LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BART-3-E(0-1)

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-BF113017.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	5.057	502	505	513	rBV	24207	28477	5.68%	0.529%
2	5.457	570	573	586	rBV	404895	395060	78.87%	7.334%
3	6.451	740	742	743	rBV	8763	6613	1.32%	0.123%
4	6.475	743	746	758	rVB	456543	409433	81.74%	7.601%
5	6.616	766	770	773	rBV	520845	439750	87.79%	8.164%
6	6.845	806	809	813	rBV	318884	249203	49.75%	4.626%
7	6.998	832	835	839	rBV	412098	359514	71.77%	6.674%
8	7.410	901	905	917	rBV	290739	254824	50.87%	4.731%
9	8.128	1024	1027	1034	rBV	368698	298456	59.58%	5.541%
10	9.198	1206	1209	1220	rBV	558027	500925	100.00%	9.299%
11	9.275	1220	1222	1225	rVB	7989	6299	1.26%	0.117%
12	9.598	1270	1277	1283	rBV	29187	30151	6.02%	0.560%
13	9.804	1309	1312	1314	rBV	16449	11964	2.39%	0.222%
14	9.886	1322	1326	1330	rBV	309344	295830	59.06%	5.492%
15	10.304	1394	1397	1399	rVB	15898	12270	2.45%	0.228%
16	10.674	1456	1460	1467	rBV	194005	172539	34.44%	3.203%
17	10.774	1474	1477	1482	rBV	12952	13768	2.75%	0.256%
18	11.374	1575	1579	1581	rBV	305343	253201	50.55%	4.700%
19	11.398	1581	1583	1589	rVB	63492	50613	10.10%	0.940%
20	11.610	1615	1619	1623	rBV	6174	7055	1.41%	0.131%
21	11.886	1662	1666	1668	rBV2	8011	13510	2.70%	0.251%
22	11.986	1680	1683	1686	rBV2	11503	10915	2.18%	0.203%
23	12.168	1709	1714	1717	rBV4	5643	6658	1.33%	0.124%
24	12.204	1717	1720	1724	rVB2	13255	11373	2.27%	0.211%
25	12.586	1782	1785	1789	rVB	115932	93896	18.74%	1.743%
26	12.674	1798	1800	1805	rBV6	3324	5735	1.14%	0.106%
27	12.815	1818	1824	1831	rBV	86296	100809	20.12%	1.871%
28	12.957	1844	1848	1851	rBV	444209	379102	75.68%	7.038%
29	13.039	1858	1862	1865	rVB5	6486	9012	1.80%	0.167%
30	13.145	1874	1880	1883	rBV2	14886	24821	4.96%	0.461%
31	13.215	1889	1892	1894	rVB2	8409	7374	1.47%	0.137%
32	13.245	1894	1897	1901	rBV4	9169	12805	2.56%	0.238%
33	13.339	1911	1913	1917	rVB3	7304	8895	1.78%	0.165%
34	13.374	1917	1919	1922	rBV3	6607	8018	1.60%	0.149%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BART-3-E(0-1)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.515	1940	1943	1945	rBV4	5130	7312	1.46%	0.136%
36	13.657	1965	1967	1970	rBV2	8371	7044	1.41%	0.131%
37	13.768	1983	1986	1988	rBV	15494	14474	2.89%	0.269%
38	13.792	1988	1990	1992	rVB2	8308	6006	1.20%	0.111%
39	13.845	1993	1999	2001	rVV6	26350	34899	6.97%	0.648%
40	13.868	2001	2003	2006	rVV2	12645	12202	2.44%	0.227%
41	13.933	2012	2014	2017	rBV4	8602	9462	1.89%	0.176%
42	13.980	2020	2022	2024	rBV2	21778	20602	4.11%	0.382%
43	14.021	2024	2029	2031	rVV2	300543	334925	66.86%	6.218%
44	14.045	2031	2033	2035	rVB	45771	37243	7.43%	0.691%
45	15.062	2204	2206	2211	rBV	36379	53545	10.69%	0.994%
46	15.498	2276	2280	2284	rVB	179125	229674	45.85%	4.264%
47	16.180	2393	2396	2406	rVB3	64460	130494	26.05%	2.422%

