LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090319\
Data File : BM022500.D
Acq On : 03 Sep 2019 13:27
Operator : HP/JU
Sample : K4619-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP4-COMP

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-BM082919.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	5.128	358	364	376	rBV	365132	550169	45.08%	8.363%
2	6.704	626	632	652	rBV	338956	579928	47.51%	8.816%
3	7.040	683	689	703	rBV	434675	653646	53.55%	9.936%
4	7.504	763	768	777	rBB	83586	126252	10.34%	1.919%
5	7.810	814	820	831	rBB	326328	511496	41.91%	7.775%
6	8.681	961	968	995	rBV	172623	356646	29.22%	5.421%
7	10.281	1234	1240	1261	rBB	57414	134159	10.99%	2.039%
8	12.769	1657	1663	1683	rBV	469593	762821	62.50%	11.596%
9	13.657	1810	1814	1826	rBV	23529	39584	3.24%	0.602%
10	14.169	1896	1901	1912	rBV	103629	169636	13.90%	2.579%
11	15.686	2153	2159	2177	rBB	404151	694502	56.90%	10.557%
12	16.945	2368	2373	2388	rBV2	92141	178504	14.63%	2.713%
13	17.833	2518	2524	2535	rBV2	34434	59892	4.91%	0.910%
14	19.127	2739	2744	2753	rBV3	15009	29495	2.42%	0.448%
15	19.580	2816	2821	2834	rBV	1049032	1220538	100.00%	18.553%
16	20.845	3032	3036	3043	rBV4	28939	45571	3.73%	0.693%
17	21.162	3085	3090	3098	rBV2	128998	212154	17.38%	3.225%
18	21.697	3178	3181	3184	rBV4	14067	17081	1.40%	0.260%
19	22.144	3254	3257	3262	rVB4	17055	20277	1.66%	0.308%
20	22.627	3336	3339	3343	rVB3	19980	24534	2.01%	0.373%
21	23.344	3456	3461	3472	rVB	92722	191606	15.70%	2.913%

