LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

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-BG071519.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	3.197	13	18	32	rVB	369105	639765	8.35%	1.527%
2	5.612	422	429	439	rBV	1791797	2946711	38.46%	7.032%
3	7.198	691	699	714	rBV	1907665	3329038	43.45%	7.945%
4	7.580	755	764	773	rBV	1821245	3215420	41.97%	7.674%
5	8.050	836	844	851	rBV	359579	624549	8.15%	1.491%
6	8.373	890	899	910	rBV	1393126	2448407	31.96%	5.843%
7	9.202	1028	1040	1053	rBV	1123241	2009926	26.23%	4.797%
8	10.853	1313	1321	1329	rBV	462791	858396	11.20%	2.049%
9	13.297	1729	1737	1754	rBV	2746949	4567826	59.62%	10.901%
10	14.114	1870	1876	1884	rVB	351753	506834	6.62%	1.210%
11	14.666	1963	1970	1979	rVB2	722508	1180302	15.41%	2.817%
12	16.141	2214	2221	2238	rBV	2546233	3969170	51.81%	9.473%
13	17.398	2428	2435	2445	rBV2	1047083	1628568	21.26%	3.887%
14	20.007	2872	2879	2886	rBV	5580070	7661561	100.00%	18.285%
15	20.688	2989	2995	3006	rBV	120202	215791	2.82%	0.515%
16	21.317	3097	3102	3134	rBV2	158458	689472	9.00%	1.645%
17	21.646	3152	3158	3166	rVB	1220870	1992455	26.01%	4.755%
18	21.869	3193	3196	3205	rVB2	62866	104367	1.36%	0.249%
19	22.480	3295	3300	3307	rBV	92946	171537	2.24%	0.409%
20	23.179	3413	3419	3427	rVB	127008	236808	3.09%	0.565%
21	23.990	3550	3557	3565	rVB	132306	291165	3.80%	0.695%
22	24.842	3691	3702	3712	rBV2	743953	2070303	27.02%	4.941%
23	24.948	3713	3720	3731	rVB	114639	297942	3.89%	0.711%
24	26.088	3907	3914	3925	rVB2	82443	245108	3.20%	0.585%

Sum of corrected areas: 41901421

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
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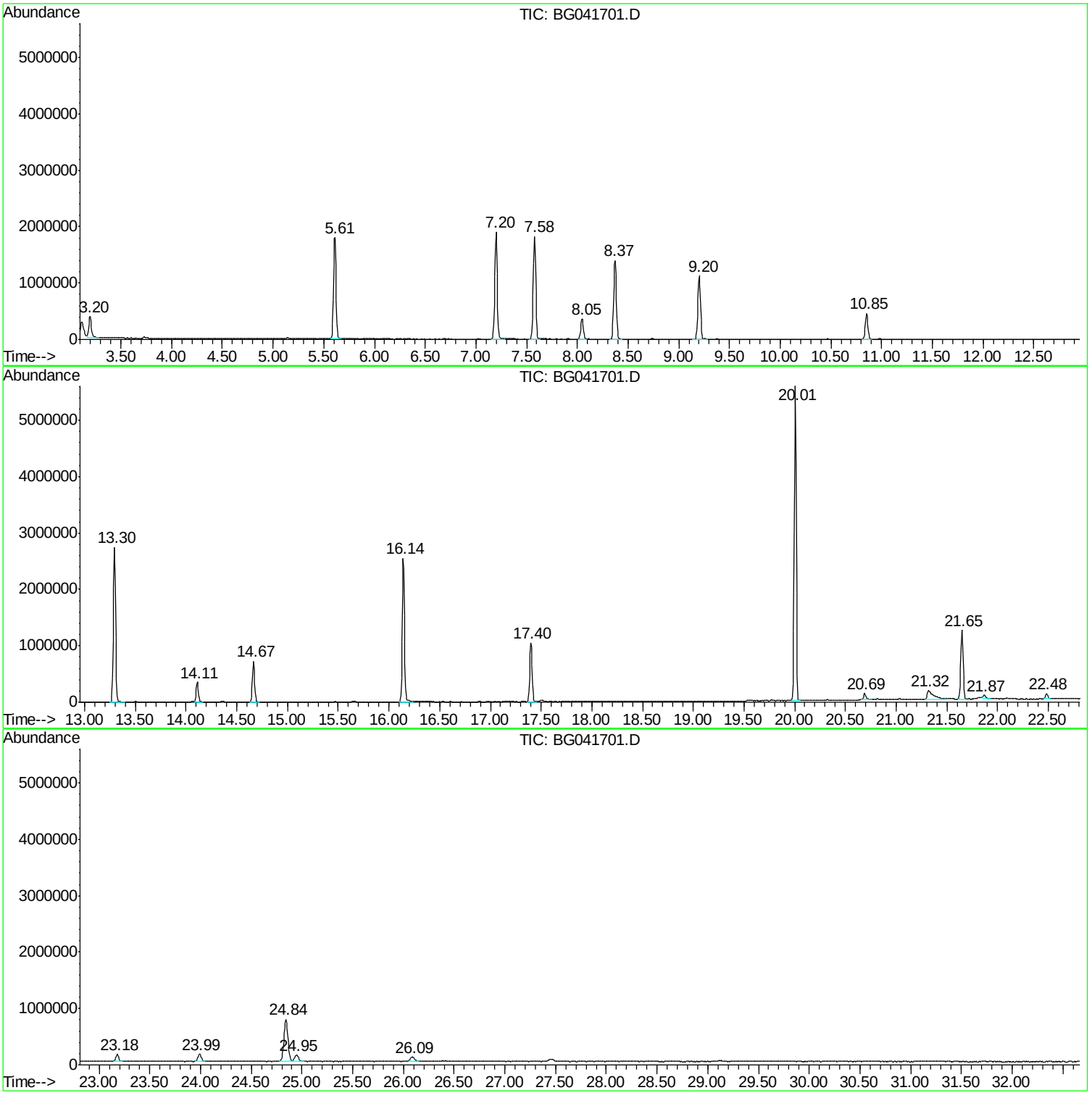
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

