LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

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-BG123019.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	5.033	325	331	342	rBV	276569	421988	8.21%	1.390%
2	5.509	405	412	423	rBV	1214962	2015833	39.20%	6.641%
3	7.107	675	684	696	rBV	1376024	2417266	47.01%	7.963%
4	7.471	737	746	758	rBV	1313487	2309483	44.92%	7.608%
5	7.936	817	825	833	rVB	312016	533134	10.37%	1.756%
6	8.259	871	880	888	rBV	934394	1662732	32.34%	5.477%
7	9.087	1012	1021	1032	rBV	763827	1394468	27.12%	4.594%
8	10.738	1293	1302	1320	rBV	436900	828460	16.11%	2.729%
9	13.194	1712	1720	1734	rBV	2265955	3723741	72.42%	12.267%
10	14.023	1855	1861	1873	rBV	40574	72503	1.41%	0.239%
11	14.569	1947	1954	1970	rVB	774912	1254270	24.39%	4.132%
12	16.056	2200	2207	2223	rBV	1713979	2759854	53.67%	9.092%
13	17.313	2414	2421	2432	rBV	861889	1359857	26.45%	4.480%
14	19.927	2860	2866	2878	rBV	3862066	5141870	100.00%	16.939%
15	21.238	3083	3089	3098	rBV	70667	162043	3.15%	0.534%
16	21.561	3137	3144	3157	rBV2	856478	1401944	27.27%	4.618%
17	22.366	3276	3281	3290	rBV	64469	108726	2.11%	0.358%
18	23.006	3383	3390	3394	rBV	216054	451909	8.79%	1.489%
19	23.224	3422	3427	3436	rVB	42989	82653	1.61%	0.272%
20	23.823	3522	3529	3538	rVB2	92846	207957	4.04%	0.685%
21	24.675	3664	3674	3681	rBV2	512621	1436871	27.94%	4.733%
22	24.739	3682	3685	3693	rVB3	96814	195185	3.80%	0.643%
23	25.832	3863	3871	3880	rVB2	71626	209685	4.08%	0.691%
24	27.137	4087	4093	4108	rVB4	56092	203330	3.95%	0.670%

Sum of corrected areas: 30355762

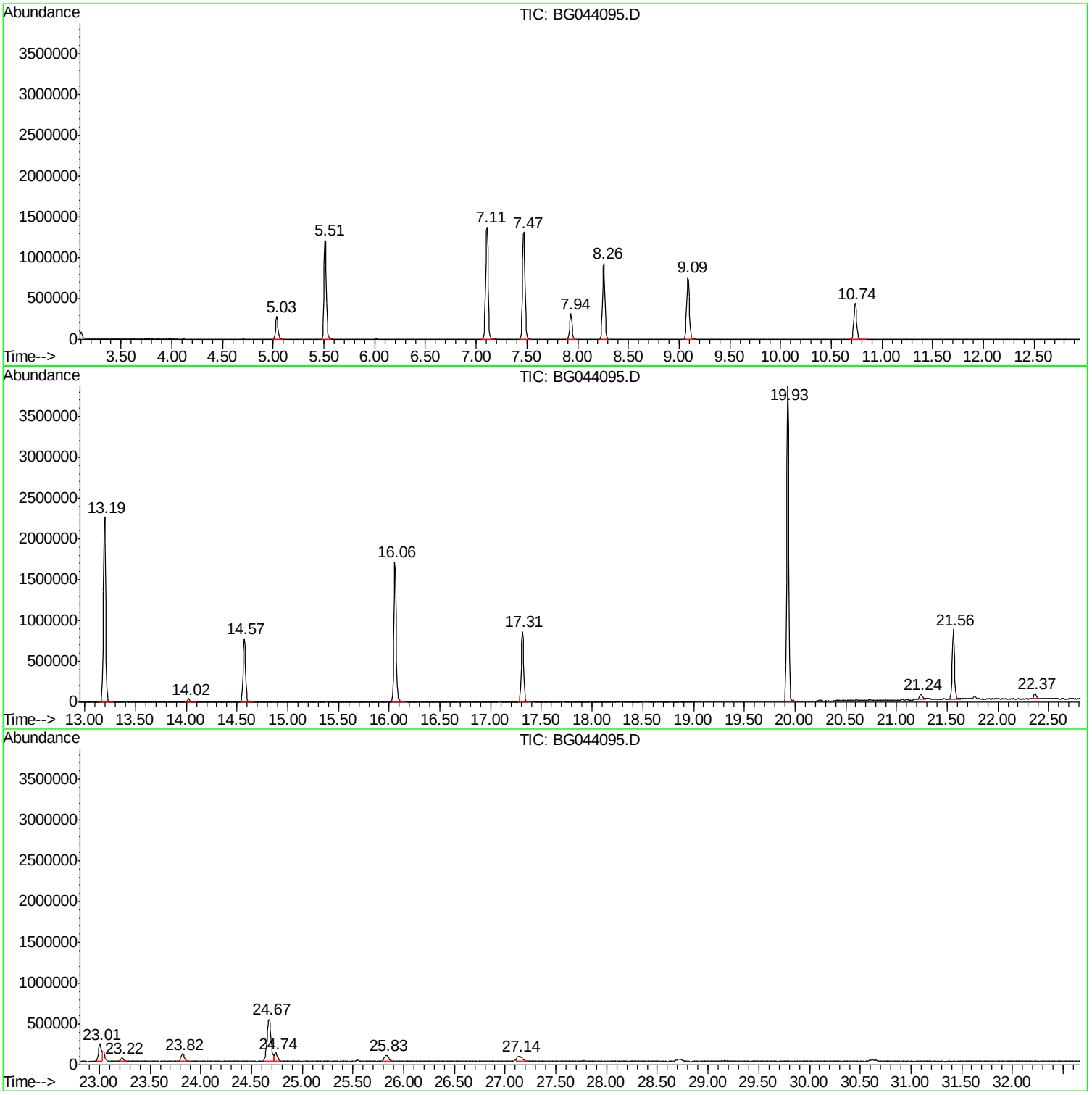
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

