LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018845.D
Acq On : 18 Feb 2019 19:11
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

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-BM021119.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	4.857	297	301	311	rBV	214664	300724	2.96%	0.381%
2	5.298	369	376	387	rBV	4753113	6767872	66.68%	8.571%
3	6.881	637	645	660	rBV	4580562	7162554	70.57%	9.071%
4	7.240	698	706	716	rBV	4776712	7475220	73.65%	9.467%
5	7.704	778	785	793	rBV	1198375	1834791	18.08%	2.324%
6	8.022	831	839	853	rBV	3522681	5575032	54.93%	7.060%
7	8.875	976	984	994	rBV	2538612	4334415	42.70%	5.489%
8	10.492	1251	1259	1273	rBV	1471065	2452005	24.16%	3.105%
9	12.969	1673	1680	1696	rBV	6140043	9521286	93.81%	12.058%
10	13.821	1818	1825	1837	rBV	143704	254799	2.51%	0.323%
11	14.351	1909	1915	1928	rBV2	1871057	2964292	29.21%	3.754%
12	15.851	2160	2170	2188	rBV	4298300	6250265	61.58%	7.915%
13	17.104	2377	2383	2397	rBV2	2131377	3125512	30.79%	3.958%
14	17.992	2529	2534	2545	rBV	540054	866131	8.53%	1.097%
15	19.280	2748	2753	2763	rBV	298030	472197	4.65%	0.598%
16	19.739	2825	2831	2840	rBV	8665866	10149942	100.00%	12.854%
17	20.997	3041	3045	3053	rBV	288203	414687	4.09%	0.525%
18	21.297	3091	3096	3103	rBV	2202489	2829658	27.88%	3.584%
19	21.433	3116	3119	3123	rVB	239134	235399	2.32%	0.298%
20	21.862	3189	3192	3198	rBV	333103	435721	4.29%	0.552%
21	22.327	3267	3271	3278	rBV	452561	604128	5.95%	0.765%
22	22.456	3290	3293	3298	rVB	246890	316965	3.12%	0.401%
23	22.839	3353	3358	3364	rBV	453336	643833	6.34%	0.815%
24	23.403	3450	3454	3461	rVB	392446	611860	6.03%	0.775%
25	23.550	3473	3479	3492	rVB	1401025	2864747	28.22%	3.628%
26	24.056	3561	3565	3572	rVB	286635	499334	4.92%	0.632%

Sum of corrected areas: 78963369

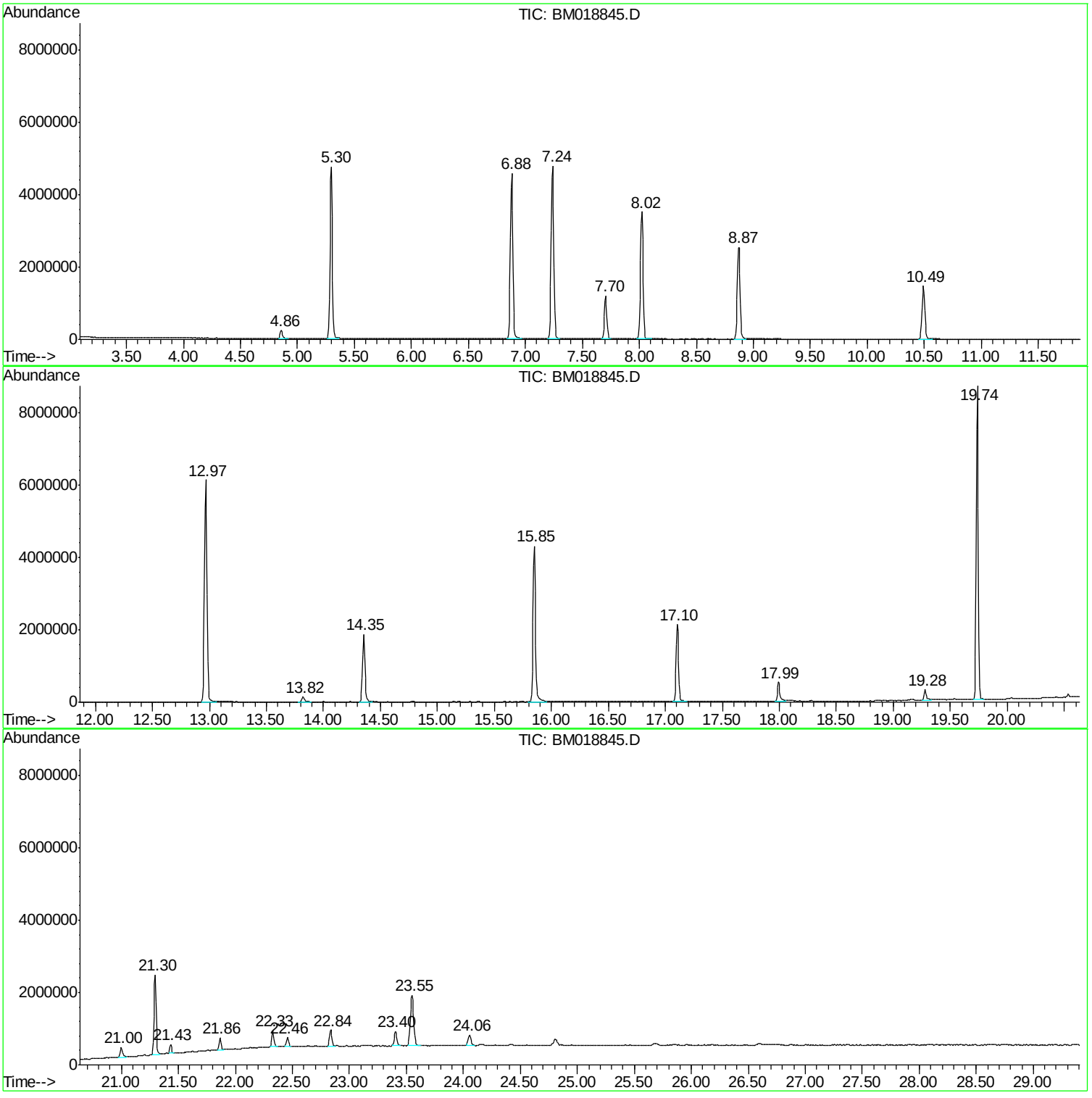
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018845.D
Acq On : 18 Feb 2019 19:11
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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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Data File : BM018845.D
Acq On : 18 Feb 2019 19:11
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

