LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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	5.040	498	502	511	rBV	50273	66940	6.36%	0.703%
2	5.445	566	571	590	rBV	834185	848276	80.58%	8.912%
3	6.463	739	744	753	rBV	942223	900314	85.52%	9.458%
4	6.598	763	767	770	rBV	1088871	908776	86.32%	9.547%
5	6.828	802	806	812	rBB	299001	259618	24.66%	2.727%
6	6.981	828	832	835	rBV	910850	742572	70.54%	7.801%
7	7.392	898	902	905	rBV	637273	529483	50.30%	5.563%
8	8.110	1020	1024	1027	rBV	344297	314811	29.90%	3.307%
9	9.181	1202	1206	1209	rBV	1165356	1052749	100.00%	11.060%
10	9.575	1270	1273	1276	rBV	100626	72216	6.86%	0.759%
11	9.786	1305	1309	1313	rVB	35888	30137	2.86%	0.317%
12	9.863	1319	1322	1326	rVB2	389141	314179	29.84%	3.301%
13	10.286	1391	1394	1397	rVB	32939	26163	2.49%	0.275%
14	10.504	1425	1431	1433	rBV2	9612	11172	1.06%	0.117%
15	10.657	1453	1457	1461	rBV	518424	424270	40.30%	4.457%
16	10.757	1471	1474	1478	rBV	26789	26733	2.54%	0.281%
17	11.357	1572	1576	1578	rBV	339964	303296	28.81%	3.186%
18	11.380	1578	1580	1584	rVV	145961	117408	11.15%	1.233%
19	11.427	1586	1588	1591	rVB	17271	15714	1.49%	0.165%
20	11.469	1591	1595	1602	rBV4	12499	16638	1.58%	0.175%
21	11.586	1609	1615	1618	rBV2	19721	24627	2.34%	0.259%
22	11.869	1655	1663	1671	rBV3	39770	86191	8.19%	0.905%
23	11.969	1677	1680	1682	rBV	29401	28529	2.71%	0.300%
24	11.992	1682	1684	1687	rVB2	13514	12125	1.15%	0.127%
25	12.151	1708	1711	1713	rVB	15385	12864	1.22%	0.135%
26	12.186	1713	1717	1720	rBV	39083	35330	3.36%	0.371%
27	12.404	1748	1754	1756	rBV3	17407	21135	2.01%	0.222%
28	12.498	1766	1770	1773	rBV3	15489	18688	1.78%	0.196%
29	12.569	1779	1782	1786	rBV	269875	237025	22.51%	2.490%
30	12.663	1795	1798	1801	rBV5	15283	21326	2.03%	0.224%
31	12.721	1804	1808	1810	rVV4	16492	20094	1.91%	0.211%
32	12.751	1810	1813	1815	rVV	52185	42417	4.03%	0.446%
33	12.804	1815	1822	1825	rVV	211493	239441	22.74%	2.515%
34	12.851	1828	1830	1835	rVB4	16704	19353	1.84%	0.203%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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	12.939	1841	1845	1848	rBV	996213	863299	82.00%	9.069%
36	12.963	1848	1849	1853	rVB2	18001	14209	1.35%	0.149%
37	13.010	1854	1857	1863	rBV5	16600	38582	3.66%	0.405%
38	13.198	1886	1889	1892	rVB	20842	17411	1.65%	0.183%
39	13.233	1892	1895	1897	rBV2	23527	27044	2.57%	0.284%
40	13.457	1931	1933	1935	rVB2	29460	19927	1.89%	0.209%
41	13.645	1963	1965	1967	rBV	24028	17417	1.65%	0.183%
42	13.751	1981	1983	1986	rBV	26332	20727	1.97%	0.218%
43	13.827	1993	1996	1998	rBV3	48303	49195	4.67%	0.517%
44	13.963	2017	2019	2022	rBV2	39815	42931	4.08%	0.451%
45	14.004	2022	2026	2029	rVV2	327996	365527	34.72%	3.840%
46	14.027	2029	2030	2033	rVB	85086	55040	5.23%	0.578%
47	15.480	2275	2277	2281	rVB	164612	186849	17.75%	1.963%

