LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031119\
Data File : BM019104.D
Acq On : 11 Mar 2019 21:49
Operator : JU/SJ
Sample : K1817-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PST-028-B007-1-030619

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	363	369	383	rBV	692317	1098040	42.02%	6.307%
2	6.840	631	638	660	rBV	694483	1284876	49.17%	7.380%
3	7.192	691	698	712	rBV	771600	1272552	48.70%	7.309%
4	7.663	771	778	789	rBV	210295	352775	13.50%	2.026%
5	7.975	825	831	842	rBV	516238	850322	32.54%	4.884%
6	8.828	969	976	989	rBV	332277	673430	25.77%	3.868%
7	10.445	1245	1251	1262	rBV	259662	496723	19.01%	2.853%
8	12.927	1667	1673	1696	rBV	983639	1559194	59.67%	8.956%
9	13.786	1812	1819	1827	rBV	55405	96886	3.71%	0.556%
10	14.316	1903	1909	1925	rVB2	443586	723868	27.70%	4.158%
11	15.815	2158	2164	2183	rBV	865065	1379074	52.77%	7.921%
12	17.068	2371	2377	2393	rBV2	563007	919631	35.19%	5.282%
13	17.957	2524	2528	2544	rBV	102669	227355	8.70%	1.306%
14	19.245	2743	2747	2758	rBV3	117413	261857	10.02%	1.504%
15	19.703	2820	2825	2839	rBV	2131724	2613138	100.00%	15.009%
16	20.968	3036	3040	3047	rBV3	112297	171688	6.57%	0.986%
17	21.268	3086	3091	3102	rBV	966212	1335149	51.09%	7.669%
18	21.833	3185	3187	3190	rBV	82955	96262	3.68%	0.553%
19	22.292	3262	3265	3269	rVB	134994	159213	6.09%	0.914%
20	22.797	3347	3351	3356	rBV	164439	230140	8.81%	1.322%
21	23.362	3444	3447	3452	rVB	146351	201753	7.72%	1.159%
22	23.503	3466	3471	3483	rVB	717515	1406271	53.82%	8.077%

Sum of corrected areas: 17410197

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031119\
Data File : BM019104.D
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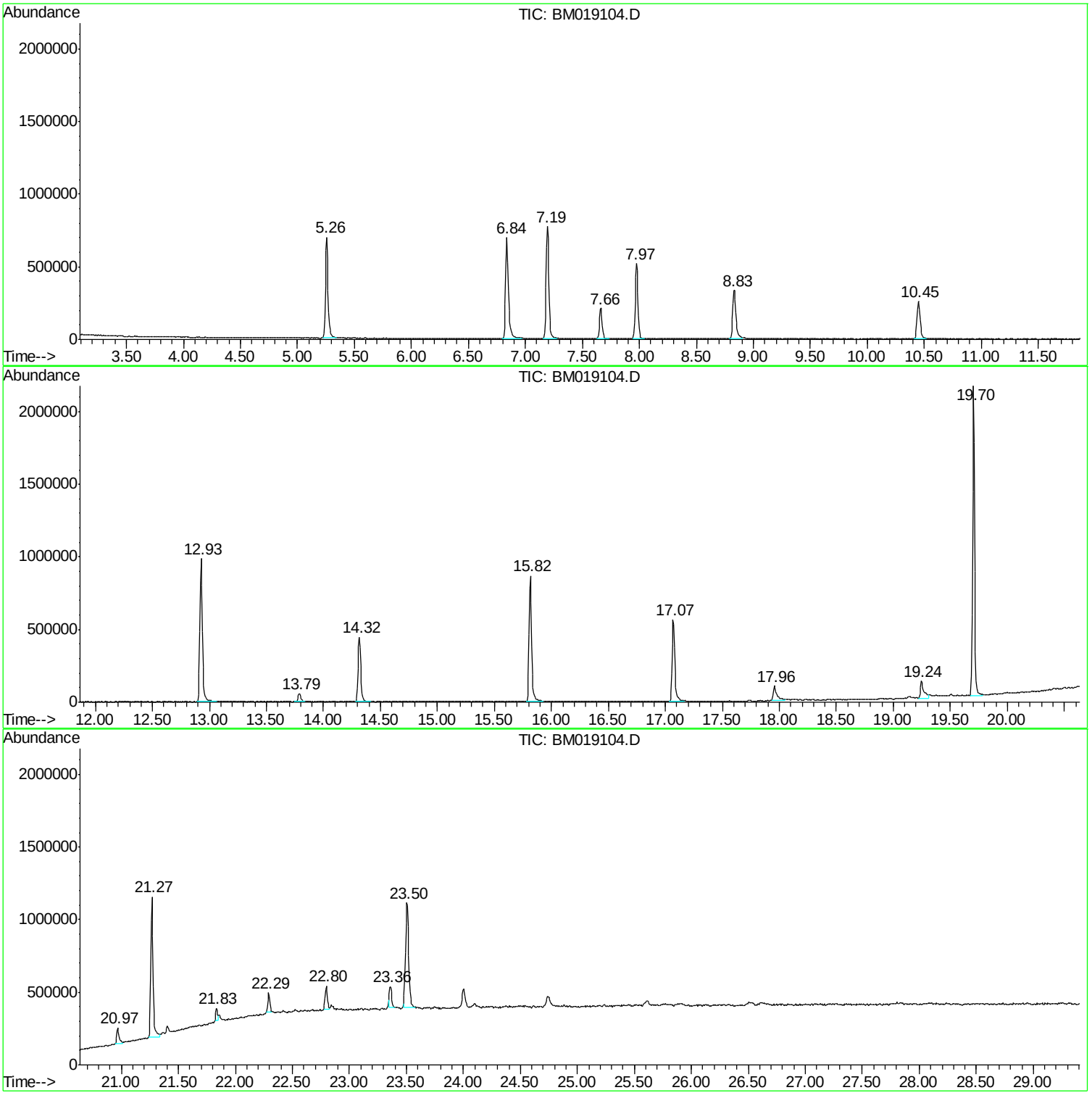
Sample : K1817-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PST-028-B007-1-030619