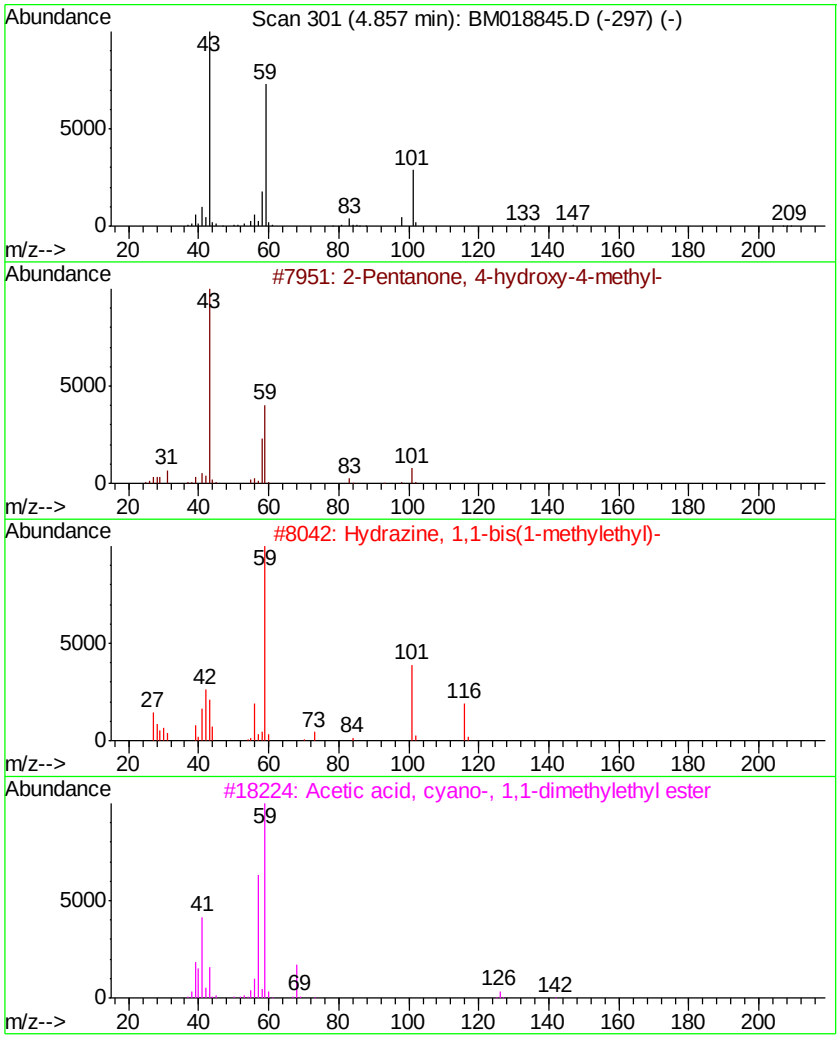
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

