LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

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_G\METHODS\8270-BG042319.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	3.140	3	9	18	rBV	657369	1180007	33.75%	5.174%
2	3.217	18	22	32	rVB	172141	263664	7.54%	1.156%
3	5.661	431	438	448	rBV	808019	1273504	36.42%	5.584%
4	7.271	704	712	722	rBV	913747	1570717	44.92%	6.887%
5	7.653	770	777	789	rBV	826246	1407447	40.25%	6.171%
6	8.129	851	858	867	rBV	186710	317027	9.07%	1.390%
7	8.452	906	913	920	rBV	520778	869216	24.86%	3.811%
8	9.304	1050	1058	1069	rBV	520880	926418	26.49%	4.062%
9	10.949	1330	1338	1346	rBV	250195	454163	12.99%	1.991%
10	13.381	1744	1752	1761	rBV	1361259	2090687	59.79%	9.166%
11	14.198	1886	1891	1898	rVB	209692	306364	8.76%	1.343%
12	14.756	1980	1986	1996	rBV2	466900	737481	21.09%	3.233%
13	16.243	2231	2239	2254	rBV	1506768	2217660	63.42%	9.723%
14	17.500	2445	2453	2460	rBV	666054	992956	28.40%	4.354%
15	18.358	2593	2599	2613	rBV	453080	642655	18.38%	2.818%
16	19.621	2809	2814	2828	rBV	256005	379186	10.84%	1.663%
17	20.097	2889	2895	2901	rBV	2675096	3496577	100.00%	15.330%
18	20.861	3021	3025	3030	rBV3	31674	42820	1.22%	0.188%
19	21.378	3108	3113	3128	rBV	228984	418534	11.97%	1.835%
20	21.783	3175	3182	3189	rBV	678559	1122682	32.11%	4.922%
21	21.936	3204	3208	3214	rVB2	56020	72279	2.07%	0.317%
22	22.559	3309	3314	3319	rBV2	74278	125093	3.58%	0.548%
23	23.276	3429	3436	3441	rBV2	96040	182057	5.21%	0.798%
24	24.104	3570	3577	3585	rVB2	96514	206503	5.91%	0.905%
25	25.126	3737	3751	3762	rBV2	381538	1297855	37.12%	5.690%
26	26.260	3936	3944	3954	rVB4	58524	179033	5.12%	0.785%
27	27.659	4177	4182	4184	rBV6	21691	35544	1.02%	0.156%

Sum of corrected areas: 22808129

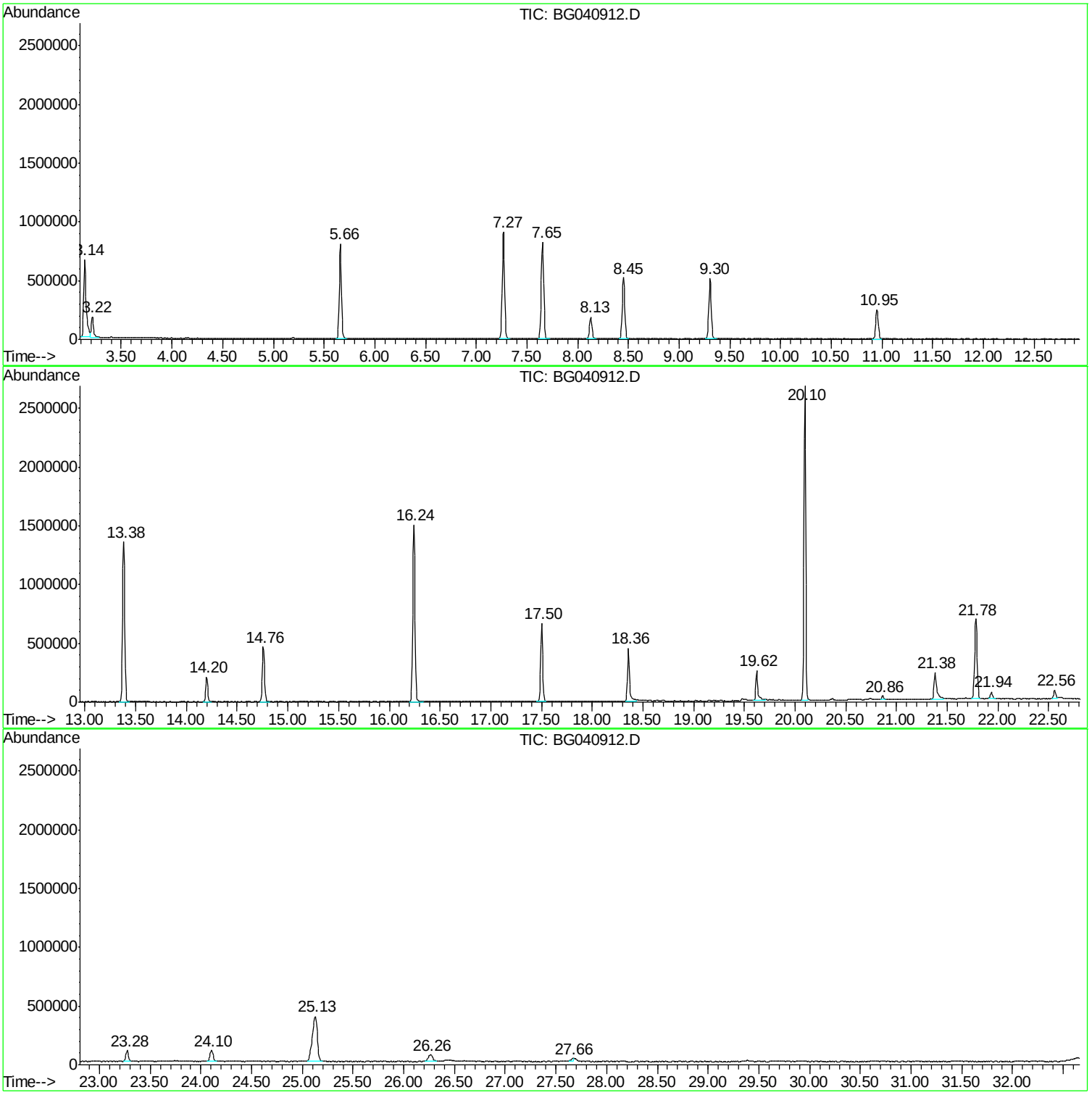
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