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\BM031119\
Data File : BM019104.D
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Operator : JU/SJ
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Instrument : BNA_M
ClientSampleId : PST-028-B007-1-030619

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

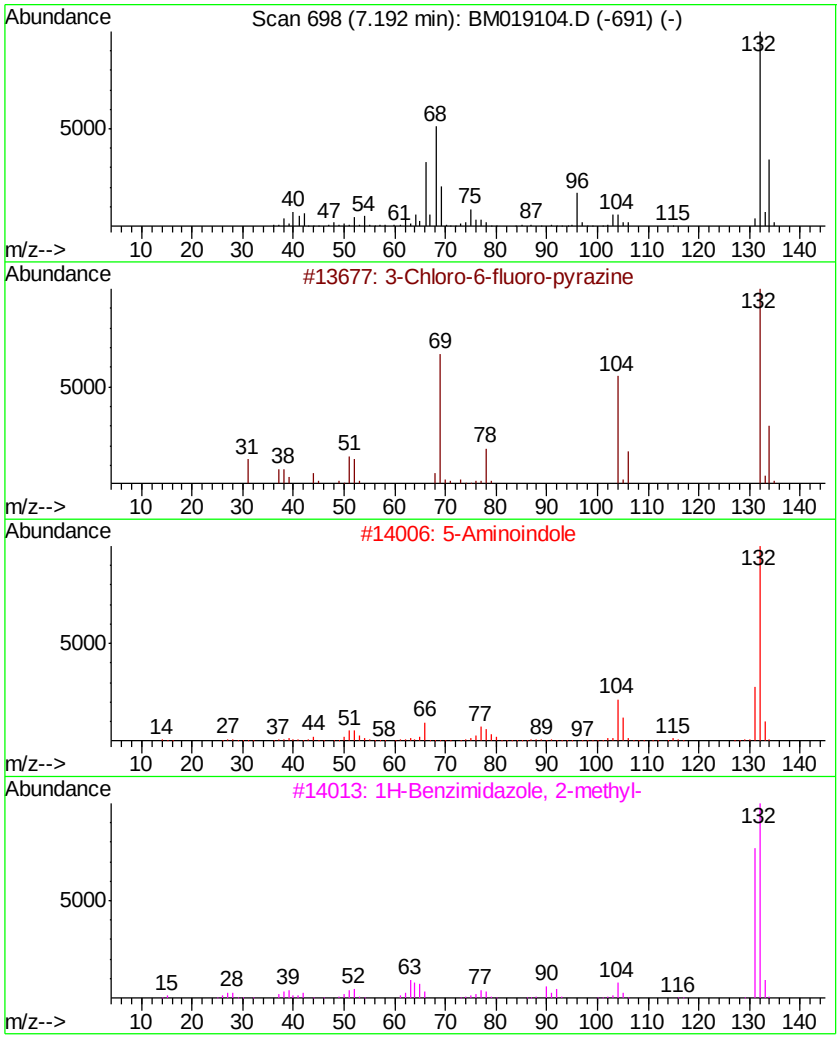
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

