LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104517.D
Acq On : 14 Apr 2018 10:39
Operator : JU/SJ
Sample : J2368-11
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

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	5.004	492	496	503	rVB	123388	124204	3.14%	0.522%
2	5.422	563	567	574	rBV	1488708	1275224	32.26%	5.361%
3	6.033	667	671	680	rBV	55479	59319	1.50%	0.249%
4	6.439	736	740	746	rVB	844175	825964	20.90%	3.472%
5	6.575	759	763	767	rBV	2321416	2243955	56.77%	9.434%
6	6.804	799	802	806	rBV	919629	838438	21.21%	3.525%
7	6.963	825	829	833	rBV	2865440	2810992	71.11%	11.817%
8	7.375	893	899	902	rBV	2107828	2053502	51.95%	8.633%
9	8.092	1017	1021	1024	rBV	1144104	942951	23.85%	3.964%
10	9.169	1198	1204	1207	rBV	4115578	3952899	100.00%	16.618%
11	9.557	1267	1270	1274	rBV	219130	206993	5.24%	0.870%
12	9.774	1304	1307	1310	rBV	148472	110497	2.80%	0.465%
13	9.845	1315	1319	1328	rVB2	1356937	1223235	30.95%	5.142%
14	10.274	1389	1392	1395	rVB2	172261	134812	3.41%	0.567%
15	10.492	1424	1429	1432	rBV	41284	54554	1.38%	0.229%
16	10.639	1447	1454	1457	rBV	1439523	1444346	36.54%	6.072%
17	10.745	1469	1472	1474	rBV	140236	118513	3.00%	0.498%
18	10.774	1474	1477	1487	rVB2	321732	384752	9.73%	1.617%
19	11.198	1545	1549	1551	rBV	65060	54514	1.38%	0.229%
20	11.333	1568	1572	1576	rBV	1118210	947183	23.96%	3.982%
21	12.739	1808	1811	1817	rVB	92748	71791	1.82%	0.302%
22	12.927	1838	1843	1846	rBV	2693659	2476931	62.66%	10.413%
23	13.445	1928	1931	1935	rVB	51230	43816	1.11%	0.184%
24	13.815	1991	1994	2003	rBV	216484	234111	5.92%	0.984%
25	13.974	2018	2021	2025	rBV	646455	645767	16.34%	2.715%
26	15.439	2265	2270	2280	rVB	397753	507640	12.84%	2.134%

Sum of corrected areas: 23786903

LSC Report - Integrated Chromatogram

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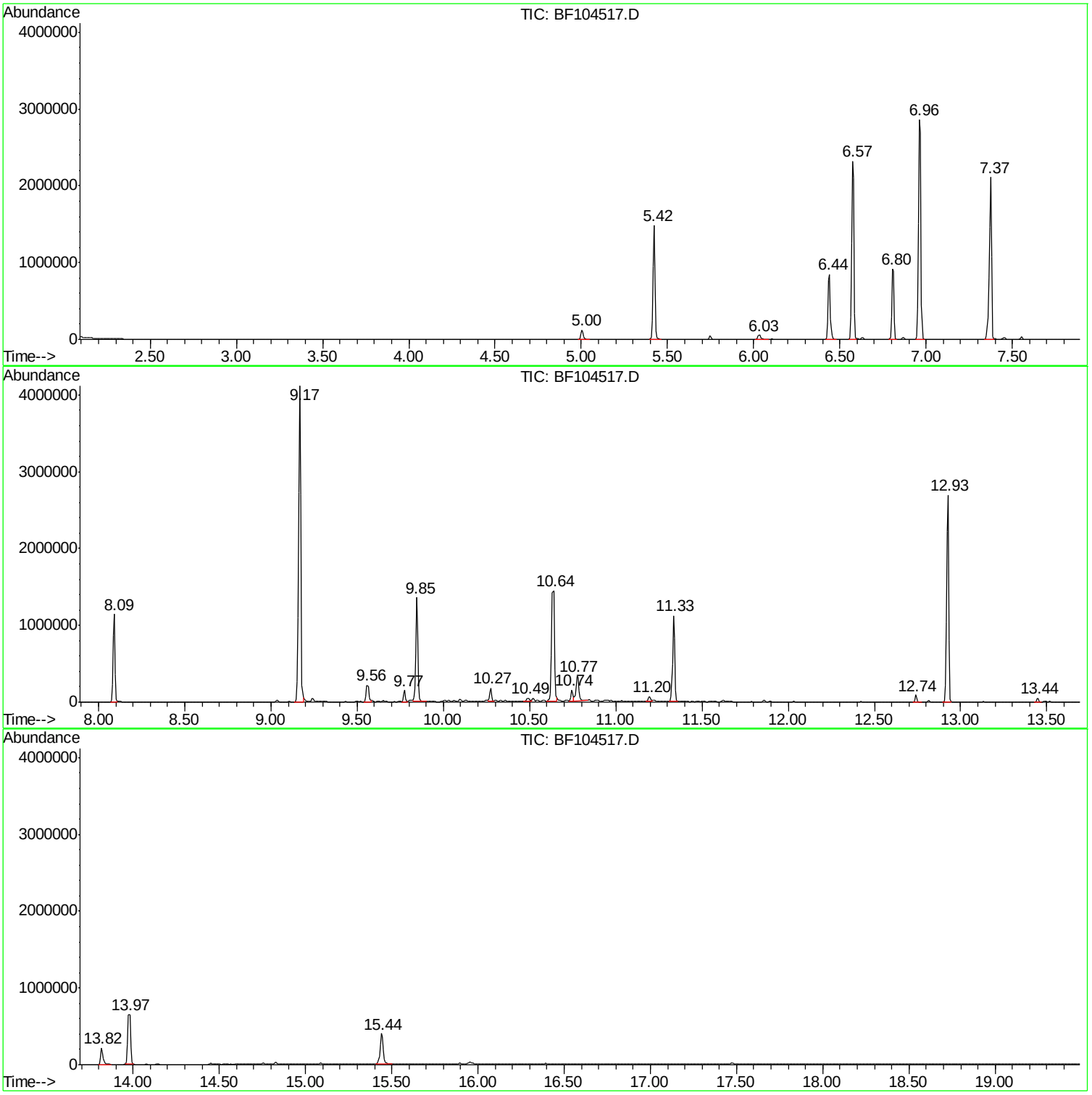
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

