LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043739.D
Acq On : 20 Nov 2019 22:23
Operator : JU
Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 13-(0-2)

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-BG102119.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	3.146	6	10	25	rVB	80766	125071	5.38%	1.007%
2	5.090	334	341	355	rBV	89496	150448	6.47%	1.212%
3	5.578	417	424	447	rBV	446045	784653	33.76%	6.321%
4	7.182	689	697	709	rBV	460308	890744	38.33%	7.175%
5	7.529	748	756	769	rBV	475391	868668	37.38%	6.997%
6	7.987	827	834	841	rBV	83658	144681	6.23%	1.165%
7	8.310	881	889	900	rBV	347542	621041	26.72%	5.003%
8	9.150	1023	1032	1052	rBV	231925	502658	21.63%	4.049%
9	10.796	1305	1312	1321	rBV	79047	176326	7.59%	1.420%
10	13.240	1721	1728	1744	rBV	714762	1198072	51.55%	9.651%
11	14.074	1864	1870	1882	rBV	51881	101695	4.38%	0.819%
12	14.620	1957	1963	1971	rBV	184076	311564	13.41%	2.510%
13	16.113	2210	2217	2238	rBV	659813	1186997	51.08%	9.562%
14	17.364	2424	2430	2434	rBV	251604	413046	17.77%	3.327%
15	17.405	2434	2437	2446	rVV	90422	158024	6.80%	1.273%
16	17.488	2446	2451	2461	rVB4	30542	70304	3.03%	0.566%
17	18.257	2576	2582	2585	rBV5	23948	45556	1.96%	0.367%
18	18.445	2607	2614	2617	rBV4	18691	36746	1.58%	0.296%
19	19.421	2774	2780	2786	rBV	122067	180810	7.78%	1.456%
20	19.779	2837	2841	2851	rVB	103103	155259	6.68%	1.251%
21	19.973	2868	2874	2884	rBV	1670598	2323982	100.00%	18.720%
22	20.273	2921	2925	2931	rVB2	22847	34570	1.49%	0.278%
23	20.378	2934	2943	2948	rBV3	13910	31953	1.37%	0.257%
24	21.630	3145	3156	3161	rBV3	309481	645957	27.80%	5.203%
25	22.405	3283	3288	3294	rVB4	23528	38821	1.67%	0.313%
26	23.081	3394	3403	3410	rVB2	25653	60162	2.59%	0.485%
27	23.804	3517	3526	3531	rBV2	27496	84914	3.65%	0.684%
28	23.868	3531	3537	3544	rVB2	71951	161423	6.95%	1.300%
29	24.656	3663	3671	3683	rVB3	24975	71627	3.08%	0.577%
30	24.803	3686	3696	3706	rBV2	198691	600665	25.85%	4.839%
31	25.901	3874	3883	3894	rVB3	45019	127075	5.47%	1.024%
32	28.821	4372	4380	4387	rVB10	9238	27632	1.19%	0.223%
33	30.784	4708	4714	4722	rVB10	16789	54603	2.35%	0.440%
34	31.800	4880	4887	4888	rBV7	15000	28459	1.22%	0.229%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043739.D
Acq On : 20 Nov 2019 22:23
Operator : JU
Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
13-(0-2)

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-BG102119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

