LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

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-BF092317.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	4.446	398	401	411	rBV	60543	87495	4.90%	0.540%
2	5.063	502	506	522	rBV	342519	424793	23.79%	2.621%
3	5.463	571	574	603	rVB	1573267	1513781	84.77%	9.340%
4	6.481	743	747	760	rBV	1507248	1595112	89.33%	9.842%
5	6.616	766	770	773	rBV	1814977	1611525	90.25%	9.943%
6	6.669	776	779	782	rVB2	26235	21636	1.21%	0.133%
7	6.845	805	809	816	rVB	537056	489835	27.43%	3.022%
8	6.998	831	835	844	rBV	1585659	1314391	73.61%	8.110%
9	7.410	901	905	908	rBV	1038266	970832	54.37%	5.990%
10	8.122	1023	1026	1034	rBV	760131	662589	37.11%	4.088%
11	8.681	1118	1121	1130	rBV	191282	148949	8.34%	0.919%
12	9.198	1205	1209	1212	rBV	2232072	1785684	100.00%	11.017%
13	9.592	1273	1276	1283	rVB	506717	378254	21.18%	2.334%
14	9.881	1321	1325	1329	rVB	803805	670431	37.54%	4.136%
15	10.592	1442	1446	1449	rBV	718829	597378	33.45%	3.686%
16	10.669	1455	1459	1467	rBV	777823	652545	36.54%	4.026%
17	10.922	1499	1502	1507	rVB	38075	30351	1.70%	0.187%
18	10.975	1507	1511	1514	rBV	166940	162625	9.11%	1.003%
19	11.016	1514	1518	1521	rVV	26006	43543	2.44%	0.269%
20	11.369	1574	1578	1581	rBV	652373	562878	31.52%	3.473%
21	12.398	1750	1753	1765	rBV3	67475	90943	5.09%	0.561%
22	12.580	1781	1784	1789	rBV	51547	49306	2.76%	0.304%
23	12.810	1818	1823	1829	rBV	55719	72854	4.08%	0.450%
24	12.945	1842	1846	1850	rBV	1187231	1067833	59.80%	6.588%
25	13.833	1993	1997	2001	rBV2	41779	46088	2.58%	0.284%
26	13.969	2017	2020	2023	rBV	37121	36672	2.05%	0.226%
27	14.010	2023	2027	2030	rBV	493097	441826	24.74%	2.726%
28	14.833	2165	2167	2172	rVB	23178	21465	1.20%	0.132%
29	15.051	2202	2204	2208	rBV2	22204	30405	1.70%	0.188%
30	15.480	2272	2277	2290	rVB	393946	526994	29.51%	3.251%
31	16.145	2388	2390	2399	rVB9	21339	41529	2.33%	0.256%
32	16.974	2527	2531	2536	rVB7	18824	35588	1.99%	0.220%
33	17.415	2604	2606	2612	rVB6	11718	21619	1.21%	0.133%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-116-8(0-5)