Sum of corrected areas: 6578491

LSC Report - Integrated Chromatogram

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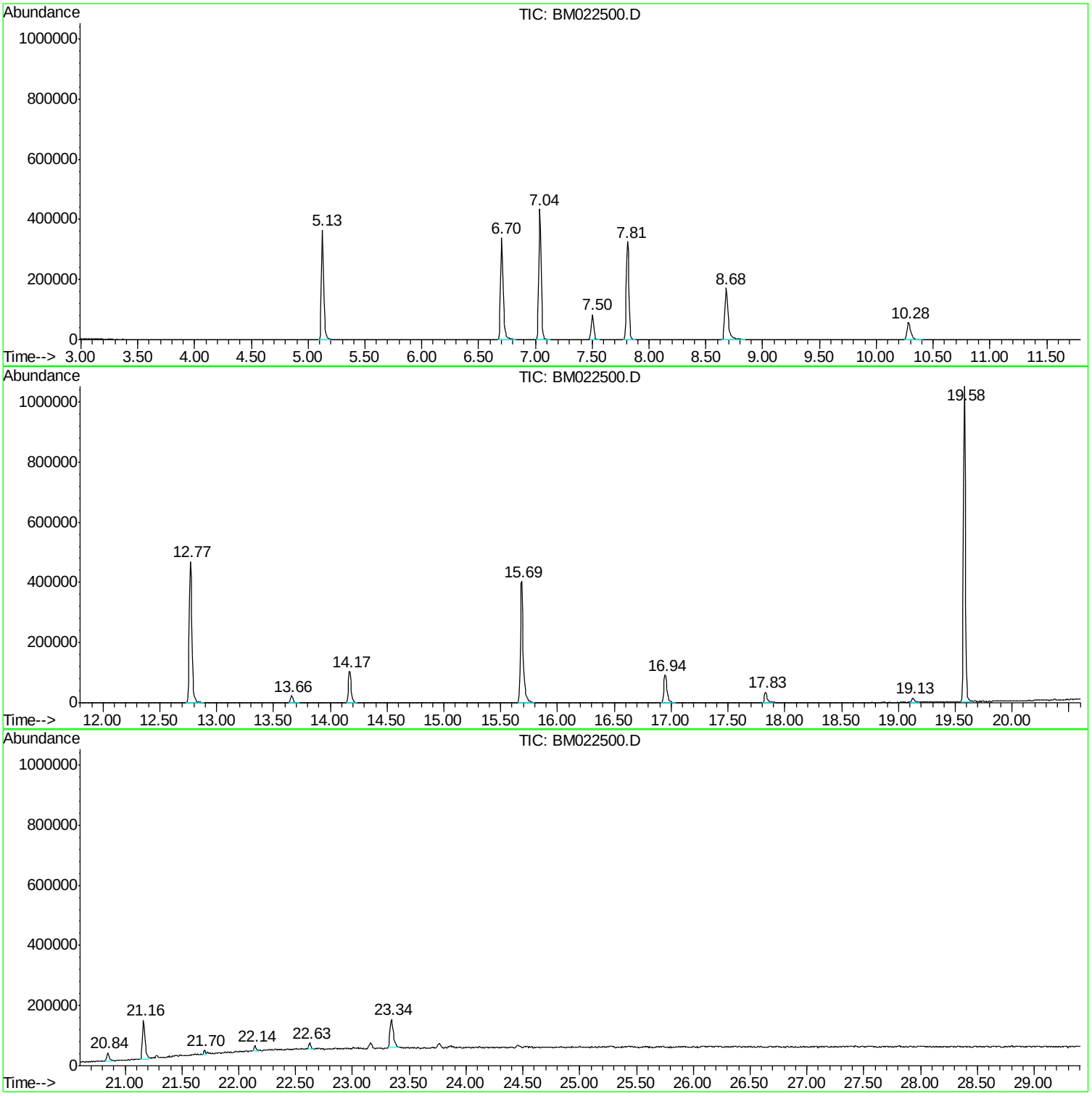
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP4-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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BNA_M
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

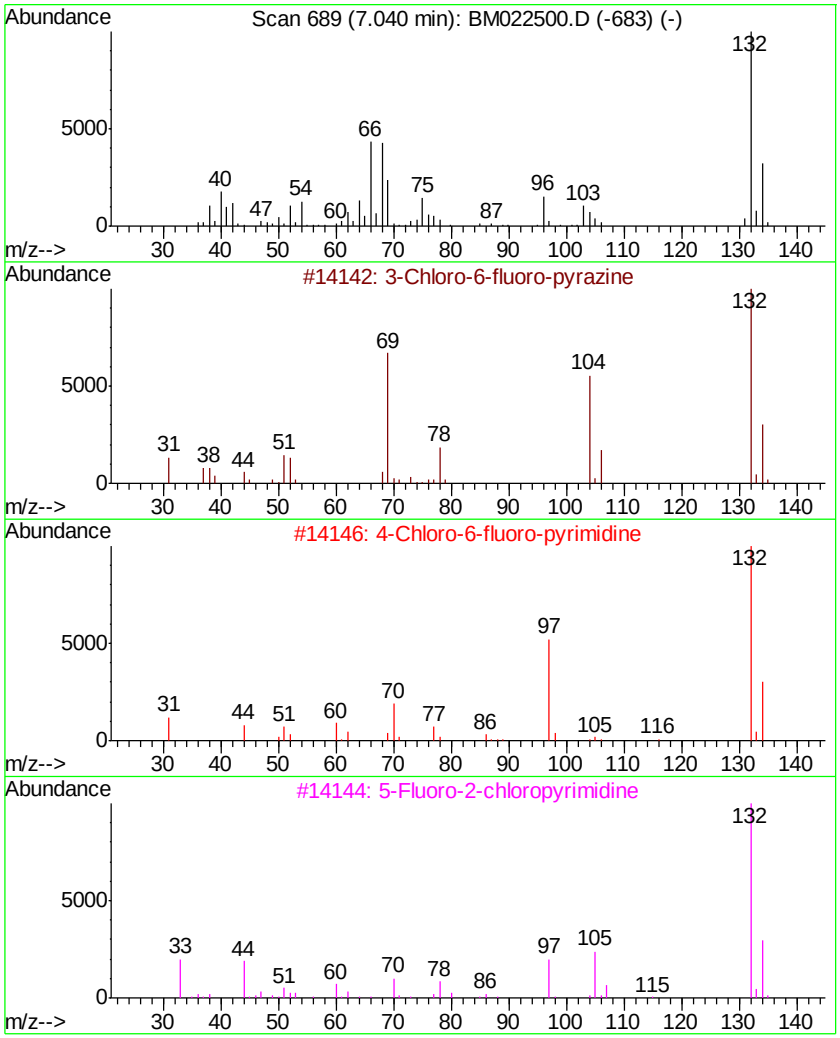
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

