LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094694.D
Acq On : 28 Apr 2017 20:04
Operator : SJ/MA
Sample : I2895-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

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-BF041717.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	3.943	337	341	353	rBV	466654	582626	17.67%	2.158%
2	4.331	403	407	422	rBV	3074272	3205377	97.21%	11.873%
3	4.713	468	472	480	rBV	34876	36804	1.12%	0.136%
4	5.407	584	590	605	rBV	2723079	3238819	98.22%	11.997%
5	5.525	606	610	614	rBV	3109375	3297397	100.00%	12.214%
6	5.772	648	652	660	rBV	685545	642174	19.48%	2.379%
7	5.948	677	682	685	rBV	2716314	2520944	76.45%	9.338%
8	6.425	757	763	766	rBV	1806763	1978542	60.00%	7.329%
9	7.260	901	905	913	rBV	919191	827109	25.08%	3.064%
10	8.583	1125	1130	1133	rBV	3255040	3223219	97.75%	11.939%
11	9.083	1212	1215	1220	rBV	253296	231709	7.03%	0.858%
12	9.395	1258	1268	1279	rBV2	856283	871583	26.43%	3.228%
13	9.989	1365	1369	1374	rBV	48221	45186	1.37%	0.167%
14	10.377	1430	1435	1438	rBV	1506167	1657873	50.28%	6.141%
15	10.577	1465	1469	1476	rBV	57159	79713	2.42%	0.295%
16	11.130	1559	1563	1566	rBV	42026	40637	1.23%	0.151%
17	11.219	1574	1578	1582	rBV	749290	693373	21.03%	2.568%
18	11.954	1699	1703	1711	rBV2	94173	115301	3.50%	0.427%
19	13.195	1909	1914	1918	rBV	2014079	2245340	68.09%	8.317%
20	14.360	2107	2112	2122	rBV4	61190	123369	3.74%	0.457%