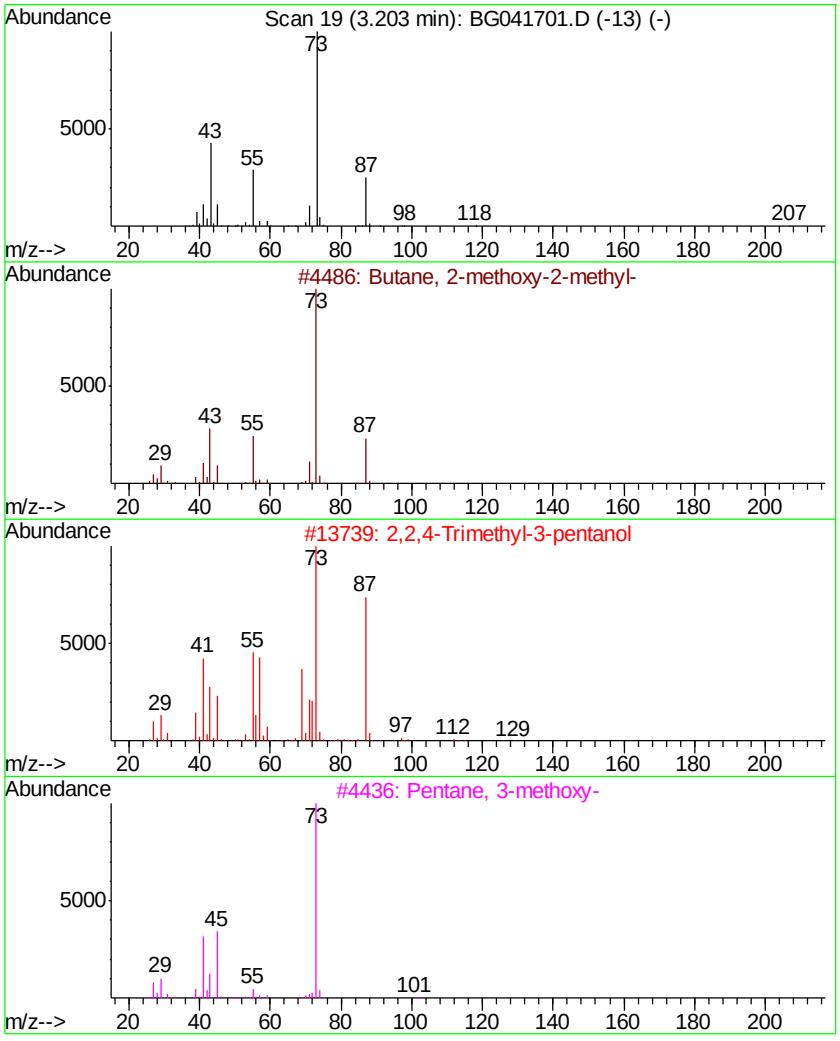
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

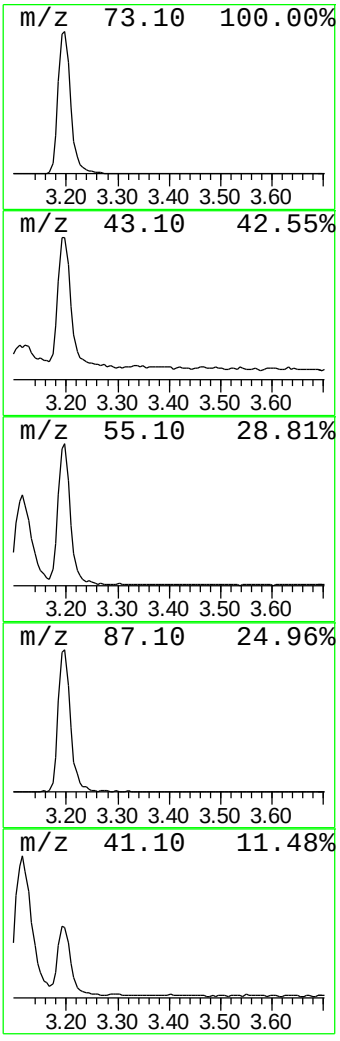
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	20.49 ng	639765	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