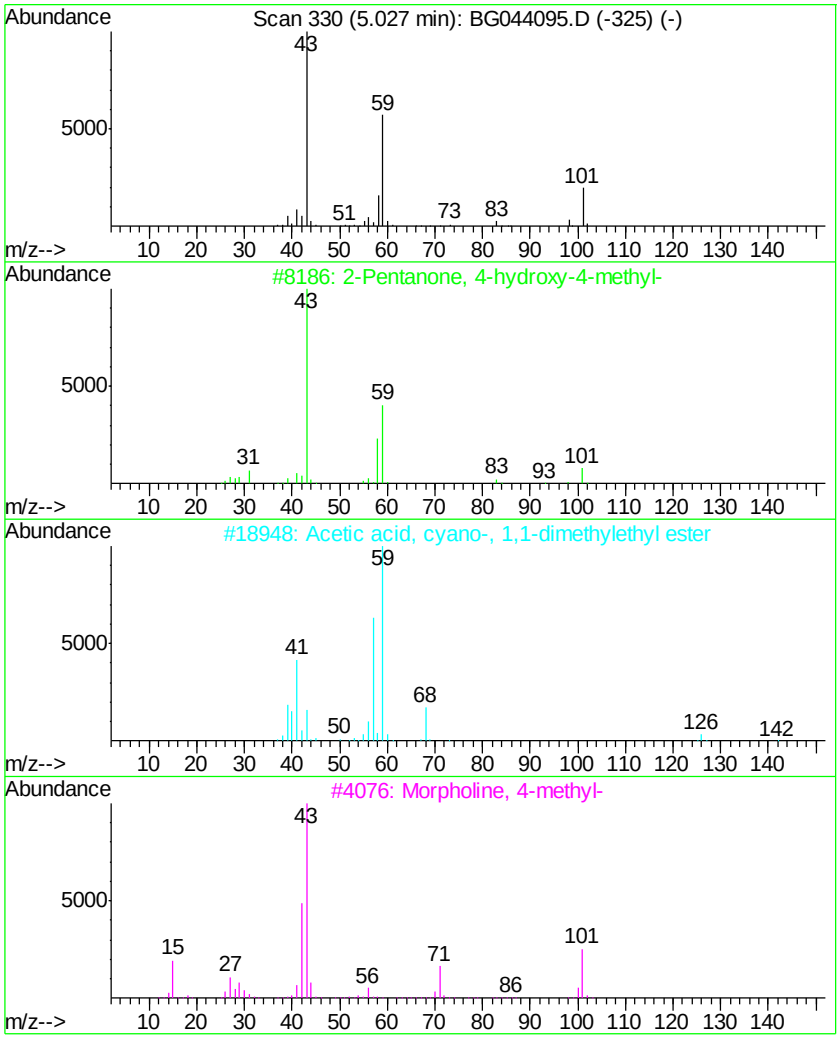
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

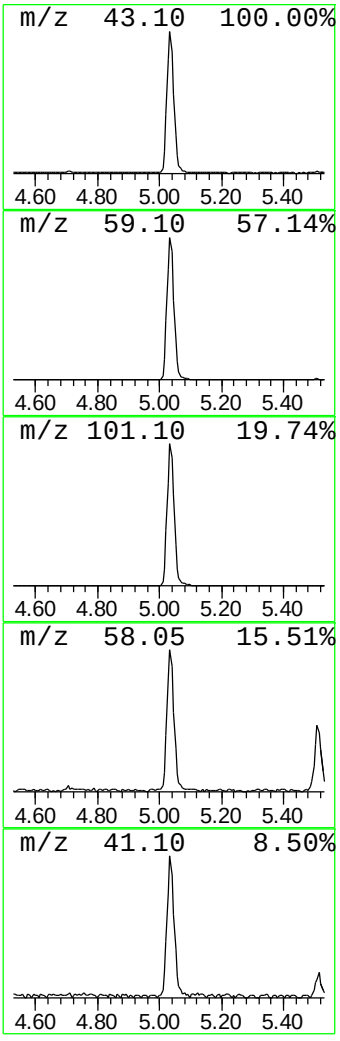
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	15.83 ng	421988	1,4-Dichlorobenzene-d4	7.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

