LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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	5.063	502	506	515	rBV	46858	79988	5.58%	0.650%
2	5.457	568	573	576	rBV	1369284	1308295	91.32%	10.634%
3	6.475	741	746	759	rBV	1167560	1407852	98.27%	11.443%
4	6.604	764	768	771	rBV	1429843	1395637	97.42%	11.343%
5	6.828	803	806	812	rBV	314904	263389	18.38%	2.141%
6	6.987	829	833	836	rBV	1267669	1095995	76.50%	8.908%
7	7.398	898	903	906	rBV	823081	808210	56.41%	6.569%
8	7.498	917	920	926	rBV	12736	15176	1.06%	0.123%
9	8.110	1021	1024	1031	rBV	367110	310407	21.67%	2.523%
10	9.186	1203	1207	1210	rBV	1573701	1432635	100.00%	11.644%
11	9.257	1217	1219	1222	rBV	22191	15928	1.11%	0.129%
12	9.580	1268	1274	1281	rVB	123080	110515	7.71%	0.898%
13	9.786	1305	1309	1312	rBV	48509	37938	2.65%	0.308%
14	9.869	1319	1323	1327	rVB2	370471	307168	21.44%	2.497%
15	10.286	1391	1394	1397	rVB	49989	38206	2.67%	0.311%
16	10.504	1426	1431	1434	rBV3	17594	19885	1.39%	0.162%
17	10.663	1454	1458	1462	rBV	713369	675759	47.17%	5.492%
18	10.763	1472	1475	1480	rBV	35069	42353	2.96%	0.344%
19	11.210	1548	1551	1553	rBV	24578	17540	1.22%	0.143%
20	11.363	1573	1577	1579	rBV	322337	282271	19.70%	2.294%
21	11.386	1579	1581	1584	rVB	43403	35578	2.48%	0.289%
22	11.874	1660	1664	1670	rBV2	56366	71127	4.96%	0.578%
23	12.298	1732	1736	1739	rBV	28851	27612	1.93%	0.224%
24	12.580	1780	1784	1786	rBV	85053	77666	5.42%	0.631%
25	12.610	1786	1789	1793	rVB	134393	119015	8.31%	0.967%
26	12.810	1820	1823	1825	rVB	59433	46232	3.23%	0.376%
27	12.945	1842	1846	1850	rBV	1122249	1084413	75.69%	8.814%
28	13.198	1885	1889	1892	rBV6	16892	29584	2.07%	0.240%
29	13.321	1908	1910	1913	rBV3	15566	17068	1.19%	0.139%
30	13.474	1932	1936	1939	rBV	493485	426878	29.80%	3.470%
31	13.833	1994	1997	2001	rBV3	80460	81334	5.68%	0.661%
32	13.968	2018	2020	2022	rBV	49650	38499	2.69%	0.313%
33	14.010	2023	2027	2030	rBV	306156	300549	20.98%	2.443%
34	14.127	2044	2047	2050	rBV3	30536	45081	3.15%	0.366%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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	14.168	2052	2054	2056	rVV	43146	34951	2.44%	0.284%
36	14.192	2056	2058	2061	rVV	30974	27718	1.93%	0.225%
37	15.492	2275	2279	2282	rVB	148620	175047	12.22%	1.423%

Sum of corrected areas: 12303499

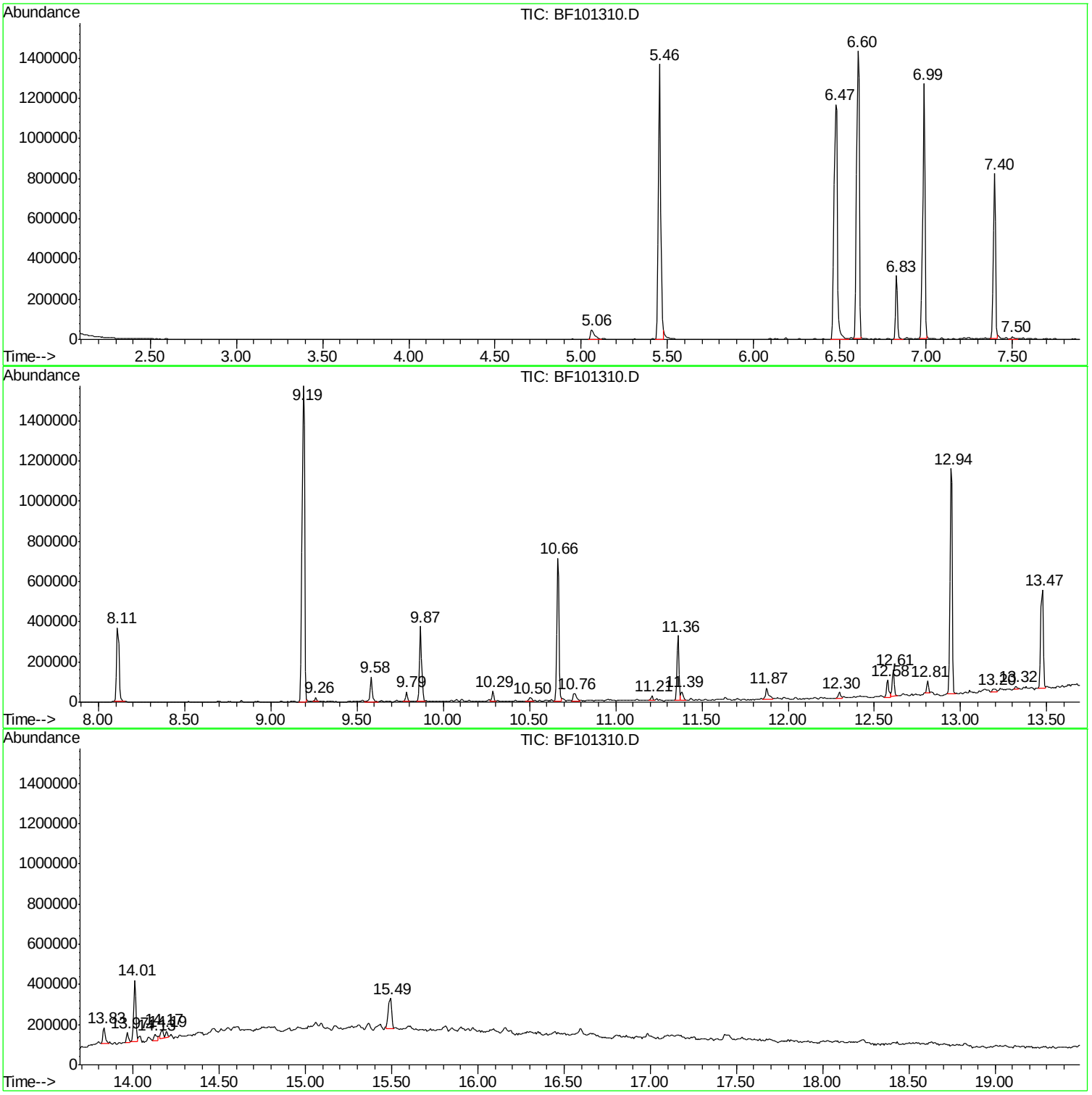
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
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Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