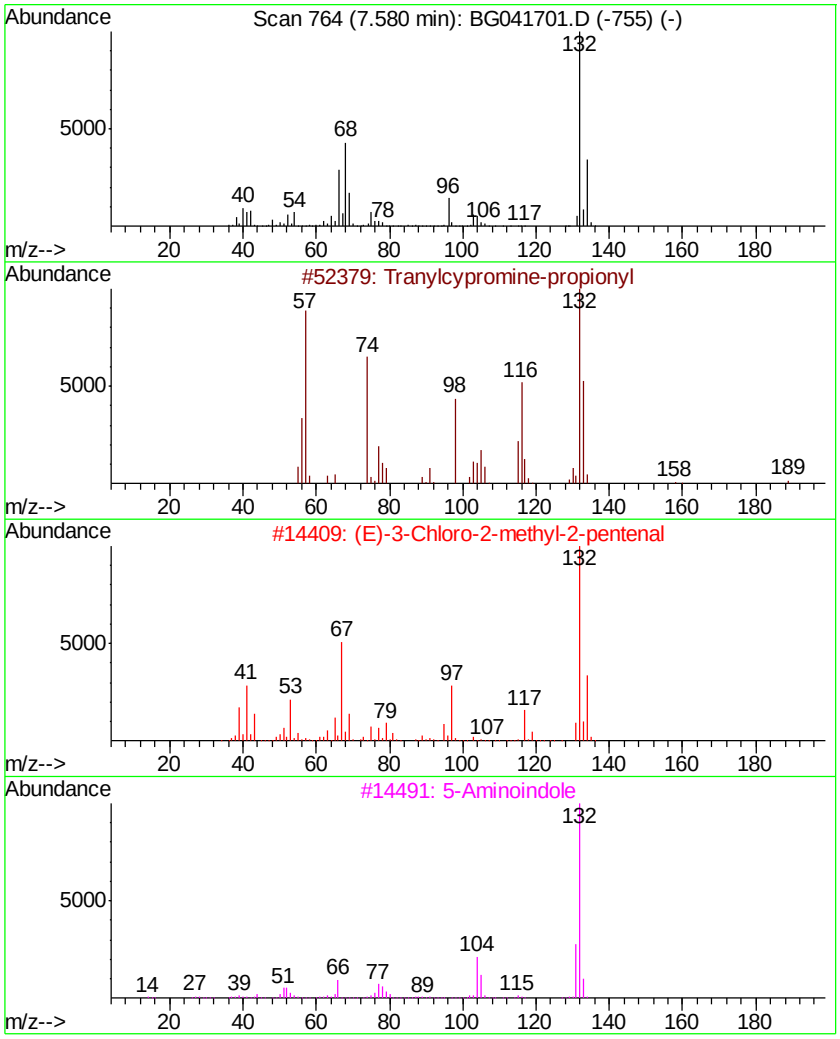
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

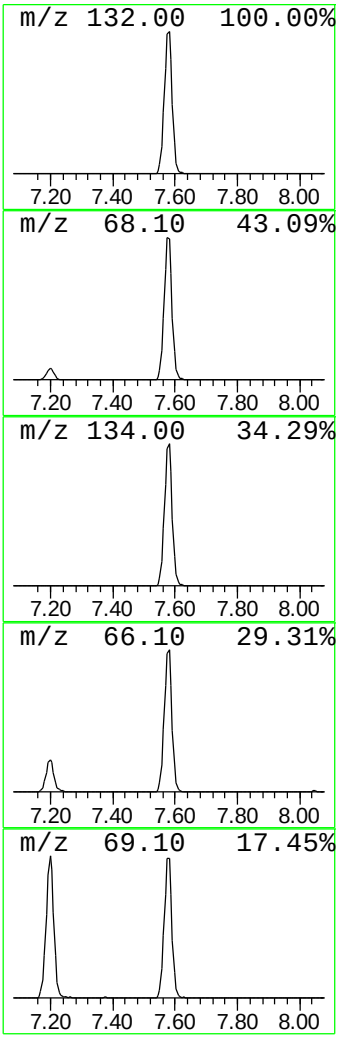
****

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	102.97 ng	3215420	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

