LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
Data File : BM019178.D
Acq On : 14 Mar 2019 20:31
Operator : JU/SJ
Sample : K1897-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-1

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	5.258	379	386	406	rBV	4176457	6141377	36.72%	6.919%
2	6.840	647	655	675	rBV	4648179	7533834	45.04%	8.488%
3	7.193	707	715	729	rBV	4628748	7169340	42.86%	8.077%
4	7.657	787	794	803	rBV	736152	1203260	7.19%	1.356%
5	7.969	839	847	858	rBV	3050862	4792247	28.65%	5.399%
6	8.828	985	993	1010	rBV	2400602	4161556	24.88%	4.688%
7	10.440	1258	1267	1281	rBV	980049	1731522	10.35%	1.951%
8	12.922	1682	1689	1711	rBV	7193047	10401161	62.19%	11.718%
9	13.775	1829	1834	1849	rBV	402545	642292	3.84%	0.724%
10	14.310	1917	1925	1939	rBV2	1765158	2738922	16.38%	3.086%
11	15.810	2173	2180	2199	rBV	6792688	9971772	59.62%	11.234%
12	17.063	2387	2393	2409	rBV2	2443284	3523881	21.07%	3.970%
13	17.951	2539	2544	2556	rBV	269757	483716	2.89%	0.545%
14	19.704	2836	2842	2854	rBV	14455440	16725519	100.00%	18.843%
15	20.962	3051	3056	3064	rBV	1027768	1283480	7.67%	1.446%
16	21.262	3101	3107	3120	rBV	3090379	4118823	24.63%	4.640%
17	21.398	3127	3130	3136	rBV	259240	290295	1.74%	0.327%
18	21.827	3200	3203	3211	rBV2	285055	487130	2.91%	0.549%
19	22.286	3277	3281	3287	rBV	307704	386809	2.31%	0.436%
20	22.415	3300	3303	3308	rVB	190260	237524	1.42%	0.268%
21	22.786	3362	3366	3371	rBV	363420	508475	3.04%	0.573%
22	23.350	3458	3462	3467	rVB	242185	354769	2.12%	0.400%
23	23.497	3481	3487	3498	rVB	1739225	3249655	19.43%	3.661%
24	23.992	3567	3571	3577	rVB	358486	623975	3.73%	0.703%

Sum of corrected areas: 88761334

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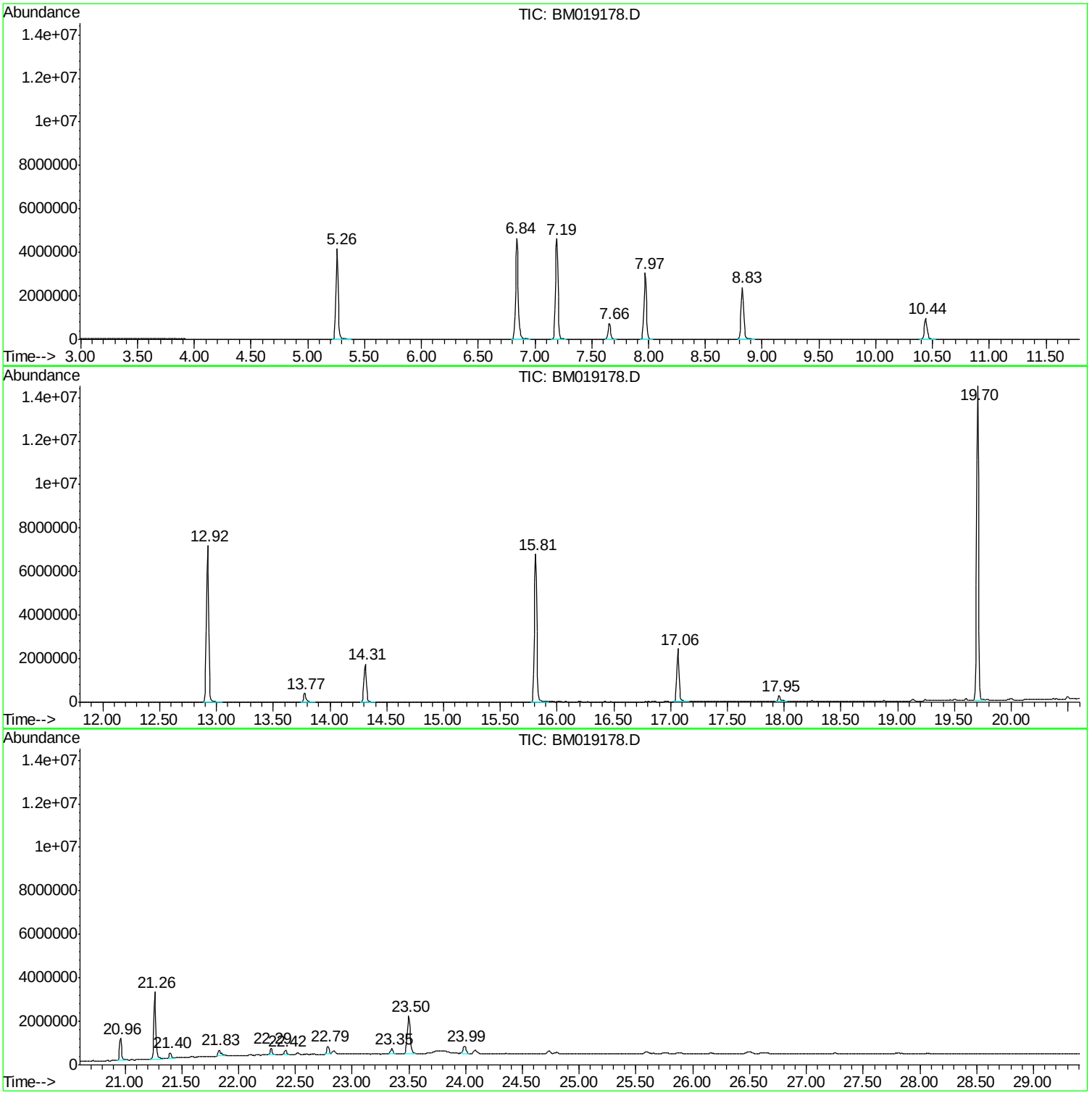
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-1