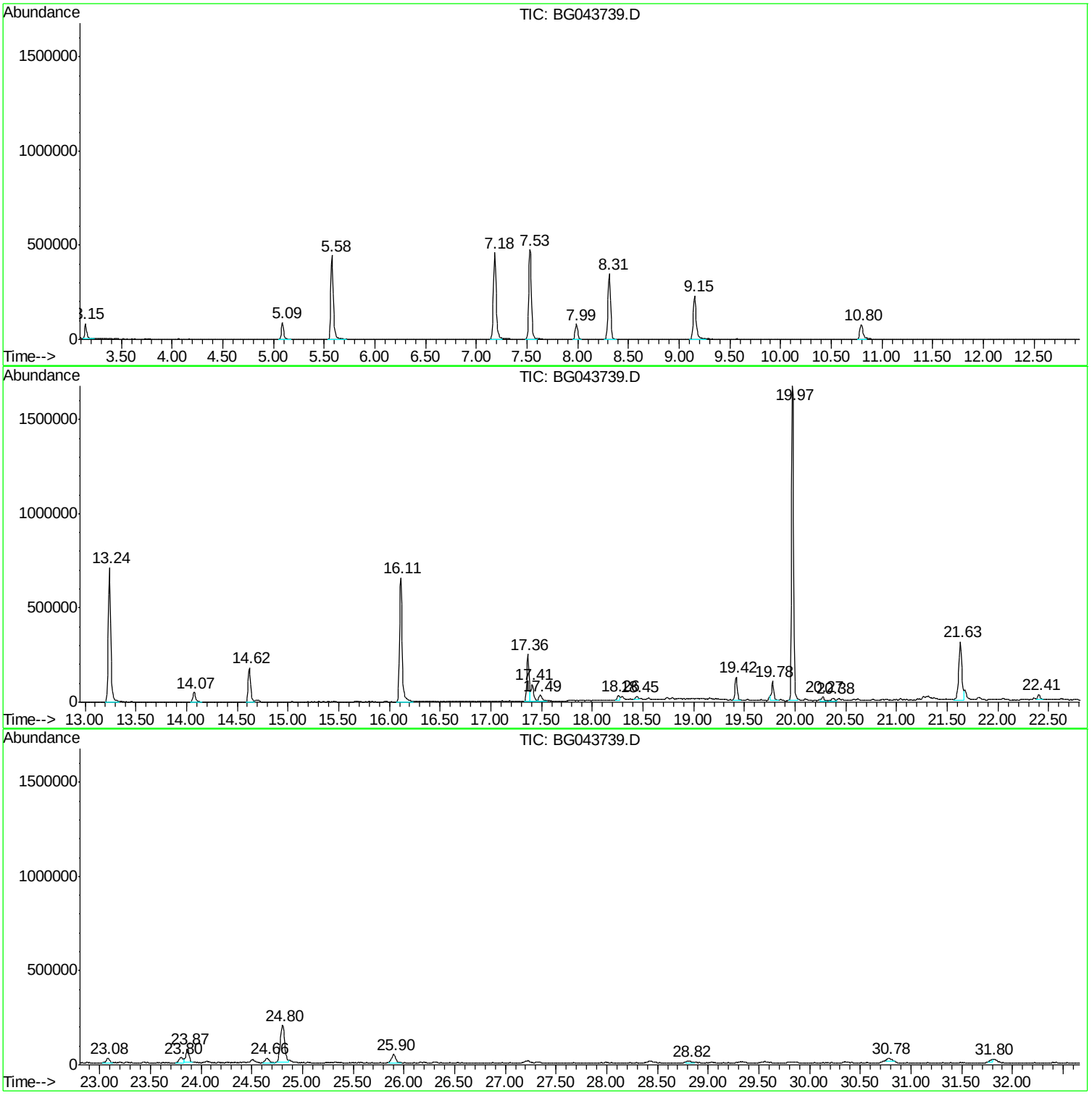
Sum of corrected areas: 12414206

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043739.D
Acq On : 20 Nov 2019 22:23
Operator : JU
Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
13-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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\BG112019\
Data File : BG043739.D
Acq On : 20 Nov 2019 22:23
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Sample : K5904-16
Misc :
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

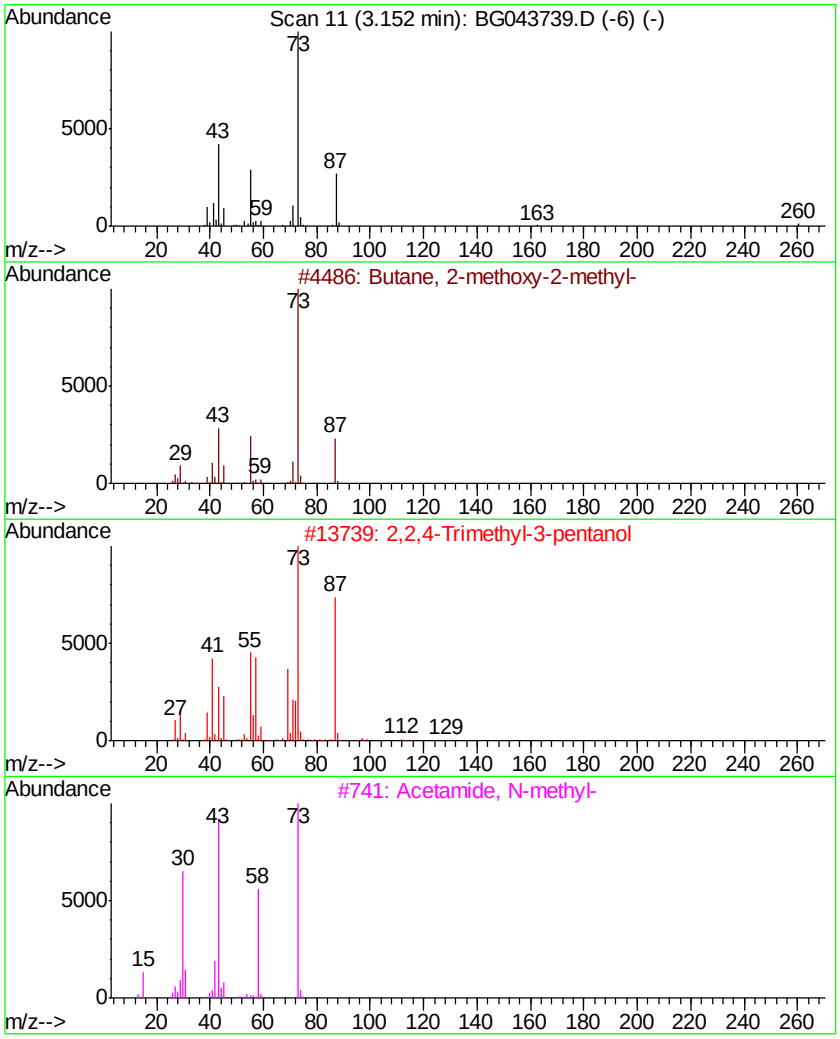
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

