LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031319\
Data File : BM019154.D
Acq On : 13 Mar 2019 20:06
Operator : JU/SJ
Sample : K1861-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BF-10-031119

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	5.257	380	386	408	rBV	4309906	6170016	39.54%	7.324%
2	6.840	648	655	679	rBV	4345479	7405059	47.45%	8.790%
3	7.193	708	715	730	rBV	4489816	7034020	45.07%	8.349%
4	7.657	787	794	803	rBV	782504	1215823	7.79%	1.443%
5	7.975	835	848	862	rBV	3032360	4846002	31.05%	5.752%
6	8.828	985	993	1016	rBV	2366203	4033191	25.84%	4.787%
7	10.445	1261	1268	1286	rBV	941643	1698988	10.89%	2.017%
8	12.928	1682	1690	1710	rBV	6749660	10086866	64.64%	11.973%
9	13.780	1828	1835	1850	rBV	399280	651874	4.18%	0.774%
10	14.310	1918	1925	1940	rBV2	1677890	2598831	16.65%	3.085%
11	15.810	2174	2180	2198	rBV	6141537	9144871	58.60%	10.855%
12	17.068	2386	2394	2407	rBV	2183500	3293542	21.10%	3.909%
13	17.957	2539	2545	2556	rBV	283136	484636	3.11%	0.575%
14	19.704	2836	2842	2853	rBV	13001476	15605548	100.00%	18.524%
15	20.962	3052	3056	3065	rBV	774117	967061	6.20%	1.148%
16	21.262	3102	3107	3117	rBV	2600050	3464820	22.20%	4.113%
17	21.398	3127	3130	3138	rBV	267895	332881	2.13%	0.395%
18	21.833	3200	3204	3206	rBV	353938	440431	2.82%	0.523%
19	22.286	3278	3281	3290	rVB	398585	512753	3.29%	0.609%
20	22.792	3363	3367	3372	rVB	401500	541345	3.47%	0.643%
21	23.350	3458	3462	3470	rVB	312249	503906	3.23%	0.598%
22	23.503	3481	3488	3500	rBV	1454619	2795555	17.91%	3.318%
23	23.991	3568	3571	3579	rVB	228496	417254	2.67%	0.495%

Sum of corrected areas: 84245273

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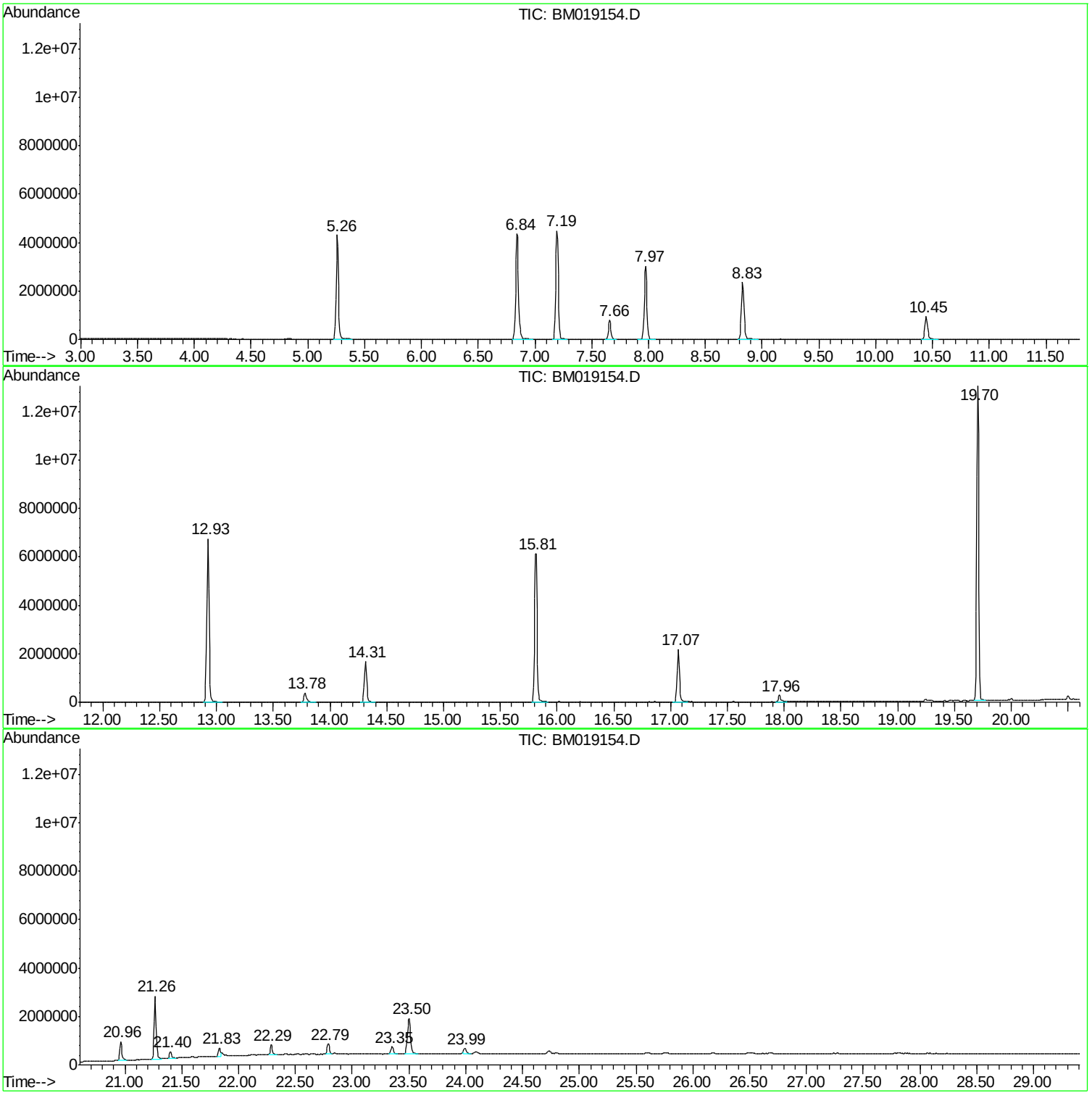
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BF-10-031119