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

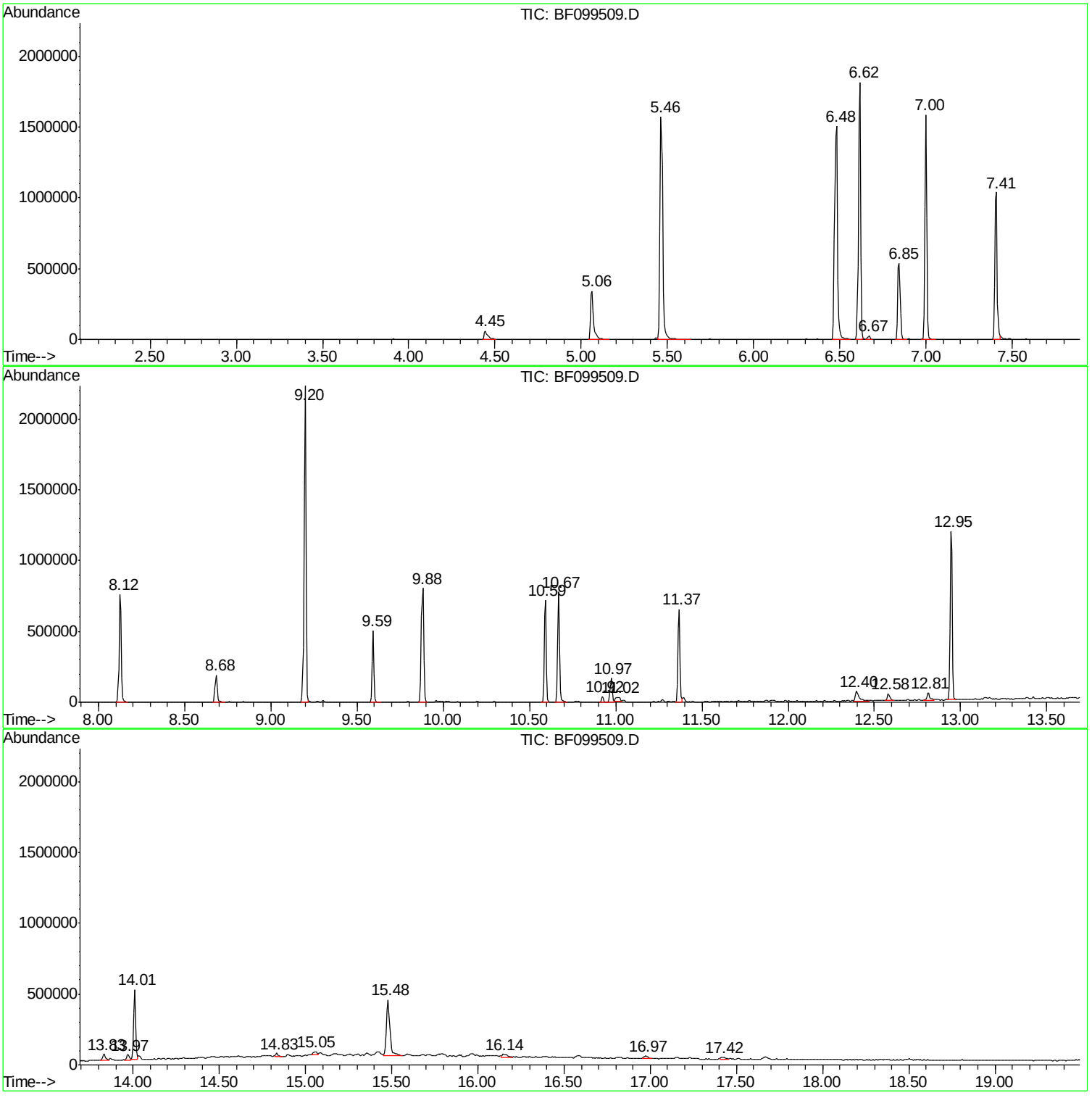
Sum of corrected areas: 16207749

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

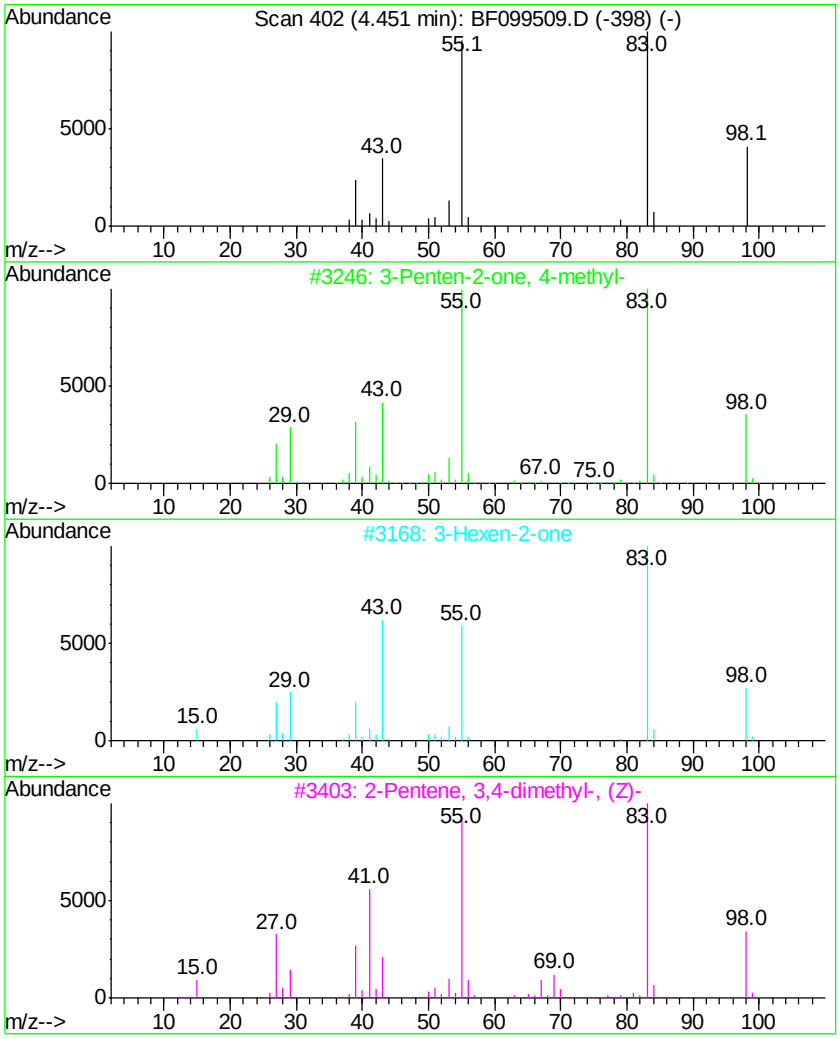
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

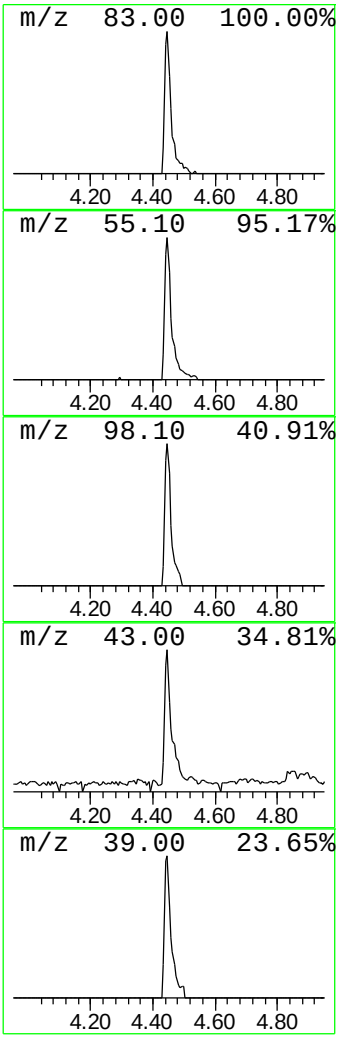
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	3.57 ng	87495	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

