LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
Data File : BM019163.D
Acq On : 14 Mar 2019 11:25
Operator : JU/SJ
Sample : K1824-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-24

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.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	4.816	307	311	325	rVB	107664	169785	1.04%	0.200%
2	5.257	379	386	401	rBV	4220593	6088738	37.45%	7.166%
3	6.840	647	655	671	rBV	4512571	7427811	45.69%	8.742%
4	7.193	707	715	736	rBV	4462911	7038014	43.29%	8.283%
5	7.657	787	794	802	rBV	777897	1239613	7.62%	1.459%
6	7.969	839	847	864	rBV	3003423	4810756	29.59%	5.662%
7	8.828	983	993	1013	rBV	2343137	4070001	25.03%	4.790%
8	10.439	1260	1267	1281	rBV	992067	1754999	10.80%	2.066%
9	12.922	1682	1689	1709	rBV	6879391	10187569	62.66%	11.990%
10	13.775	1824	1834	1848	rBV	483525	798990	4.91%	0.940%
11	14.310	1918	1925	1936	rBV2	1772229	2719042	16.73%	3.200%
12	15.810	2169	2180	2199	rBV	6721211	9364933	57.60%	11.022%
13	17.063	2387	2393	2411	rBV2	2366605	3508329	21.58%	4.129%
14	17.957	2539	2545	2558	rBV	209669	406208	2.50%	0.478%
15	19.704	2836	2842	2854	rBV	13178177	16257260	100.00%	19.134%
16	20.962	3052	3056	3067	rBV	595001	841333	5.18%	0.990%
17	21.262	3102	3107	3118	rBV	2910788	3801946	23.39%	4.475%
18	21.827	3200	3203	3207	rBV	150649	192020	1.18%	0.226%
19	22.286	3277	3281	3287	rBV	211312	281508	1.73%	0.331%
20	22.786	3363	3366	3372	rVB	240343	320219	1.97%	0.377%
21	23.350	3458	3462	3468	rVB	218676	334900	2.06%	0.394%
22	23.497	3481	3487	3499	rVB	1559915	3035497	18.67%	3.573%
23	23.992	3567	3571	3577	rVB	181307	316259	1.95%	0.372%

Sum of corrected areas: 84965730

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
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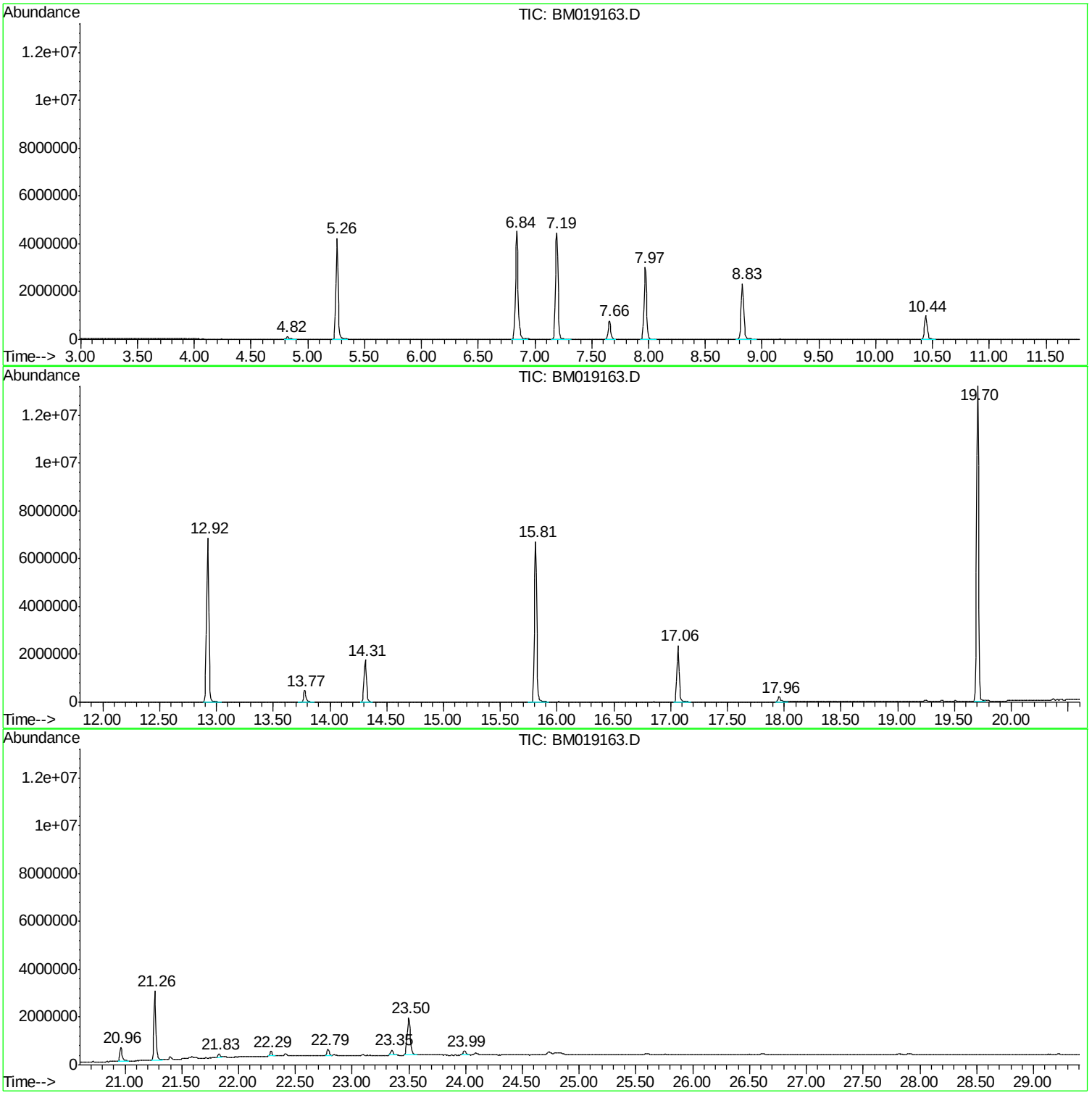
Sample : K1824-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
Data File : BM019163.D
Acq On : 14 Mar 2019 11:25
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Sample : K1824-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

