%
30	13.957	2016	2018	2020	rBV	181519	202799	6.75%	0.767%
31	13.980	2020	2022	2025	rVB	849099	667792	22.24%	2.524%
32	15.451	2268	2272	2281	rVB	501265	706773	23.54%	2.671%
33	17.468	2611	2615	2624	rVB4	155586	373315	12.43%	1.411%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 26457708

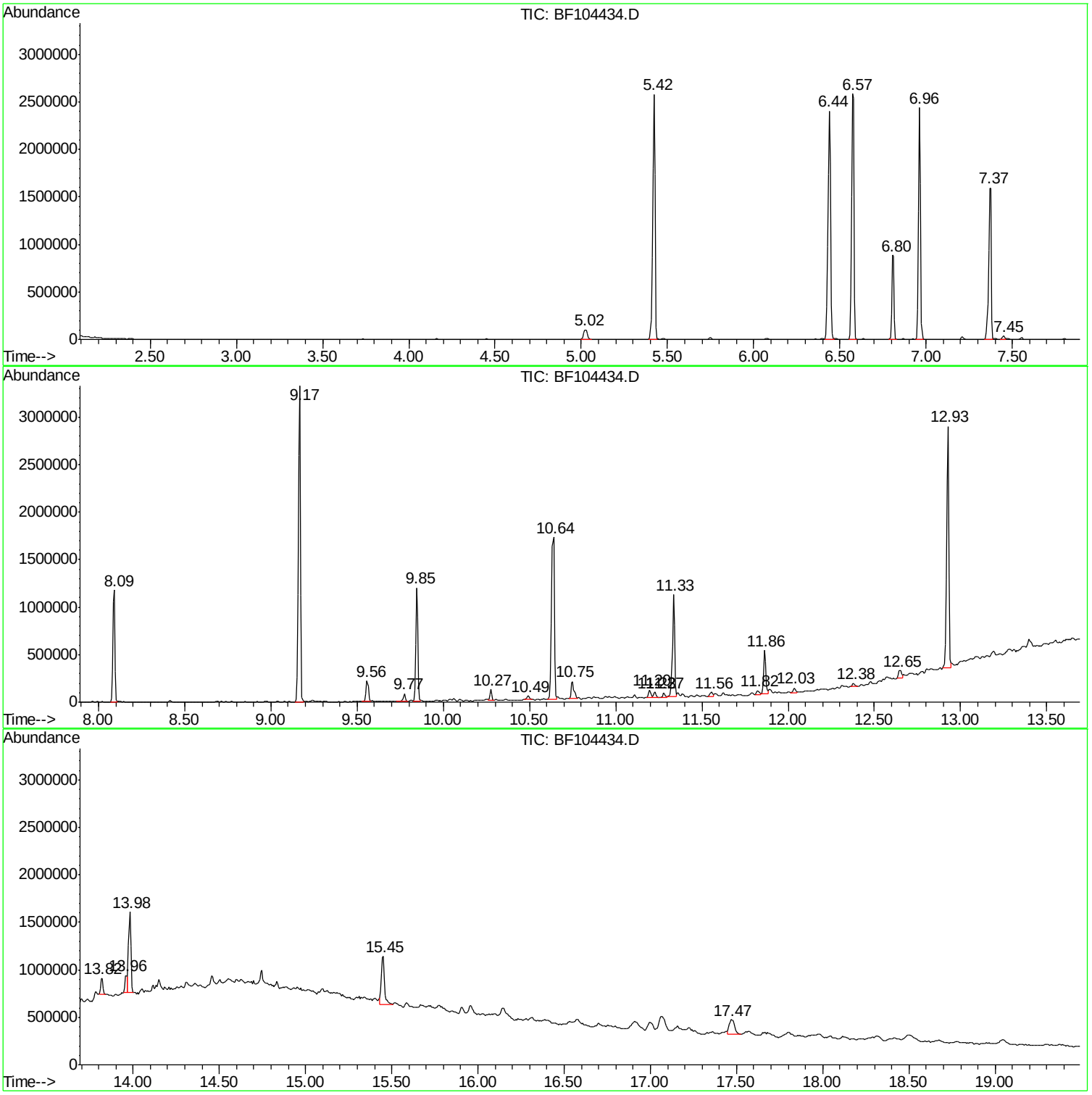
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S003-0001-02

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\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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