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\BM031319\
Data File : BM019154.D
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Operator : JU/SJ
Sample : K1861-05
Misc :
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Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

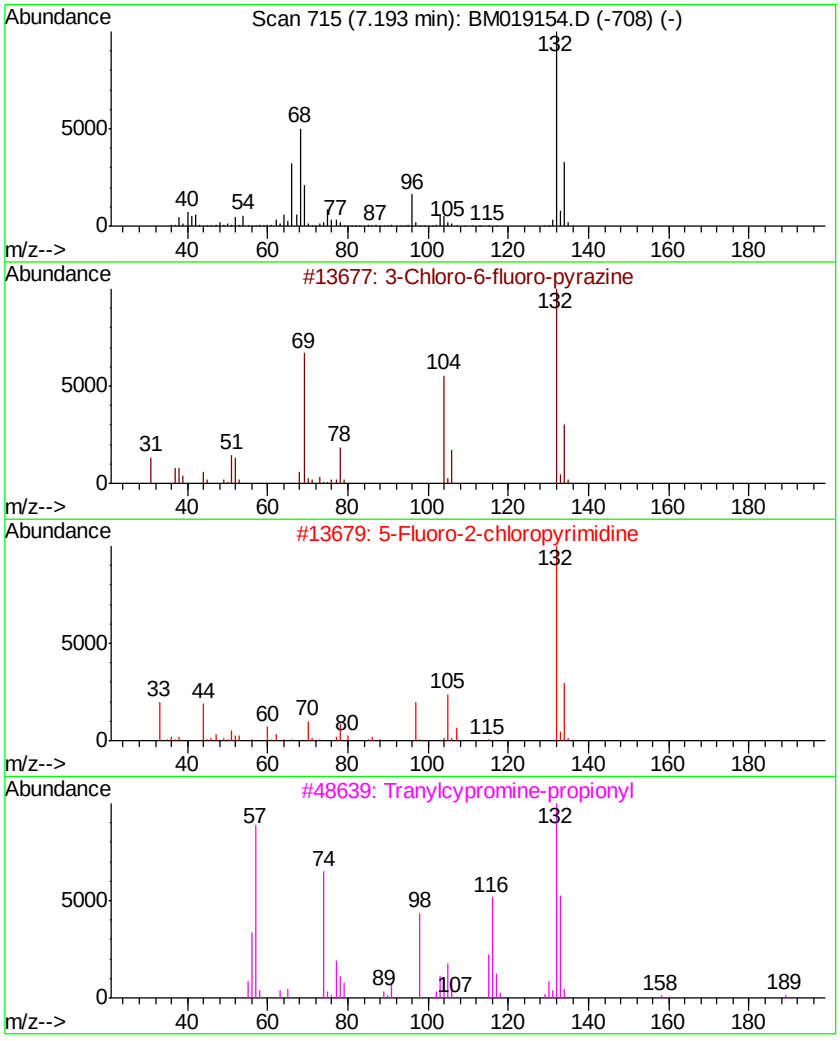
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

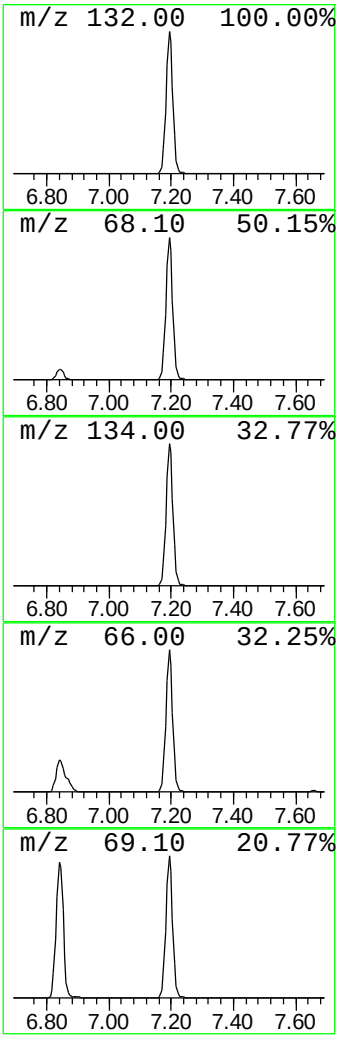
****

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	115.71 ng	7034020	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11