Sum of corrected areas: 9518768

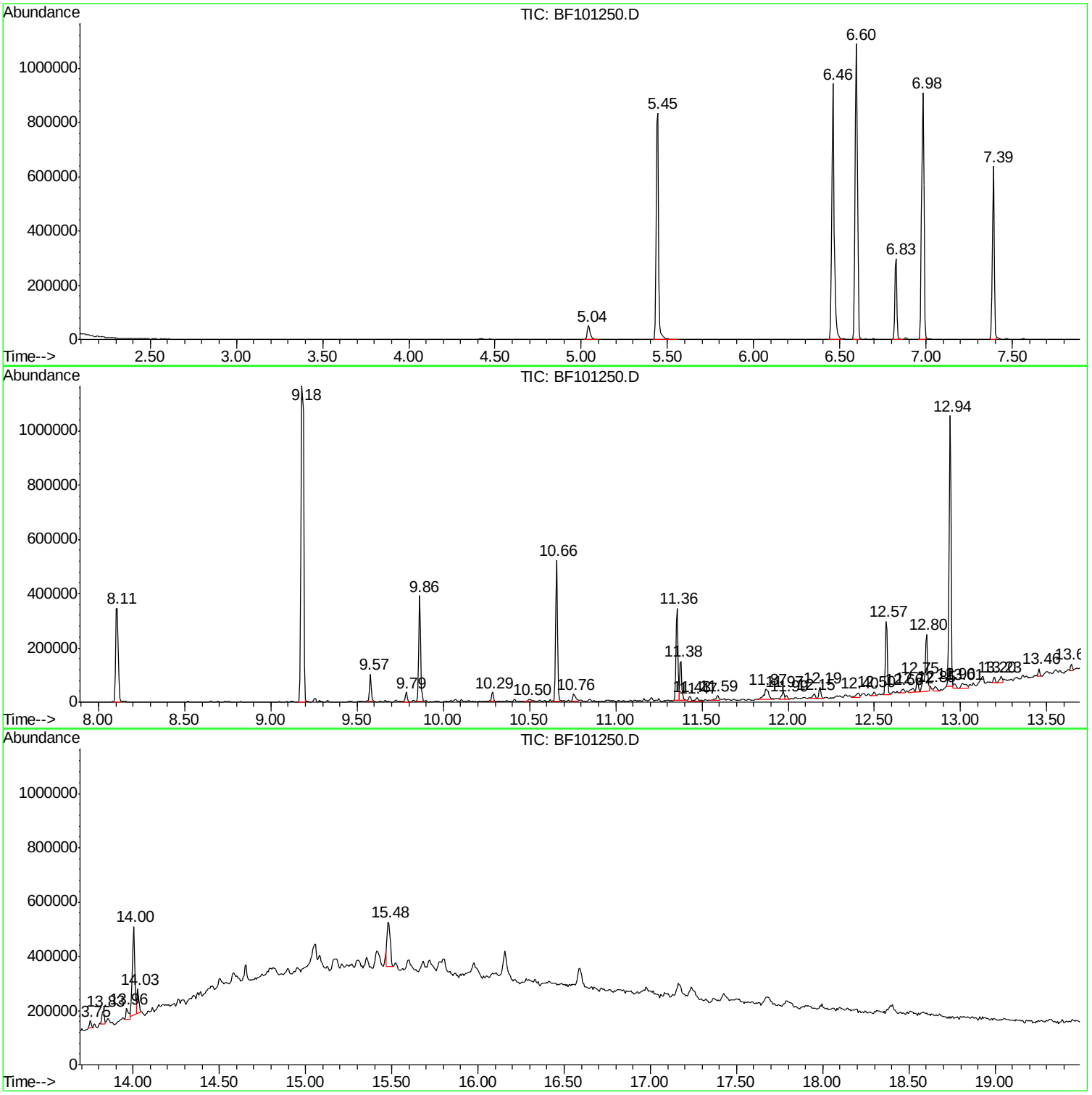
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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\BF120817\
Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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

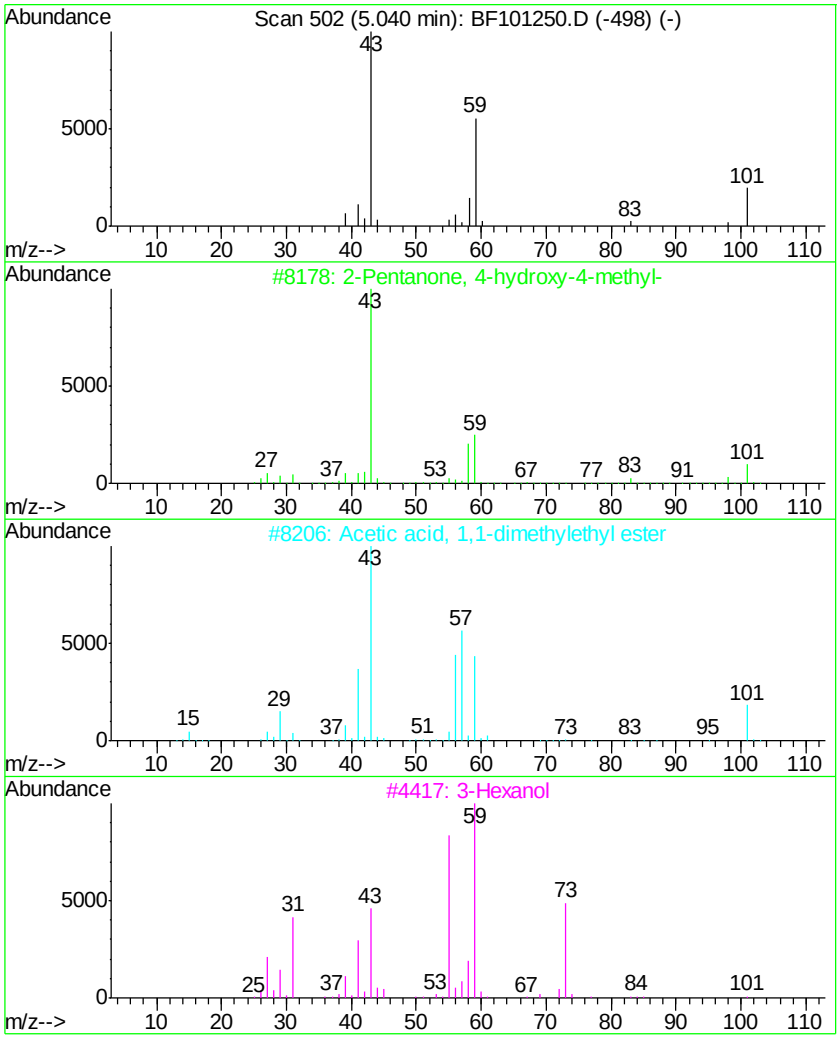
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