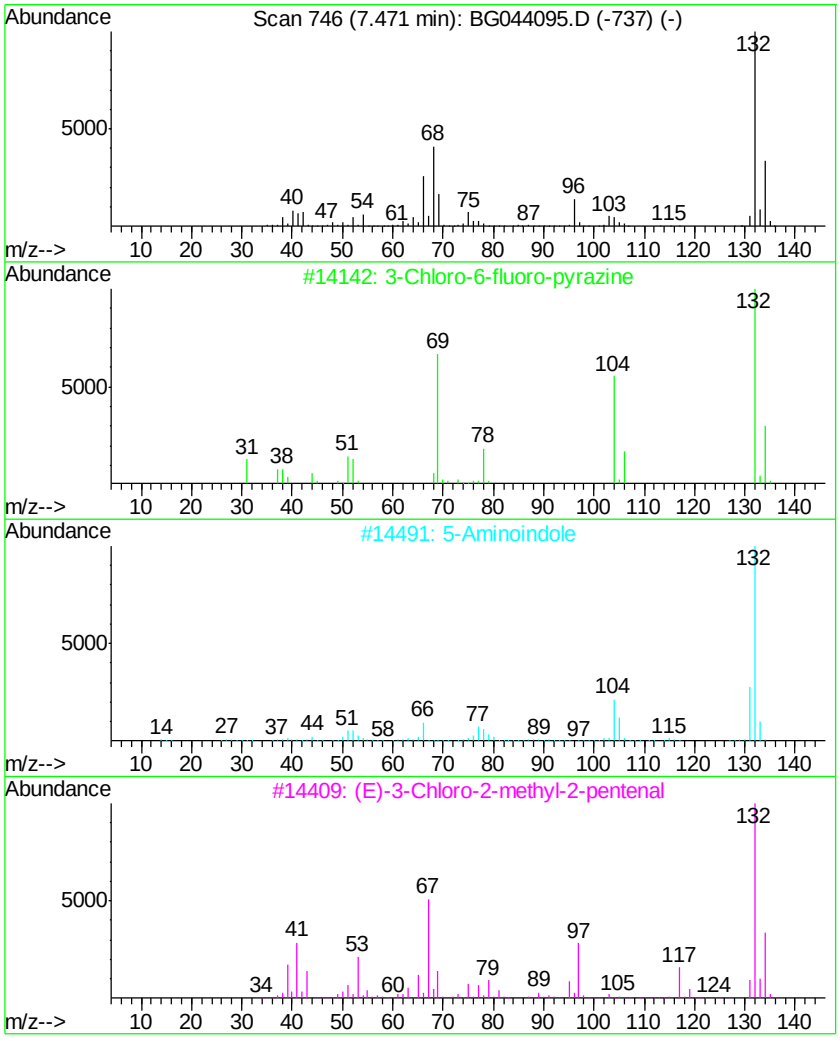
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

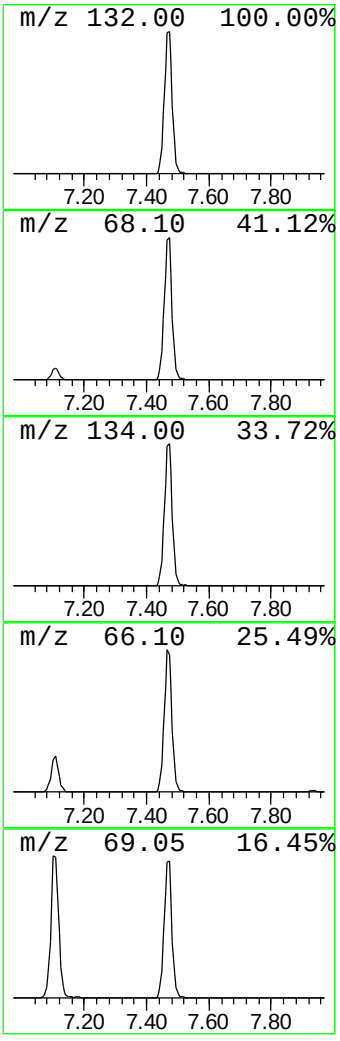
****

Peak Number 2 unknown7.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	86.64 ng	2309480	1,4-Dichlorobenzene-d4	7.94

