LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019947.D
Acq On : 17 Apr 2019 20:28
Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

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	5.140	360	366	382	rBV	2452120	3696209	76.41%	9.787%
2	6.722	628	635	665	rBV	2326857	3889039	80.40%	10.297%
3	7.063	686	693	707	rBV	2687604	4117936	85.13%	10.903%
4	7.528	763	772	780	rBV	505090	808627	16.72%	2.141%
5	7.840	818	825	838	rBV	1865951	2960551	61.20%	7.839%
6	8.699	964	971	993	rBV	1152914	2238878	46.28%	5.928%
7	10.304	1235	1244	1262	rBV	492491	1000387	20.68%	2.649%
8	12.798	1661	1668	1689	rBV	2927919	4563114	94.33%	12.082%
9	13.675	1812	1817	1828	rBV	112446	215015	4.44%	0.569%
10	14.192	1899	1905	1921	rBV2	692476	1119313	23.14%	2.964%
11	15.704	2156	2162	2182	rBV	1908073	3042169	62.89%	8.055%
12	16.957	2369	2375	2396	rBV2	632019	1131781	23.40%	2.997%
13	17.857	2520	2528	2534	rBV3	41325	90500	1.87%	0.240%
14	19.604	2819	2825	2837	rBV	3989330	4837393	100.00%	12.808%
15	20.392	2956	2959	2963	rBV2	46289	51266	1.06%	0.136%
16	20.862	3035	3039	3047	rBV3	112327	198278	4.10%	0.525%
17	21.174	3087	3092	3104	rBV	971343	1339157	27.68%	3.546%
18	21.298	3110	3113	3117	rBV2	97962	110481	2.28%	0.293%
19	21.721	3182	3185	3189	rBV	126826	135857	2.81%	0.360%
20	22.168	3258	3261	3265	rVB	130289	146066	3.02%	0.387%
21	22.656	3340	3344	3348	rVB	137551	183918	3.80%	0.487%
22	23.198	3433	3436	3441	rVB	137871	192677	3.98%	0.510%
23	23.368	3459	3465	3474	rVB	785828	1513010	31.28%	4.006%
24	23.809	3537	3540	3547	rVB2	115159	186147	3.85%	0.493%

Sum of corrected areas: 37767769

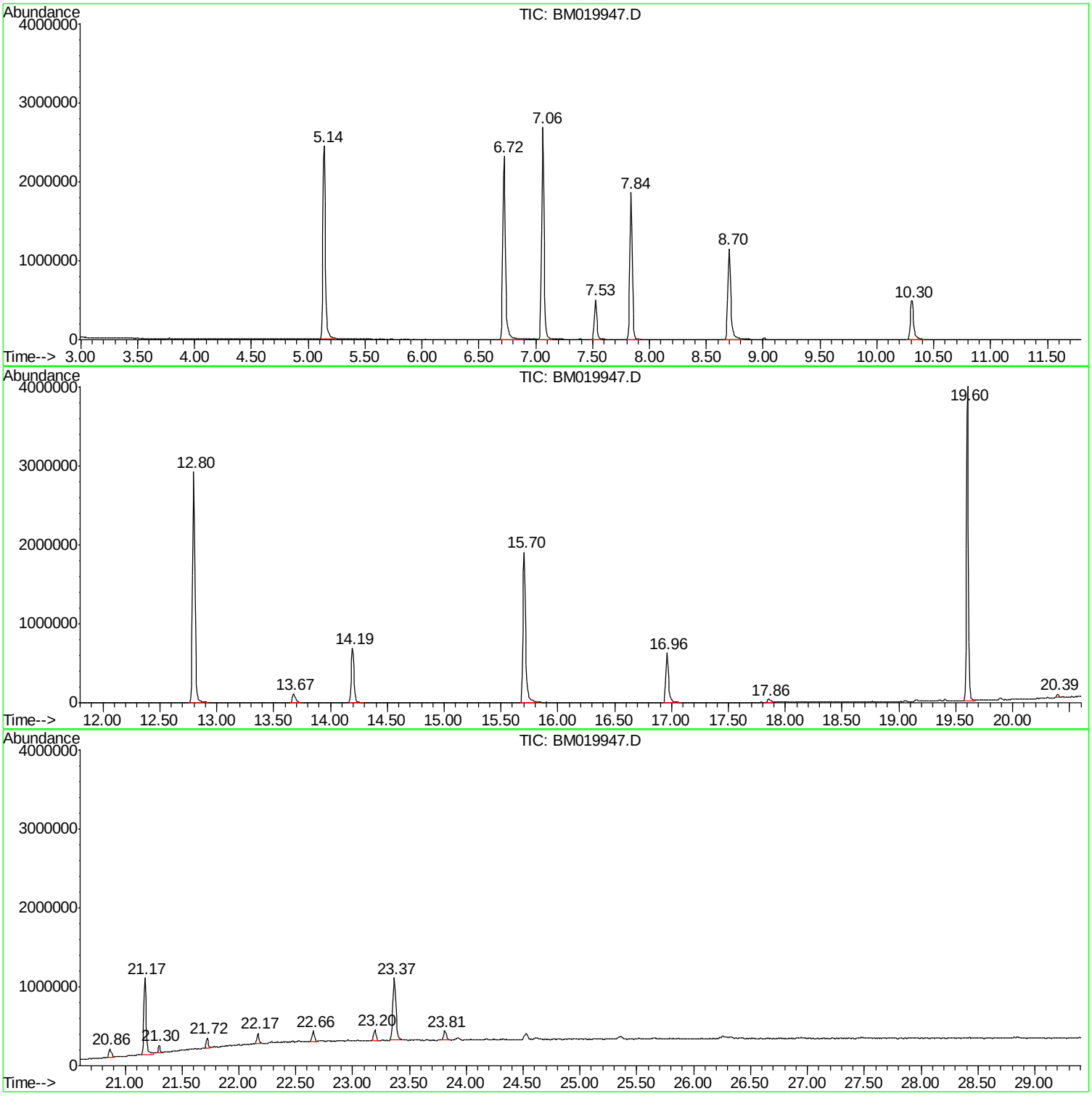
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019947.D
Acq On : 17 Apr 2019 20:28
Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