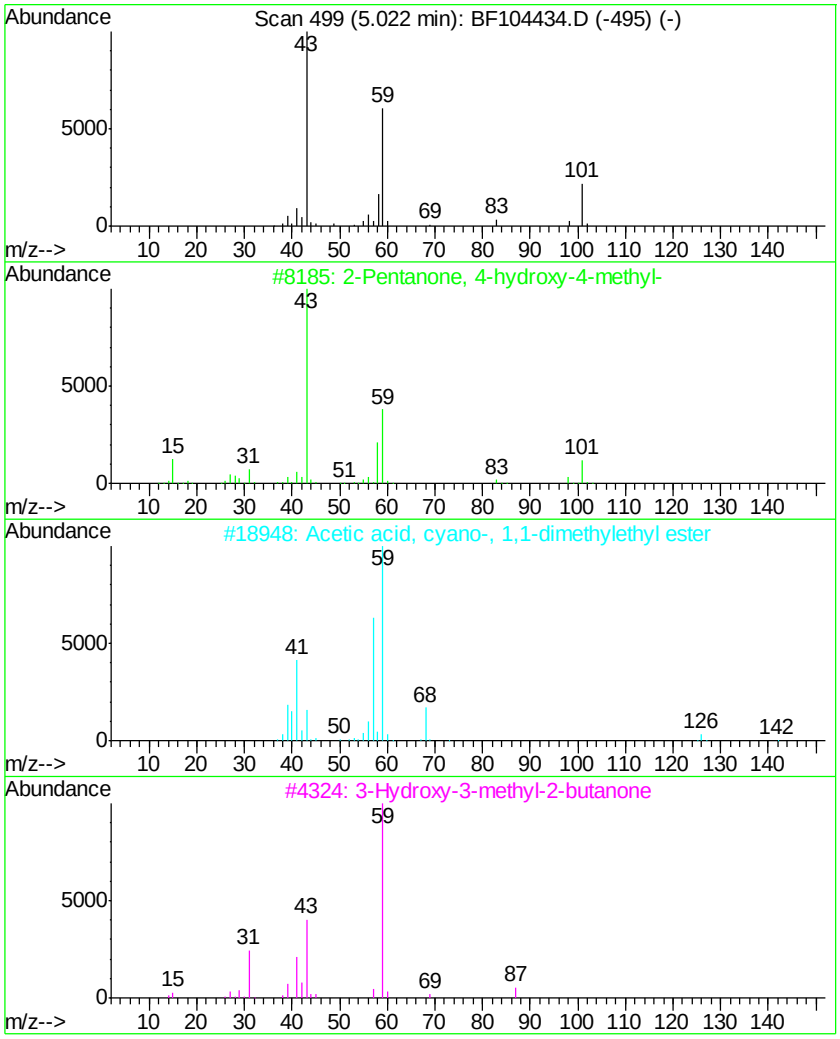
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

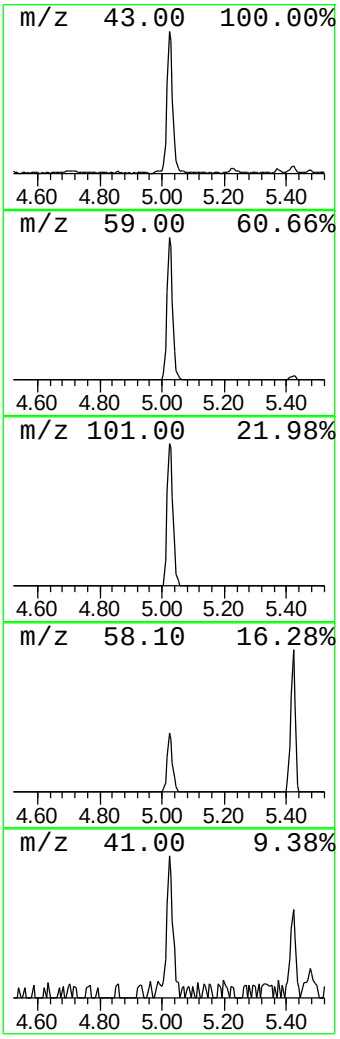
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.16 ng	126011	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	12
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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

