LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

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-BM041519.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	379	rBV	748608	1267850	22.73%	4.186%
2	6.716	627	634	650	rBV	363360	803267	14.40%	2.652%
3	7.046	684	690	707	rBV	1505776	2454888	44.01%	8.105%
4	7.510	763	769	780	rBV	372217	593592	10.64%	1.960%
5	7.822	815	822	834	rBV	1293247	2086496	37.41%	6.889%
6	8.687	962	969	986	rBV	838040	1637207	29.35%	5.405%
7	10.292	1234	1242	1262	rBV	357476	741824	13.30%	2.449%
8	12.780	1659	1665	1686	rBV	2290169	3637494	65.22%	12.009%
9	14.180	1897	1903	1918	rVB2	543848	937356	16.81%	3.095%
10	15.692	2153	2160	2181	rBV	1681868	2916564	52.29%	9.629%
11	16.945	2367	2373	2387	rBV2	683628	1096196	19.65%	3.619%
12	17.833	2518	2524	2536	rBV	184133	345494	6.19%	1.141%
13	19.133	2740	2745	2754	rBV	137379	237453	4.26%	0.784%
14	19.592	2817	2823	2833	rBV	4406329	5577689	100.00%	18.415%
15	20.856	3033	3038	3047	rBV	211637	330051	5.92%	1.090%
16	21.162	3085	3090	3099	rBV	894513	1283998	23.02%	4.239%
17	21.286	3108	3111	3116	rBV	154258	167479	3.00%	0.553%
18	21.709	3179	3183	3187	rBV	288604	332651	5.96%	1.098%
19	22.150	3254	3258	3264	rVB	403397	484531	8.69%	1.600%
20	22.639	3336	3341	3347	rBV	422886	587867	10.54%	1.941%
21	23.174	3428	3432	3440	rVB	445177	733280	13.15%	2.421%
22	23.350	3456	3462	3473	rVB	715819	1504892	26.98%	4.969%
23	23.792	3532	3537	3544	rVB	304724	530366	9.51%	1.751%

Sum of corrected areas: 30288485

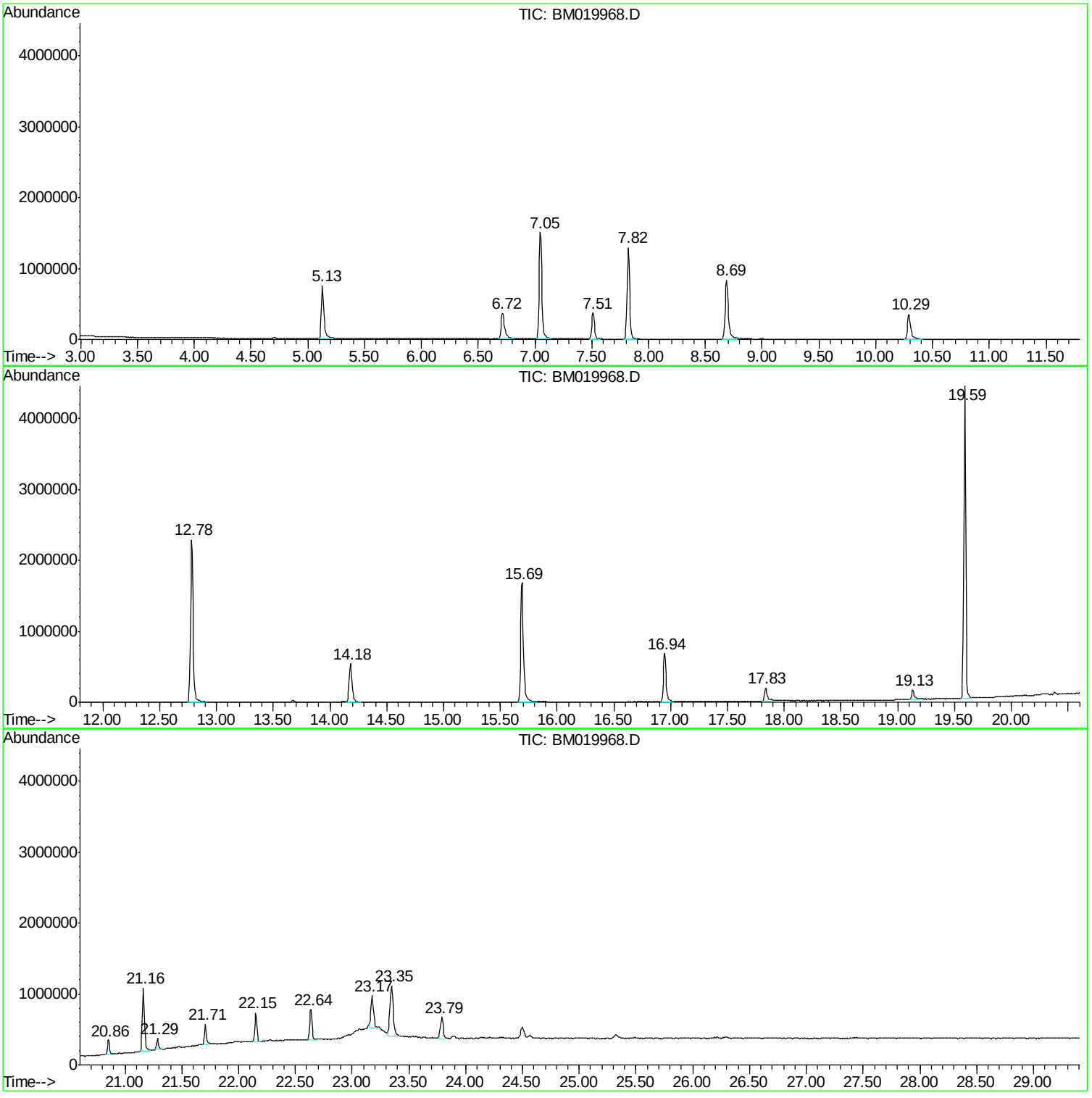
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
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Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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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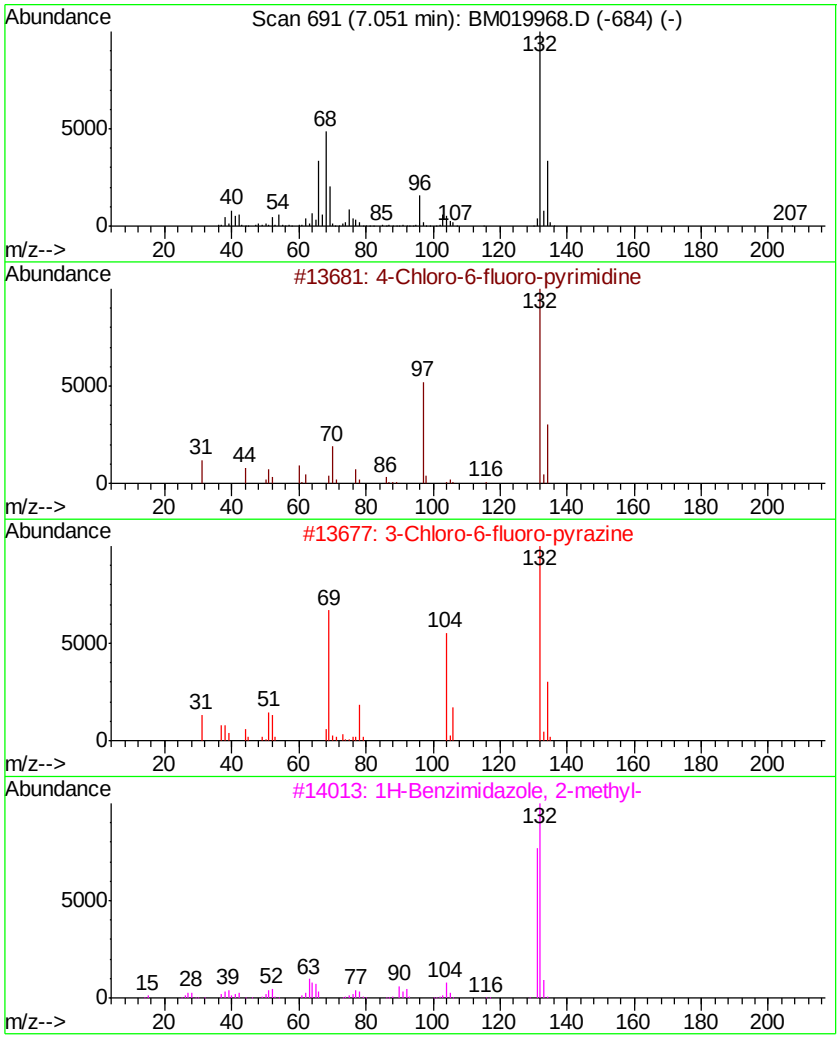
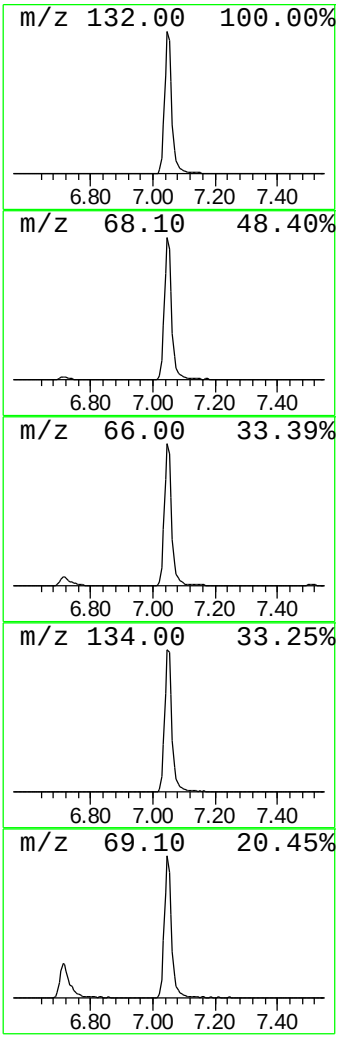
Peak Number 1 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	82.71 ng	2454890	1,4-Dichlorobenzene-d4	7.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13