21	14.471	2126	2131	2135	rBV	590098	622506	18.88%	2.306%
22	15.142	2241	2245	2253	rBV	39594	58802	1.78%	0.218%
23	15.859	2363	2367	2372	rBV	87920	96865	2.94%	0.359%
24	16.101	2403	2408	2419	rVB	420225	504676	15.31%	1.869%
25	16.583	2487	2490	2496	rVB	38375	56780	1.72%	0.210%

Sum of corrected areas: 26996724

LSC Report - Integrated Chromatogram

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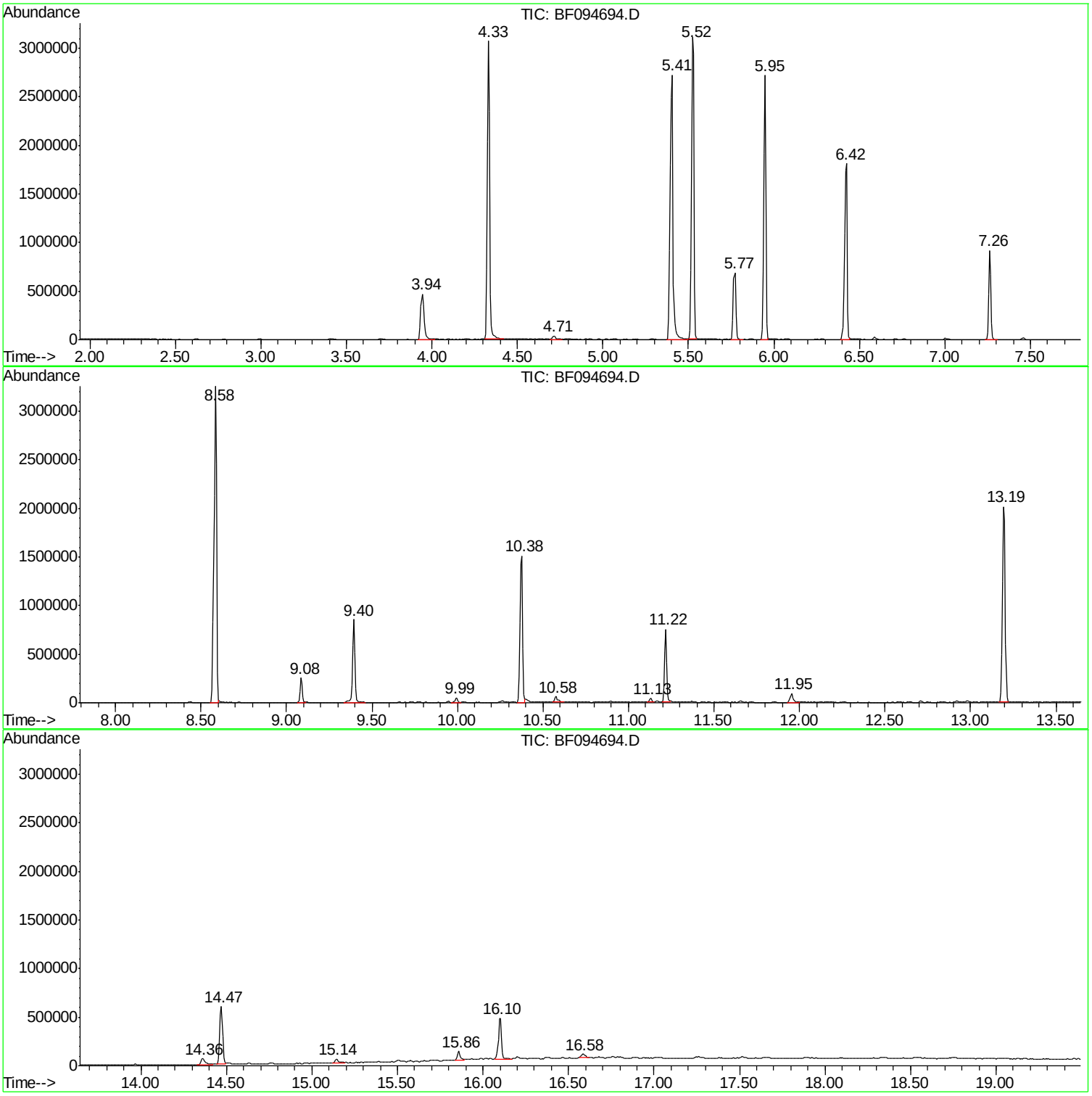
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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\BF042817\
Data File : BF094694.D
Acq On : 28 Apr 2017 20:04
Operator : SJ/MA
Sample : I2895-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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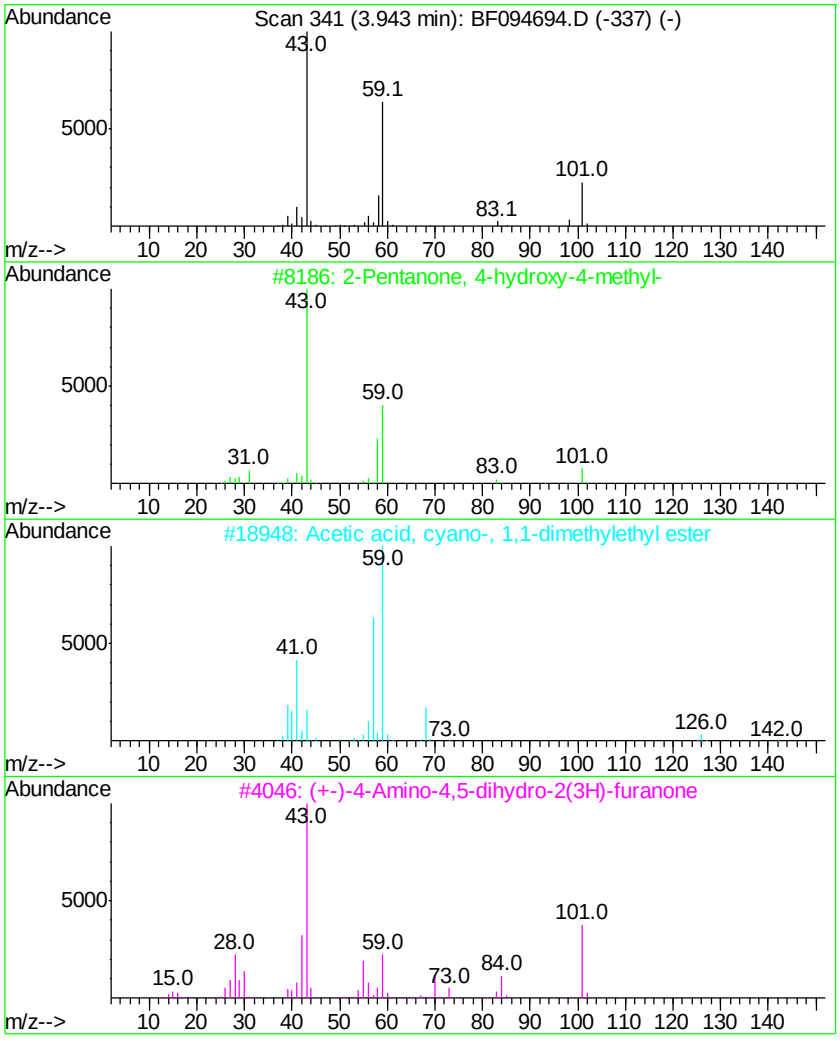
