LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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	5.016	494	498	506	rVB	104022	133065	4.36%	0.468%
2	5.422	561	567	570	rBV	2307157	2489620	81.53%	8.750%
3	6.439	734	740	743	rBV	2457818	2561118	83.87%	9.001%
4	6.575	758	763	766	rBV	2758657	2601322	85.19%	9.143%
5	6.804	799	802	806	rVB	988303	810293	26.54%	2.848%
6	6.963	825	829	832	rBV	2370529	2027730	66.41%	7.127%
7	7.369	893	898	901	rBV	1683479	1630230	53.39%	5.730%
8	8.086	1016	1020	1024	rBV	1222011	1103334	36.13%	3.878%
9	9.169	1199	1204	1207	rBV	3266138	3053519	100.00%	10.732%
10	9.228	1210	1214	1219	rVB3	53768	56886	1.86%	0.200%
11	9.557	1264	1270	1274	rBV	205024	214690	7.03%	0.755%
12	9.757	1300	1304	1305	rBV	56124	49942	1.64%	0.176%
13	9.775	1305	1307	1310	rVB	81011	56866	1.86%	0.200%
14	9.845	1315	1319	1322	rVV2	1352578	1161885	38.05%	4.084%
15	9.869	1322	1323	1329	rVB2	45584	44310	1.45%	0.156%
16	9.963	1335	1339	1343	rBV2	76961	85104	2.79%	0.299%
17	10.004	1343	1346	1349	rVV2	41033	38211	1.25%	0.134%
18	10.063	1353	1356	1359	rVB	58928	58081	1.90%	0.204%
19	10.275	1389	1392	1395	rVB	106035	79285	2.60%	0.279%
20	10.363	1404	1407	1412	rBV6	29405	37325	1.22%	0.131%
21	10.492	1426	1429	1434	rVB2	59885	72737	2.38%	0.256%
22	10.633	1445	1453	1457	rBV	1691782	1747667	57.23%	6.142%
23	10.669	1457	1459	1464	rVB4	49058	57704	1.89%	0.203%
24	10.751	1470	1473	1478	rBV2	187657	254478	8.33%	0.894%
25	11.198	1546	1549	1551	rBV	90172	73225	2.40%	0.257%
26	11.227	1551	1554	1560	rVB	123887	119509	3.91%	0.420%
27	11.280	1560	1563	1566	rBV2	62414	63506	2.08%	0.223%
28	11.333	1568	1572	1575	rVV	1139421	958612	31.39%	3.369%
29	11.363	1575	1577	1579	rVB	69804	50478	1.65%	0.177%
30	11.557	1606	1610	1611	rBV2	36897	46719	1.53%	0.164%
31	11.580	1611	1614	1617	rVB	50667	55201	1.81%	0.194%
32	11.827	1653	1656	1658	rBV3	47150	48951	1.60%	0.172%
33	11.863	1658	1662	1666	rBV	534650	563223	18.45%	1.979%
34	12.033	1689	1691	1695	rBV	61169	64437	2.11%	0.226%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

35	12.316	1737	1739	1741	rBV2	56281	50519	1.65%	0.178%
36	12.651	1794	1796	1798	rBV	99080	85708	2.81%	0.301%
37	12.927	1838	1843	1846	rBV	2314108	2322159	76.05%	8.161%
38	13.821	1993	1995	1999	rVB	392792	359014	11.76%	1.262%
39	13.963	2017	2019	2021	rBV	460606	487549	15.97%	1.714%
40	13.986	2021	2023	2026	rVB	806286	629987	20.63%	2.214%
41	15.462	2271	2274	2283	rVB	602266	829499	27.17%	2.915%
42	17.086	2546	2550	2559	rVB6	266477	622514	20.39%	2.188%
43	17.498	2616	2620	2630	rVB3	306307	596580	19.54%	2.097%