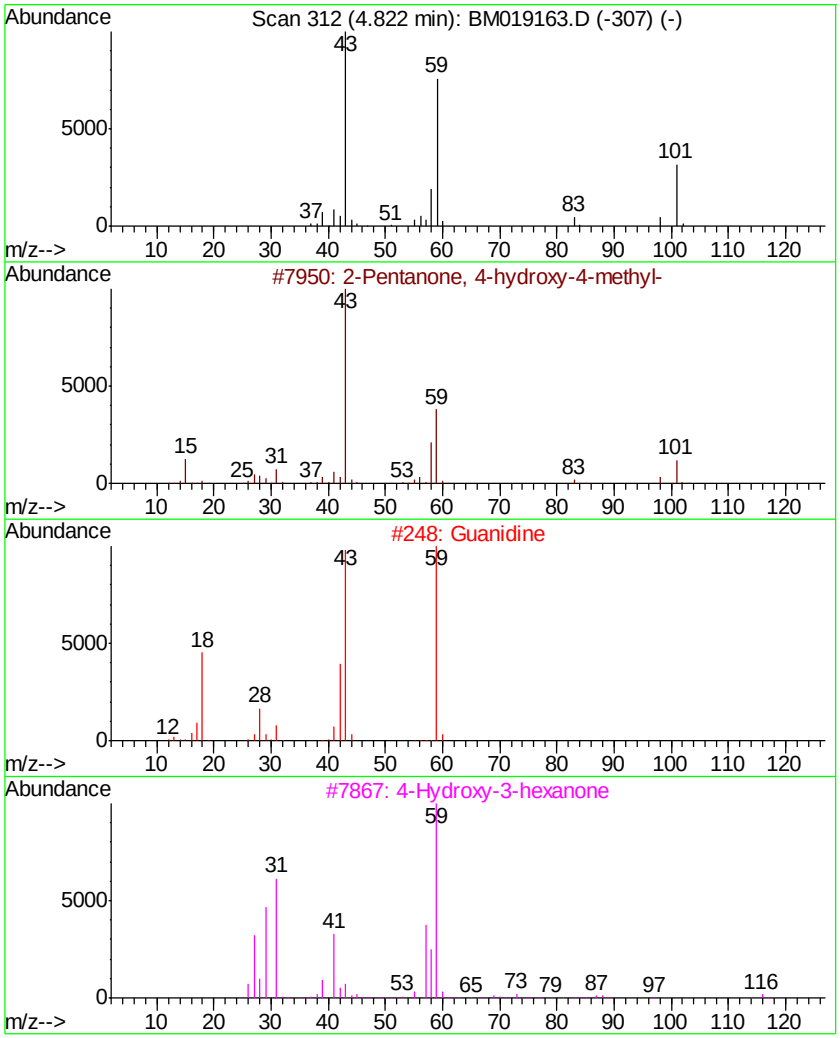
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