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\BM041719\
Data File : BM019947.D
Acq On : 17 Apr 2019 20:28
Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

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

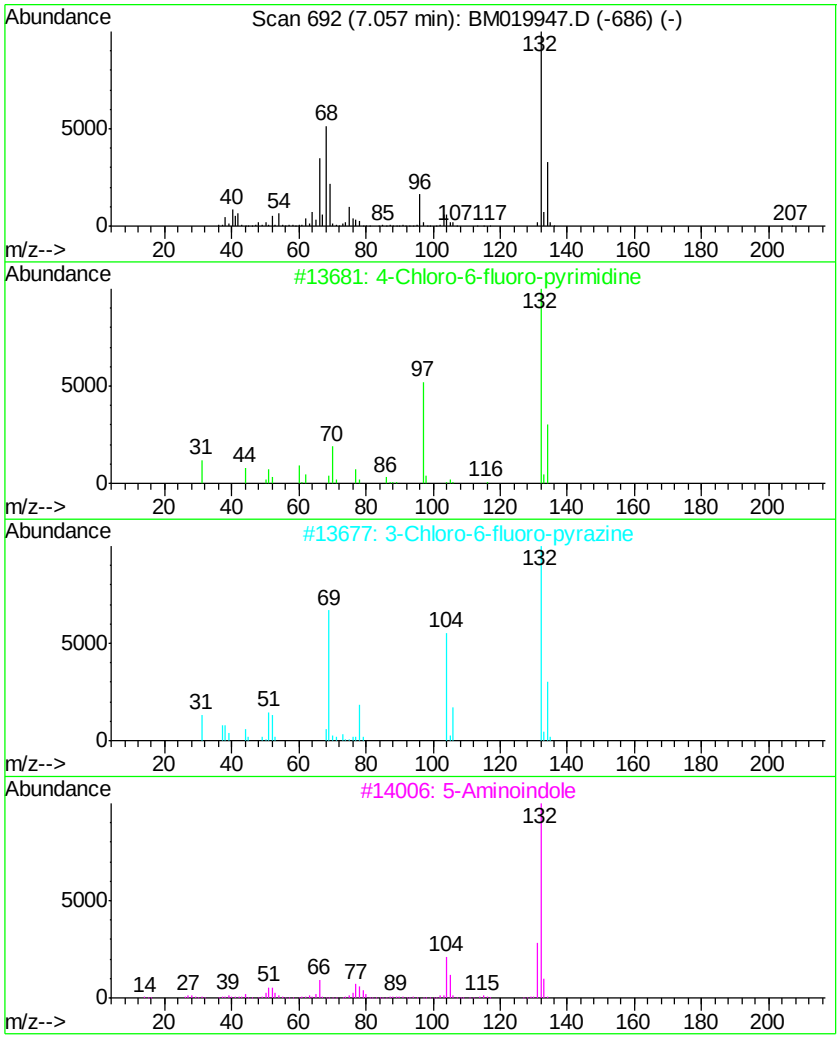
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