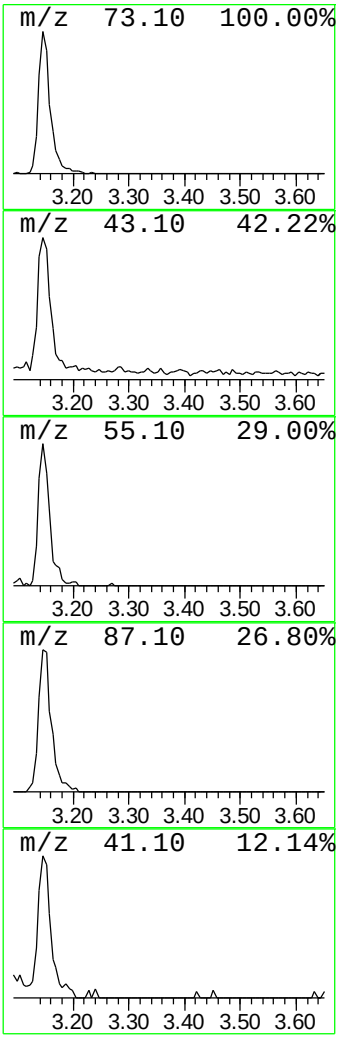
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	17.29 ng	125071	1,4-Dichlorobenzene-d4	7.99

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	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043739.D
Acq On : 20 Nov 2019 22:23
Operator : JU
Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 13-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

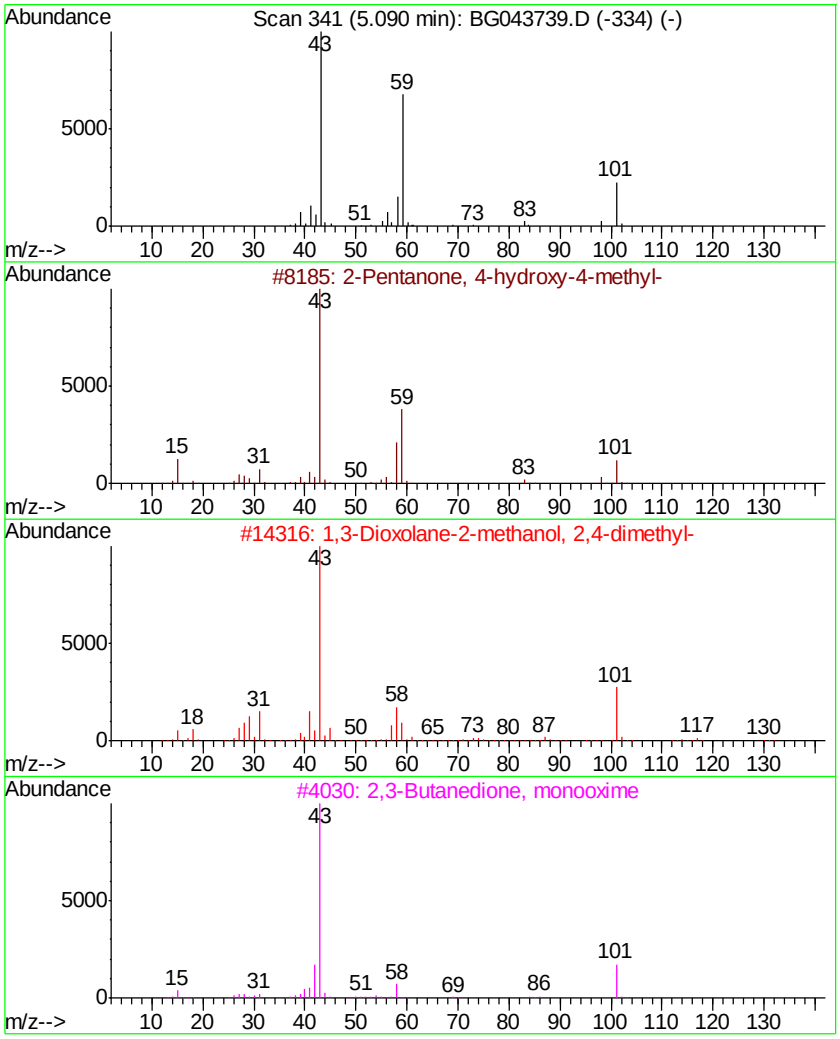
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

