LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\
Data File : BF098618.D
Acq On : 18 Sep 2017 22:49
Operator : SJ/JU
Sample : I5260-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091317-SIDI-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-BF091117.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	4.804	459	462	473	rBV	180358	230385	5.00%	0.801%
2	5.245	533	537	552	rBV	1290179	1409156	30.55%	4.896%
3	6.286	711	714	728	rBV	909767	983999	21.34%	3.419%
4	6.410	731	735	744	rVB	2929746	2568814	55.70%	8.926%
5	6.633	769	773	780	rBV	1172905	976040	21.16%	3.391%
6	6.792	795	800	803	rBV	3540896	3077629	66.73%	10.694%
7	7.210	865	871	874	rBV	2699836	2739888	59.41%	9.520%
8	7.922	988	992	995	rBV	1253848	1158054	25.11%	4.024%
9	8.998	1170	1175	1178	rBV	4929552	4611957	100.00%	16.025%
10	9.392	1239	1242	1246	rBV	135527	109755	2.38%	0.381%
11	9.669	1285	1289	1293	rBV	1431152	1176971	25.52%	4.090%
12	10.463	1419	1424	1427	rBV	1644218	1536216	33.31%	5.338%
13	10.574	1440	1443	1451	rVB	45481	47016	1.02%	0.163%
14	11.151	1537	1541	1545	rBV	1420657	1119244	24.27%	3.889%
15	12.739	1806	1811	1814	rBV	3777155	3500084	75.89%	12.162%
16	13.627	1958	1962	1967	rBV	71514	96514	2.09%	0.335%
17	13.786	1985	1989	1995	rVB	1089462	959589	20.81%	3.334%
18	14.545	2116	2118	2121	rVB	54940	49457	1.07%	0.172%
19	14.851	2167	2170	2174	rBV	98632	104529	2.27%	0.363%
20	15.186	2222	2227	2236	rBV2	786981	1065067	23.09%	3.701%