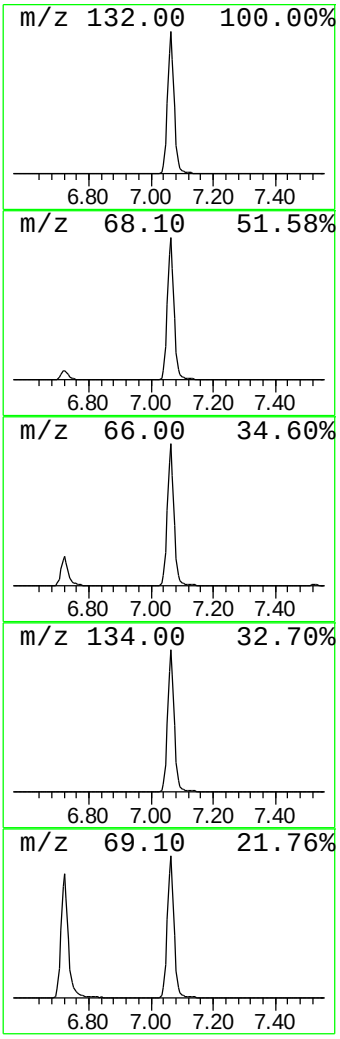
****

Peak Number 1 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	101.85 ng	4117940	1,4-Dichlorobenzene-d4	7.53

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	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13





Library Search Compound Report

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Data File : BM019947.D
Acq On : 17 Apr 2019 20:28
Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

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

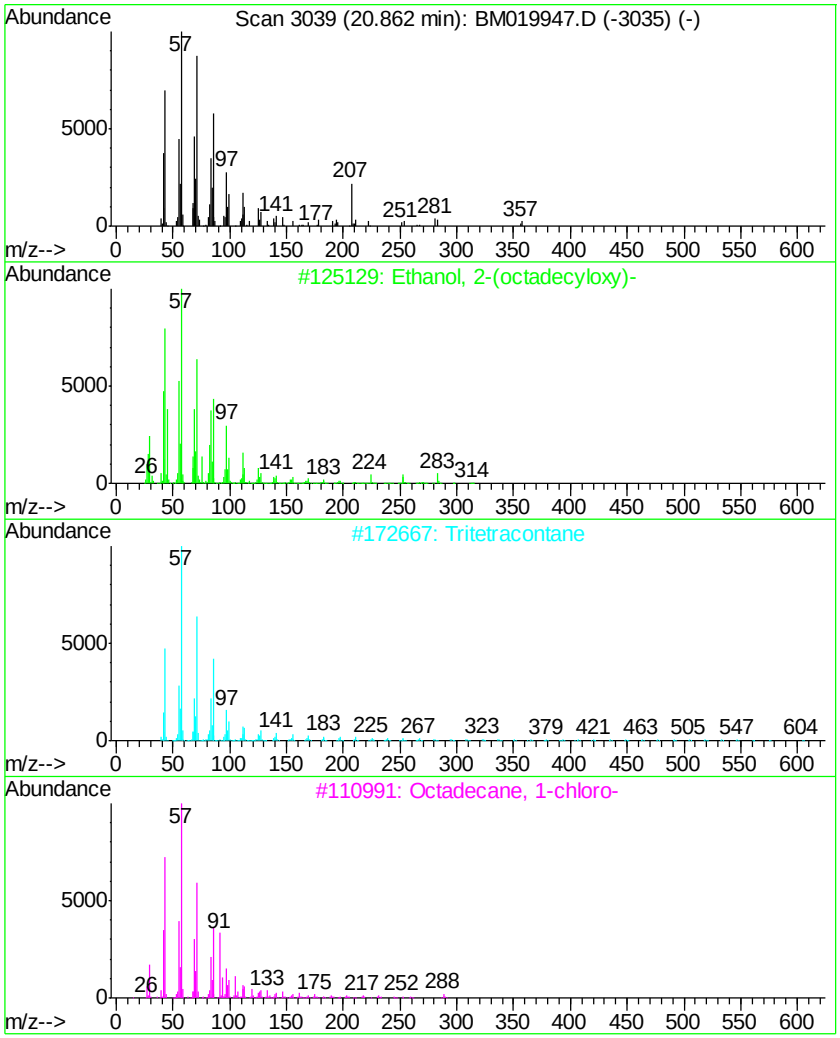
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