Library Search Compound Report

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Data File : BM019968.D
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Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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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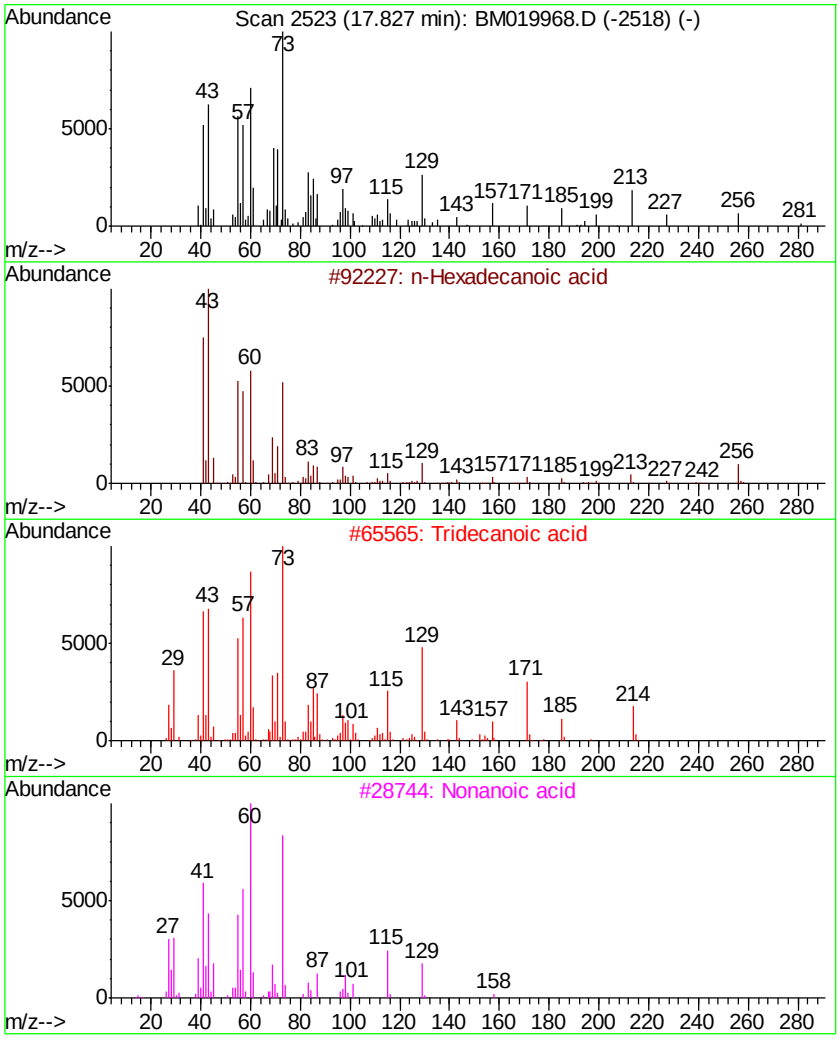
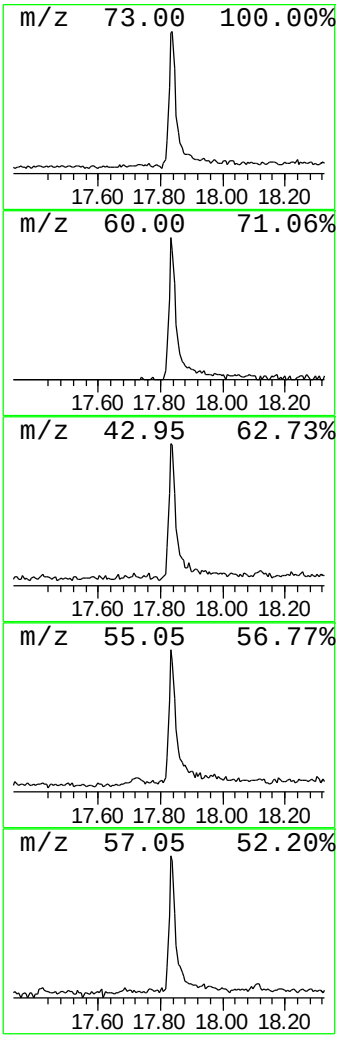
Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	6.30 ng	345494	Phenanthrene-d10	16.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Nonanoic acid	158	C9H18O2	000112-05-0	30
4	d-Glucitol, 4-O-nonyl-	308	C15H32O6	132591-06-1	22
5	Pentadecane	212	C15H32	000629-62-9	11