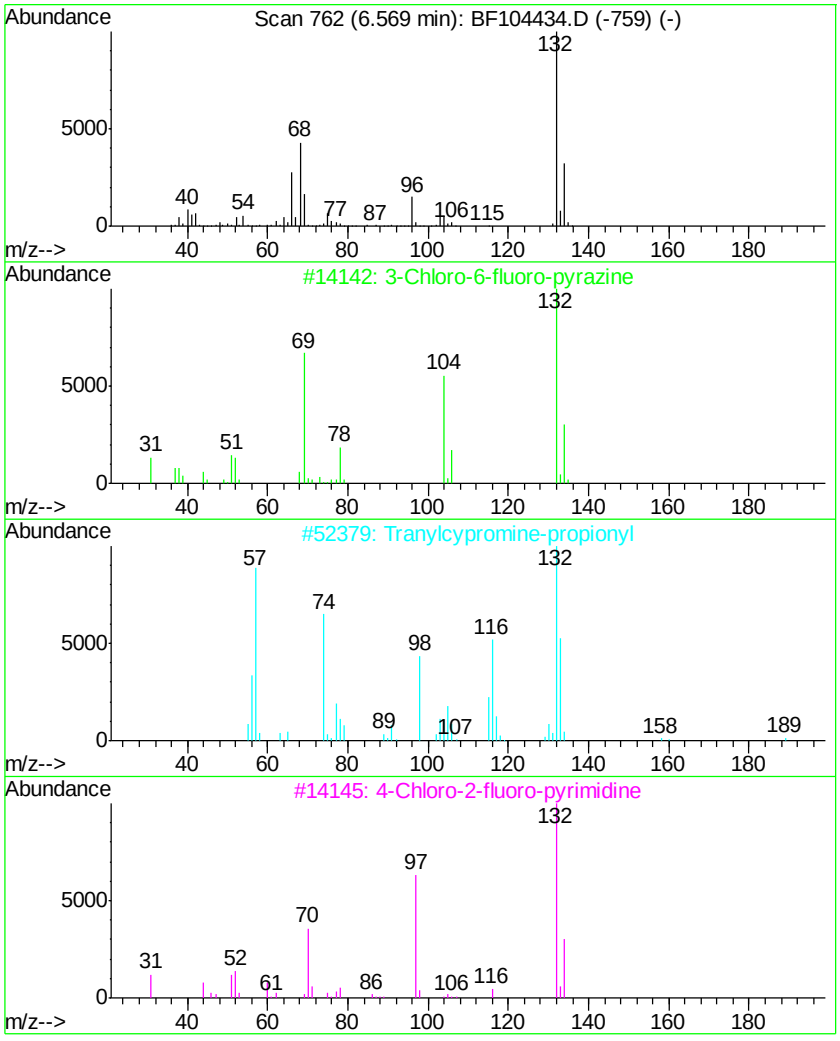
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

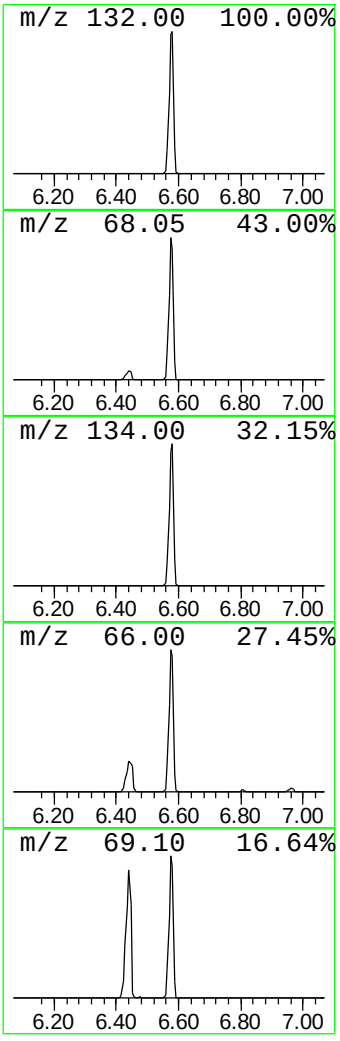
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	67.20 ng	2676860	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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