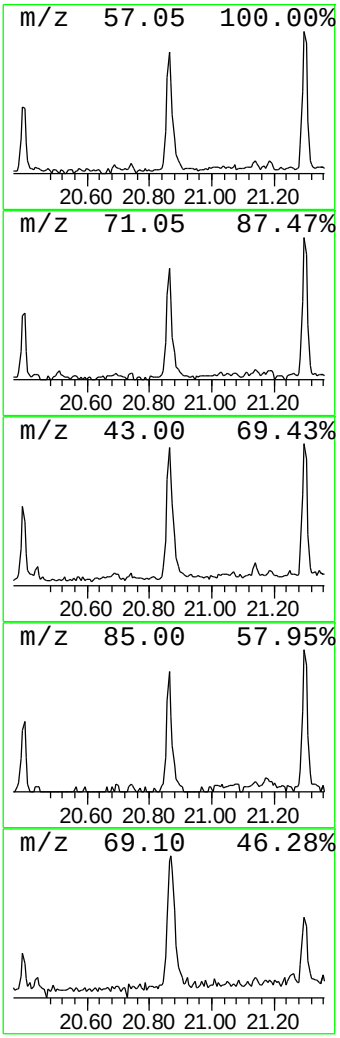
****

Peak Number 3 Ethanol, 2-(octadecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.96 ng	198278	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	80
2	Tritetracontane	605	C43H88	007098-21-7	72
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	72
4	1-Pentadecene	210	C15H30	013360-61-7	60
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019947.D
Acq On : 17 Apr 2019 20:28
Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

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

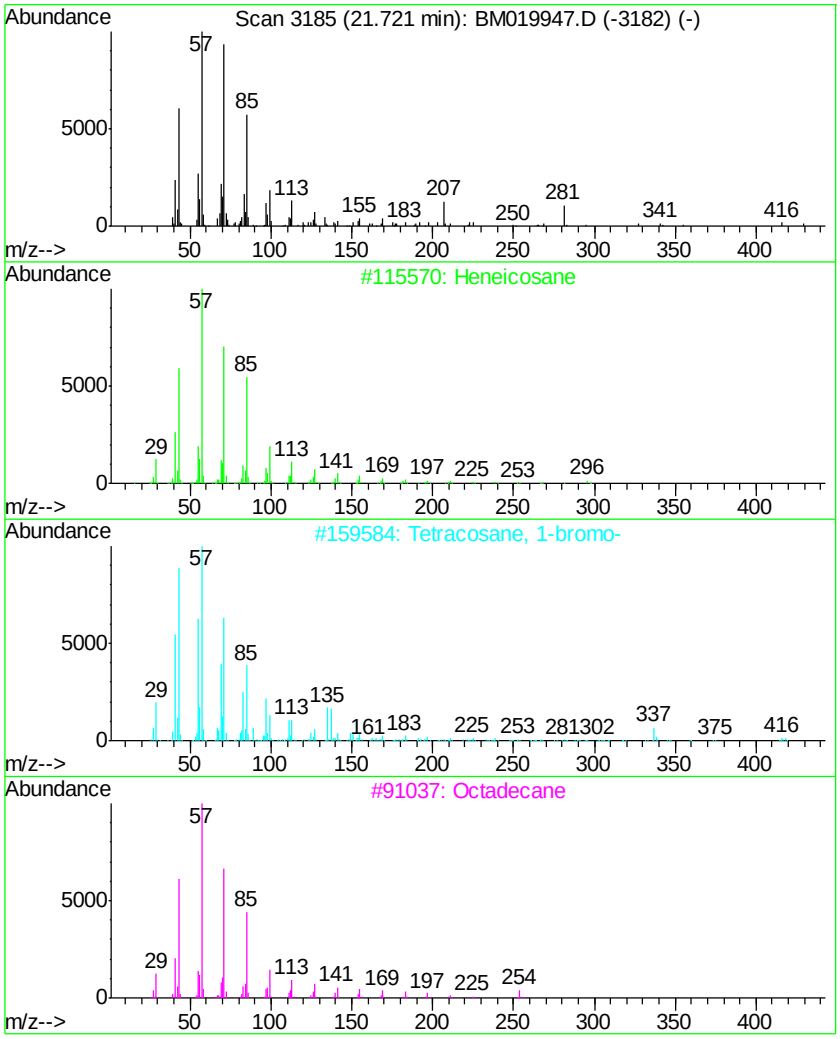
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