Library Search Compound Report

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Operator : JU/SJ
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Instrument : BNA_M
ClientSampleId : BF-10-031119

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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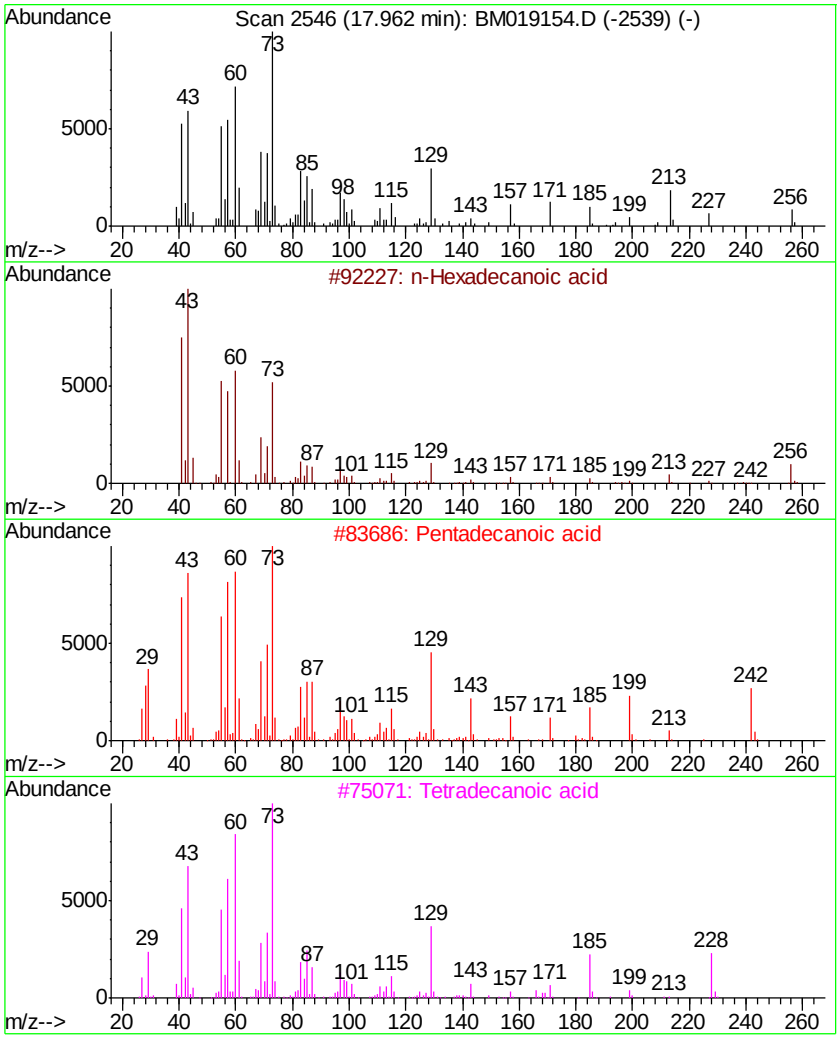
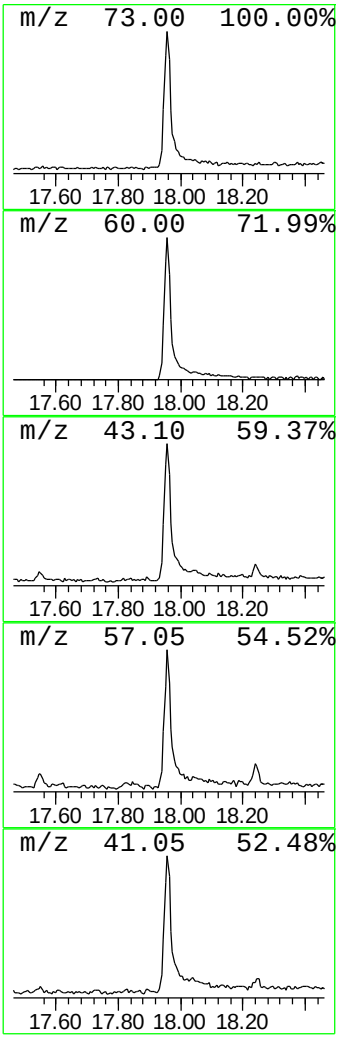
Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	2.94 ng	484636	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	38
5	Tridecane	184	C13H28	000629-50-5	11





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031319\
Data File : BM019154.D
Acq On : 13 Mar 2019 20:06
Operator : JU/SJ
Sample : K1861-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BF-10-031119