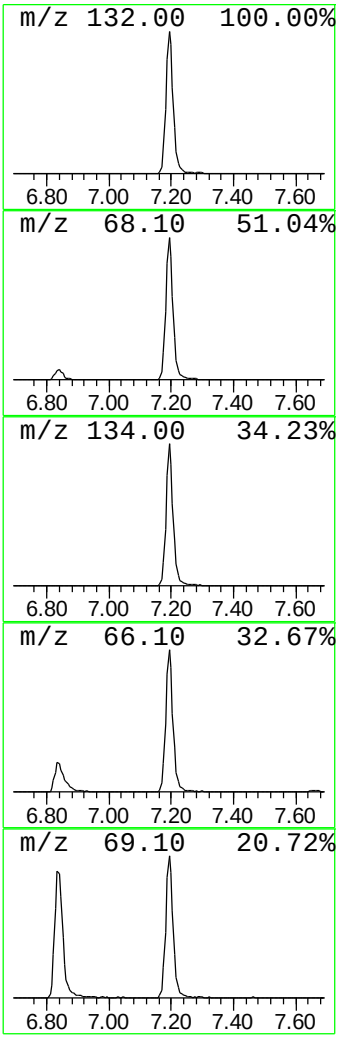
****

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	72.15 ng	1272550	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-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : PST-028-B007-1-030619

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

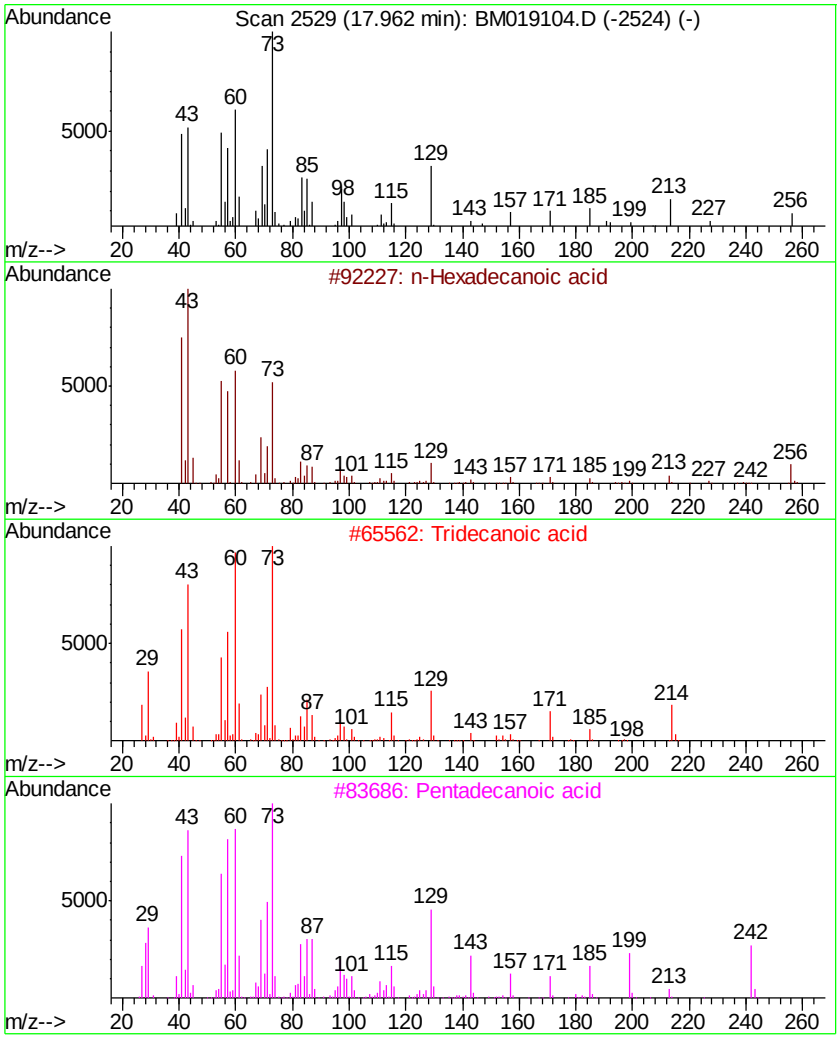
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