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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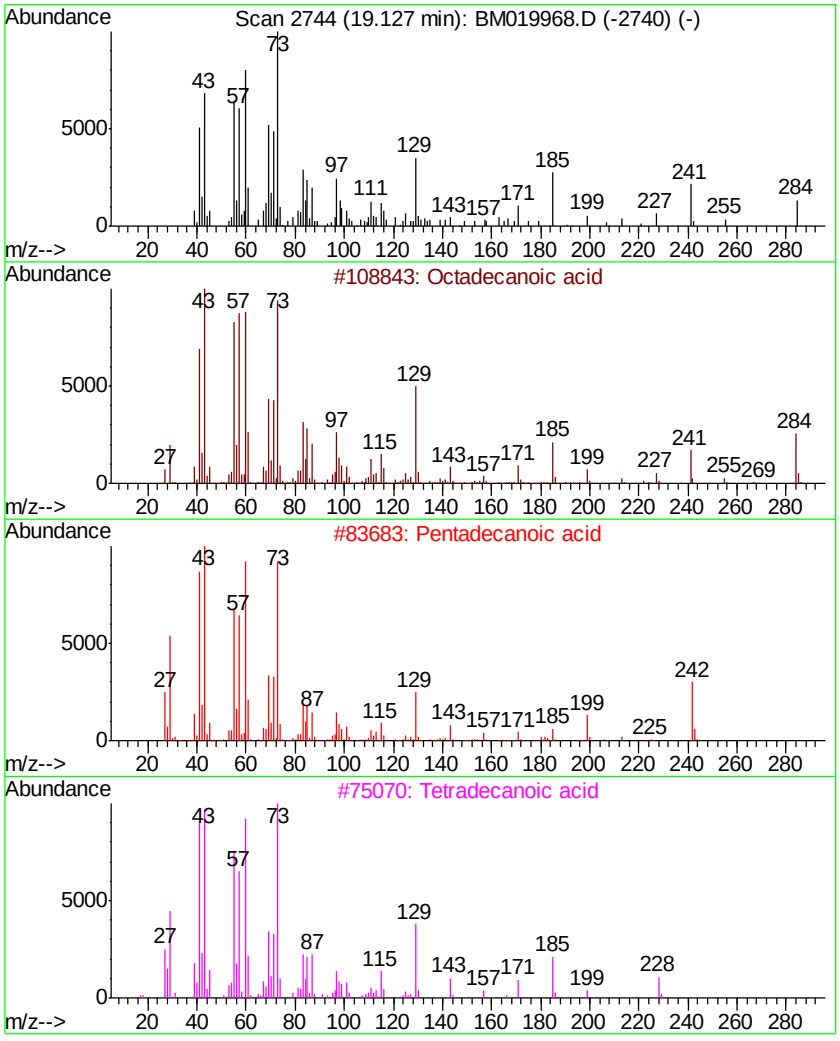
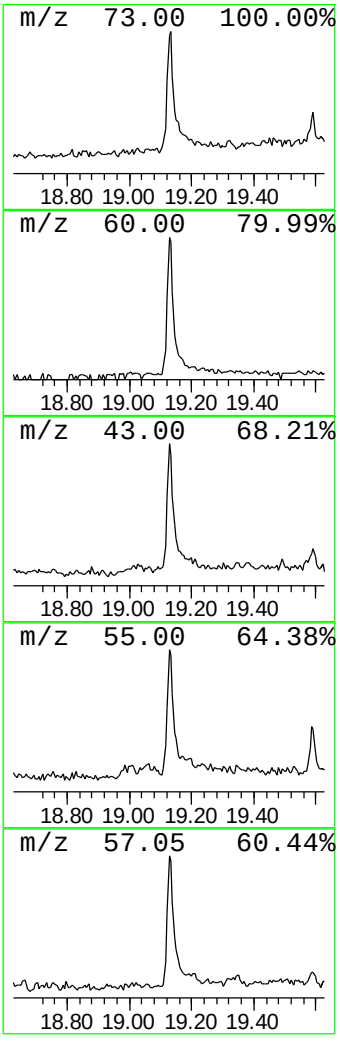
Peak Number 4 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	3.70 ng	237453	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tetratetracontane	619	C44H90	007098-22-8	11