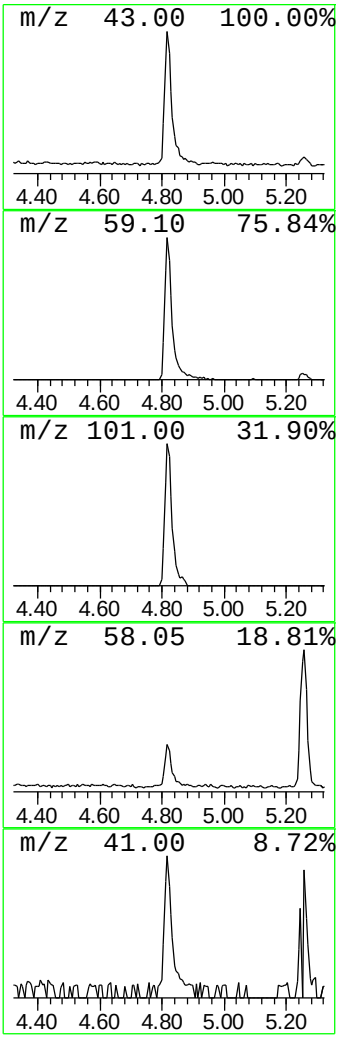
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	2.74 ng	169785	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	50
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	38
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
5	3-Hexanol	102	C6H14O	000623-37-0	33





Library Search Compound Report

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

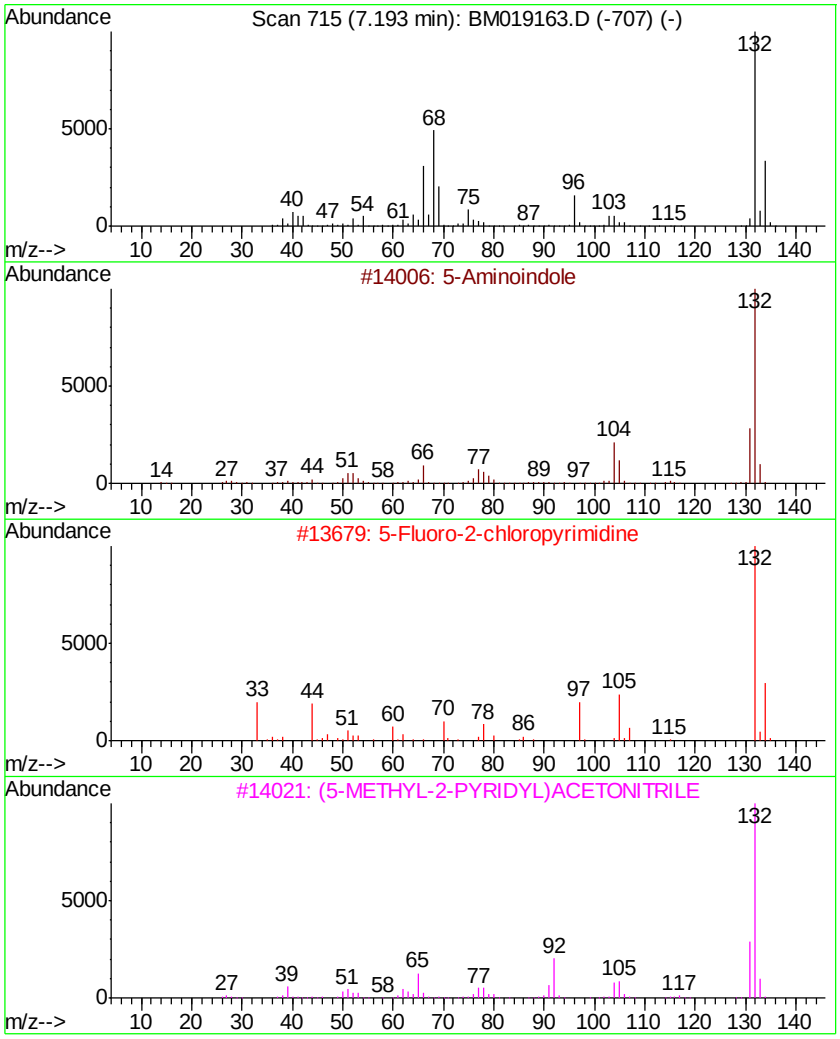
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