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
Data File : BM019178.D
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Operator : JU/SJ
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-1

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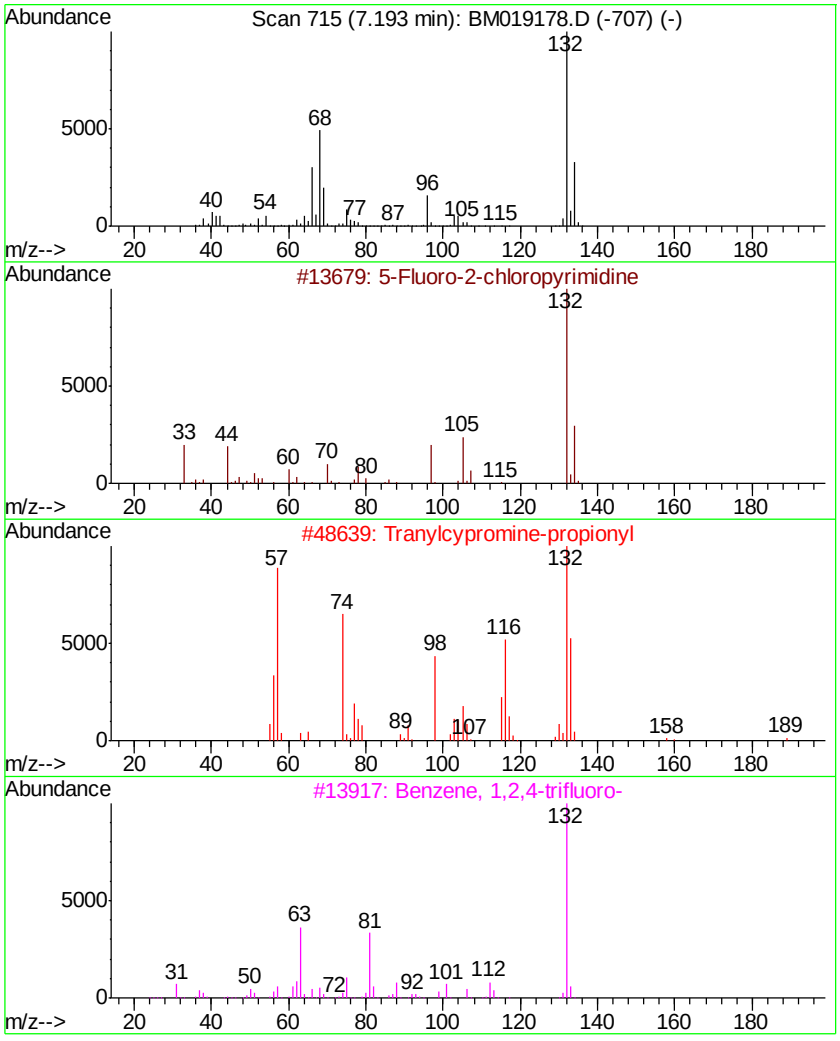
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