21	15.580	2290	2294	2300	rVB	170475	231817	5.03%	0.806%
22	16.027	2364	2370	2377	rBV	179191	298832	6.48%	1.038%
23	16.545	2452	2458	2466	rBV	129611	265663	5.76%	0.923%
24	17.156	2557	2562	2574	rVB3	110981	265285	5.75%	0.922%
25	17.886	2679	2686	2697	rBV3	66293	197095	4.27%	0.685%

Sum of corrected areas: 28779056

LSC Report - Integrated Chromatogram

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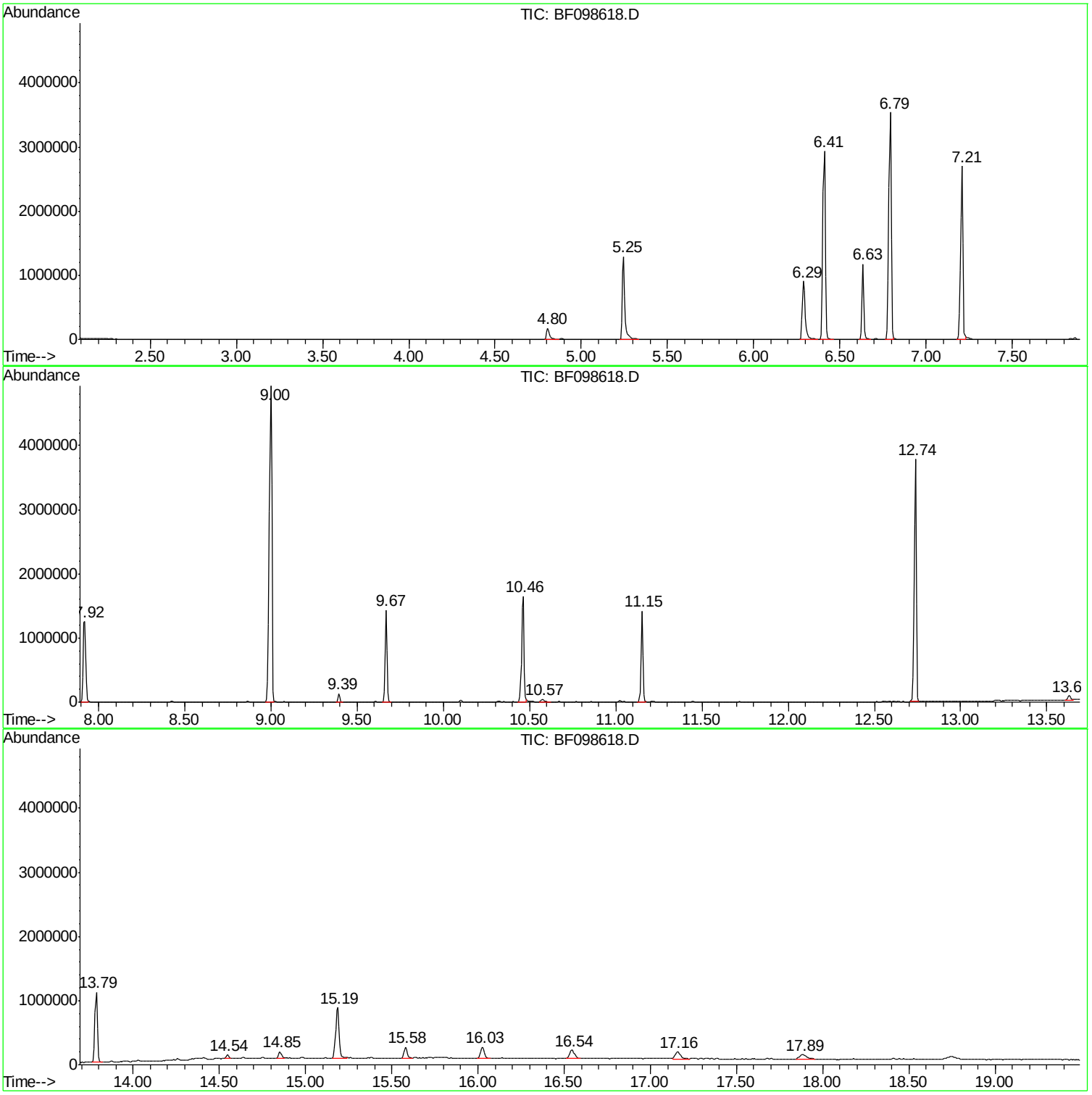
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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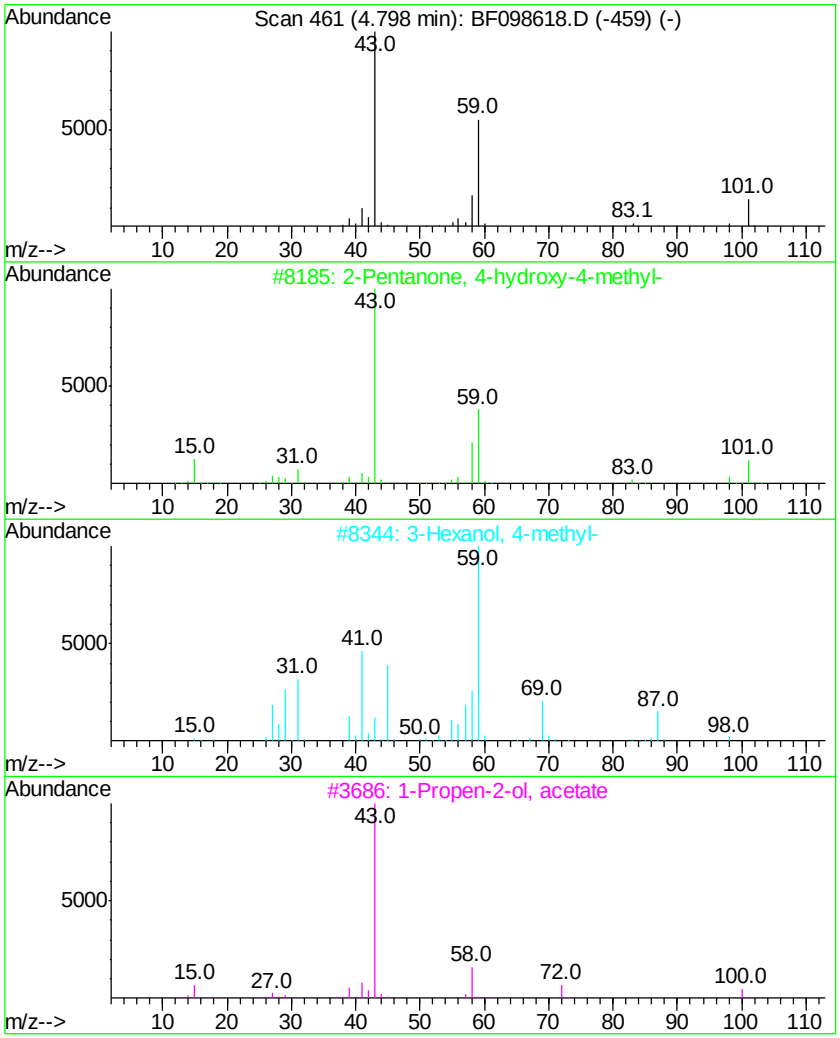
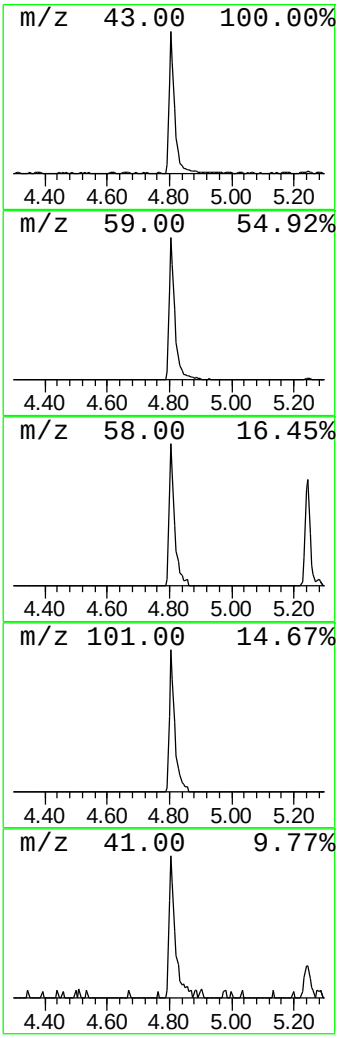