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\BF041318\
Data File : BF104517.D
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Operator : JU/SJ
Sample : J2368-11
Misc :
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Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

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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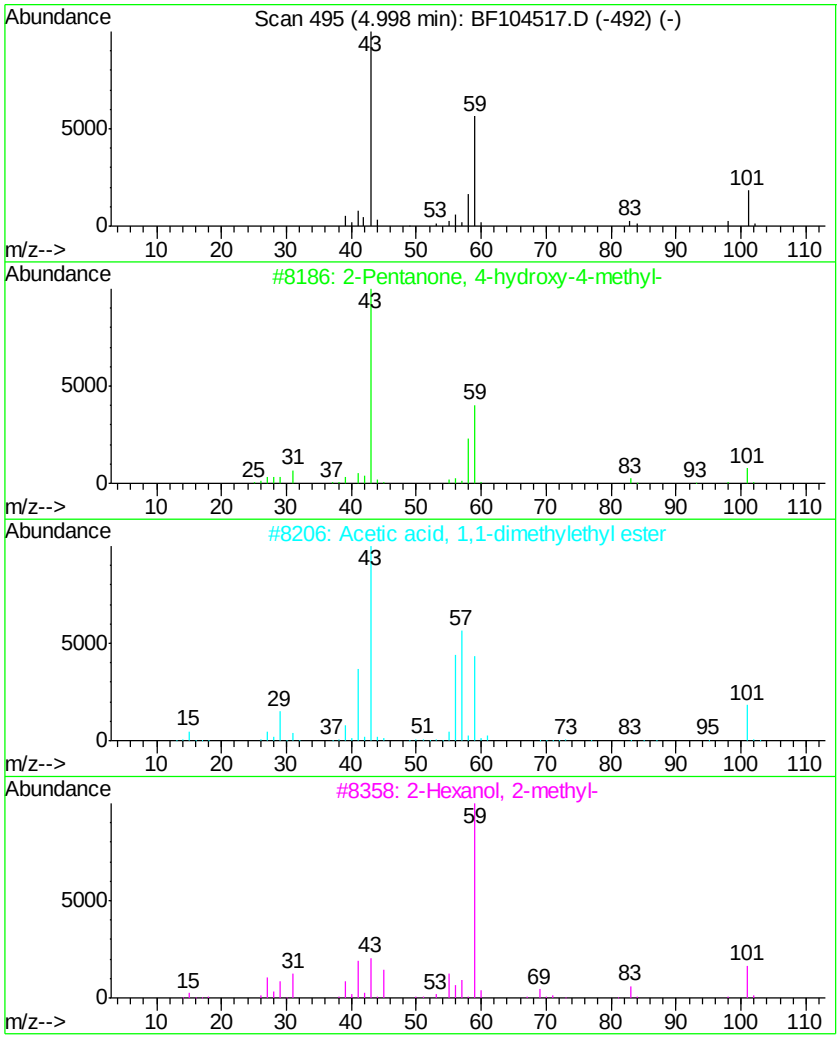
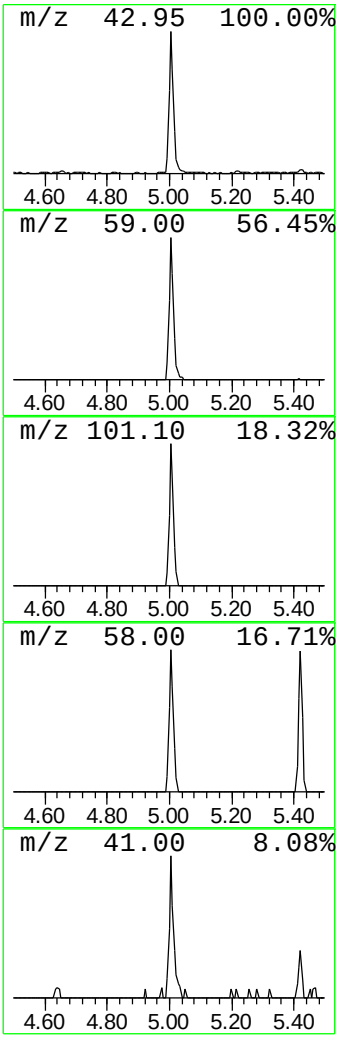
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.96 ng	124204	1,4-Dichlorobenzene-d4	6.81