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

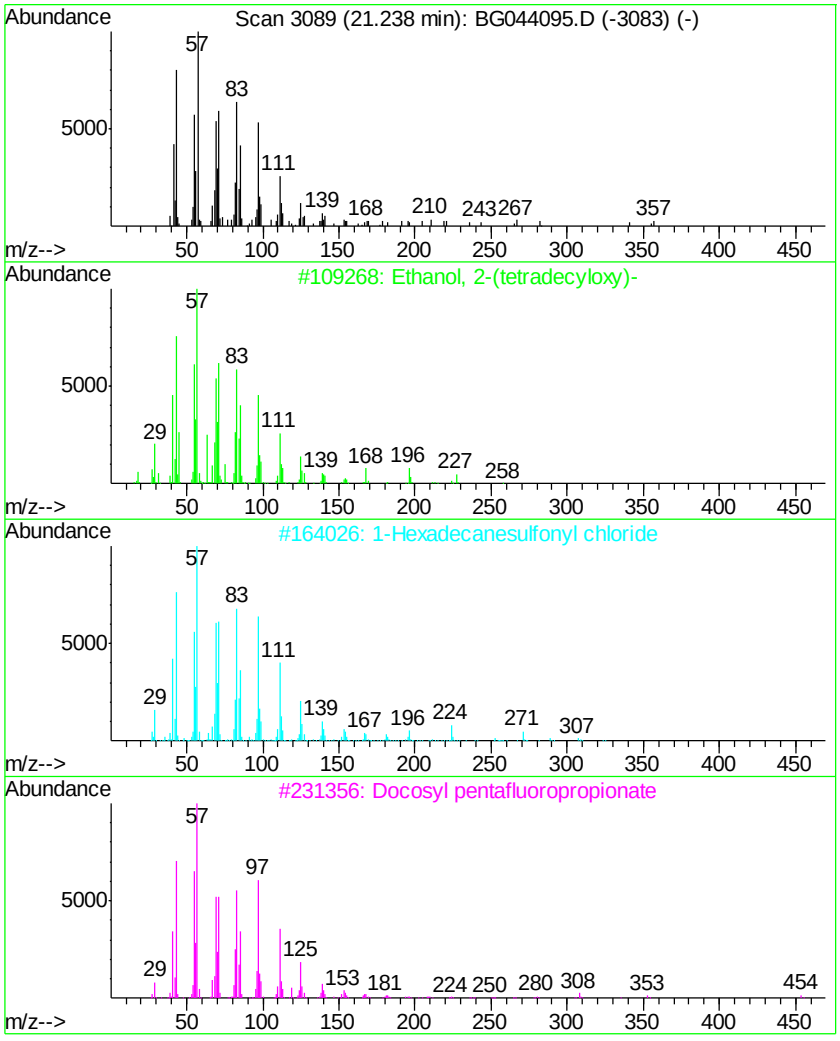
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

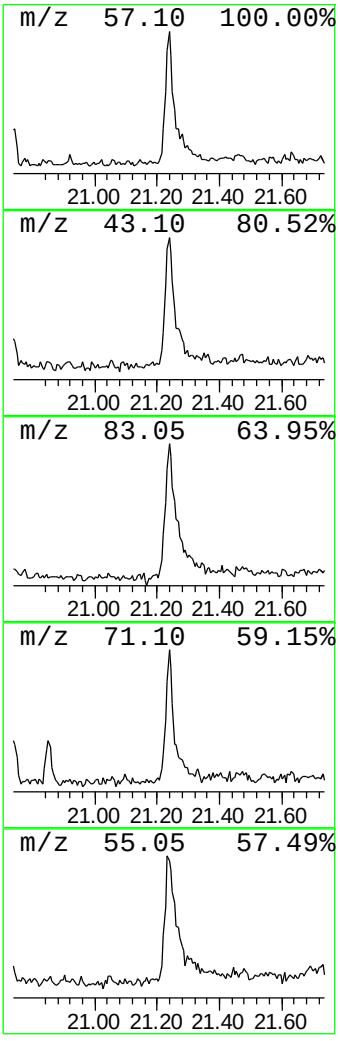
****

Peak Number 4 Ethanol, 2-(tetradecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.24	2.31 ng	162043	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	83
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	83
5	17-Pentatriacontene	491	C35H70	006971-40-0	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

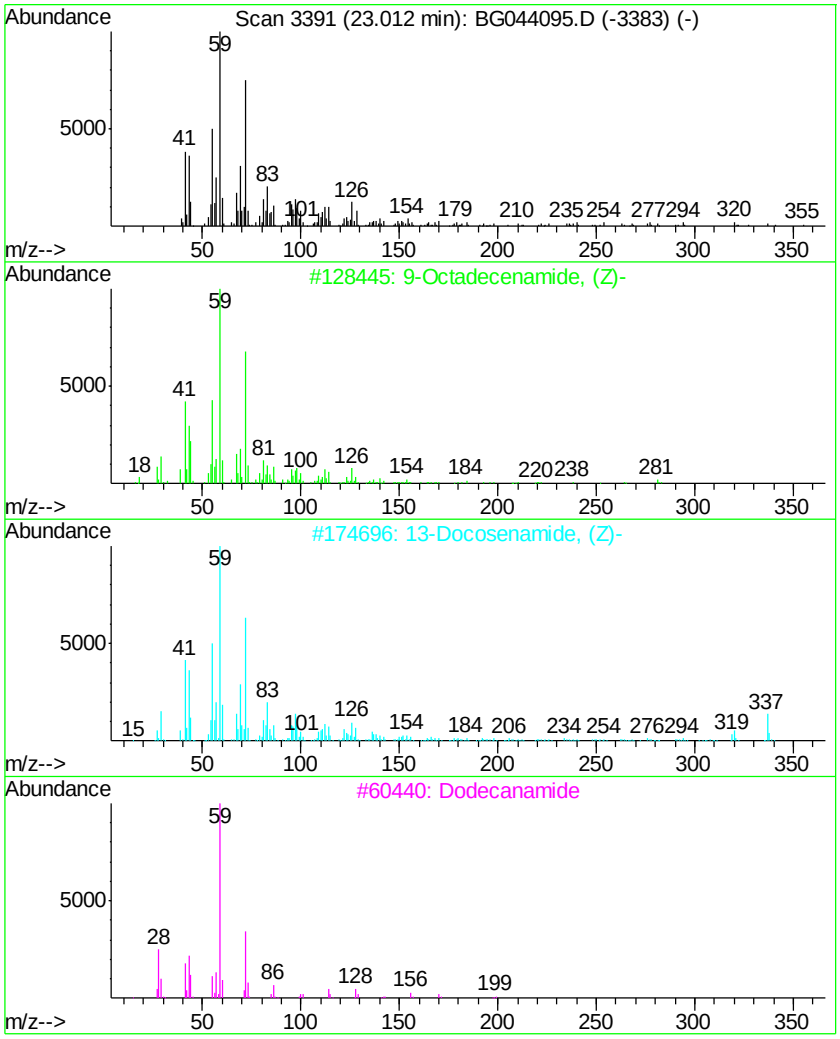
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