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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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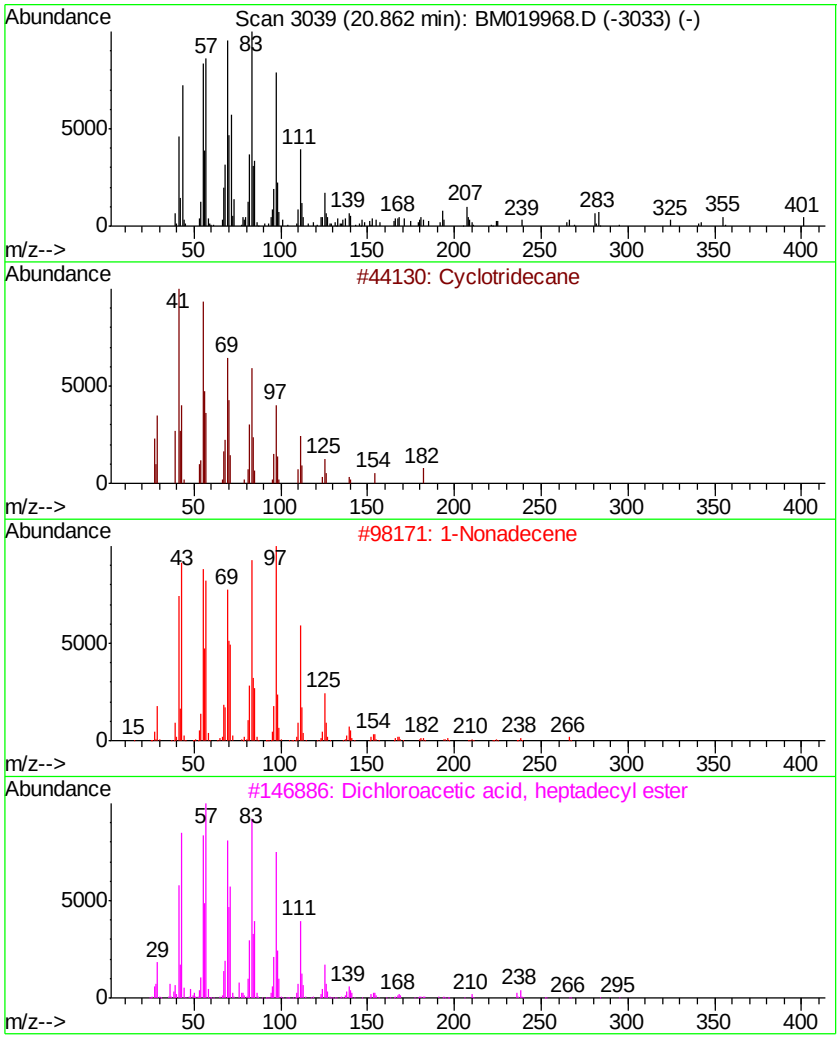
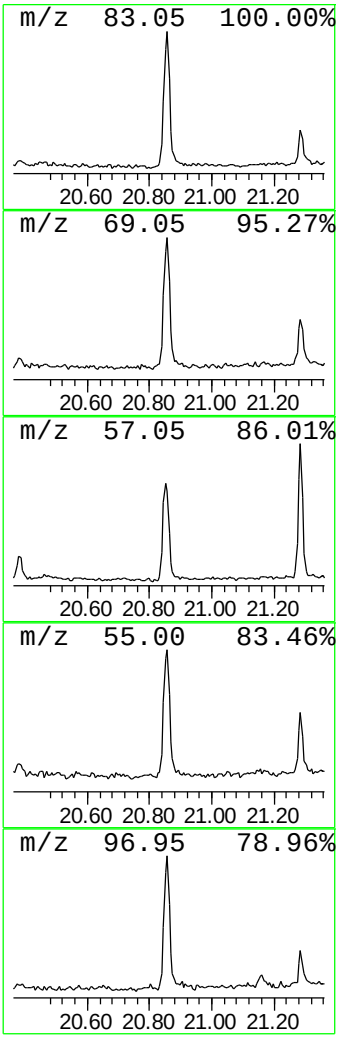
Peak Number 5 Cyclotridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	5.14 ng	330051	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotridecane	182	C13H26	000295-02-3	95
2	1-Nonadecene	266	C19H38	018435-45-5	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4	Cyclotetradecane	196	C14H28	000295-17-0	94
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94





Library Search Compound Report

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Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

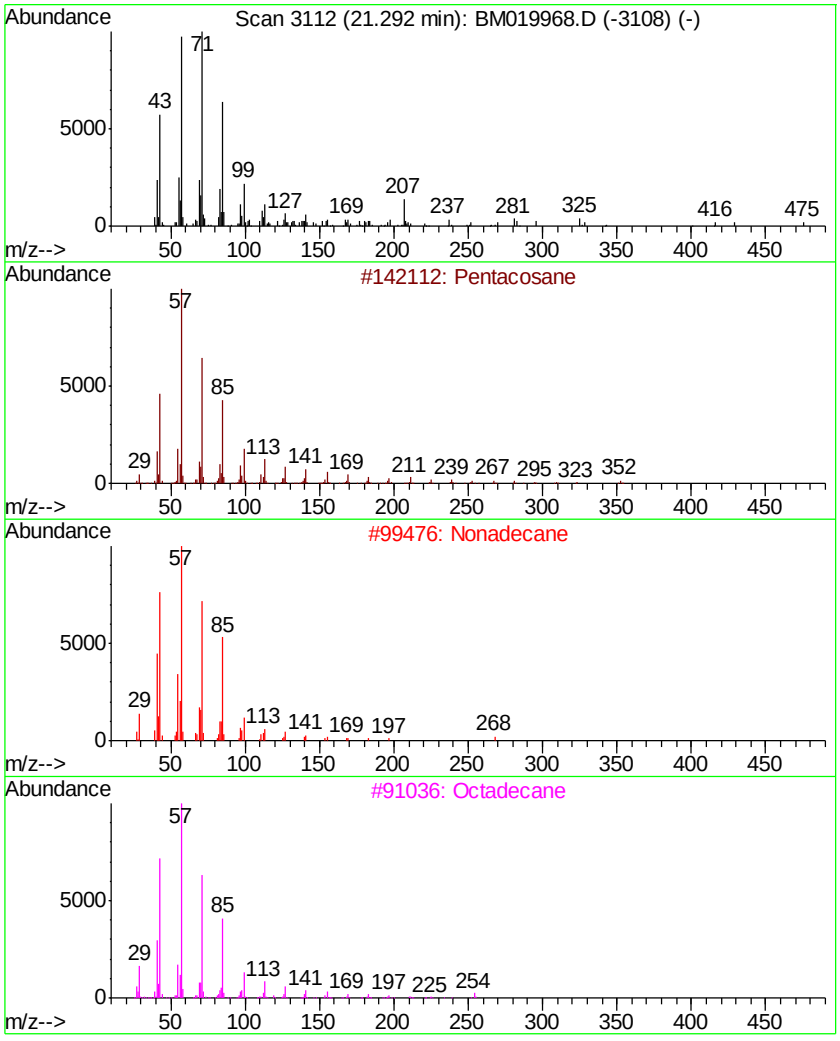
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