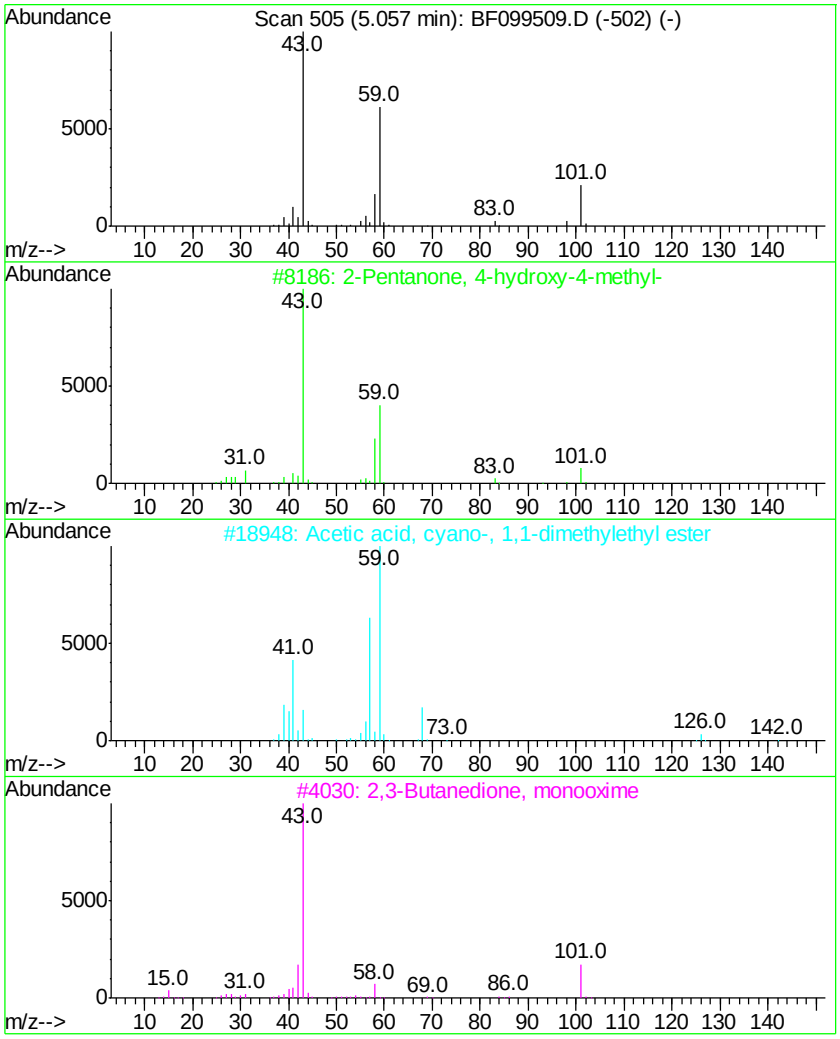
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

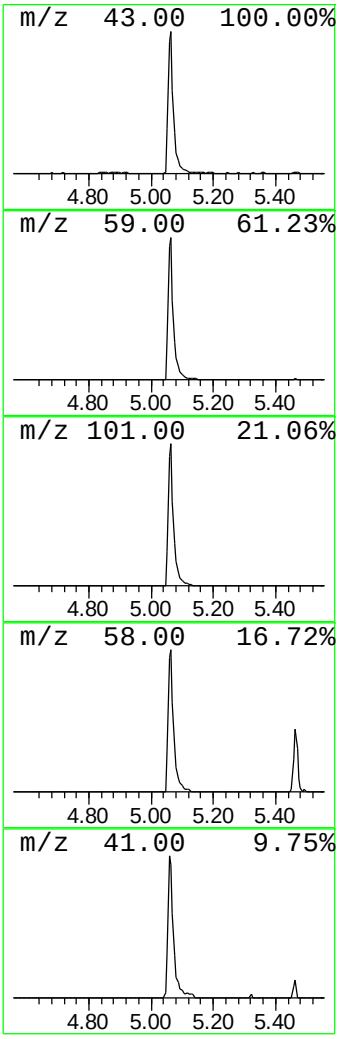
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	17.34 ng	424793	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