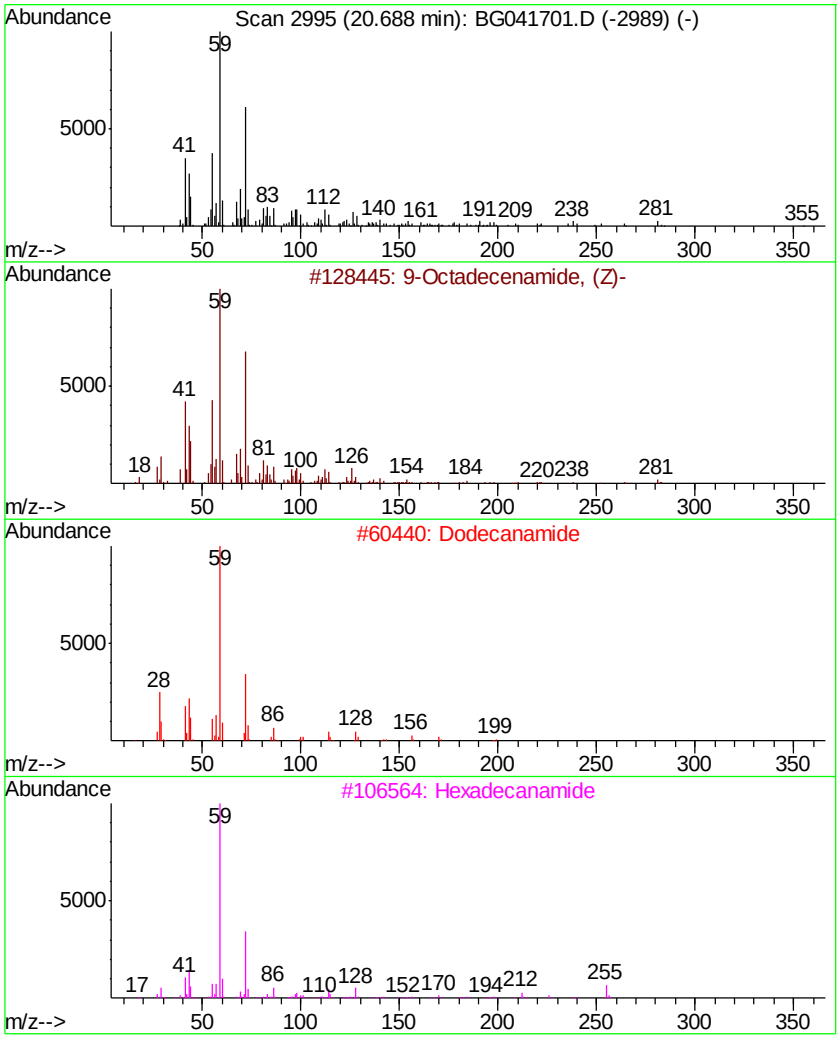
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

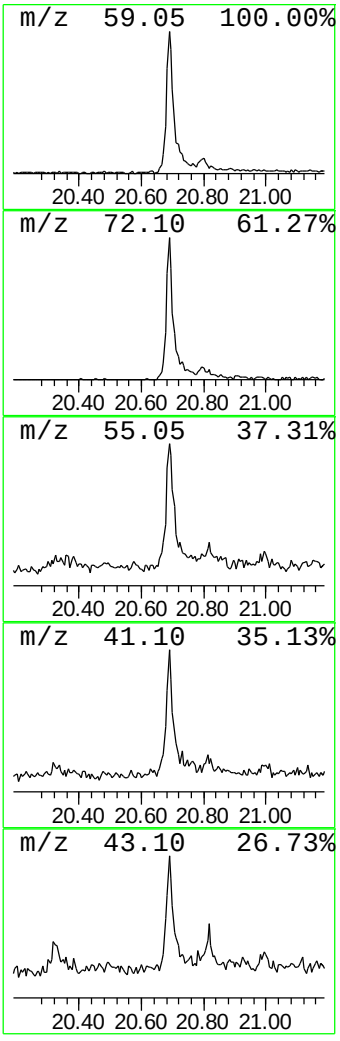
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	2.17 ng	215791	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Dodecanamide	199	C12H25NO	001120-16-7	81
3	Hexadecanamide	255	C16H33NO	000629-54-9	64
4	Octadecanamide	283	C18H37NO	000124-26-5	64
5	Nonanamide	157	C9H19NO	001120-07-6	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

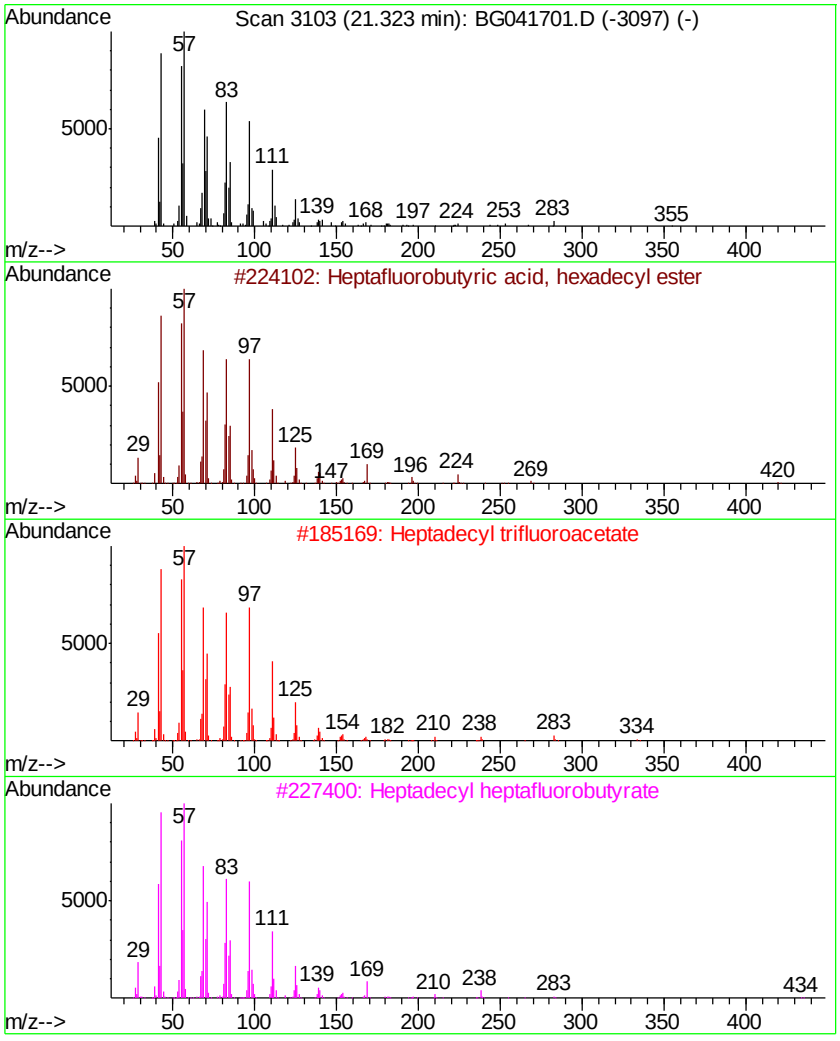
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