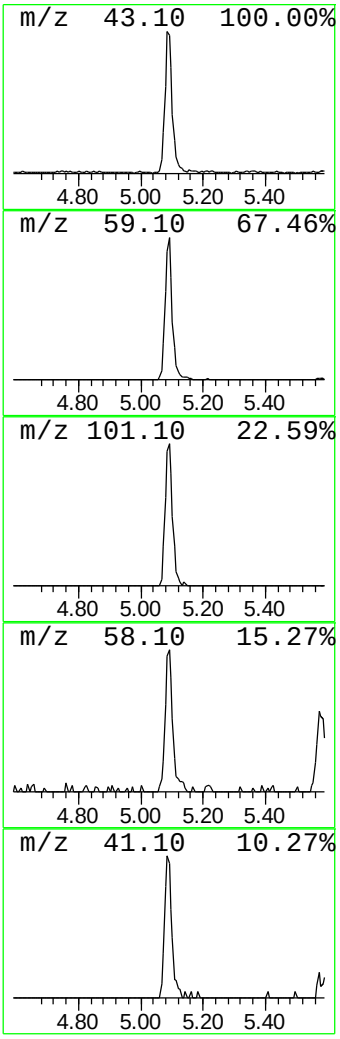
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	20.80 ng	150448	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043739.D
Acq On : 20 Nov 2019 22:23
Operator : JU
Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 13-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

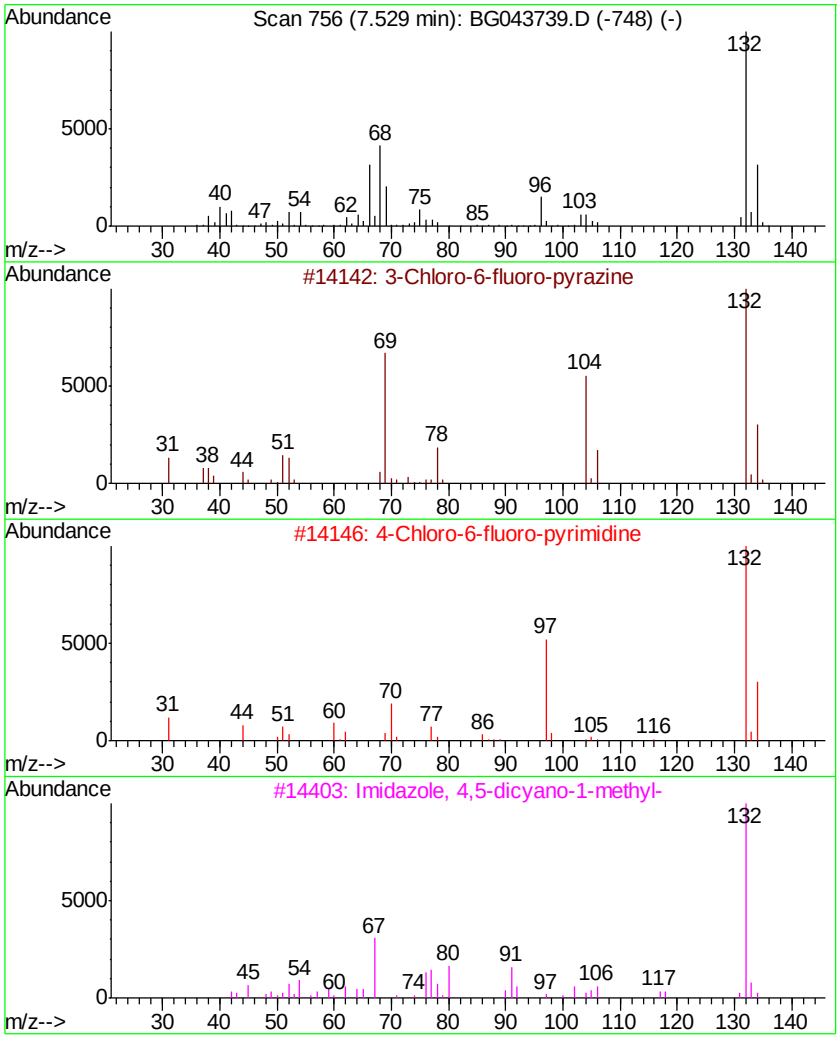
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