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

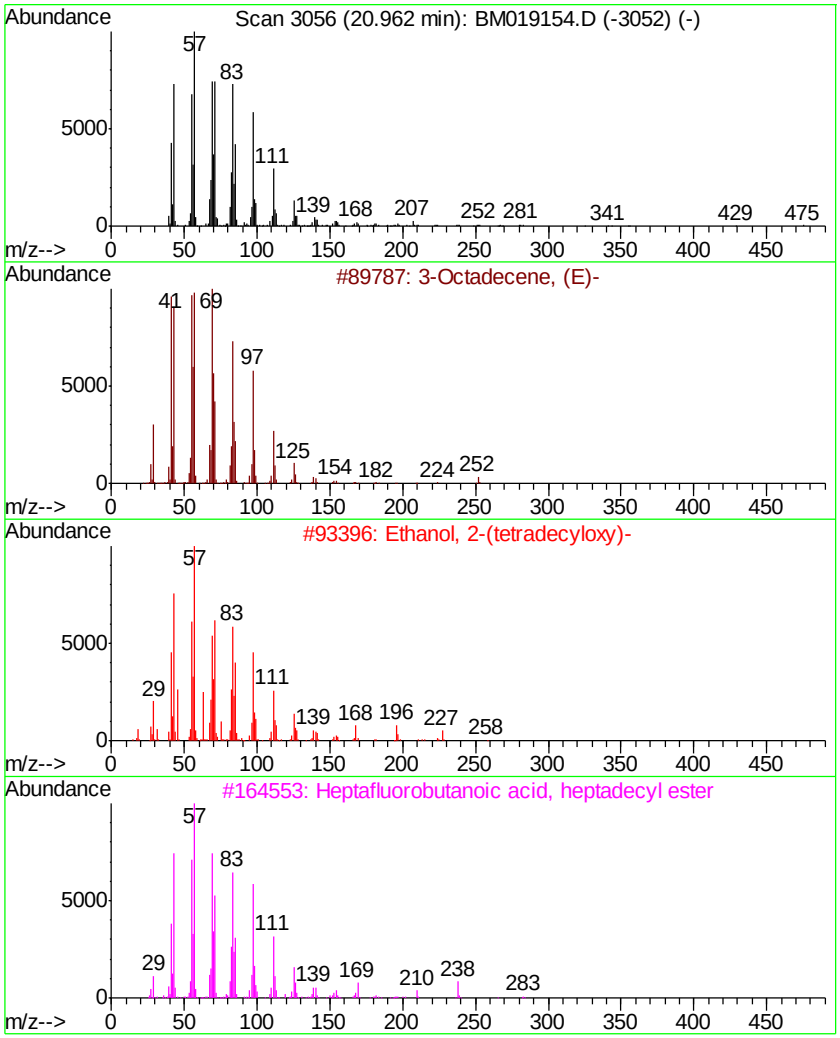
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

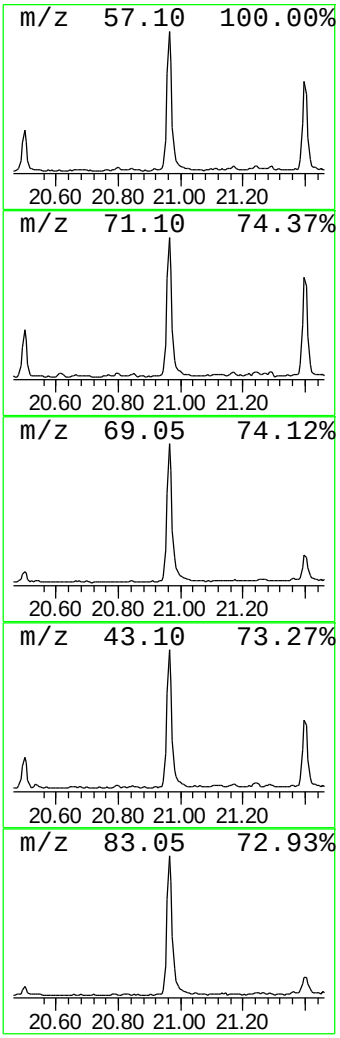
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.96	5.58 ng	967061	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	95
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	76
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	74
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	74
5	1-Octadecanol	270	C18H38O	000112-92-5	70





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Data File : BM019154.D
Acq On : 13 Mar 2019 20:06
Operator : JU/SJ
Sample : K1861-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BF-10-031119