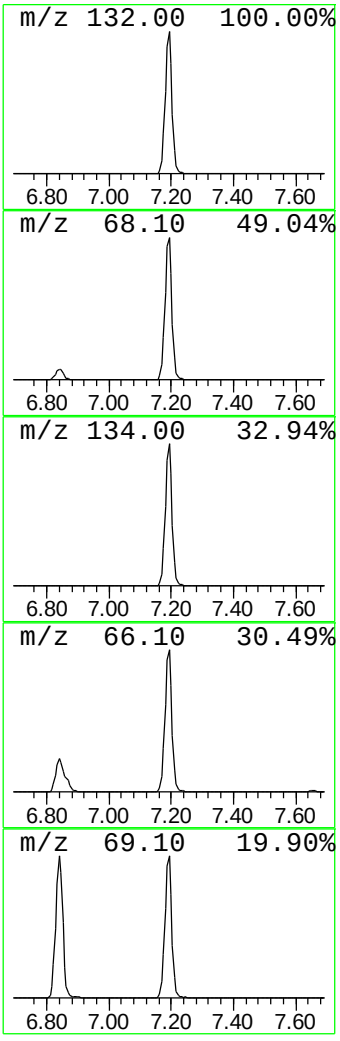
****

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	119.17 ng	7169340	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BM019178.D
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Operator : JU/SJ
Sample : K1897-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-1

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

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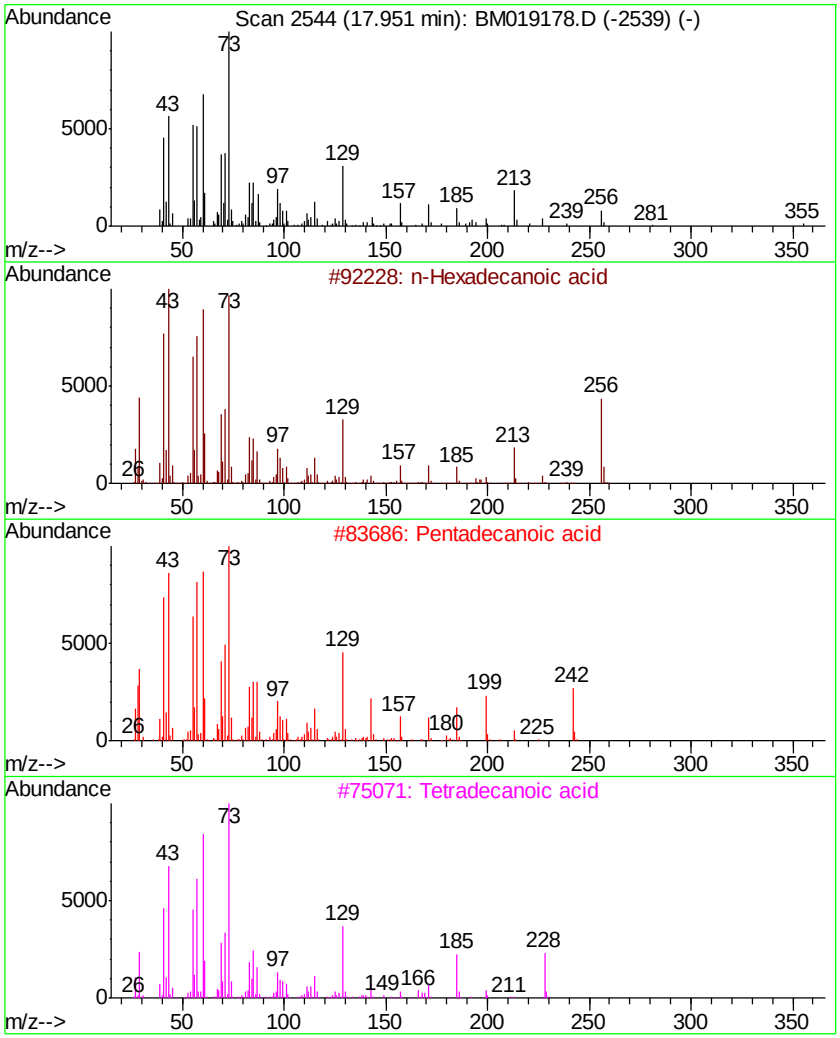
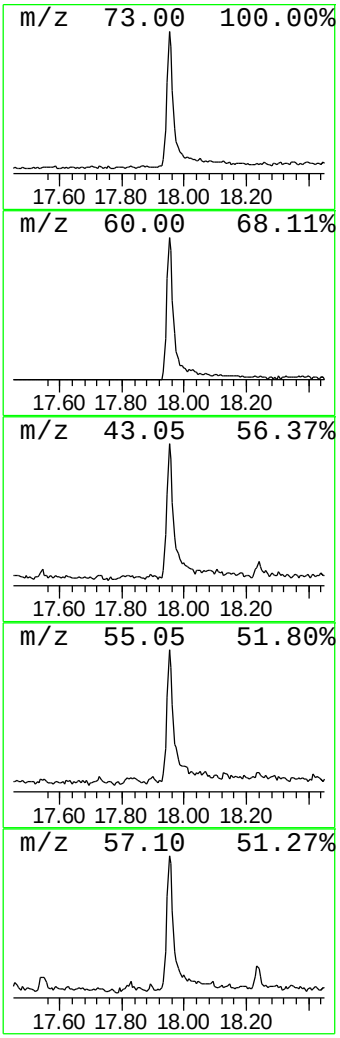
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	2.75 ng	483716	Phenanthrene-d10	17.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
Data File : BM019178.D
Acq On : 14 Mar 2019 20:31
Operator : JU/SJ
Sample : K1897-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-1