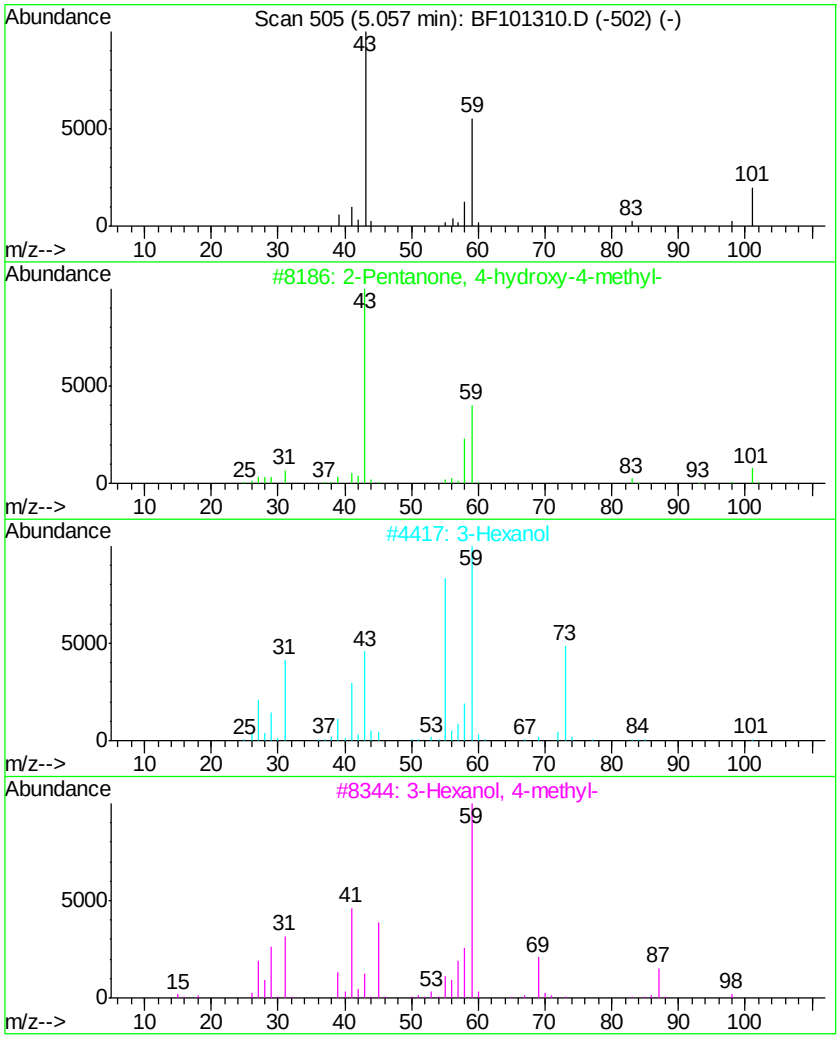
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

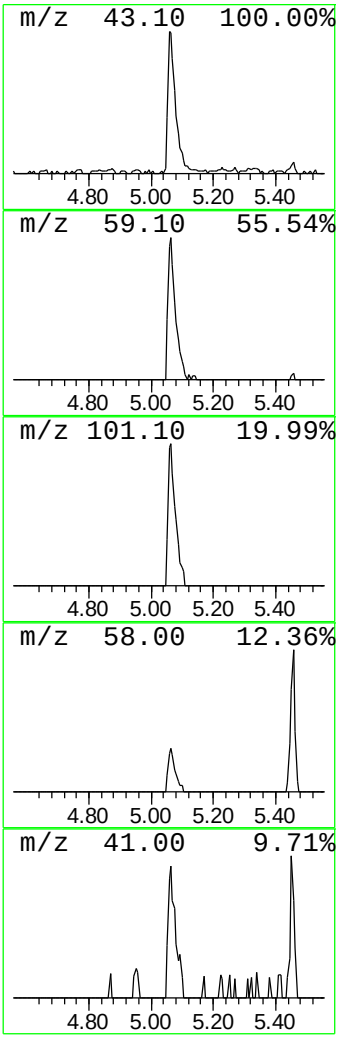
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	6.07 ng	79988	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	3-Hexanol	102	C6H14O	000623-37-0	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

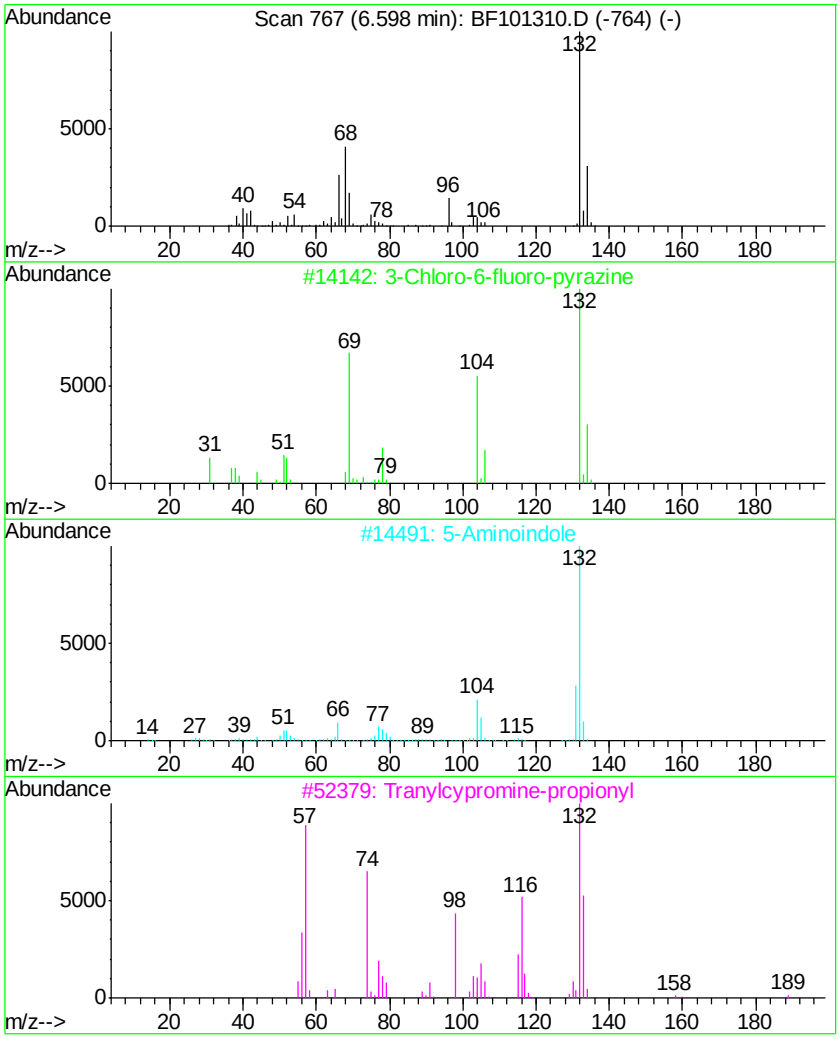
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

