LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043043.D
Acq On : 5 Oct 2019 00:39
Operator : JU
Sample : K5154-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105I

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-BG092519.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	3.173	7	14	22	rBV2	202953	511848	8.95%	1.735%
2	3.255	22	28	44	rVB	738915	1321009	23.10%	4.478%
3	5.646	427	435	446	rBV	776203	1283147	22.44%	4.350%
4	7.233	697	705	720	rBV	550562	1059783	18.53%	3.593%
5	7.603	759	768	778	rBV	1145681	1998584	34.95%	6.775%
6	8.061	838	846	853	rBV	253258	445672	7.79%	1.511%
7	8.384	893	901	910	rBV	752961	1342108	23.47%	4.550%
8	9.224	1036	1044	1053	rBV	661738	1231813	21.54%	4.176%
9	10.864	1315	1323	1334	rBV	327612	600894	10.51%	2.037%
10	13.308	1730	1739	1751	rBV	1915012	2894334	50.61%	9.812%
11	14.130	1873	1879	1890	rBV	250733	368321	6.44%	1.249%
12	14.683	1966	1973	1981	rVB	553892	892211	15.60%	3.025%
13	16.169	2218	2226	2240	rBV	1803314	2847758	49.80%	9.654%
14	17.421	2431	2439	2447	rBV2	710864	1178091	20.60%	3.994%
15	18.314	2586	2591	2599	rBV	288528	381031	6.66%	1.292%
16	19.583	2802	2807	2814	rBV3	80384	121757	2.13%	0.413%
17	20.035	2877	2884	2892	rBV	4353203	5718698	100.00%	19.386%
18	20.828	3014	3019	3023	rBV3	38712	59084	1.03%	0.200%
19	21.340	3101	3106	3116	rBV	245690	489153	8.55%	1.658%
20	21.692	3159	3166	3179	rVB	823453	1446864	25.30%	4.905%
21	21.886	3195	3199	3204	rBV2	82281	114660	2.01%	0.389%
22	22.497	3298	3303	3308	rBV2	119643	189826	3.32%	0.644%
23	23.190	3415	3421	3429	rVB	160173	294685	5.15%	0.999%
24	23.995	3551	3558	3566	rBV	161458	342129	5.98%	1.160%
25	24.912	3704	3714	3730	rVB3	508926	1824870	31.91%	6.186%
26	26.081	3904	3913	3923	rVB2	119185	371723	6.50%	1.260%
27	27.444	4136	4145	4154	rVB4	52059	168606	2.95%	0.572%

Sum of corrected areas: 29498659

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
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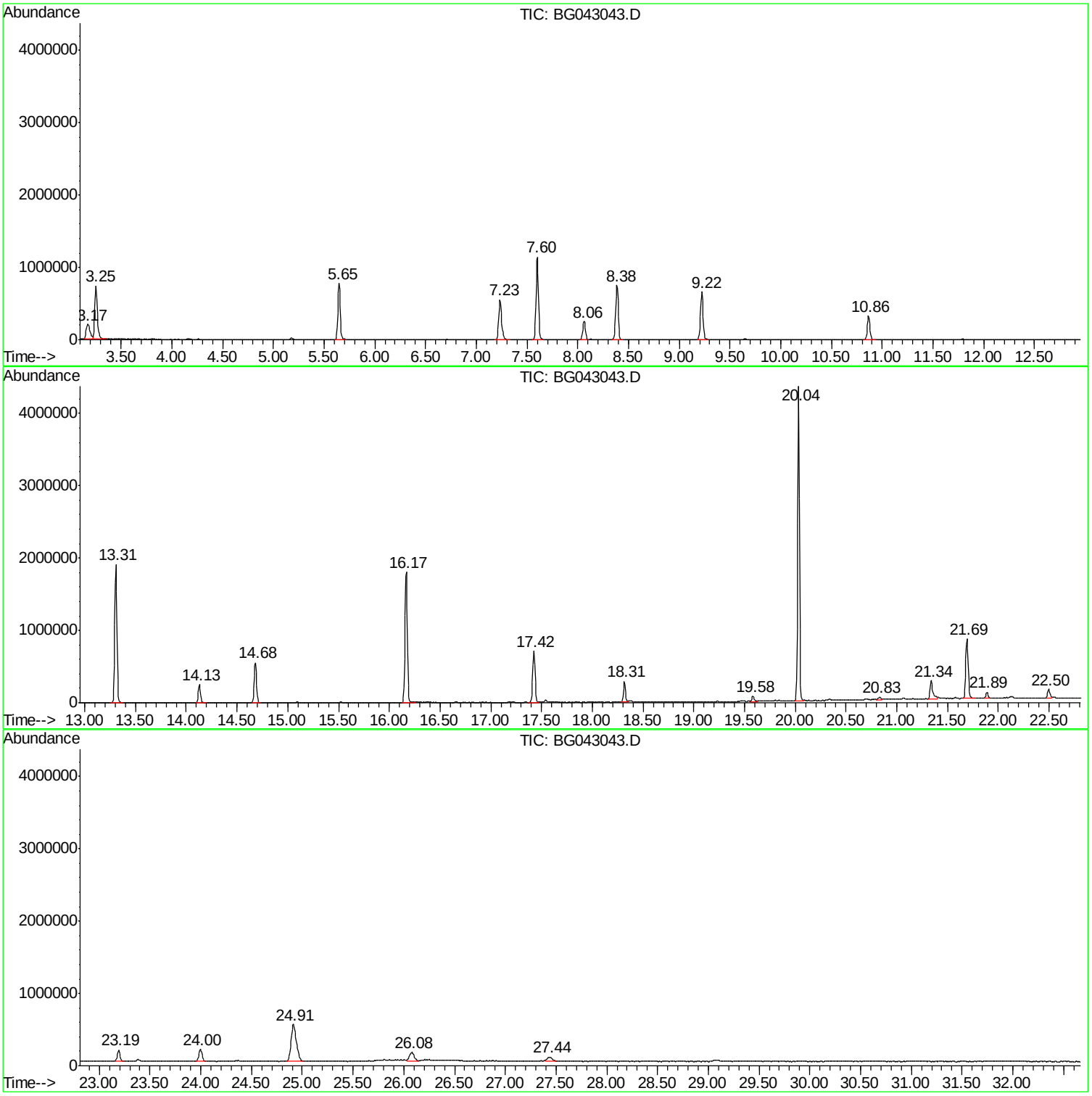
Acq On : 5 Oct 2019 00:39
Operator : JU
Sample : K5154-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