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	4.72 ng	230385	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Library Search Compound Report

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Operator : SJ/JU
Sample : I5260-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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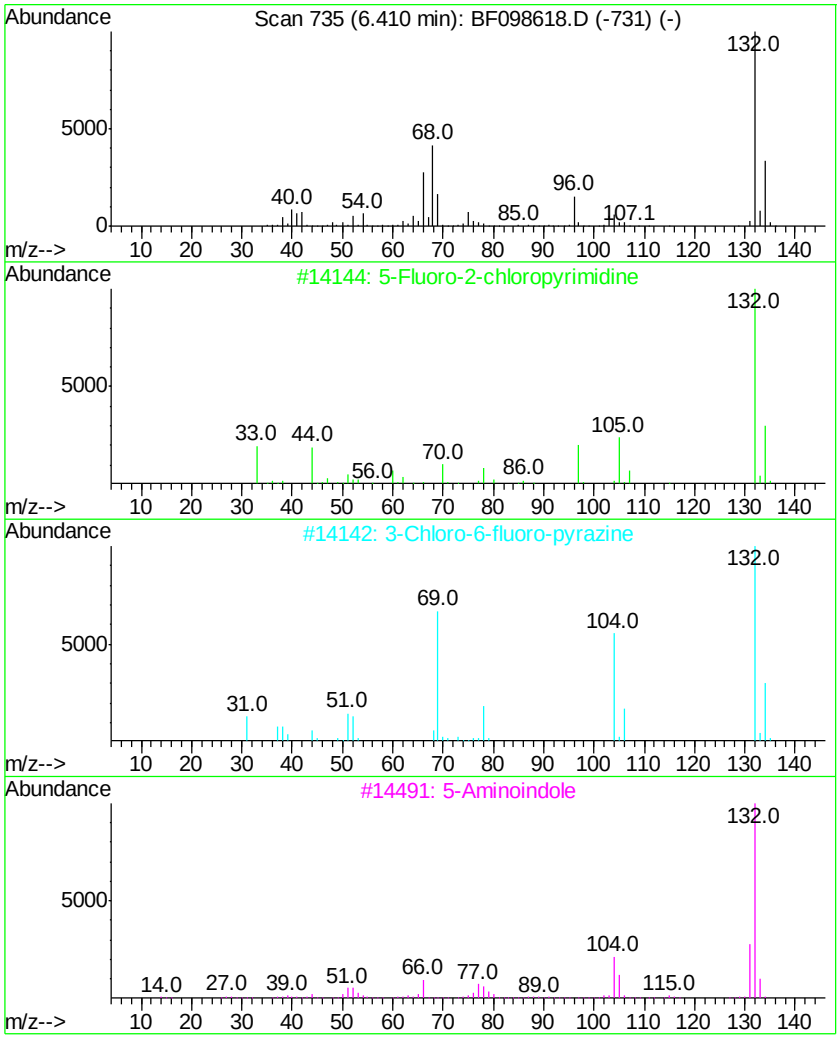
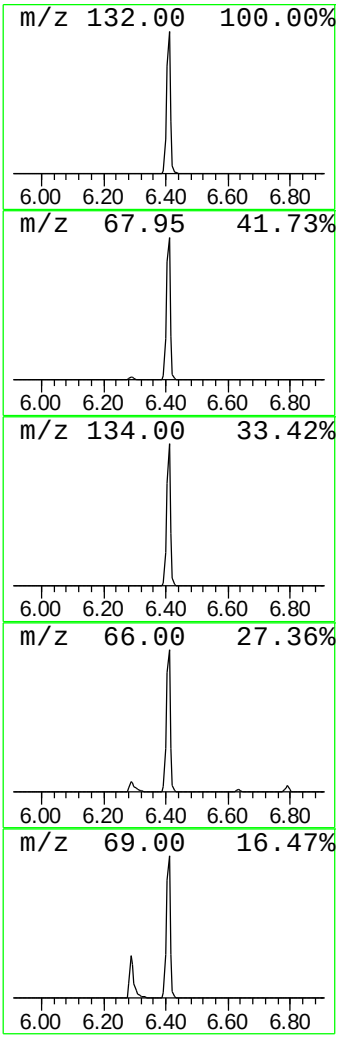
Peak Number 2 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	52.64 ng	2568810	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\
Data File : BF098618.D
Acq On : 18 Sep 2017 22:49
Operator : SJ/JU
Sample : I5260-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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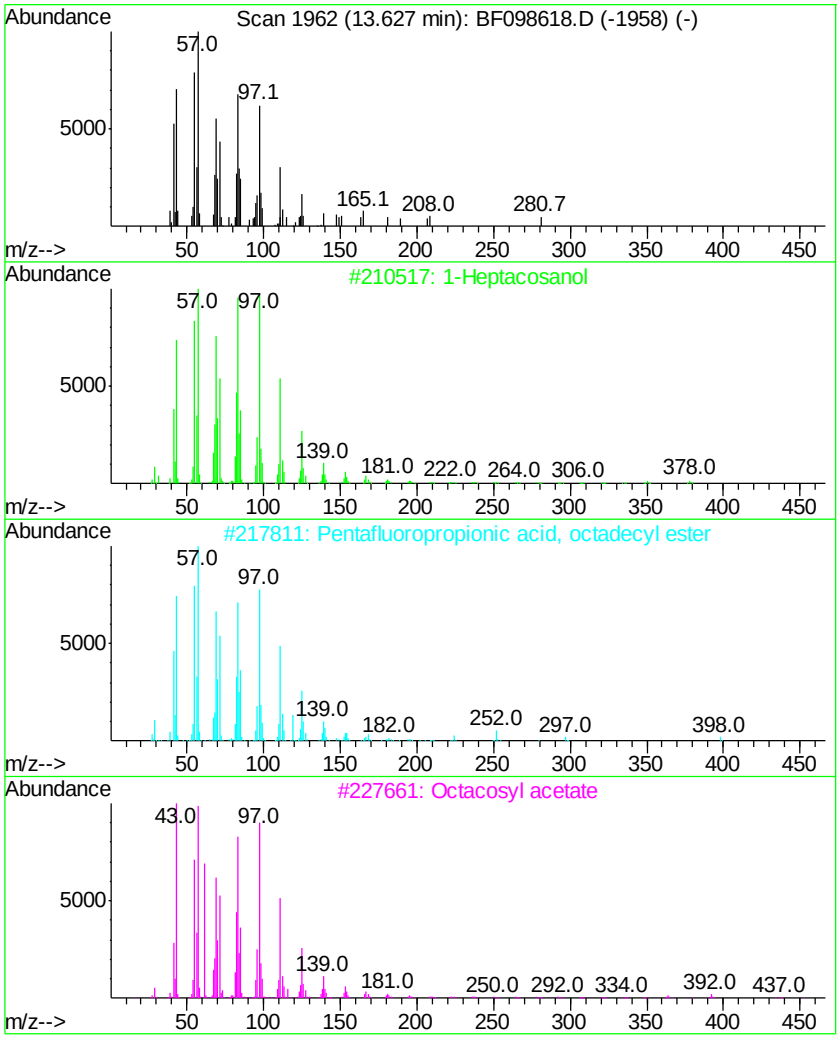