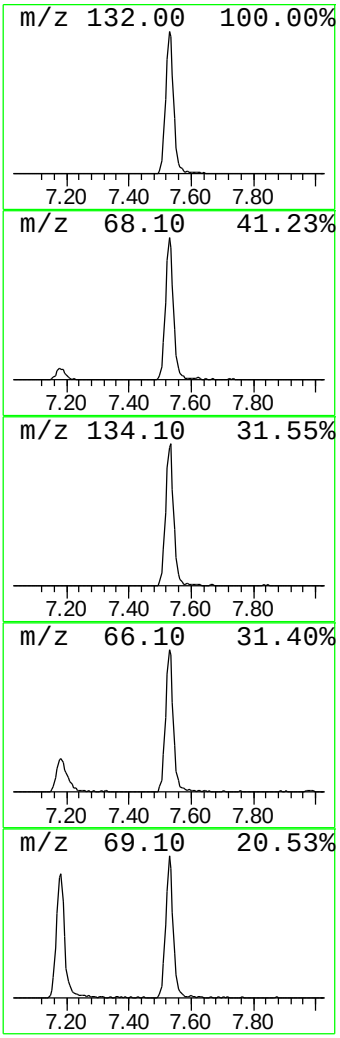
****

Peak Number 3 unknown7.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	120.08 ng	868668	1,4-Dichlorobenzene-d4	7.99

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	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





Library Search Compound Report

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Operator : JU
Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 13-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

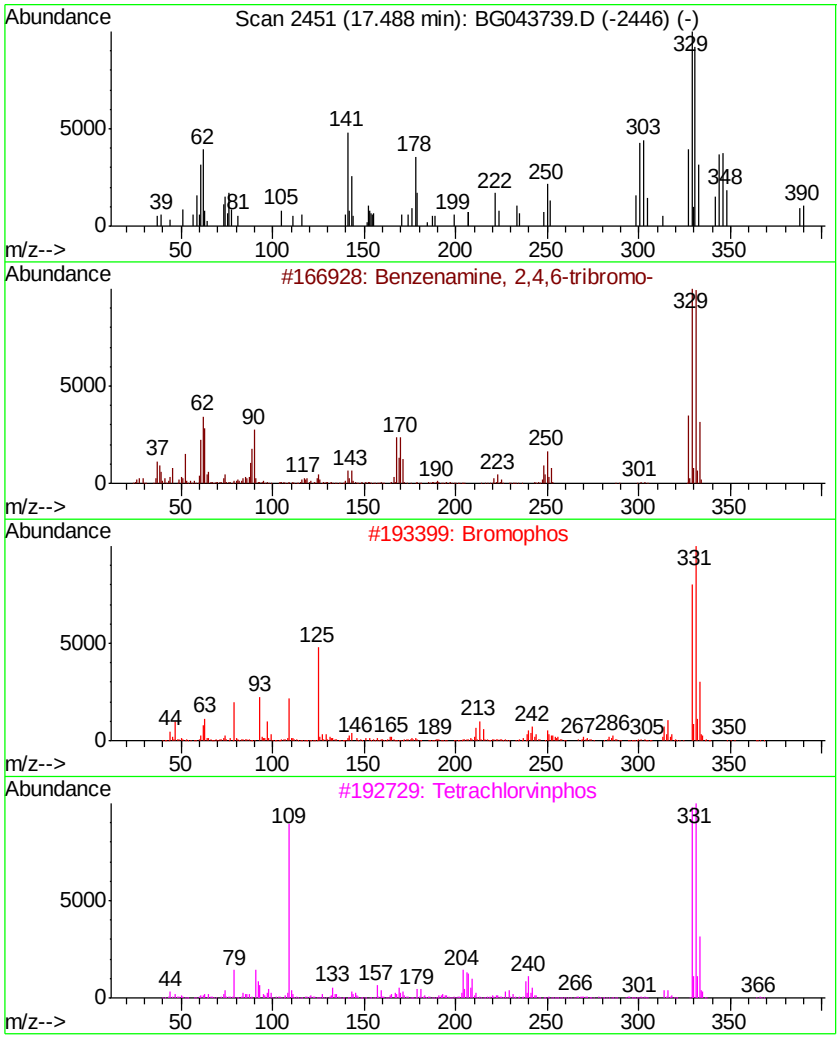
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

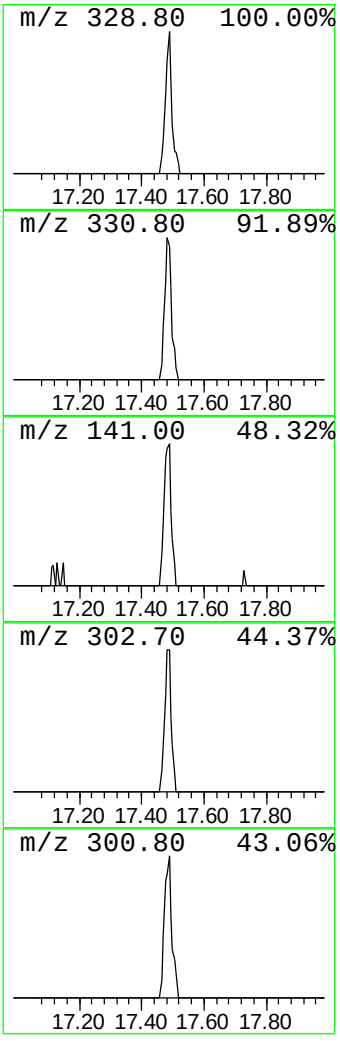
****

Peak Number 5 Benzenamine, 2,4,6-tribromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.49	3.40 ng	70304	Phenanthrene-d10	17.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	68
2	Bromophos	364	C8H8BrCl2O3PS	002104-96-3	12
3	Tetrachlorvinphos	364	C10H9Cl4O4P	022248-79-9	12
4	1,3,4-Oxadiazol-2-amine, 5-(2-br...	329	C11H12BrN3O4	1000350-74-8	10
5	2,5-Di(trifluoroacetyloxy)acetop...	344	C12H6F6O5	1000365-30-5	10