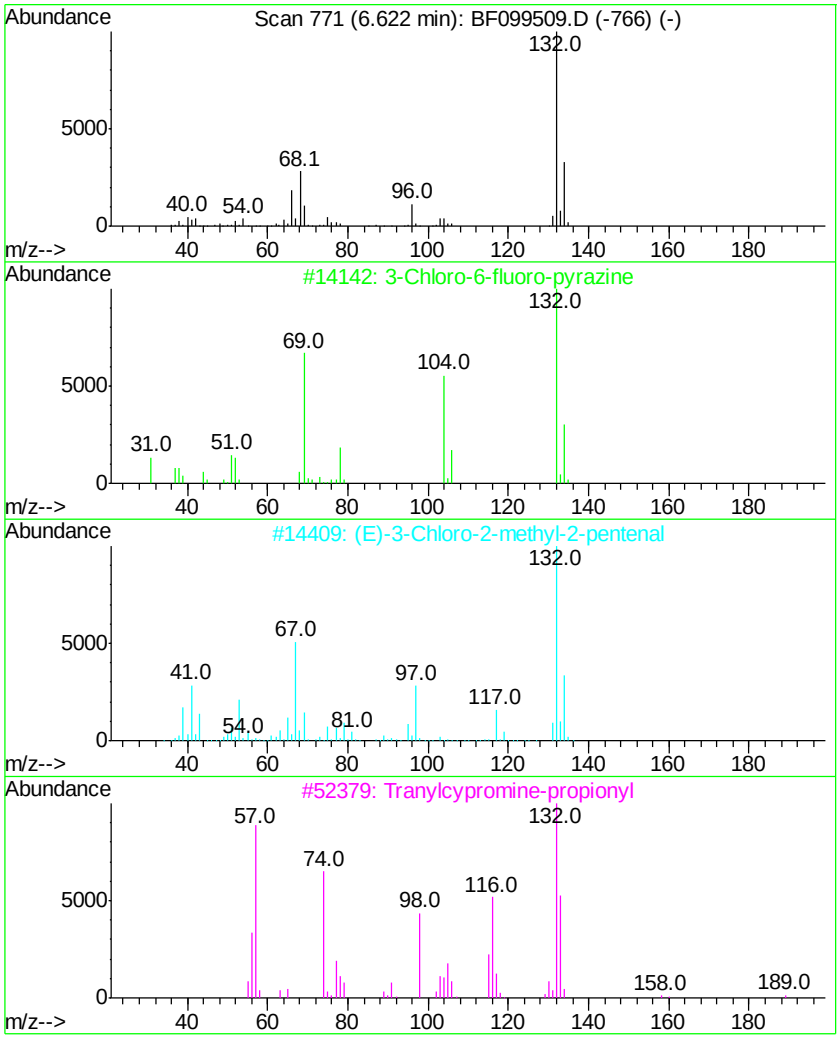
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

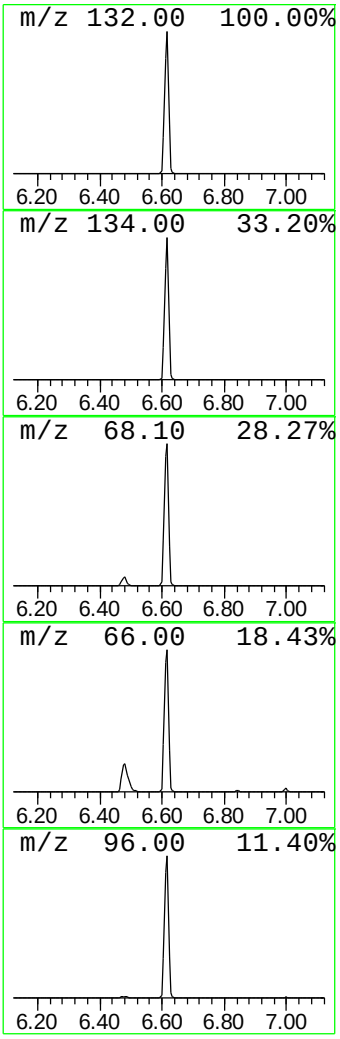
****

Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	65.80 ng	1611530	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

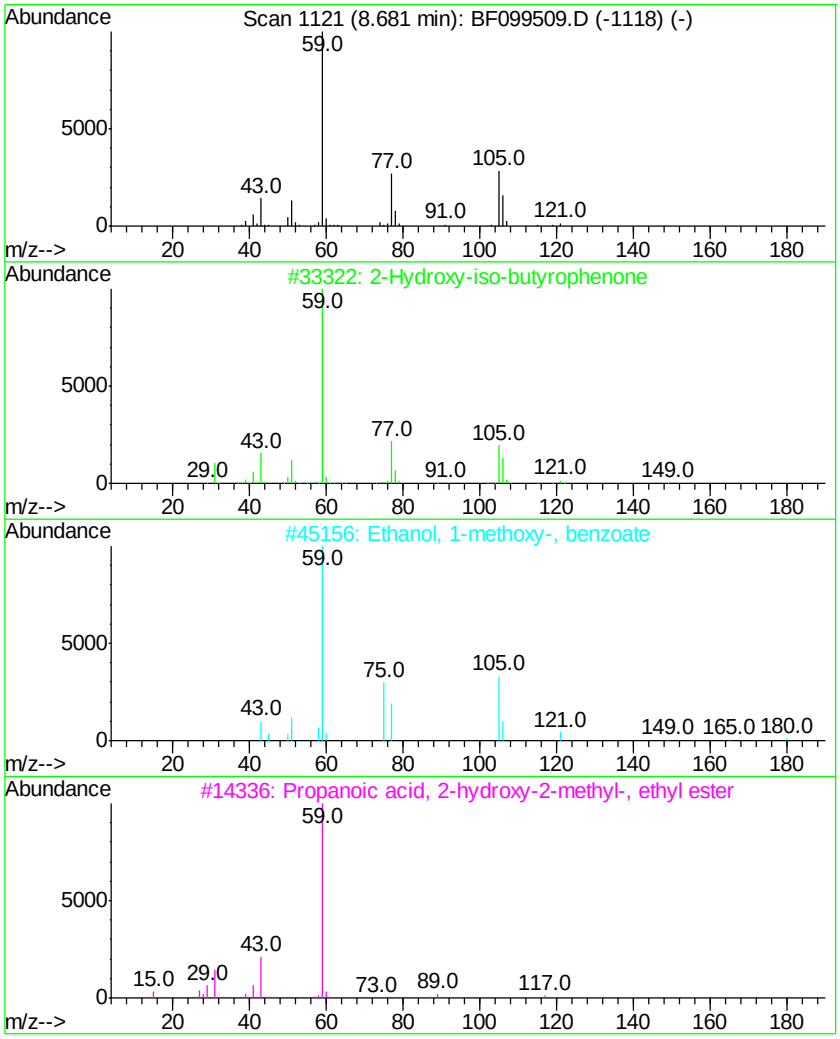
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