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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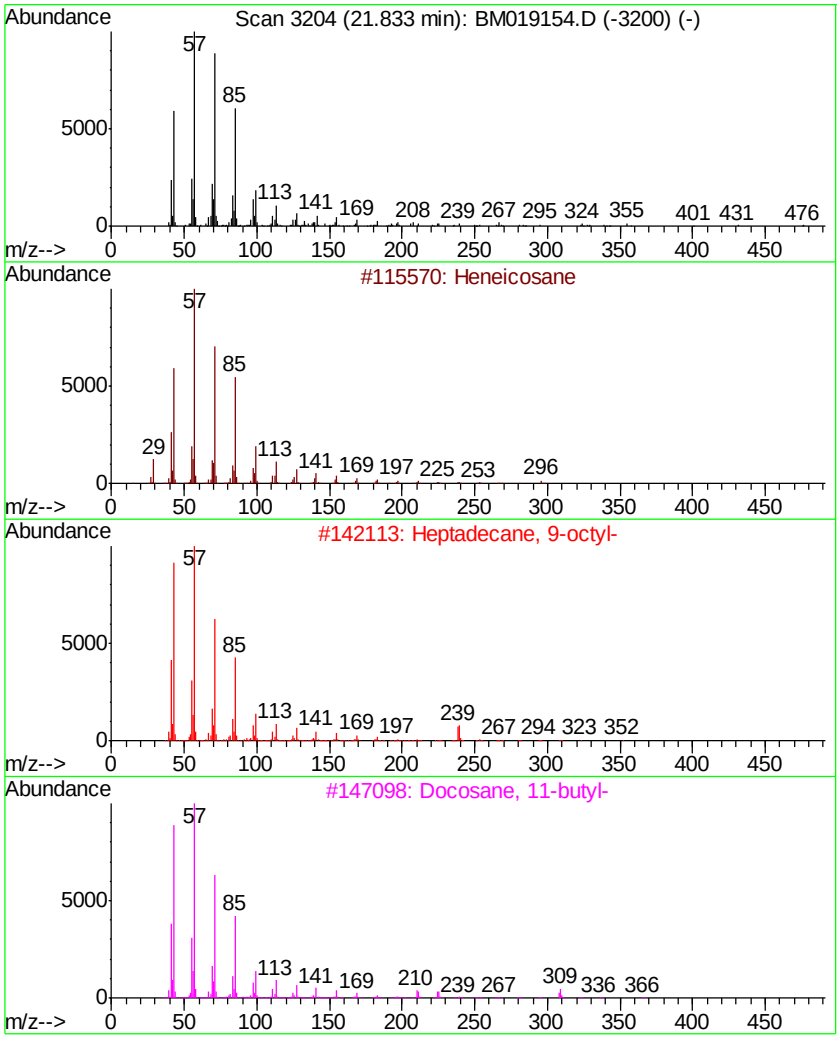
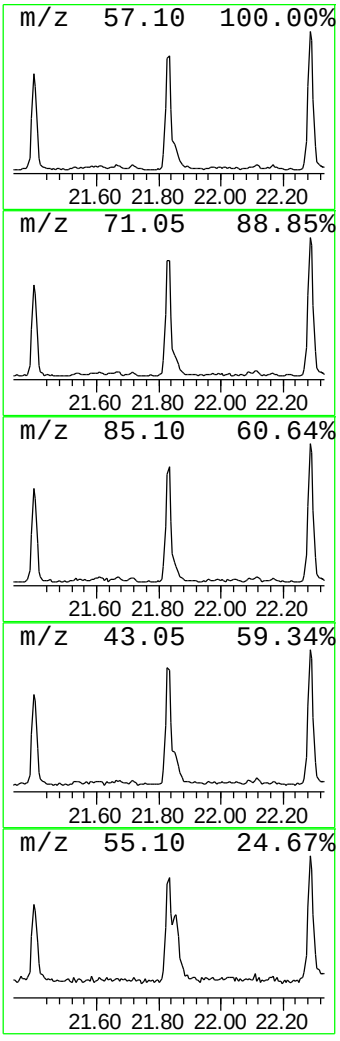
Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.83	2.54 ng	440431	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91





Library Search Compound Report

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Acq On : 13 Mar 2019 20:06
Operator : JU/SJ
Sample : K1861-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BF-10-031119

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
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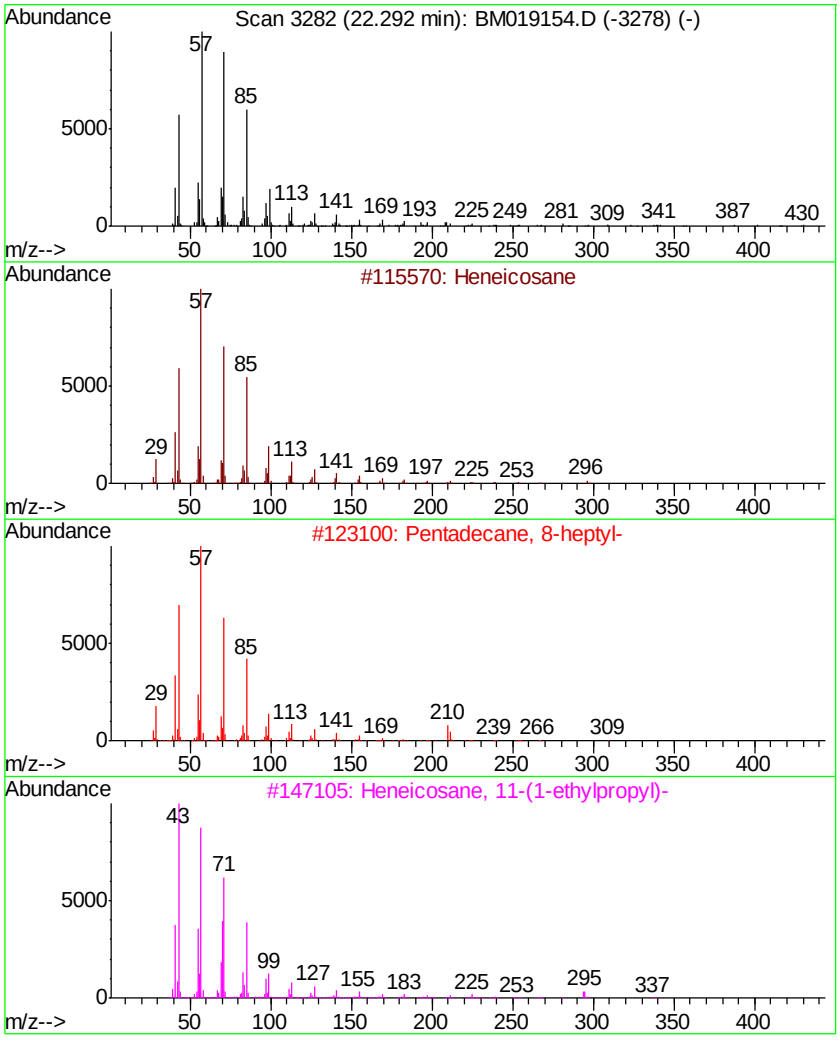
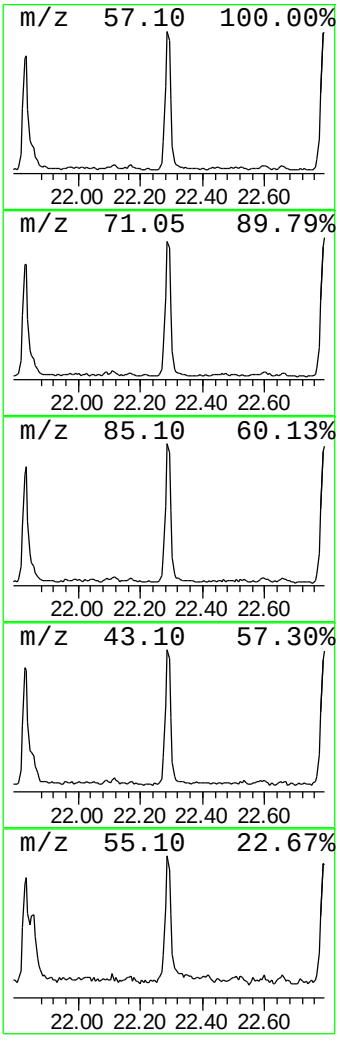
****