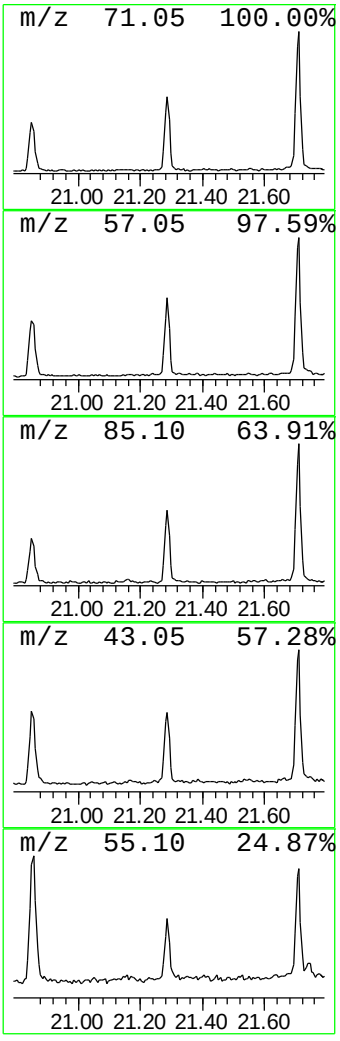
****

Peak Number 6 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	2.61 ng	167479	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Nonadecane	268	C19H40	000629-92-5	90
3	Octadecane	254	C18H38	000593-45-3	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
5	Eicosane	282	C20H42	000112-95-8	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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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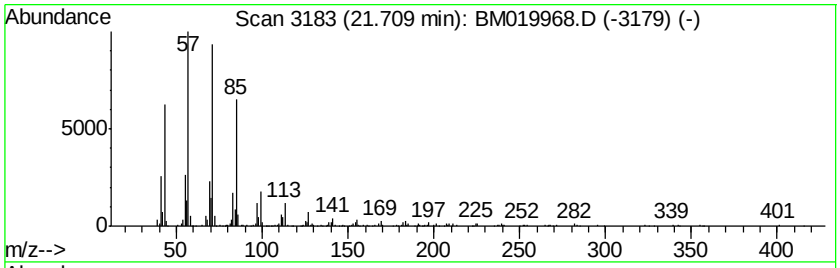
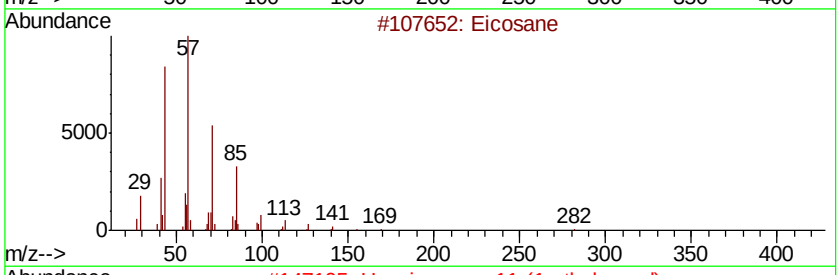
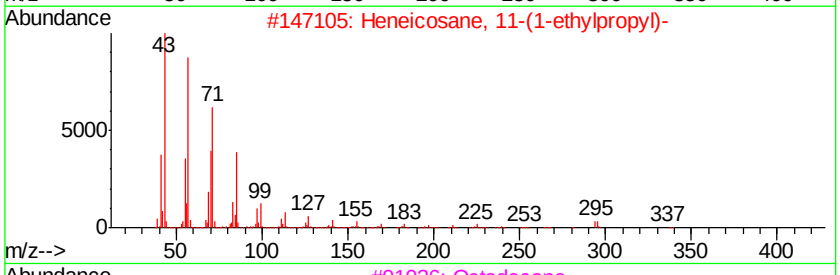
Peak Number 7 Eicosane Concentration Rank 8

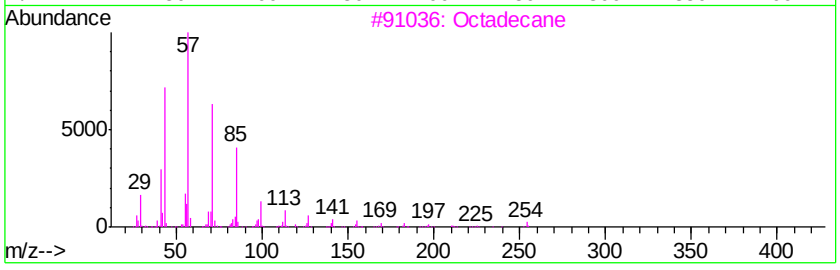
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.71	5.18 ng	332651	Chrysene-d12	21.16

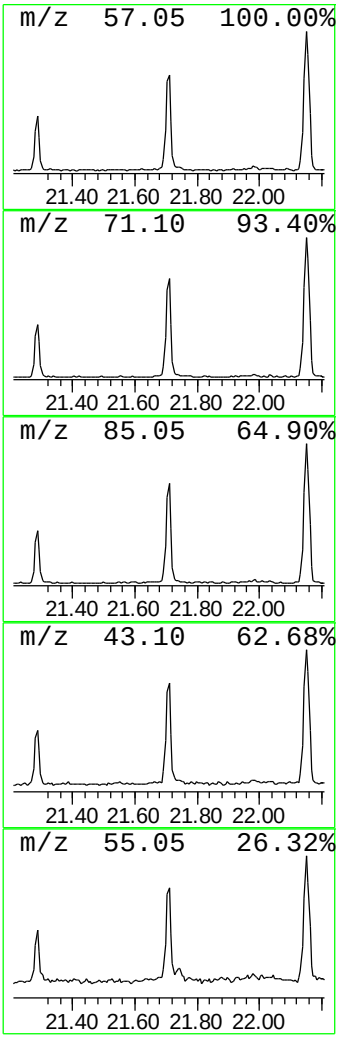
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3	Octadecane	254	C18H38	000593-45-3	87
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5	Nonadecane	268	C19H40	000629-92-5	86