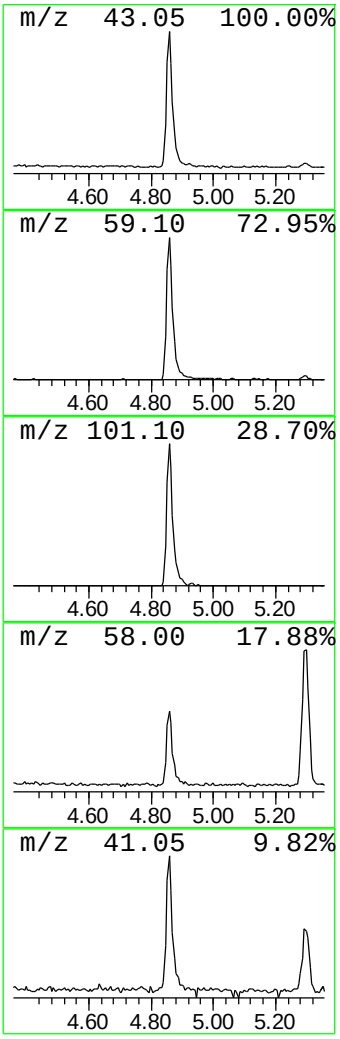
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	3.28 ng	300724	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Data File : BM018845.D
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Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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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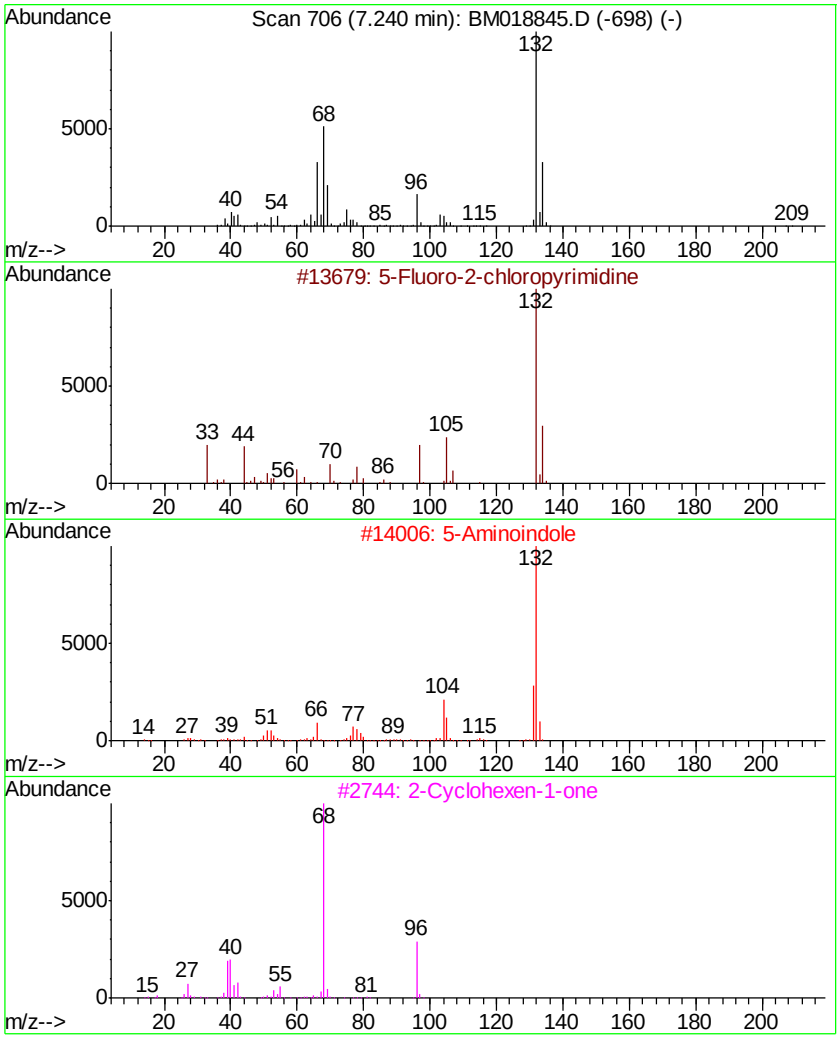
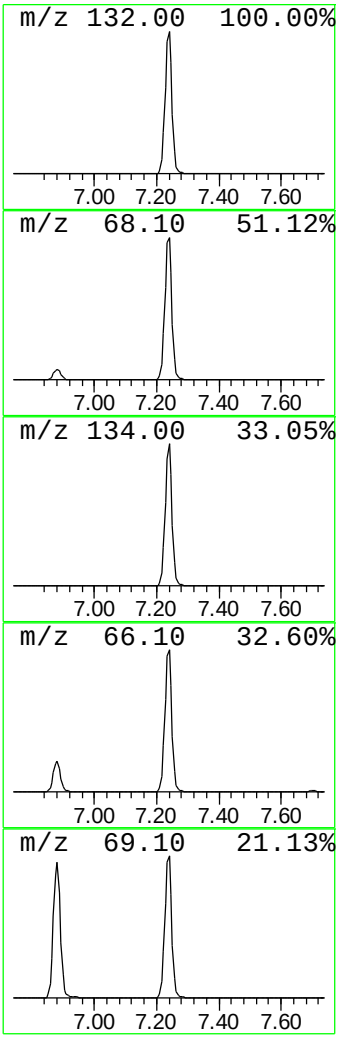
Peak Number 2 unknown7.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	81.48 ng	7475220	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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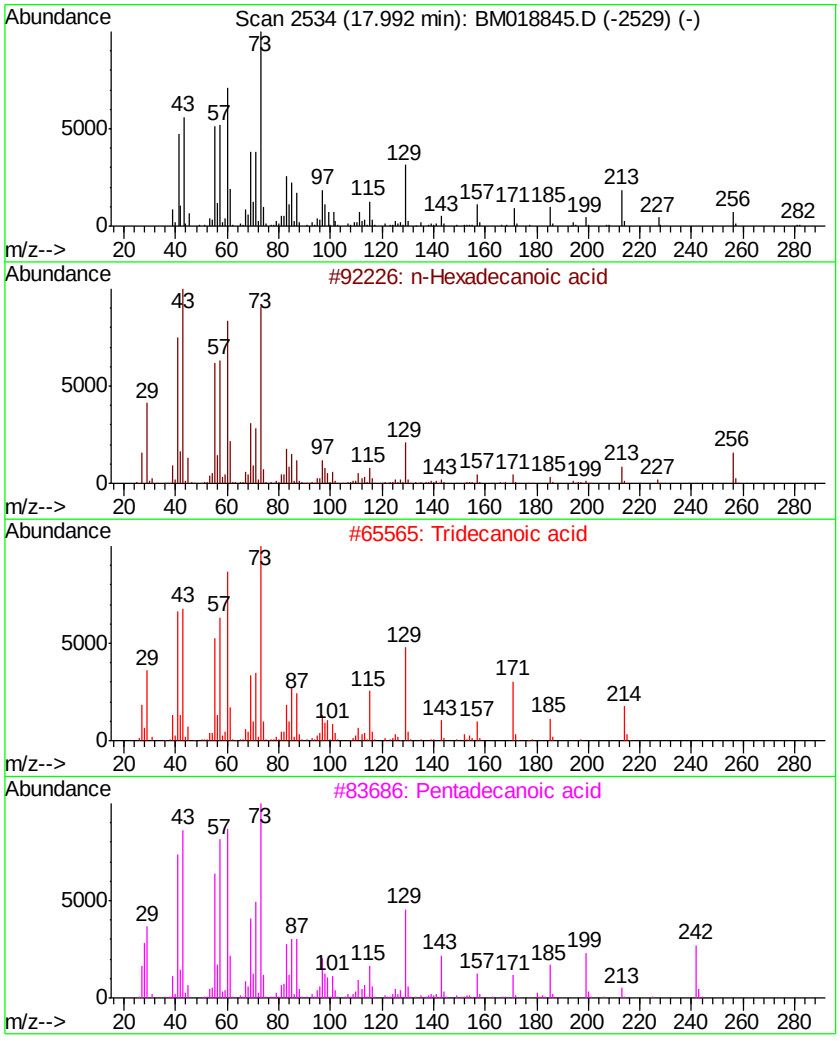
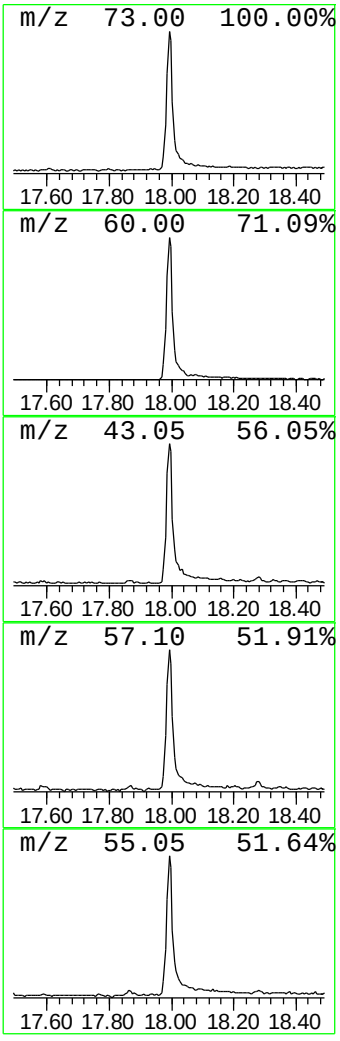
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	5.54 ng	866131	Phenanthrene-d10	17.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Data File : BM018845.D
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Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