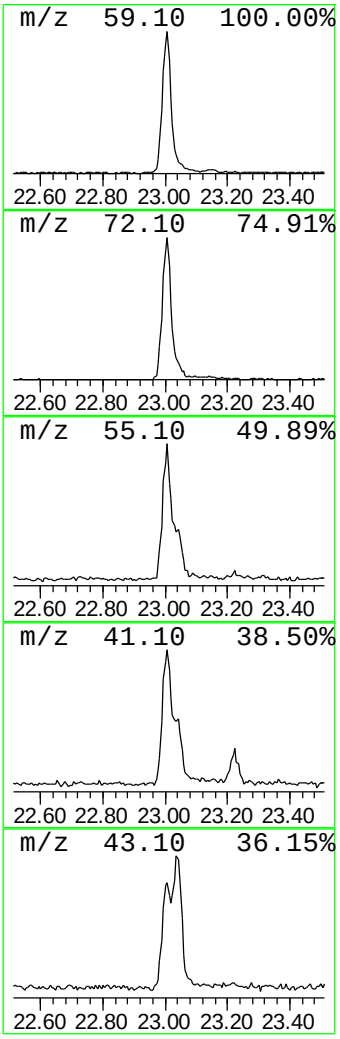
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.01	6.45 ng	451909	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	53
3	Dodecanamide	199	C12H25NO	001120-16-7	38
4	Decanamide-	171	C10H21NO	002319-29-1	38
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

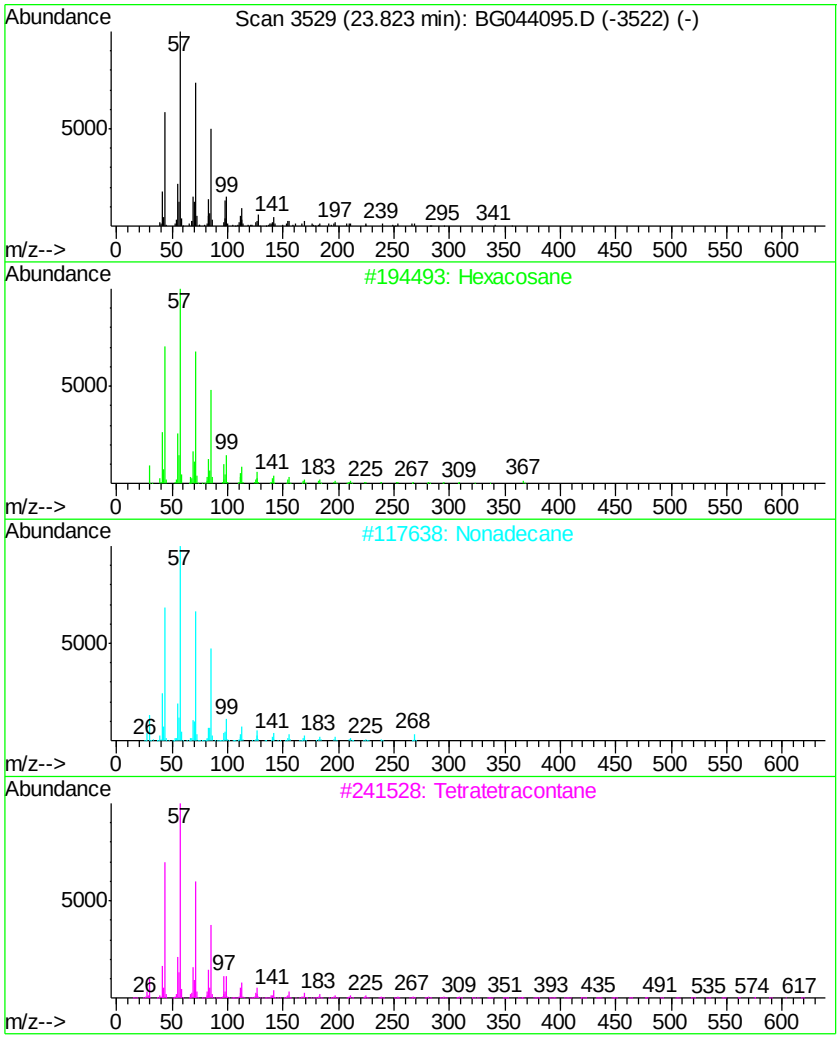
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