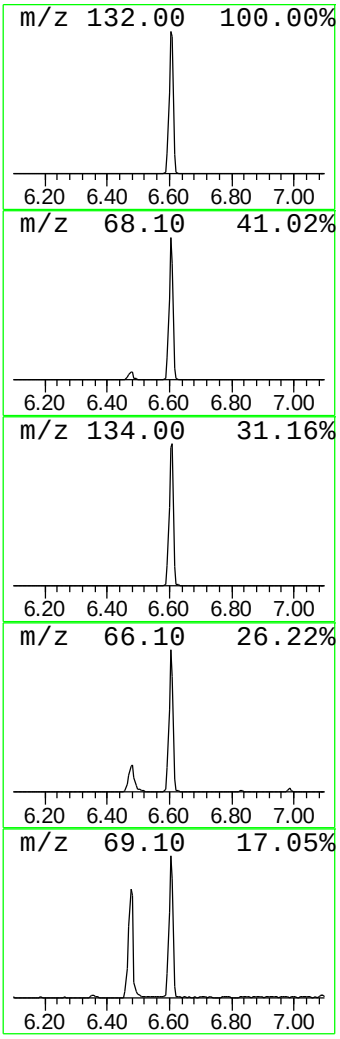
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	105.98 ng	1395640	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	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

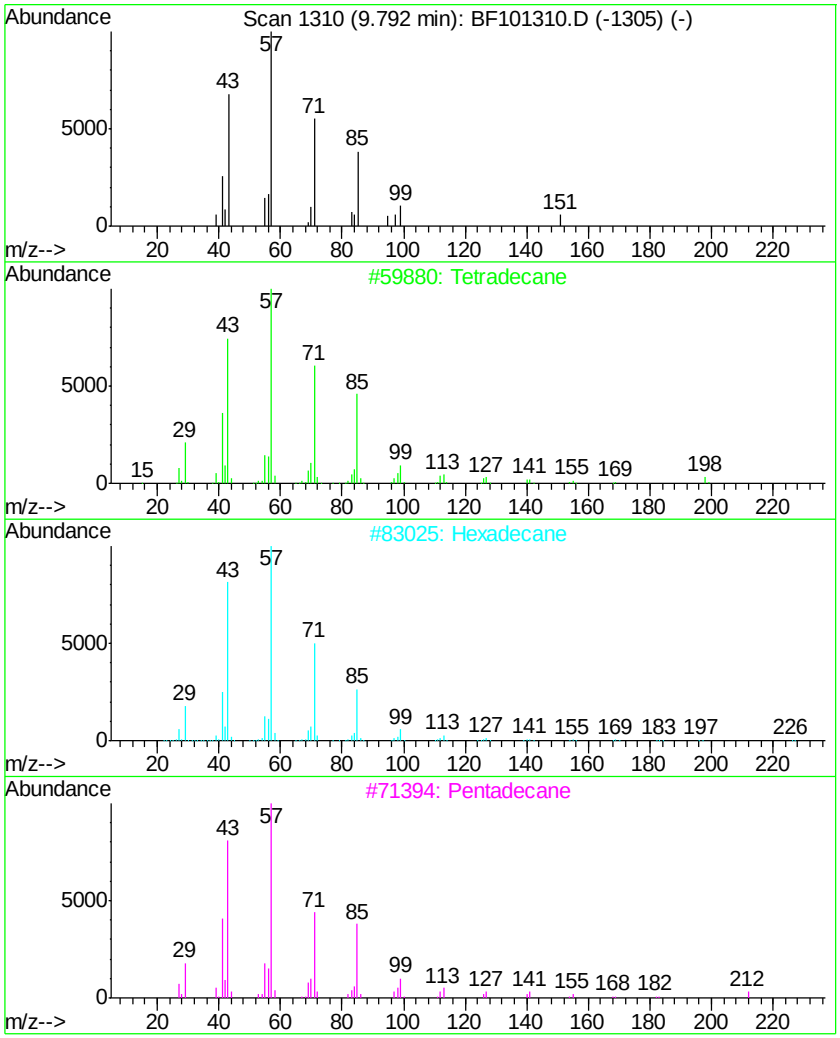
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

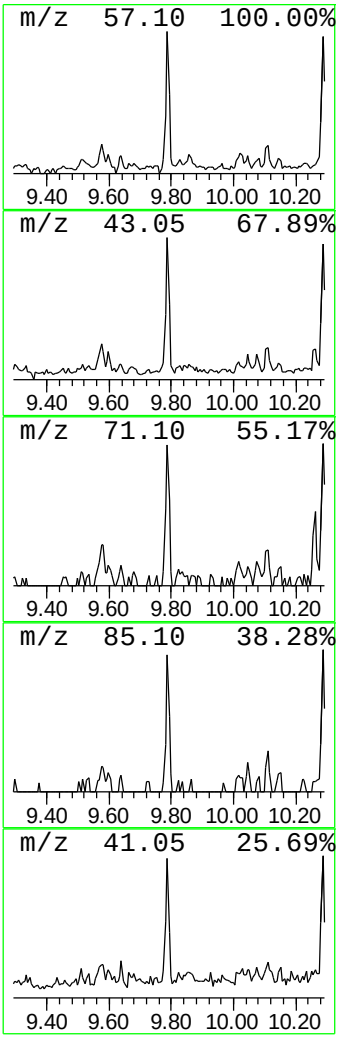
****

Peak Number 4 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	2.47 ng	37938	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	78
2	Hexadecane	226	C16H34	000544-76-3	72
3	Pentadecane	212	C15H32	000629-62-9	64
4	Decane, 2-methyl-	156	C11H24	006975-98-0	64
5	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