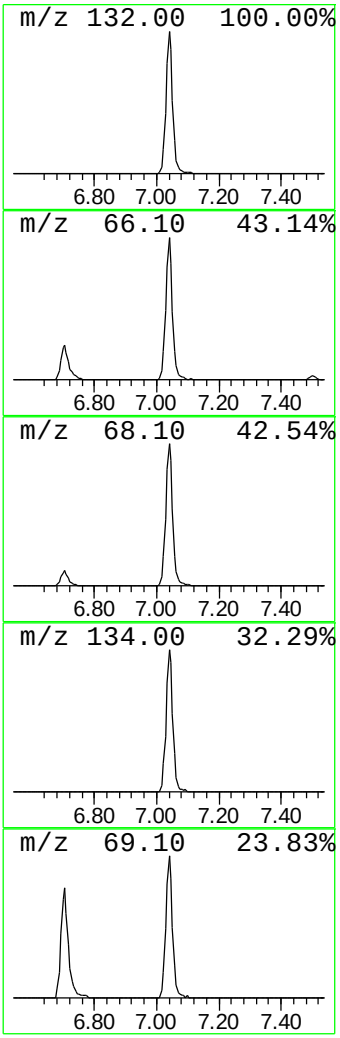
****

Peak Number 1 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	103.55 ng	653646	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14