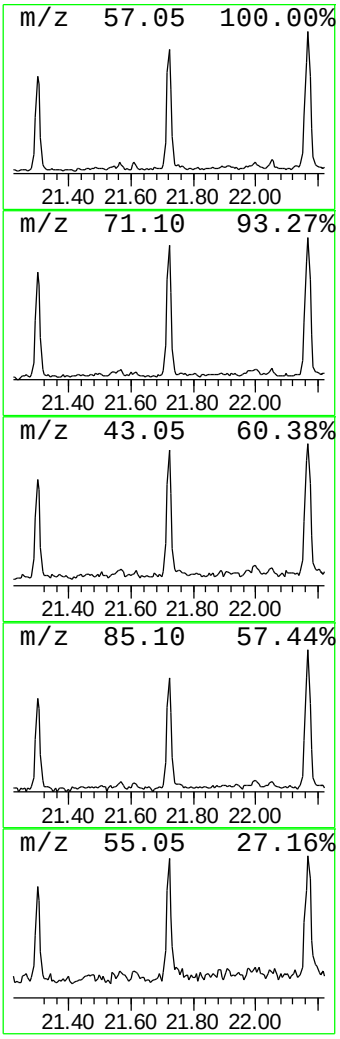
****

Peak Number 4 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	2.03 ng	135857	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	83
2	Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	81
3	Octadecane	254	C18H38	000593-45-3	80
4	Nonacosane	408	C29H60	000630-03-5	80
5	Hexadecane	226	C16H34	000544-76-3	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019947.D
Acq On : 17 Apr 2019 20:28
Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

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

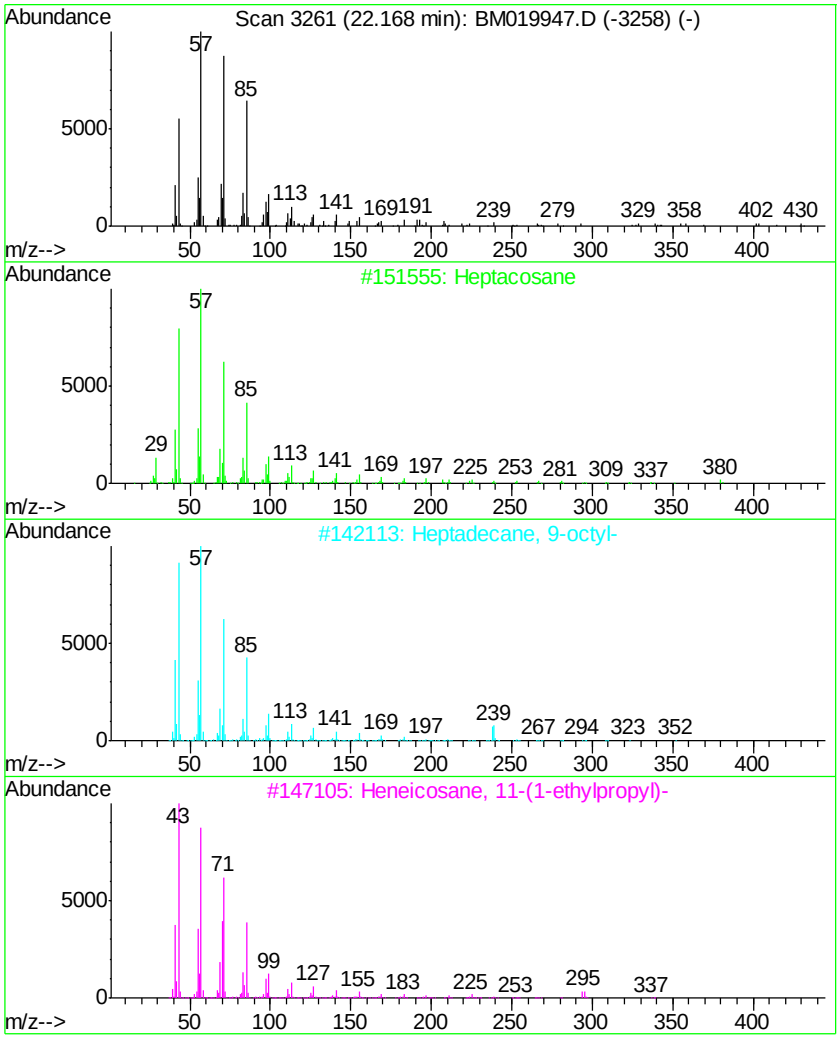
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

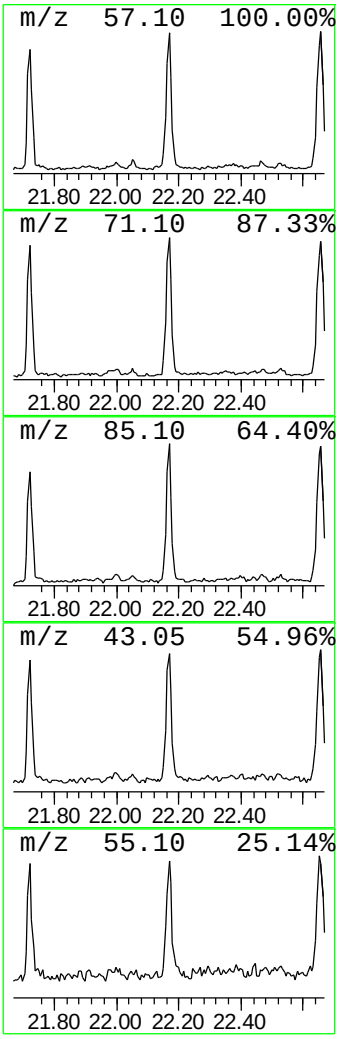
****

Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.17	2.18 ng	146066	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Heptadecane	240	C17H36	000629-78-7	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019947.D
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Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