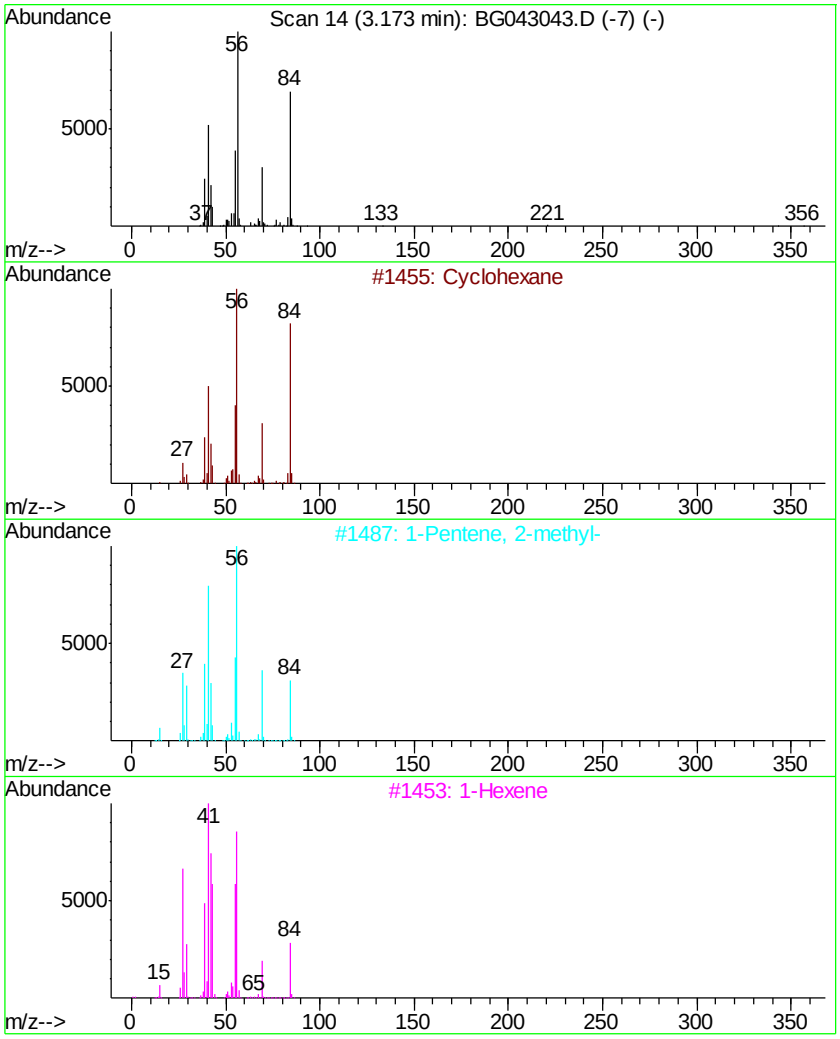
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

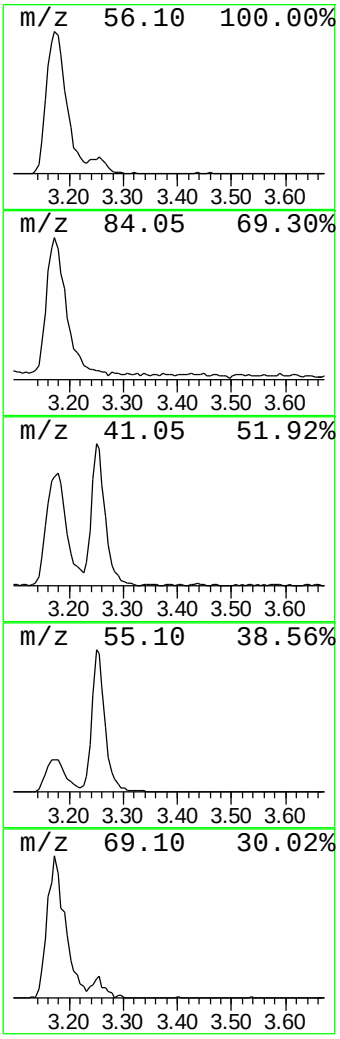
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	22.97 ng	511848	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	1-Hexene	84	C6H12	000592-41-6	50
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
5	Pyridine-D5-	84	C5D5N	007291-22-7	50





Library Search Compound Report

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Data File : BG043043.D
Acq On : 5 Oct 2019 00:39
Operator : JU
Sample : K5154-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