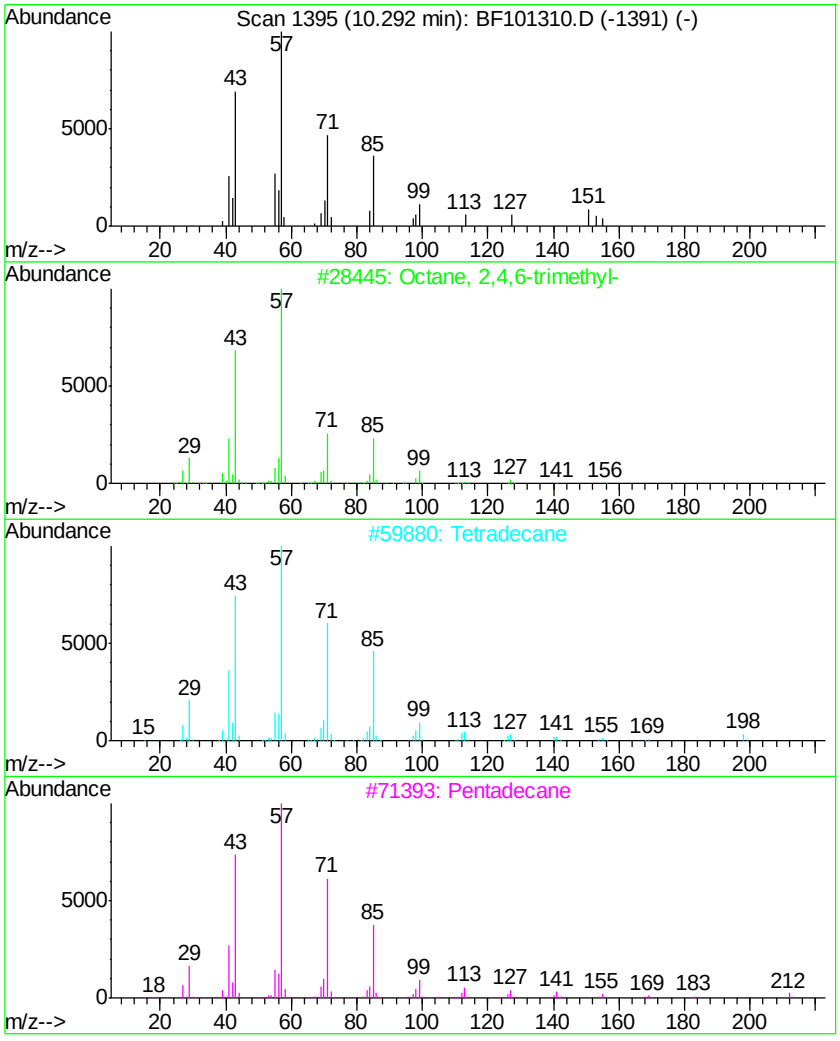
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

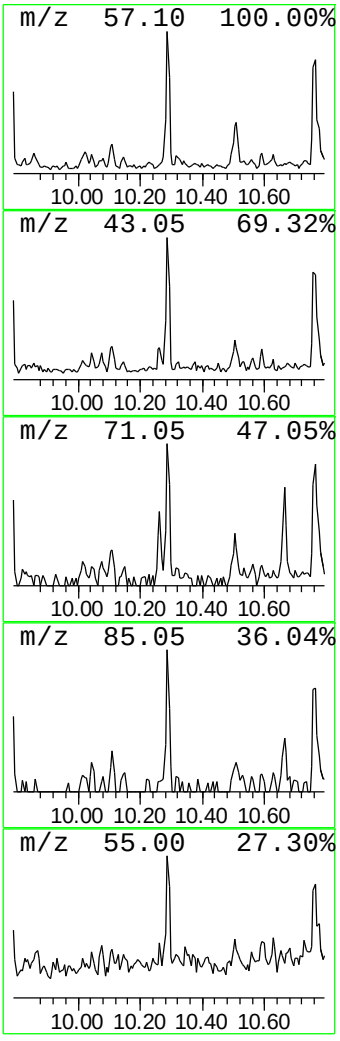
****

Peak Number 5 Octane, 2,4,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.29	2.49 ng	38206	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
2	Tetradecane	198	C14H30	000629-59-4	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Heptadecane	240	C17H36	000629-78-7	72
5	Eicosane	282	C20H42	000112-95-8	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