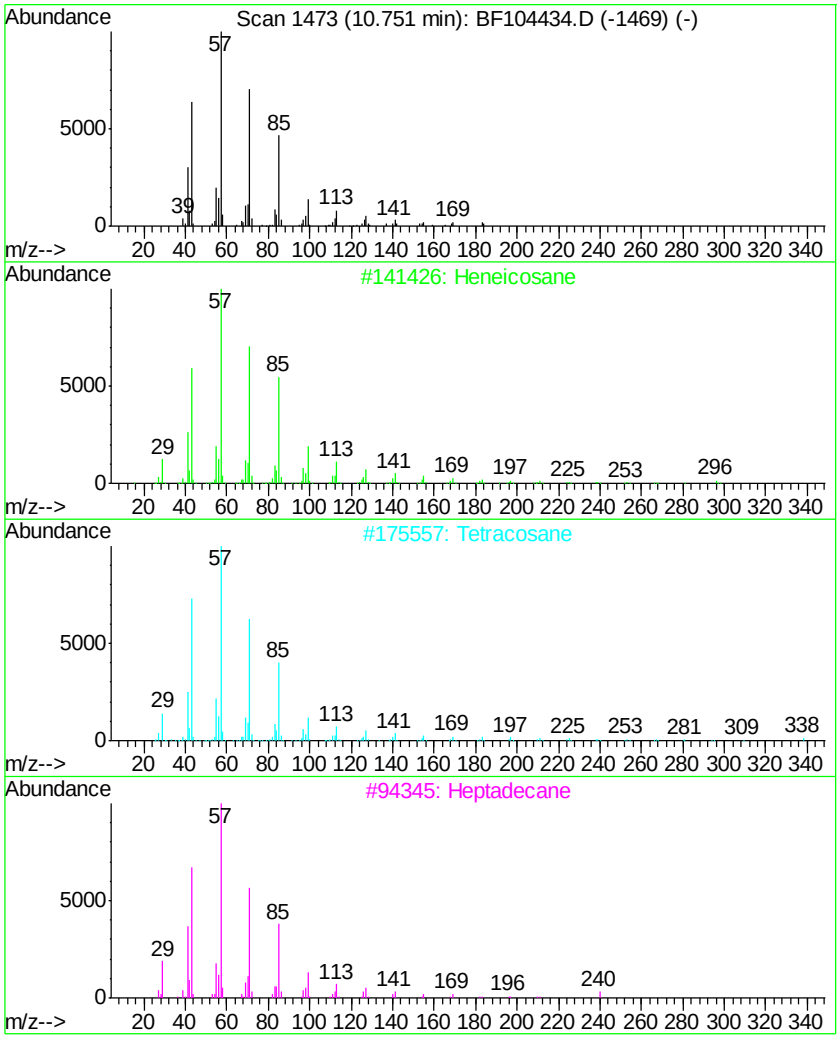
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

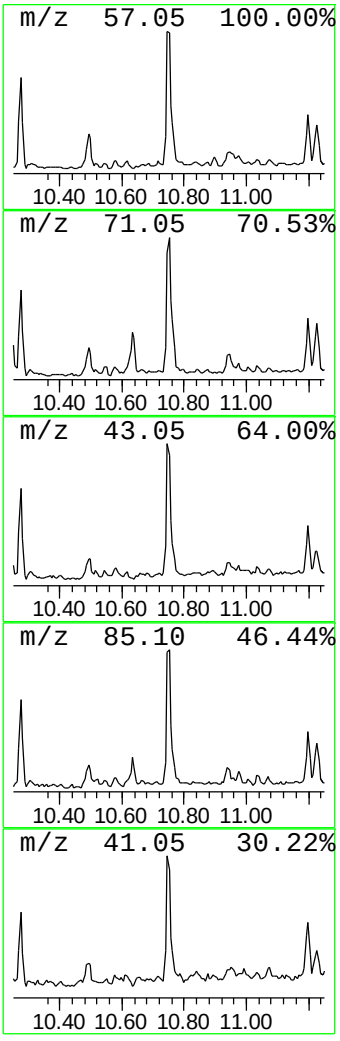
****

Peak Number 4 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	4.35 ng	203290	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Hexadecane	226	C16H34	000544-76-3	91
5	Pentadecane	212	C15H32	000629-62-9	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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