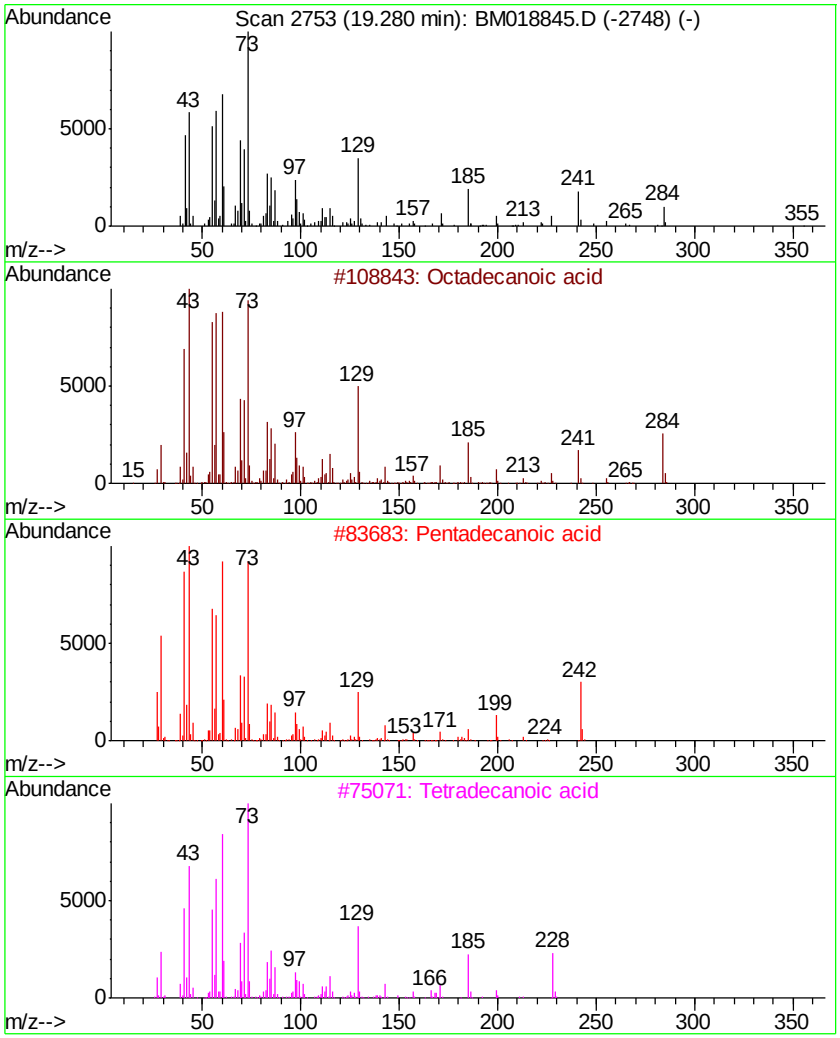
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

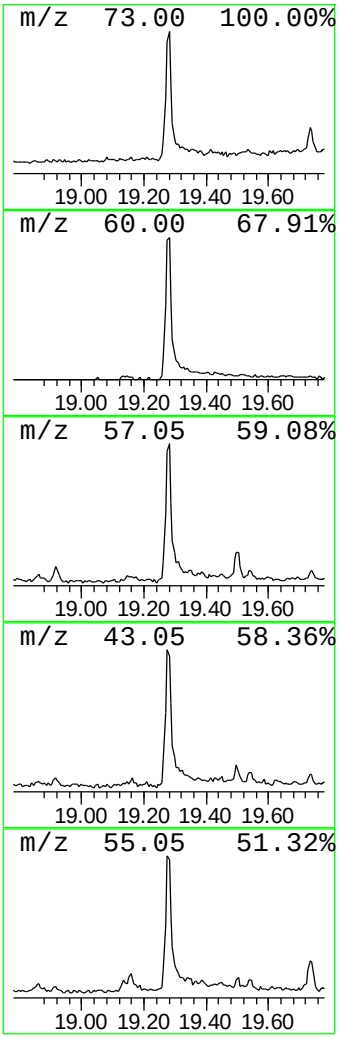
****

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	3.34 ng	472197	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Tetratetracontane	619	C44H90	007098-22-8	18
5	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
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Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

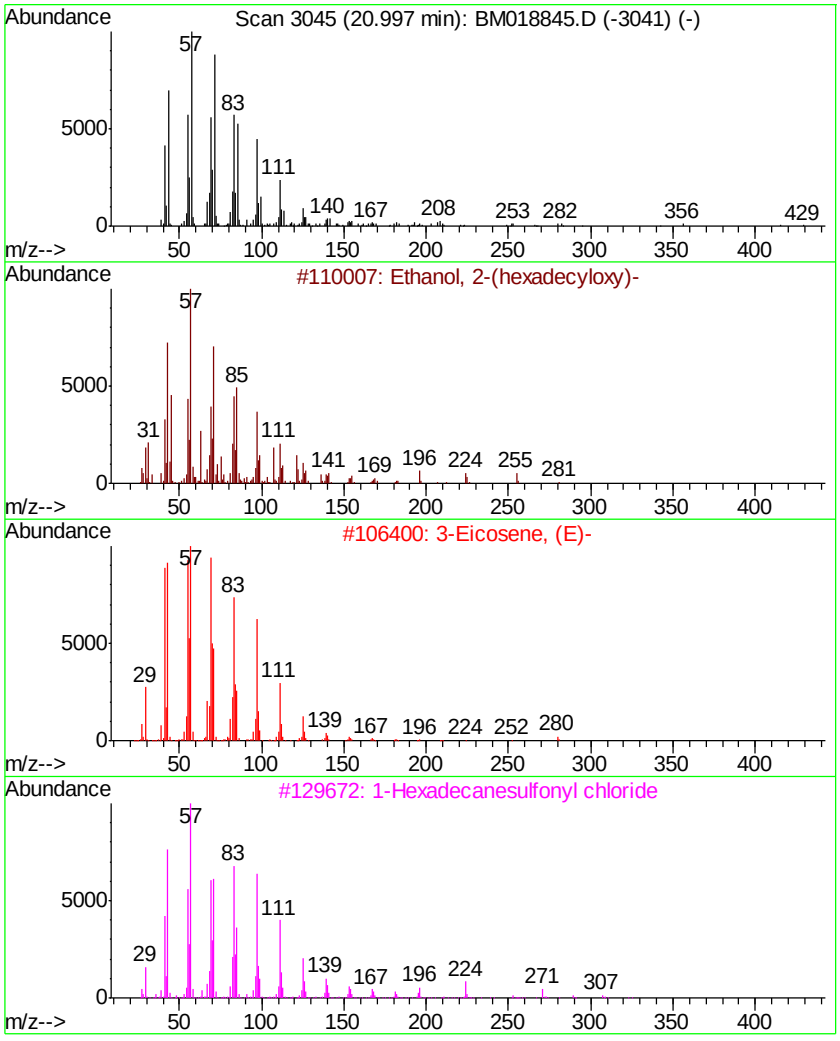
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