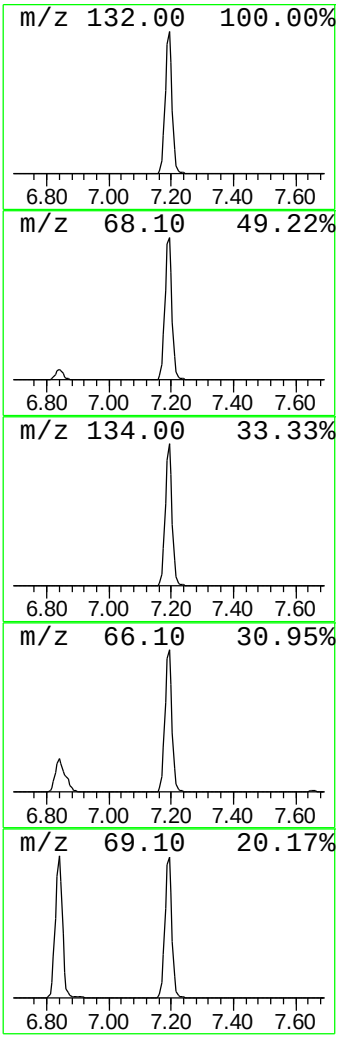
****

Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	113.55 ng	7038010	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
Data File : BM019163.D
Acq On : 14 Mar 2019 11:25
Operator : JU/SJ
Sample : K1824-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

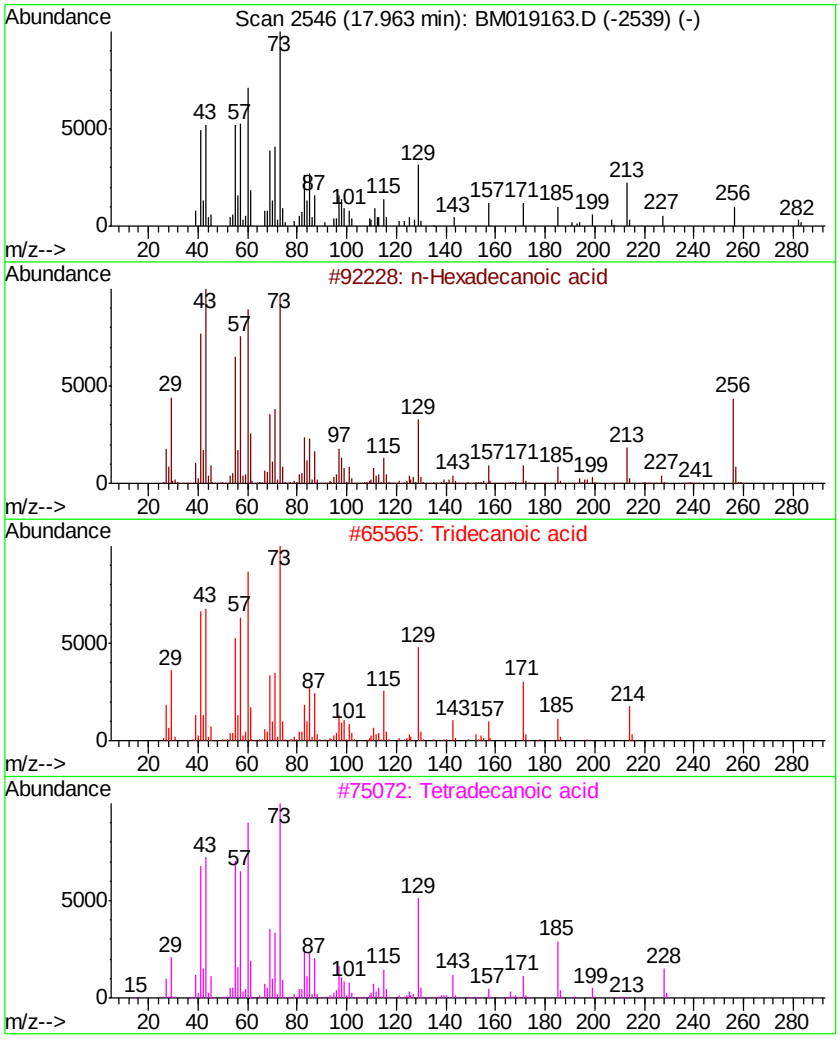
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

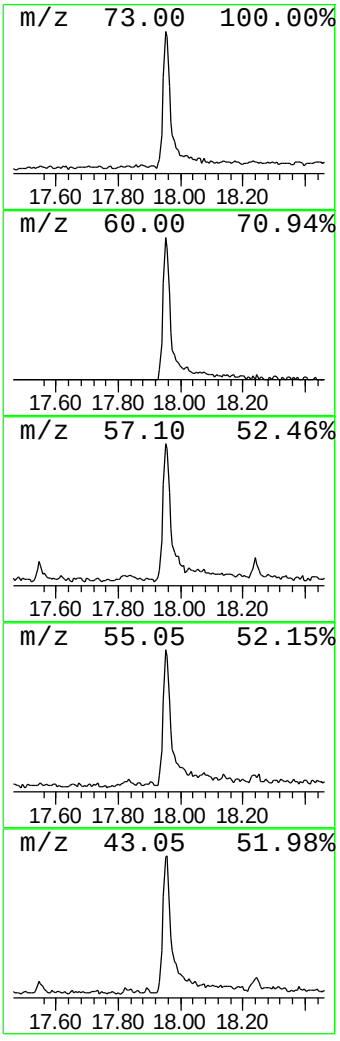
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	2.32 ng	406208	Phenanthrene-d10	17.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	49
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	45
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Library Search Compound Report