Library Search Compound Report

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

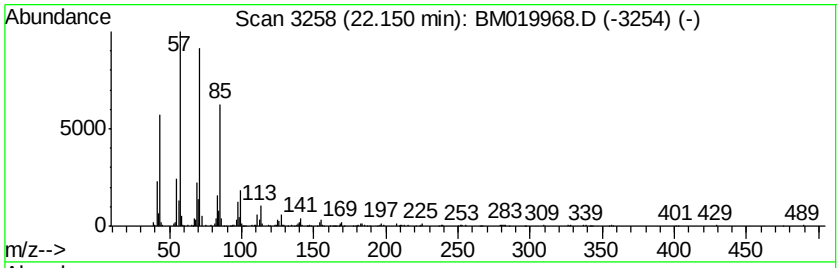
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

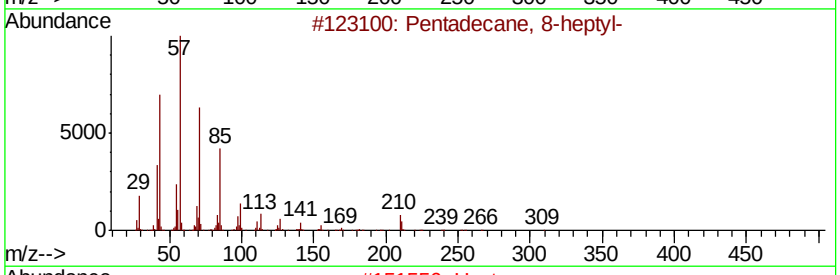
****

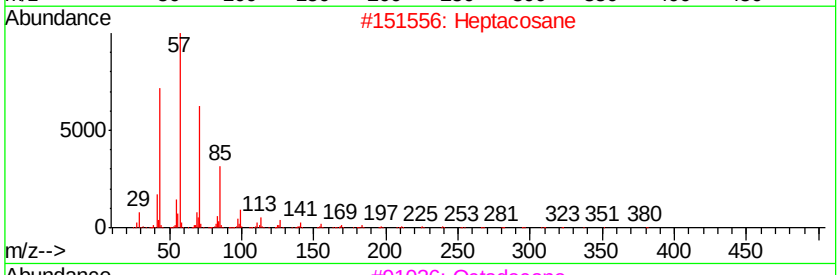
Peak Number 8 Pentadecane, 8-heptyl- Concentration Rank 5

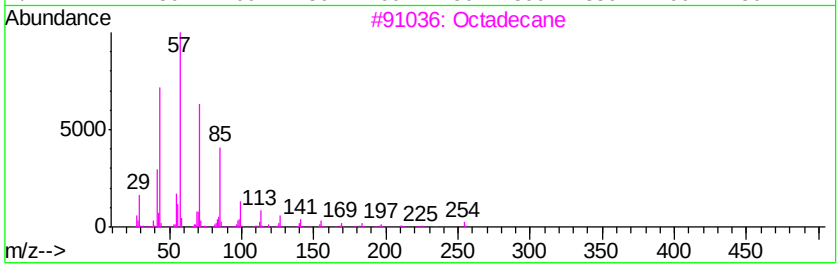
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.15	7.55 ng	484531	Chrysene-d12	21.16

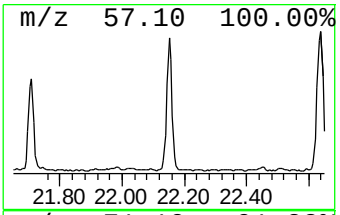
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	Octadecane	254	C18H38	000593-45-3	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86