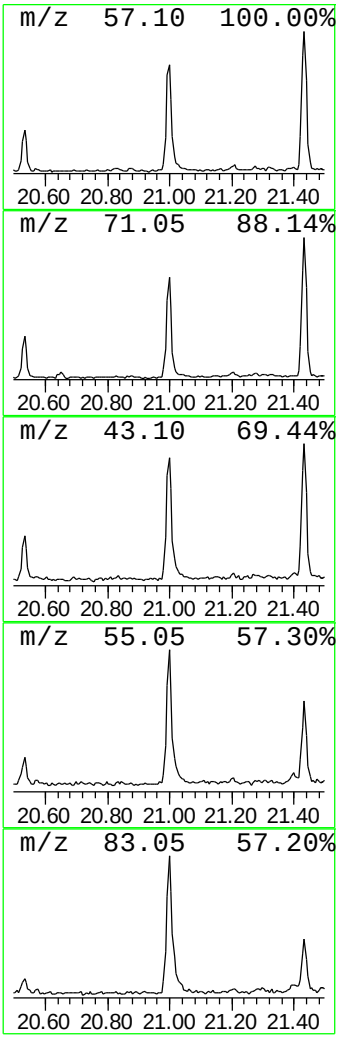
****

Peak Number 6 Ethanol, 2-(hexadecyloxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	2.93 ng	414687	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	83
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	64
4	Cyclotetradecane	196	C14H28	000295-17-0	64
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	58





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Operator : JU/SJ
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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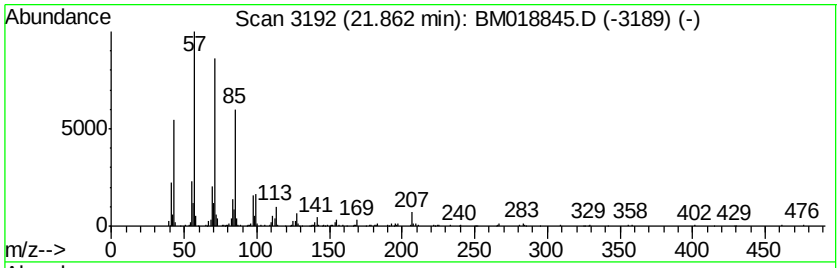
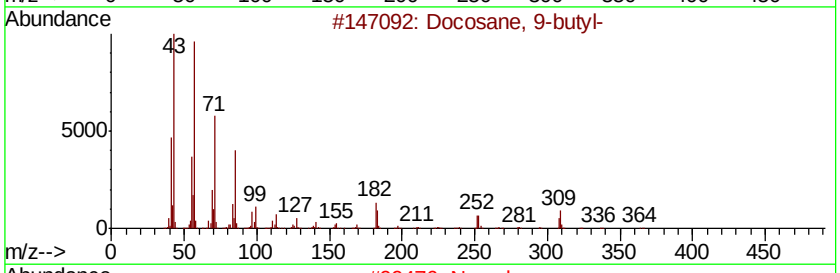
****

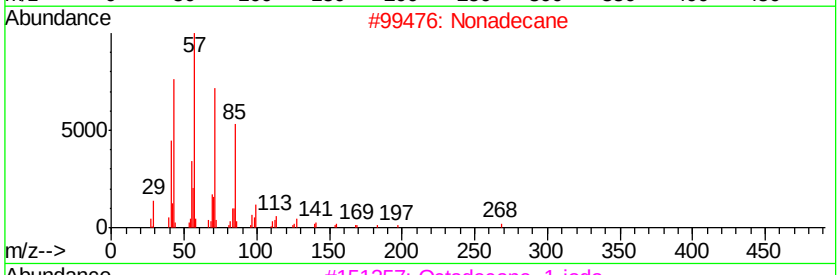
Peak Number 7 Docosane, 9-butyl- Concentration Rank 10

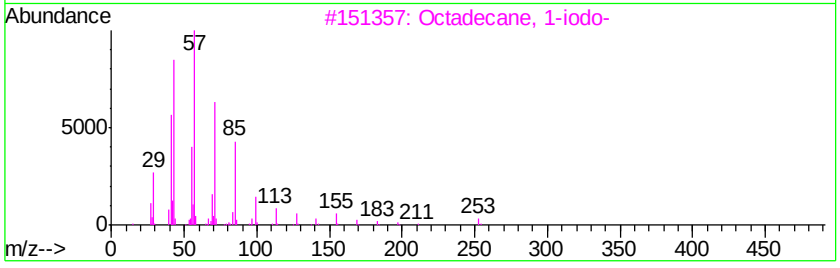
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	3.08 ng	435721	Chrysene-d12	21.30

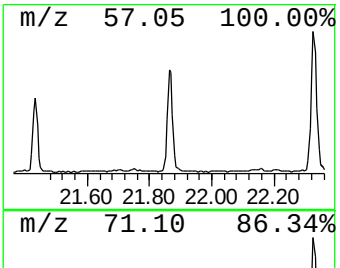
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 9-butyl-	366	C26H54	055282-14-9	90
2	Nonadecane	268	C19H40	000629-92-5	86
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86