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Operator : JU/SJ
Sample : K1824-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-24

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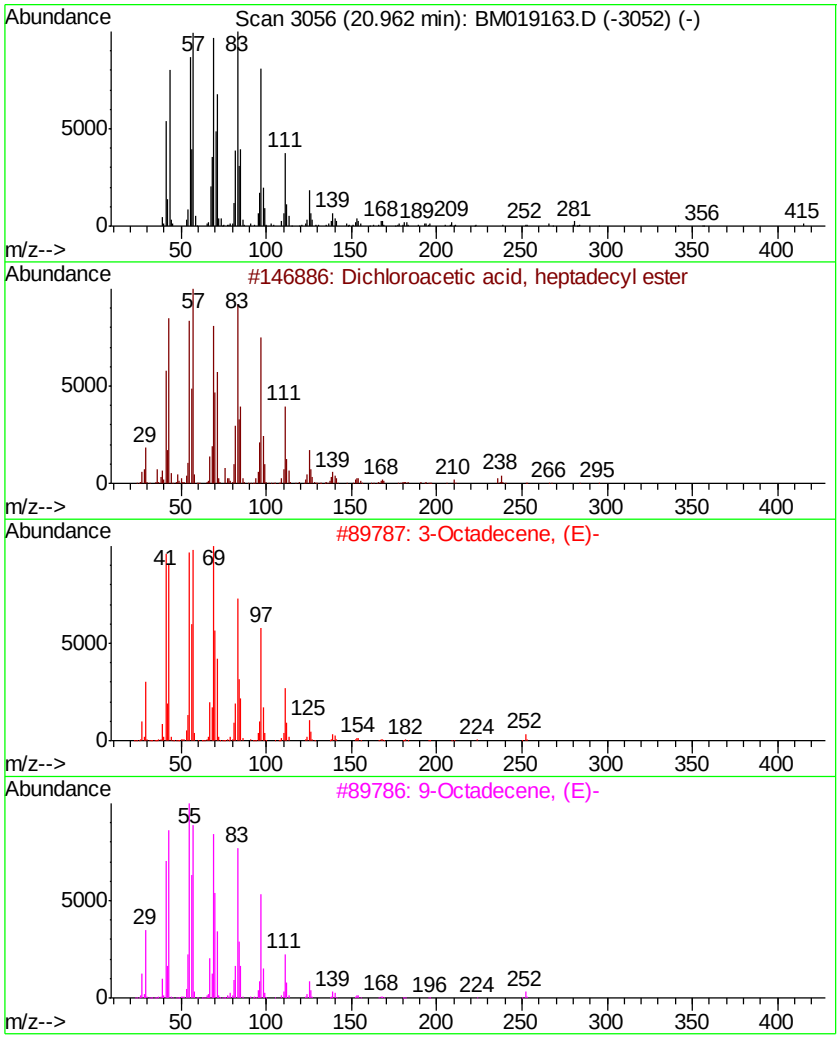
TIC Integration Parameters: LSCINT.P

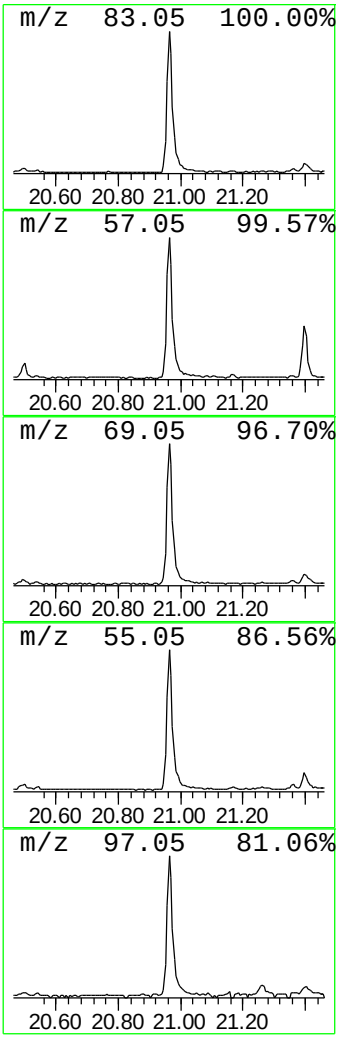
****

Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.96	4.43 ng	841333	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	3-Octadecene, (E)-	252	C18H36	007206-19-1	94
3	9-Octadecene, (E)-	252	C18H36	007206-25-9	93
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91