Sum of corrected areas: 28452792

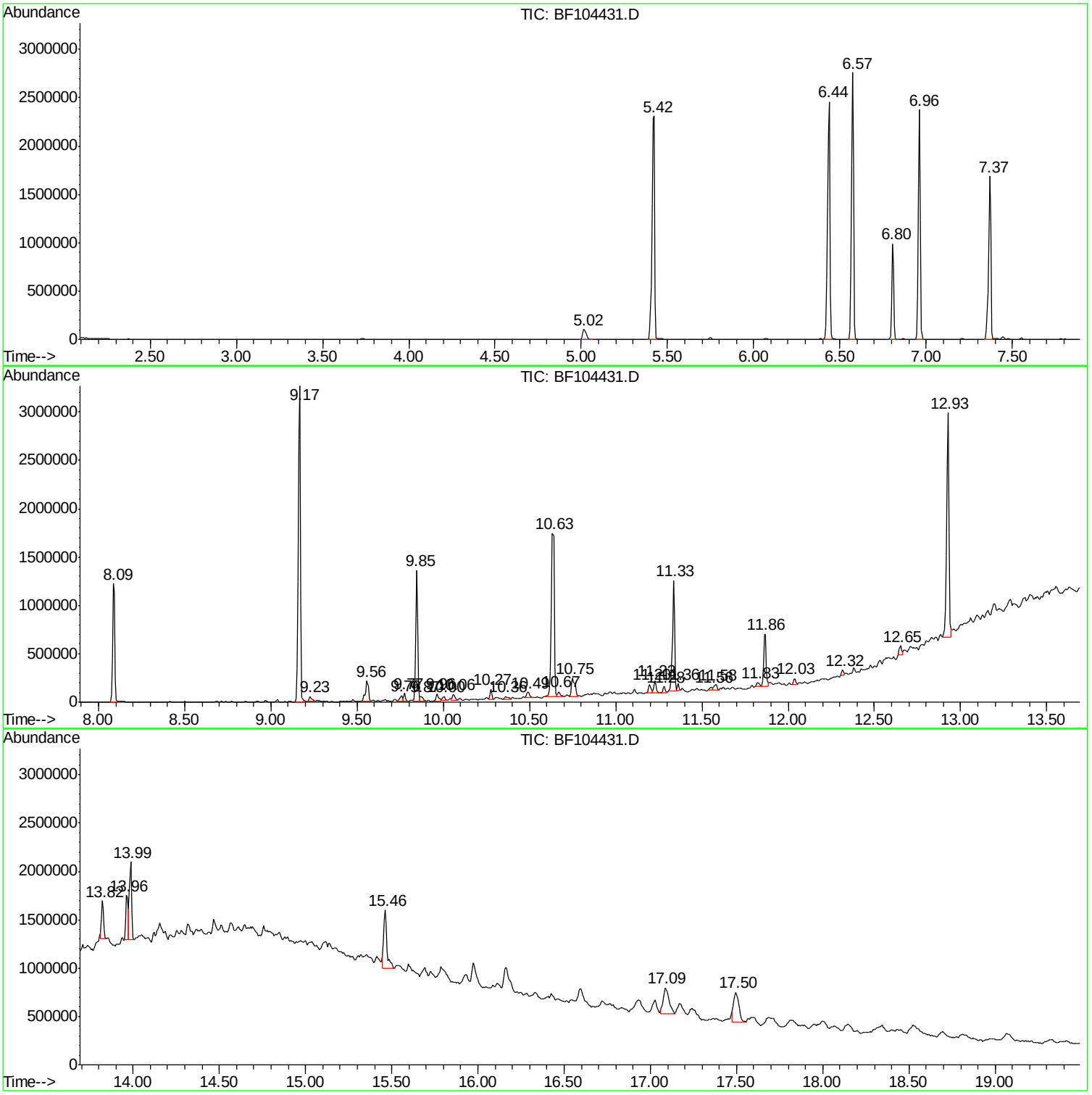
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

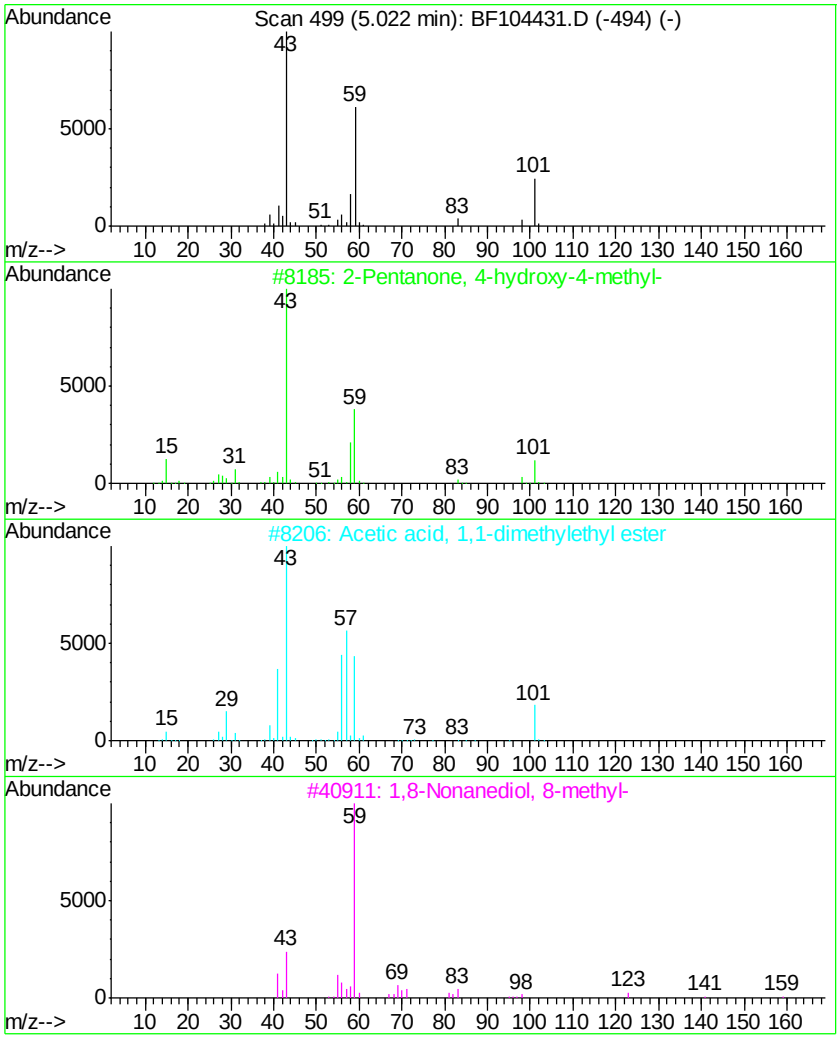
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