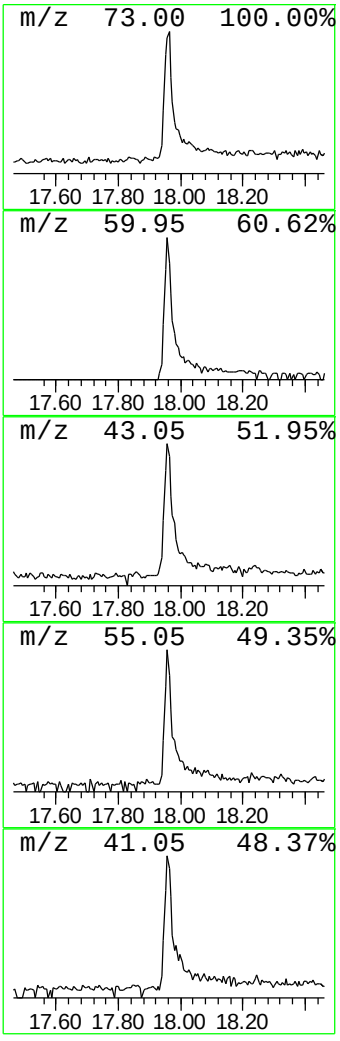
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	4.94 ng	227355	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	59
5	Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031119\
Data File : BM019104.D
Acq On : 11 Mar 2019 21:49
Operator : JU/SJ
Sample : K1817-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PST-028-B007-1-030619

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

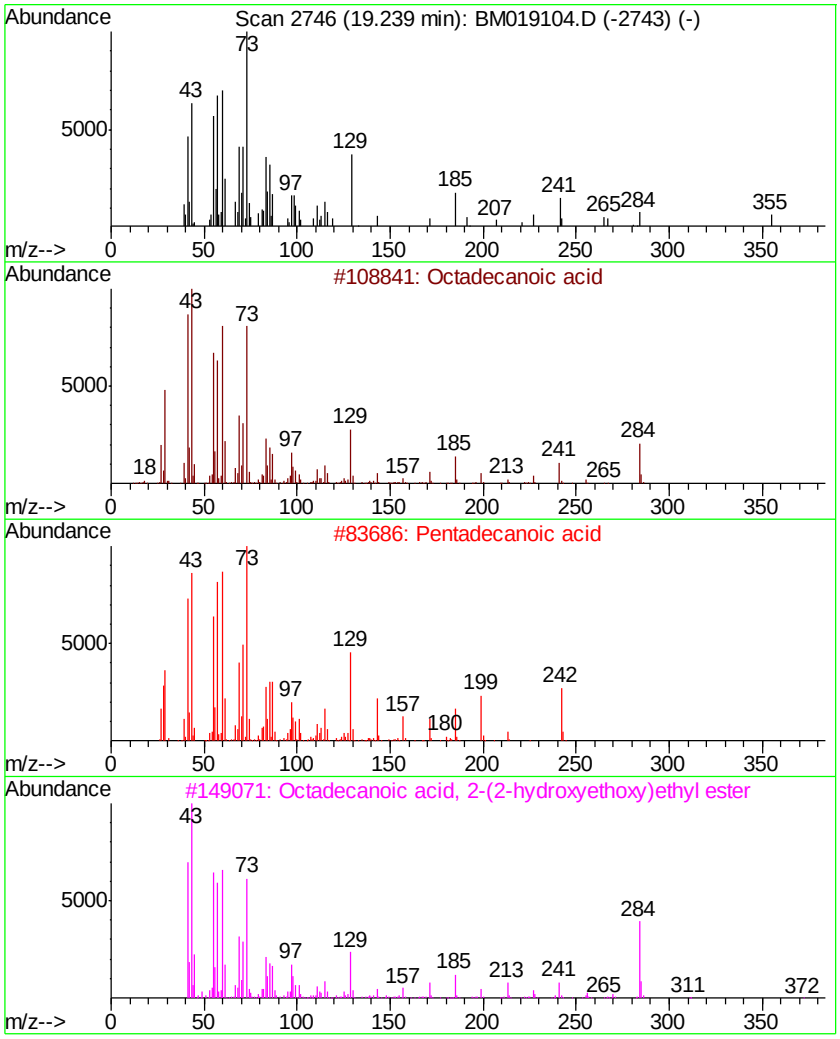
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

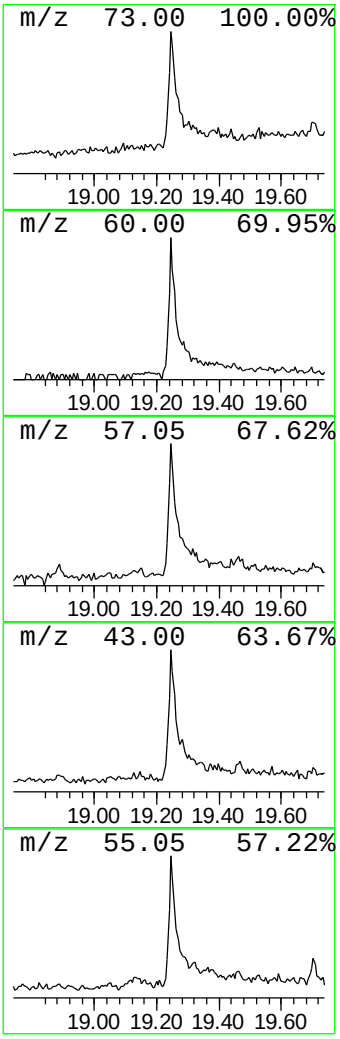
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	3.92 ng	261857	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tritetracontane	605	C43H88	007098-21-7	11