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Instrument : BNA_M
ClientSampleId : TP-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
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TIC Library : C:\DATABASE\NIST02.L
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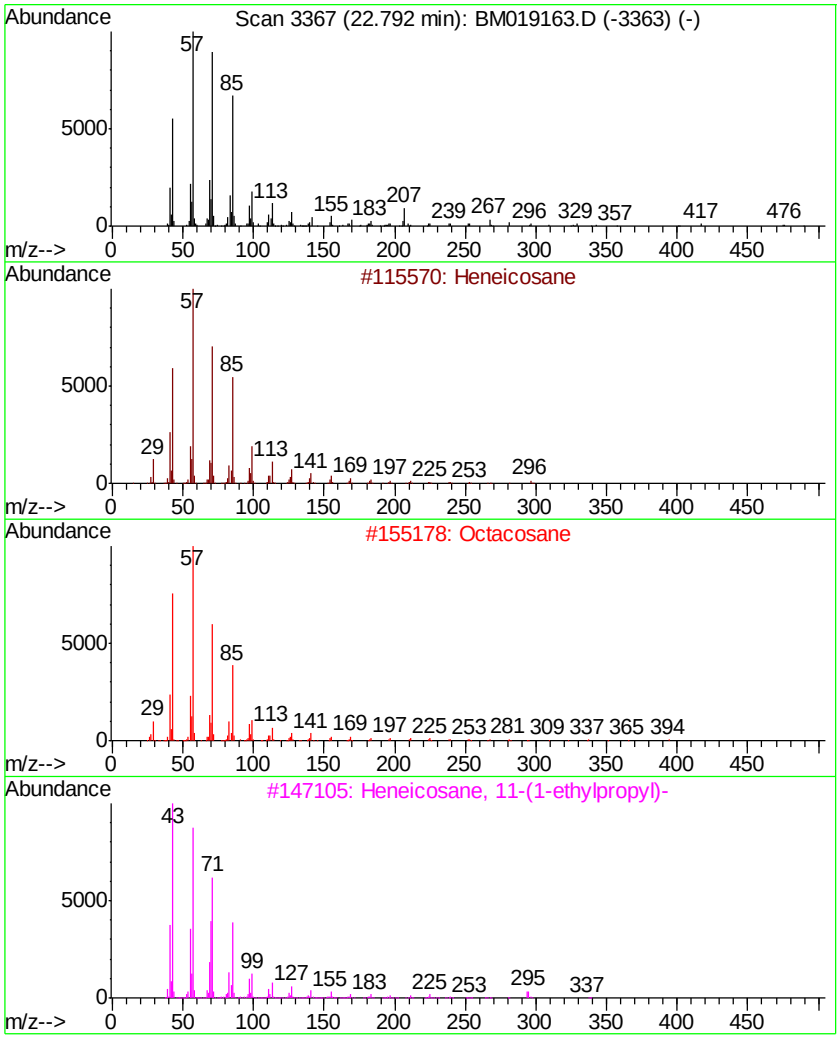
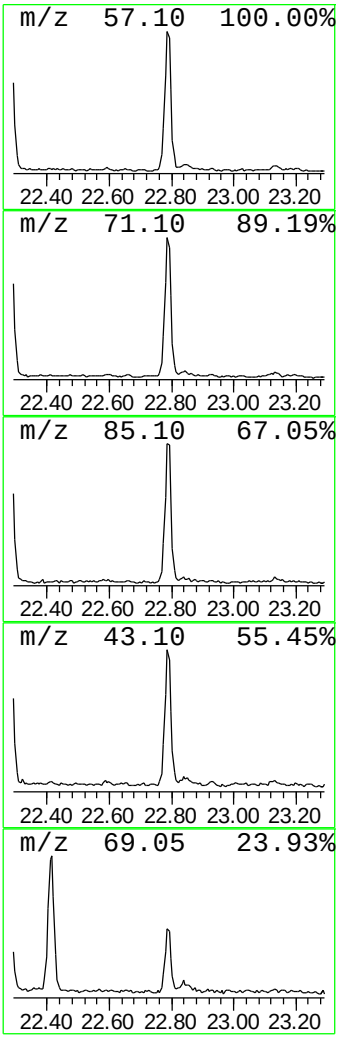
****

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.79	2.11 ng	320219	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4	Nonacosane	408	C29H60	000630-03-5	83
5	Heptadecane	240	C17H36	000629-78-7	80





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Instrument : BNA_M
ClientSampleId : TP-24