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	50
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Sample : J2368-11
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

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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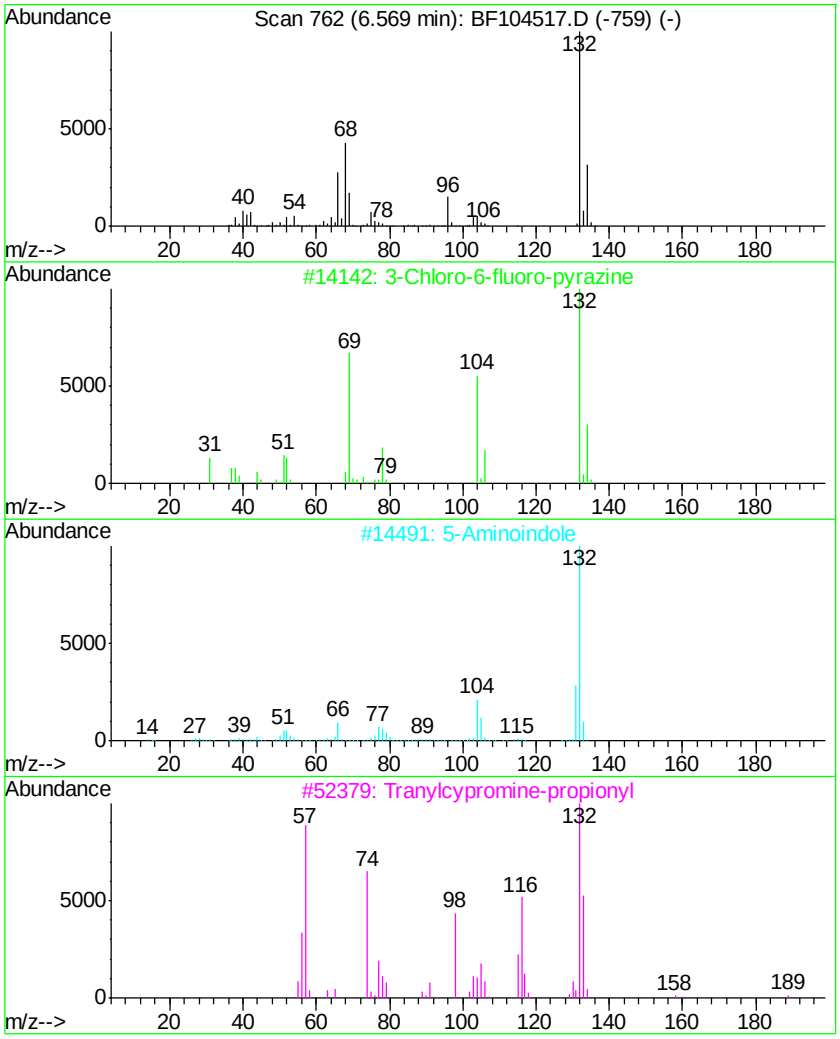
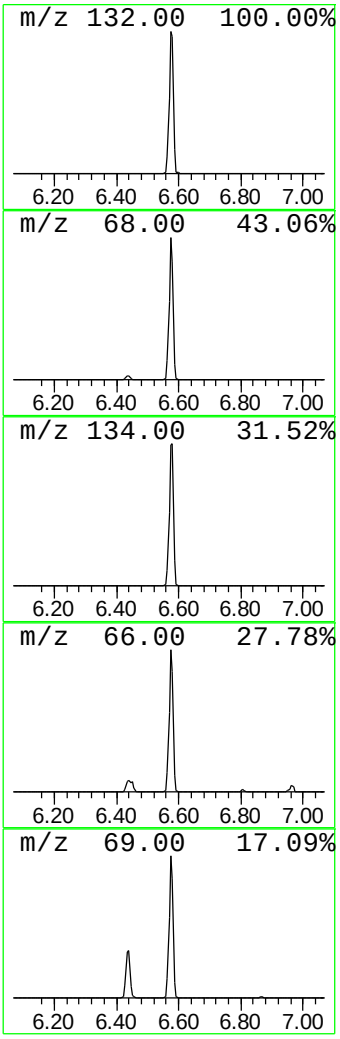
Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	53.53 ng	2243960	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
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\BF041318\
Data File : BF104517.D
Acq On : 14 Apr 2018 10:39
Operator : JU/SJ
Sample : J2368-11
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