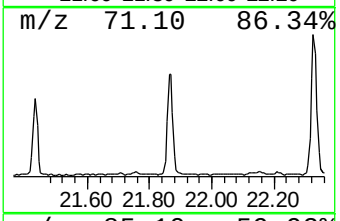


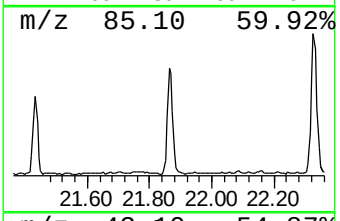


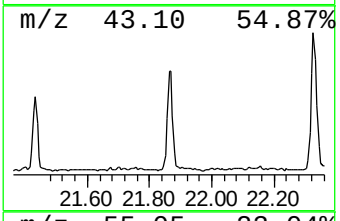


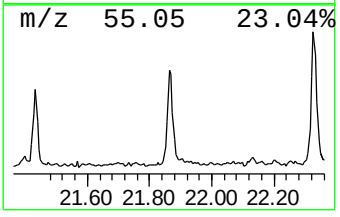












Library Search Compound Report

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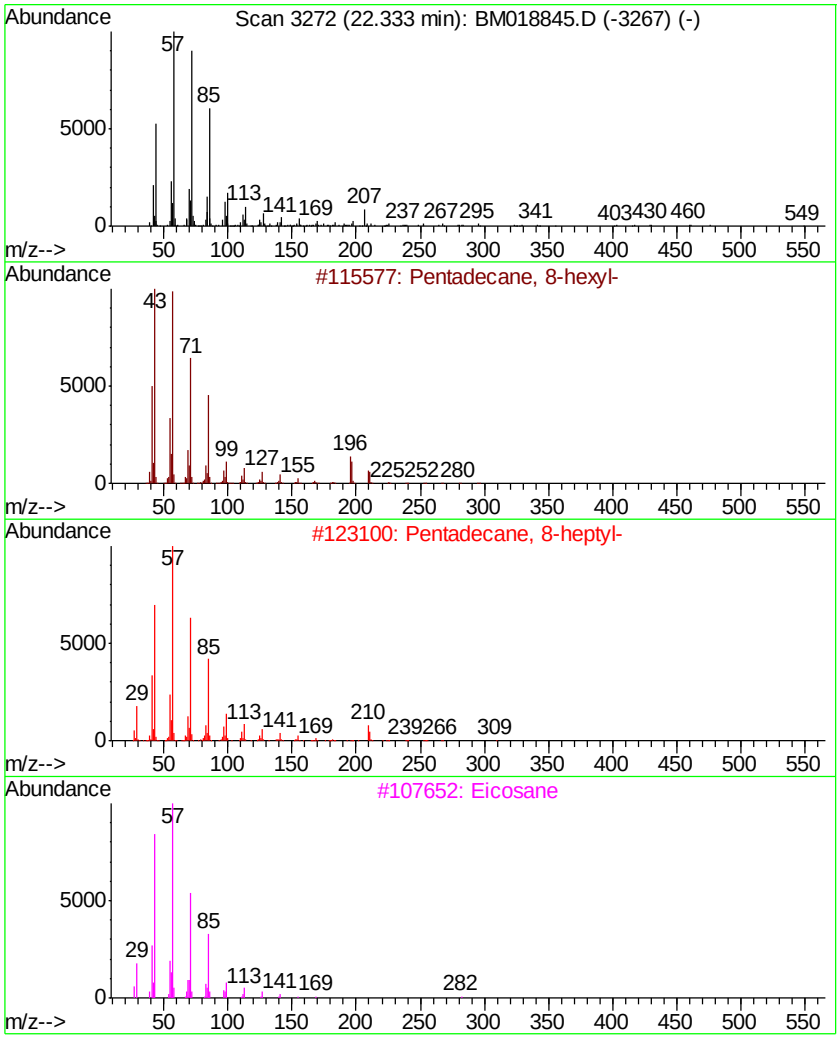
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