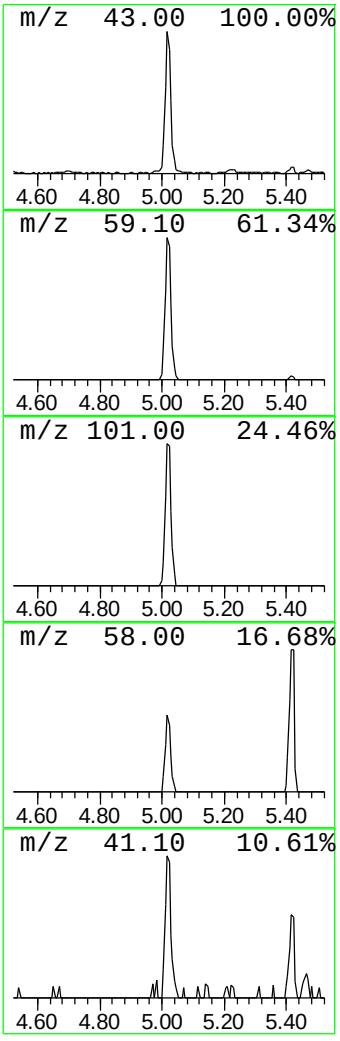
****

Peak Number 1 unknown5.02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.28 ng	133065	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	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

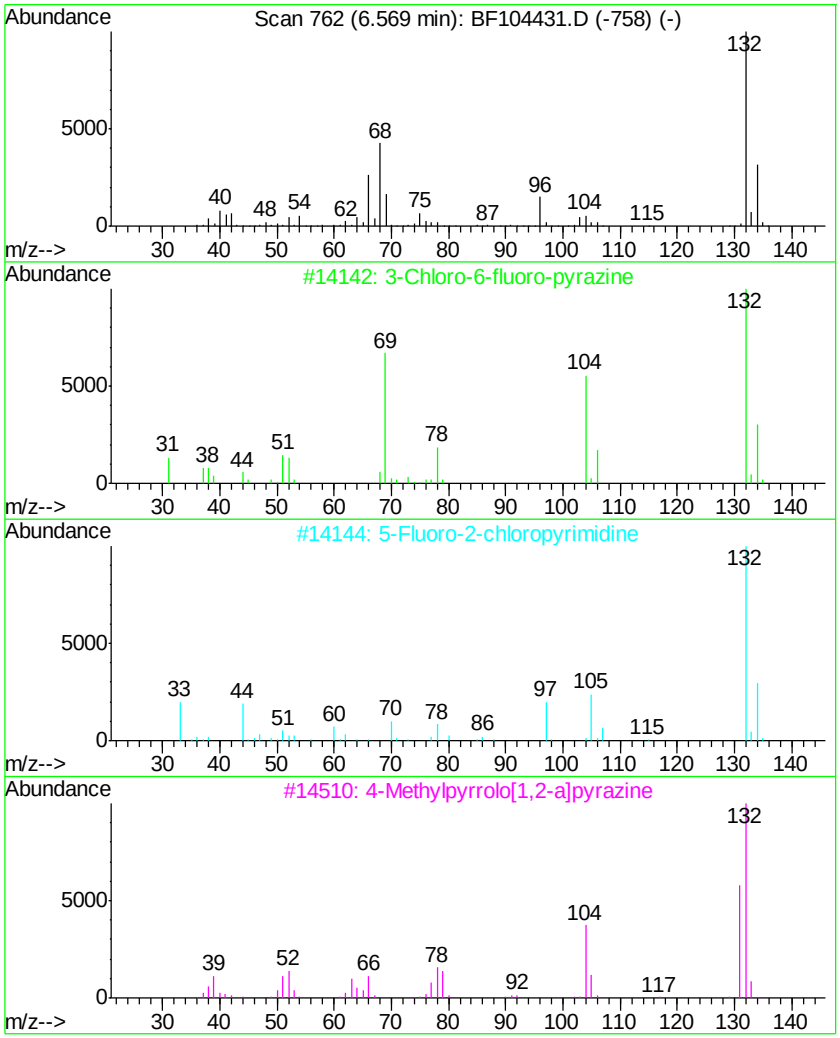
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

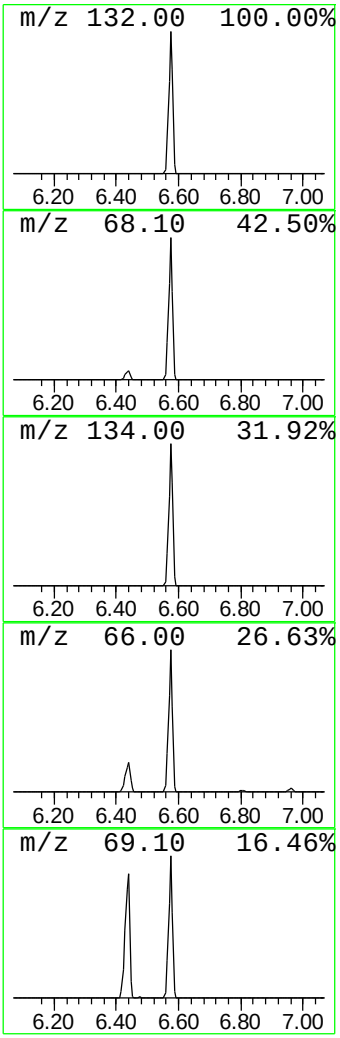
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	64.21 ng	2601320	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