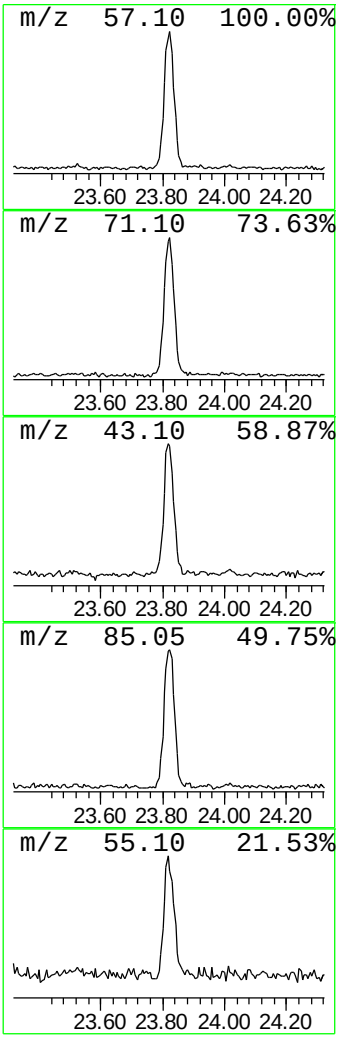
****

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.82	2.89 ng	207957	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Nonadecane	268	C19H40	000629-92-5	93
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Octacosane	394	C28H58	000630-02-4	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
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Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

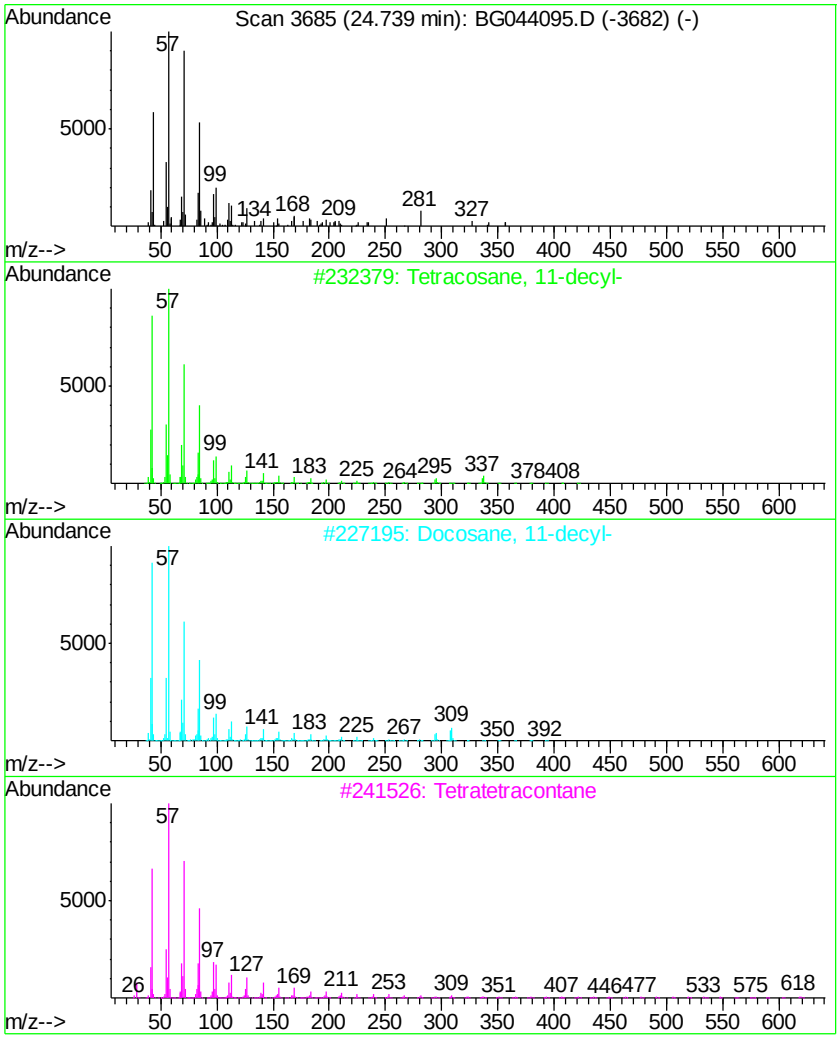
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