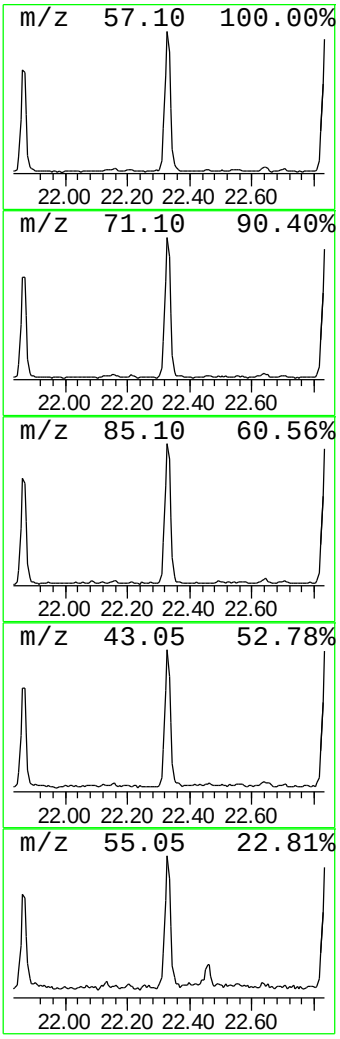
****

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	4.27 ng	604128	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Eicosane	282	C20H42	000112-95-8	90
4	Octadecane	254	C18H38	000593-45-3	83
5	Heptacosane	380	C27H56	000593-49-7	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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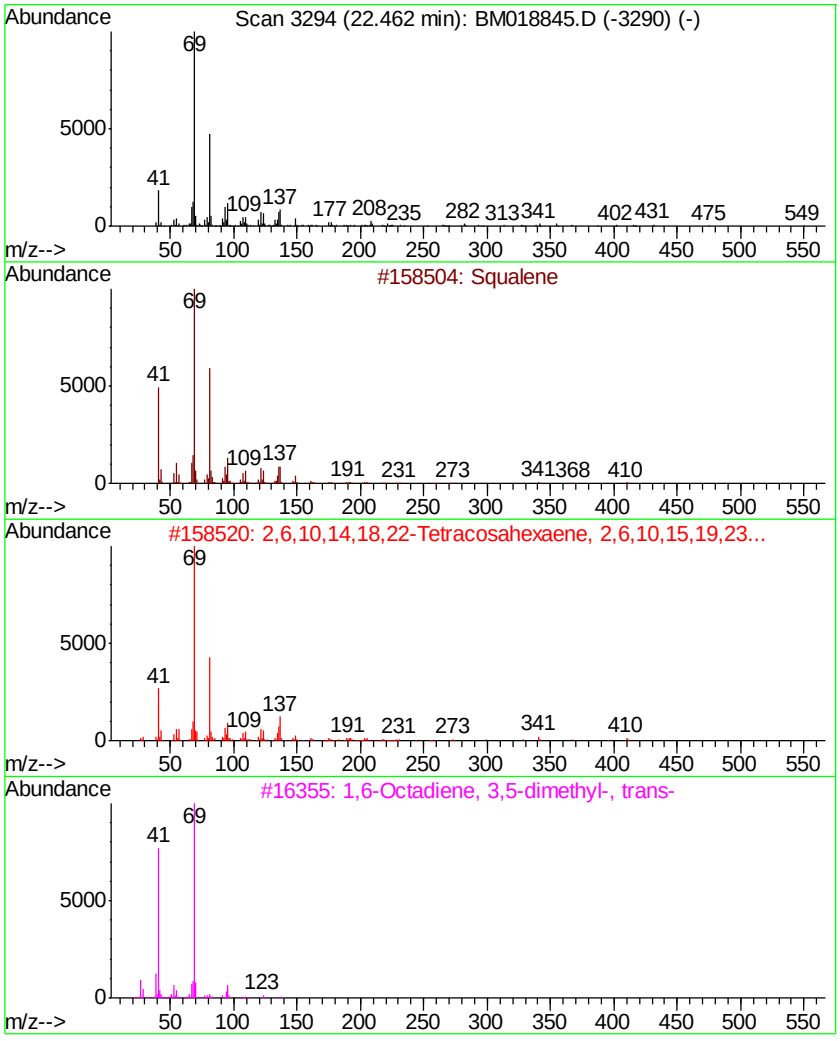
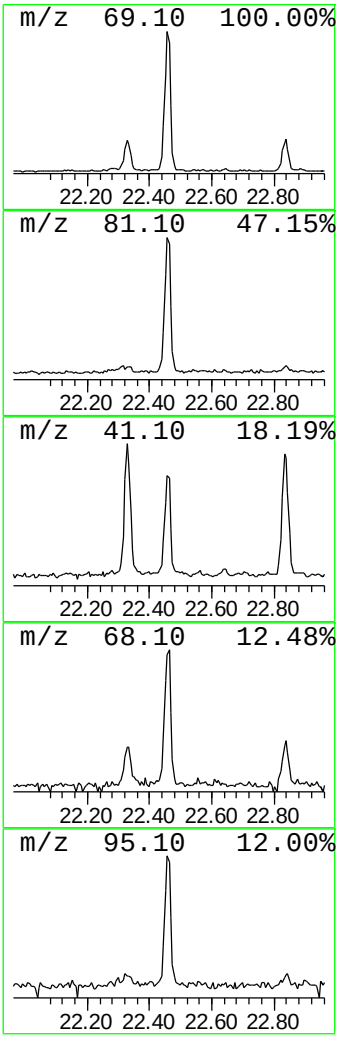
Peak Number 9 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.46	2.21 ng	316965	Perylene-d12	23.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	81
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
3	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	59
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	58





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Acq On : 18 Feb 2019 19:11
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

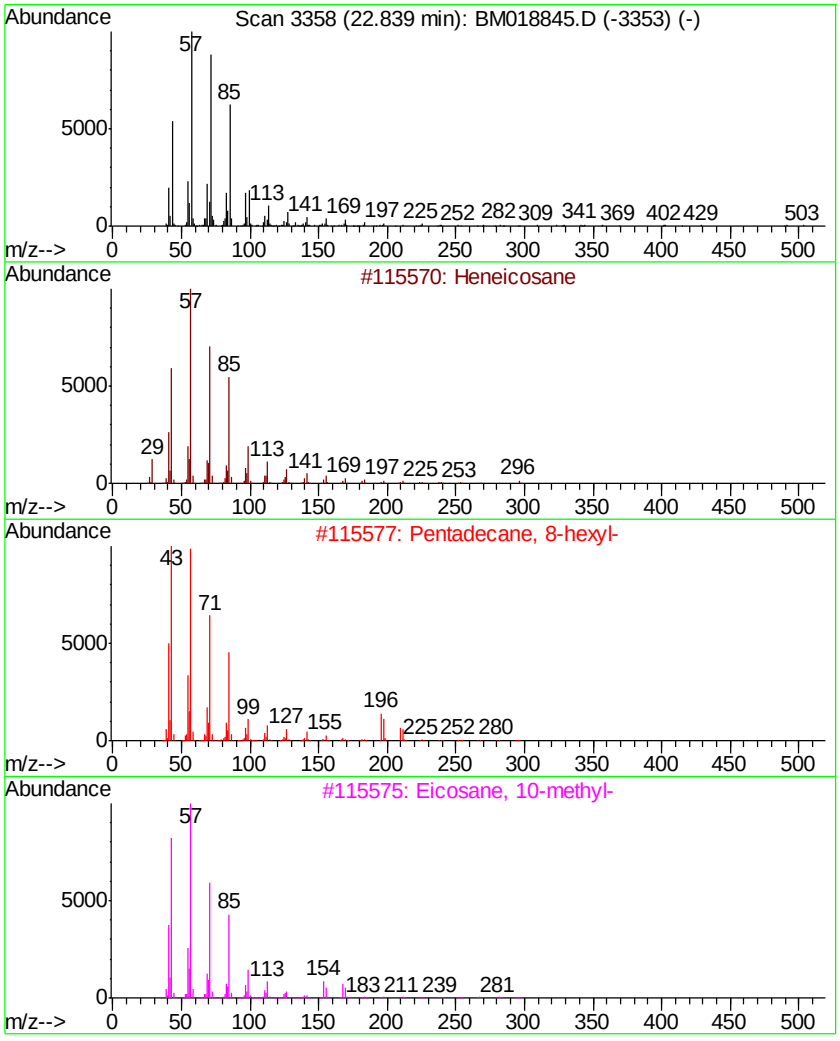
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