Library Search Compound Report

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Data File : BM019104.D
Acq On : 11 Mar 2019 21:49
Operator : JU/SJ
Sample : K1817-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PST-028-B007-1-030619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
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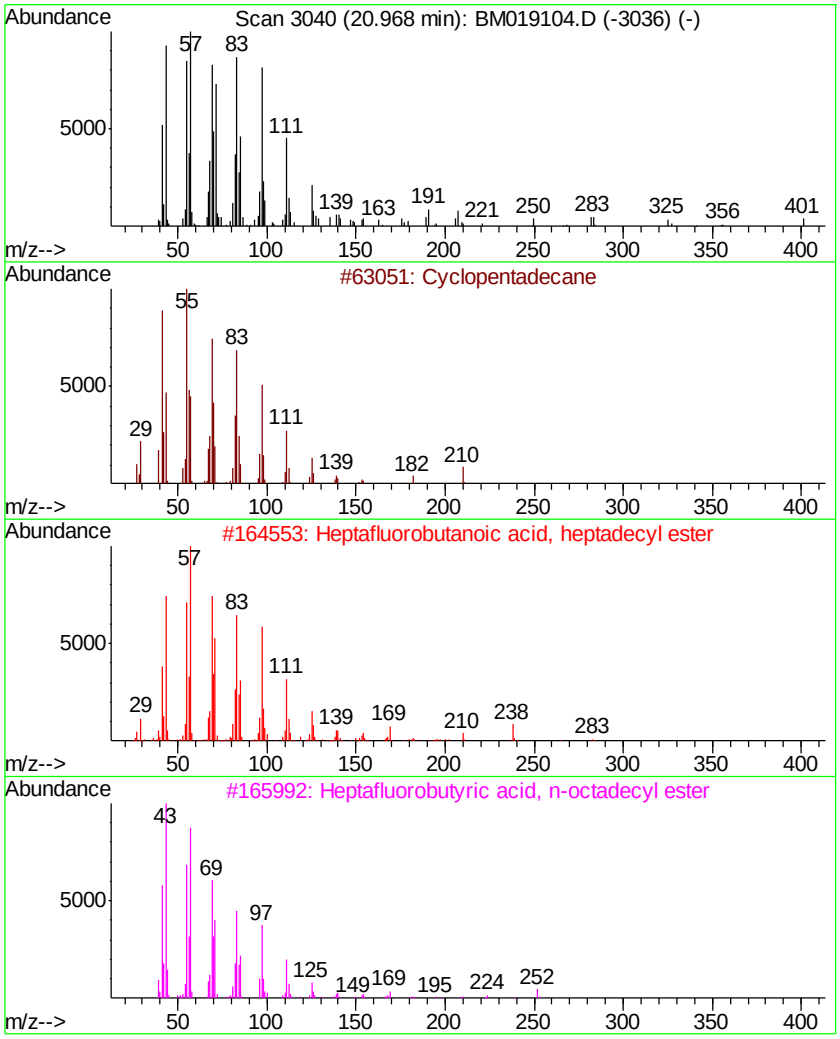
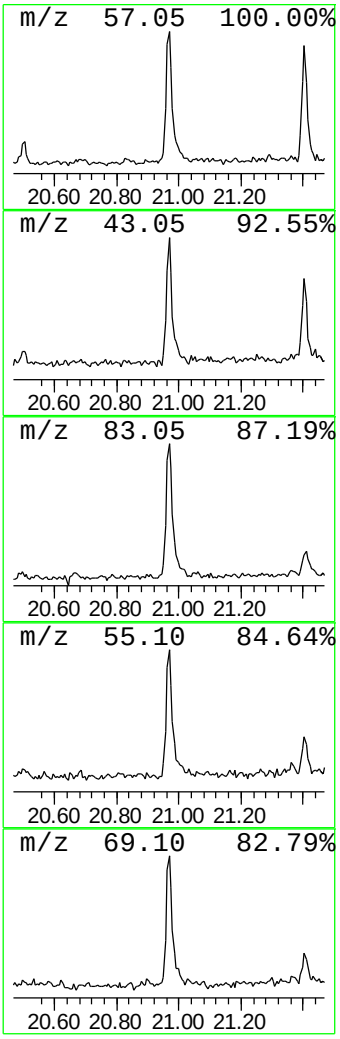
****

Peak Number 5 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	2.57 ng	171688	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	83