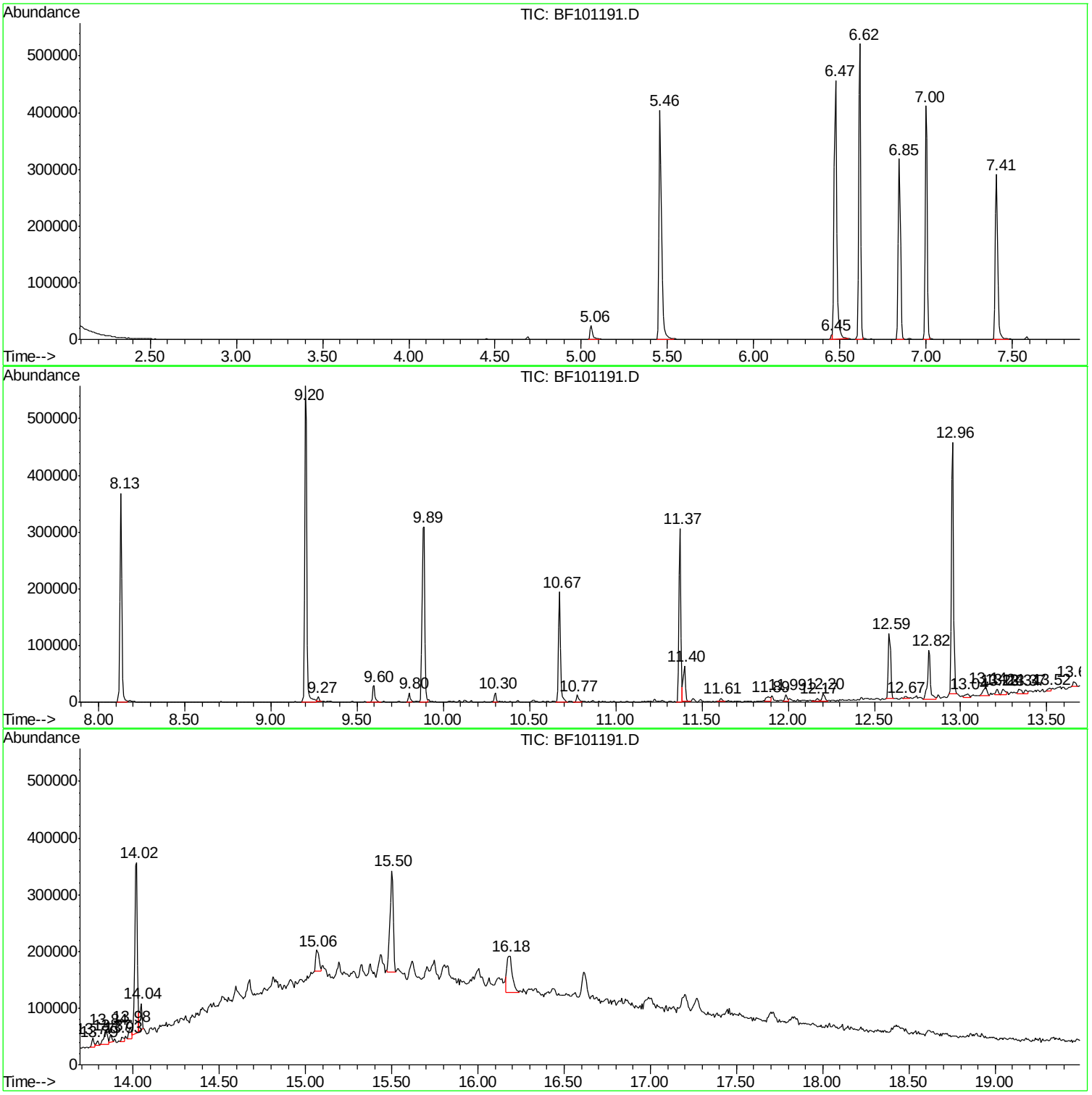
Sum of corrected areas: 5386750

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BART-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BART-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