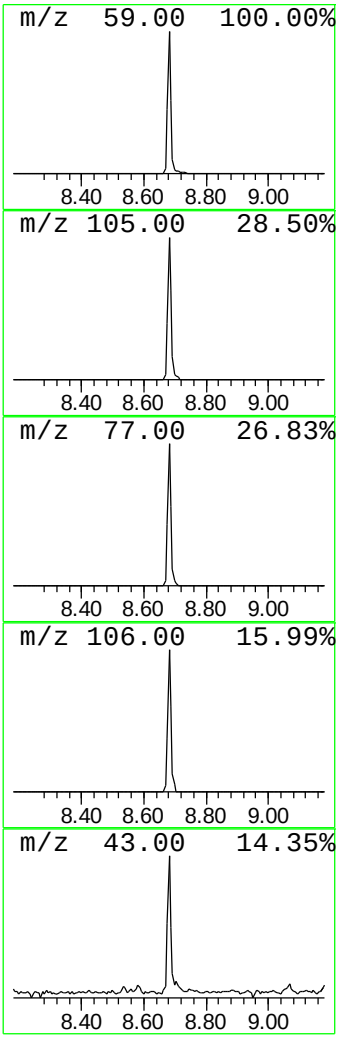
****

Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	4.50 ng	148949	Naphthalene-d8	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	7
5	Guanidine	59	CH5N3	000113-00-8	7





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

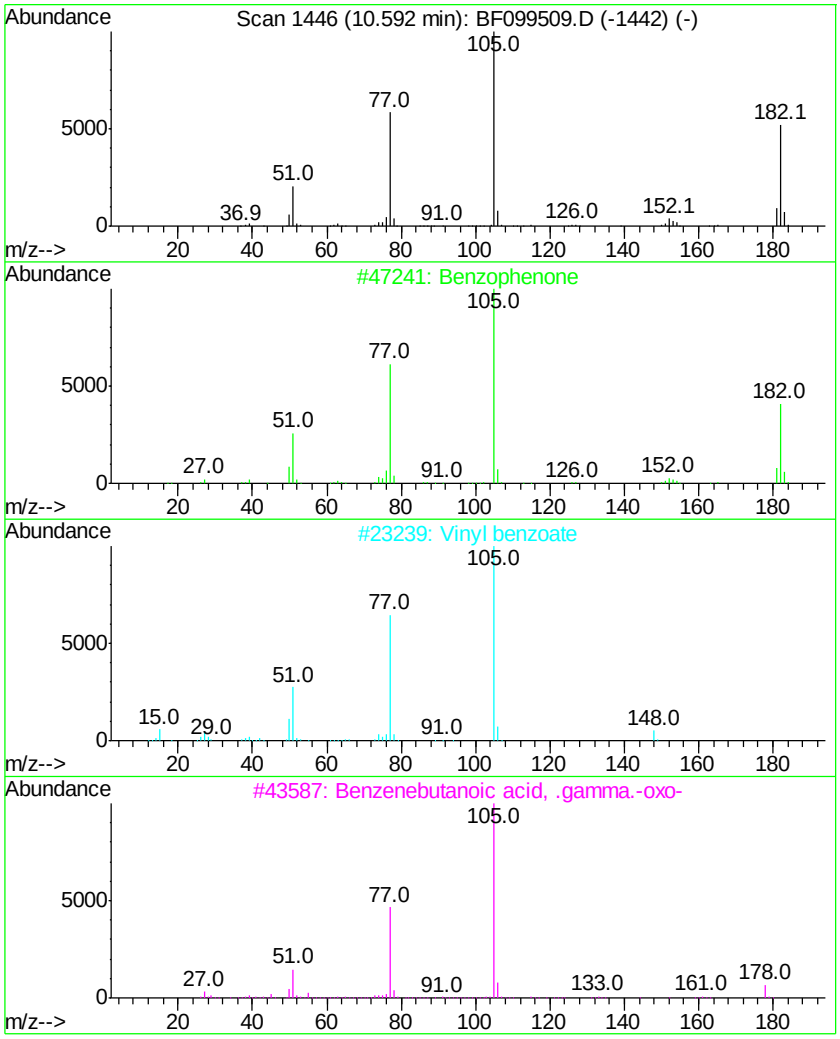
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