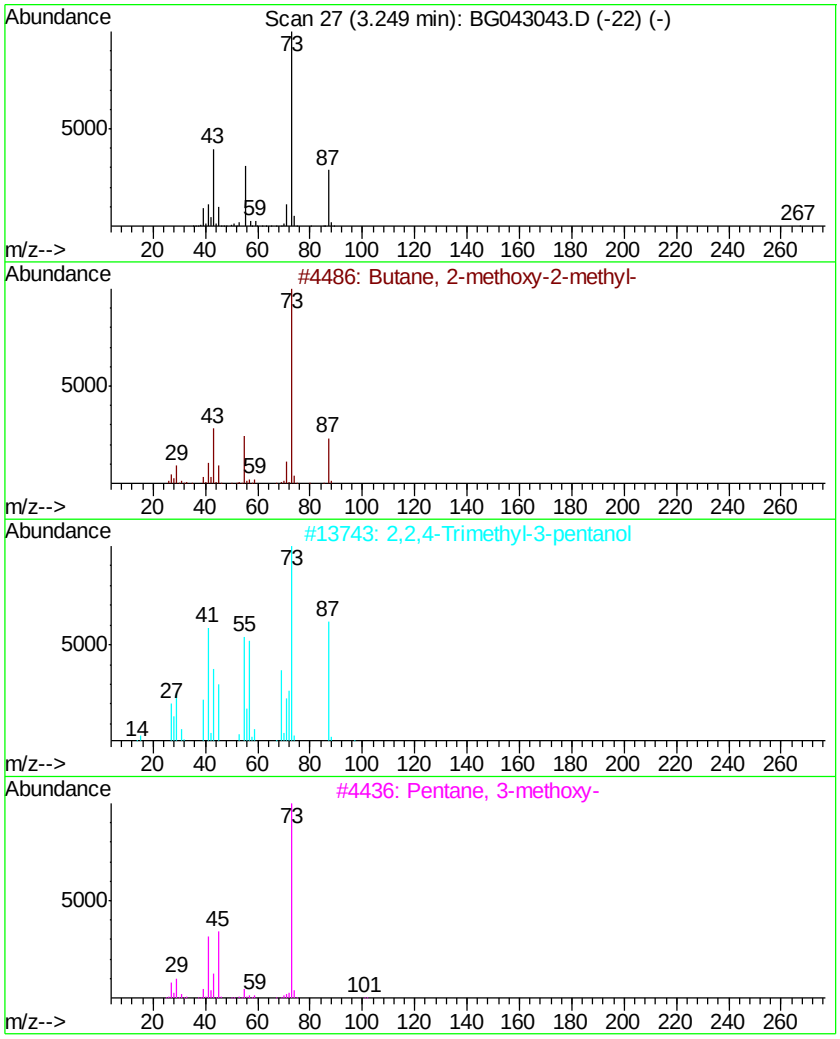
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

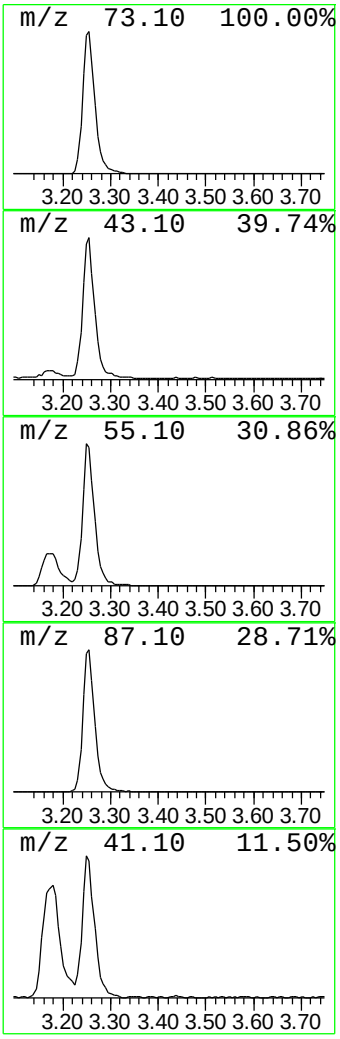
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.25	59.28 ng	1321010	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
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Acq On : 5 Oct 2019 00:39
Operator : JU
Sample : K5154-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

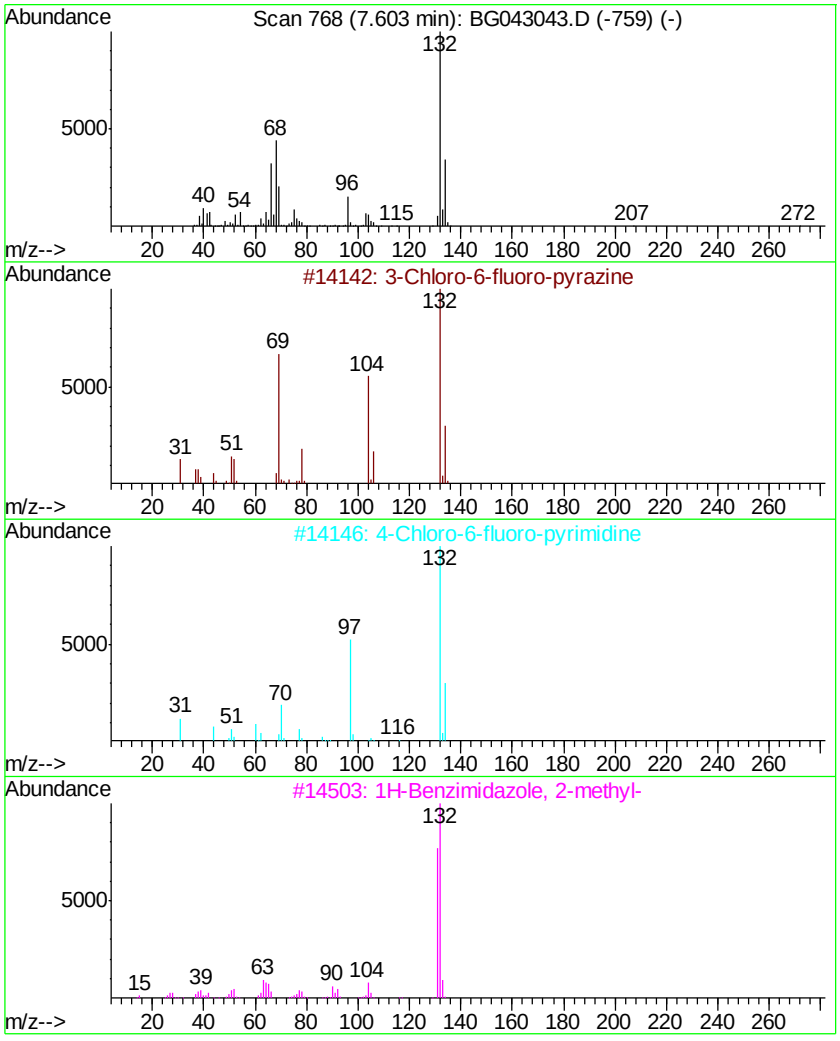
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

