LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM111318\
Data File : BM017633.D
Acq On : 13 Nov 2018 22:37
Operator : MJ/SJ
Sample : J5920-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DSN001

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-BM111218.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	4.793	302	307	318	rBV	295754	411969	2.82%	0.570%
2	5.240	377	383	396	rBV	1822904	2606548	17.86%	3.609%
3	6.798	642	648	663	rBV	1005380	1648757	11.30%	2.283%
4	7.151	700	708	721	rBV	3462425	5537711	37.94%	7.668%
5	7.616	780	787	796	rBV	967351	1530377	10.49%	2.119%
6	7.928	832	840	852	rBV	3326570	5375065	36.83%	7.443%
7	8.769	975	983	1003	rBV	2689682	4565997	31.29%	6.322%
8	10.386	1251	1258	1276	rBV	1120211	2063846	14.14%	2.858%
9	12.874	1673	1681	1700	rBV	6683903	10131326	69.42%	14.029%
10	13.733	1820	1827	1834	rBV	136747	239721	1.64%	0.332%
11	14.263	1910	1917	1932	rBV2	1696486	2716193	18.61%	3.761%
12	15.757	2165	2171	2201	rVB	4933314	7933994	54.36%	10.986%
13	17.015	2378	2385	2400	rBV	2210601	3337391	22.87%	4.621%
14	17.921	2533	2539	2549	rBV	512718	730372	5.00%	1.011%
15	19.209	2753	2758	2767	rBV	302417	457062	3.13%	0.633%
16	19.656	2828	2834	2847	rBV	12622084	14594793	100.00%	20.209%
17	20.939	3049	3052	3059	rBV2	114090	157061	1.08%	0.217%
18	21.215	3093	3099	3111	rBV	2649295	3768691	25.82%	5.218%
19	21.803	3195	3199	3202	rBV	188990	228988	1.57%	0.317%
20	22.256	3272	3276	3281	rVB	274897	371892	2.55%	0.515%
21	22.744	3356	3359	3365	rVB	318712	447880	3.07%	0.620%
22	23.297	3449	3453	3459	rVB	324656	492547	3.37%	0.682%