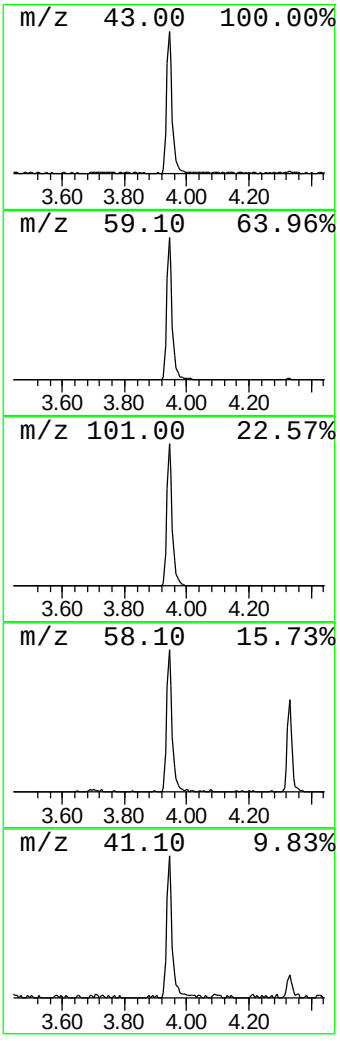
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	18.15 ng	582626	1,4-Dichlorobenzene-d4	5.77

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	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Data File : BF094694.D
Acq On : 28 Apr 2017 20:04
Operator : SJ/MA
Sample : I2895-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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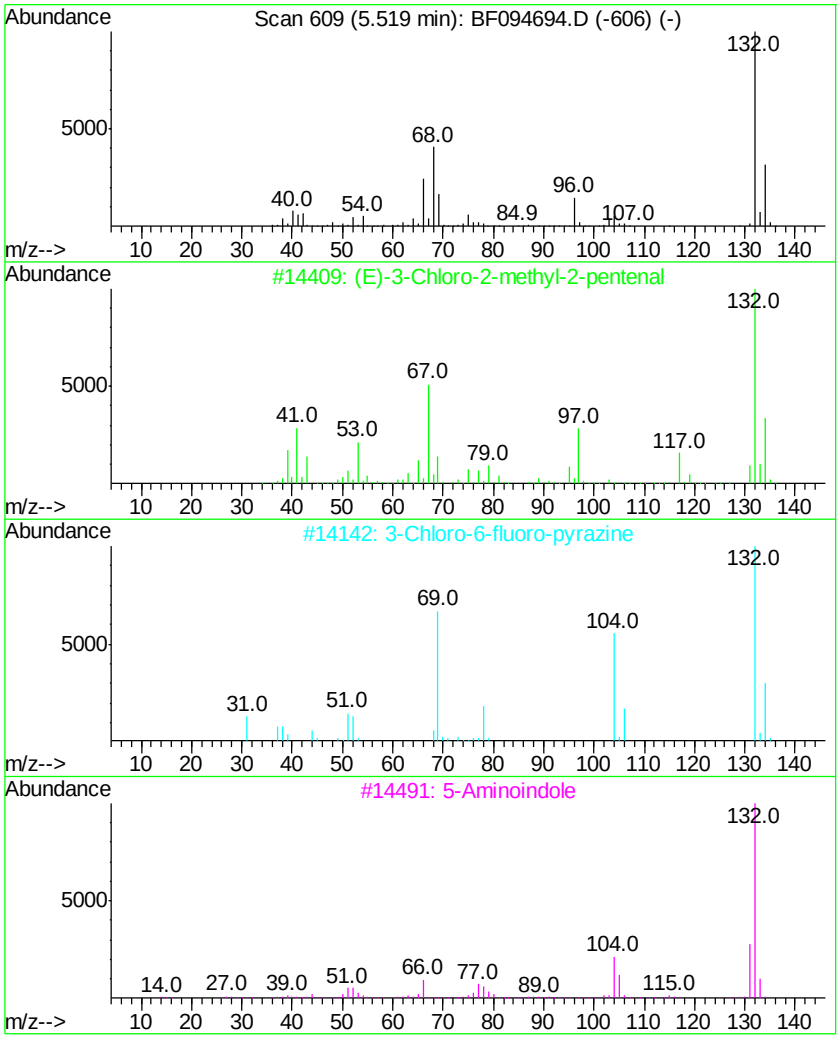
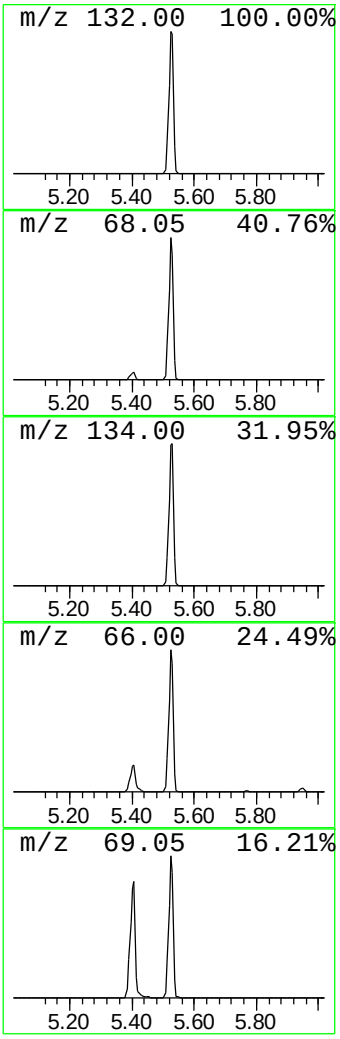
Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	102.70 ng	3297400	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Acq On : 28 Apr 2017 20:04