Peak Number 6 Pentadecane, 8-heptyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.29	2.96 ng	512753	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BF-10-031119

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

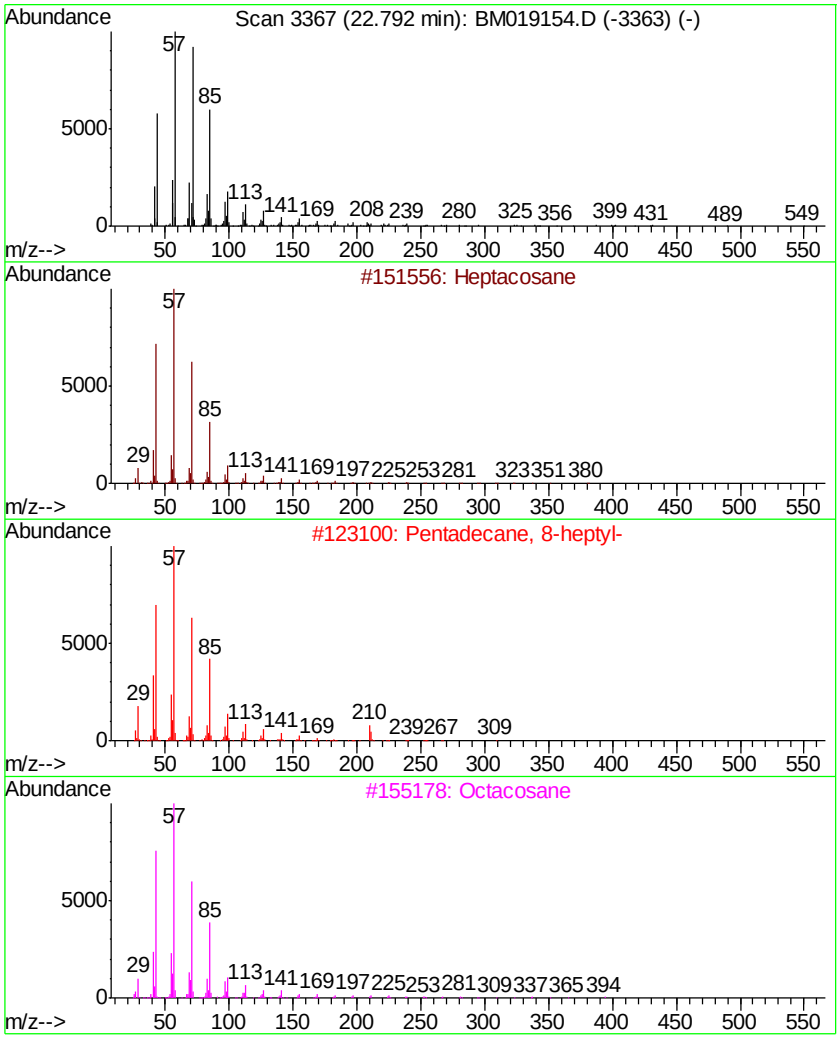
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