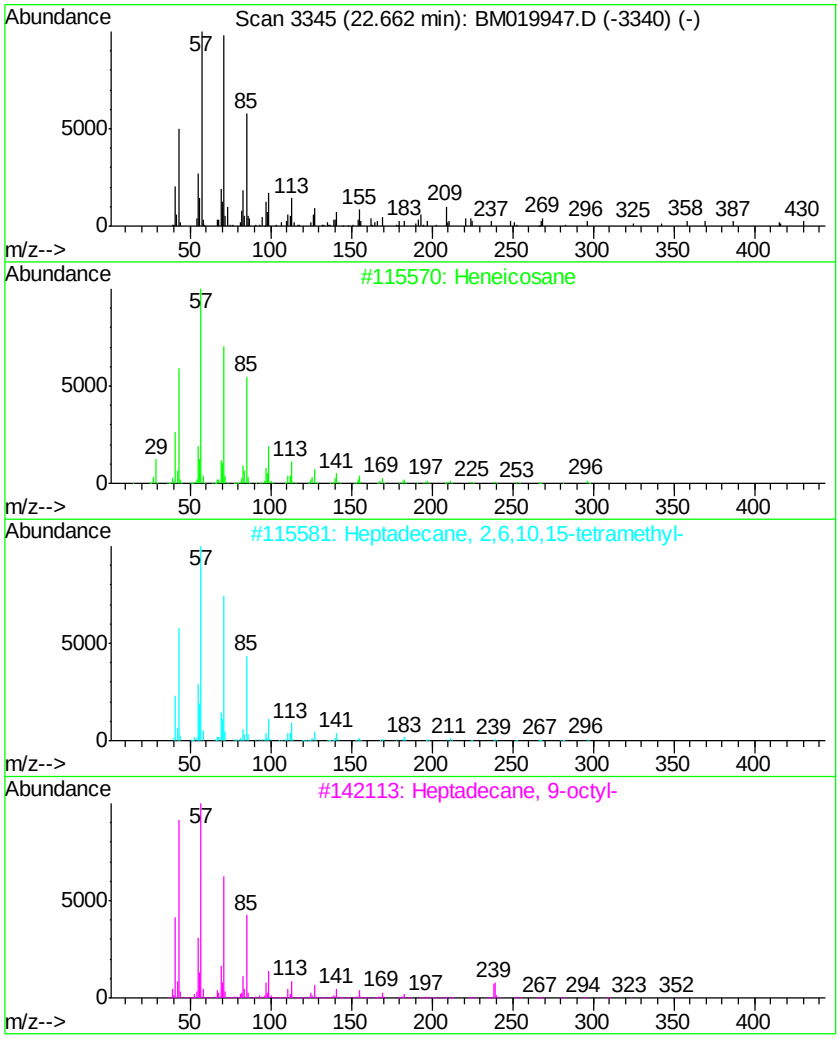
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

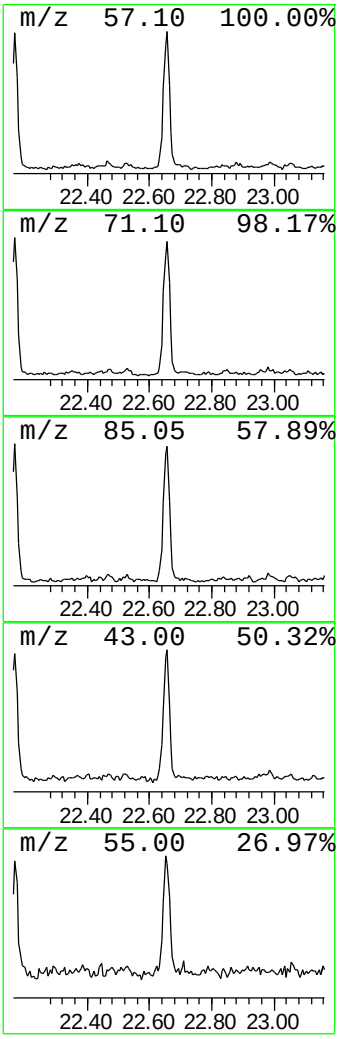
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.66	2.43 ng	183918	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Docosane, 7-butyl-	366	C26H54	055282-15-0	87
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86





Library Search Compound Report

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Data File : BM019947.D
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Operator : JU/SJ
Sample : K2422-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP1-D