Operator : SJ/MA
Sample : I2895-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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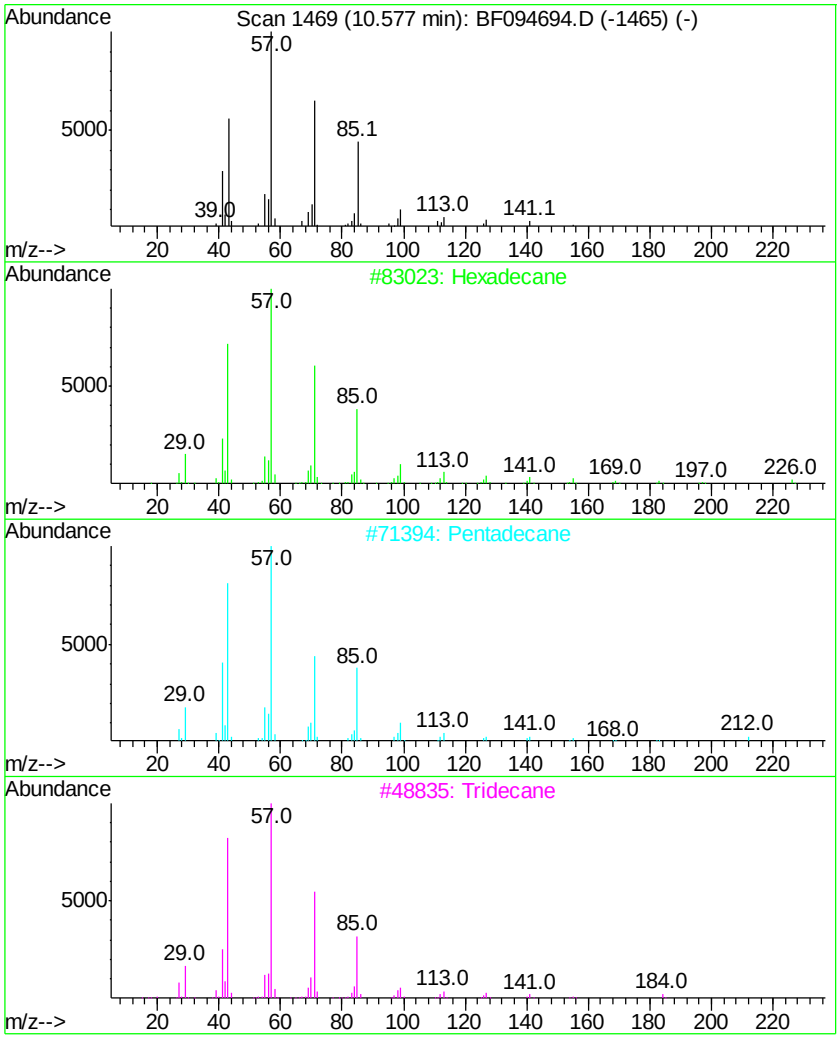
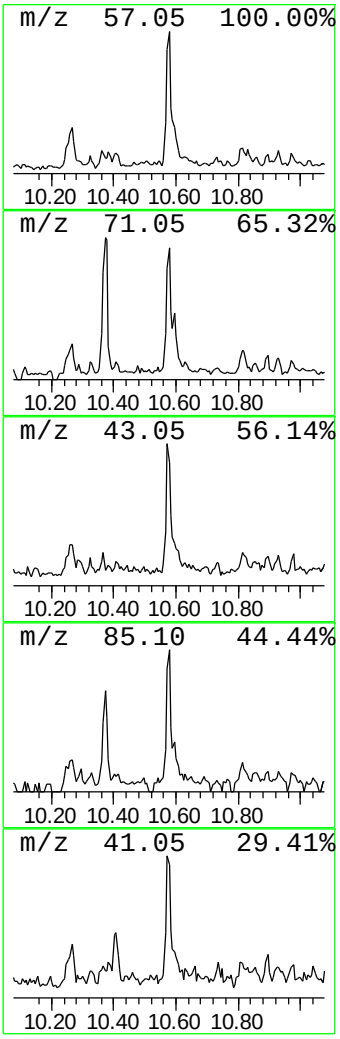
Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	2.30 ng	79713	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Heptadecane	240	C17H36	000629-78-7	86
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094694.D
Acq On : 28 Apr 2017 20:04
Operator : SJ/MA
Sample : I2895-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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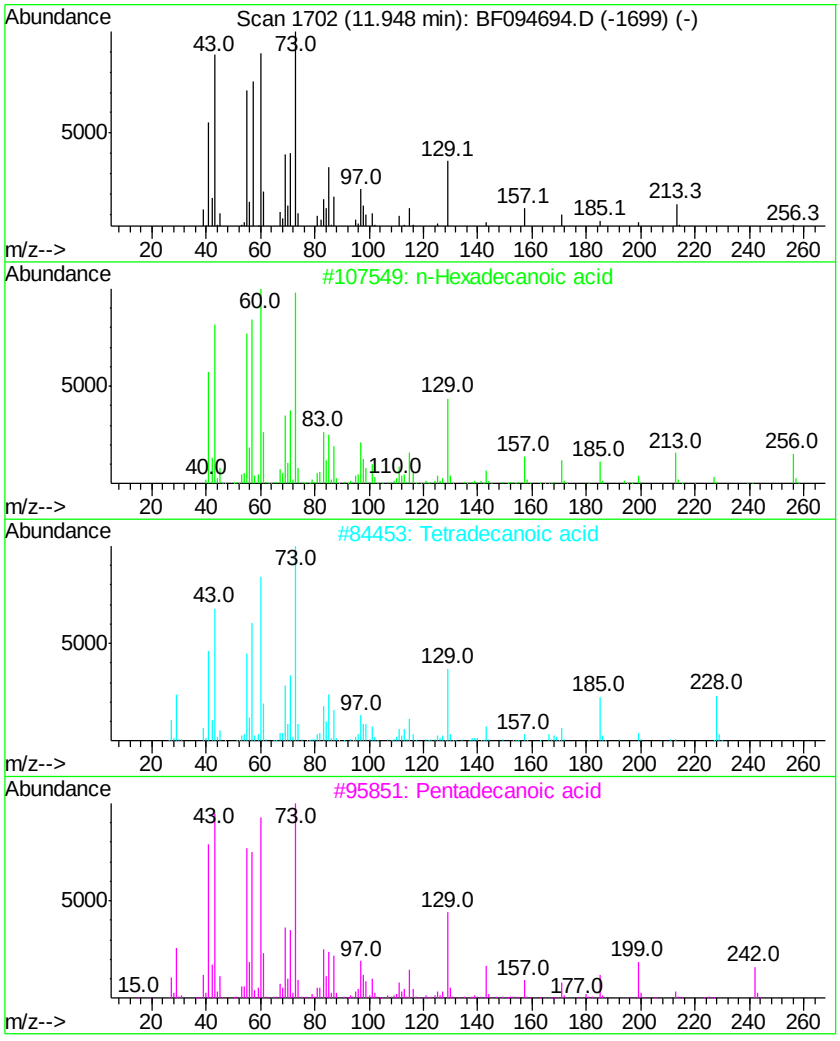
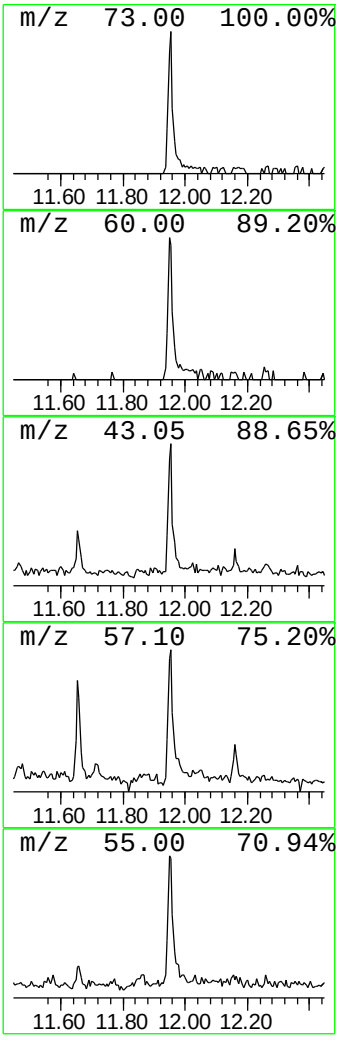