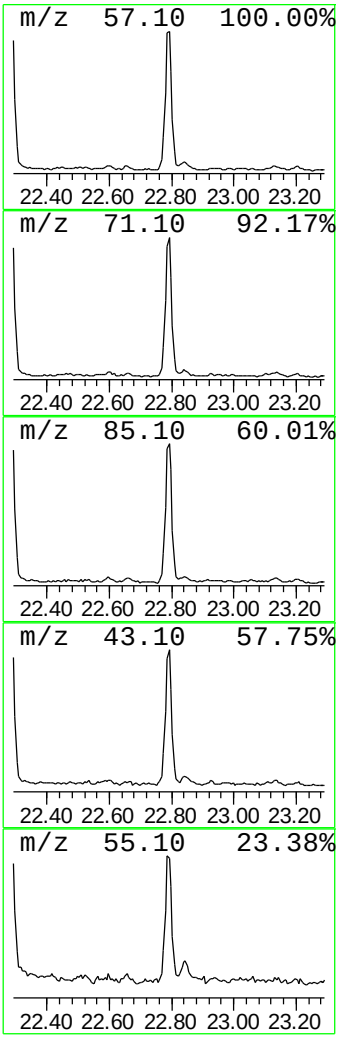
****

Peak Number 7 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.79	3.87 ng	541345	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Octacosane	394	C28H58	000630-02-4	83
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80
5	Heneicosane	296	C21H44	000629-94-7	70





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Instrument : BNA_M
ClientSampleId : BF-10-031119

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

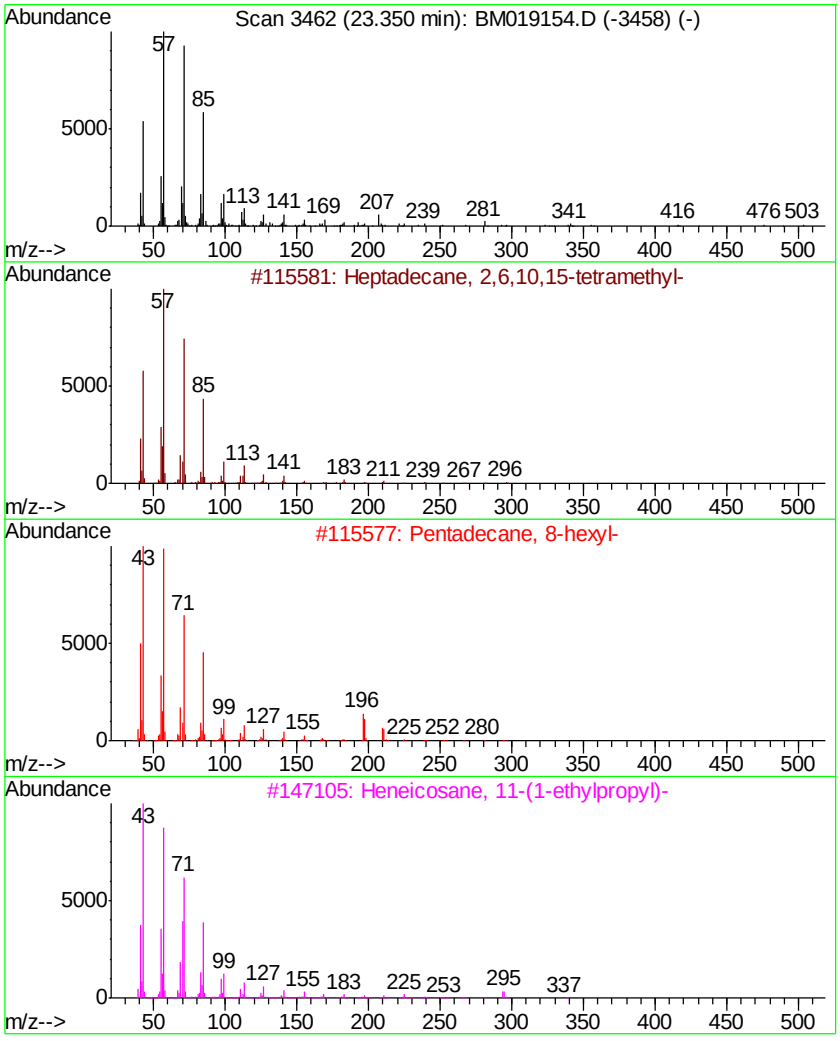
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

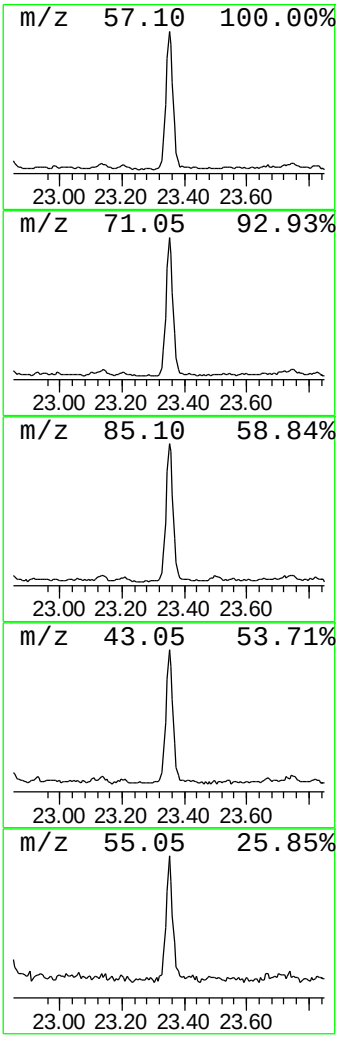
****

Peak Number 8 Heptadecane, 2,6,10,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	3.61 ng	503906	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90