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Data File : BG043739.D
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Operator : JU
Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 13-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

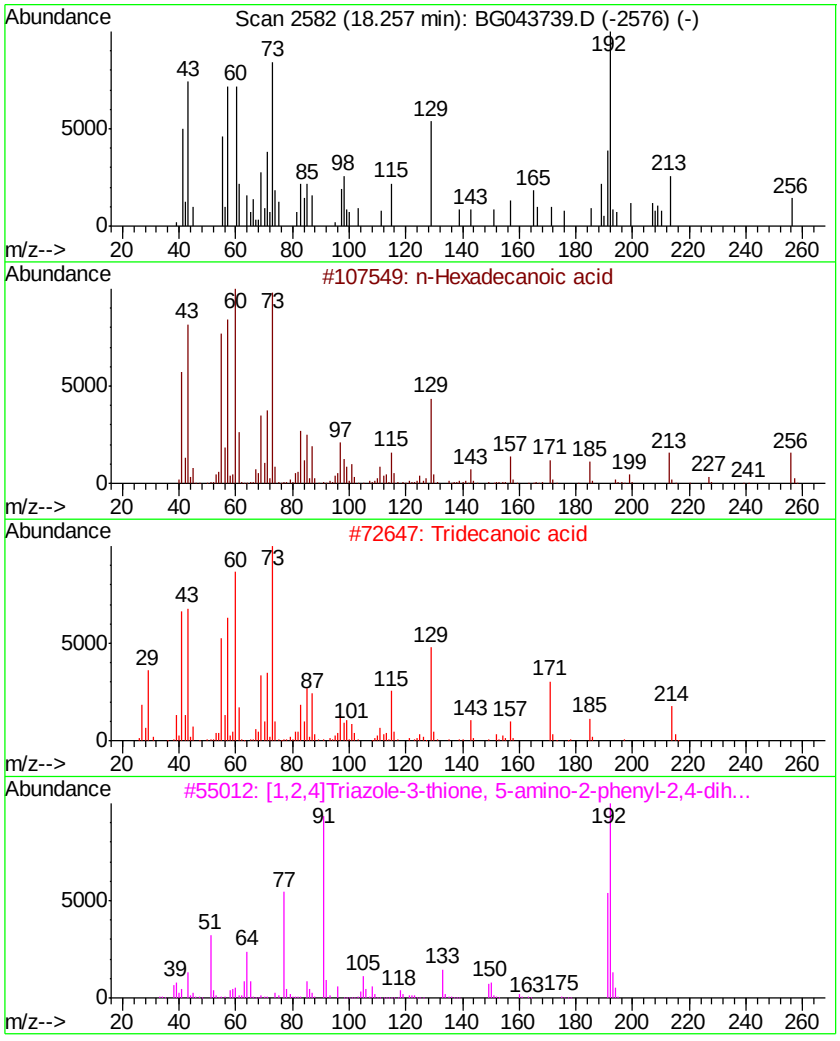
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

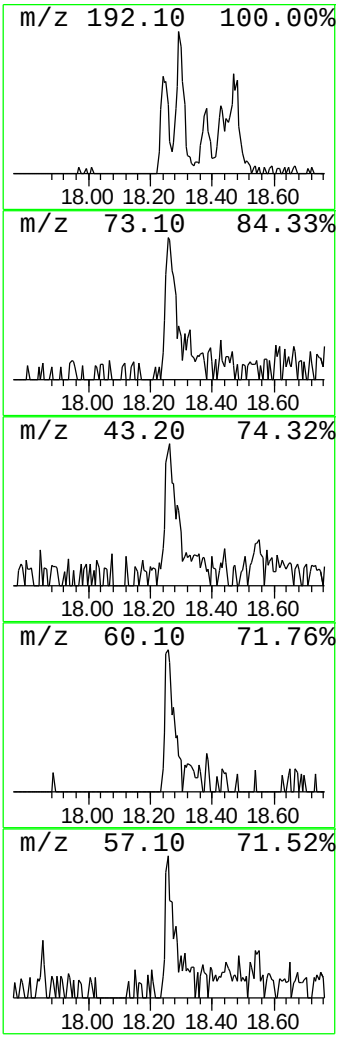
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.21 ng	45556	Phenanthrene-d10	17.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	30
3	[1,2,4]Triazole-3-thione, 5-amin...	192	C8H8N4S	1000303-72-9	22
4	n-Decanoic acid	172	C10H20O2	000334-48-5	22
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	22