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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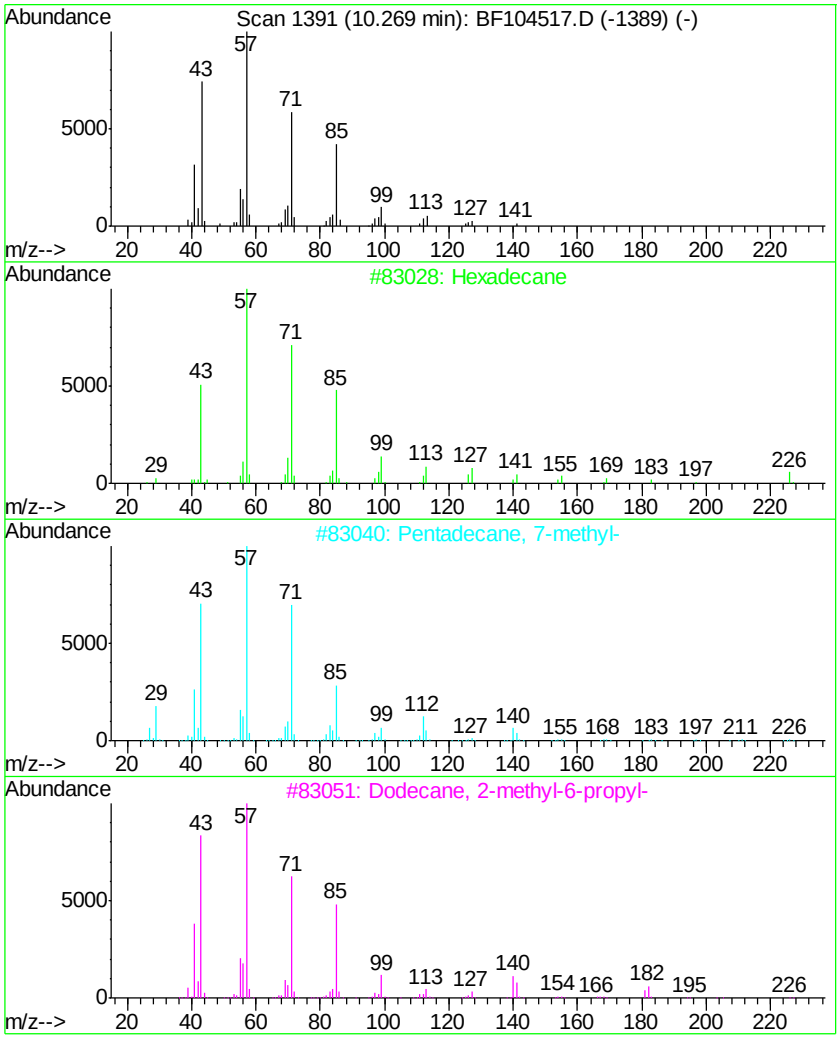
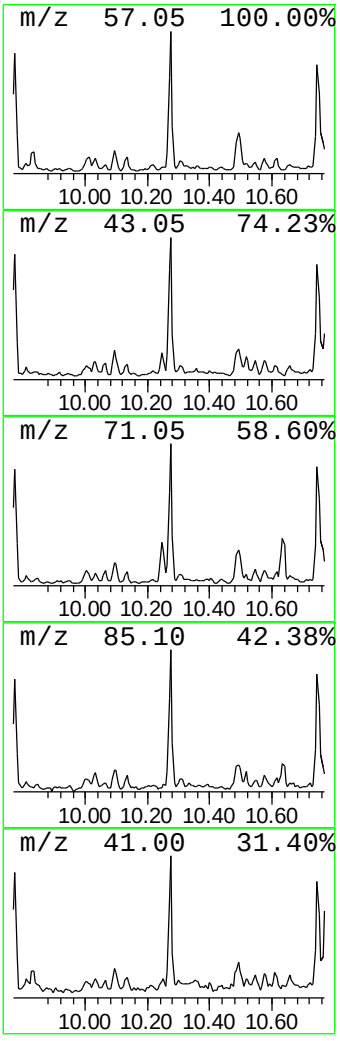
Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.20 ng	134812	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	87
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	72
5	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	64