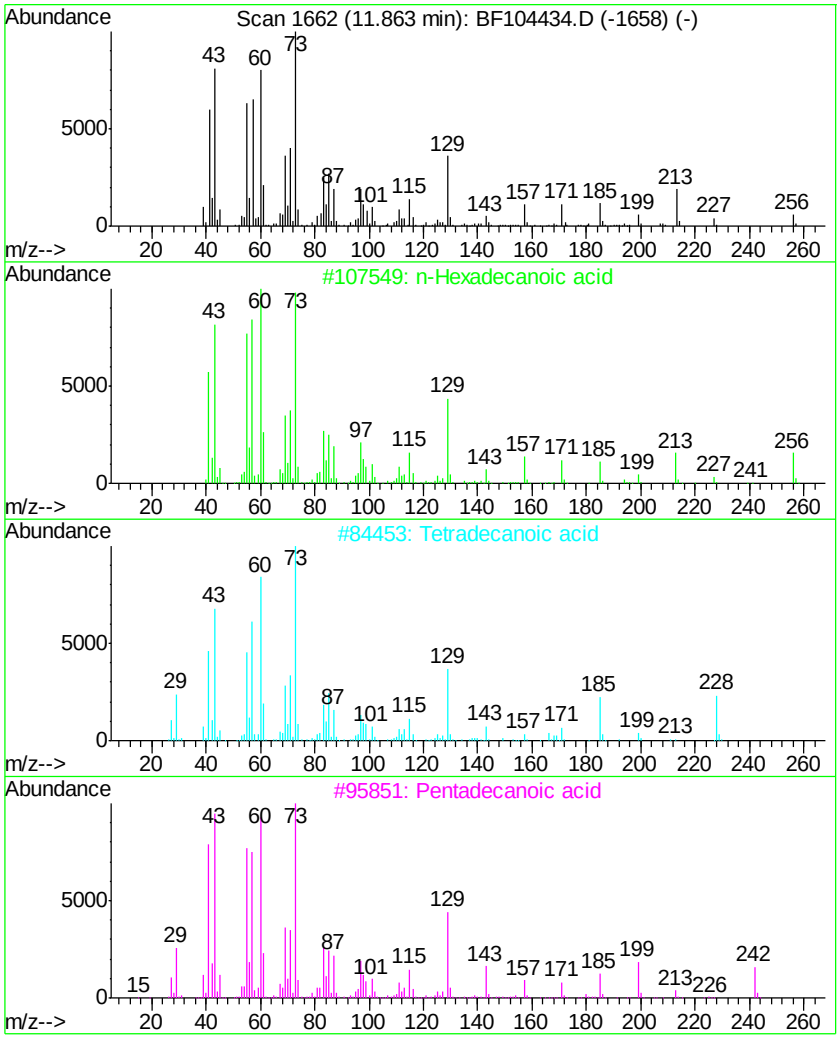
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

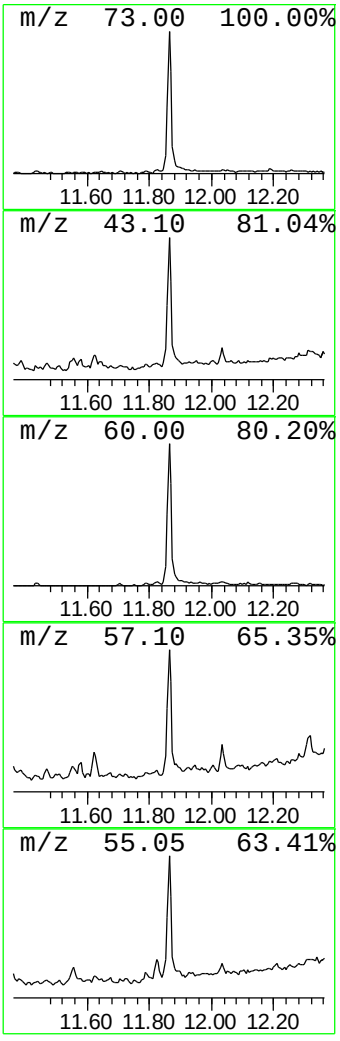
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	9.42 ng	440065	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	93
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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