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Acq On : 20 Nov 2019 22:23
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Sample : K5904-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 13-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

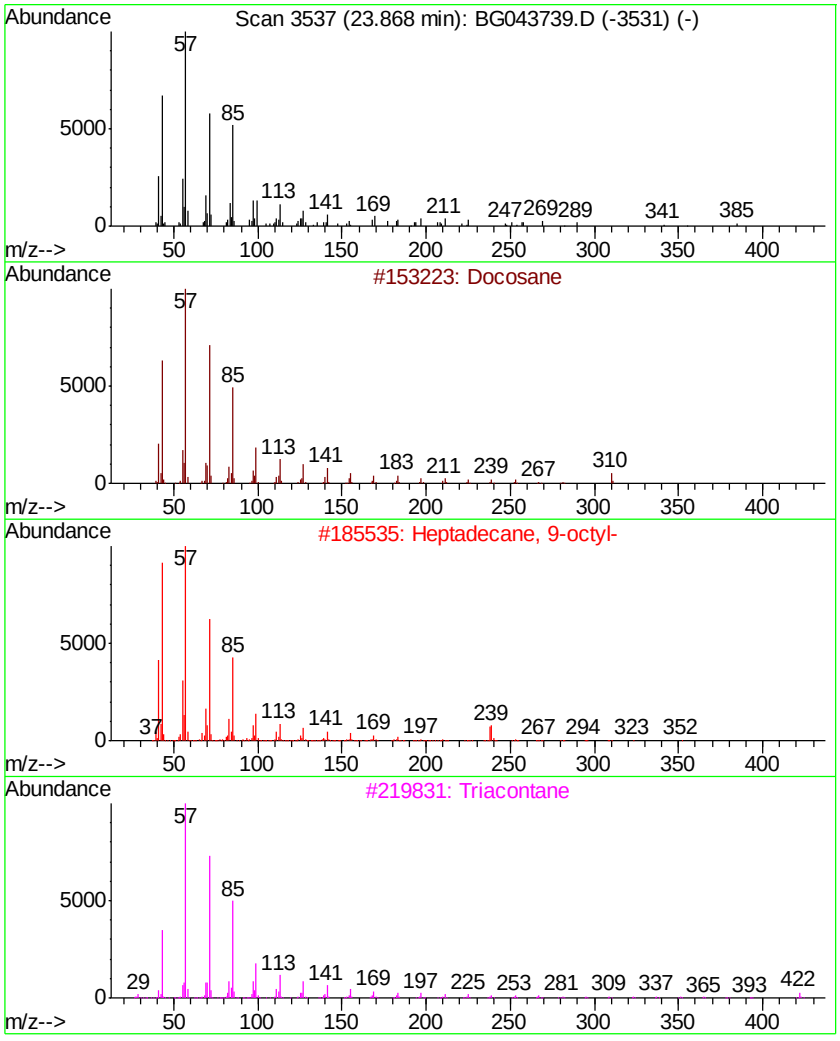
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

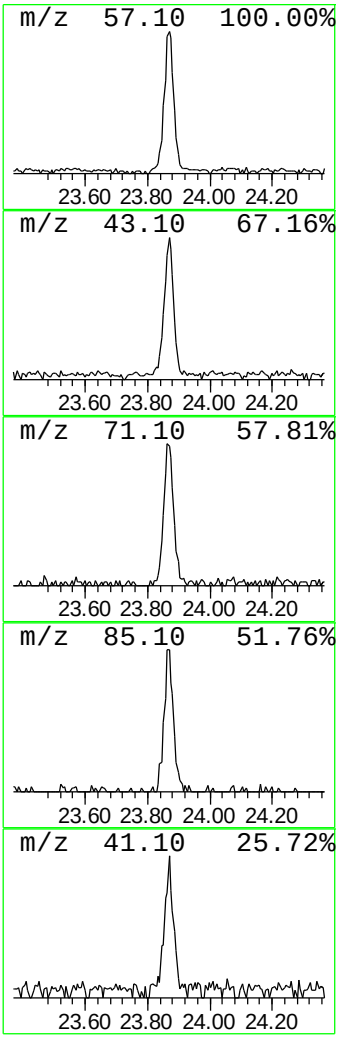
****

Peak Number 7 Docosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	5.37 ng	161423	Perylene-d12	24.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	87
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Triacontane	422	C30H62	000638-68-6	86
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 13-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