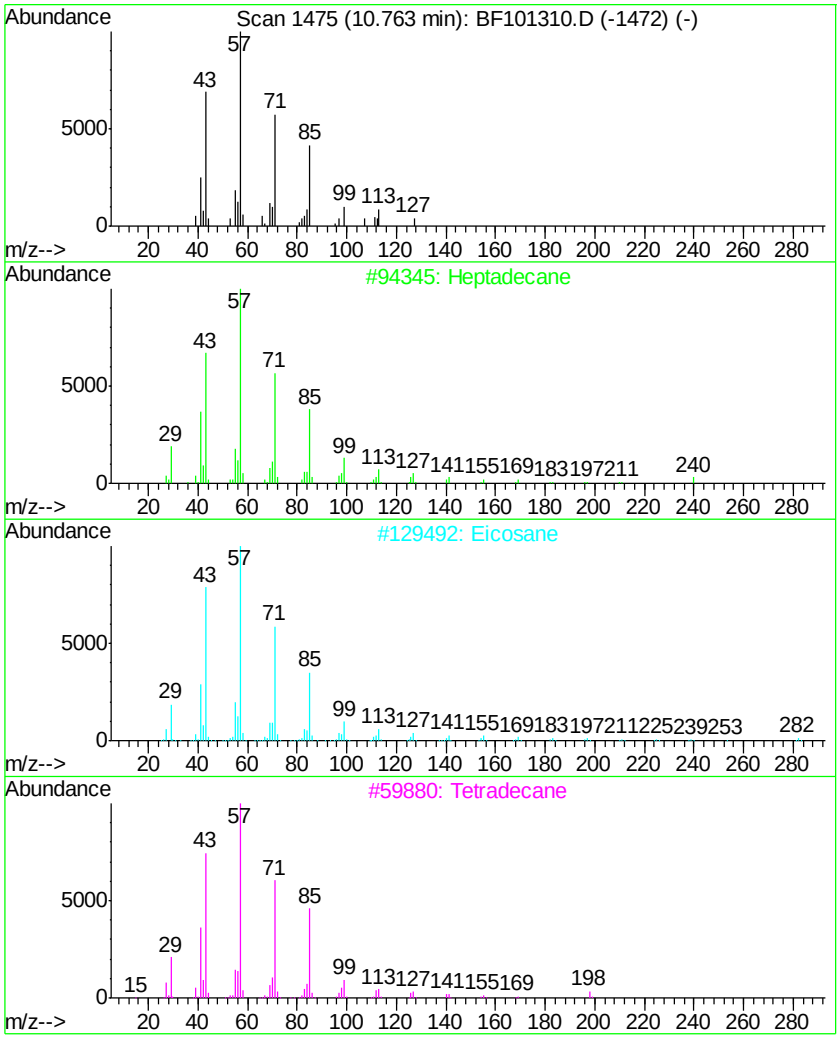
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

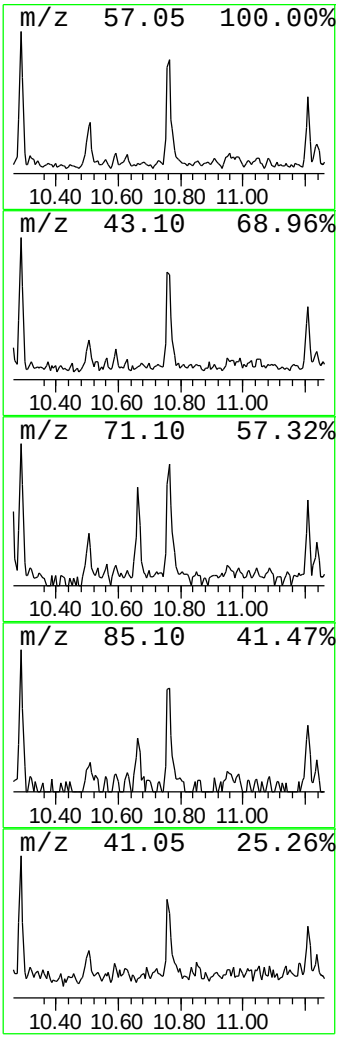
****

Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	3.00 ng	42353	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Eicosane	282	C20H42	000112-95-8	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Pentadecane	212	C15H32	000629-62-9	78
5	Tridecane	184	C13H28	000629-50-5	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

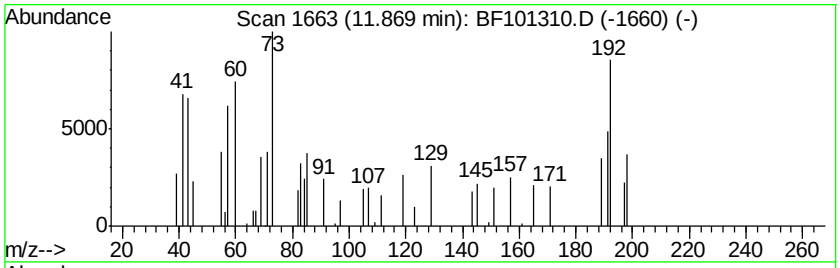
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

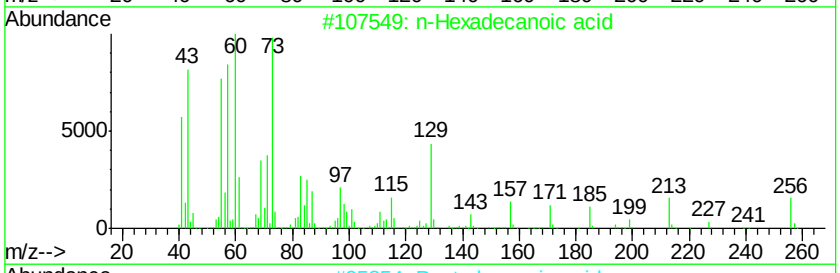
****

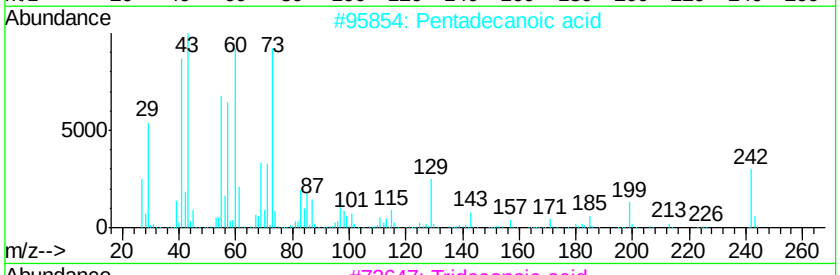
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

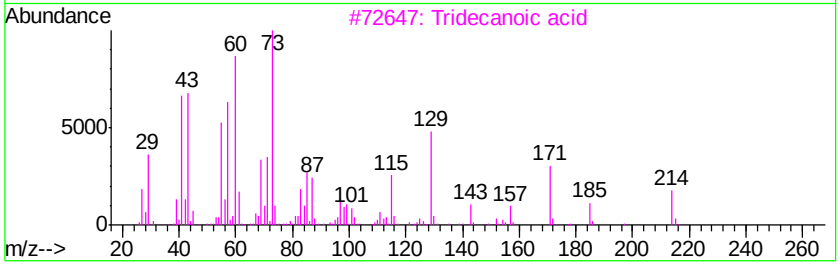
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	5.04 ng	71127	Phenanthrene-d10	11.36