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.33 ng	115301	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
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Sample : I2895-04
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Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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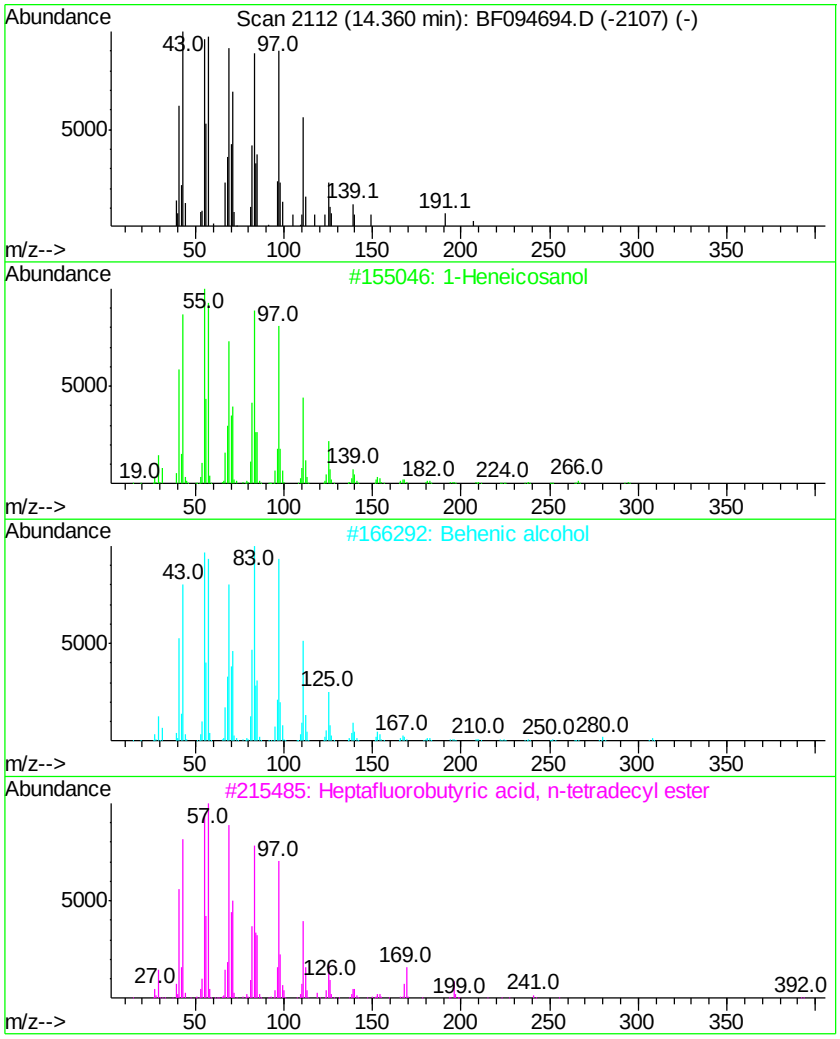
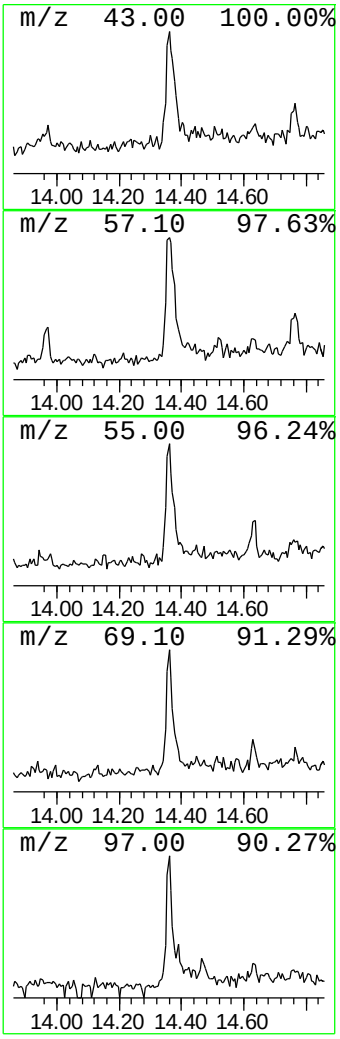
Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	3.96 ng	123369	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94





Library Search Compound Report

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Sample : I2895-04
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Instrument : BNA_F