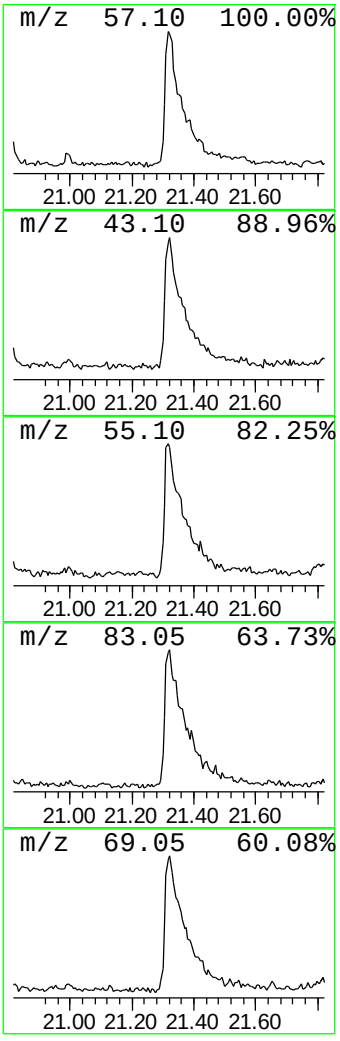
****

Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	6.92 ng	689472	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

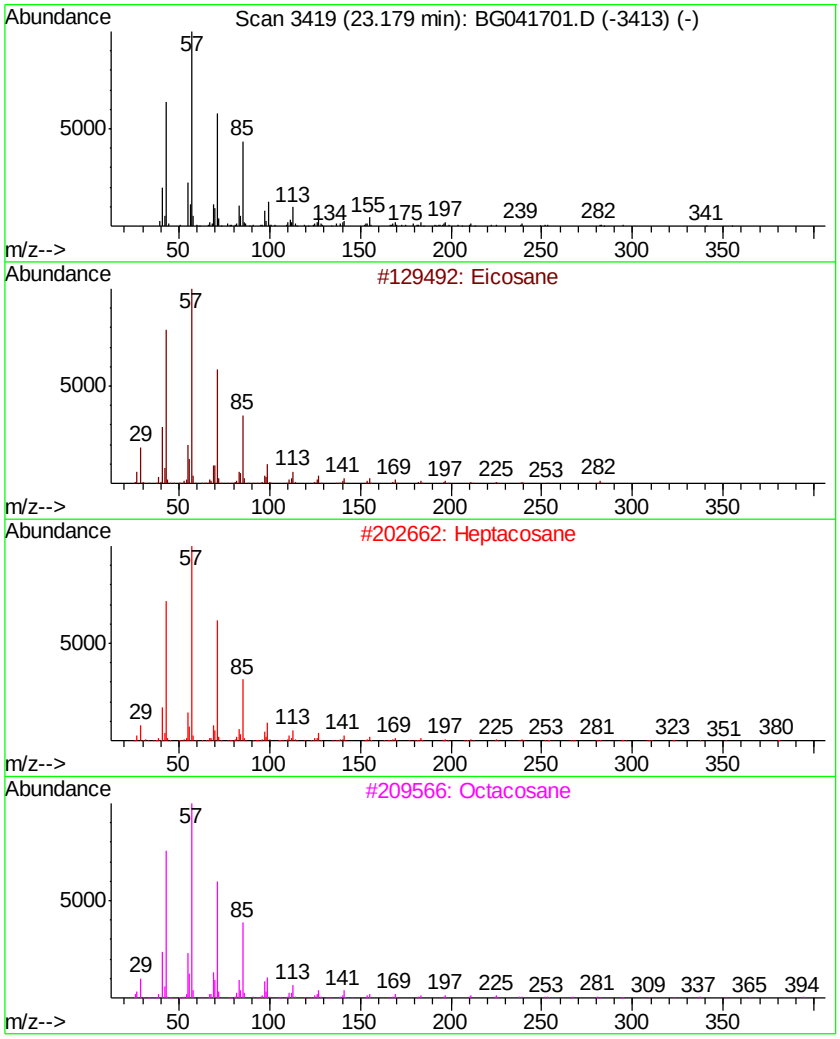
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