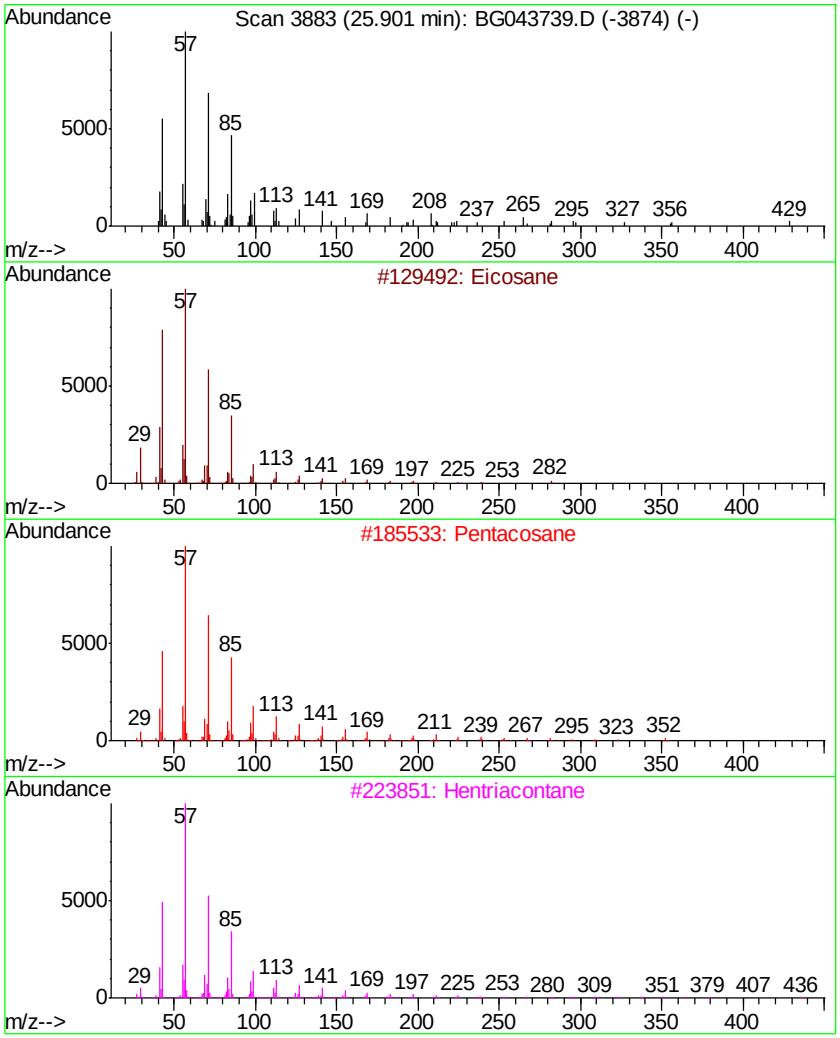
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

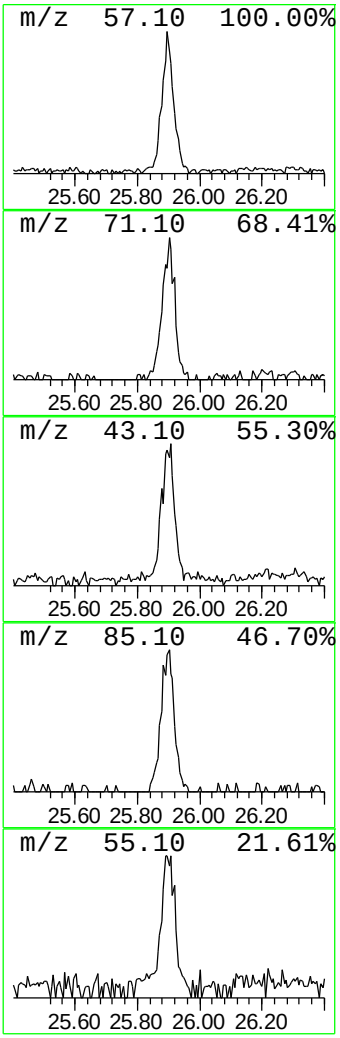
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.90	4.23 ng	127075	Perylene-d12	24.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Pentacosane	352	C25H52	000629-99-2	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Tetratetracontane	619	C44H90	007098-22-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG112019\
Data File : BG043739.D
Acq On : 20 Nov 2019 22:23
Operator : JU
Sample : K5904-16
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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...	3.15	17.3	ng	125071	1	7.99	144681	20.0
2-Pentanone, 4-hy...	5.09	20.8	ng	150448	1	7.99	144681	20.0
unknown7.53	7.53	120.1	ng	868668	1	7.99	144681	20.0
Benzenamine, 2,4,...	17.49	3.4	ng	70304	4	17.36	413046	20.0
n-Hexadecanoic acid	18.26	2.2	ng	45556	4	17.36	413046	20.0
Docosane	23.87	5.4	ng	161423	6	24.80	600665	20.0
Eicosane	25.90	4.2	ng	127075	6	24.80	600665	20.0