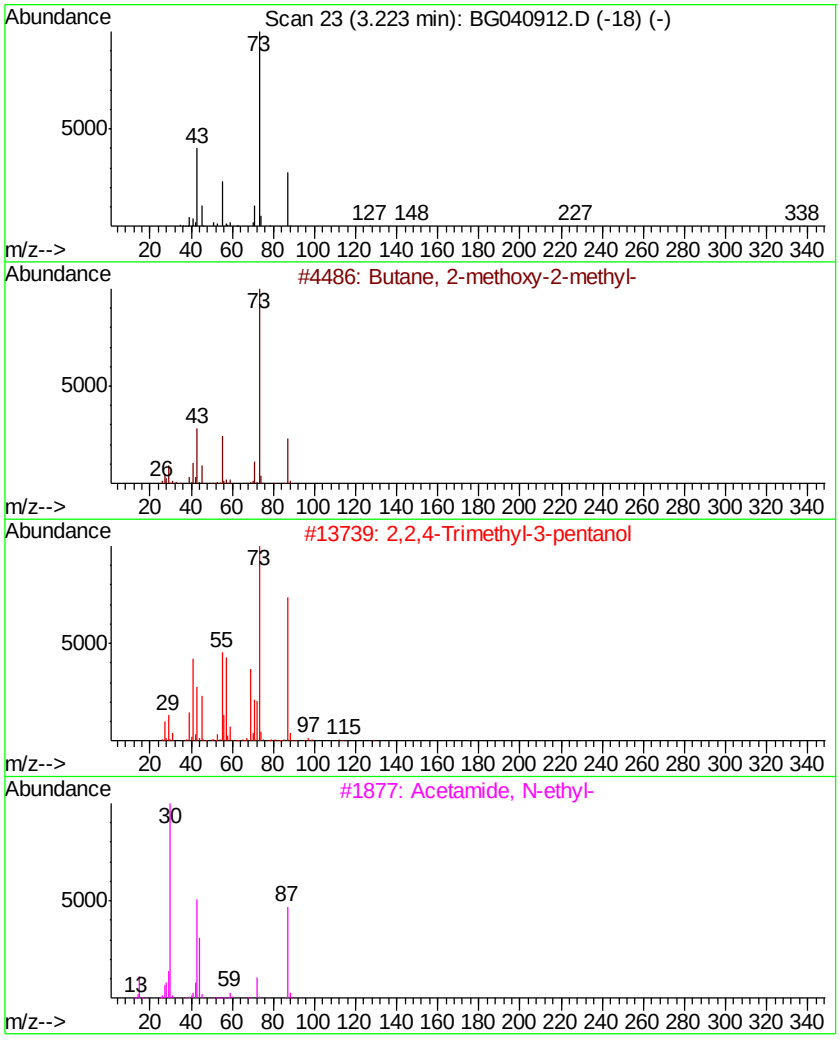
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

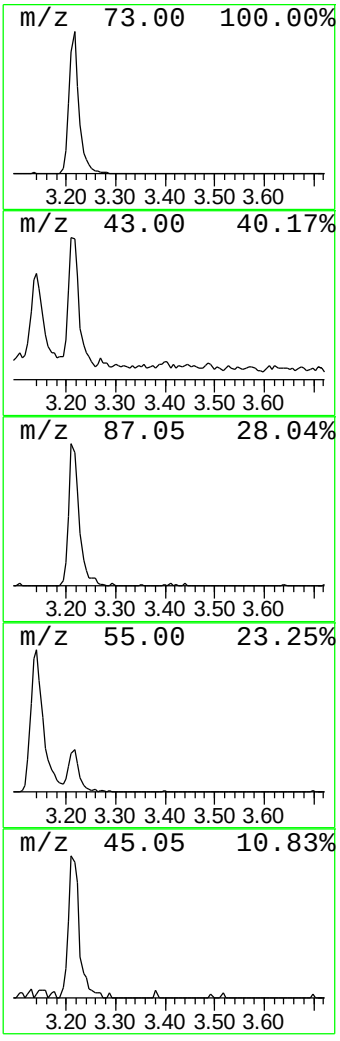
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	16.63 ng	263664	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