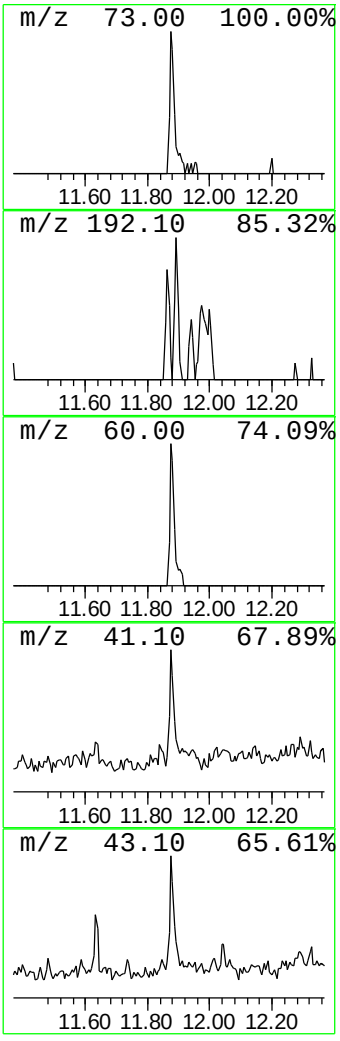
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53











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Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

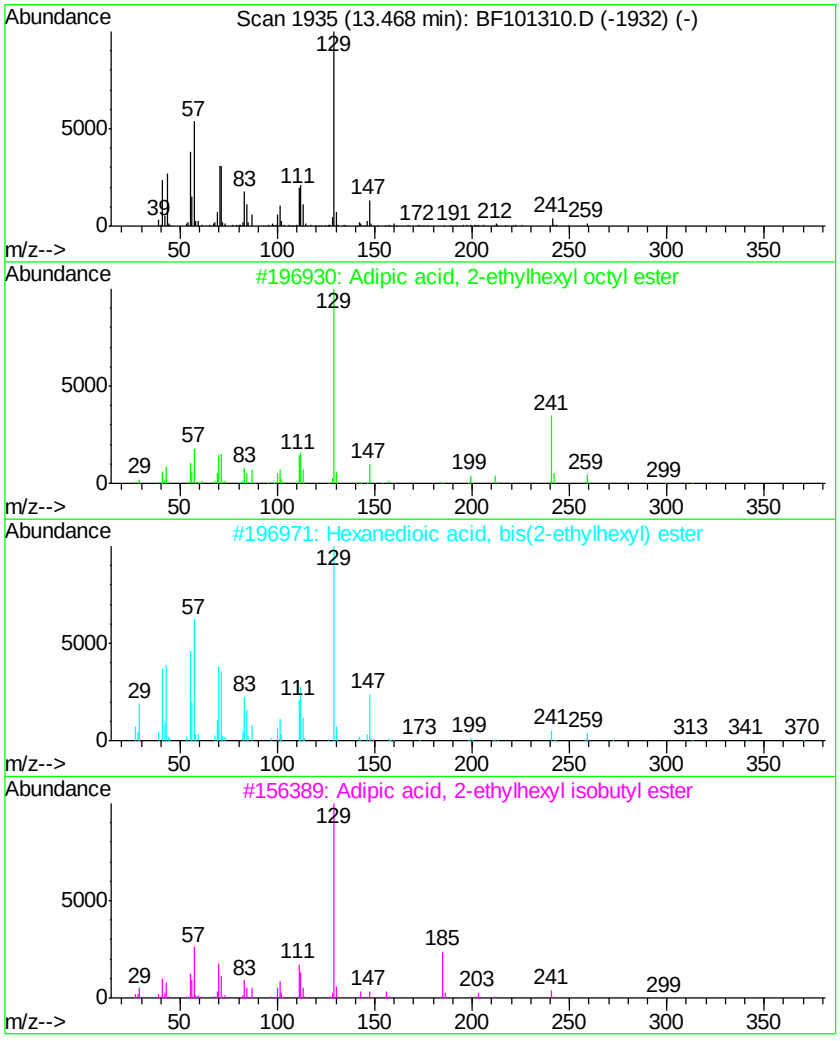
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