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Data File : BF104517.D
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Operator : JU/SJ
Sample : J2368-11
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

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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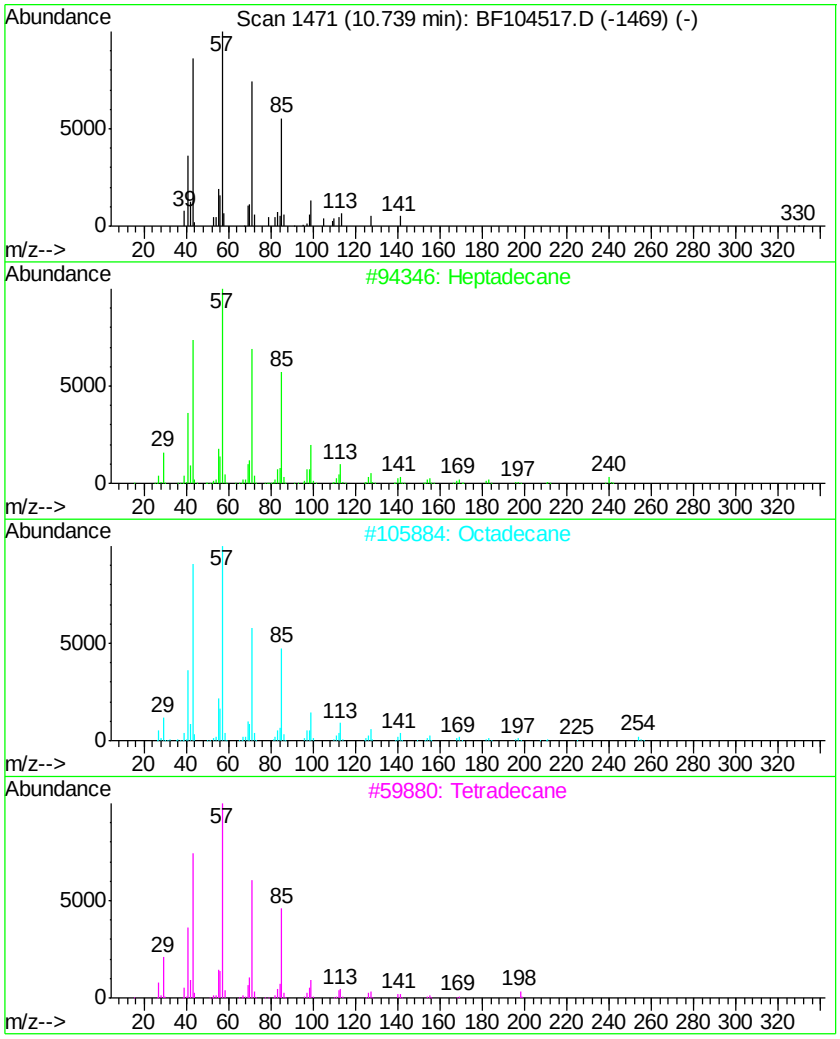
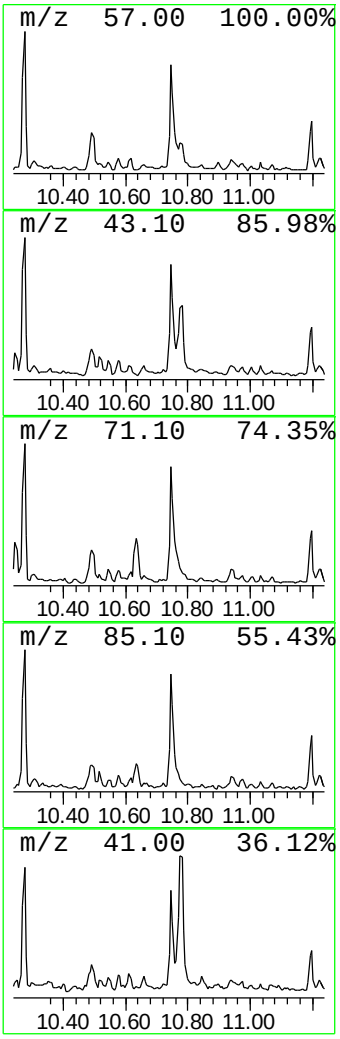
Peak Number 5 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.50 ng	118513	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Octadecane	254	C18H38	000593-45-3	90
3	Tetradecane	198	C14H30	000629-59-4	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86