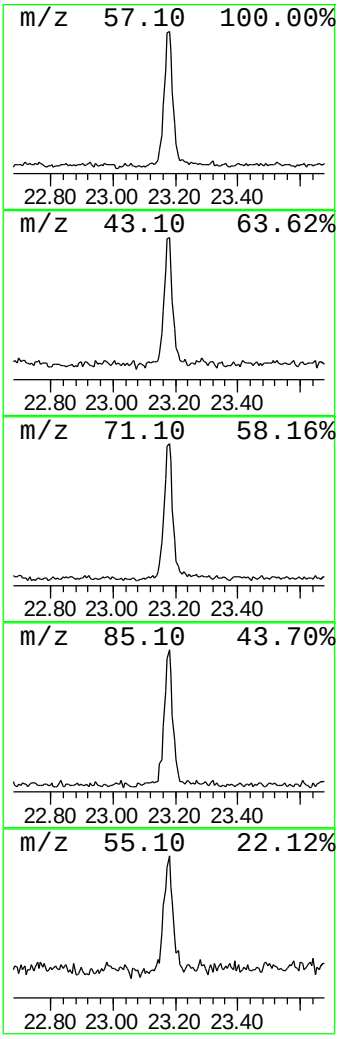
****

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	2.38 ng	236808	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
5	Pentacosane	352	C25H52	000629-99-2	90





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Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

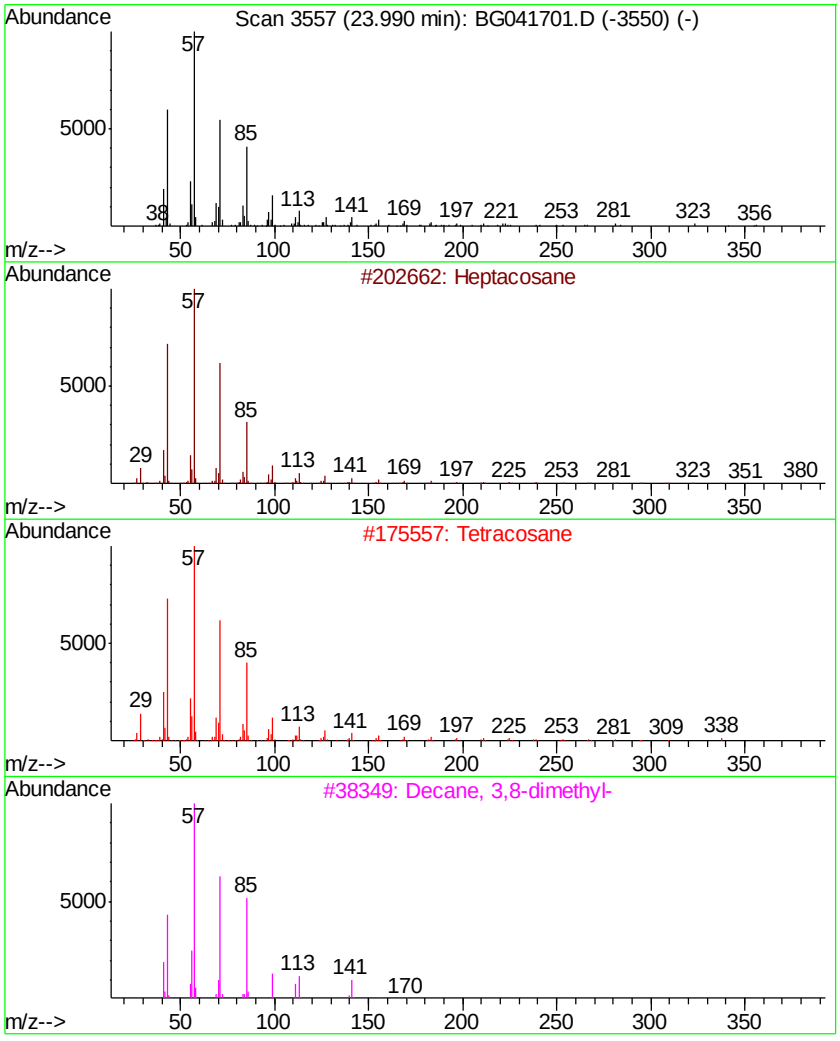
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