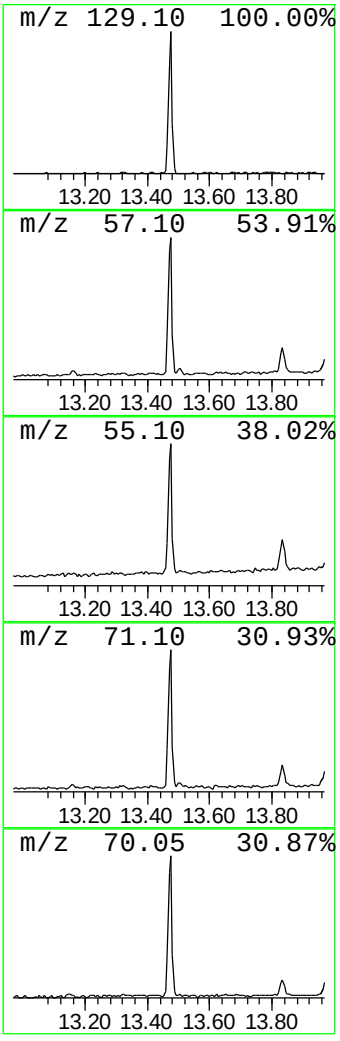
****

Peak Number 8 Adipic acid, 2-ethylhexyl o... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	28.41 ng	426878	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	81
3	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	64
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	62
5	Diisooctyl adipate	370	C22H42O4	001330-86-5	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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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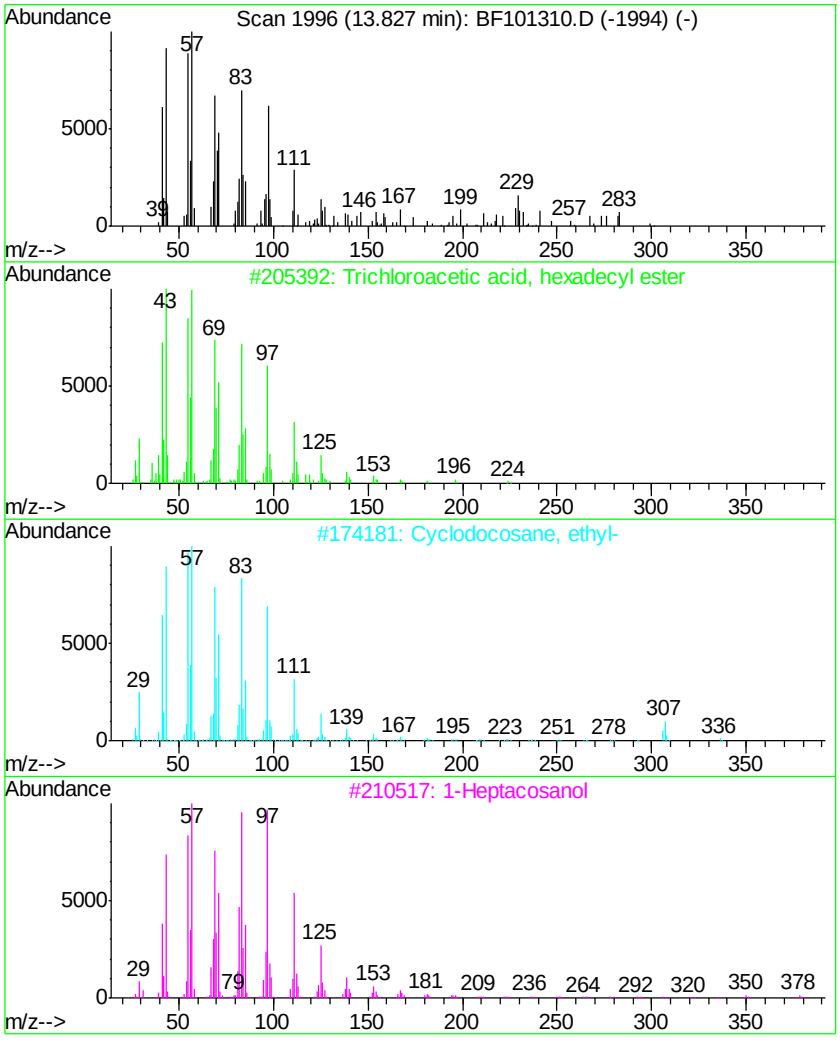
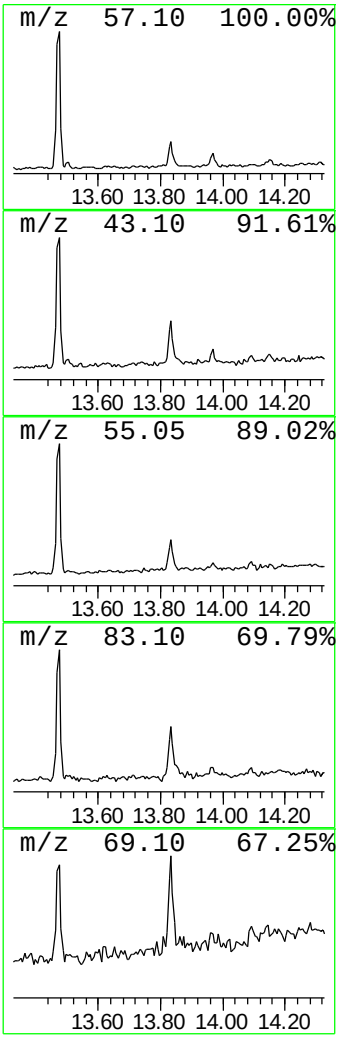
Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.41 ng	81334	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	87
3	1-Heptacosanol	396	C27H56O	002004-39-9	87
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87





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Data File : BF101310.D
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Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

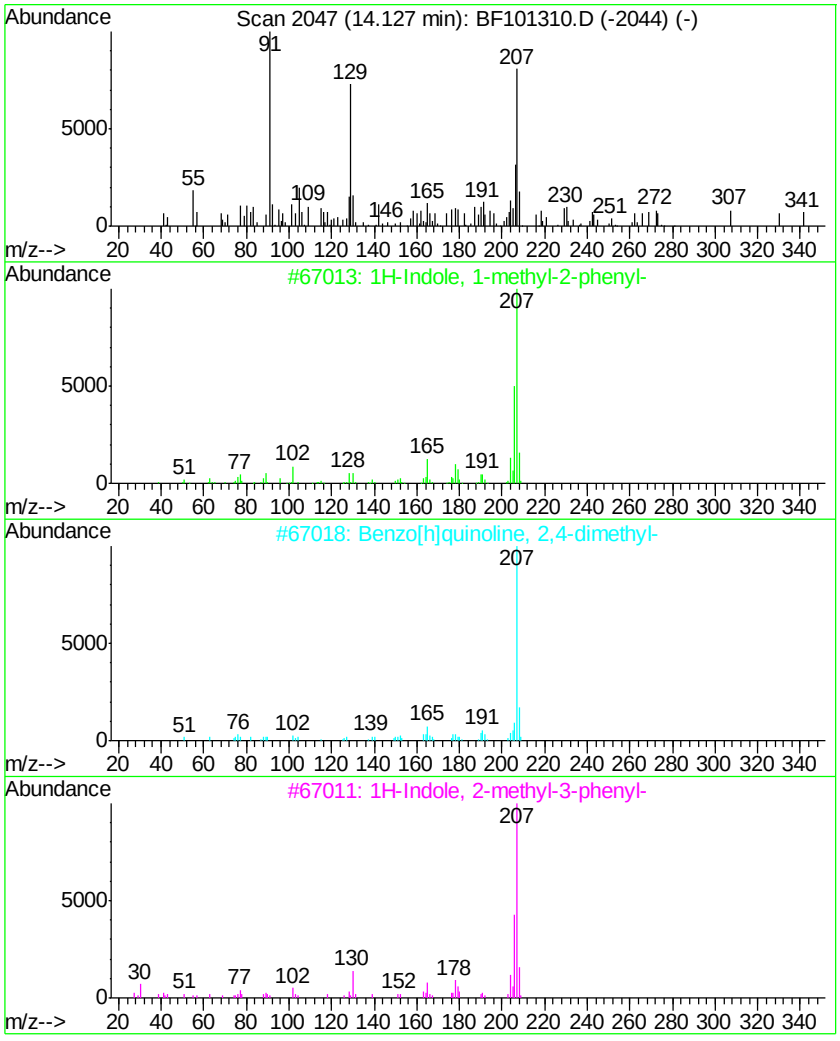
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