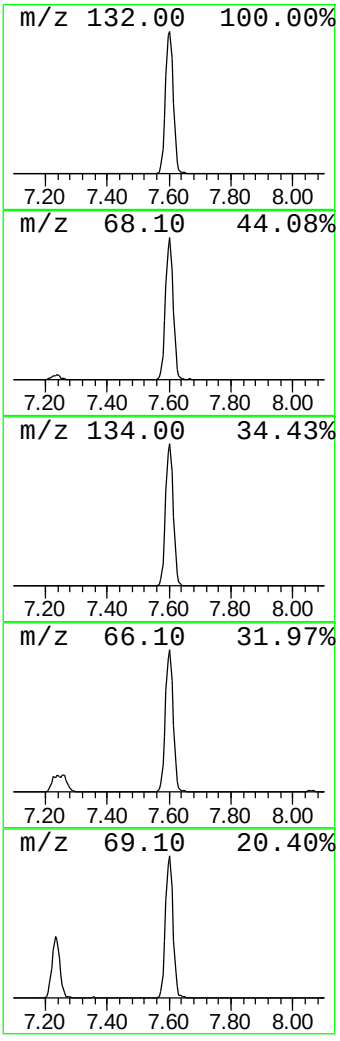
****

Peak Number 3 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	89.69 ng	1998580	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

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Data File : BG043043.D
Acq On : 5 Oct 2019 00:39
Operator : JU
Sample : K5154-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

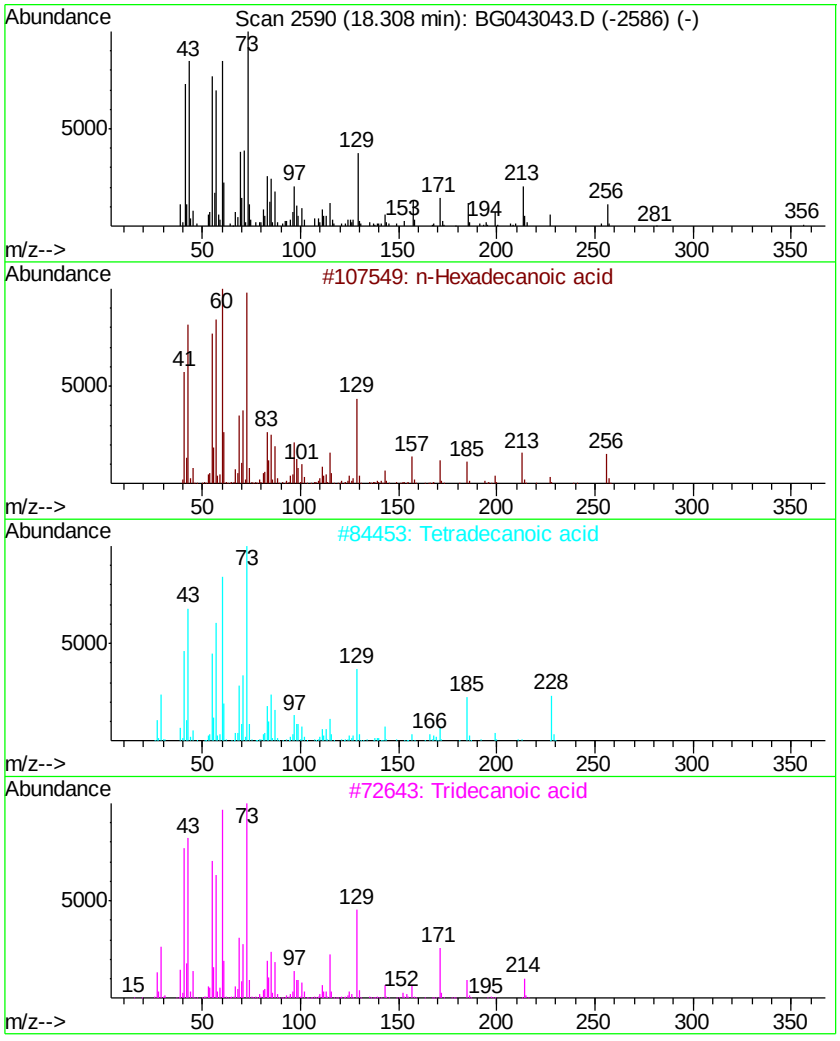
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

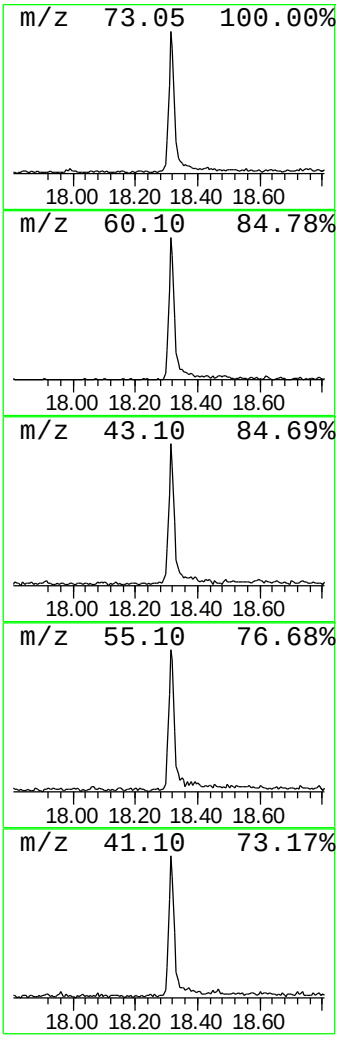
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	6.47 ng	381031	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043043.D
Acq On : 5 Oct 2019 00:39
Operator : JU
Sample : K5154-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