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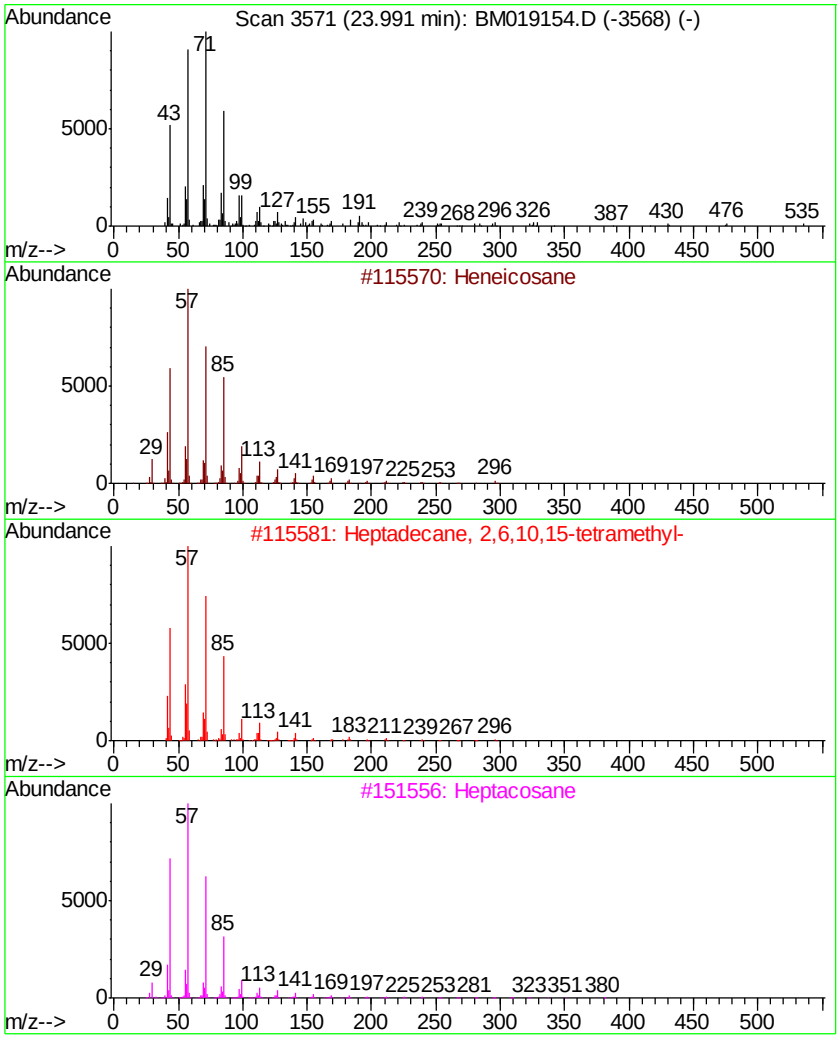
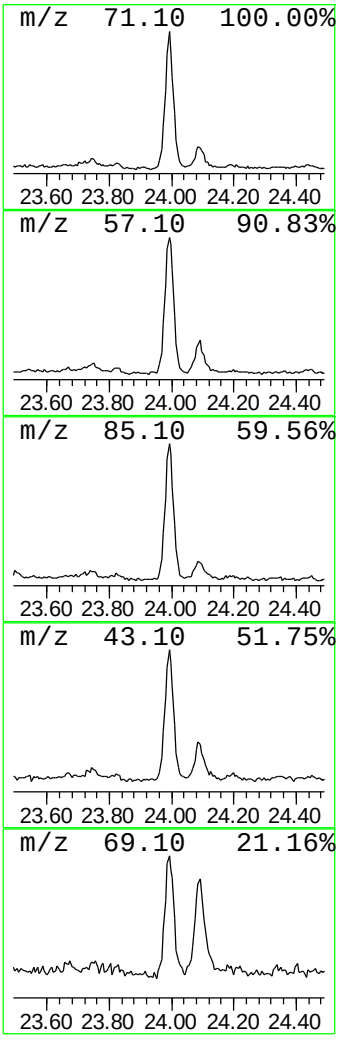
****

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.99 ng	417254	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Heptacosane	380	C27H56	000593-49-7	74
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	72
5	Octacosane	394	C28H58	000630-02-4	72





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
unknown7.19	7.19	115.7	ng	7034020	1	7.66	1215820	20.0
n-Hexadecanoic acid	17.96	2.9	ng	484636	4	17.07	3293540	20.0
3-Octadecene, (E)-	20.96	5.6	ng	967061	5	21.26	3464820	20.0
Heneicosane	21.83	2.5	ng	440431	5	21.26	3464820	20.0
Pentadecane, 8-he...	22.29	3.0	ng	512753	5	21.26	3464820	20.0
Heptacosane	22.79	3.9	ng	541345	6	23.50	2795560	20.0
Heptadecane, 2,6,...	23.35	3.6	ng	503906	6	23.50	2795560	20.0
Eicosane, 7-hexyl-	23.99	3.0	ng	417254	6	23.50	2795560	20.0