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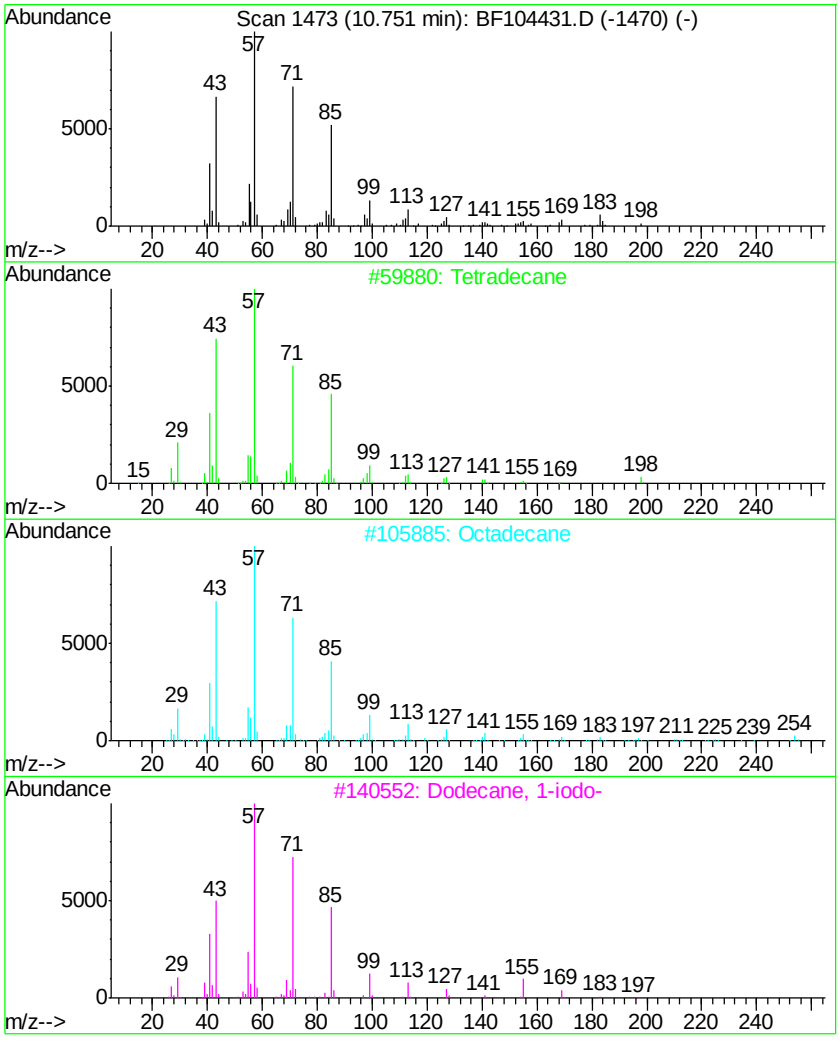
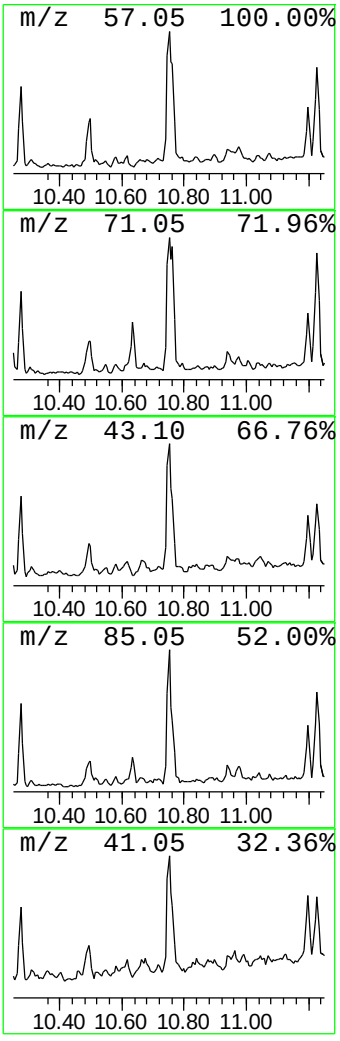
Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	5.31 ng	254478	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Octadecane	254	C18H38	000593-45-3	90
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
4	Tetracosane	338	C24H50	000646-31-1	86
5	Hexadecane	226	C16H34	000544-76-3	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