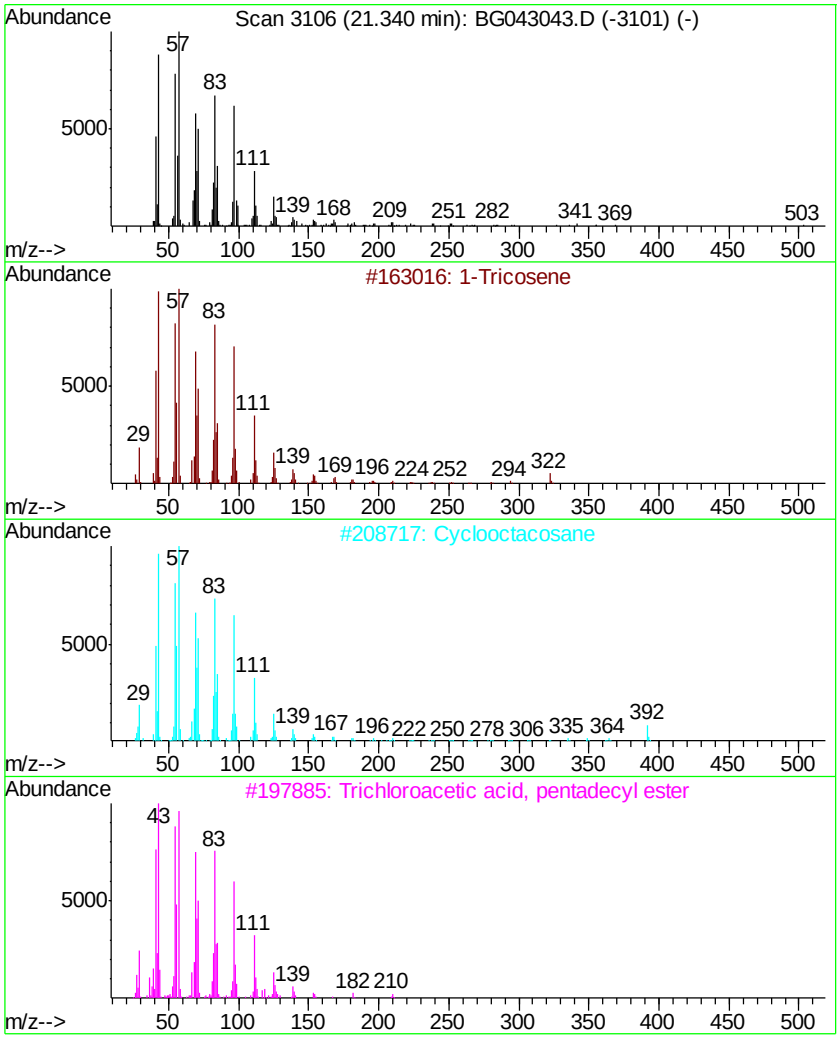
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

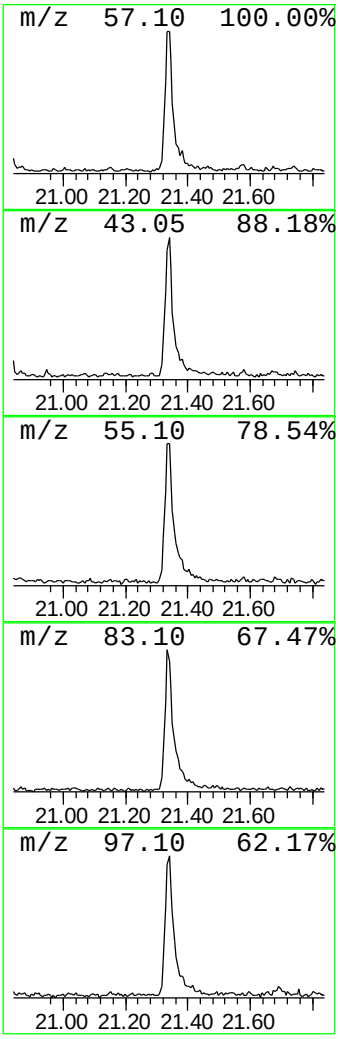
****

Peak Number 6 1-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.34	6.76 ng	489153	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	Cyclooctacosane	392	C28H56	000297-24-5	94
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94





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Instrument : BNA_G
ClientSampleId : MW-105I