ClientSampleId : SB-02-COMP(0-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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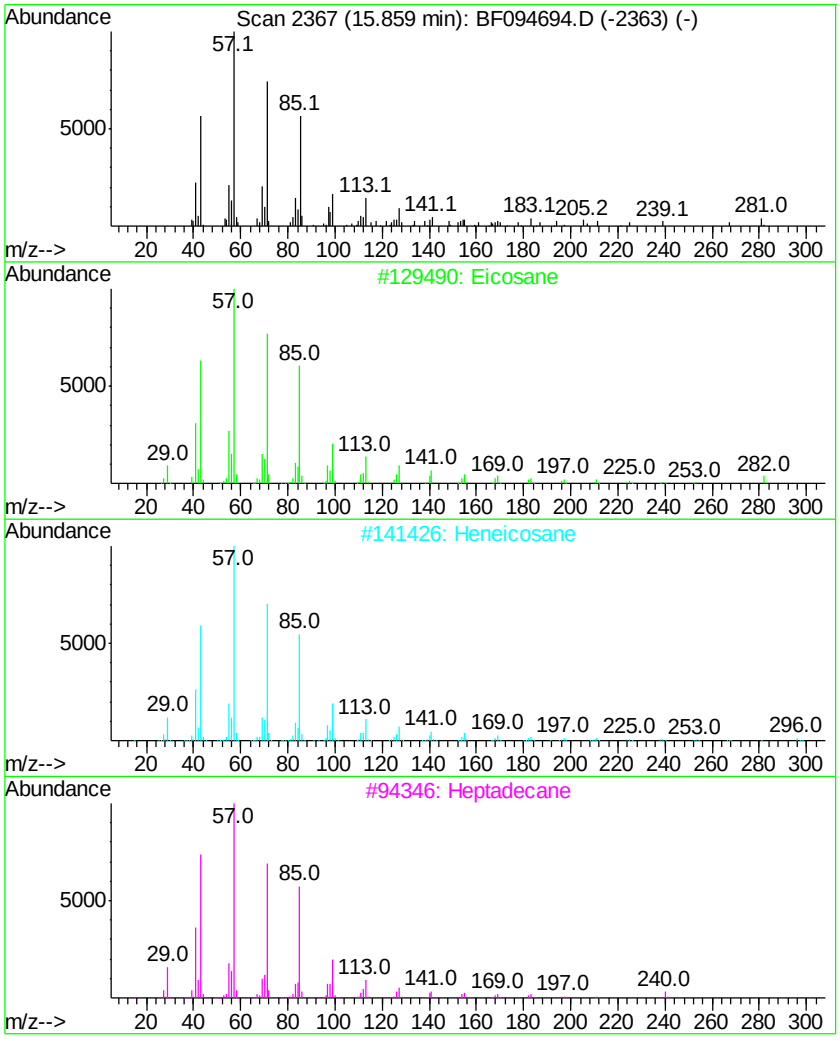
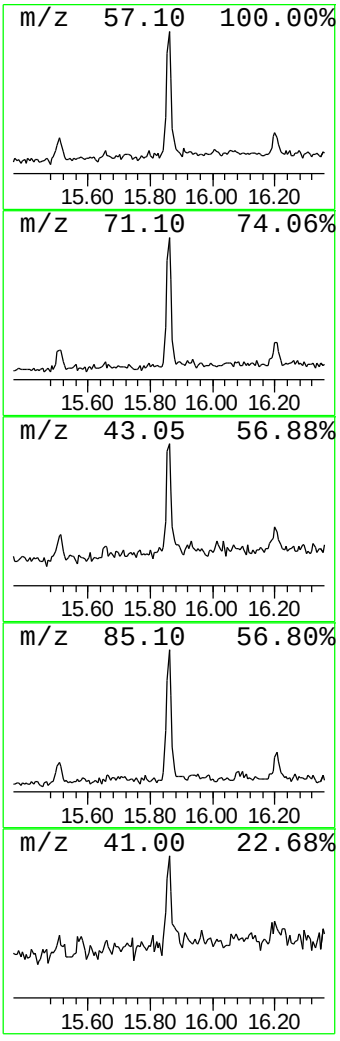
Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.84 ng	96865	Perylene-d12	16.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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

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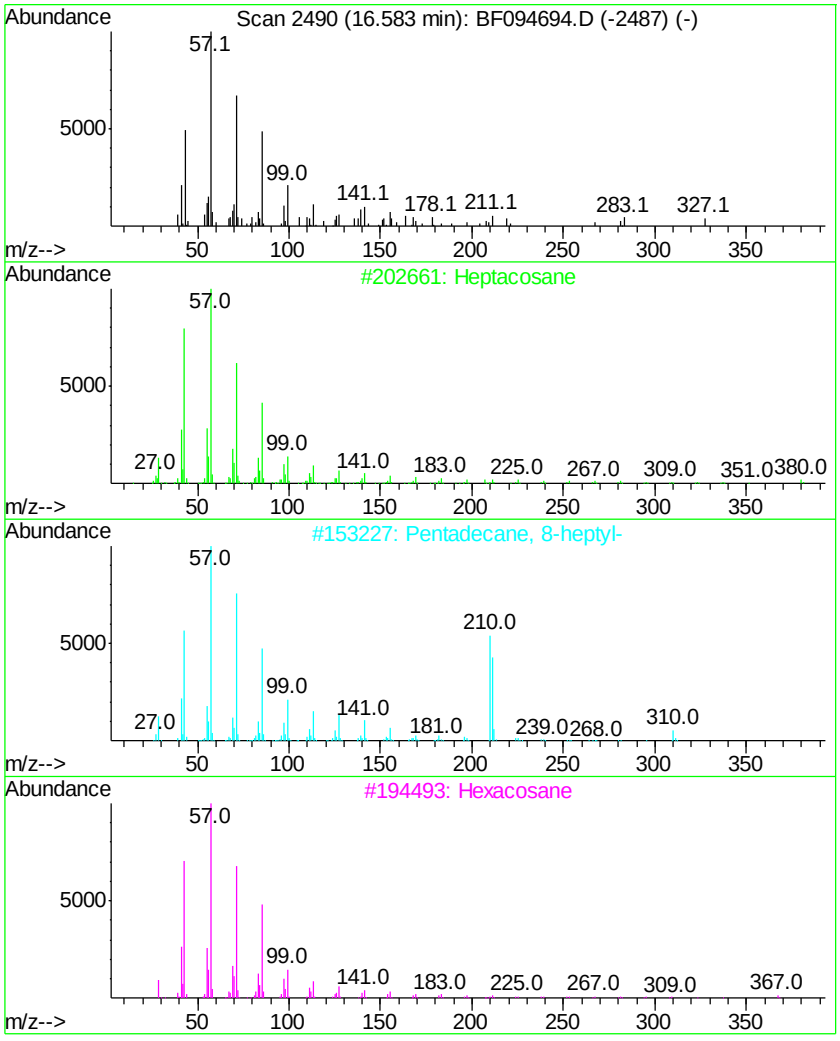
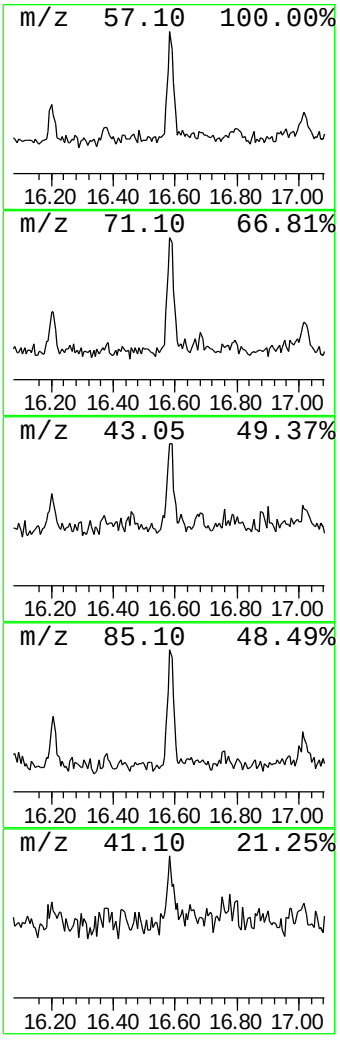
Peak Number 8 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	2.25 ng	56780	Perylene-d12	16.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	86
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	78
3	Hexacosane	366	C26H54	000630-01-3	72
4	Triacontane	422	C30H62	000638-68-6	59
5	1-Iodoundecane	282	C11H23I	004282-44-4	59





Tentatively Identified Compound (LSC) summary

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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...	3.94	18.1	ng	582626	1	5.77	642174	20.0
unknown5.52	5.52	102.7	ng	3297400	1	5.77	642174	20.0
Hexadecane	10.58	2.3	ng	79713	4	11.22	693373	20.0
n-Hexadecanoic acid	11.95	3.3	ng	115301	4	11.22	693373	20.0
1-Heneicosanol	14.36	4.0	ng	123369	5	14.47	622506	20.0
Eicosane	15.86	3.8	ng	96865	6	16.10	504676	20.0
Heptacosane	16.58	2.3	ng	56780	6	16.10	504676	20.0