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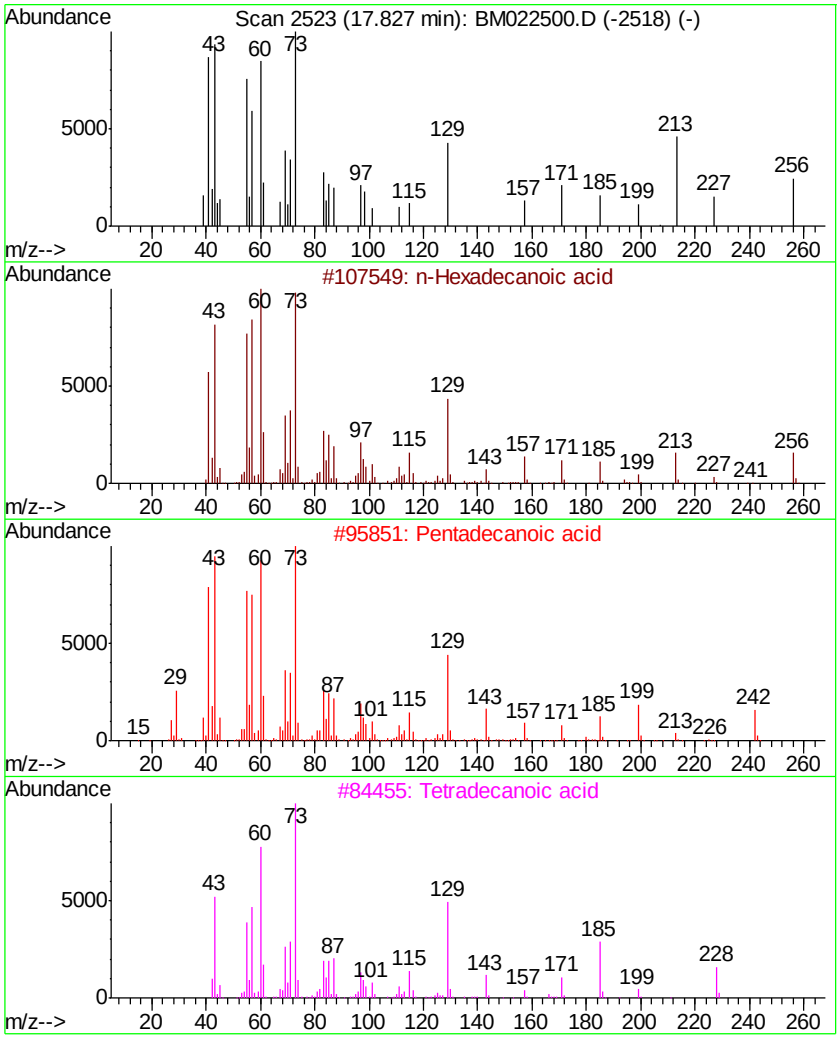
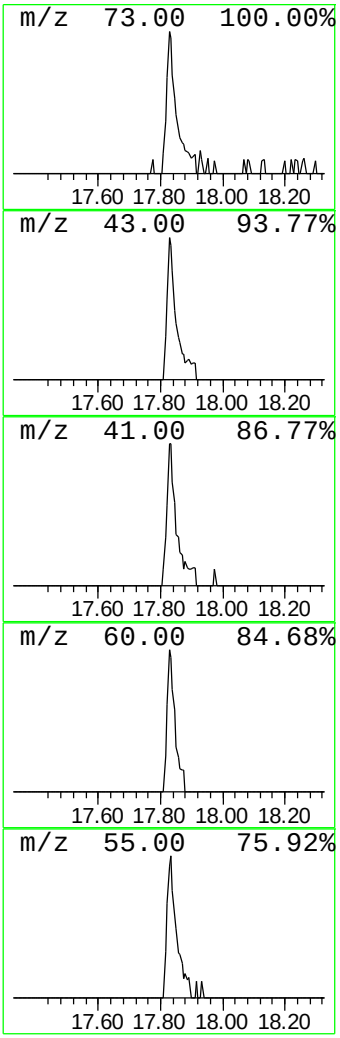
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	6.71 ng	59892	Phenanthrene-d10	16.94

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	58
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Library Search Compound Report