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

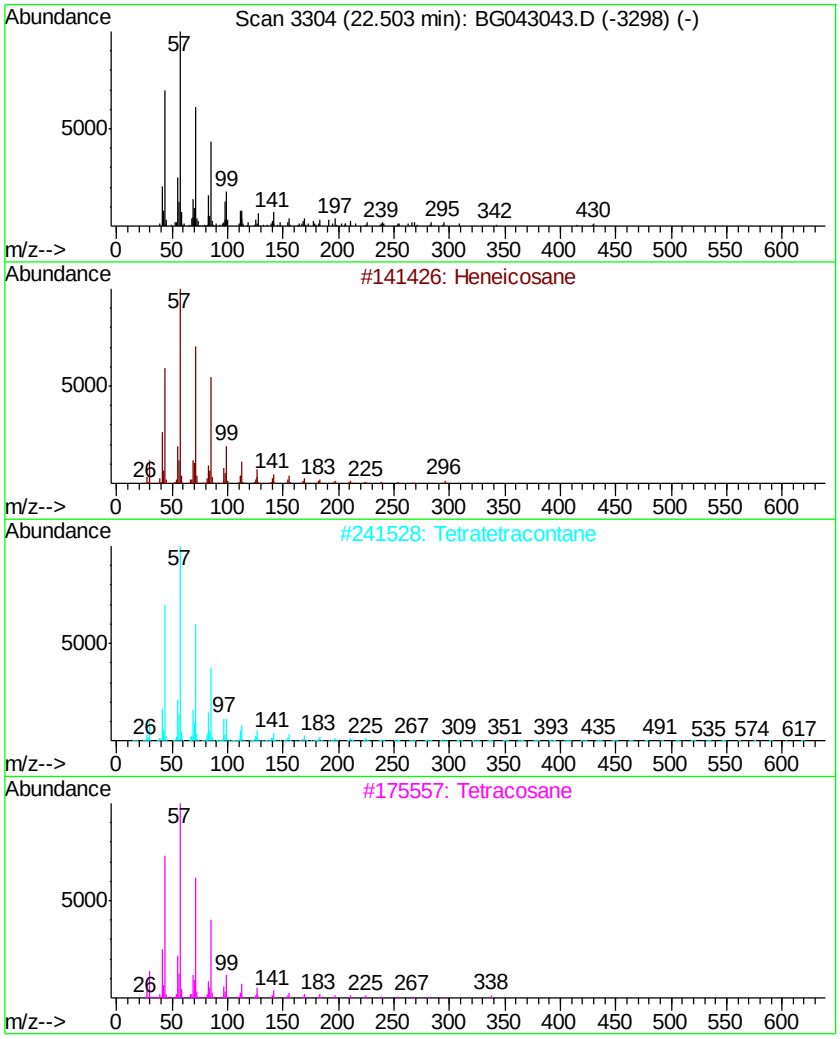
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

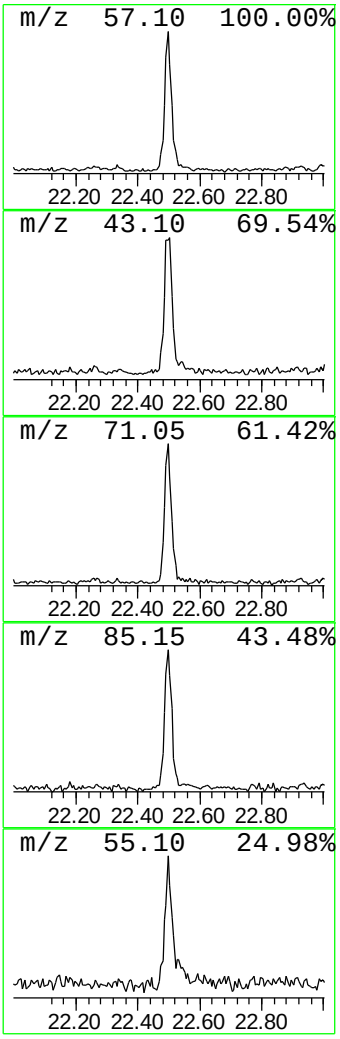
****

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	2.62 ng	189826	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Octacosane	394	C28H58	000630-02-4	87





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Instrument : BNA_G
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

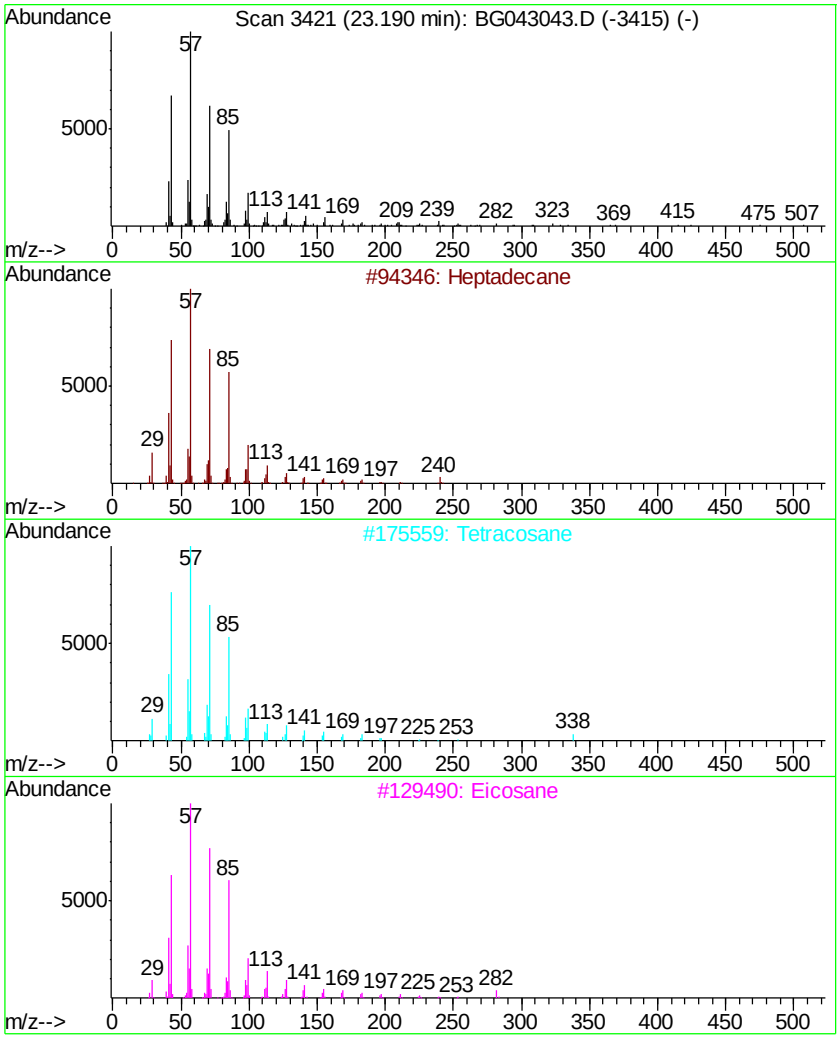
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