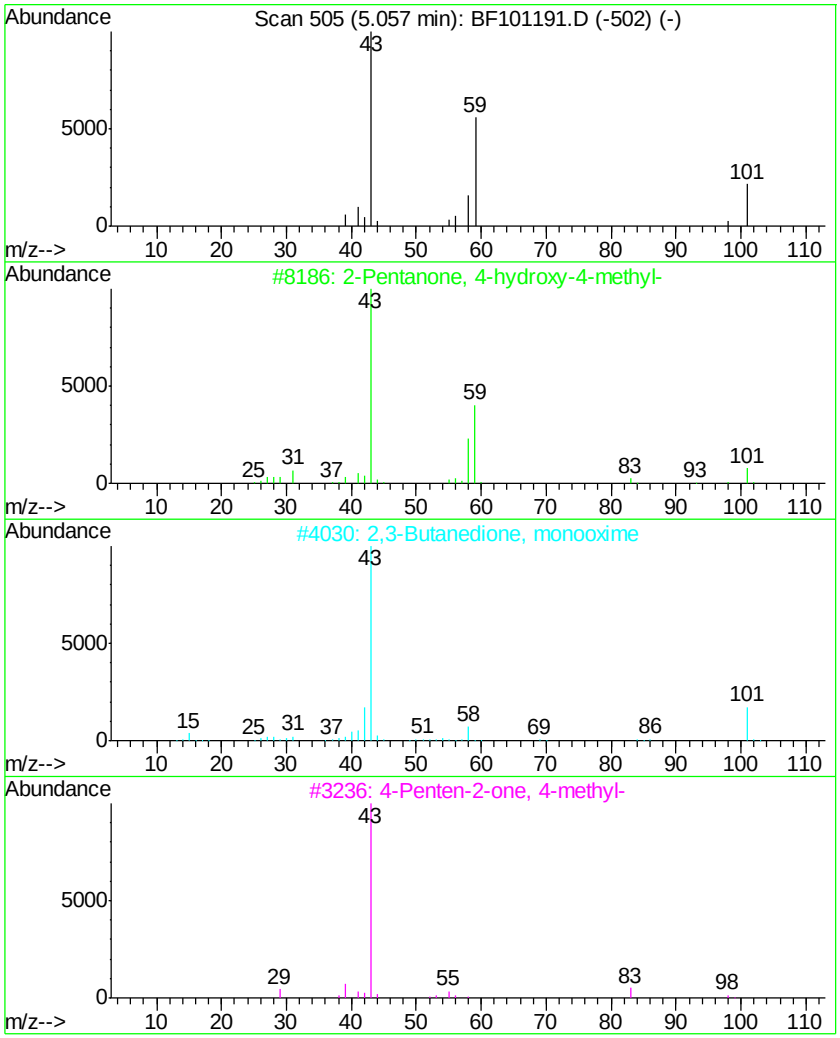
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

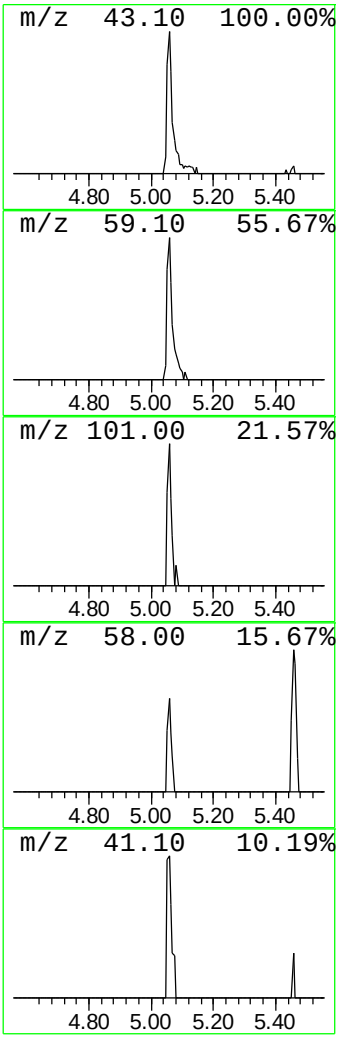
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	2.29 ng	28477	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BART-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