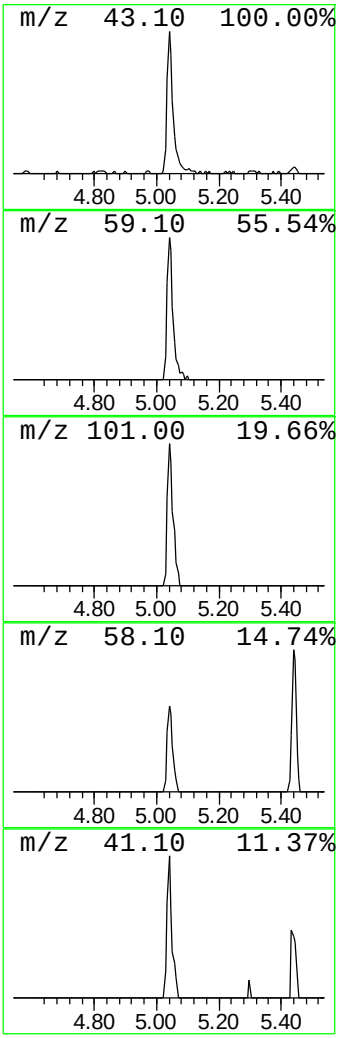
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	5.16 ng	66940	1,4-Dichlorobenzene-d4	6.83

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
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Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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

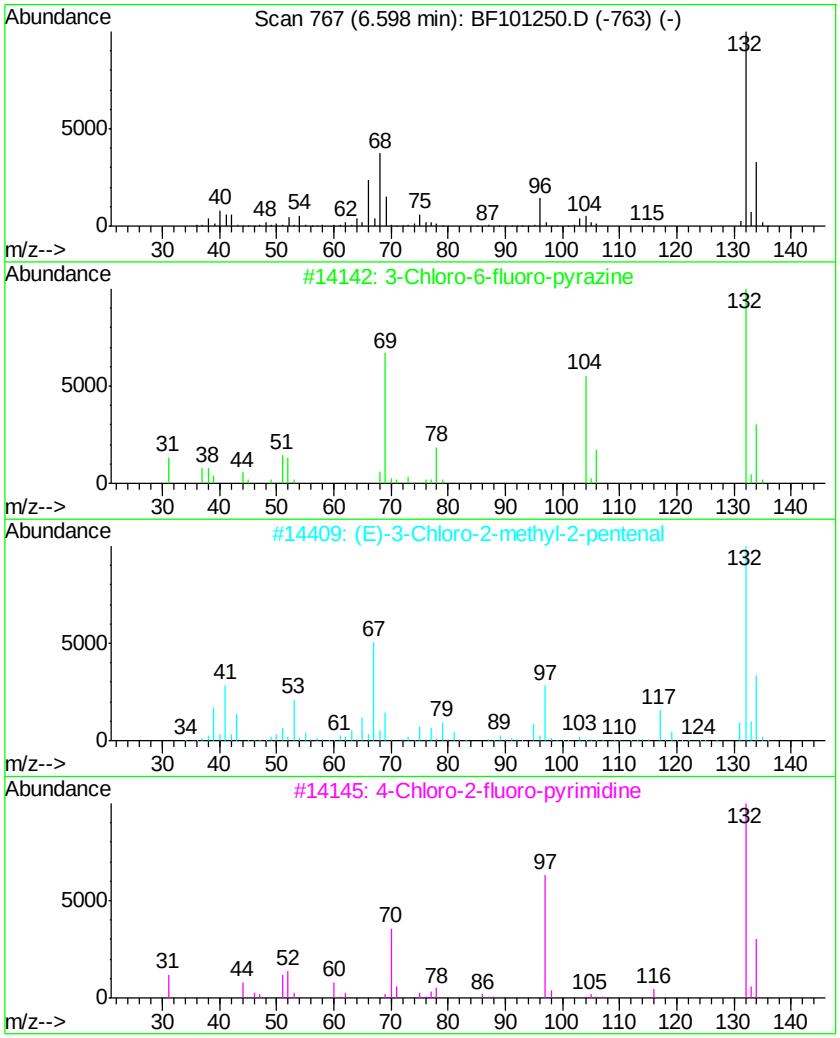
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