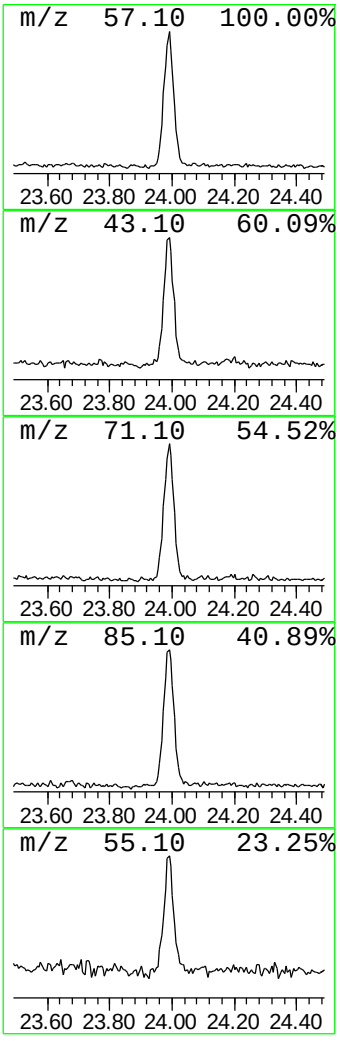
****

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.81 ng	291165	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	90
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5	Docosane	310	C22H46	000629-97-0	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
Sample : K3835-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

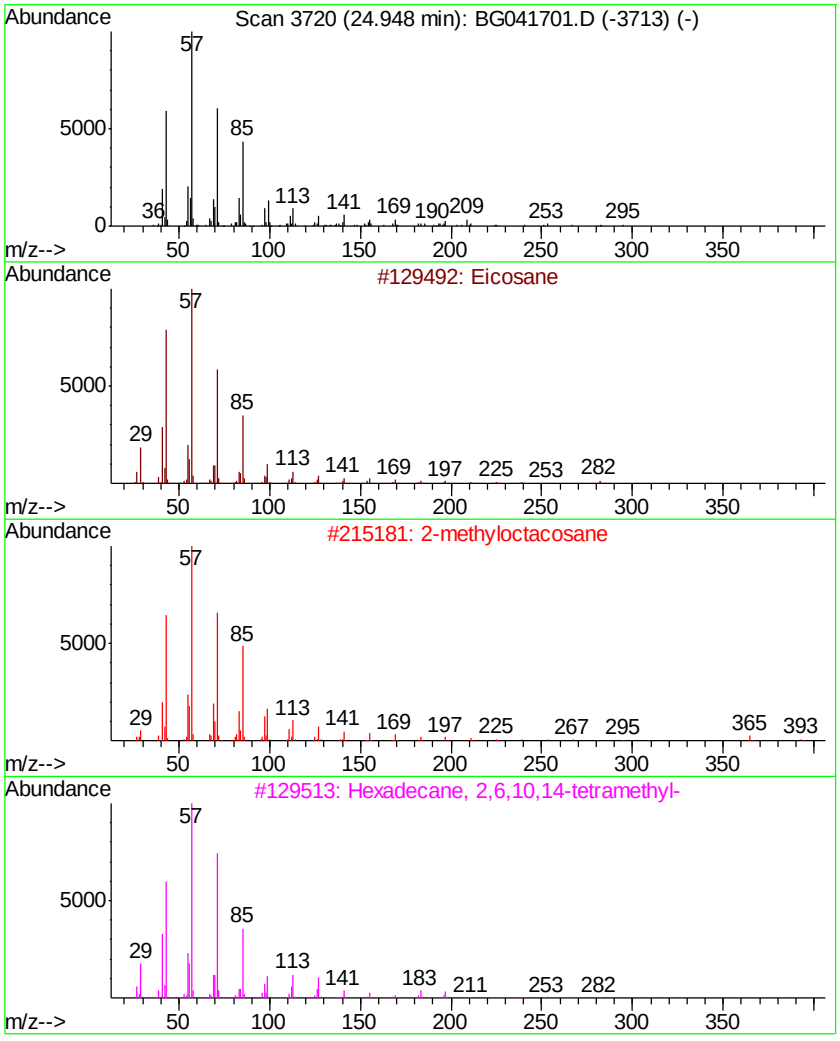
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

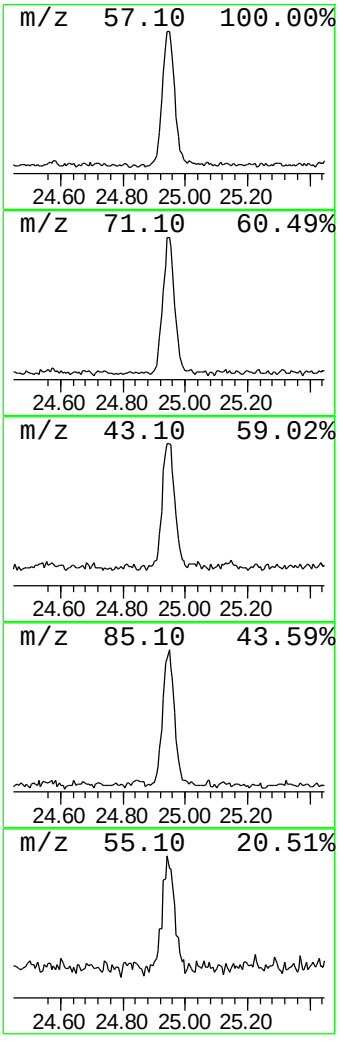
****

Peak Number 8 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.95	2.88 ng	297942	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	89
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5	Hexatriacontane	507	C36H74	000630-06-8	87