Library Search Compound Report

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Operator : JU/SJ
Sample : K1817-20
Misc :
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Instrument : BNA_M
ClientSampleId : PST-028-B007-1-030619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
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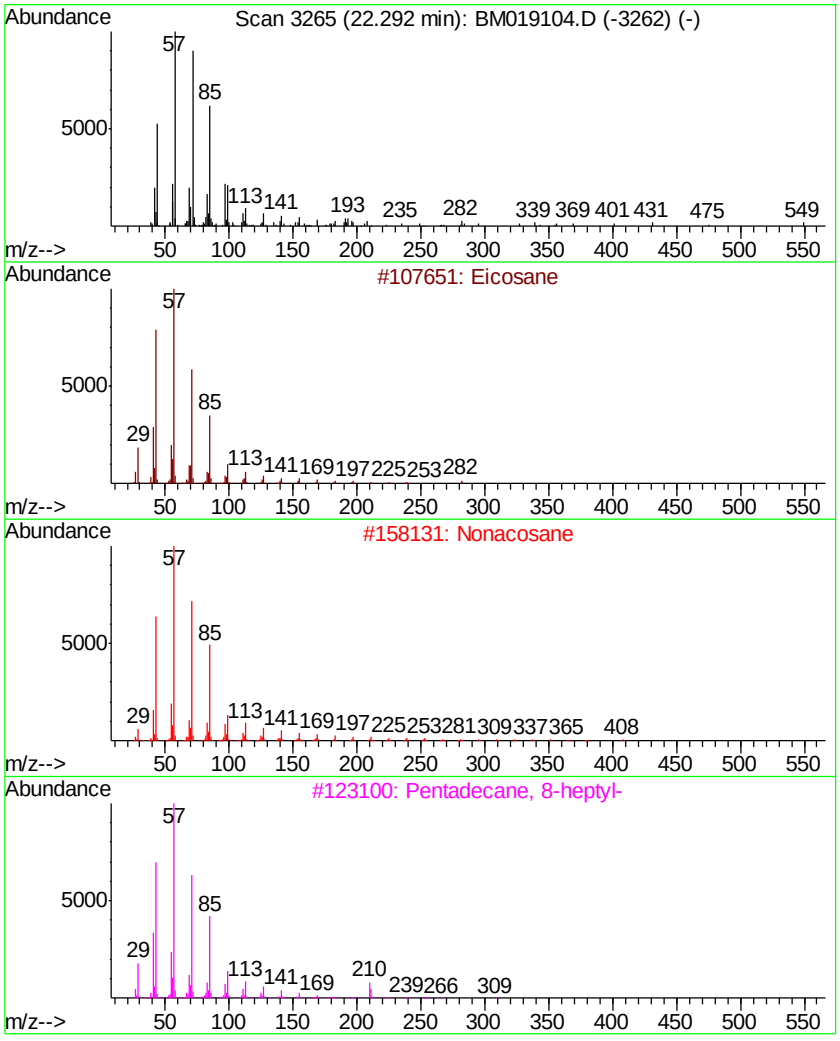
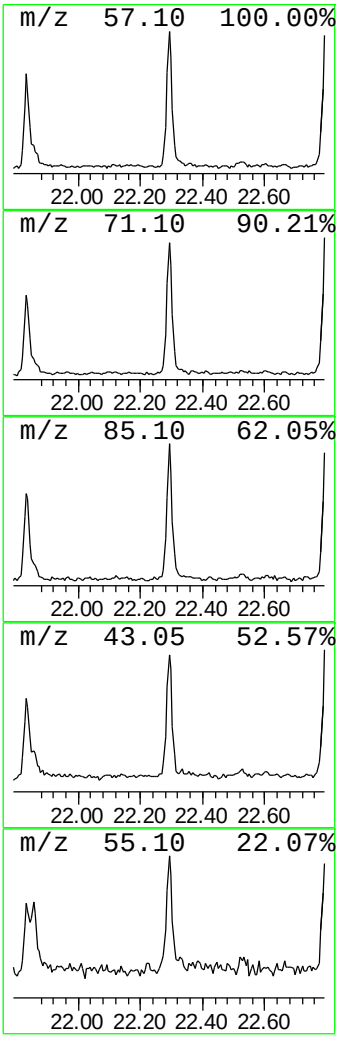
Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.29	2.38 ng	159213	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Nonacosane	408	C29H60	000630-03-5	72
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	72
4	Octadecane, 4-methyl-	268	C19H40	010544-95-3	62
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59





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Misc :
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Instrument : BNA_M
ClientSampleId : PST-028-B007-1-030619