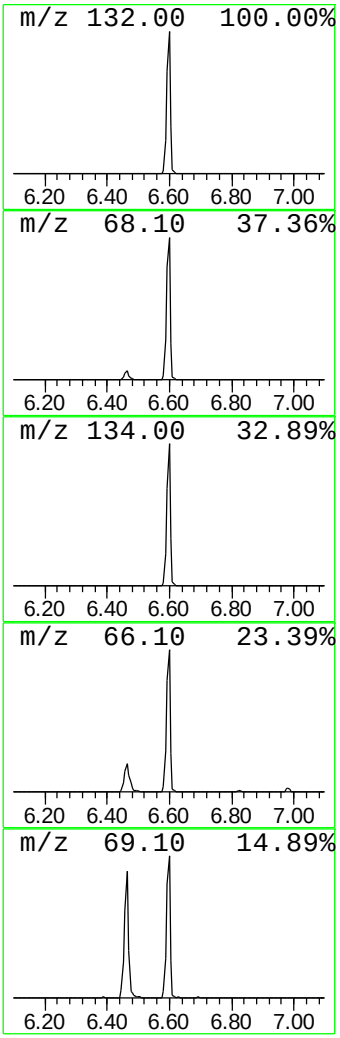
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	70.01 ng	908776	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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

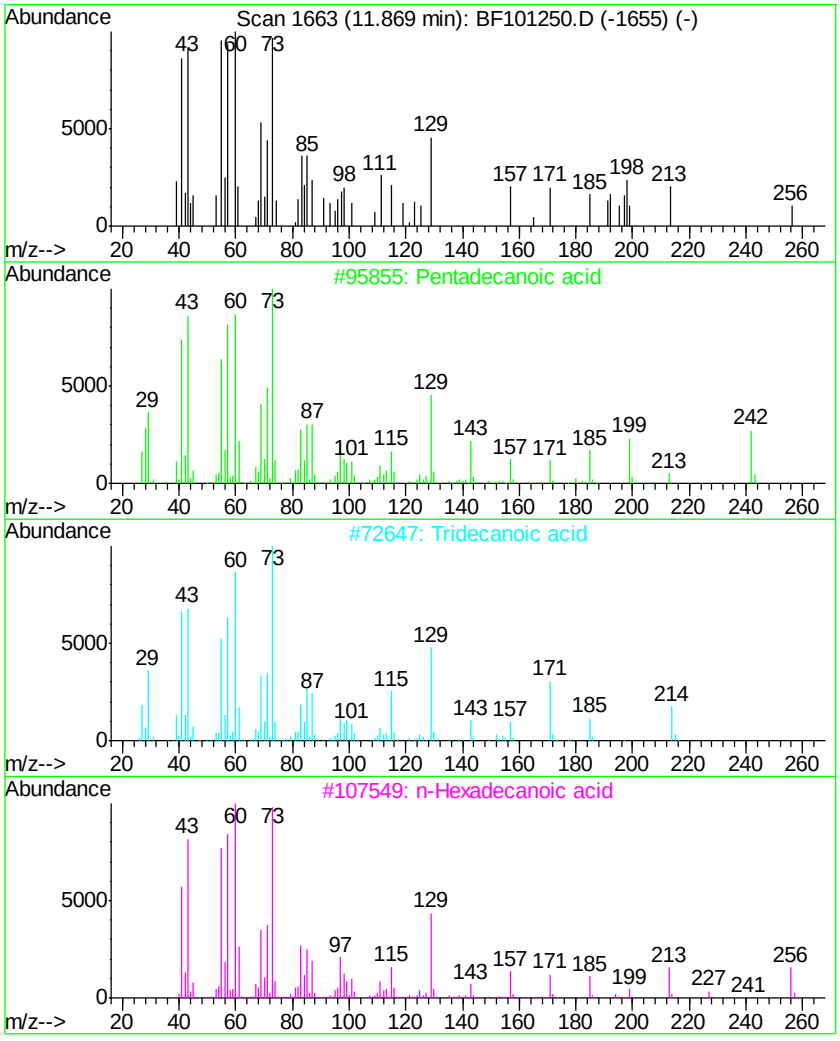
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