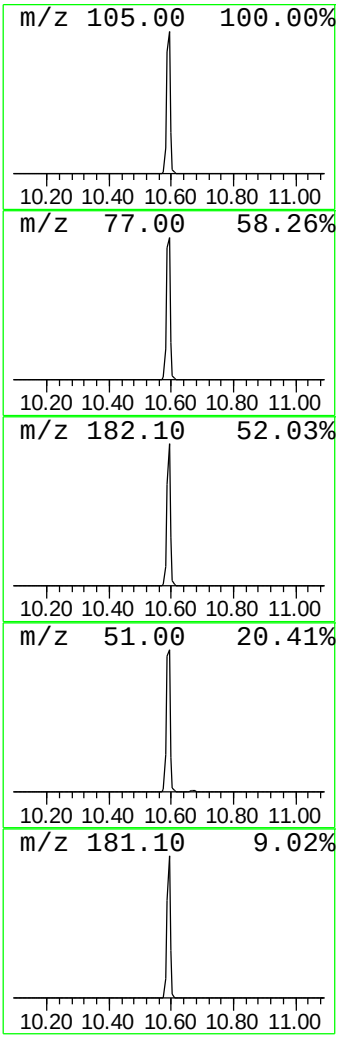
****

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	17.82 ng	597378	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Vinyl benzoate	148	C9H8O2	000769-78-8	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

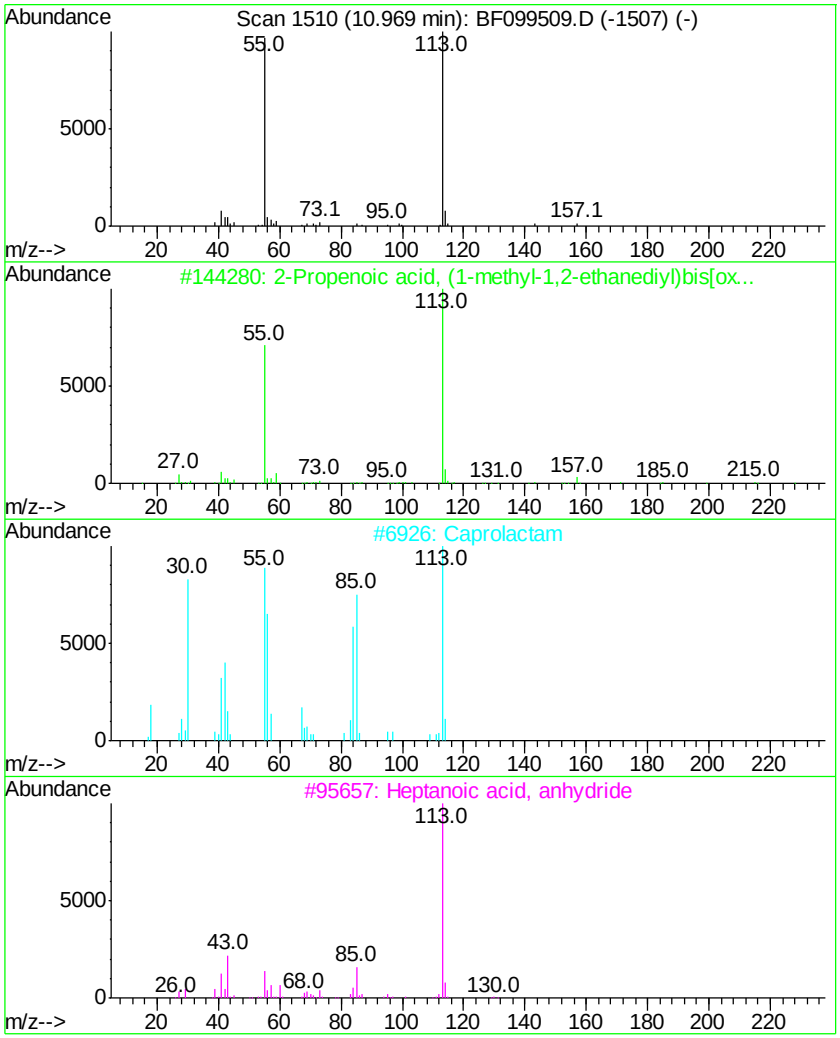
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