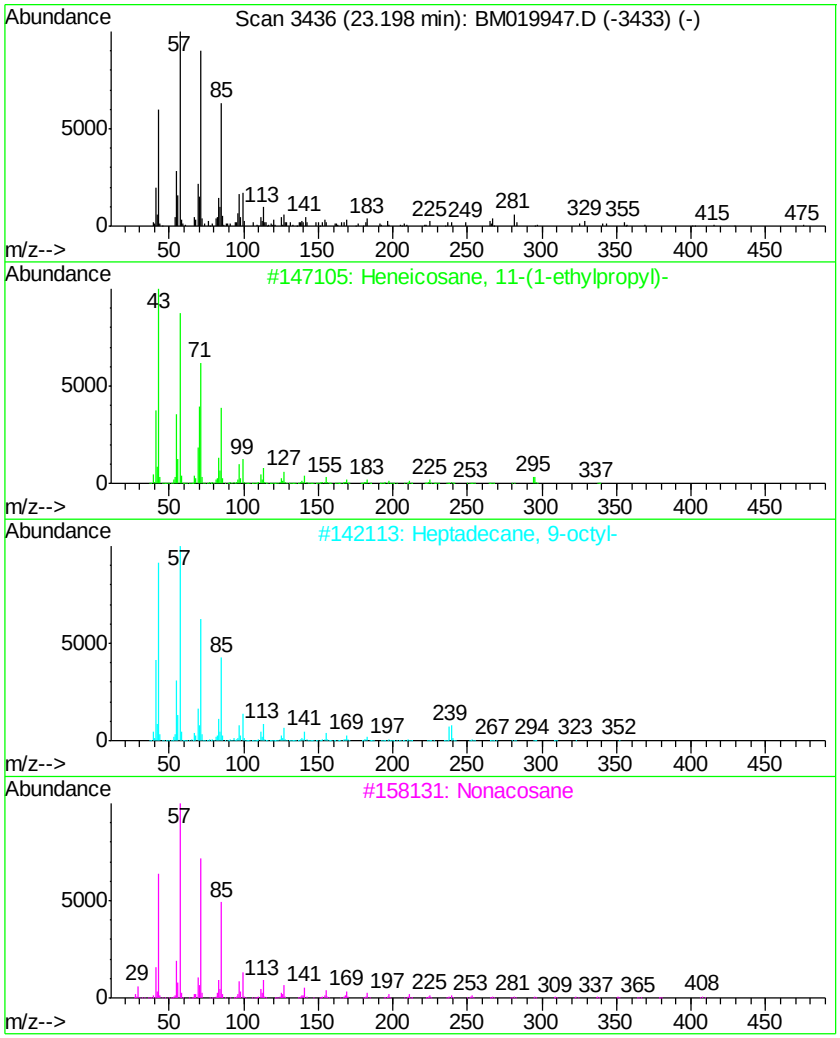
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

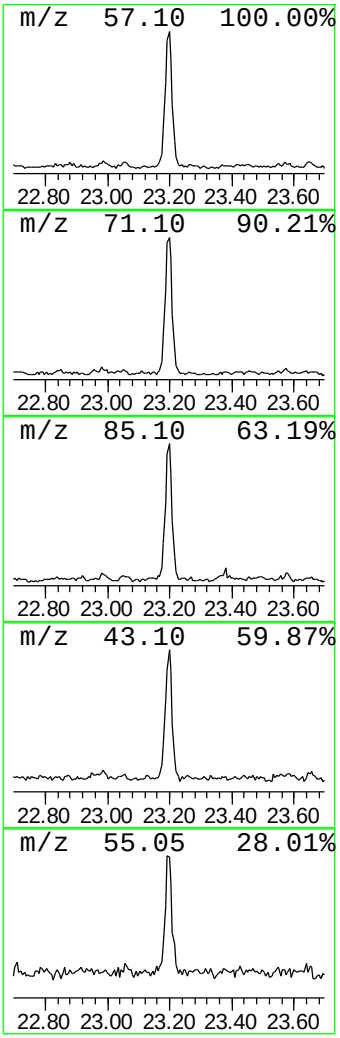
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heneicosane, 11-(1-ethylpro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.20	2.55 ng	192677	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3	Nonacosane	408	C29H60	000630-03-5	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Docosane	310	C22H46	000629-97-0	78





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BNA_M
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TP1-D