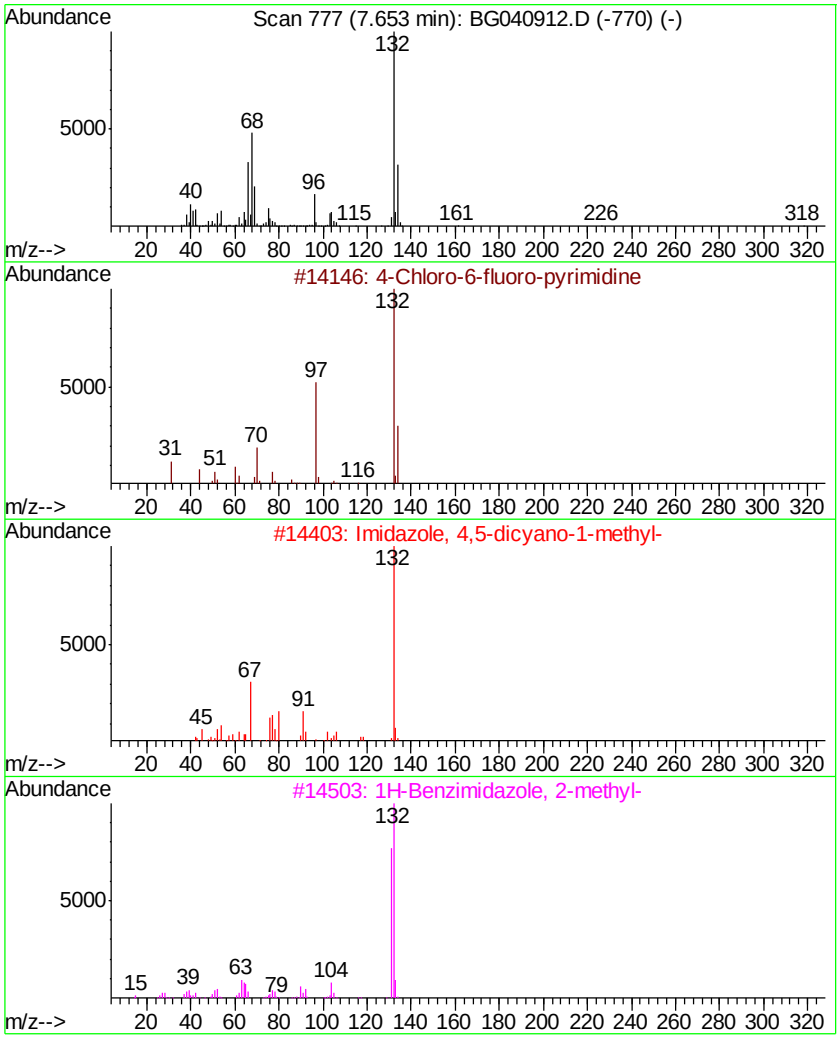
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

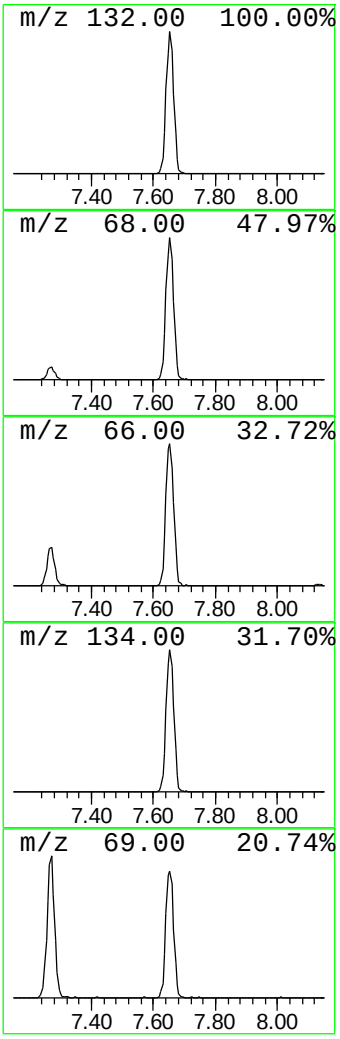
****

Peak Number 3 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	88.79 ng	1407450	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

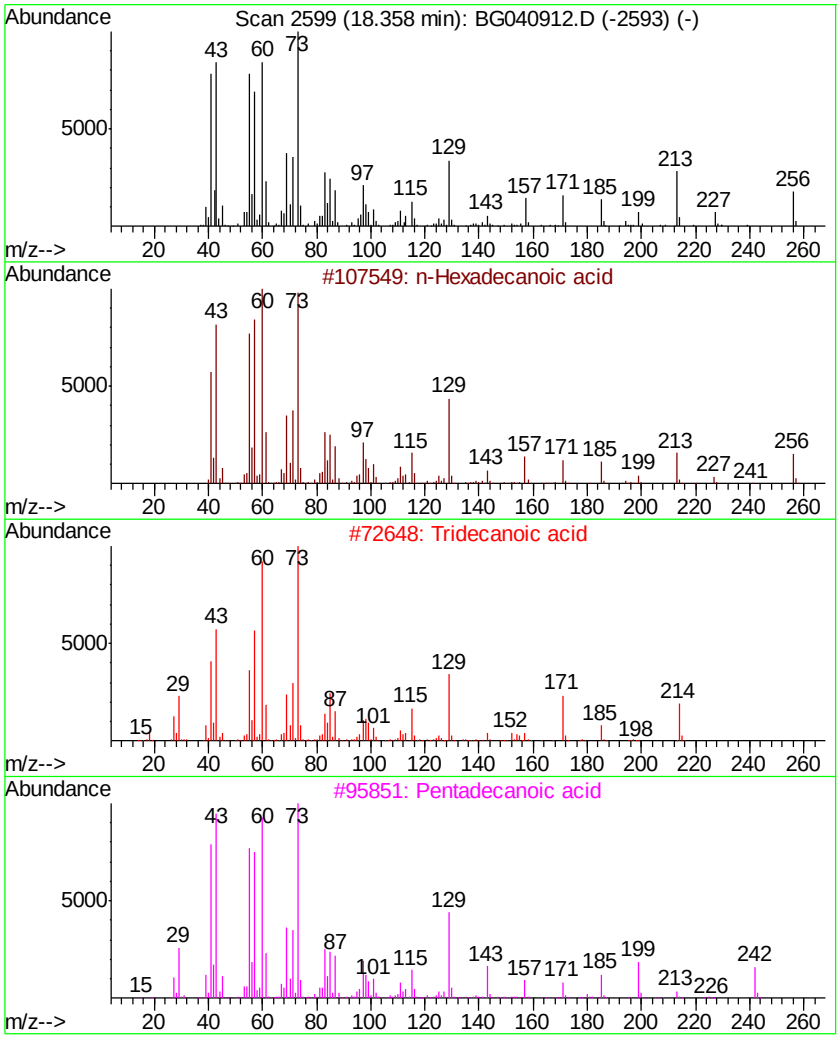
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