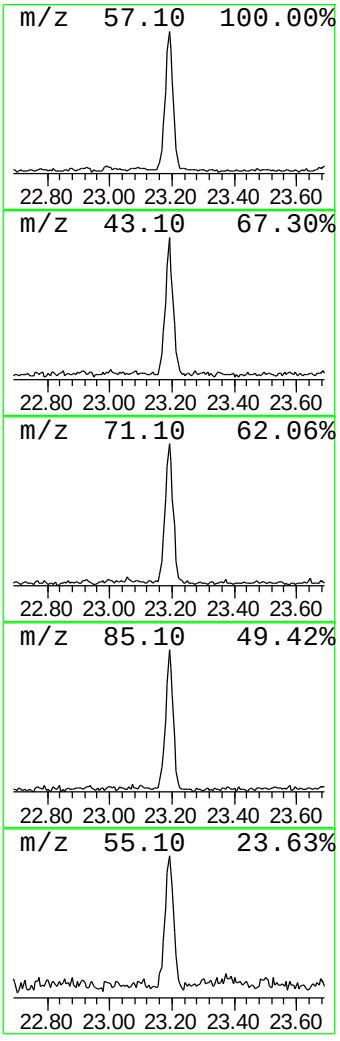
****

Peak Number 8 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	4.07 ng	294685	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	83
2	Tetracosane	338	C24H50	000646-31-1	83
3	Eicosane	282	C20H42	000112-95-8	80
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	80
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72





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Instrument : BNA_G
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TIC Library : C:\Database\NIST11.L
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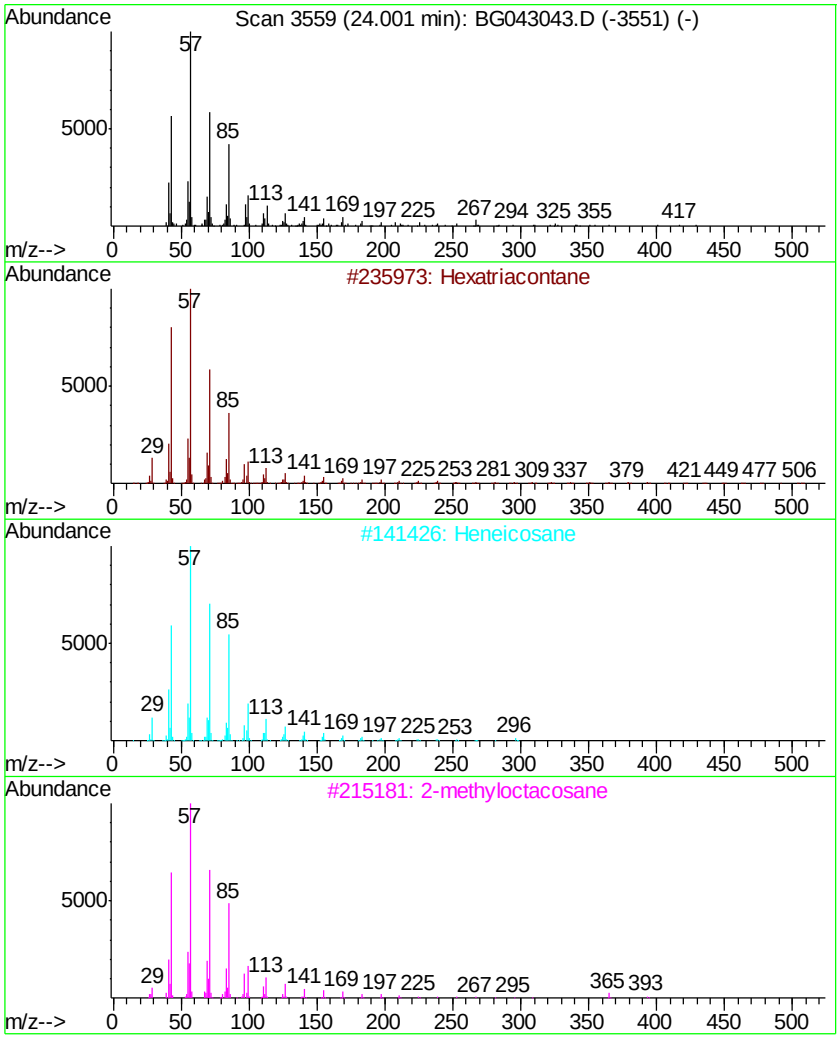
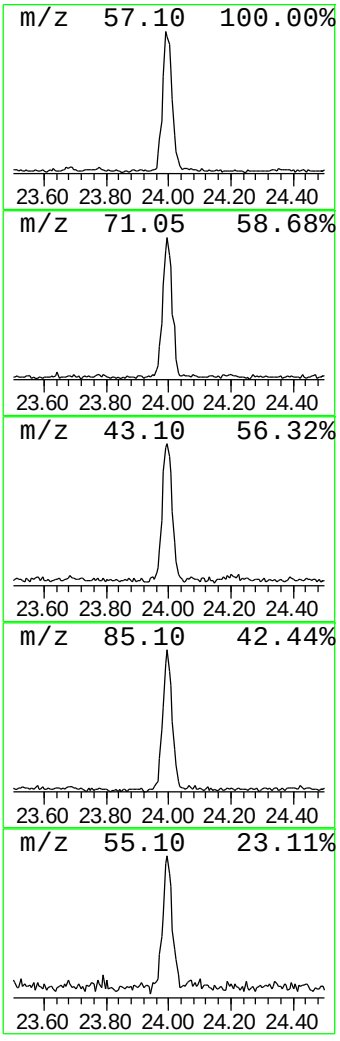
****