23	23.403	3466	3471	3484	rVB2	1225860	2470360	16.93%	3.421%
24	23.921	3555	3559	3568	rVB2	213344	400441	2.74%	0.554%

Sum of corrected areas: 72218982

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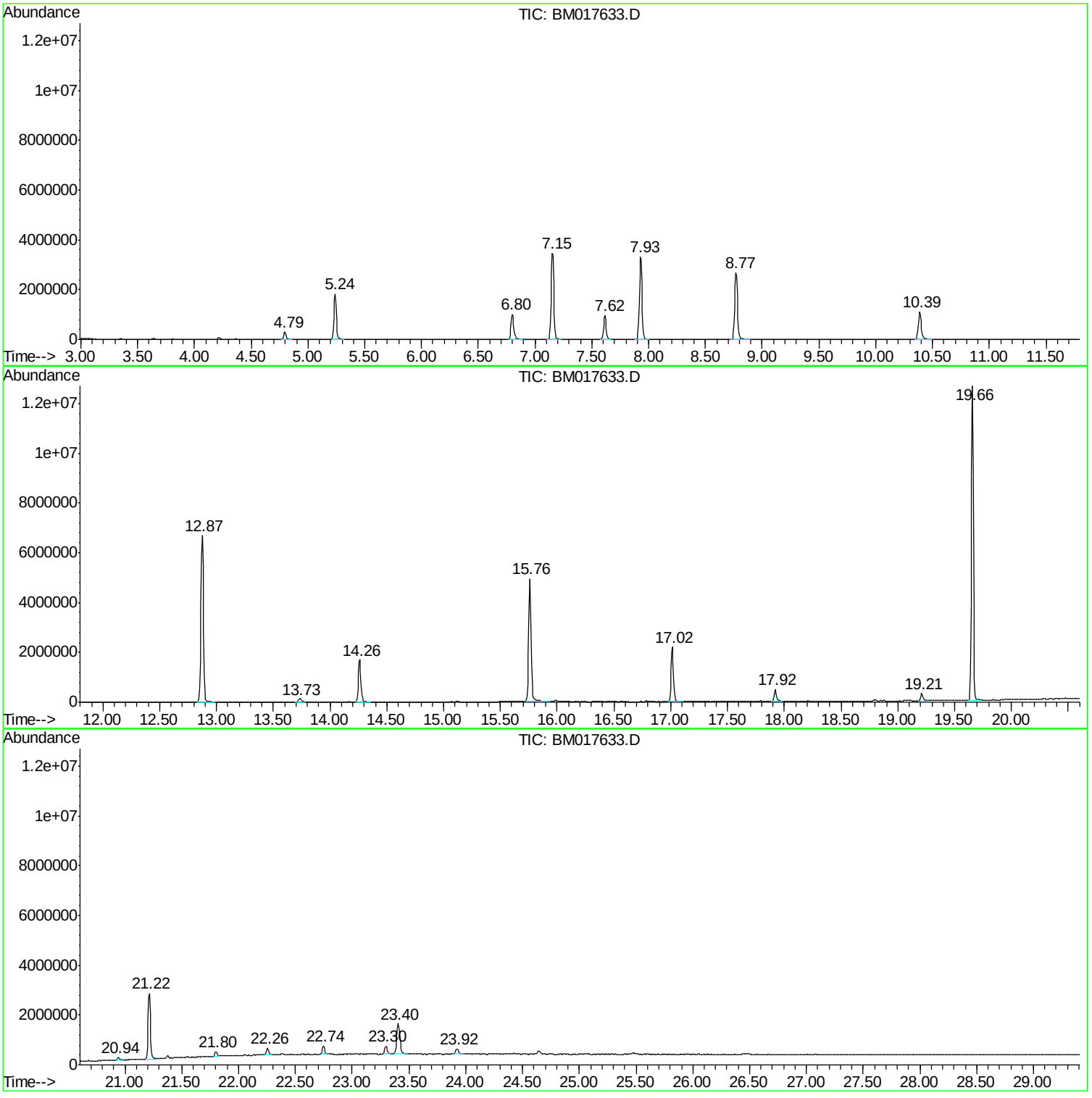
Instrument :
BNA_M
ClientSampleId :
DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.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\BM111318\
Data File : BM017633.D
Acq On : 13 Nov 2018 22:37
Operator : MJ/SJ
Sample : J5920-01
Misc :
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Instrument : BNA_M
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

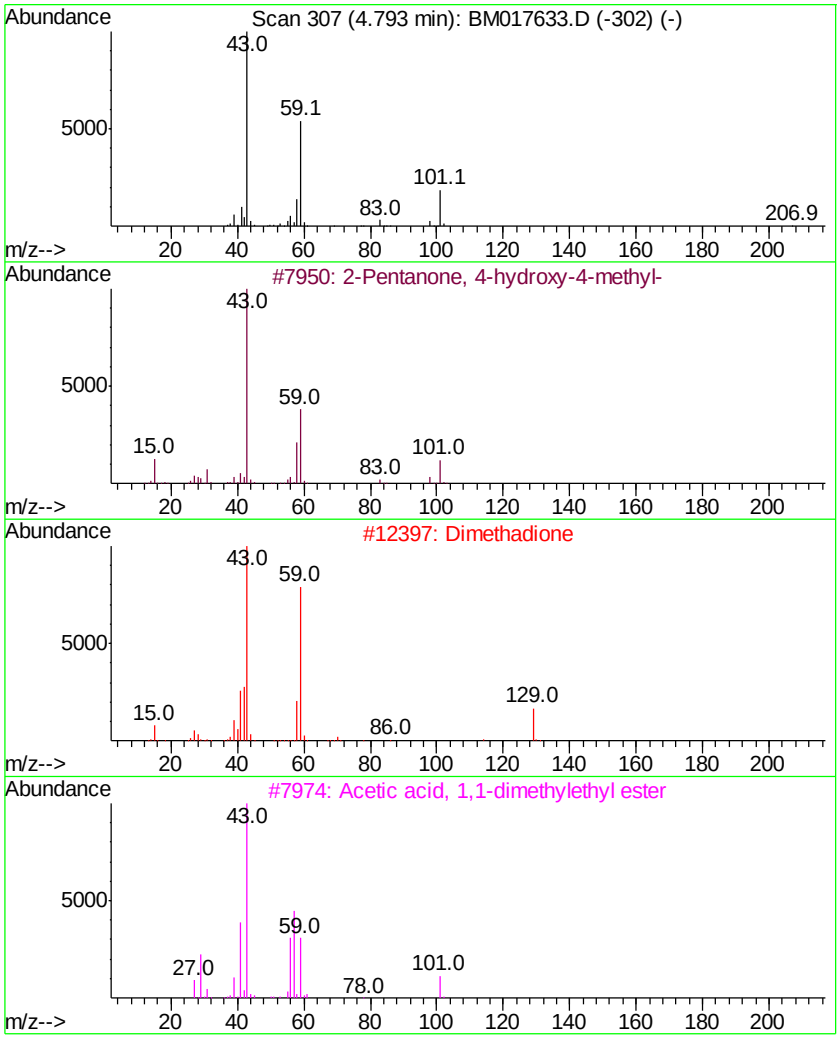
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

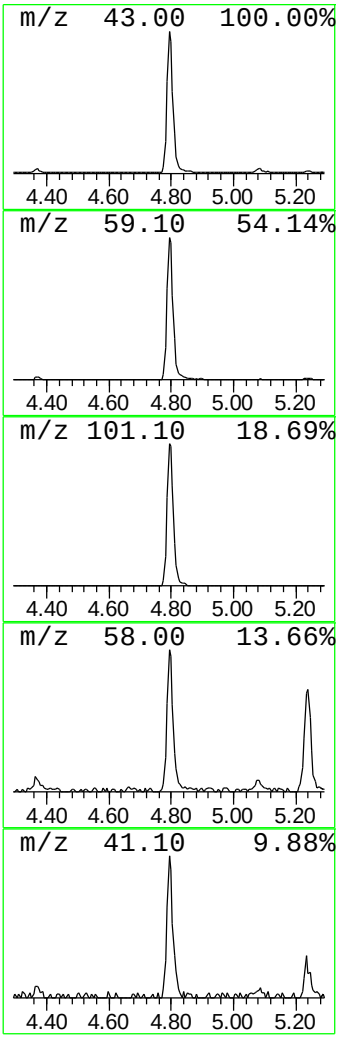