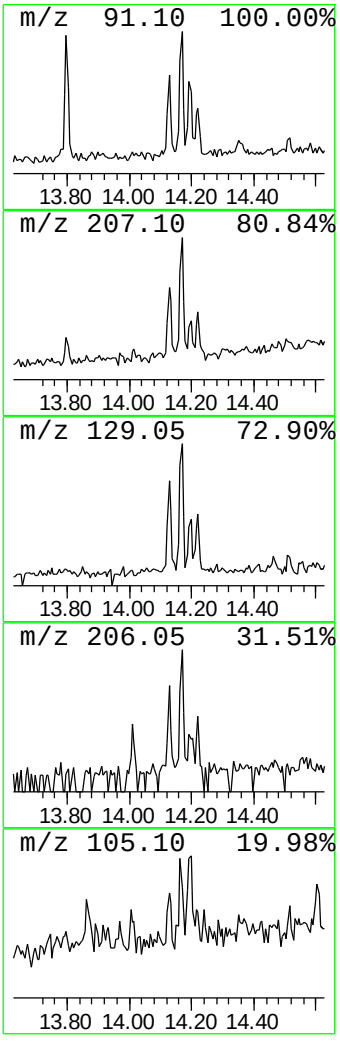
****

Peak Number 10 1H-Indole, 1-methyl-2-phenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	3.00 ng	45081	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	53
2	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	50
3	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	49
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	49
5	Indolizine, 2-(4-methylphenyl)-	207	C15H13N	007496-81-3	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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

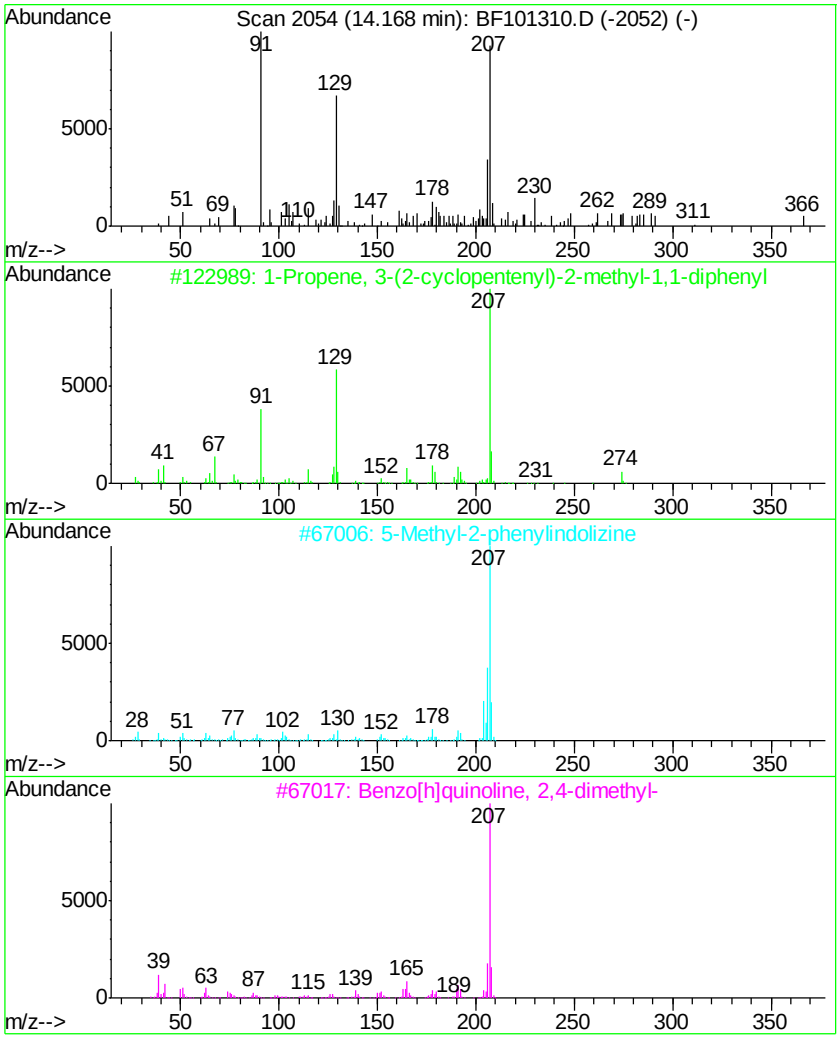
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

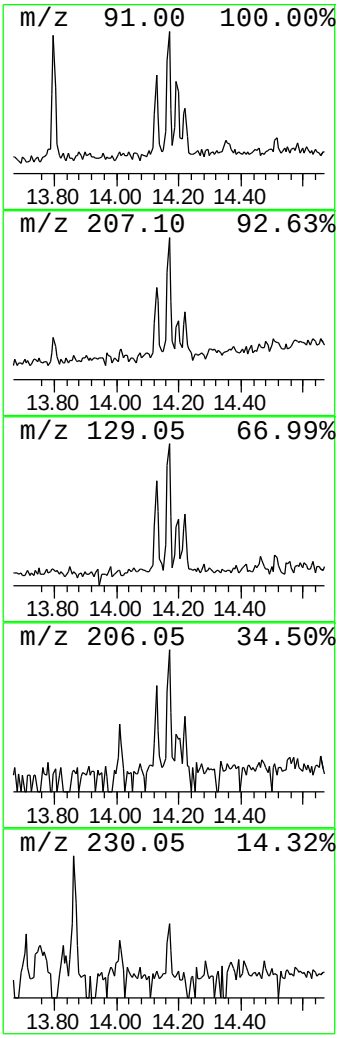
****

Peak Number 11 1-Propene, 3-(2-cyclopenten... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	2.33 ng	34951	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	58
2	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	47
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	43
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	43
5	2-Bromo-4-chloroaniline	205	C6H5BrClN	000873-38-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121117\
Data File : BF101310.D
Acq On : 12 Dec 2017 3:22
Operator : SJ/JU
Sample : I6744-10
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PROS-1-E(3-4)

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	6.1	ng	79988	1	6.83	263389	20.0
unknown6.60	6.60	106.0	ng	1395640	1	6.83	263389	20.0
Tetradecane	9.79	2.5	ng	37938	3	9.87	307168	20.0
Octane, 2,4,6-tri...	10.29	2.5	ng	38206	3	9.87	307168	20.0
Heptadecane	10.76	3.0	ng	42353	4	11.36	282271	20.0
n-Hexadecanoic acid	11.87	5.0	ng	71127	4	11.36	282271	20.0
Adipic acid, 2-et...	13.47	28.4	ng	426878	5	14.01	300549	20.0
Trichloroacetic a...	13.83	5.4	ng	81334	5	14.01	300549	20.0
1H-Indole, 1-meth...	14.13	3.0	ng	45081	5	14.01	300549	20.0
1-Propene, 3-(2-c...	14.17	2.3	ng	34951	5	14.01	300549	20.0