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

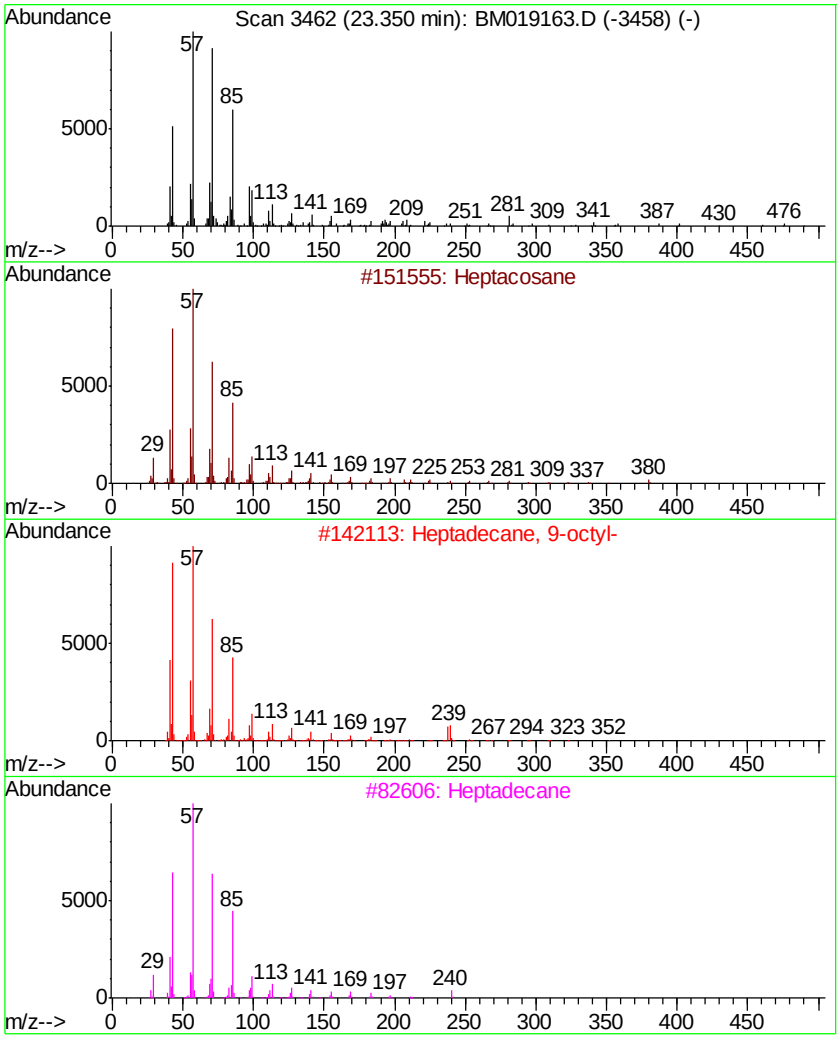
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

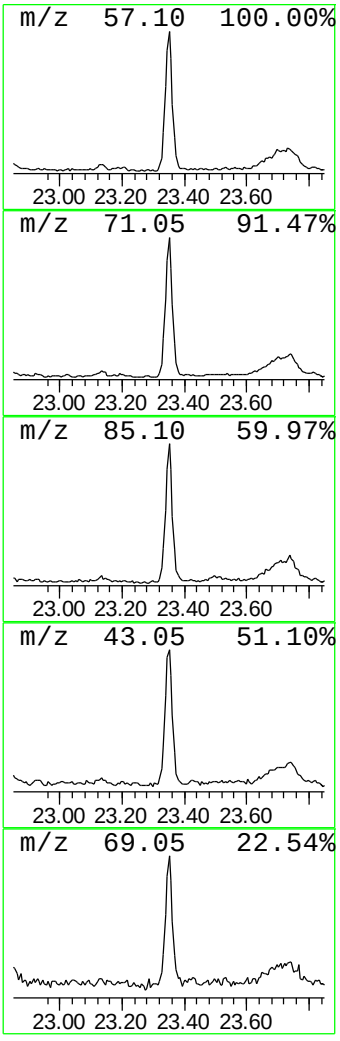
****

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	2.21 ng	334900	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
5	Hexadecane	226	C16H34	000544-76-3	80