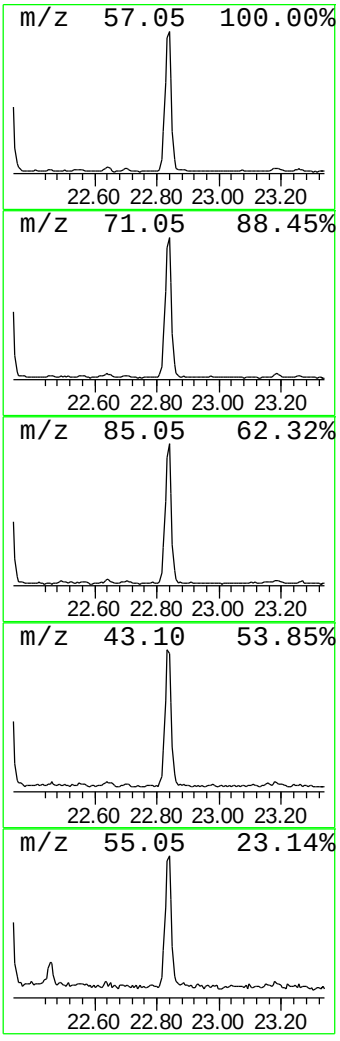
****

Peak Number 10 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.84	4.49 ng	643833	Perylene-d12	23.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018845.D
Acq On : 18 Feb 2019 19:11
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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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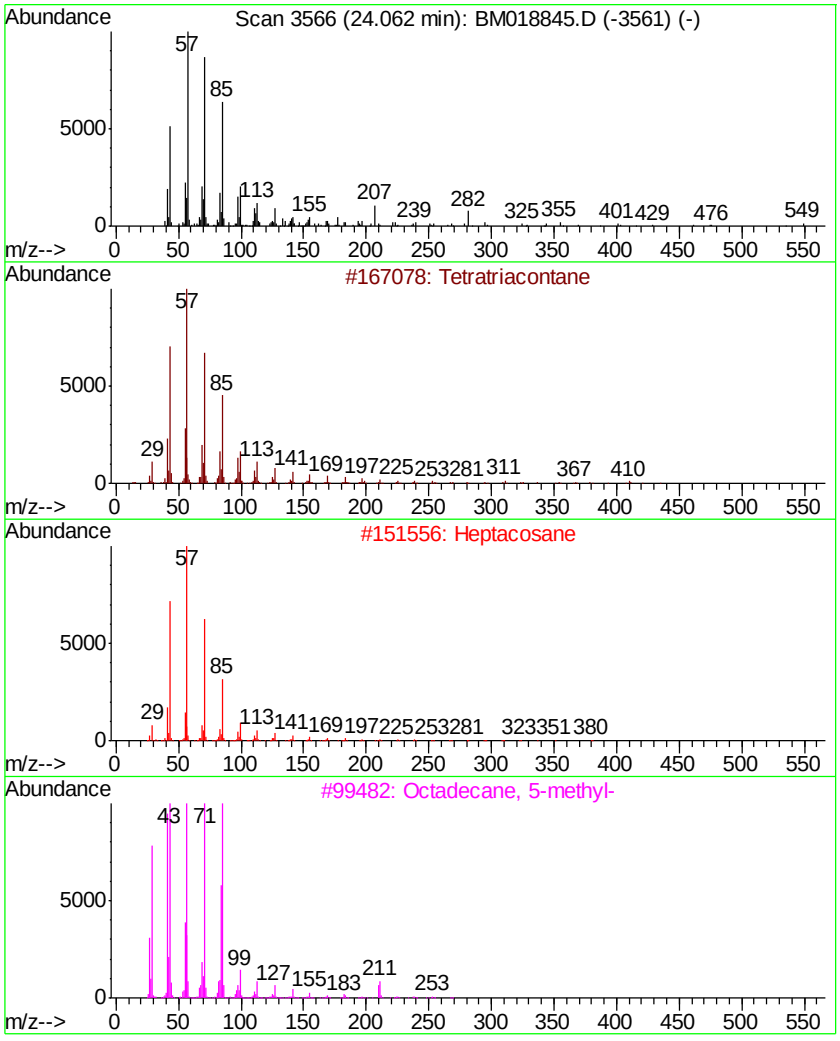
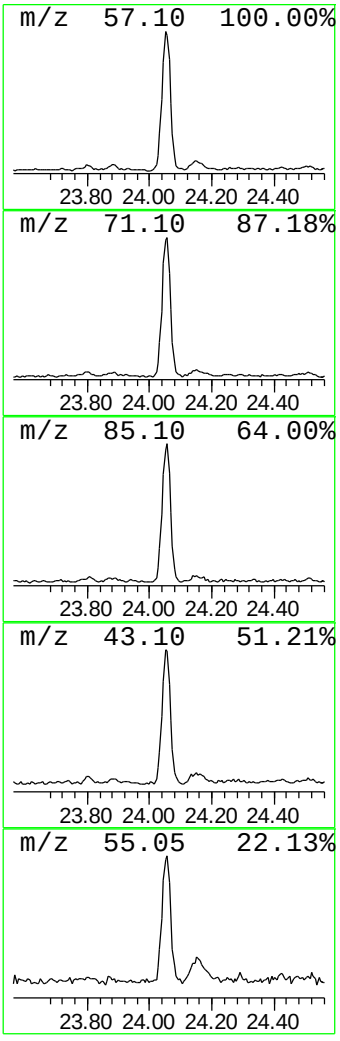
Peak Number 12 Tetratriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.06	3.49 ng	499334	Perylene-d12	23.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	87
2	Heptacosane	380	C27H56	000593-49-7	74
3	Octadecane, 5-methyl-	268	C19H40	025117-35-5	72
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	72
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM021819\
Data File : BM018845.D
Acq On : 18 Feb 2019 19:11
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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...	4.86	3.3	ng	300724	1	7.70	1834790	20.0
unknown7.24	7.24	81.5	ng	7475220	1	7.70	1834790	20.0
n-Hexadecanoic acid	17.99	5.5	ng	866131	4	17.10	3125510	20.0
Octadecanoic acid	19.28	3.3	ng	472197	5	21.30	2829660	20.0
Ethanol, 2-(hexad...	21.00	2.9	ng	414687	5	21.30	2829660	20.0
Docosane, 9-butyl-	21.86	3.1	ng	435721	5	21.30	2829660	20.0
Pentadecane, 8-he...	22.33	4.3	ng	604128	5	21.30	2829660	20.0
Squalene	22.46	2.2	ng	316965	6	23.55	2864750	20.0
Heneicosane	22.84	4.5	ng	643833	6	23.55	2864750	20.0
Tetratriacontane	24.06	3.5	ng	499334	6	23.55	2864750	20.0