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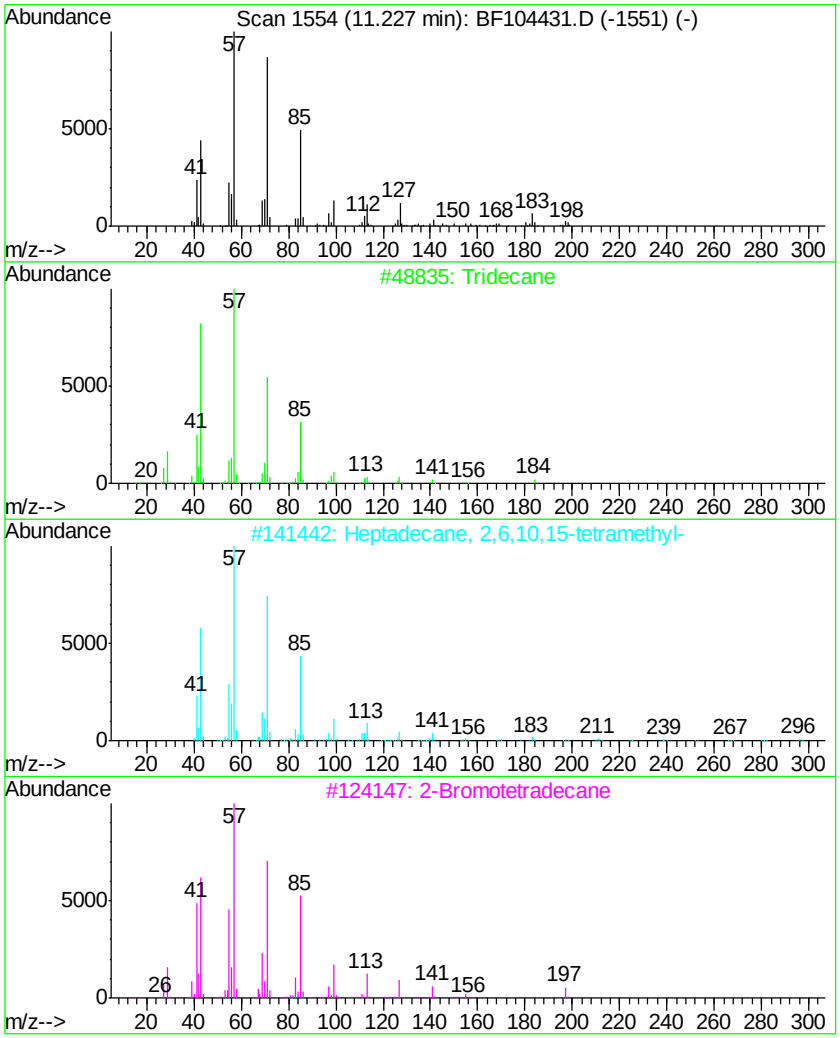
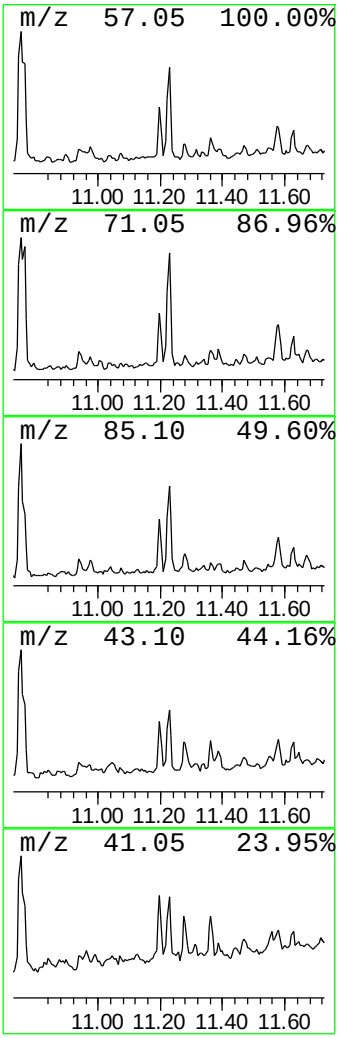
Peak Number 5 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.23	2.49 ng	119509	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
4	Tetradecane	198	C14H30	000629-59-4	78
5	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

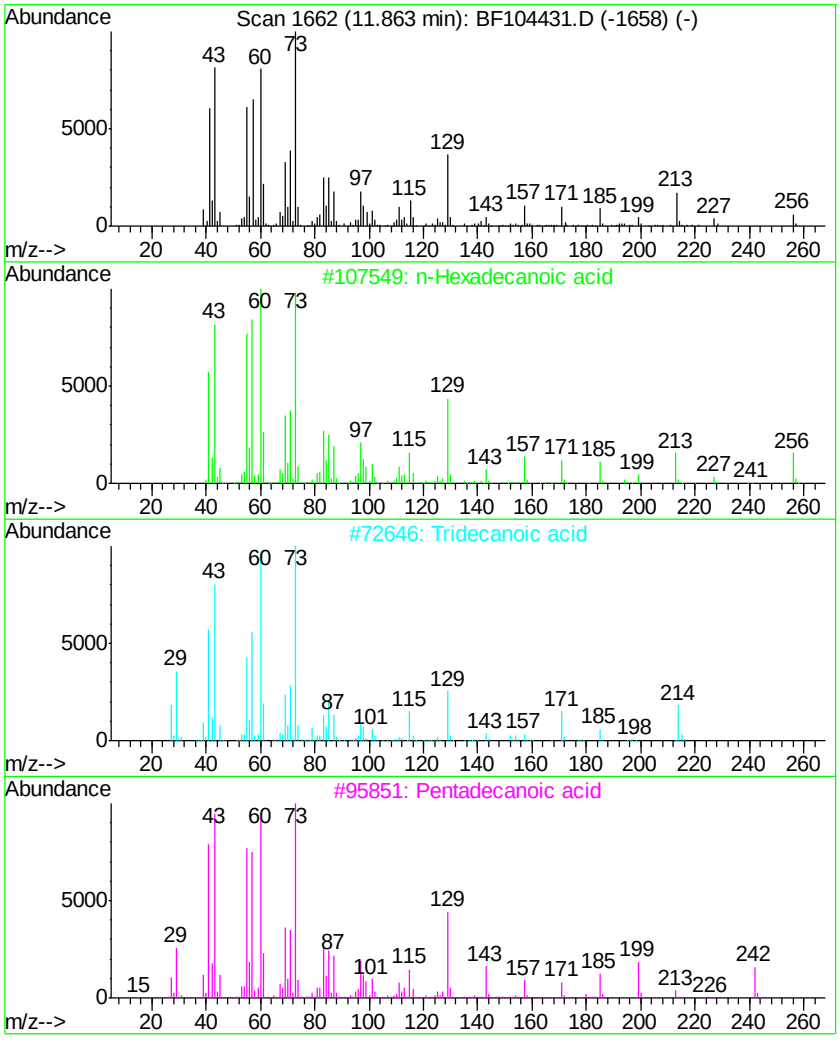
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