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

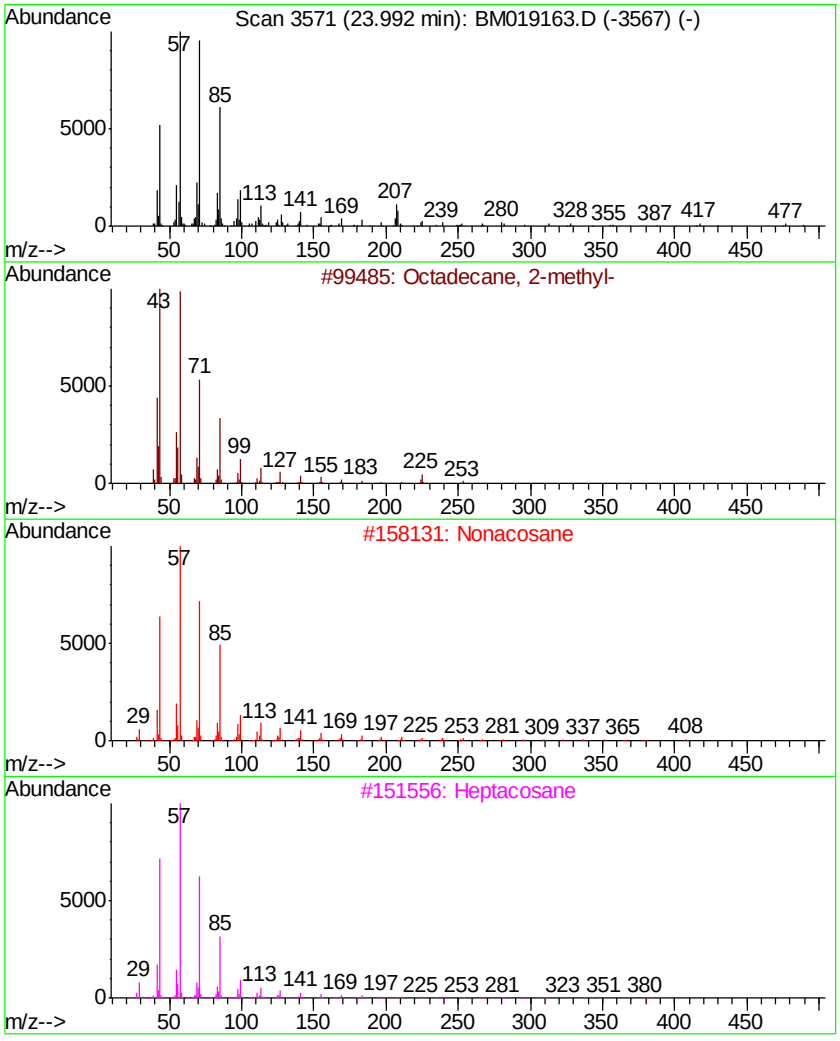
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

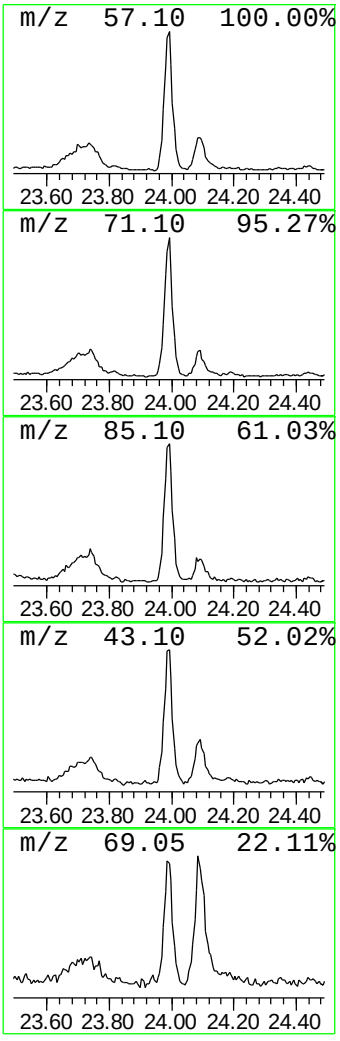
****

Peak Number 8 Octadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.08 ng	316259	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
2	Nonacosane	408	C29H60	000630-03-5	83
3	Heptacosane	380	C27H56	000593-49-7	80
4	Octadecane, 4-methyl-	268	C19H40	010544-95-3	58
5	Tetracosane	338	C24H50	000646-31-1	49





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.82	2.7	ng	169785	1	7.66	1239610	20.0
unknown7.19	7.19	113.6	ng	7038010	1	7.66	1239610	20.0
n-Hexadecanoic acid	17.96	2.3	ng	406208	4	17.06	3508330	20.0
Dichloroacetic ac...	20.96	4.4	ng	841333	5	21.26	3801950	20.0
Heneicosane	22.79	2.1	ng	320219	6	23.50	3035500	20.0
Heptacosane	23.35	2.2	ng	334900	6	23.50	3035500	20.0
Octadecane, 2-met...	23.99	2.1	ng	316259	6	23.50	3035500	20.0