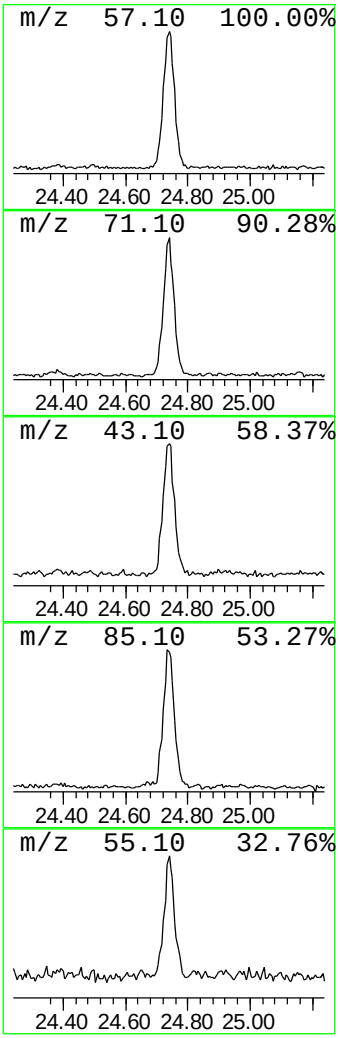
****

Peak Number 7 Tetracosane, 11-decyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.74	2.72 ng	195185	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	83
3	Tetratetracontane	619	C44H90	007098-22-8	83
4	Triacontane	422	C30H62	000638-68-6	78
5	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

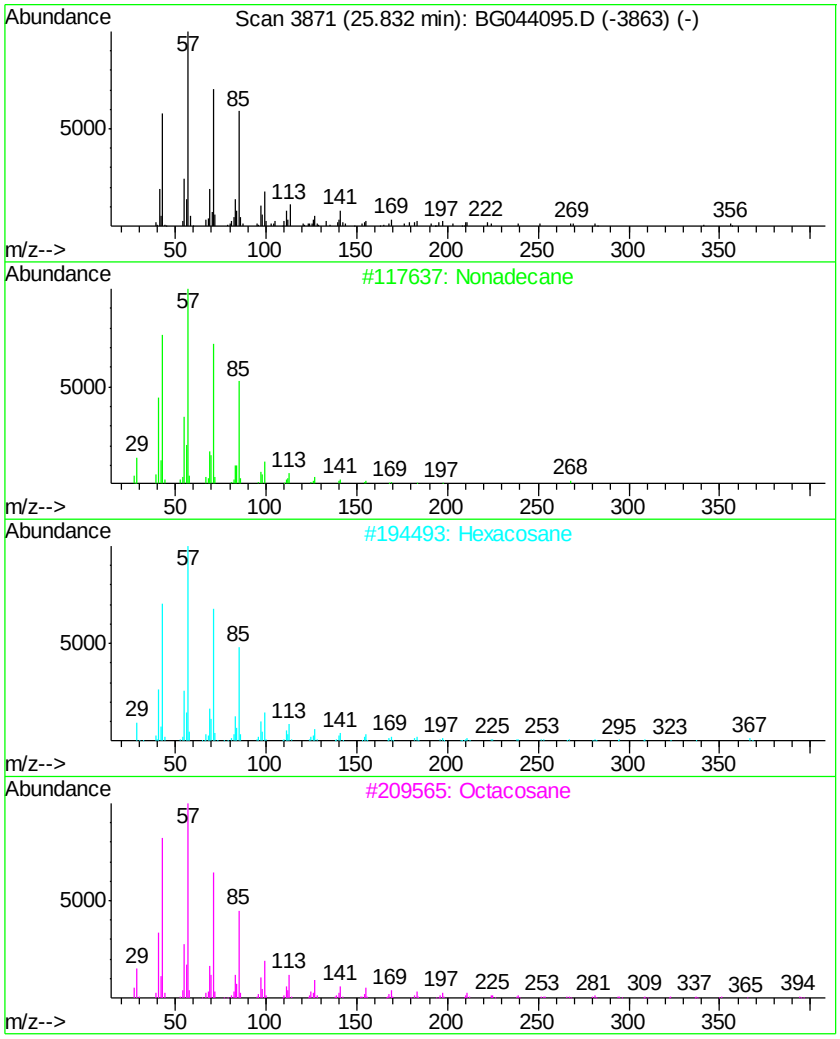
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

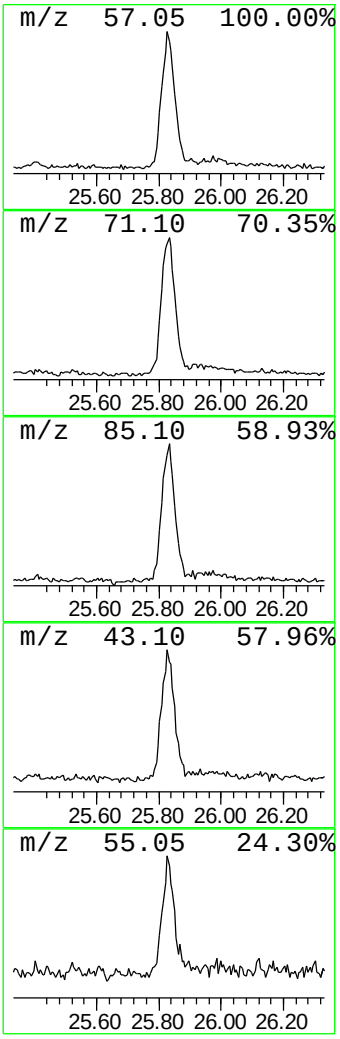
****

Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.83	2.92 ng	209685	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Docosane	310	C22H46	000629-97-0	87





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Data File : BG044095.D
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Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