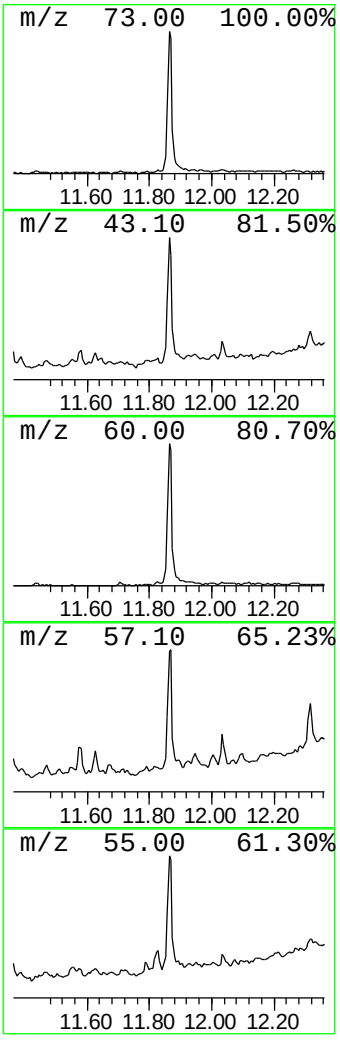
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	11.75 ng	563223	Phenanthrene-d10	11.33

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
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Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

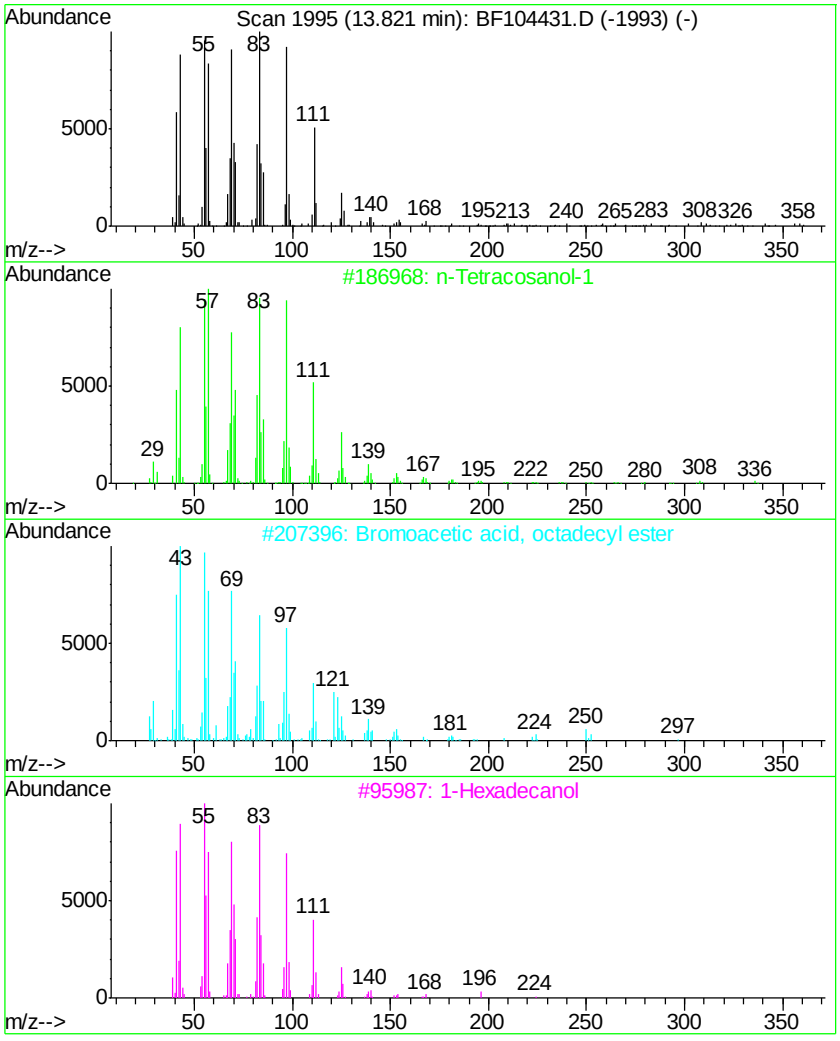
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