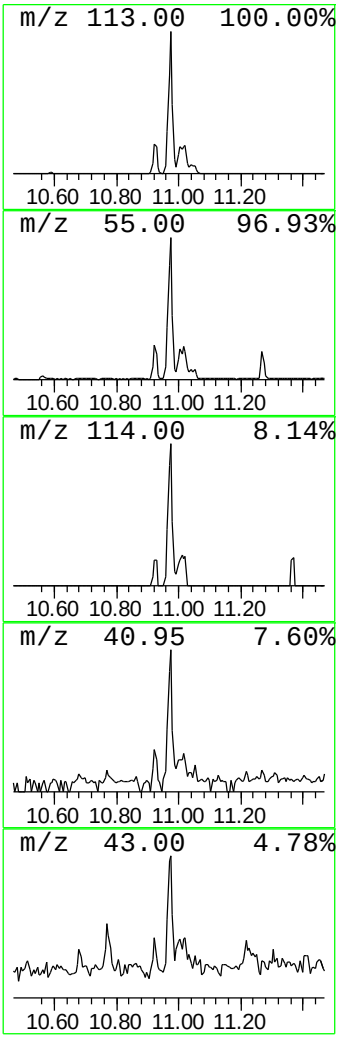
****

Peak Number 7 2-Propenoic acid, (1-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	5.78 ng	162625	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, (1-methyl-1,2-...	300	C15H24O6	042978-66-5	74
2	Caprolactam	113	C6H11NO	000105-60-2	50
3	Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	38
4	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	9
5	Piperidine-2,5-dione	113	C5H7NO2	052065-78-8	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

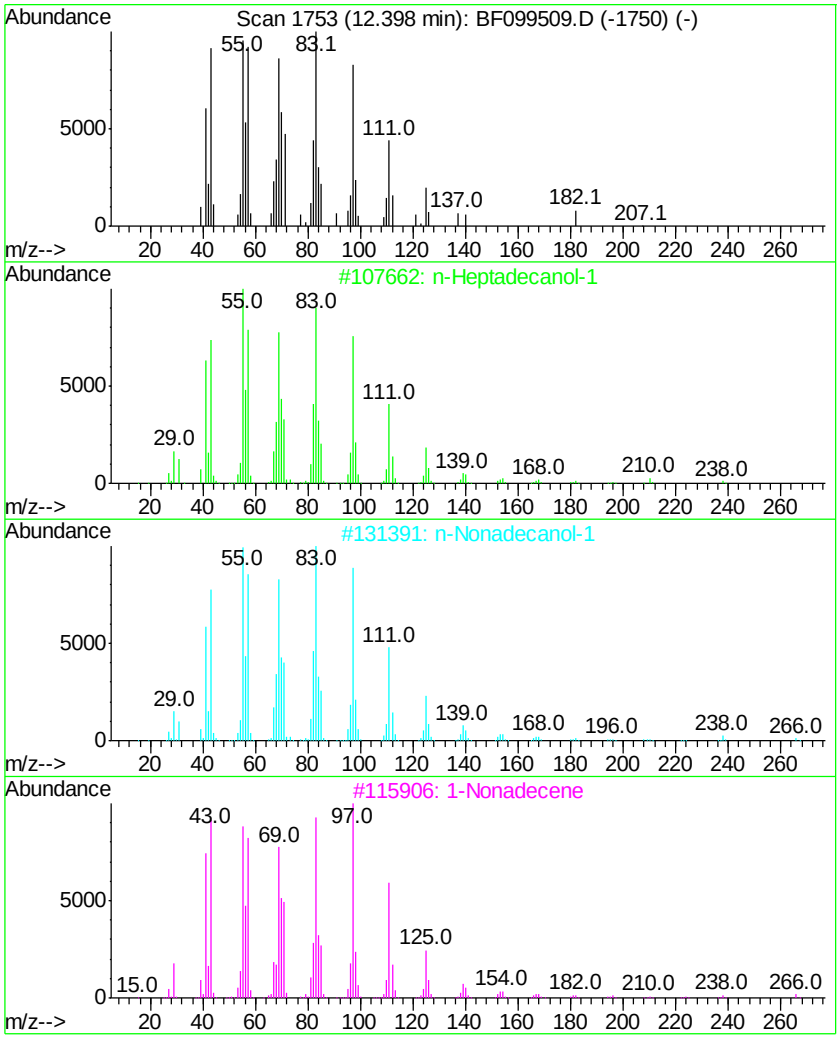
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

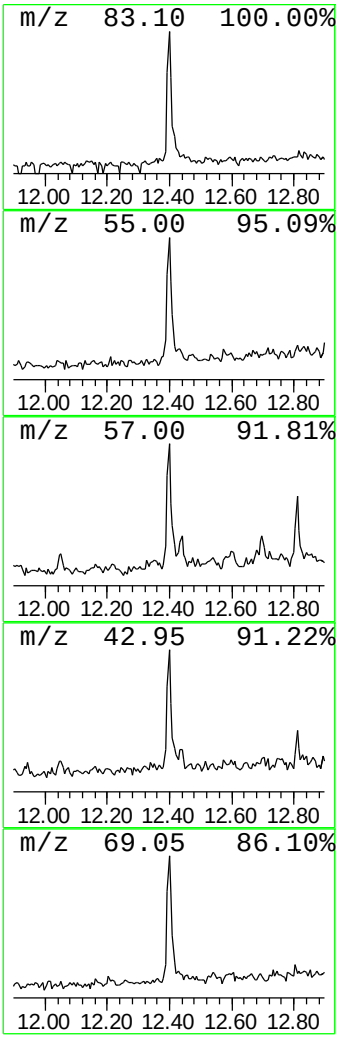
****

Peak Number 8 n-Heptadecanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	3.23 ng	90943	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