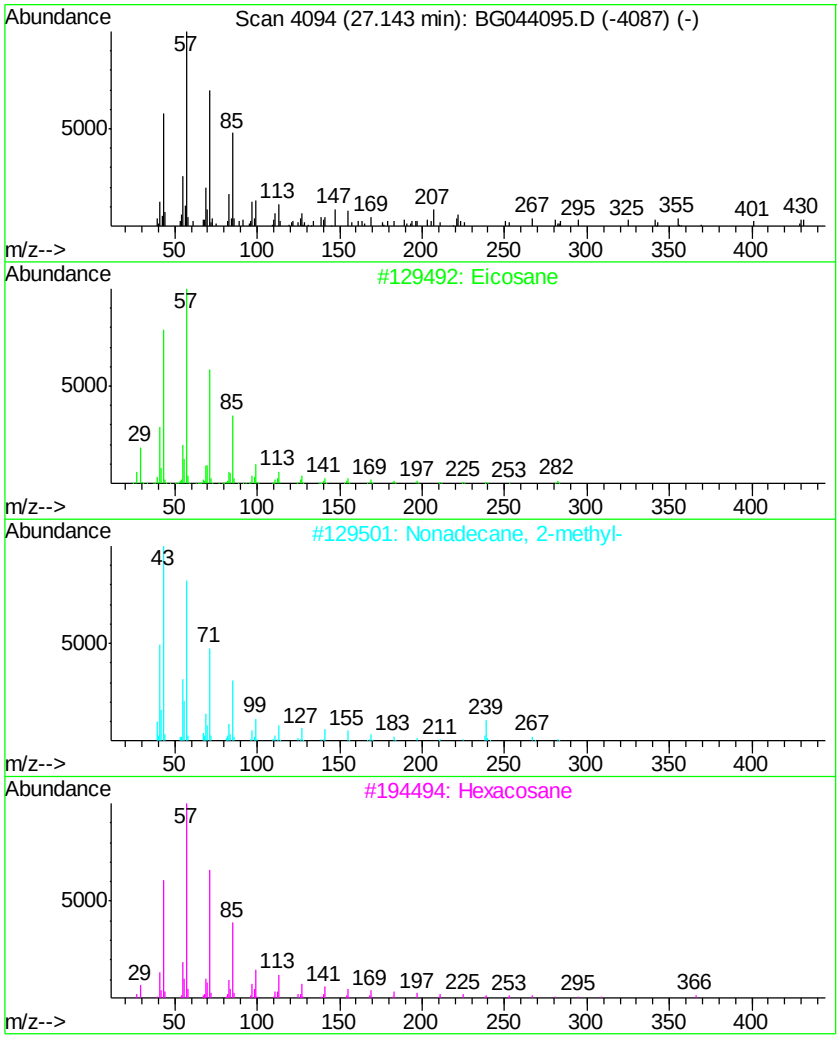
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

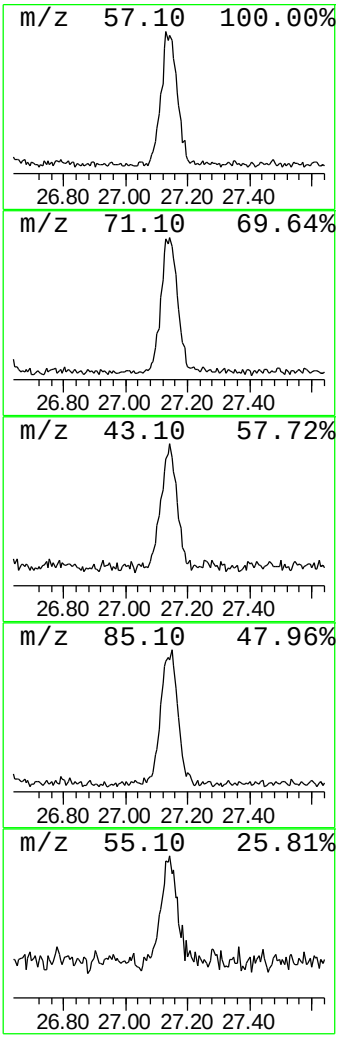
****

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.14	2.83 ng	203330	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	64
3	Hexacosane	366	C26H54	000630-01-3	64
4	Hentriacontane	437	C31H64	000630-04-6	58
5	Docosane	310	C22H46	000629-97-0	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG012020\
Data File : BG044095.D
Acq On : 20 Jan 2020 13:08
Operator : JU
Sample : PB126166BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126166BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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
2-Pentanone, 4-hy...	5.03	15.8	ng	421988	1	7.94	533134	20.0
unknown7.47	7.47	86.6	ng	2309480	1	7.94	533134	20.0
Ethanol, 2-(tetra...	21.24	2.3	ng	162043	5	21.56	1401940	20.0
9-Octadecenamide,...	23.01	6.5	ng	451909	5	21.56	1401940	20.0
Hexacosane	23.82	2.9	ng	207957	6	24.67	1436870	20.0
Tetracosane, 11-d...	24.74	2.7	ng	195185	6	24.67	1436870	20.0
Nonadecane	25.83	2.9	ng	209685	6	24.67	1436870	20.0
Eicosane	27.14	2.8	ng	203330	6	24.67	1436870	20.0