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

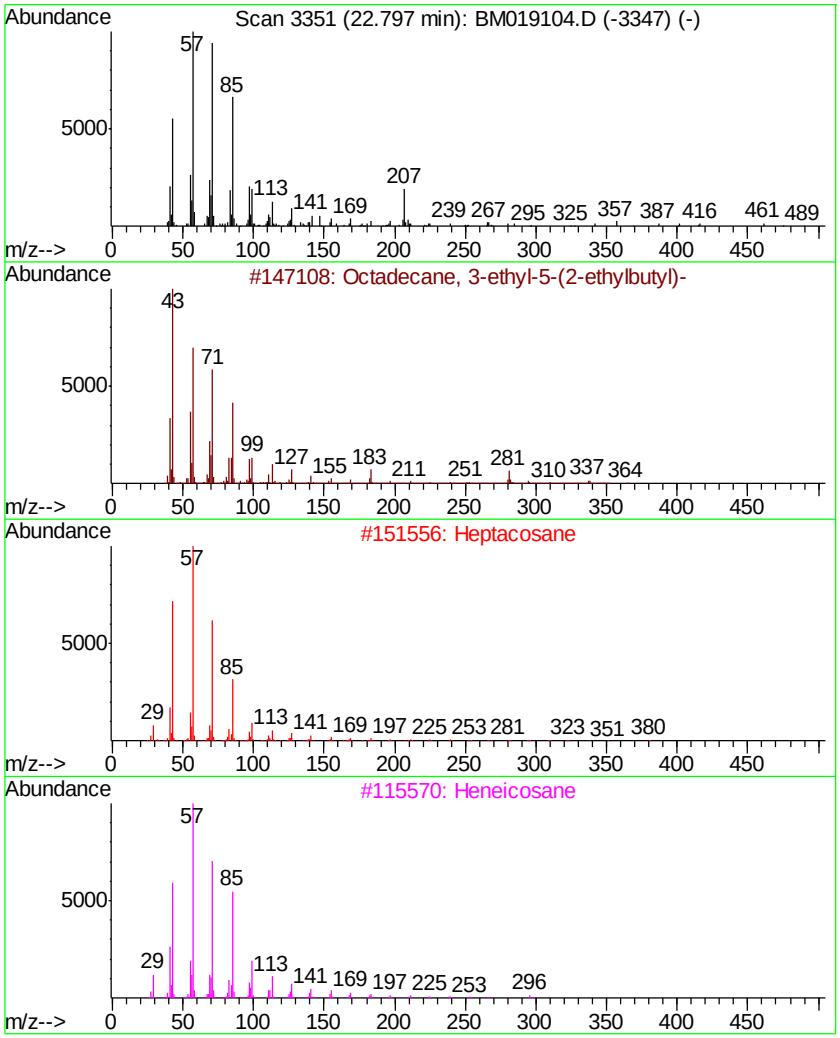
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

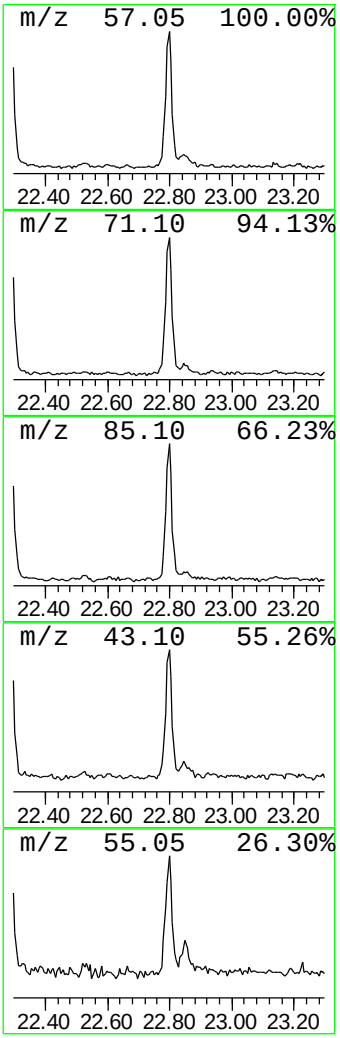
****

Peak Number 7 Octadecane, 3-ethyl-5-(2-et... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	3.27 ng	230140	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	80
2	Heptacosane	380	C27H56	000593-49-7	74
3	Heneicosane	296	C21H44	000629-94-7	74
4	Nonacosane	408	C29H60	000630-03-5	72
5	Octacosane	394	C28H58	000630-02-4	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