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

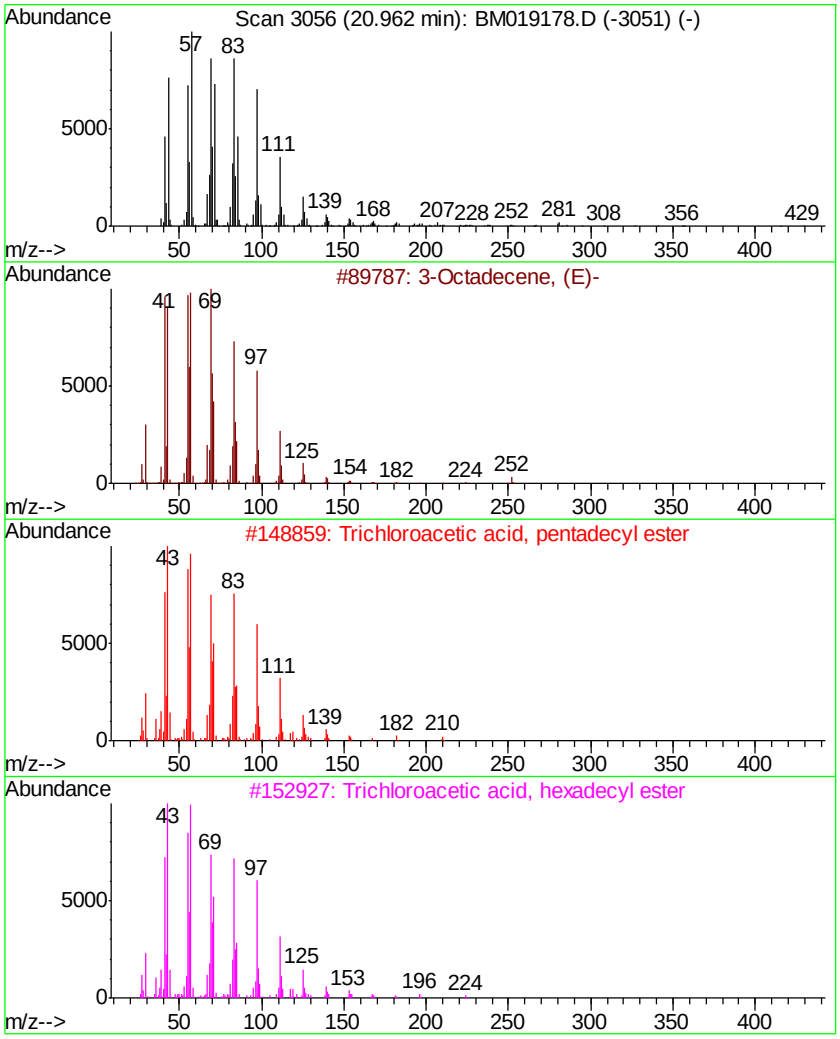
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

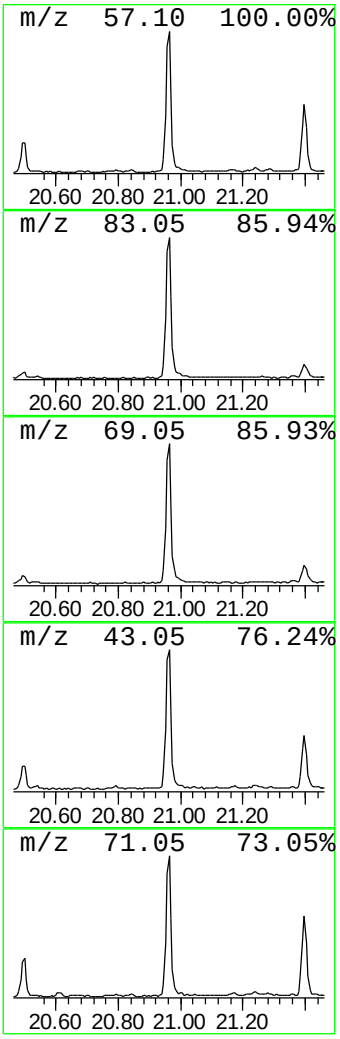
****

Peak Number 4 3-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.96	6.23 ng	1283480	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87