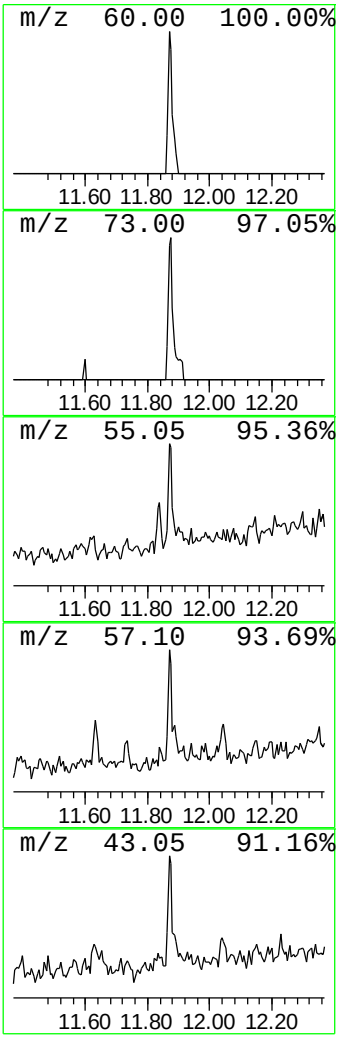
****

Peak Number 4 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	5.68 ng	86191	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
2	Tridecanoic acid	214	C13H26O2	000638-53-9	49
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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

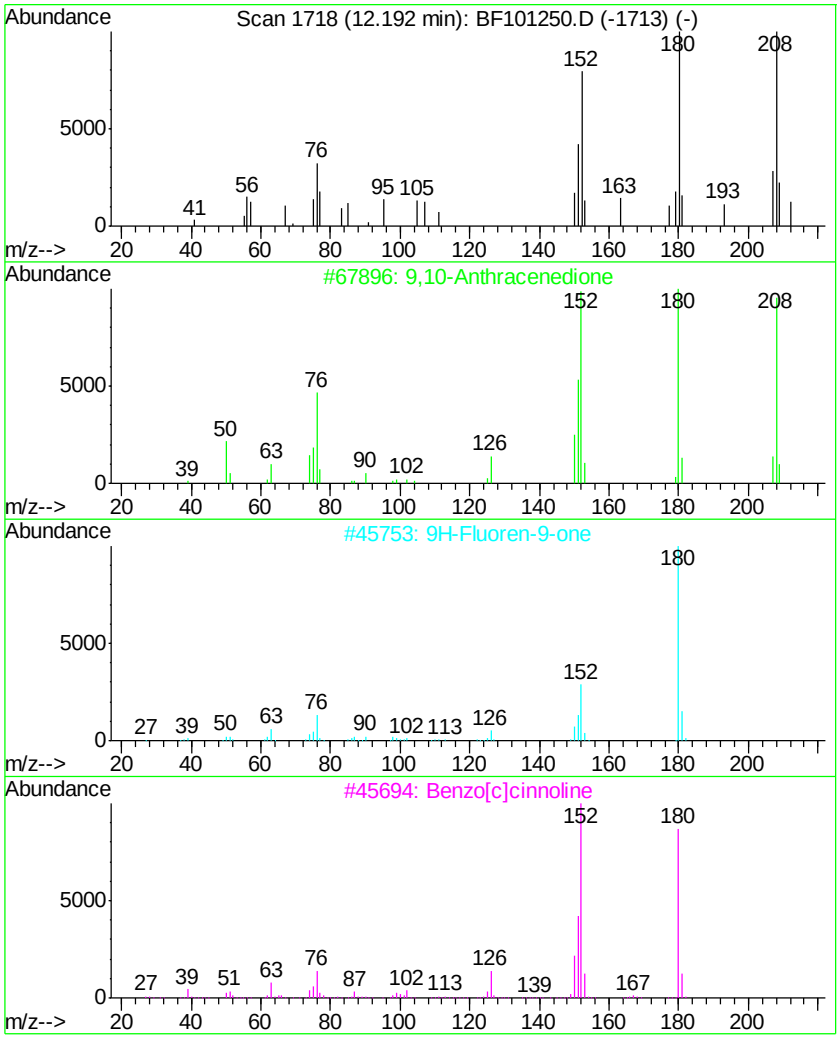
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

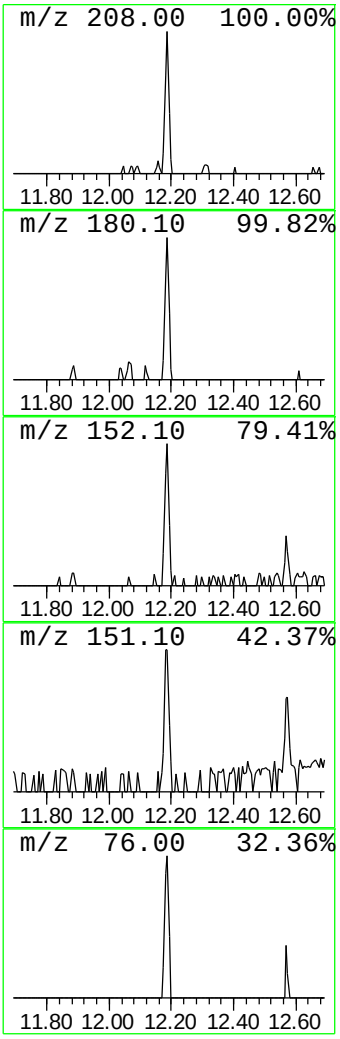
****

Peak Number 5 9,10-Anthracenedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	2.33 ng	35330	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	93
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	60
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	53
4	1,4-Anthracenedione	208	C14H8O2	000635-12-1	50
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	49