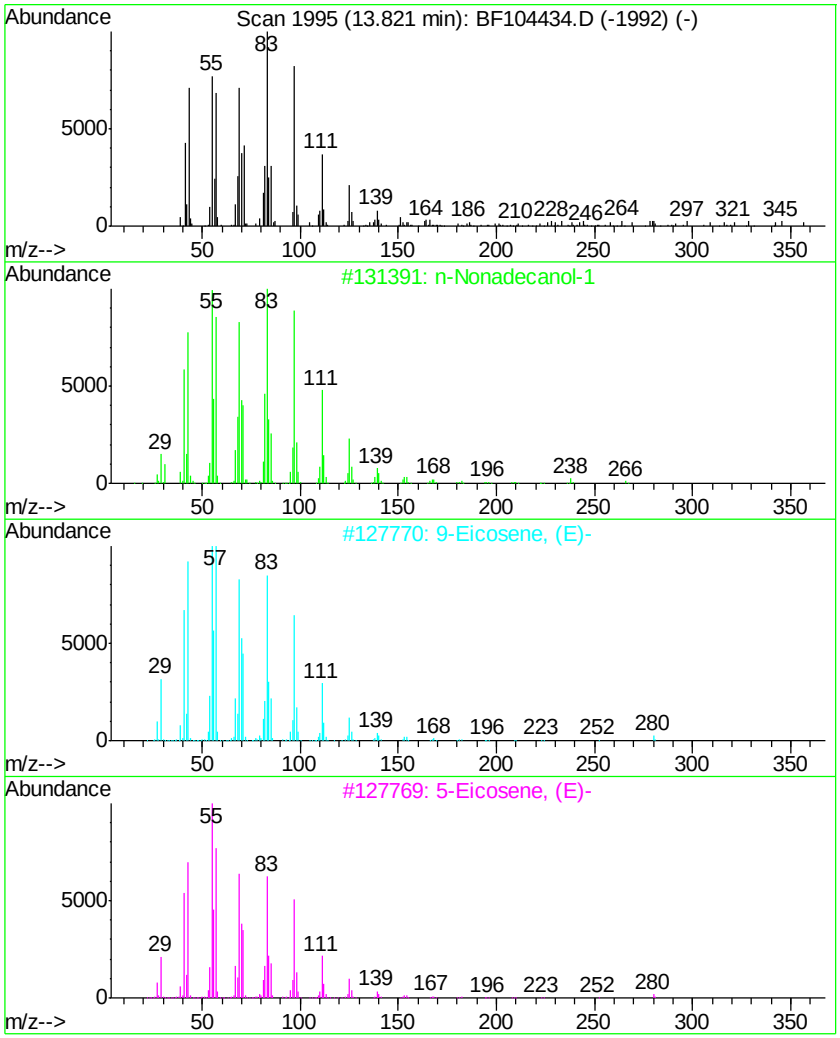
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

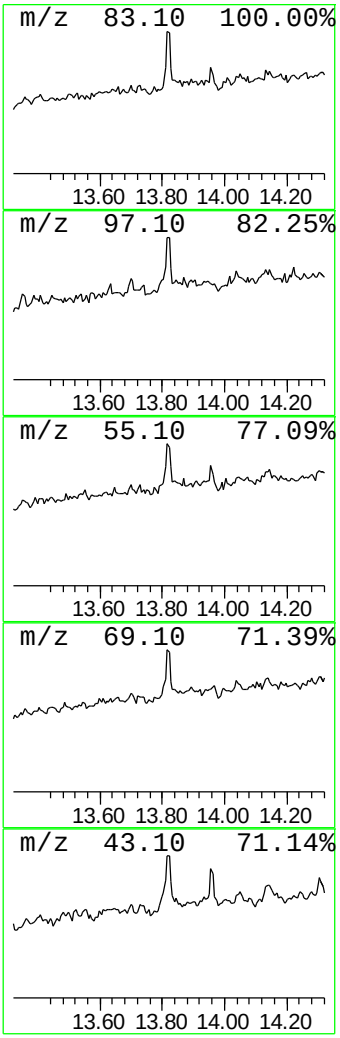
****

Peak Number 6 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.14 ng	171757	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	89
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	86
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	86
5	1-Octadecanol	270	C18H38O	000112-92-5	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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