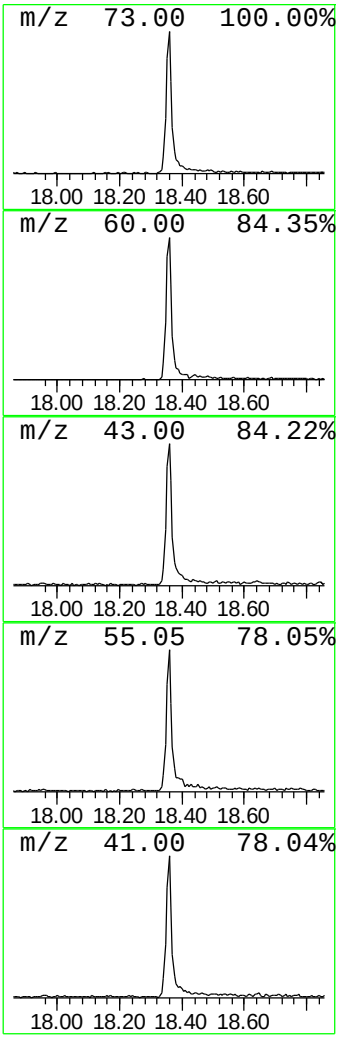
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	12.94 ng	642655	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

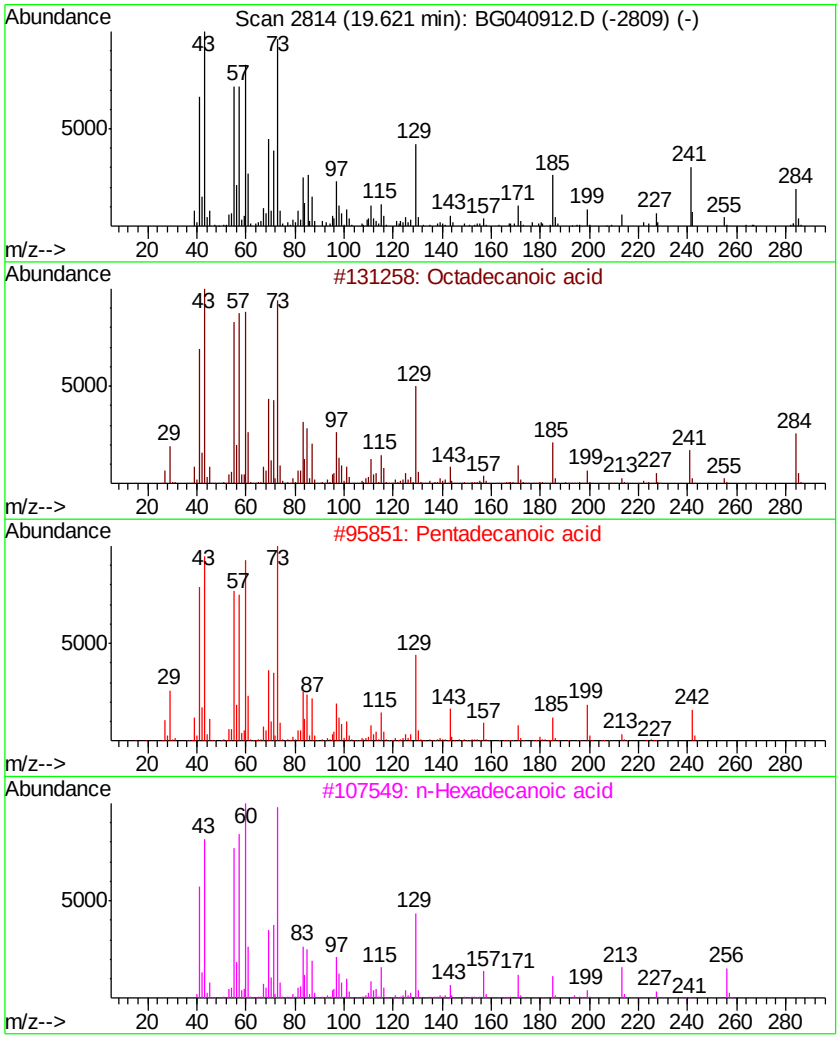
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

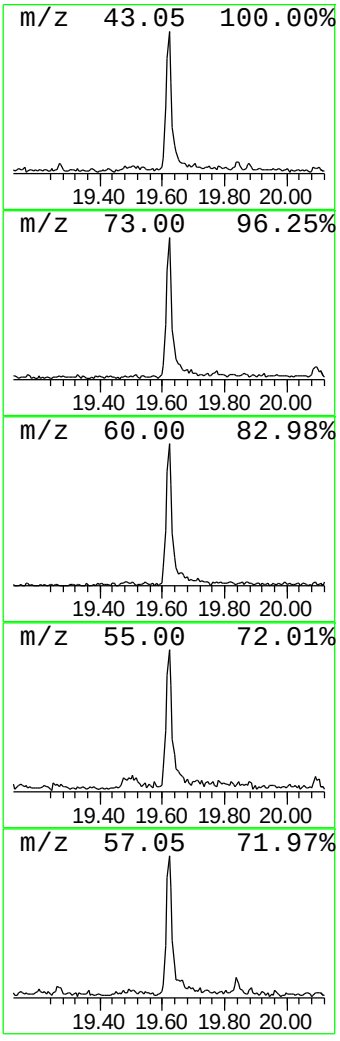
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	7.64 ng	379186	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