Peak Number 9 Hexatriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	3.75 ng	342129	Perylene-d12	24.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	87
5	Tetracosane	338	C24H50	000646-31-1	87





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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

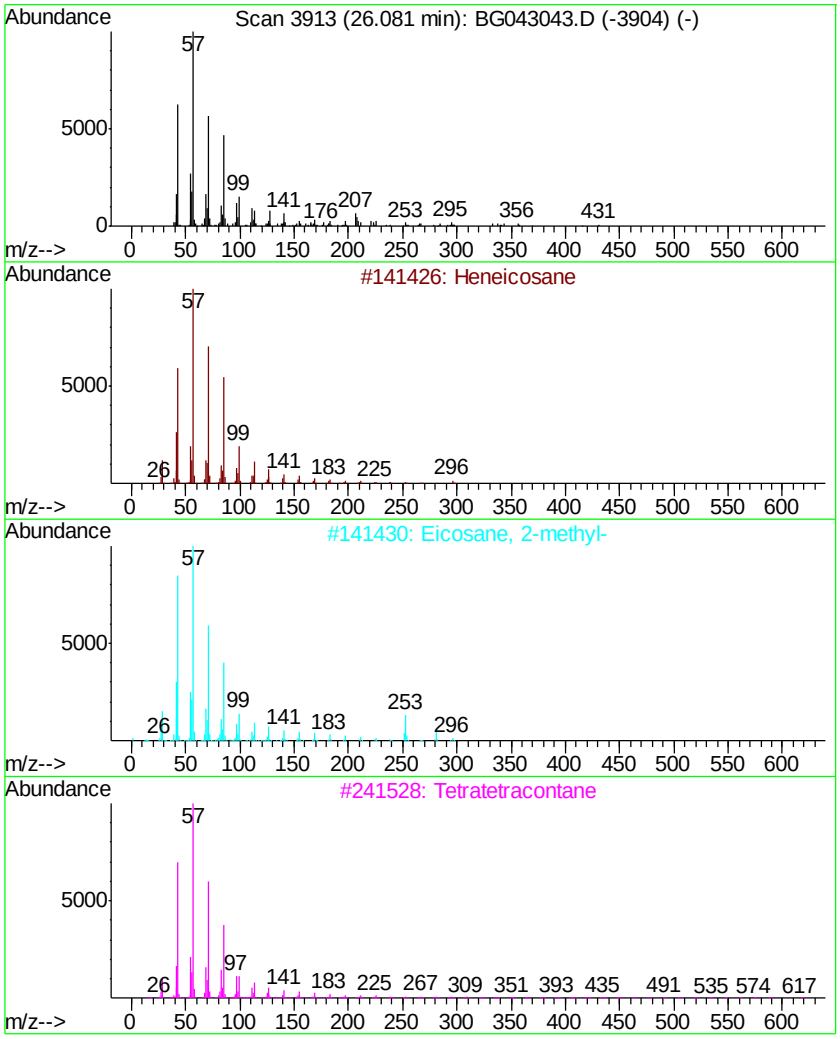
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

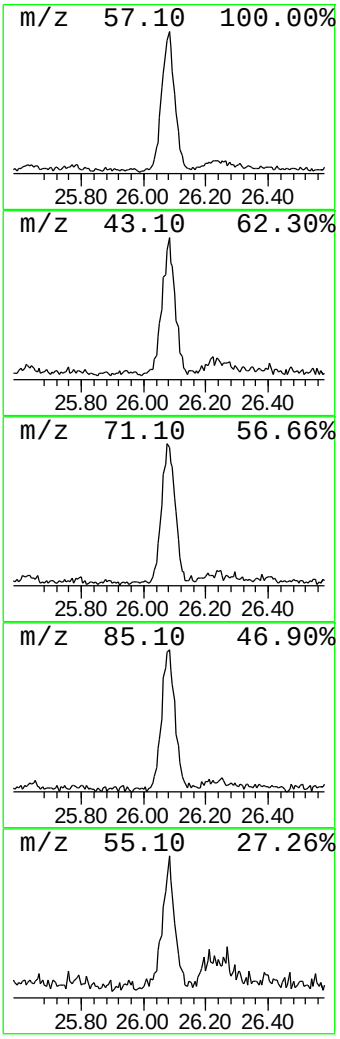
****

Peak Number 10 Eicosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.08	4.07 ng	371723	Perylene-d12	24.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Hexatriacontane	507	C36H74	000630-06-8	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100419\
Data File : BG043043.D
Acq On : 5 Oct 2019 00:39
Operator : JU
Sample : K5154-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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
1-Pentene, 2-methyl-	3.17	23.0	ng	511848	1	8.06	445672	20.0
Butane, 2-methoxy...	3.25	59.3	ng	1321010	1	8.06	445672	20.0
unknown7.60	7.60	89.7	ng	1998580	1	8.06	445672	20.0
n-Hexadecanoic acid	18.31	6.5	ng	381031	4	17.42	1178090	20.0
1-Tricosene	21.34	6.8	ng	489153	5	21.69	1446860	20.0
Heneicosane	22.50	2.6	ng	189826	5	21.69	1446860	20.0
Heptadecane	23.19	4.1	ng	294685	5	21.69	1446860	20.0
Hexatriacontane	24.00	3.8	ng	342129	6	24.91	1824870	20.0
Eicosane, 2-methyl-	26.08	4.1	ng	371723	6	24.91	1824870	20.0