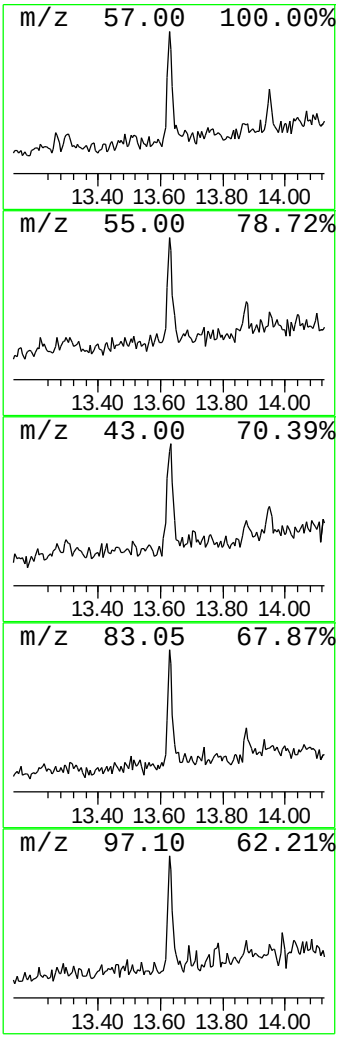
Peak Number 4 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.01 ng	96514	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	90
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
3	Octacosyl acetate	452	C30H60O2	018206-97-8	90
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
5	Triacontyl acetate	480	C32H64O2	041755-58-2	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\
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Acq On : 18 Sep 2017 22:49
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Sample : I5260-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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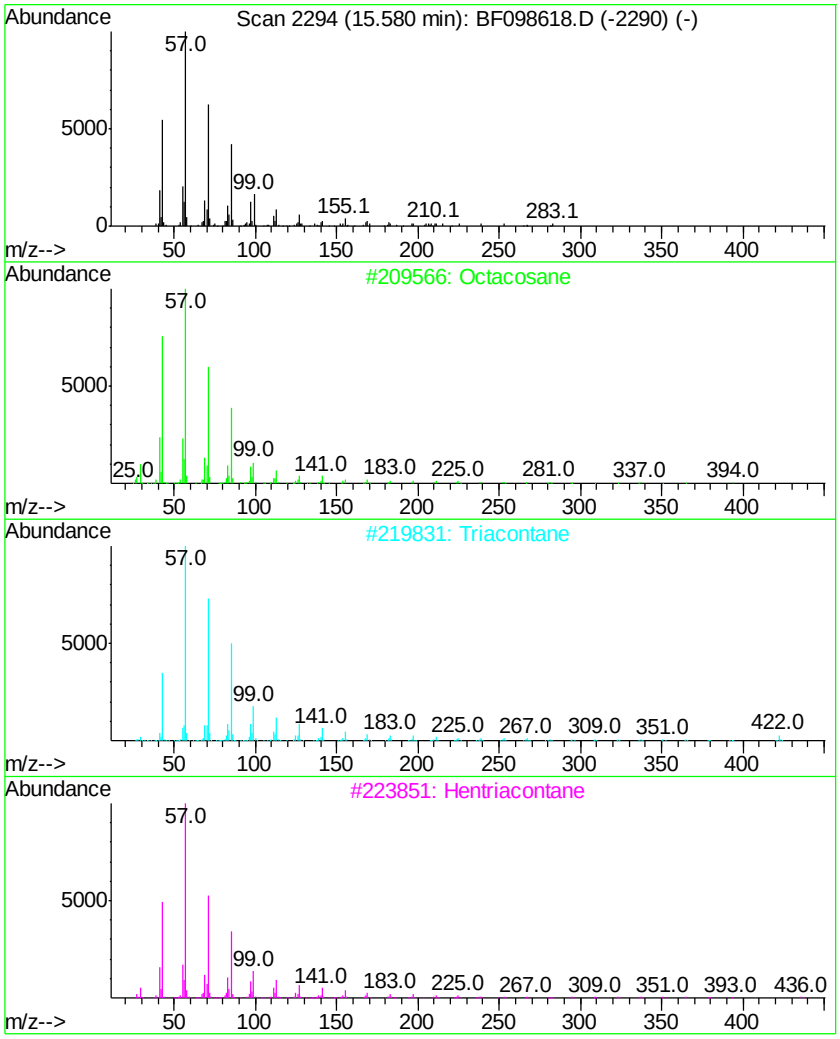