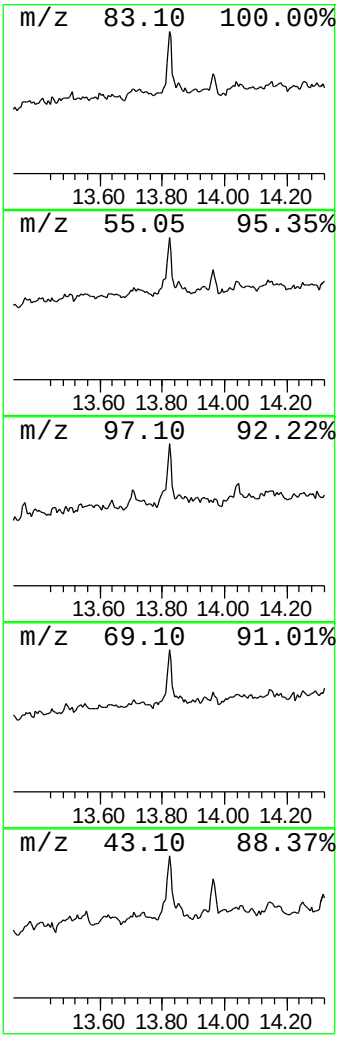
****

Peak Number 7 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	11.40 ng	359014	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Cyclopentadecane	210	C15H30	000295-48-7	87





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Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

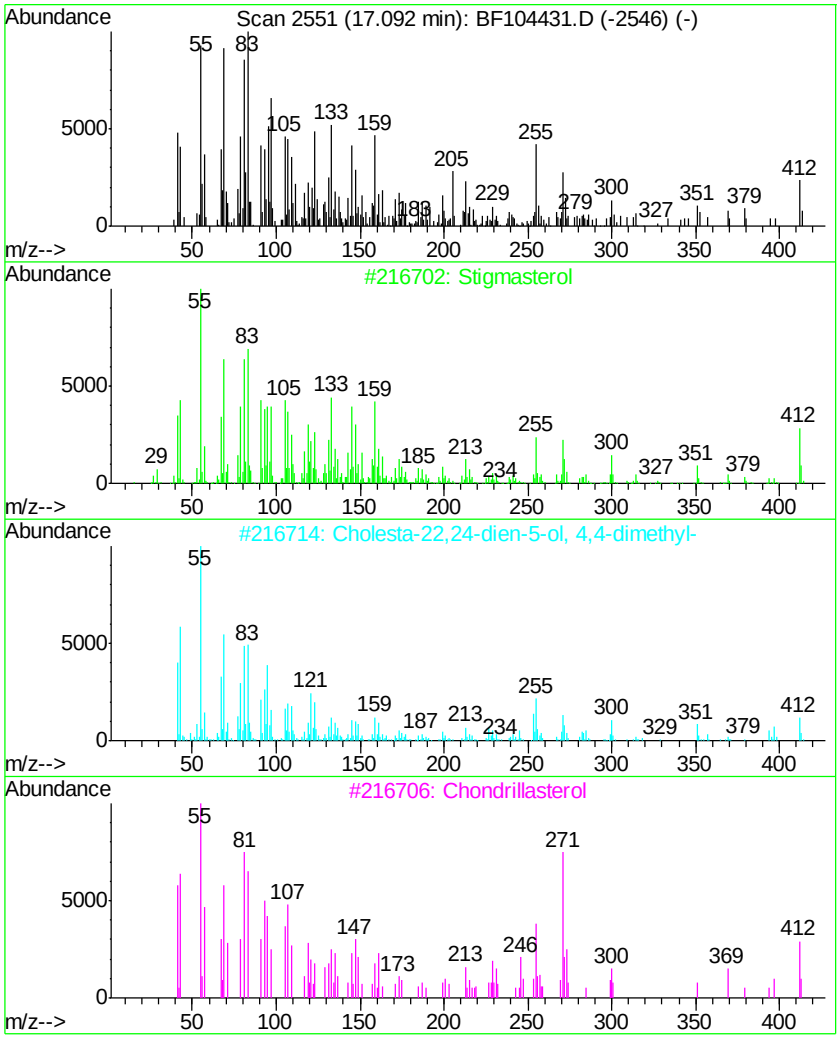
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

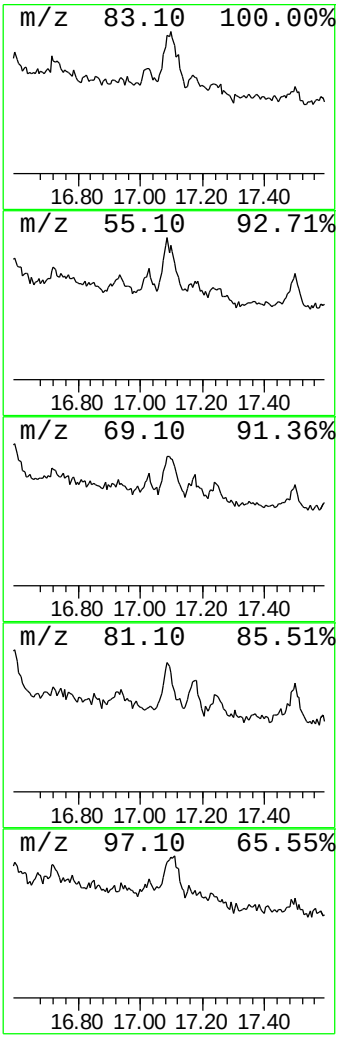
****

Peak Number 8 Stigmasterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	15.01 ng	622514	Perylene-d12	15.46

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	62
3	Chondrillasterol	412	C29H48O	000481-17-4	52
4	Stigmastan-6,22-dien, 3,5-dedihy...	394	C29H46	107304-12-1	49
5	Ergost-5,8(14)-dien-3-ol	398	C28H46O	177962-83-3	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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