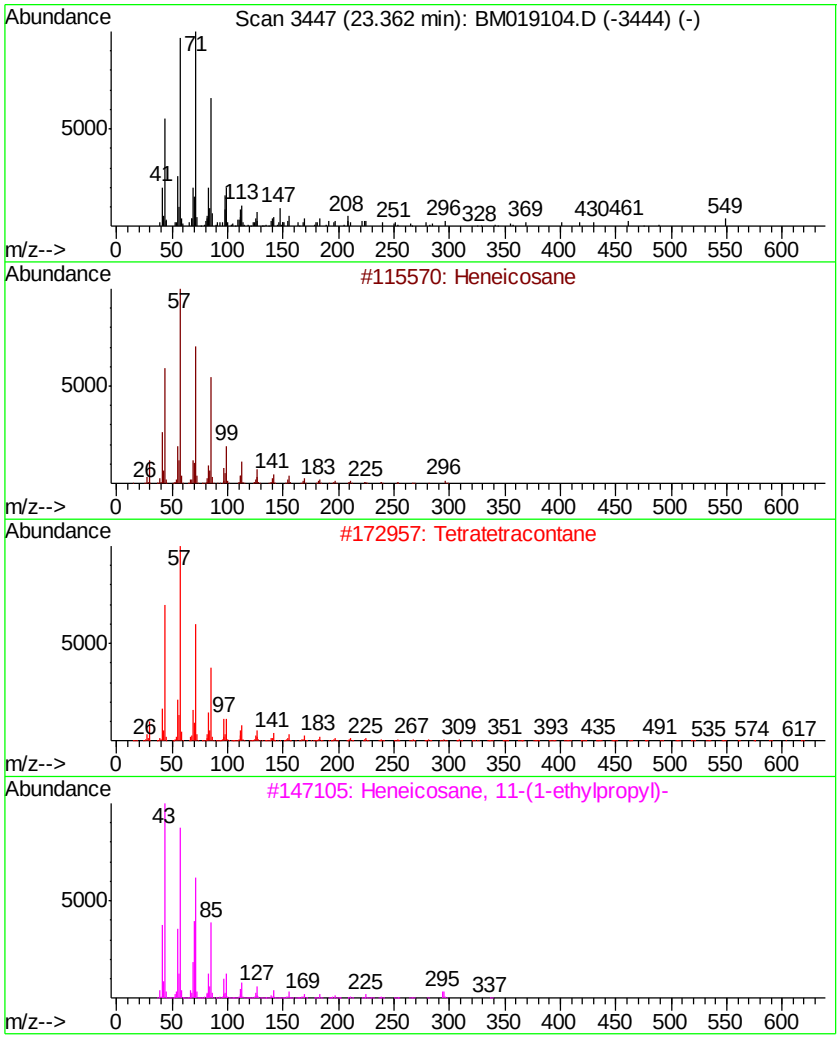
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

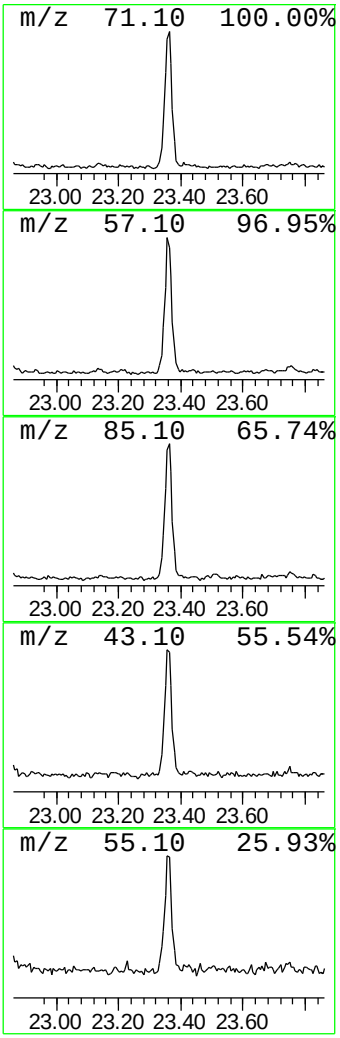
****

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	2.87 ng	201753	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Tetratetracontane	619	C44H90	007098-22-8	81
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	74
4	Octacosane	394	C28H58	000630-02-4	74
5	Tetracosane	338	C24H50	000646-31-1	74





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.19	7.19	72.2	ng	1272550	1	7.66	352775	20.0
n-Hexadecanoic acid	17.96	4.9	ng	227355	4	17.07	919631	20.0
Octadecanoic acid	19.24	3.9	ng	261857	5	21.27	1335150	20.0
Cyclopentadecane	20.97	2.6	ng	171688	5	21.27	1335150	20.0
Eicosane	22.29	2.4	ng	159213	5	21.27	1335150	20.0
Octadecane, 3-eth...	22.80	3.3	ng	230140	6	23.50	1406270	20.0
Heneicosane	23.36	2.9	ng	201753	6	23.50	1406270	20.0