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Operator : HP/JU
Sample : K4619-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP4-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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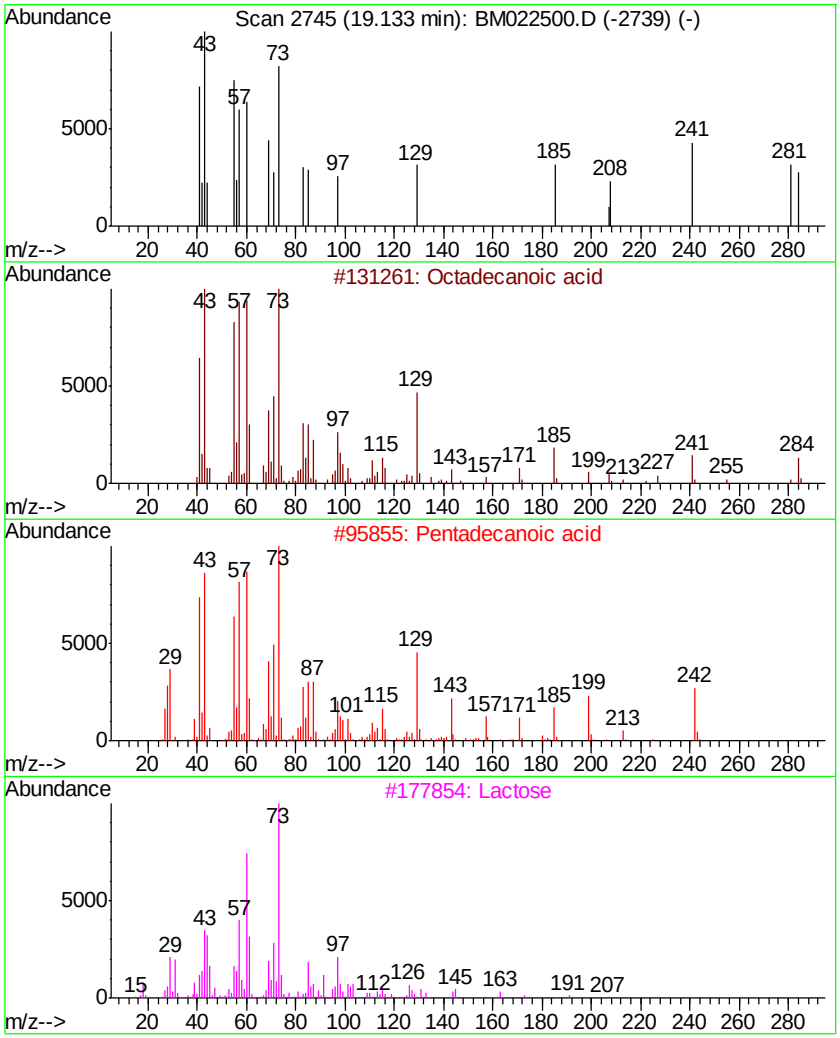
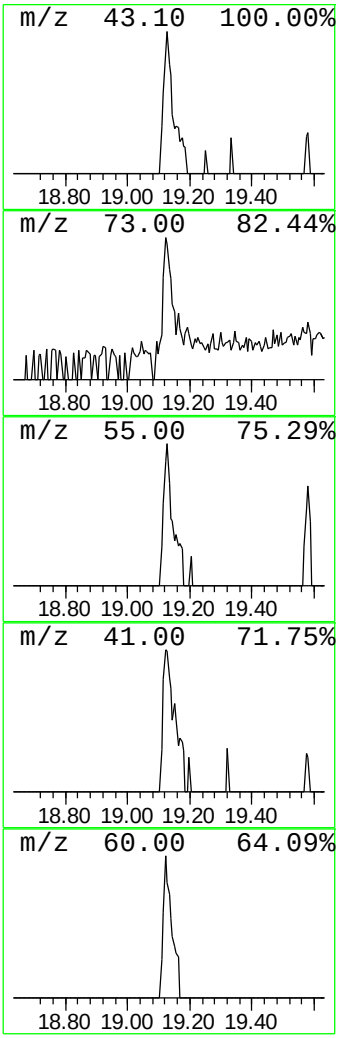
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	2.78 ng	29495	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
3	Lactose	342	C12H22O11	000063-42-3	27
4	Maltose	342	C12H22O11	000069-79-4	27
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	25