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Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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

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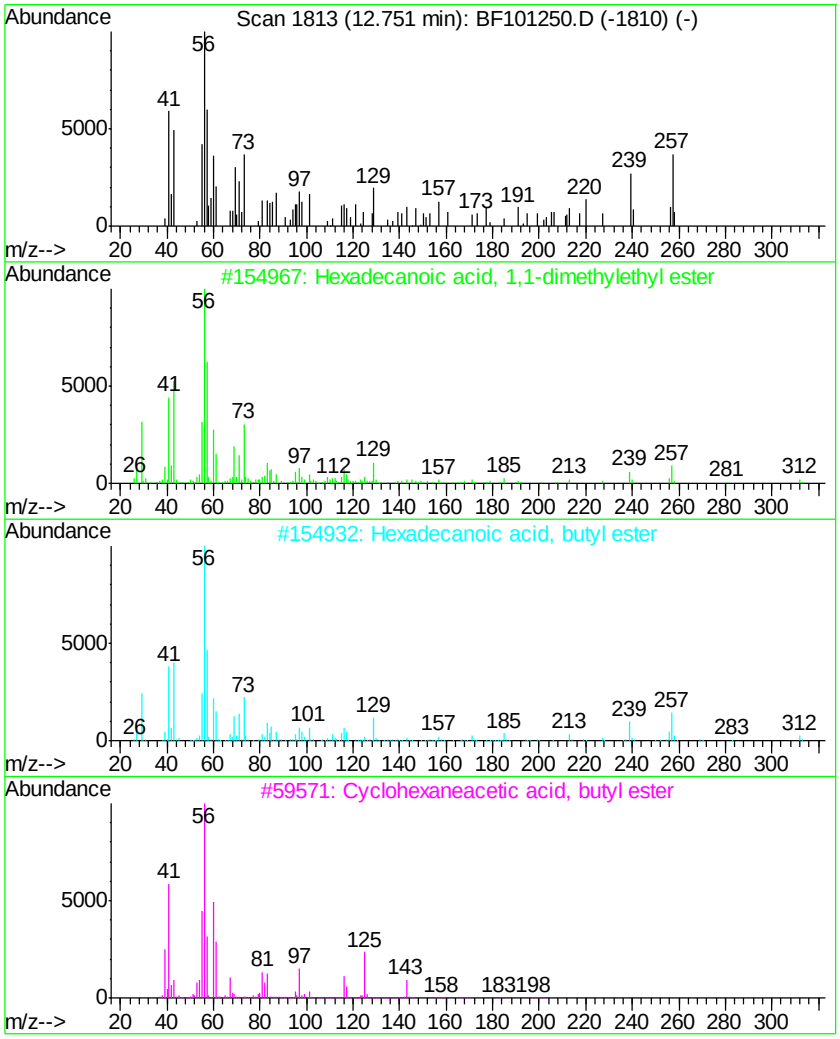
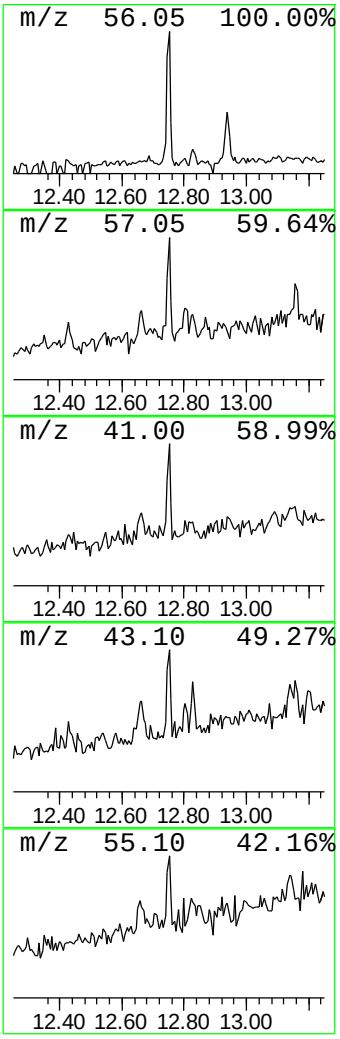
Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	2.32 ng	42417	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	43
3	Cyclohexaneacetic acid, butyl ester	198	C12H22O2	027948-12-5	38
4	Myristic acid isobutyl ester	284	C18H36O2	025263-97-2	37
5	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101250.D
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Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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