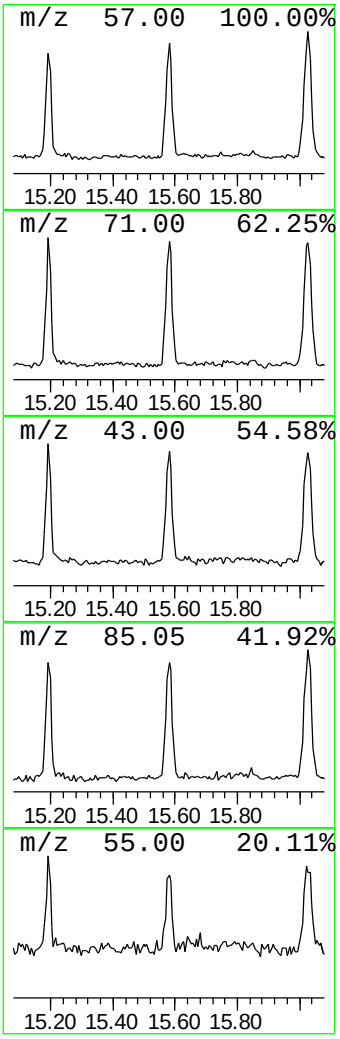
Peak Number 5 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	4.35 ng	231817	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Triacontane	422	C30H62	000638-68-6	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Heptacosane	380	C27H56	000593-49-7	83





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Sample : I5260-01
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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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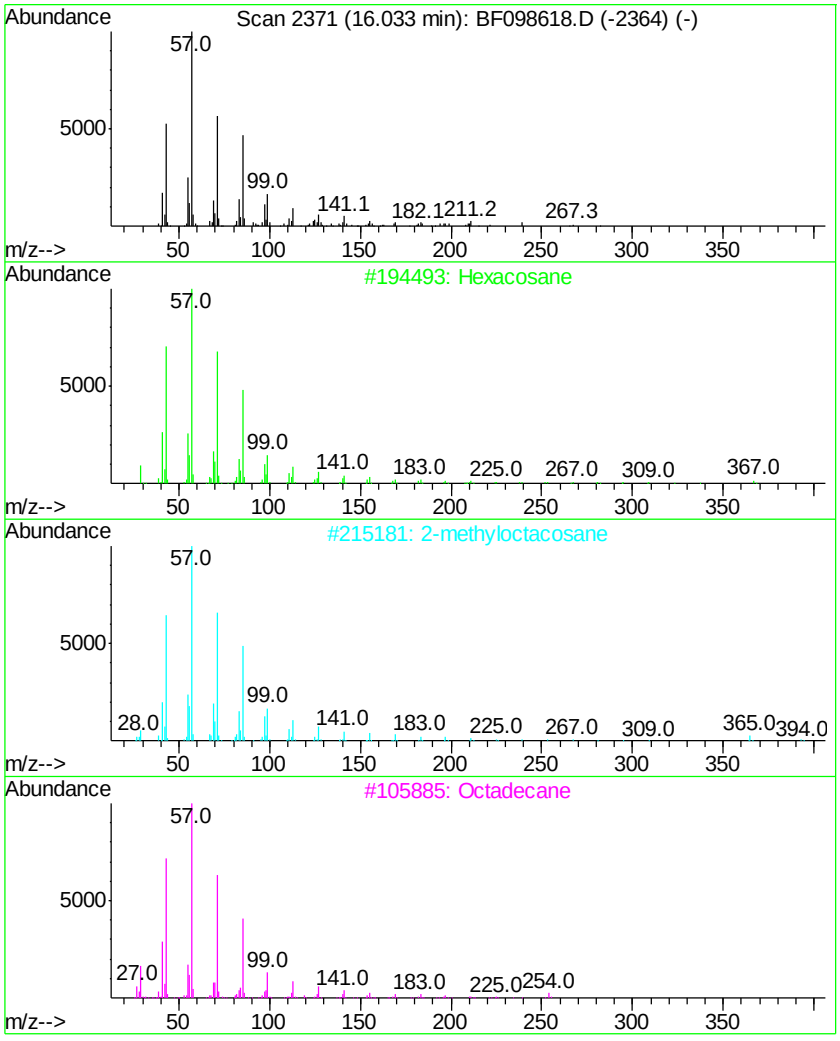
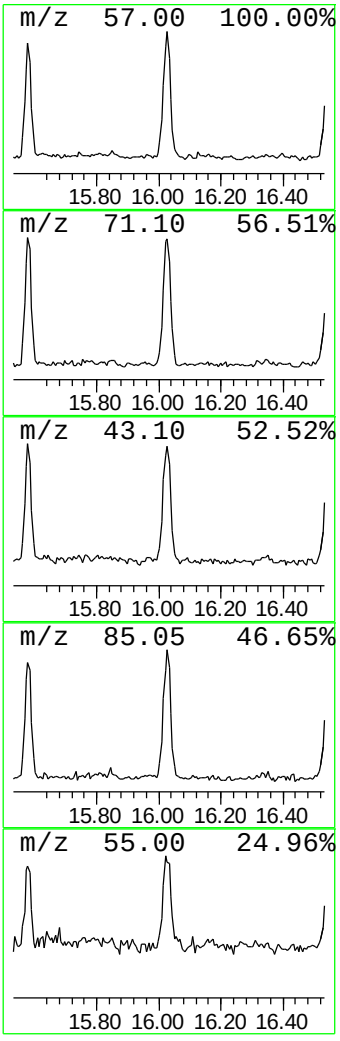