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Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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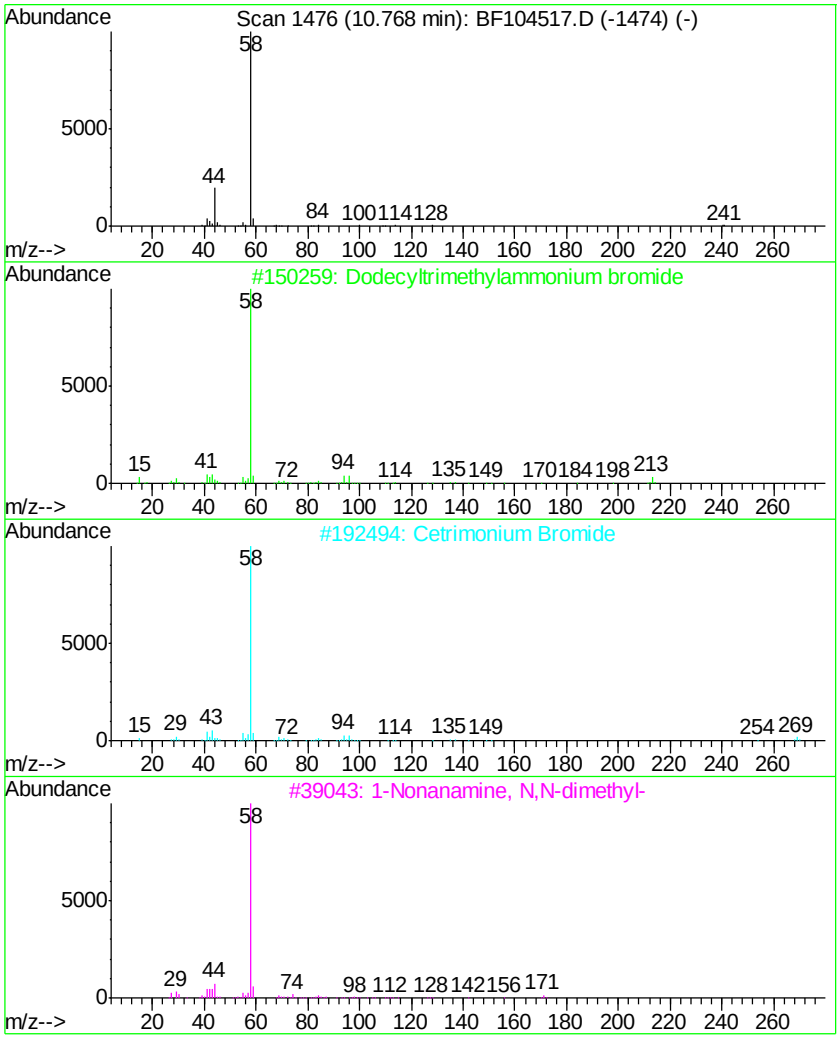
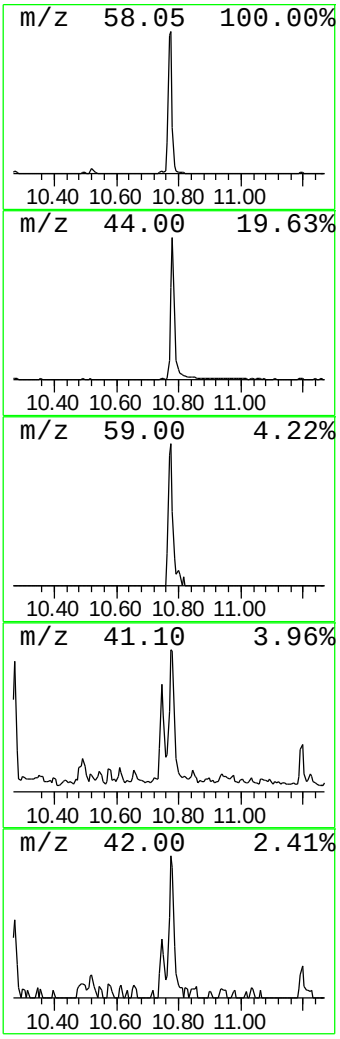
Peak Number 6 unknown10.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	8.12 ng	384752	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	38
2	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	38
3	1-Nonanamine, N,N-dimethyl-	171	C11H25N	017373-27-2	38
4	Tetradonium Bromide	335	C17H38BrN	001119-97-7	32
5	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	32