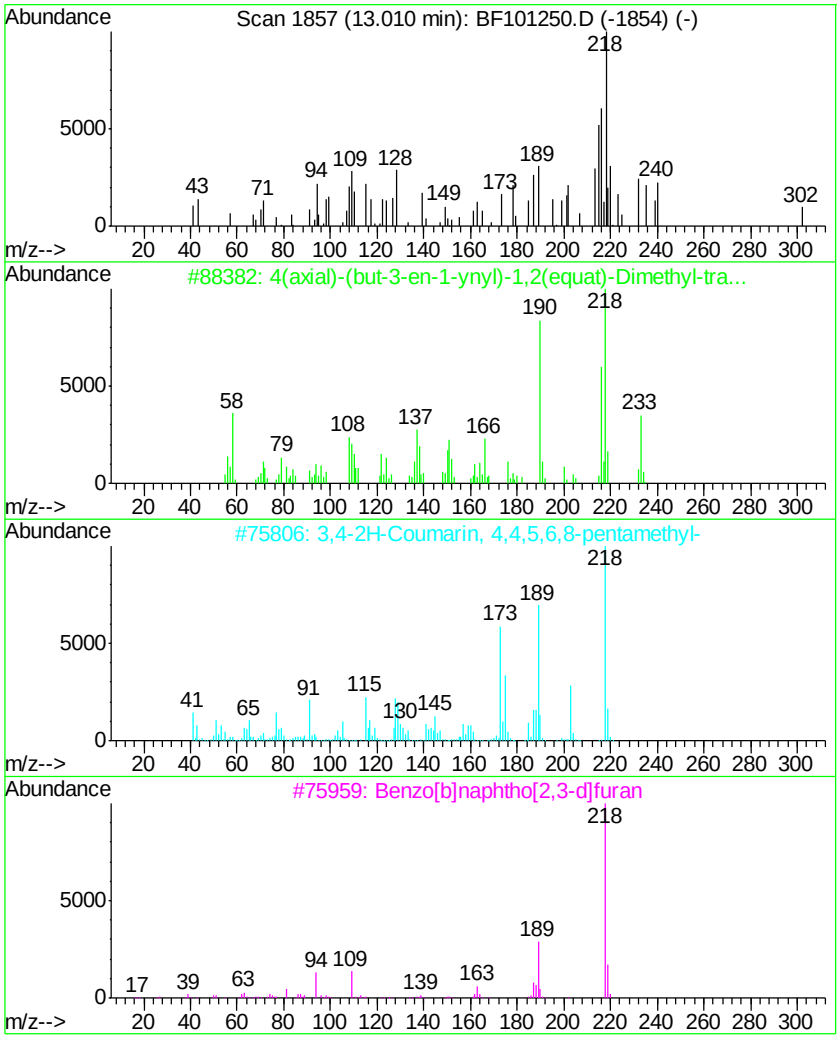
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

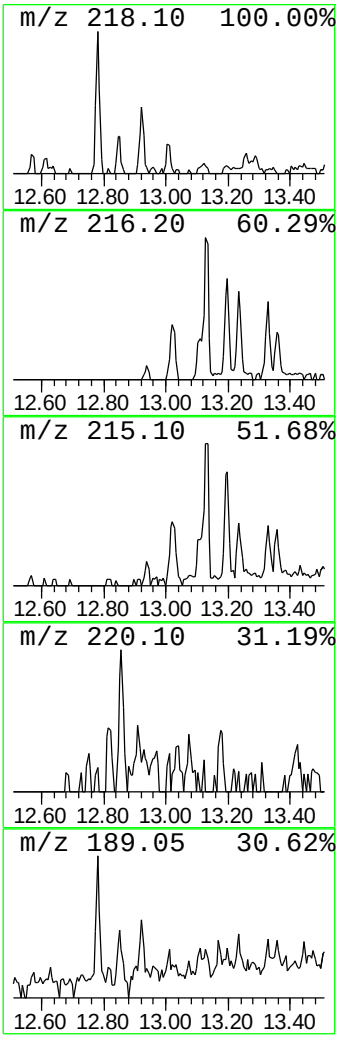
****

Peak Number 7 unknown13.01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	2.11 ng	38582	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4(axial)-(but-3-en-1-ynyl)-1,2(e...	233	C15H23NO	037993-67-2	38
2	3,4-2H-Coumarin, 4,4,5,6,8-penta...	218	C14H18O2	1000129-70-7	25
3	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	25
4	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	25
5	1H-Phenanthro[9,10-c]pyrazole	218	C15H10N2	078529-79-0	22





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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