Peak Number 6 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	5.61 ng	298832	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Docosane	310	C22H46	000629-97-0	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86





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Instrument : BNA_F
ClientSampleId : 091317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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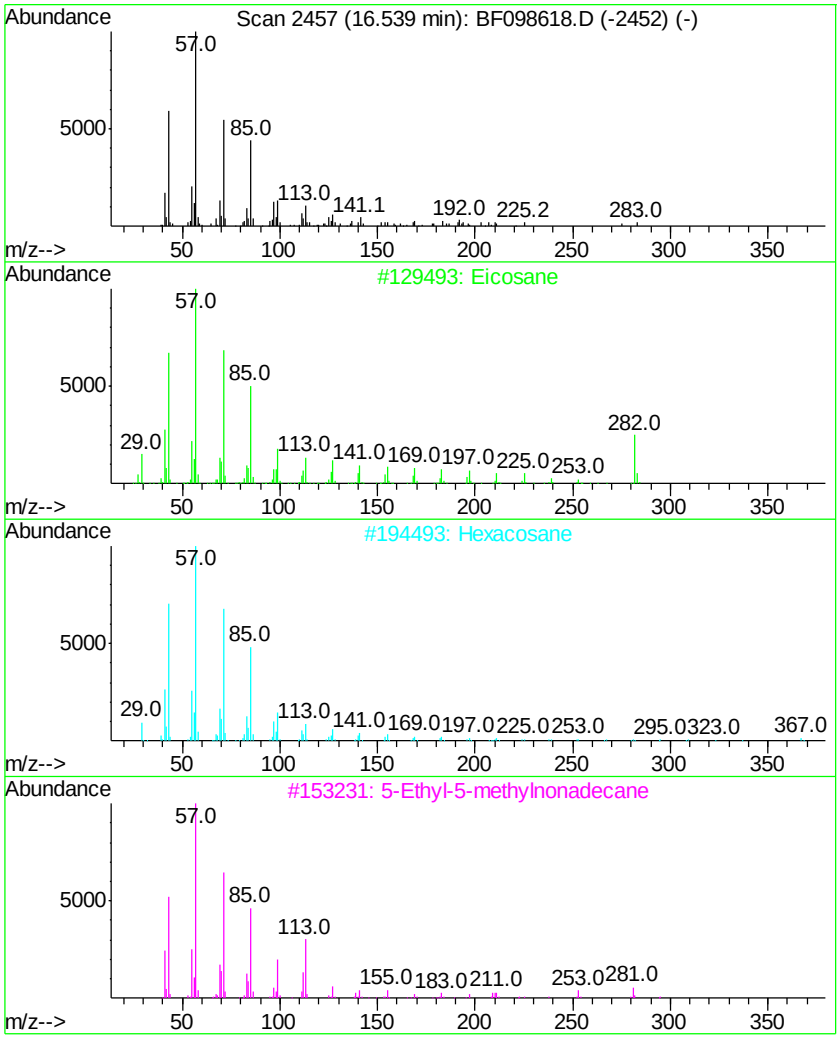
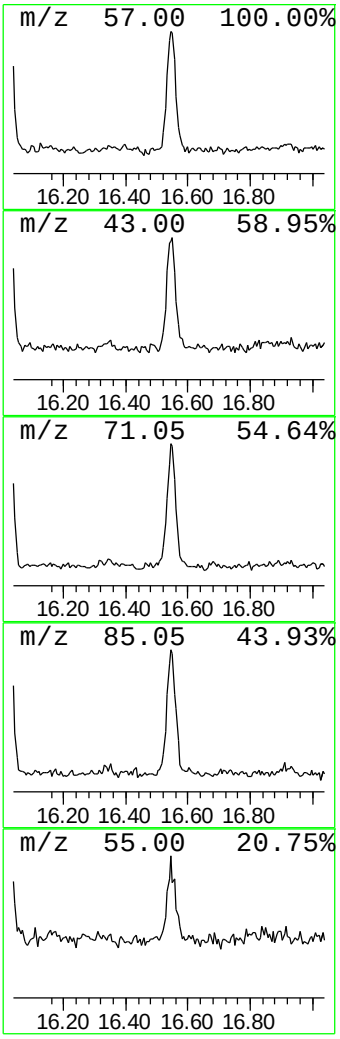
Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	4.99 ng	265663	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Octacosane	394	C28H58	000630-02-4	86





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