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Sample : J2368-11
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-B

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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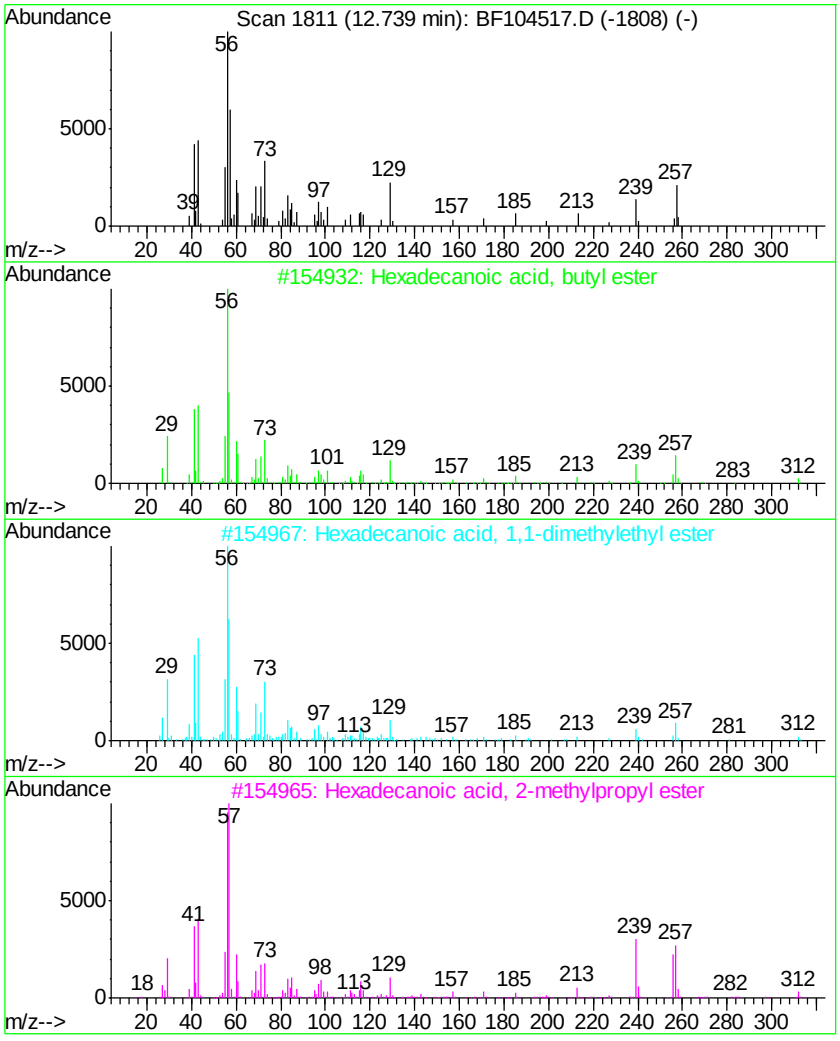
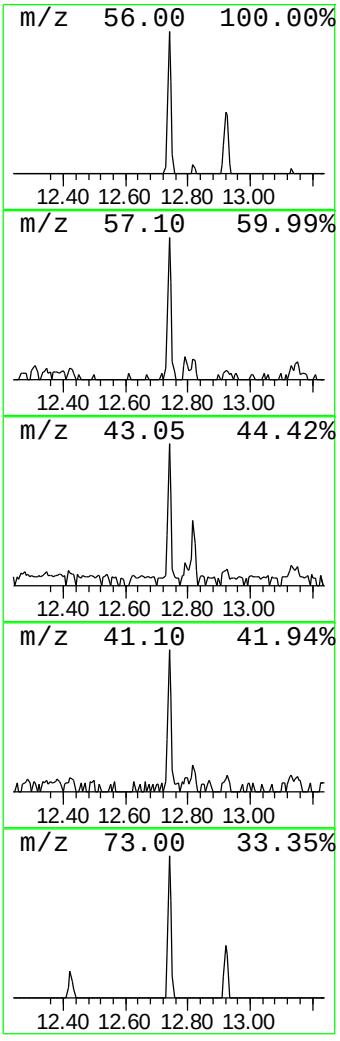
Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.22 ng	71791	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	59
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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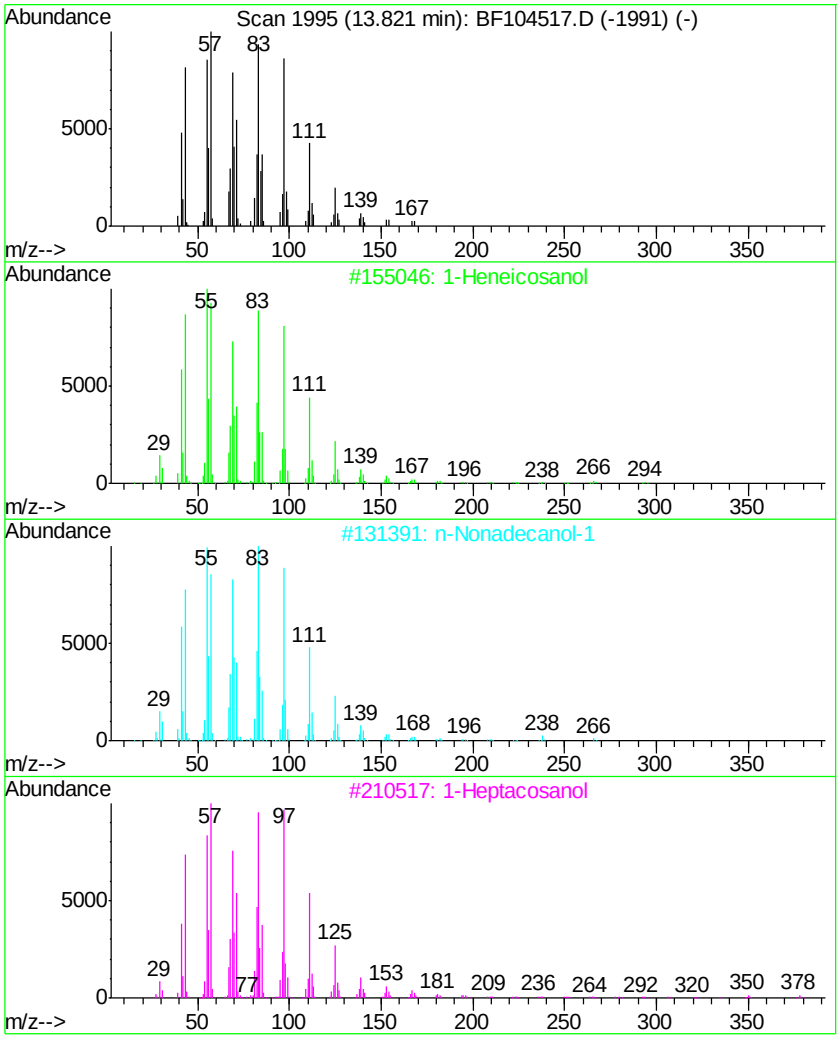
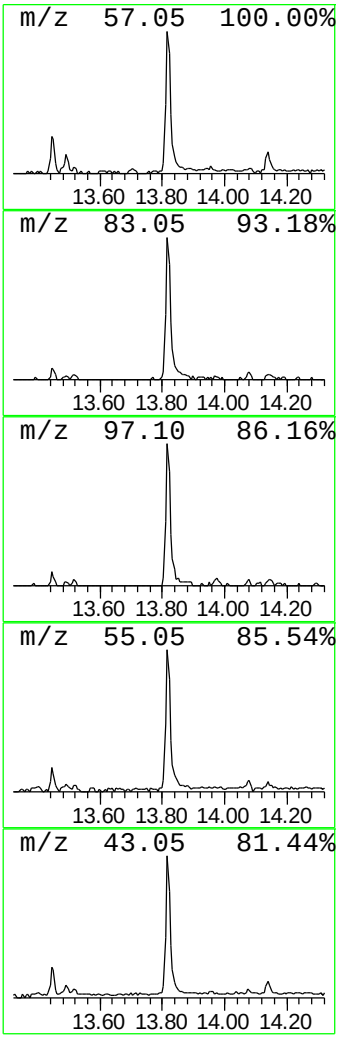
Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	7.25 ng	234111	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

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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...	5.00	3.0	ng	124204	1	6.81	838438	20.0
unknown6.57	6.57	53.5	ng	2243960	1	6.81	838438	20.0
Hexadecane	10.27	2.2	ng	134812	3	9.85	1223240	20.0
Heptadecane	10.74	2.5	ng	118513	4	11.33	947183	20.0
unknown10.77	10.77	8.1	ng	384752	4	11.33	947183	20.0
Hexadecanoic acid...	12.74	2.2	ng	71791	5	13.98	645767	20.0
1-Heneicosanol	13.82	7.3	ng	234111	5	13.98	645767	20.0