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	5.38 ng	411969	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Dimethadione	129	C5H7NO3	000695-53-4	36
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25





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Sample : J5920-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.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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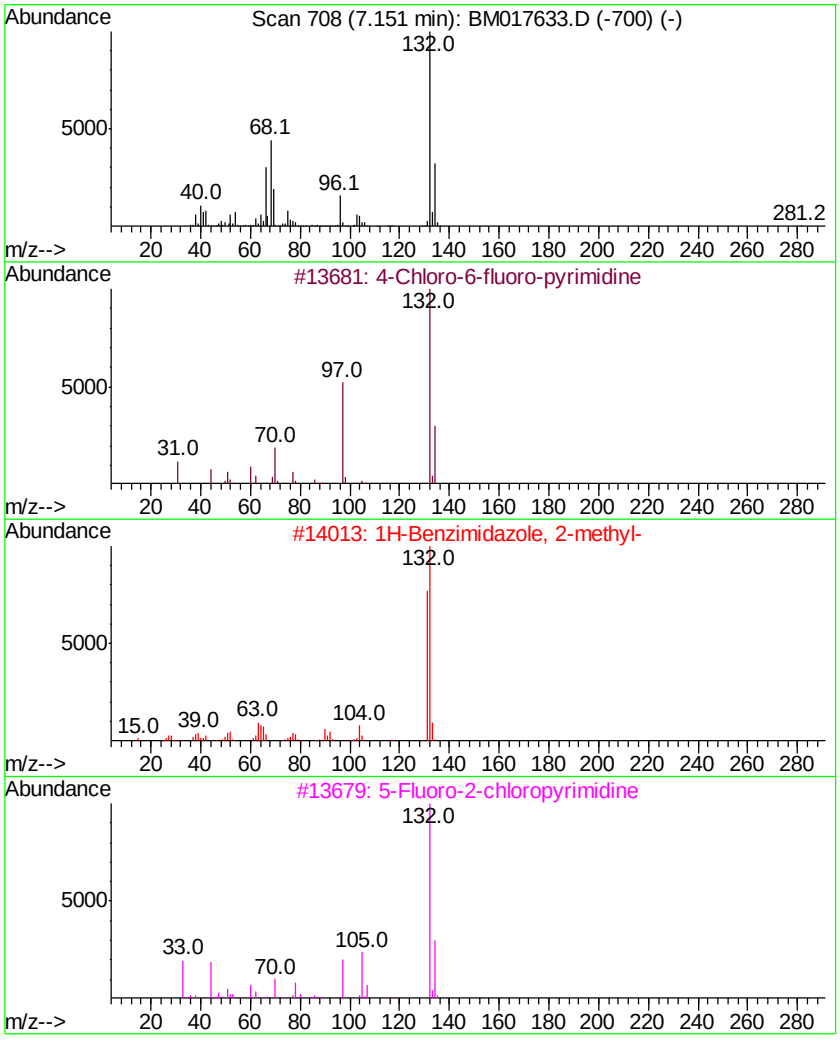
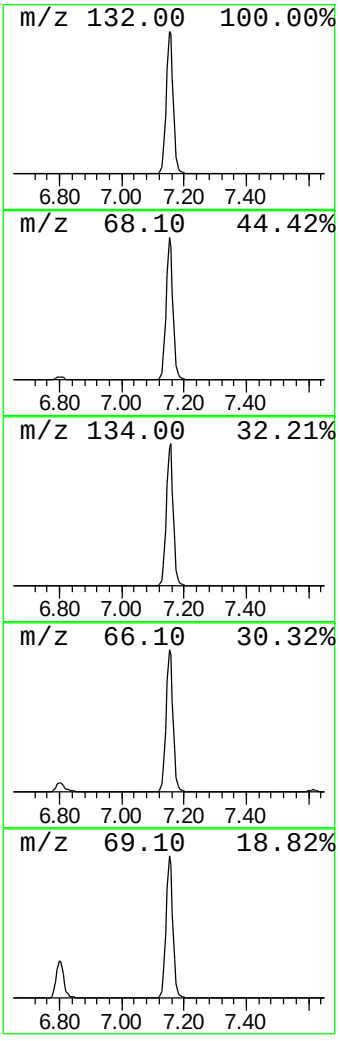
Peak Number 2 unknown7.15 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.15	72.37 ng	5537710	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





Library Search Compound Report