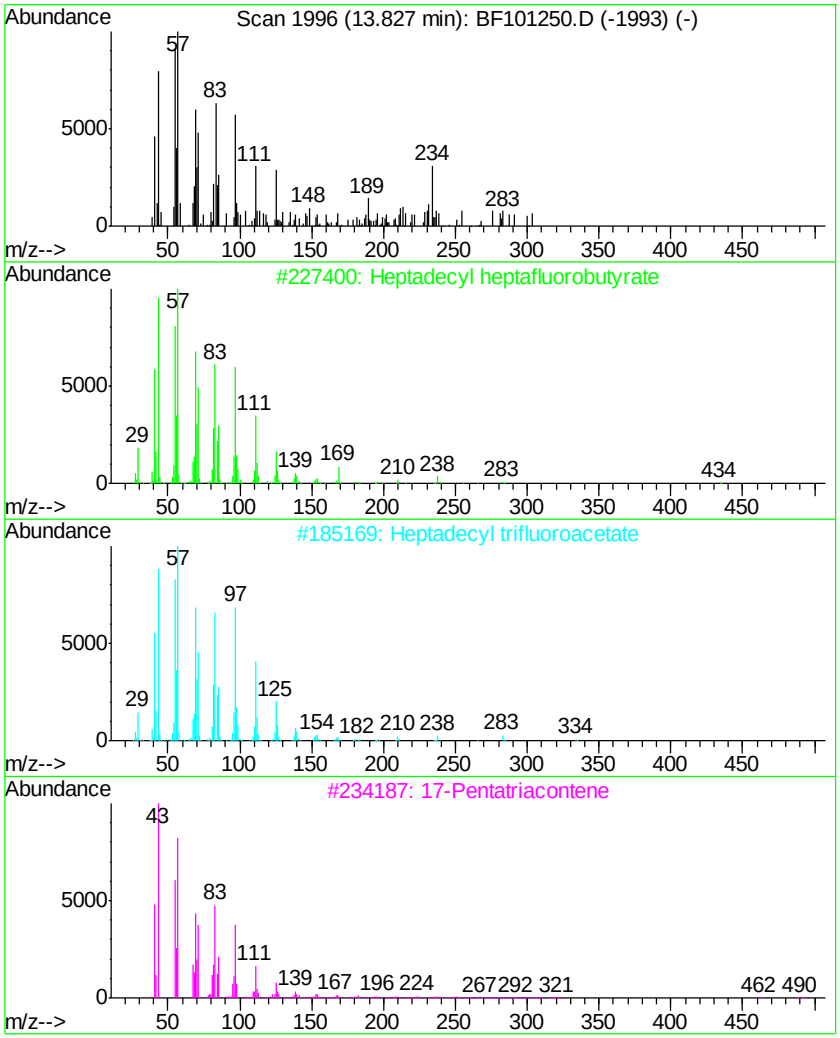
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

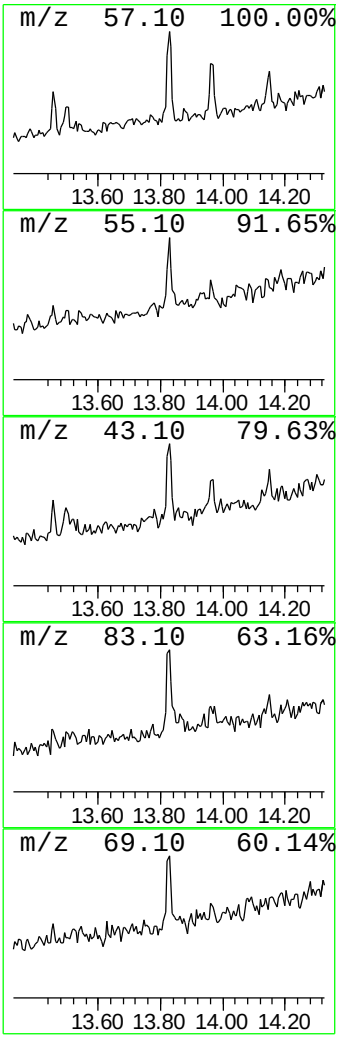
****

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.69 ng	49195	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	83
3	17-Pentatriacontene	491	C35H70	006971-40-0	83
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74
5	Cyclotetradecane	196	C14H28	000295-17-0	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101250.D
Acq On : 8 Dec 2017 21:46
Operator : SJ/JU
Sample : I6656-04
Misc :
ALS Vial : 17 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...	5.04	5.2	ng	66940	1	6.83	259618	20.0
unknown6.60	6.60	70.0	ng	908776	1	6.83	259618	20.0
Pentadecanoic acid	11.87	5.7	ng	86191	4	11.36	303296	20.0
9,10-Anthracenedione	12.19	2.3	ng	35330	4	11.36	303296	20.0
Hexadecanoic acid...	12.75	2.3	ng	42417	5	14.00	365527	20.0
unknown13.01	13.01	2.1	ng	38582	5	14.00	365527	20.0
Heptadecyl heptaf...	13.83	2.7	ng	49195	5	14.00	365527	20.0