Library Search Compound Report

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BNA_M
ClientSampleId :
TP4-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
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TIC Library : C:\DATABASE\NIST11.L
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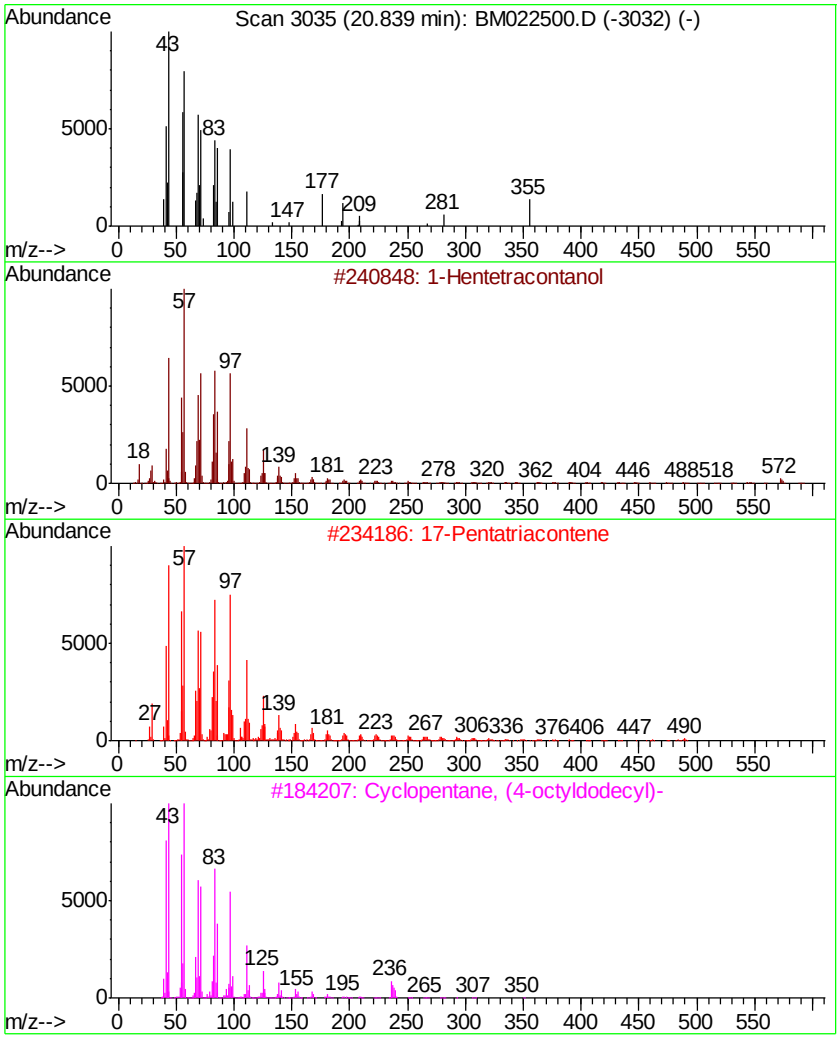
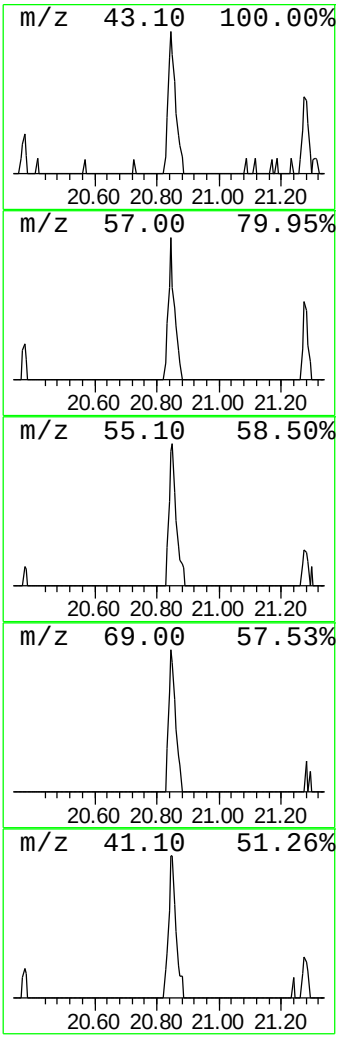
****

Peak Number 5 1-Hentetracontanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	4.30 ng	45571	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hentetracontanol	593	C41H84O	040710-42-7	80
2	17-Pentatriacontene	491	C35H70	006971-40-0	80
3	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	80
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	80
5	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	80