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Data File : BM017633.D
Acq On : 13 Nov 2018 22:37
Operator : MJ/SJ
Sample : J5920-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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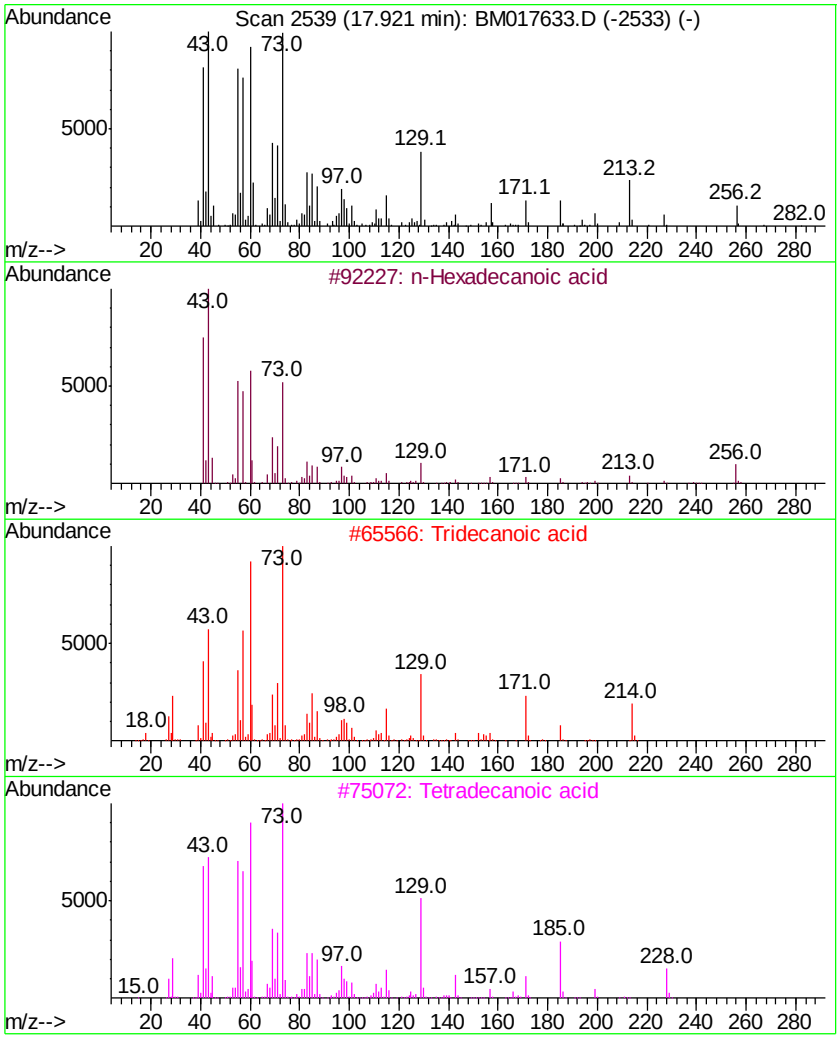
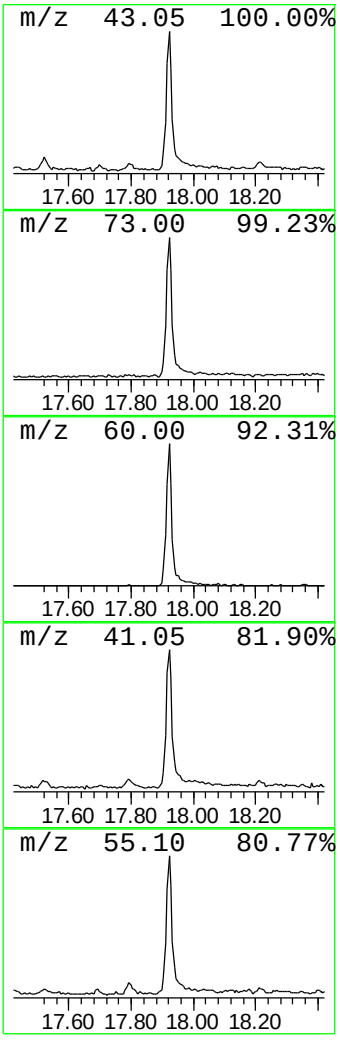
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	4.38 ng	730372	Phenanthrene-d10	17.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM111318\
Data File : BM017633.D
Acq On : 13 Nov 2018 22:37
Operator : MJ/SJ
Sample : J5920-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.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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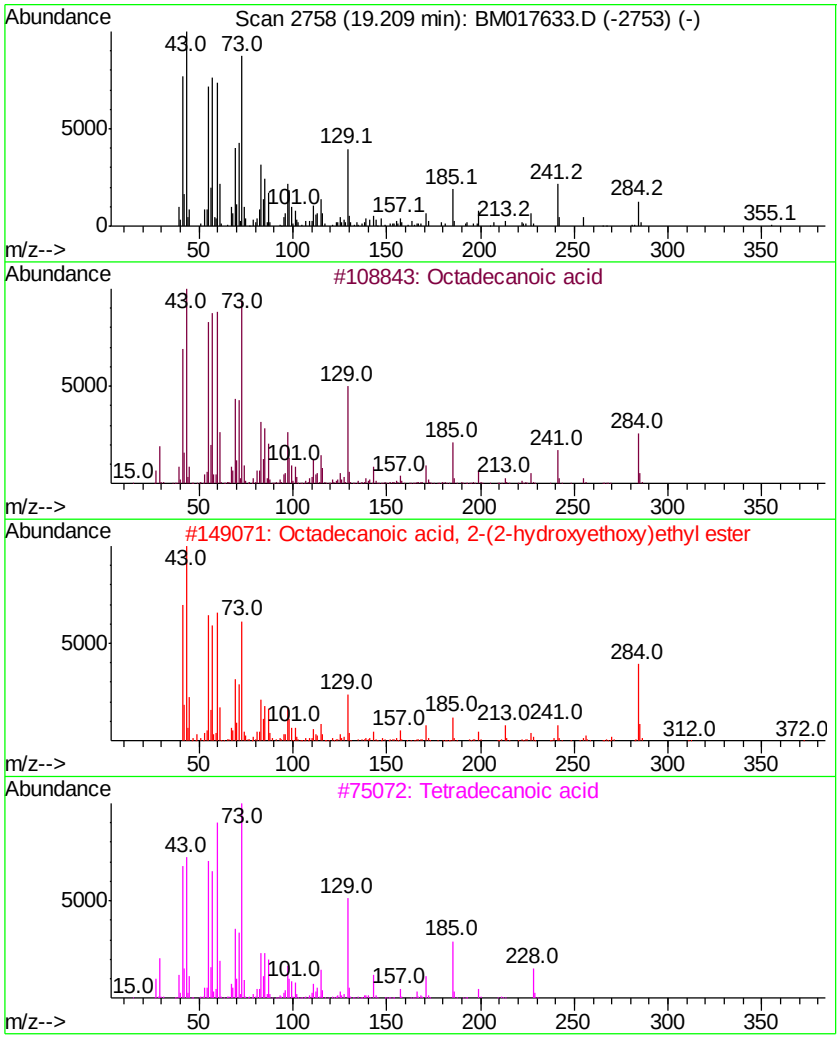
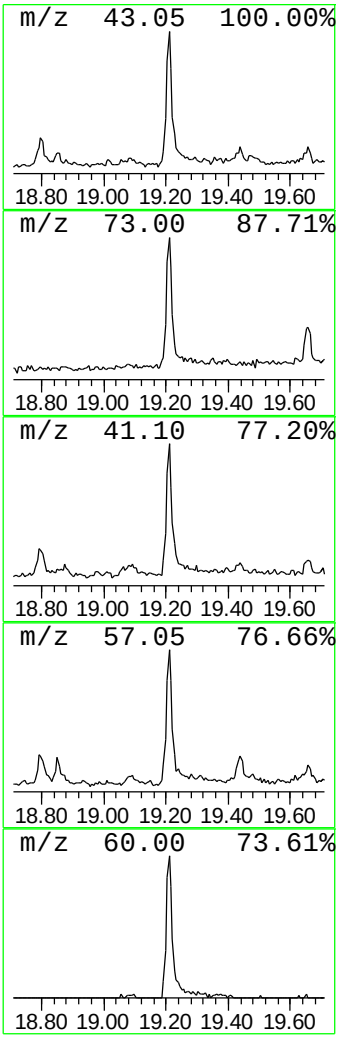
Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.21	2.43 ng	457062	Chrysene-d12	21.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM111318\
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Operator : MJ/SJ
Sample : J5920-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

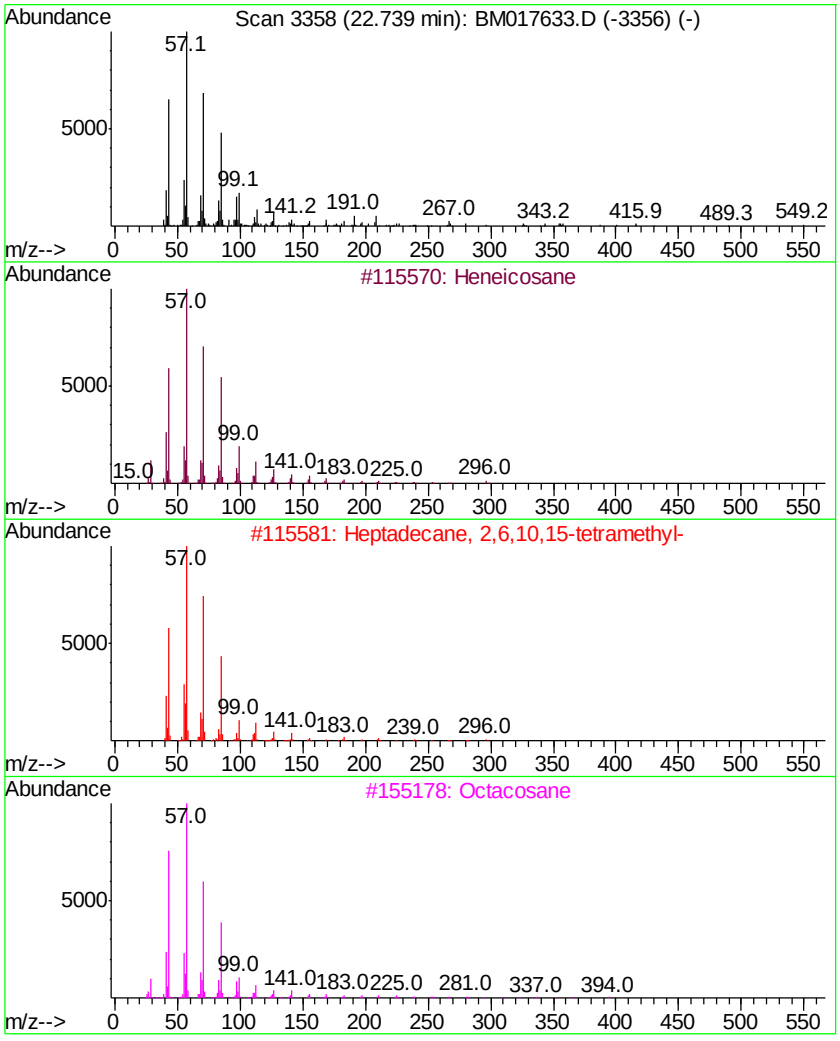
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

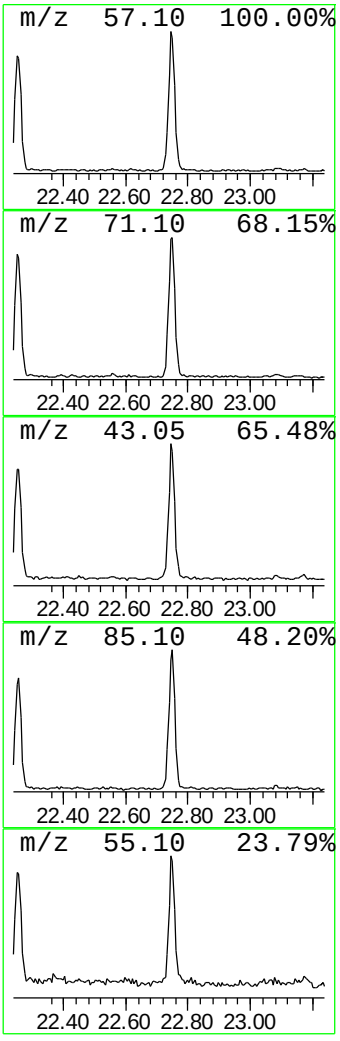
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.74	3.63 ng	447880	Perylene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Octacosane	394	C28H58	000630-02-4	90
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





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Data File : BM017633.D
Acq On : 13 Nov 2018 22:37
Operator : MJ/SJ