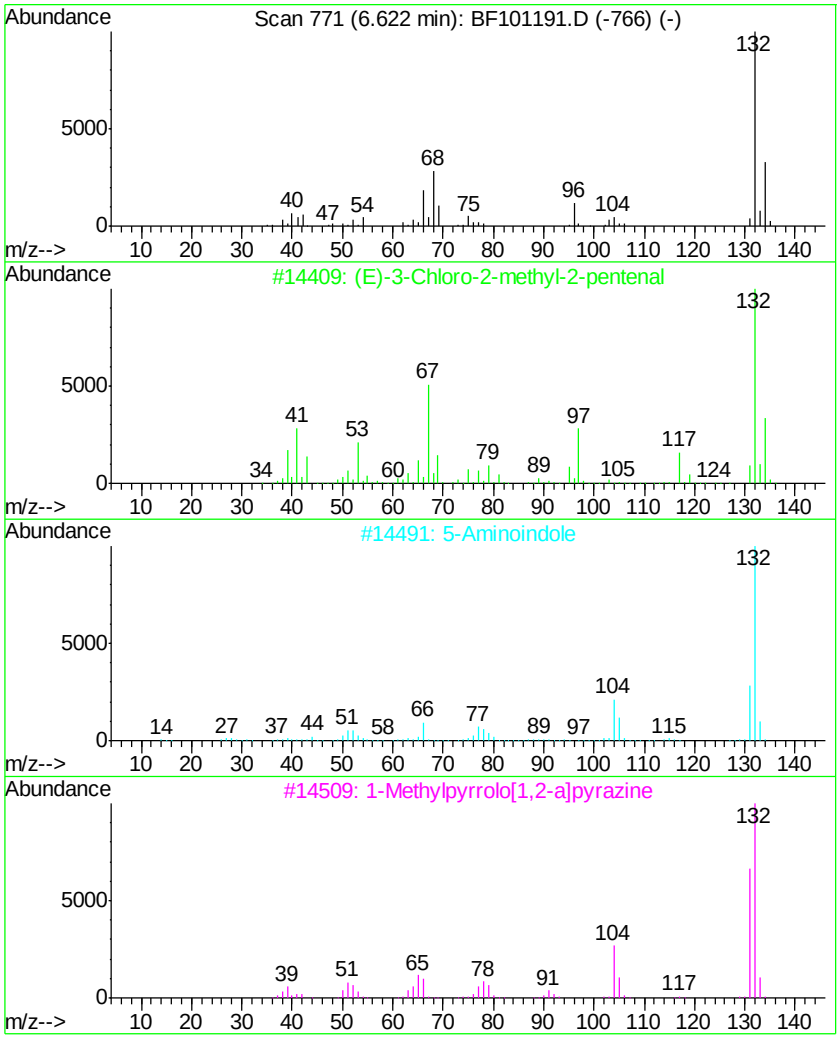
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

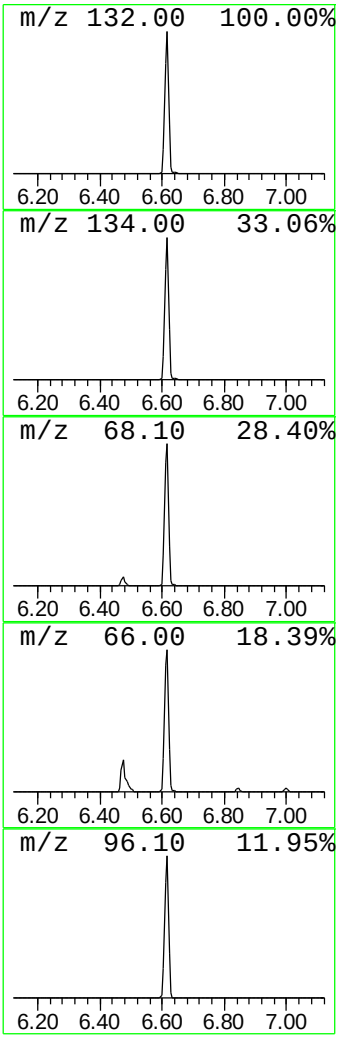
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	35.29 ng	439750	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BART-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