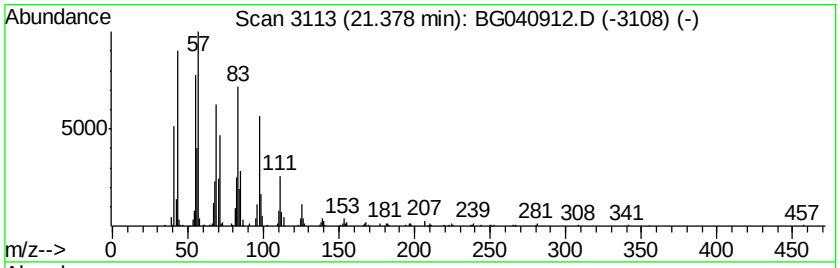
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

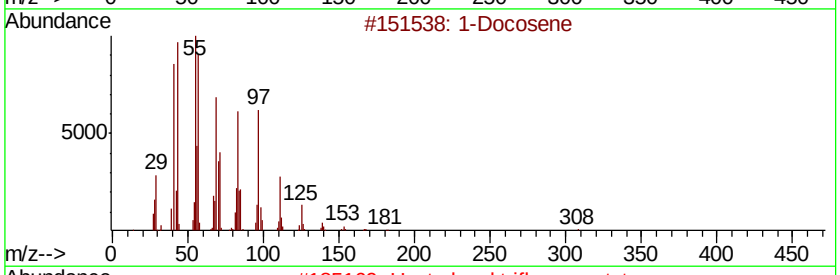
****

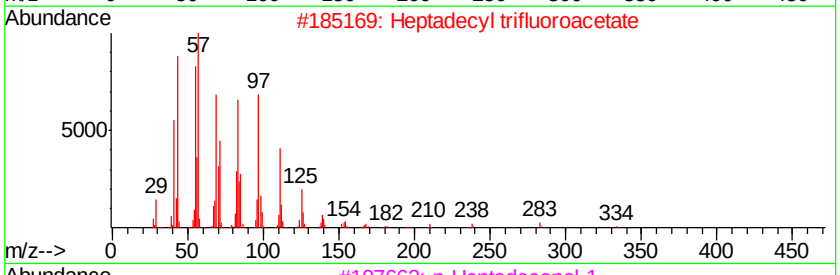
Peak Number 7 1-Docosene Concentration Rank 7

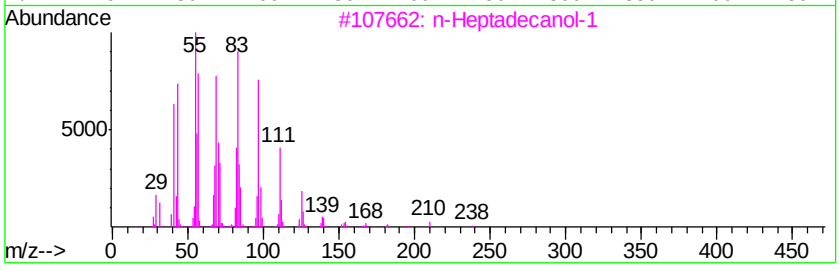
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	7.46 ng	418534	Chrysene-d12	21.78

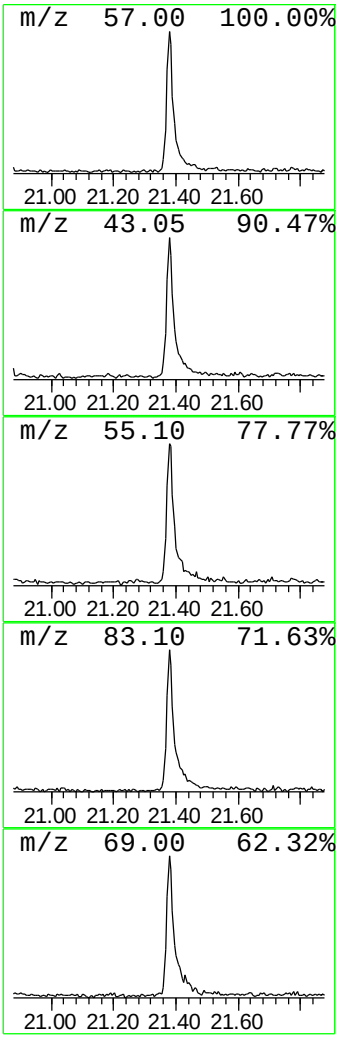
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	93
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91











Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

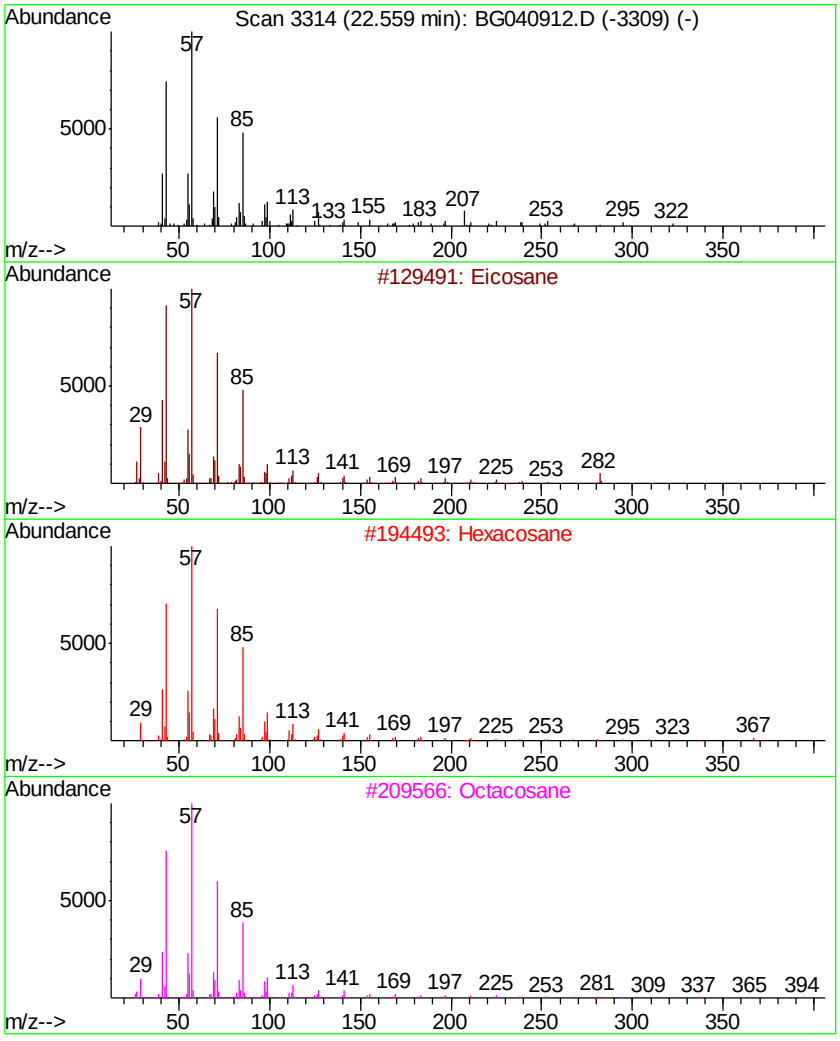
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

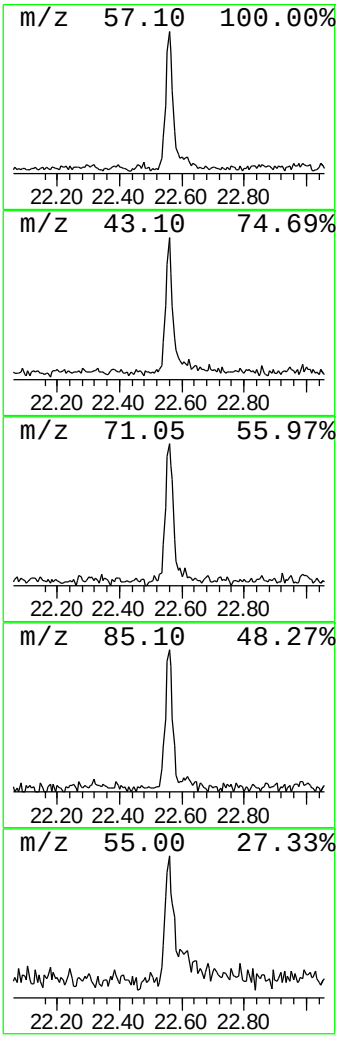
****

Peak Number 8 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.56	2.23 ng	125093	Chrysene-d12	21.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
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Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

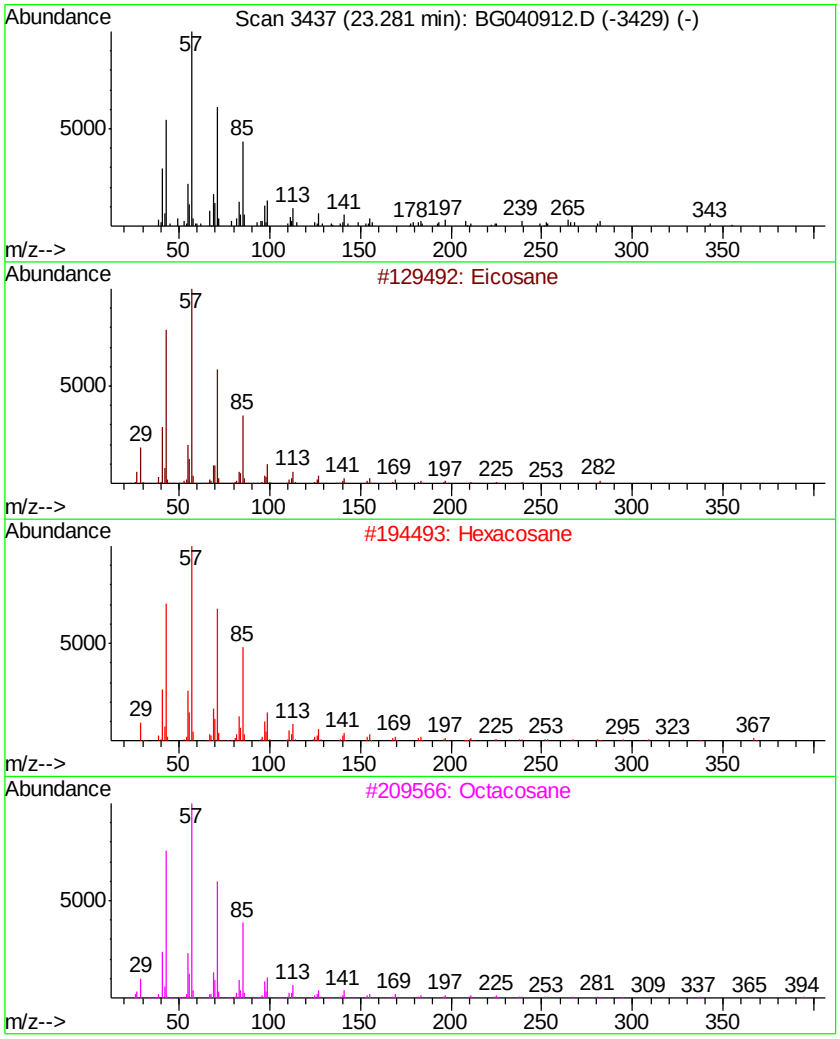
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