Sample : J5920-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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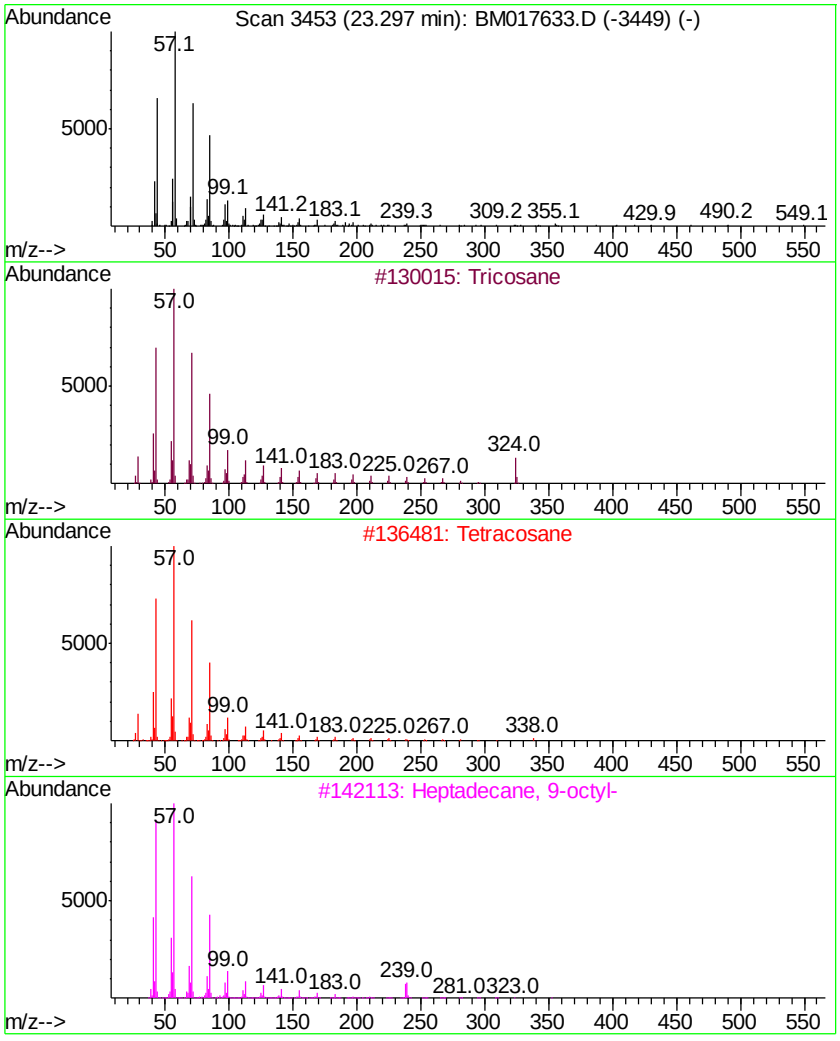
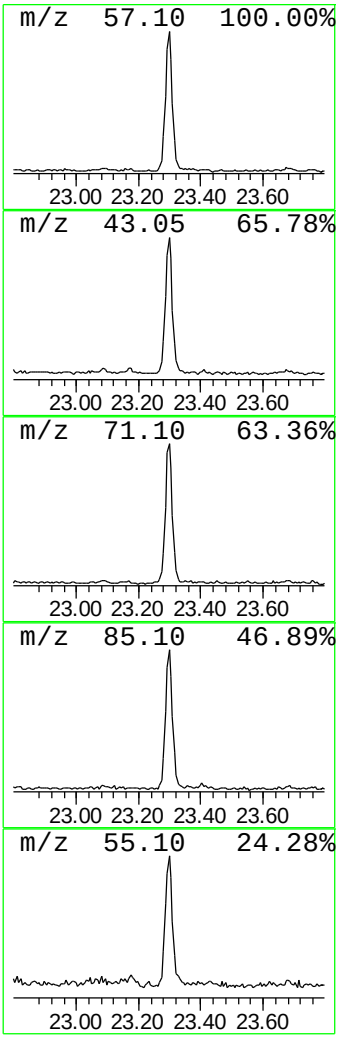
****

Peak Number 7 Tricosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	3.99 ng	492547	Perylene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	87





Library Search Compound Report

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Sample : J5920-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.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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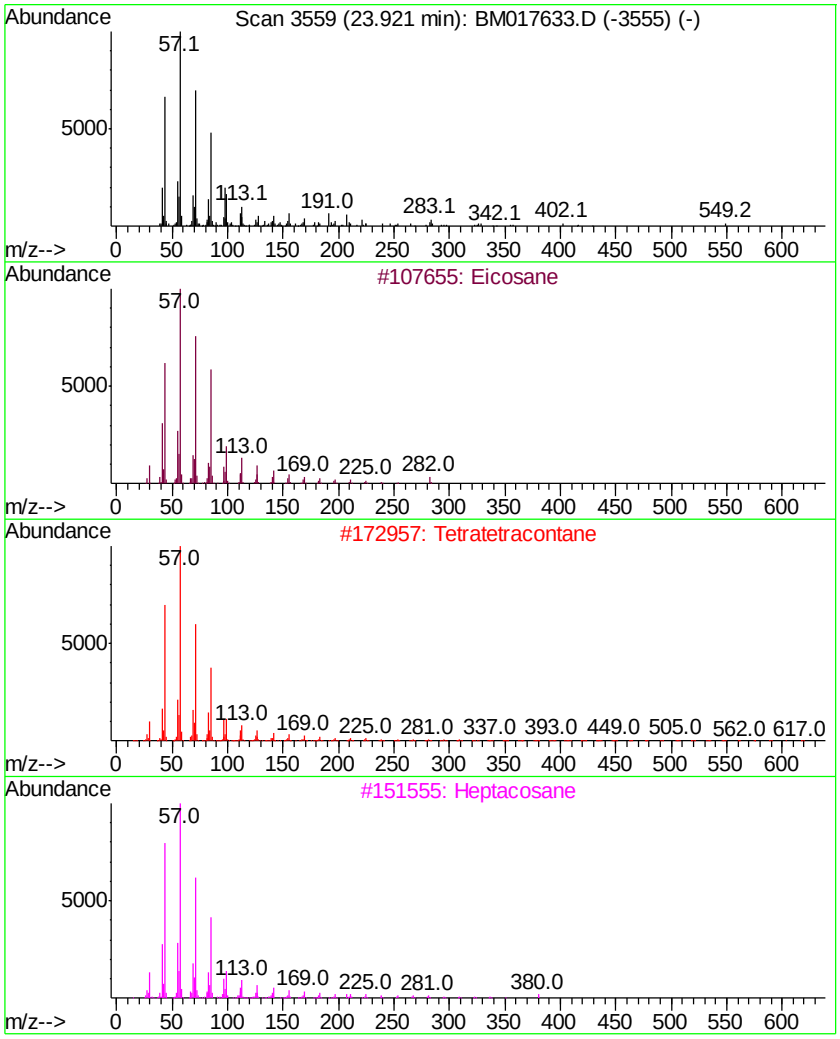
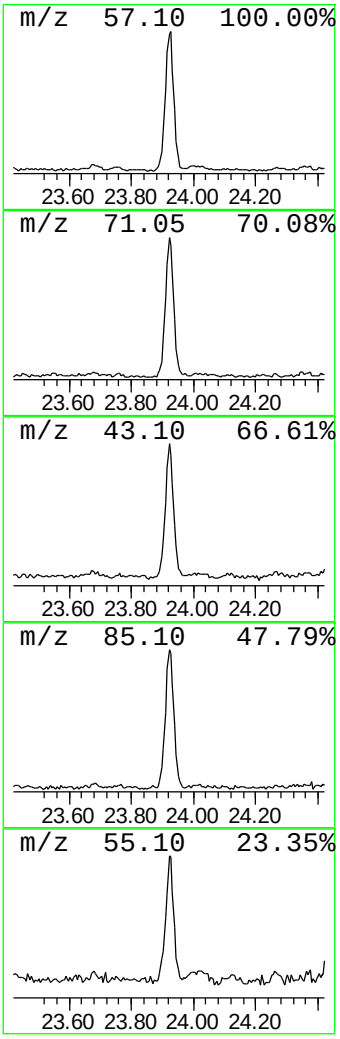
Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	3.24 ng	400441	Perylene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Heptacosane	380	C27H56	000593-49-7	81
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	81
5	Octacosane	394	C28H58	000630-02-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM111318\
Data File : BM017633.D
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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
2-Pentanone, 4-hy...	4.79	5.4	ng	411969	1	7.62	1530380	20.0
unknown7.15	7.15	72.4	ng	5537710	1	7.62	1530380	20.0
n-Hexadecanoic acid	17.92	4.4	ng	730372	4	17.02	3337390	20.0
Octadecanoic acid	19.21	2.4	ng	457062	5	21.22	3768690	20.0
Heneicosane	22.74	3.6	ng	447880	6	23.40	2470360	20.0
Tricosane	23.30	4.0	ng	492547	6	23.40	2470360	20.0
Eicosane	23.92	3.2	ng	400441	6	23.40	2470360	20.0