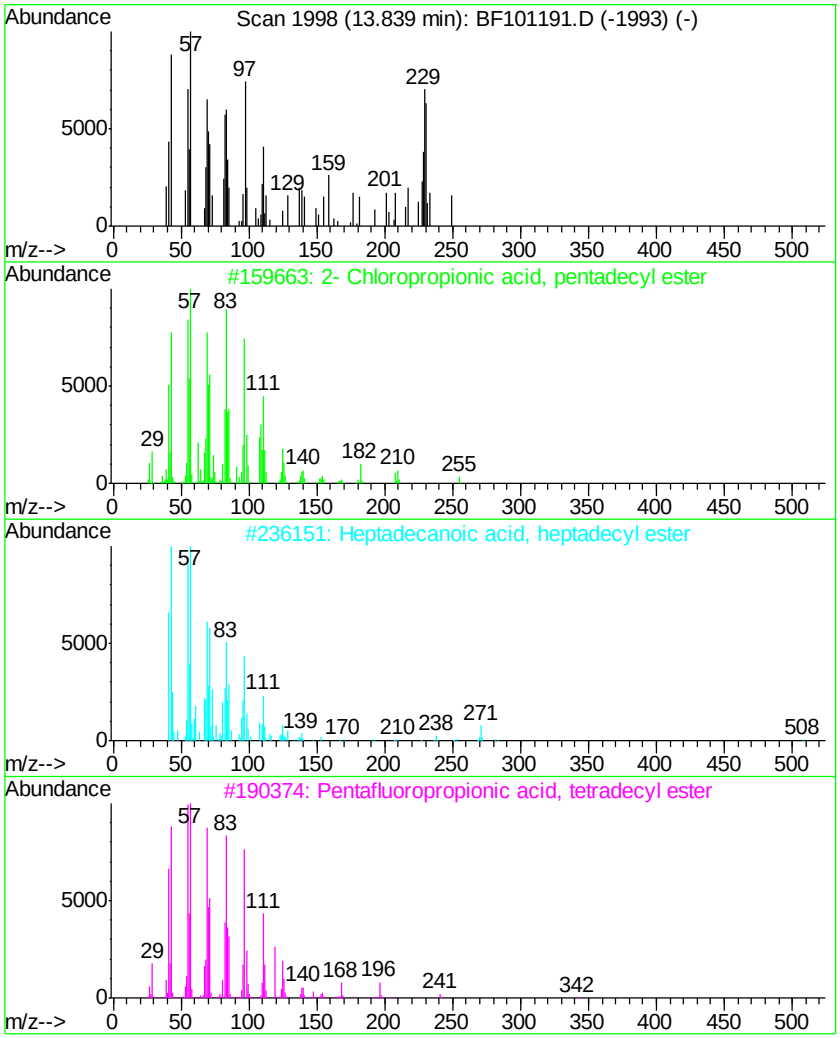
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

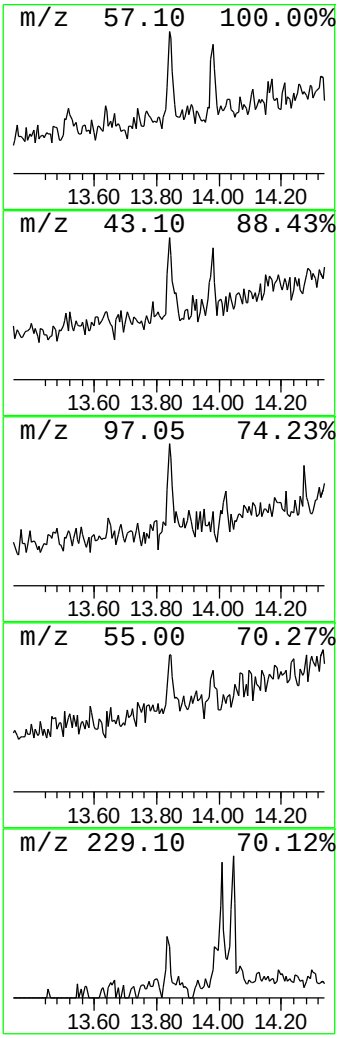
****

Peak Number 4 unknown13.84 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	2.08 ng	34899	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	38
2	Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	38
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	35
4	Trihexadecyl borate	735	C48H99BO3	002665-11-4	30
5	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BART-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