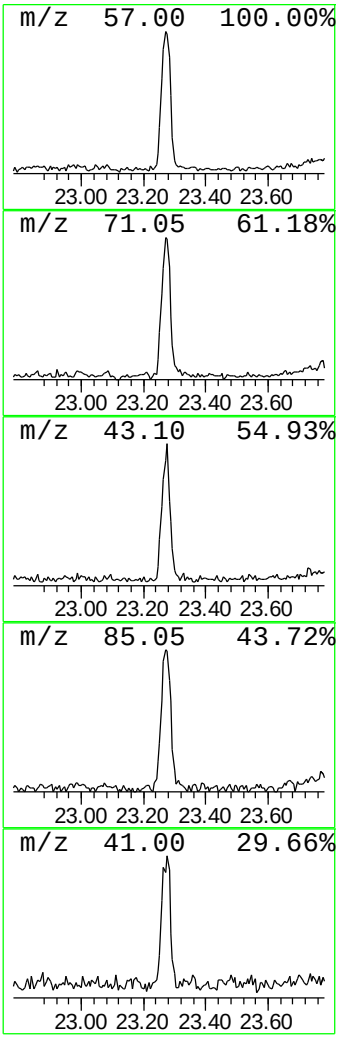
****

Peak Number 9 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	3.24 ng	182057	Chrysene-d12	21.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heneicosane	296	C21H44	000629-94-7	83





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Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

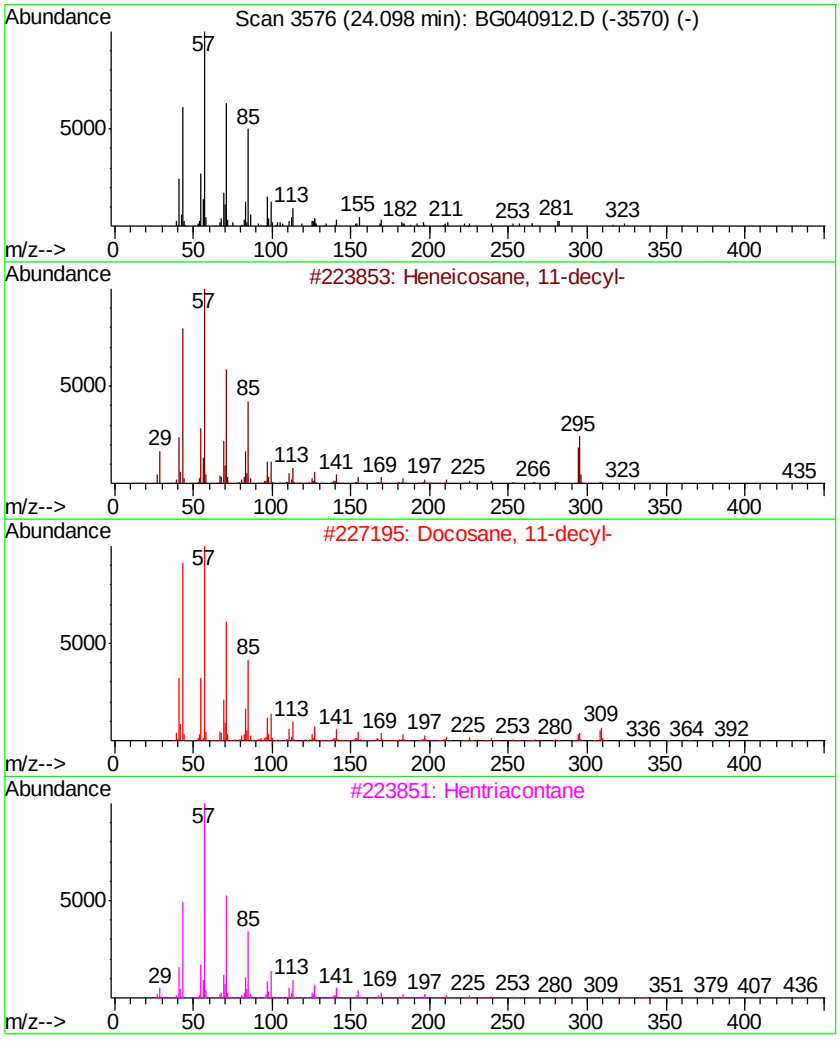
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

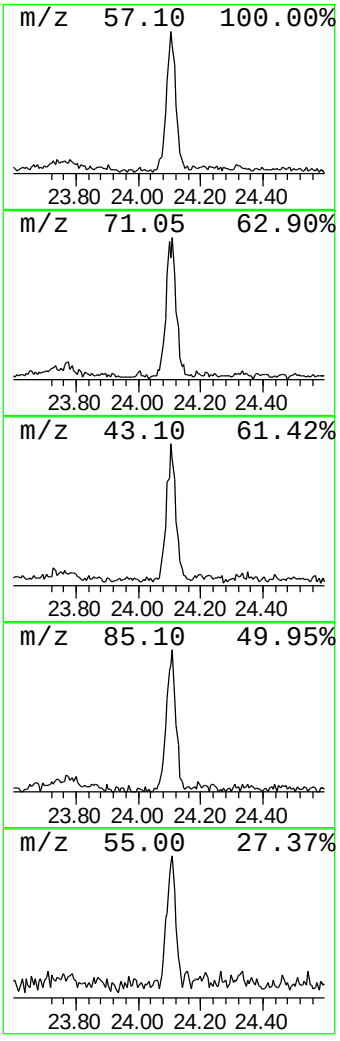
****

Peak Number 10 Heneicosane, 11-decyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.10	3.18 ng	206503	Perylene-d12	25.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Octacosane	394	C28H58	000630-02-4	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