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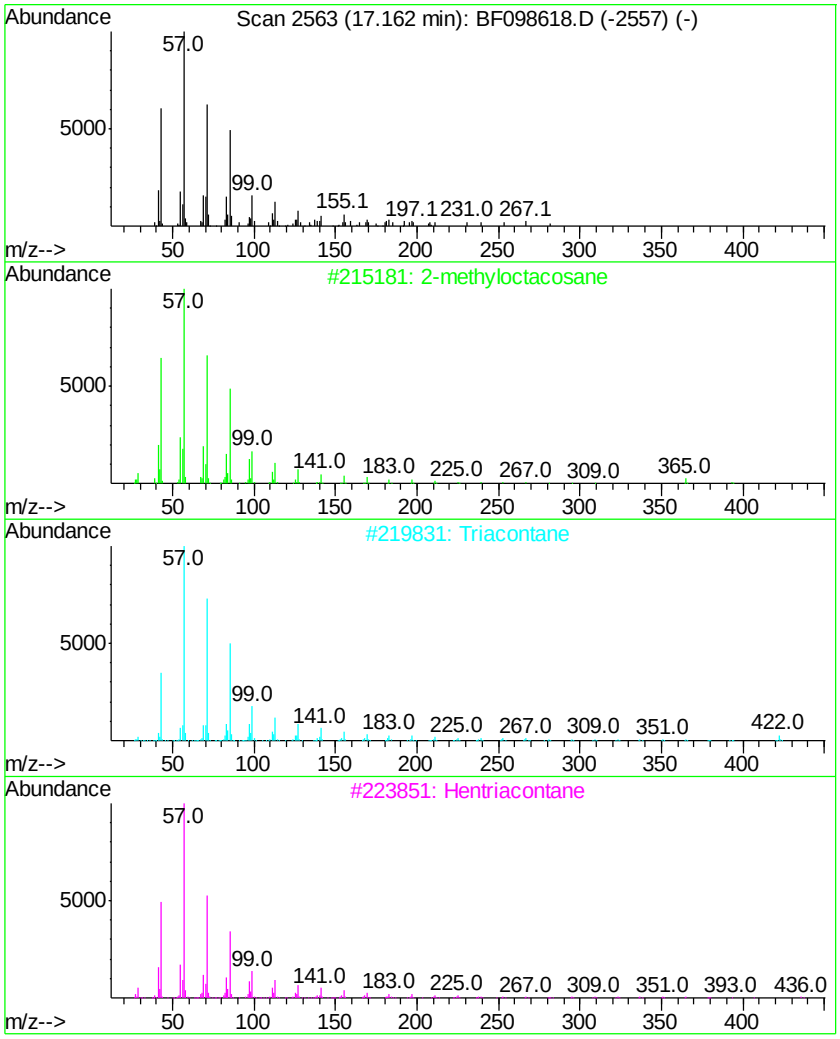
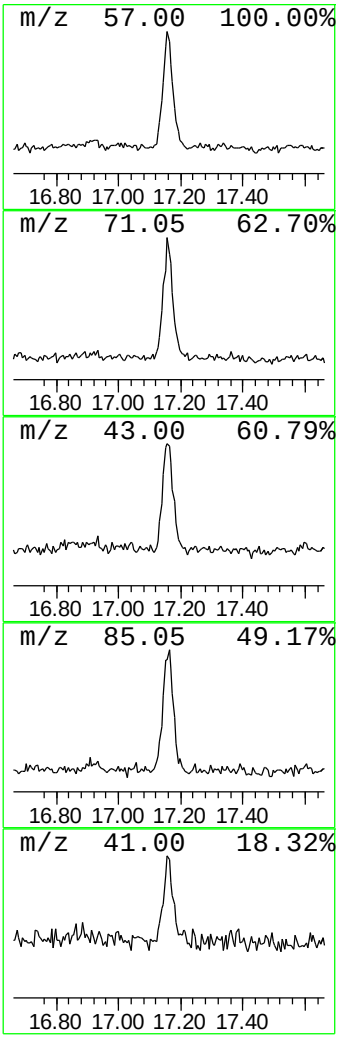
Peak Number 8 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	4.98 ng	265285	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	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...	4.80	4.7	ng	230385	1	6.63	976040	20.0
unknown6.41	6.41	52.6	ng	2568810	1	6.63	976040	20.0
1-Heptacosanol	13.63	2.0	ng	96514	5	13.79	959589	20.0
Octacosane	15.58	4.3	ng	231817	6	15.18	1065070	20.0
Hexacosane	16.03	5.6	ng	298832	6	15.18	1065070	20.0
Eicosane	16.54	5.0	ng	265663	6	15.18	1065070	20.0
2-methyloctacosane	17.16	5.0	ng	265285	6	15.18	1065070	20.0