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

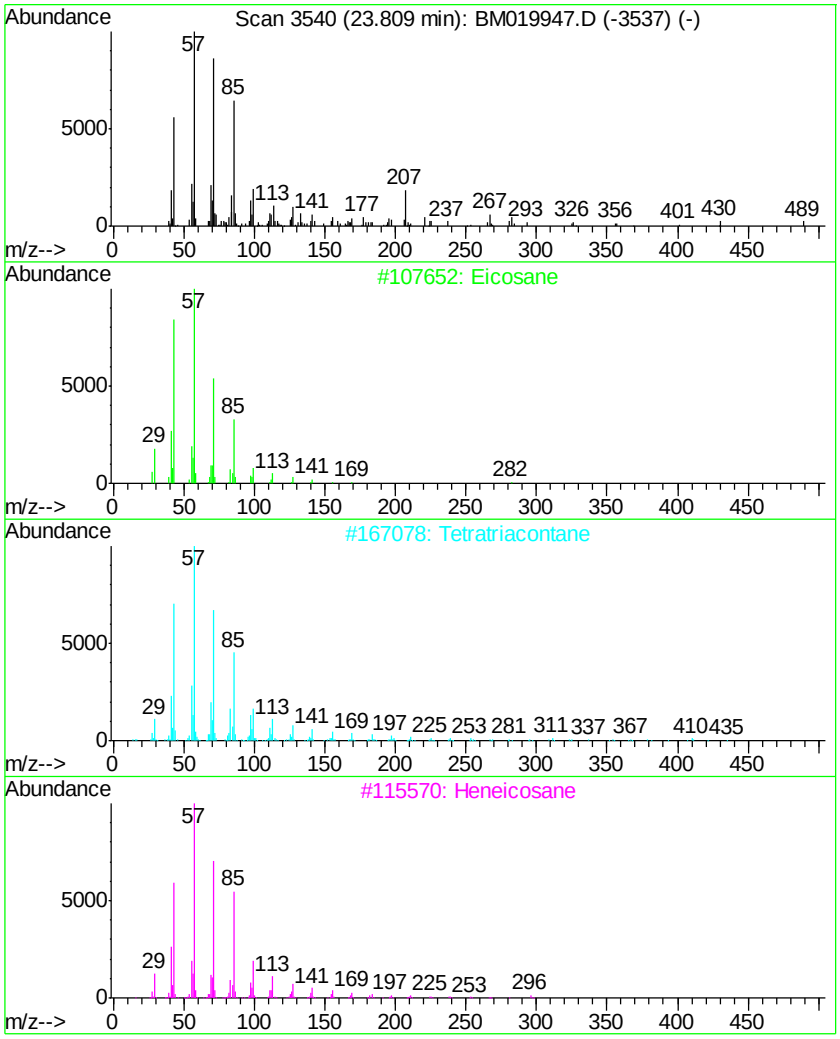
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

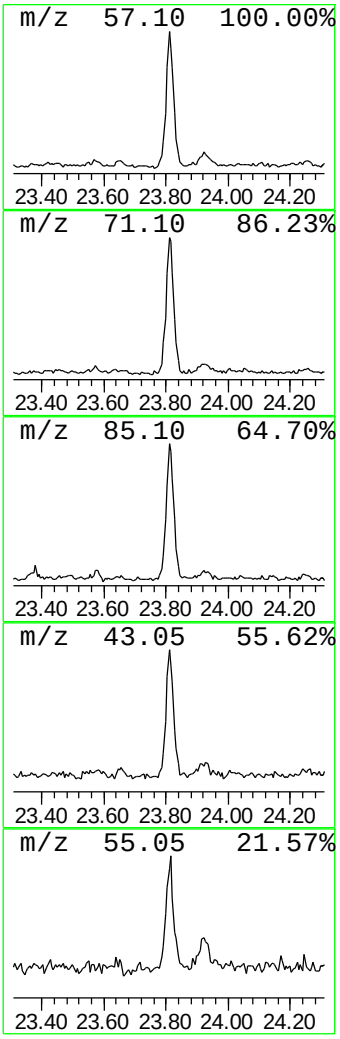
****

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.81	2.46 ng	186147	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Tetratriacontane	479	C34H70	014167-59-0	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Nonacosane	408	C29H60	000630-03-5	87
5	Hexadecane	226	C16H34	000544-76-3	87





Tentatively Identified Compound (LSC) summary

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Data File : BM019947.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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown7.06	7.06	101.8	ng	4117940	1	7.53	808627	20.0
Ethanol, 2-(octad...	20.86	3.0	ng	198278	5	21.17	1339160	20.0
Heneicosane	21.72	2.0	ng	135857	5	21.17	1339160	20.0
Heptacosane	22.17	2.2	ng	146066	5	21.17	1339160	20.0
Heptadecane, 2,6,...	22.66	2.4	ng	183918	6	23.37	1513010	20.0
Heneicosane, 11-(...	23.20	2.5	ng	192677	6	23.37	1513010	20.0
Eicosane	23.81	2.5	ng	186147	6	23.37	1513010	20.0