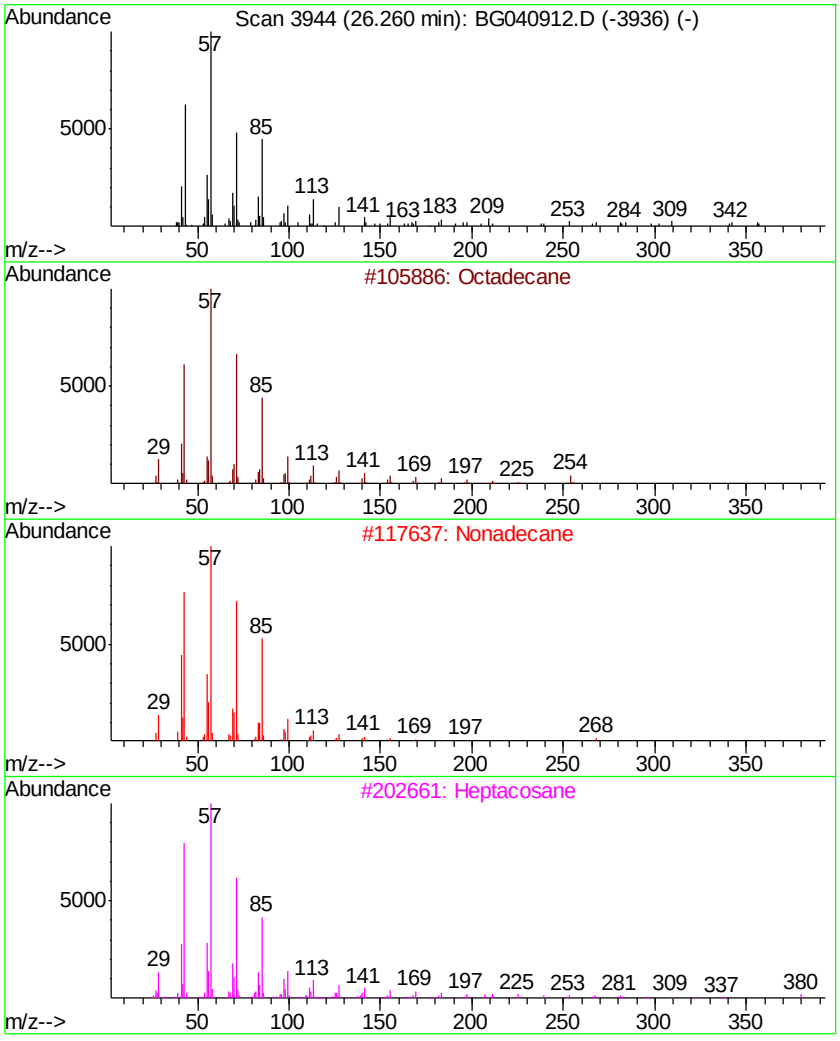
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

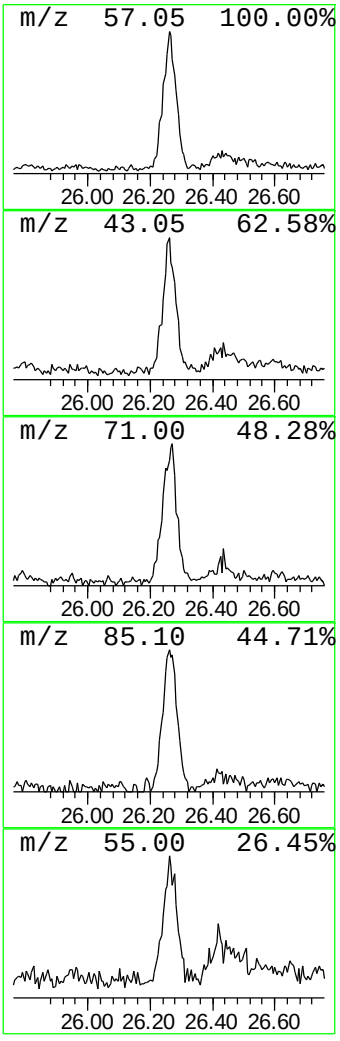
****

Peak Number 11 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.26	2.76 ng	179033	Perylene-d12	25.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Nonadecane	268	C19H40	000629-92-5	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Hexadecane	226	C16H34	000544-76-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051319\
Data File : BG040912.D
Acq On : 13 May 2019 15:39
Operator : HP/JU
Sample : K2823-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 12-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.22	16.6	ng	263664	1	8.13	317027	20.0
unknown7.65	7.65	88.8	ng	1407450	1	8.13	317027	20.0
n-Hexadecanoic acid	18.36	12.9	ng	642655	4	17.50	992956	20.0
Octadecanoic acid	19.62	7.6	ng	379186	4	17.50	992956	20.0
1-Docosene	21.38	7.5	ng	418534	5	21.78	1122680	20.0
Eicosane	22.56	2.2	ng	125093	5	21.78	1122680	20.0
Hexacosane	23.28	3.2	ng	182057	5	21.78	1122680	20.0
Heneicosane, 11-d...	24.10	3.2	ng	206503	6	25.13	1297860	20.0
Octadecane	26.26	2.8	ng	179033	6	25.13	1297860	20.0