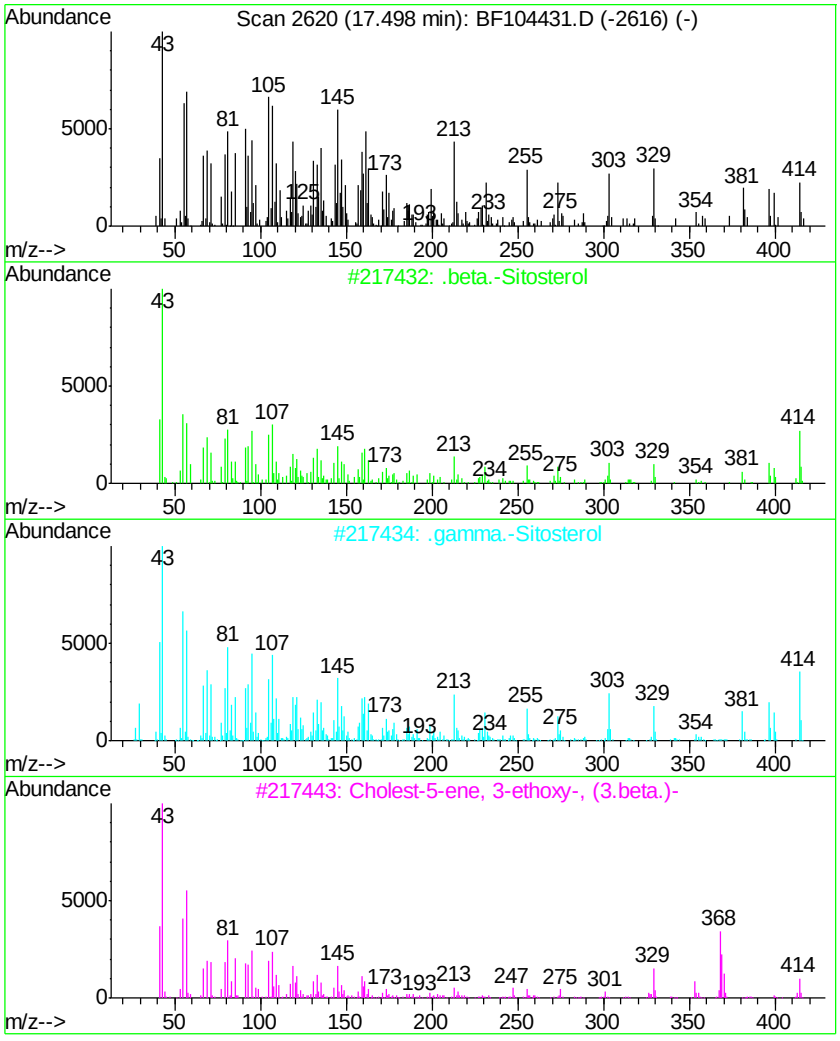
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

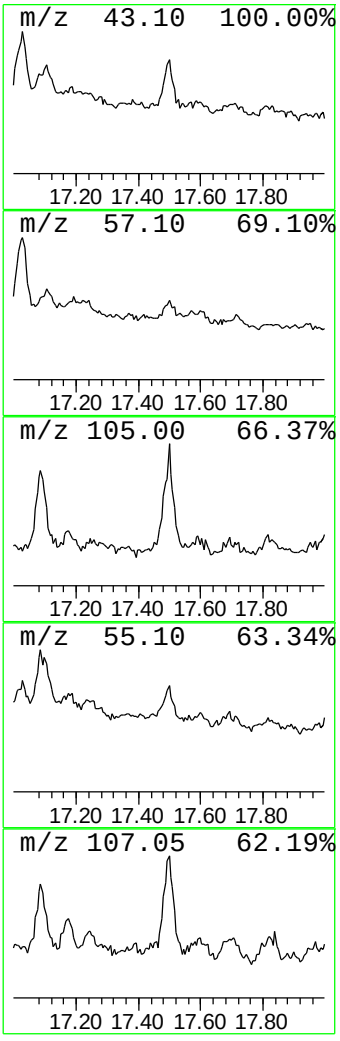
****

Peak Number 9 .beta.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.50	14.38 ng	596580	Perylene-d12	15.46

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	93
3	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	25
4	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	11
5	Benzofuran-2-carboxylic acid, (2...	303	C16H11F2NO3	1000311-07-8	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041118\
Data File : BF104431.D
Acq On : 11 Apr 2018 12:10
Operator : JU/SJ
Sample : J2310-01
Misc :
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Instrument : BNA_F
ClientSampleId : P004-S003-0001-01

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
unknown5.02	5.02	3.3	ng	133065	1	6.80	810293	20.0
unknown6.57	6.57	64.2	ng	2601320	1	6.80	810293	20.0
Tetradecane	10.75	5.3	ng	254478	4	11.33	958612	20.0
Tridecane	11.23	2.5	ng	119509	4	11.33	958612	20.0
n-Hexadecanoic acid	11.86	11.8	ng	563223	4	11.33	958612	20.0
n-Tetracosanol-1	13.82	11.4	ng	359014	5	13.99	629987	20.0
Stigmasterol	17.09	15.0	ng	622514	6	15.46	829499	20.0
.beta.-Sitosterol	17.50	14.4	ng	596580	6	15.46	829499	20.0