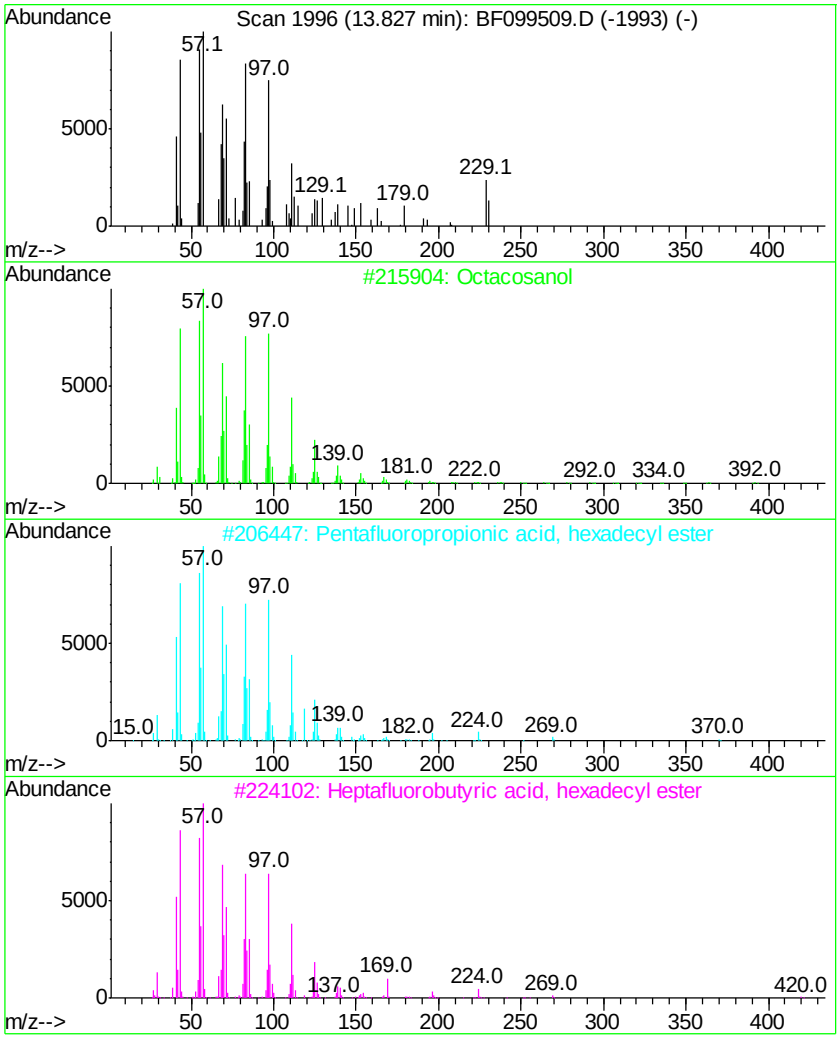
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

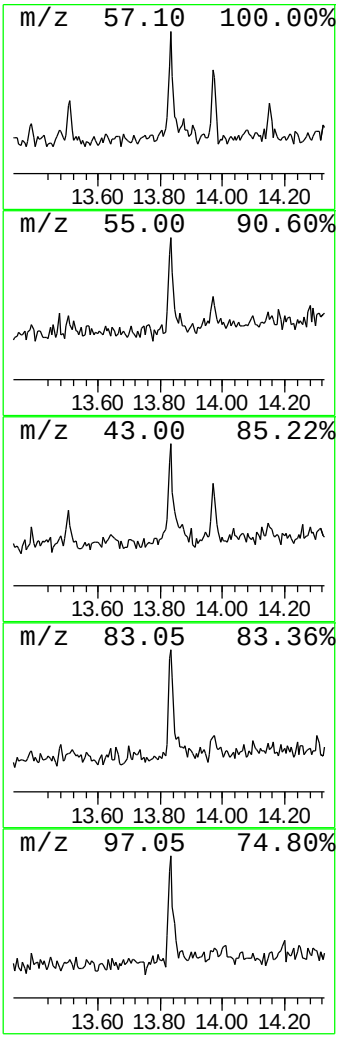
****

Peak Number 10 Octacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.09 ng	46088	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	87
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87
4	1-Heptacosanol	396	C27H56O	002004-39-9	83
5	1-Heneicosanol	312	C21H44O	015594-90-8	76





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF101517\
Data File : BF099509.D
Acq On : 15 Oct 2017 13:04
Operator : SJ/JU
Sample : I5752-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
3-Penten-2-one, 4...	4.45	3.6	ng	87495	1	6.85	489835	20.0
2-Pentanone, 4-hy...	5.06	17.3	ng	424793	1	6.85	489835	20.0
unknown6.62	6.62	65.8	ng	1611530	1	6.85	489835	20.0
2-Hydroxy-iso-but...	8.68	4.5	ng	148949	2	8.12	662589	20.0
Benzophenone	10.59	17.8	ng	597378	3	9.88	670431	20.0
2-Propenoic acid,...	10.97	5.8	ng	162625	4	11.37	562878	20.0
n-Heptadecanol-1	12.40	3.2	ng	90943	4	11.37	562878	20.0
Octacosanol	13.83	2.1	ng	46088	5	14.01	441826	20.0