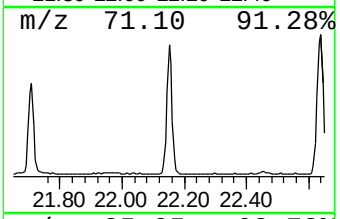


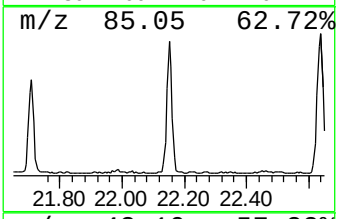


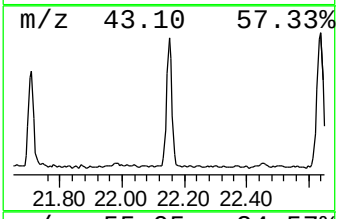


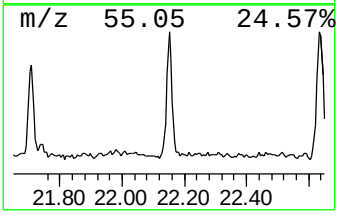












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Operator : JU/SJ
Sample : K2461-04
Misc :
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Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
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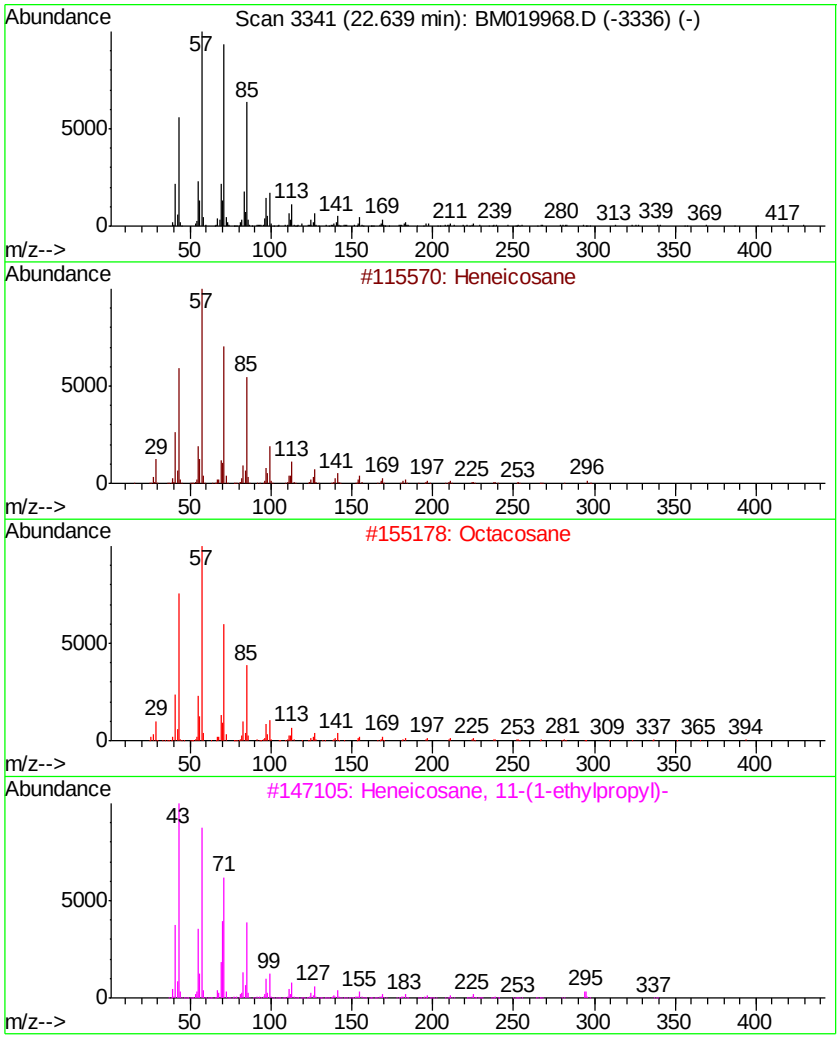
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

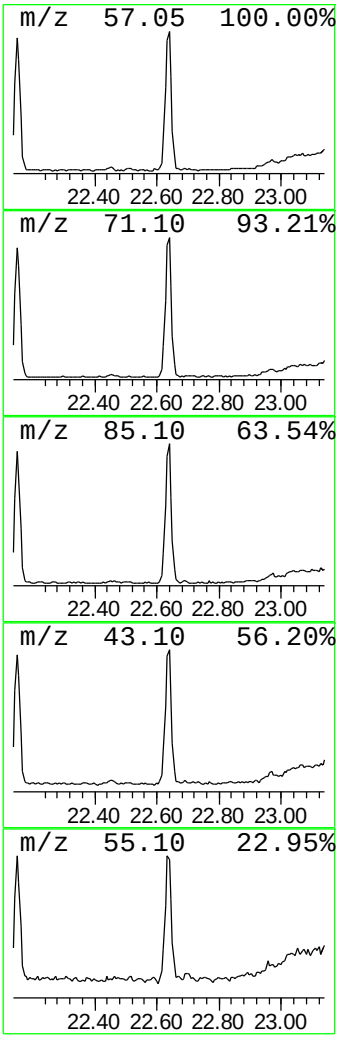
****

Peak Number 9 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.64	7.81 ng	587867	Perylene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5	Nonacosane	408	C29H60	000630-03-5	90





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Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

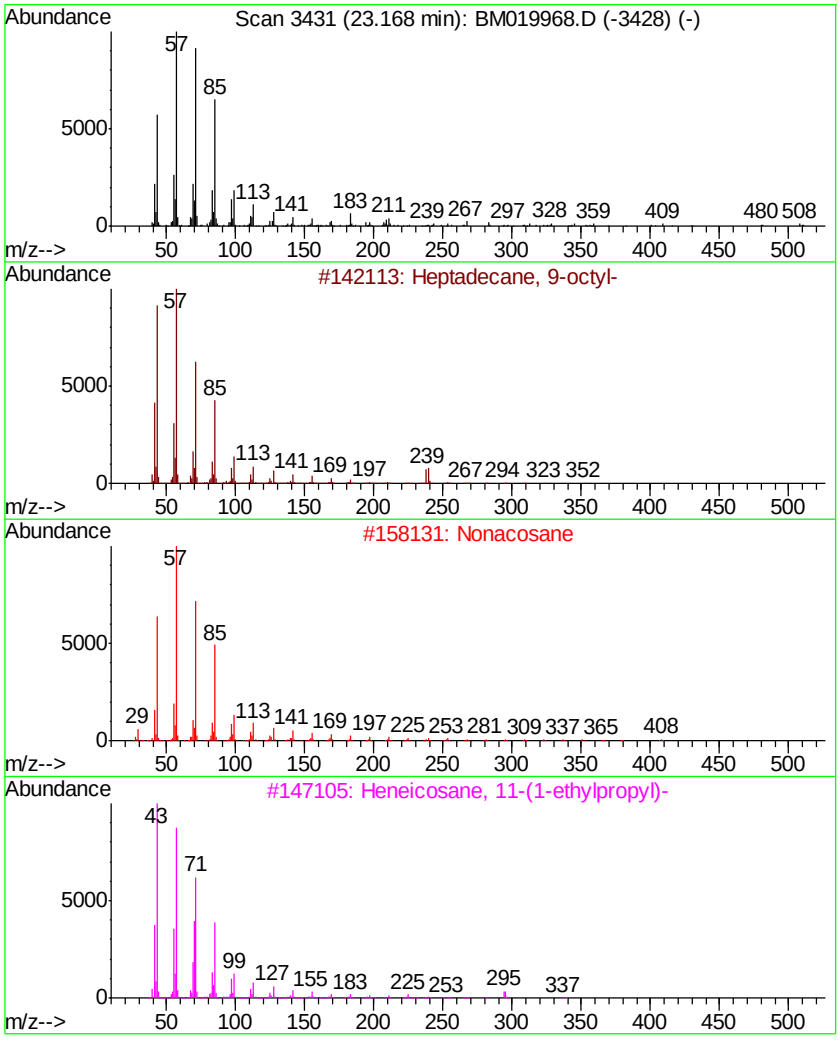
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