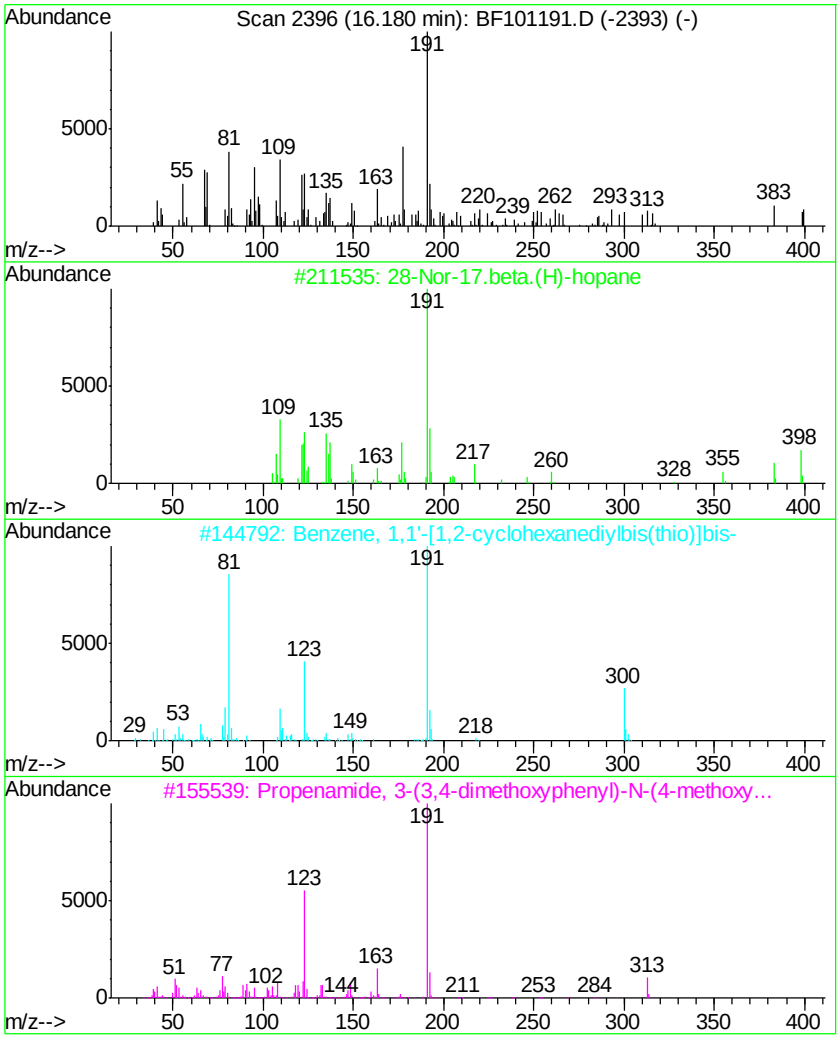
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

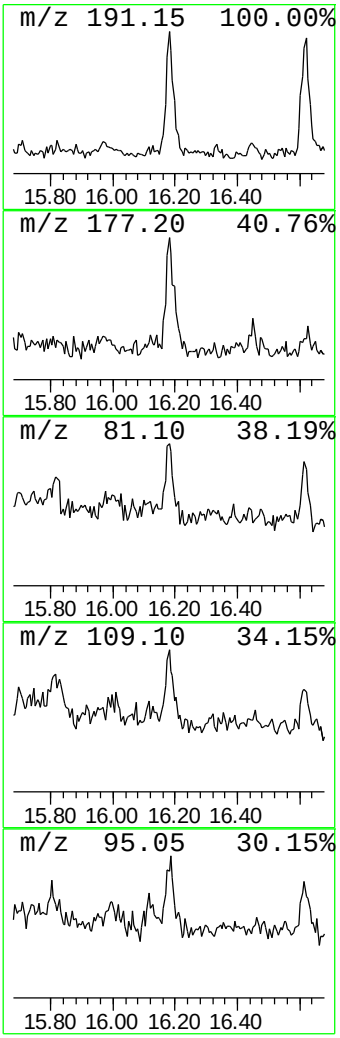
****

Peak Number 5 28-Nor-17.beta.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	11.36 ng	130494	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	62
2	Benzene, 1,1'-[1,2-cyclohexanedi...	300	C18H20S2	1000362-19-6	38
3	Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19NO4	339165-72-9	38
4	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	37
5	Anthracene, 9-butyl-	234	C18H18	001498-69-7	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120617\
Data File : BF101191.D
Acq On : 7 Dec 2017 2:45
Operator : SJ/JU
Sample : I6656-04 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BART-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.06	2.3	ng	28477	1	6.85	249203	20.0
unknown6.62	6.62	35.3	ng	439750	1	6.85	249203	20.0
unknown13.84	13.84	2.1	ng	34899	5	14.02	334925	20.0
28-Nor-17.beta.(H...	16.18	11.4	ng	130494	6	15.50	229674	20.0