Library Search Compound Report

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Data File : BM019178.D
Acq On : 14 Mar 2019 20:31
Operator : JU/SJ
Sample : K1897-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-1

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

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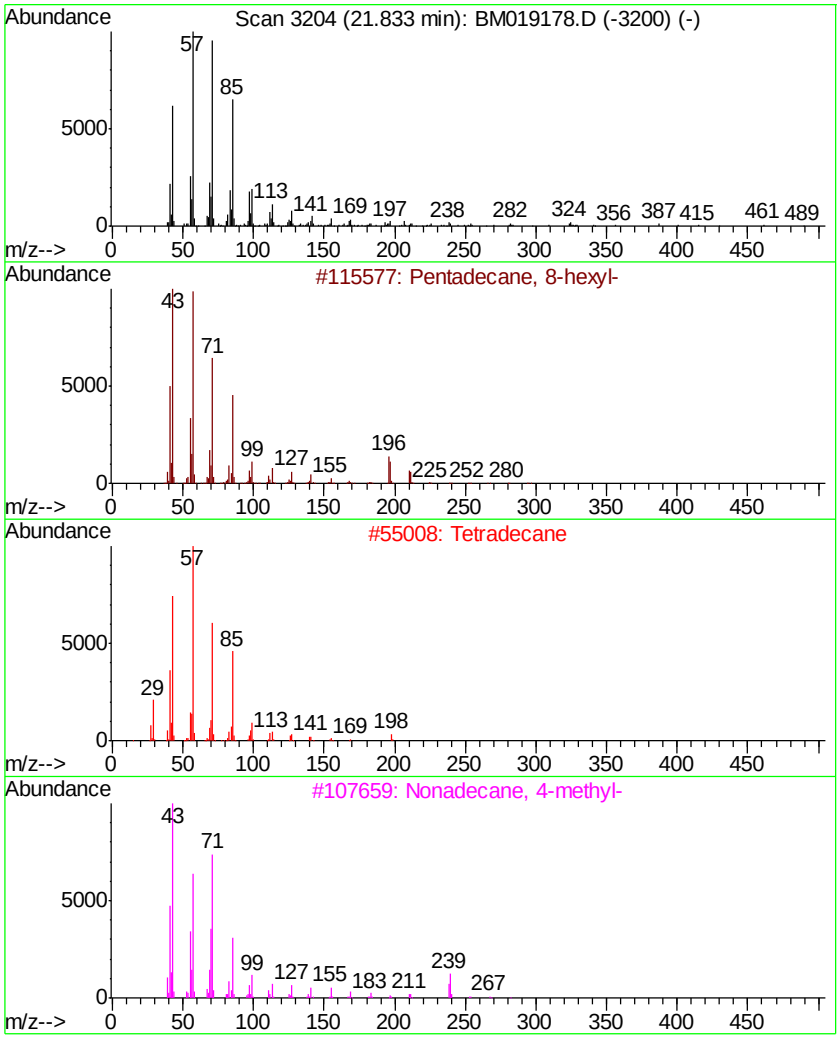
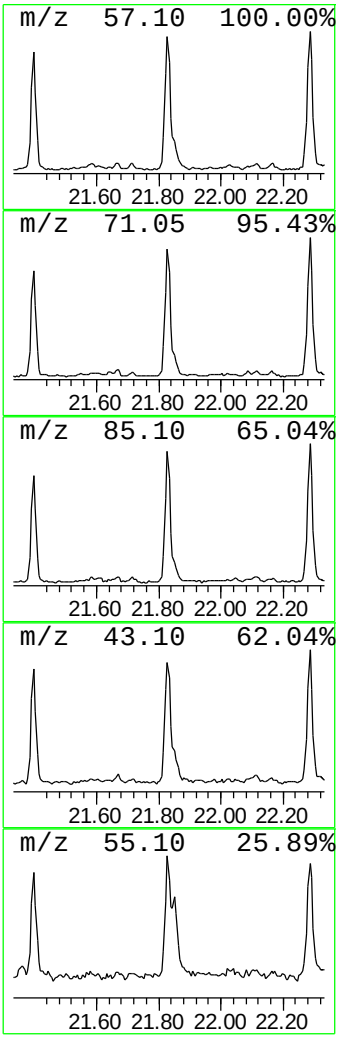
Peak Number 5 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.83	2.37 ng	487130	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
2	Tetradecane	198	C14H30	000629-59-4	87
3	Nonadecane, 4-methyl-	282	C20H42	025117-27-5	81
4	Heptacosane	380	C27H56	000593-49-7	74
5	Tridecane, 4-methyl-	198	C14H30	026730-12-1	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031419\
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Operator : JU/SJ
Sample : K1897-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-1