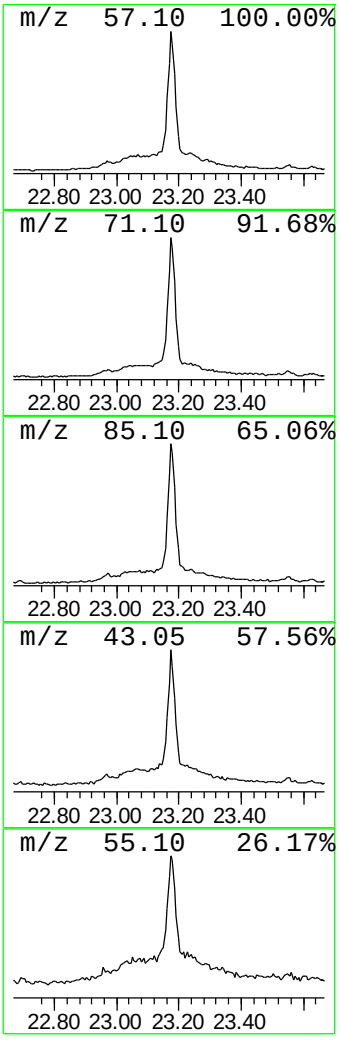
****

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	9.75 ng	733280	Perylene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Nonacosane	408	C29H60	000630-03-5	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Dodecane	170	C12H26	000112-40-3	83
5	Eicosane, 3-methyl-	296	C21H44	006418-46-8	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

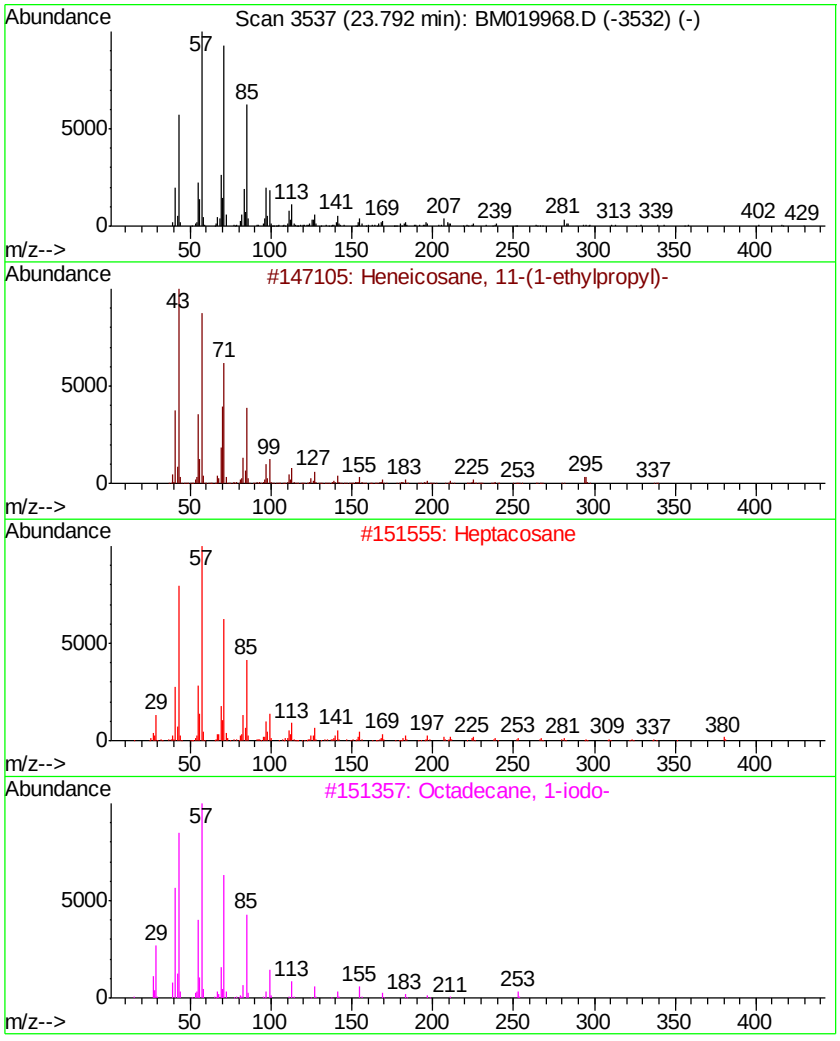
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

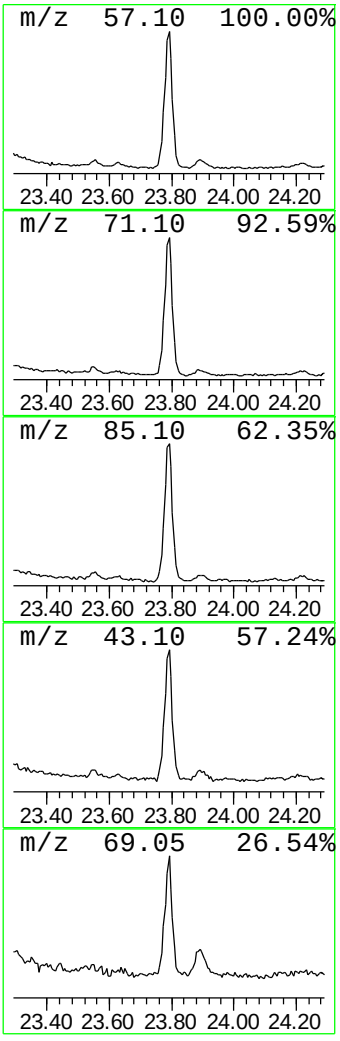
****

Peak Number 11 Heneicosane, 11-(1-ethylpro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.79	7.05 ng	530366	Perylene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
2	Heptacosane	380	C27H56	000593-49-7	86
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
4	Octacosane	394	C28H58	000630-02-4	72
5	Octadecane	254	C18H38	000593-45-3	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041819\
Data File : BM019968.D
Acq On : 18 Apr 2019 23:58
Operator : JU/SJ
Sample : K2461-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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
unknown7.05	7.05	82.7	ng	2454890	1	7.51	593592	20.0
n-Hexadecanoic acid	17.83	6.3	ng	345494	4	16.94	1096200	20.0
Octadecanoic acid	19.13	3.7	ng	237453	5	21.16	1284000	20.0
Cyclotridecane	20.86	5.1	ng	330051	5	21.16	1284000	20.0
Pentacosane	21.29	2.6	ng	167479	5	21.16	1284000	20.0
Eicosane	21.71	5.2	ng	332651	5	21.16	1284000	20.0
Pentadecane, 8-he...	22.15	7.5	ng	484531	5	21.16	1284000	20.0
Heneicosane	22.64	7.8	ng	587867	6	23.35	1504890	20.0
Heptadecane, 9-oc...	23.17	9.8	ng	733280	6	23.35	1504890	20.0
Heneicosane, 11-(...	23.79	7.0	ng	530366	6	23.35	1504890	20.0