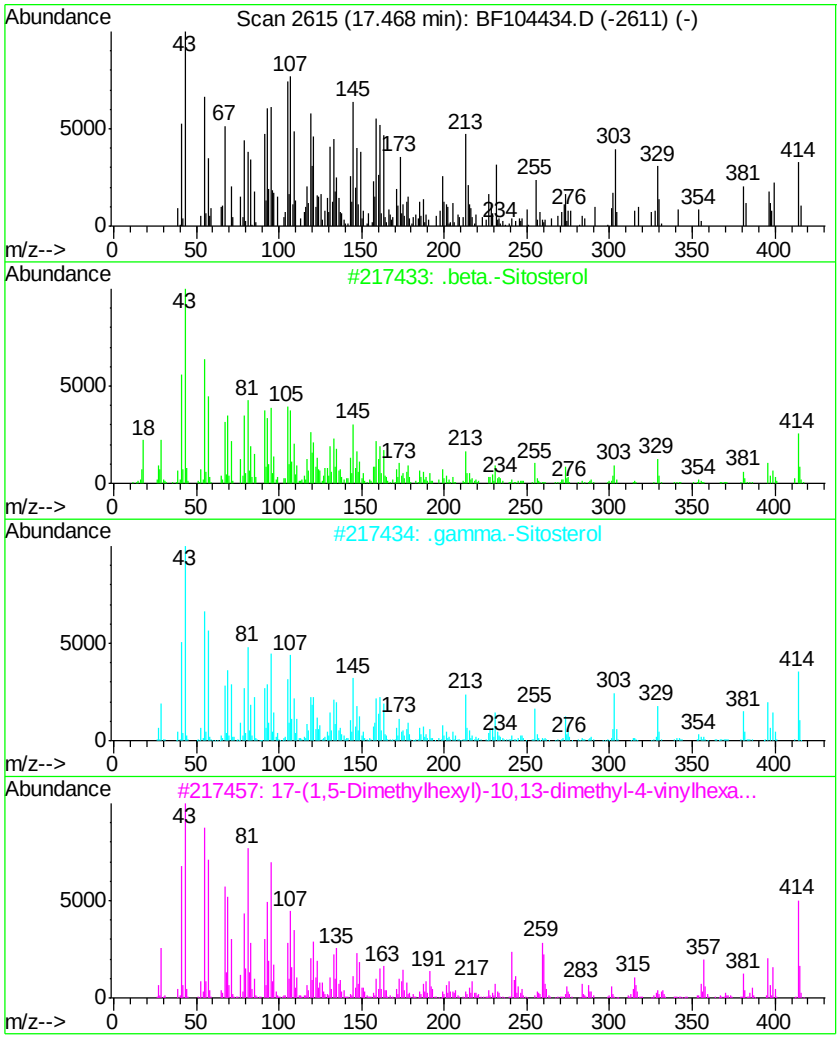
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

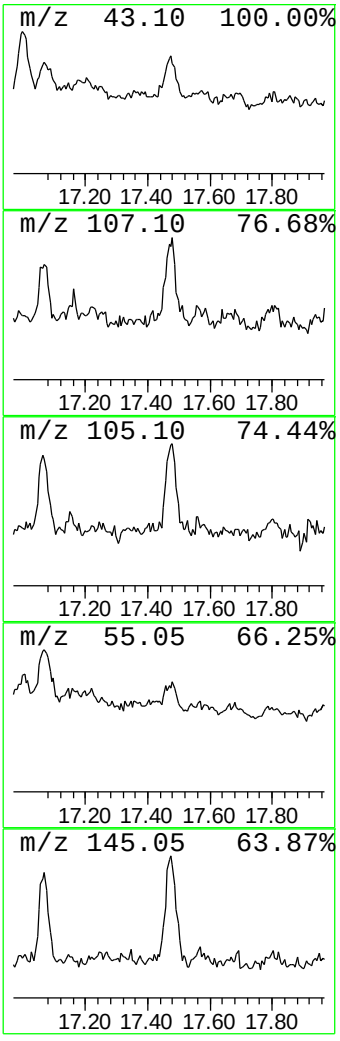
****

Peak Number 7 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	10.56 ng	373315	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	95
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	76
3	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	46
4	3-[(3,7,11,15-Tetramethylhexadec...	374	C25H46N2	067374-05-4	22
5	2,6-Bis(3-(pyrid-2-yl)-2-azaprop...	319	C19H21N5	090719-79-2	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041118\
Data File : BF104434.D
Acq On : 11 Apr 2018 13:29
Operator : JU/SJ
Sample : J2310-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-02

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...	5.02	3.2	ng	126011	1	6.81	796733	20.0
unknown6.57	6.57	67.2	ng	2676860	1	6.81	796733	20.0
Heneicosane	10.75	4.3	ng	203290	4	11.33	934118	20.0
n-Hexadecanoic acid	11.86	9.4	ng	440065	4	11.33	934118	20.0
n-Nonadecanol-1	13.82	5.1	ng	171757	5	13.98	667792	20.0
.beta.-Sitosterol	17.47	10.6	ng	373315	6	15.45	706773	20.0