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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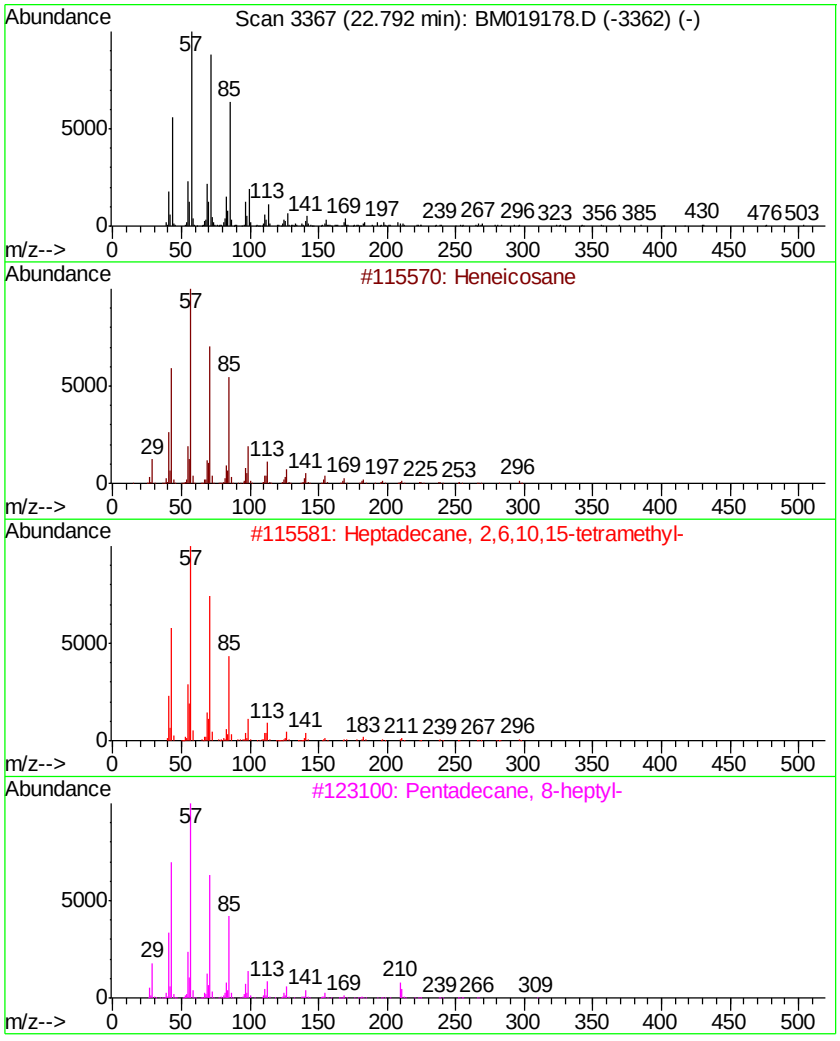
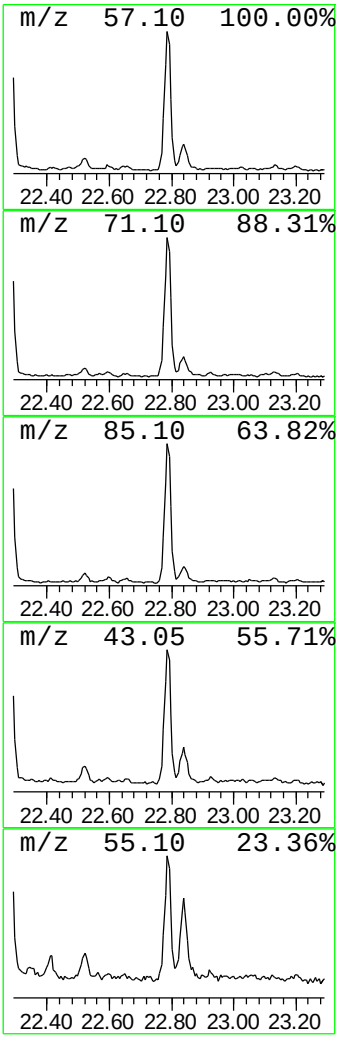
****

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.79	3.13 ng	508475	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
4	10-Methylnonadecane	282	C20H42	056862-62-5	90
5	Tetradecane	198	C14H30	000629-59-4	87