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP4-COMP

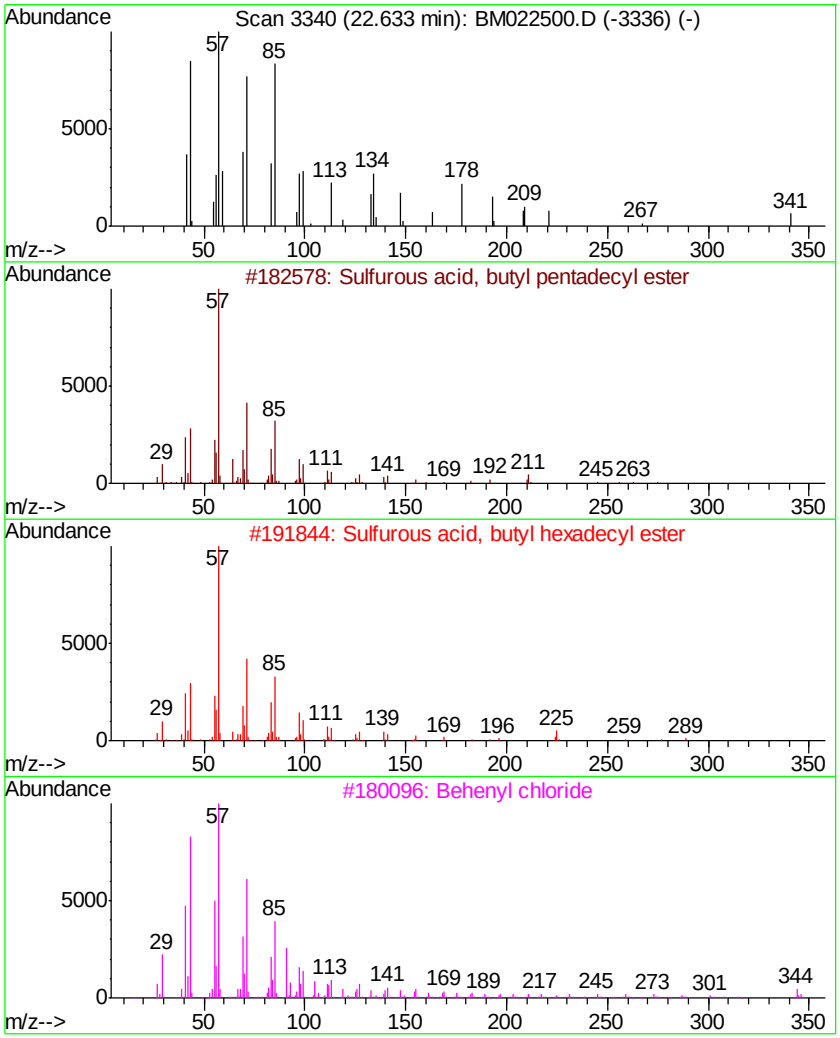
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

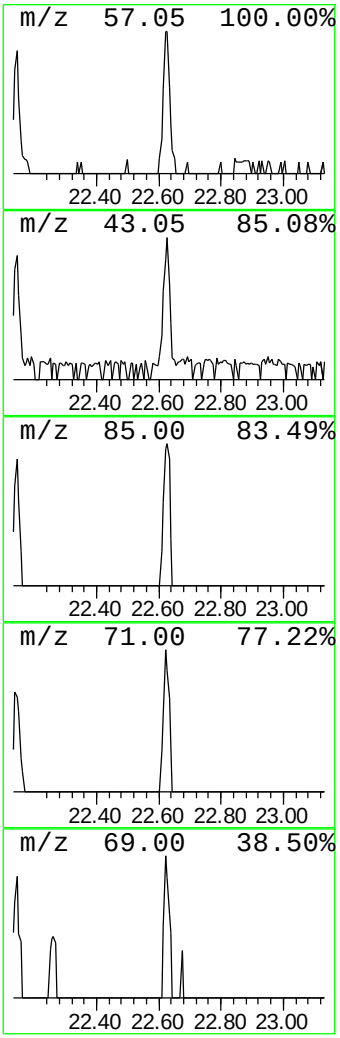
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Sulfurous acid, butyl penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	2.56 ng	24534	Perylene-d12	23.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	50
2	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	50
3	Behenyl chloride	344	C22H45Cl	042217-03-8	50
4	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	50
5	2-methylhexacosane	380	C27H56	1000376-72-7	50





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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown7.04	7.04	103.6	ng	653646	1	7.50	126252	20.0
n-Hexadecanoic acid	17.83	6.7	ng	59892	4	16.94	178504	20.0
Octadecanoic acid	19.13	2.8	ng	29495	5	21.16	212154	20.0
1-Hentetracontanol	20.84	4.3	ng	45571	5	21.16	212154	20.0
Sulfurous acid, b...	22.63	2.6	ng	24534	6	23.34	191606	20.0