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Sample : K3835-10
Misc :
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Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
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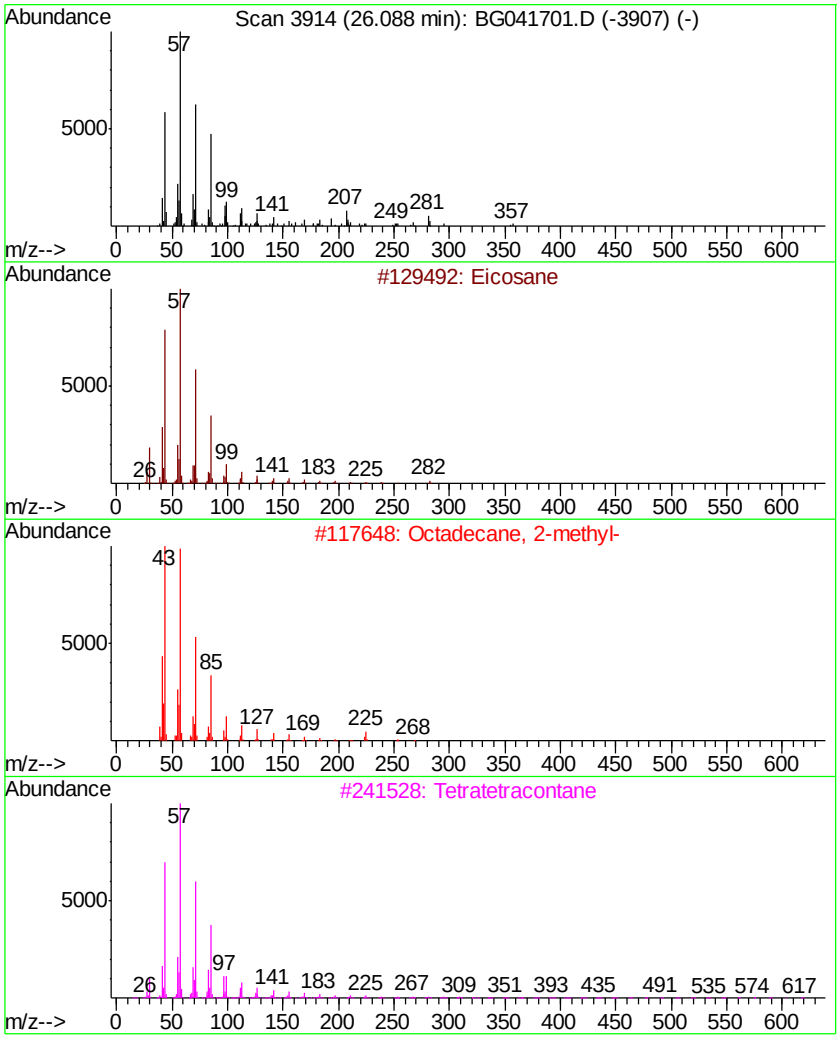
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

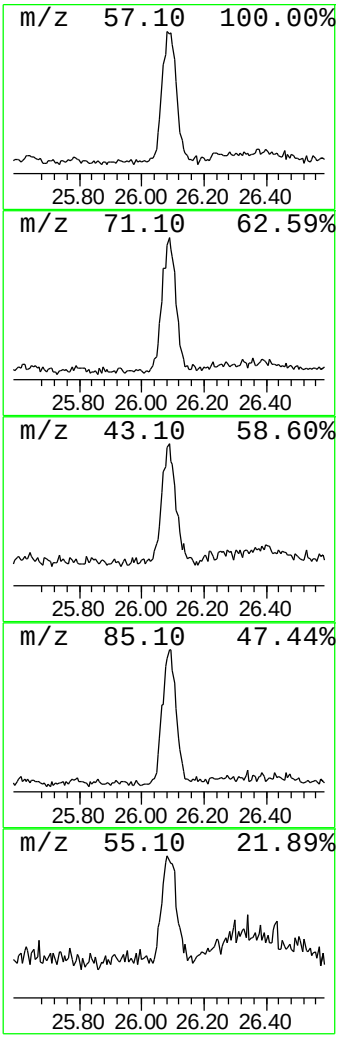
****

Peak Number 9 Octadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.09	2.37 ng	245108	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Hexatriacontane	507	C36H74	000630-06-8	87
5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071719\
Data File : BG041701.D
Acq On : 17 Jul 2019 23:33
Operator : HP/JU
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Misc :
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Instrument : BNA_G
ClientSampleId : SB-5(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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...	3.20	20.5	ng	639765	1	8.04	624549	20.0
unknown7.58	7.58	103.0	ng	3215420	1	8.04	624549	20.0
9-Octadecenamide,...	20.69	2.2	ng	215791	5	21.65	1992460	20.0
Heptafluorobutyri...	21.32	6.9	ng	689472	5	21.65	1992460	20.0
Eicosane	23.18	2.4	ng	236808	5	21.65	1992460	20.0
Heptacosane	23.99	2.8	ng	291165	6	24.84	2070300	20.0
2-methyloctacosane	24.95	2.9	ng	297942	6	24.84	2070300	20.0
Octadecane, 2-met...	26.09	2.4	ng	245108	6	24.84	2070300	20.0