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Sample : K1897-01
Misc :
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Instrument : BNA_M
ClientSampleId : TP-1

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

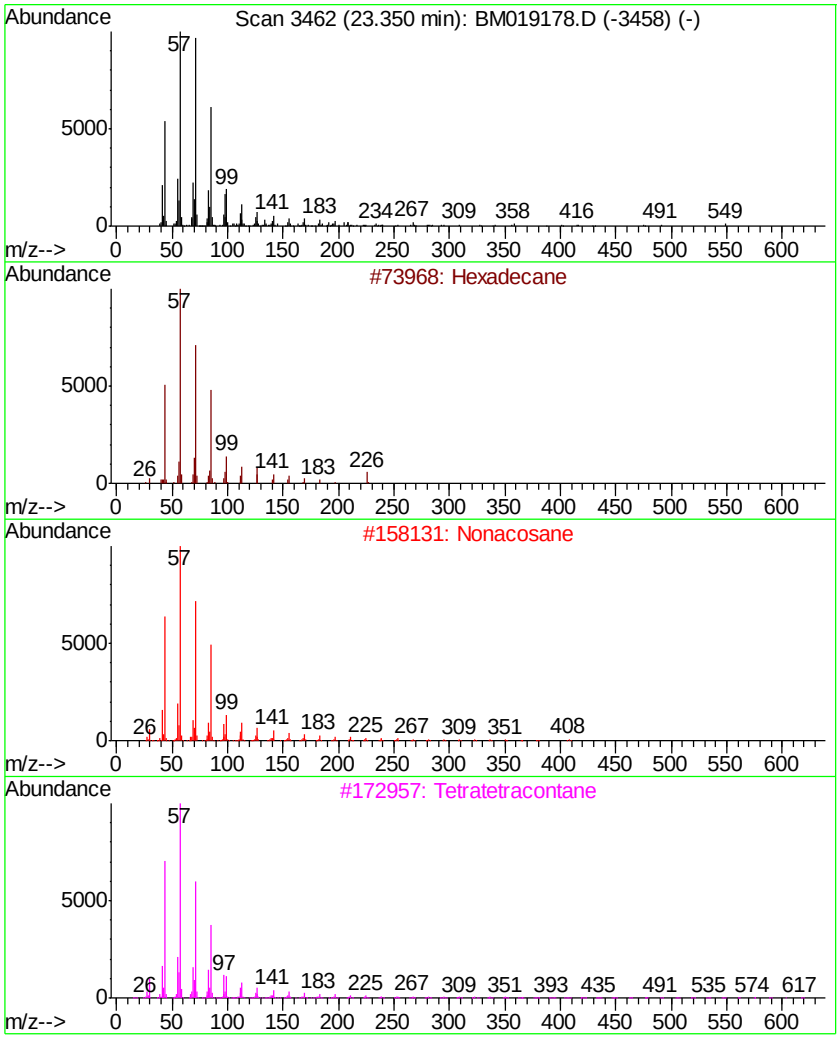
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

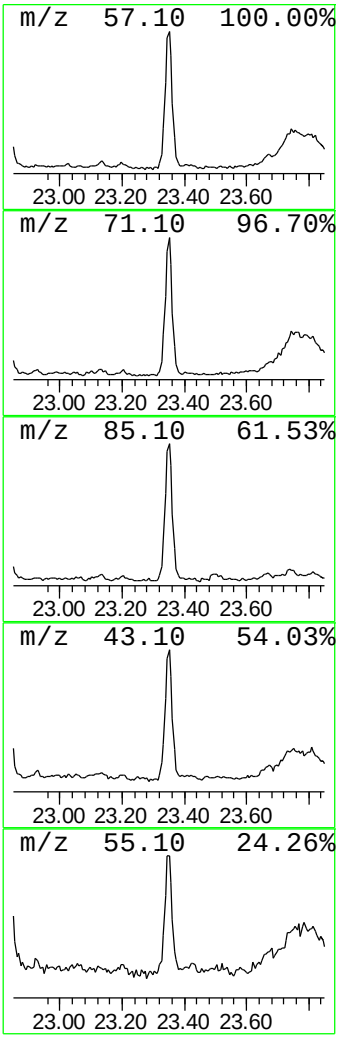
****

Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	2.18 ng	354769	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Nonacosane	408	C29H60	000630-03-5	87
3	Tetratetracontane	619	C44H90	007098-22-8	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	81





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Misc :
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Instrument : BNA_M
ClientSampleId : TP-1

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

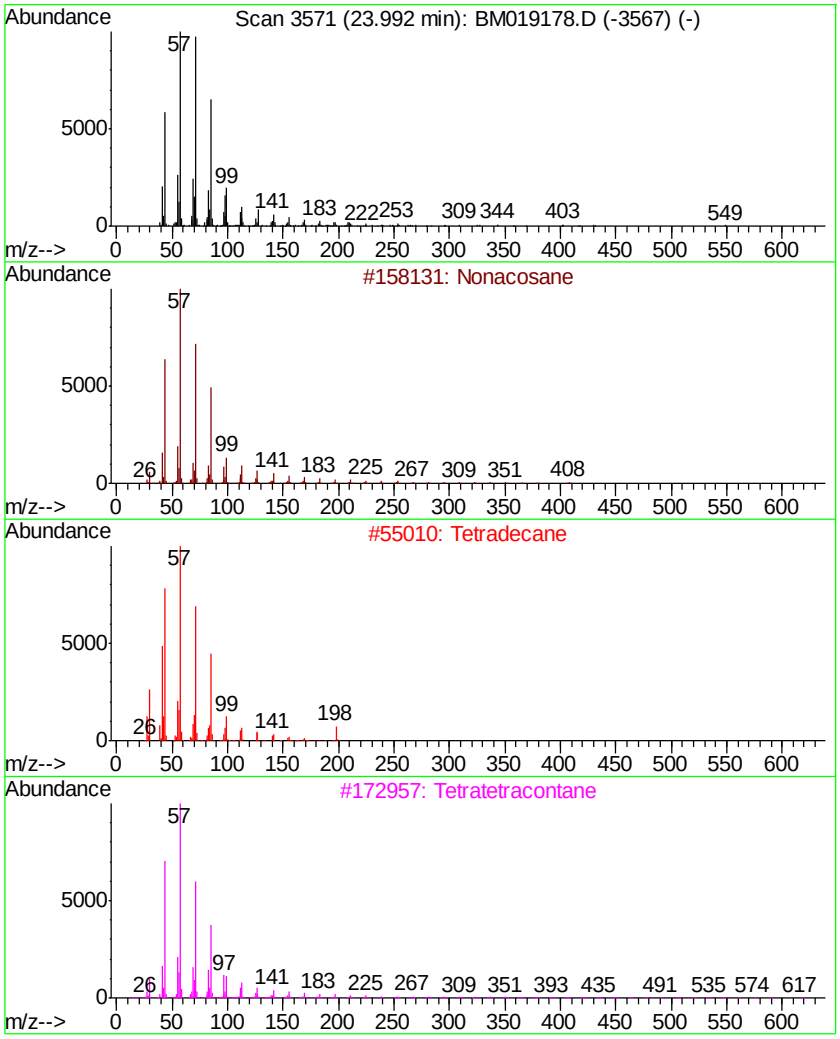
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

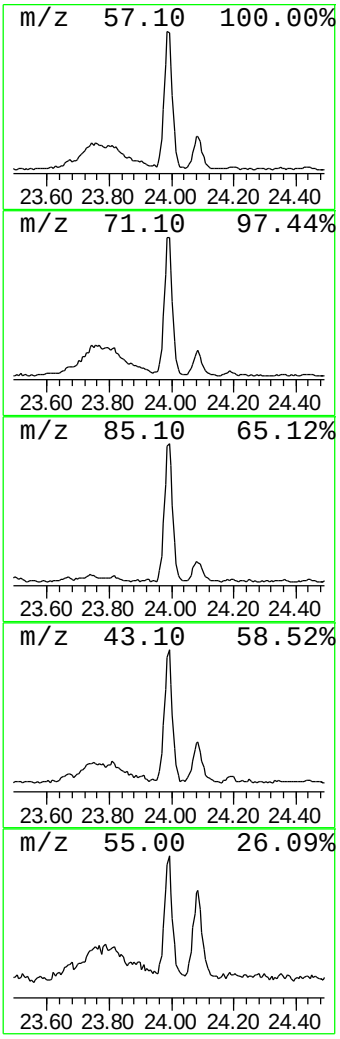
****

Peak Number 8 Nonacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	3.84 ng	623975	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5	Heptacosane	380	C27H56	000593-49-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM031419\
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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
unknown7.19	7.19	119.2	ng	7169340	1	7.66	1203260	20.0
n-Hexadecanoic acid	17.95	2.8	ng	483716	4	17.06	3523880	20.0
3-Octadecene, (E)-	20.96	6.2	ng	1283480	5	21.26	4118820	20.0
Pentadecane, 8-he...	21.83	2.4	ng	487130	5	21.26	4118820	20.0
Heneicosane	22.79	3.1	ng	508475	6	23.50	3249660	20.0
Hexadecane	23.35	2.2	ng	354769	6	23.50	3249660	20.0
Nonacosane	23.99	3.8	ng	623975	6	23.50	3249660	20.0