LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111919\
Data File : BG043703.D
Acq On : 19 Nov 2019 18:16
Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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	3.148	5	10	18	rVB	74650	103865	4.72%	0.968%
2	5.087	336	340	349	rBV	75328	118467	5.38%	1.104%
3	5.581	418	424	439	rBV	342330	606318	27.56%	5.648%
4	7.185	689	697	714	rBV	363794	725107	32.96%	6.754%
5	7.532	749	756	766	rBV	378079	686932	31.22%	6.399%
6	7.990	827	834	842	rBV	89386	158718	7.21%	1.478%
7	8.313	882	889	906	rBV	304609	537419	24.43%	5.006%
8	9.153	1023	1032	1048	rBV	182202	402903	18.31%	3.753%
9	10.798	1303	1312	1321	rBV	87576	192204	8.74%	1.790%
10	13.243	1721	1728	1741	rBV	588421	1043305	47.42%	9.719%
11	14.077	1864	1870	1885	rBV	50366	114320	5.20%	1.065%
12	14.623	1956	1963	1977	rBV2	195208	341580	15.53%	3.182%
13	16.116	2211	2217	2234	rBV	498832	949465	43.15%	8.844%
14	17.367	2423	2430	2449	rBV	233950	457504	20.79%	4.262%
15	18.266	2577	2583	2592	rBV5	19239	42914	1.95%	0.400%
16	19.976	2868	2874	2889	rBV	1572928	2200172	100.00%	20.495%
17	21.633	3150	3156	3173	rBV2	301567	611149	27.78%	5.693%
18	21.809	3182	3186	3193	rVB3	34108	50029	2.27%	0.466%
19	22.408	3282	3288	3293	rBV	59400	91158	4.14%	0.849%
20	23.084	3397	3403	3414	rVB2	74820	144409	6.56%	1.345%
21	23.877	3530	3538	3546	rBV	74613	159495	7.25%	1.486%
22	24.805	3684	3696	3713	rBV2	245902	788081	35.82%	7.341%
23	25.904	3874	3883	3894	rVB3	45564	135729	6.17%	1.264%
24	27.232	4099	4109	4117	rBV7	22775	73996	3.36%	0.689%

Sum of corrected areas: 10735239

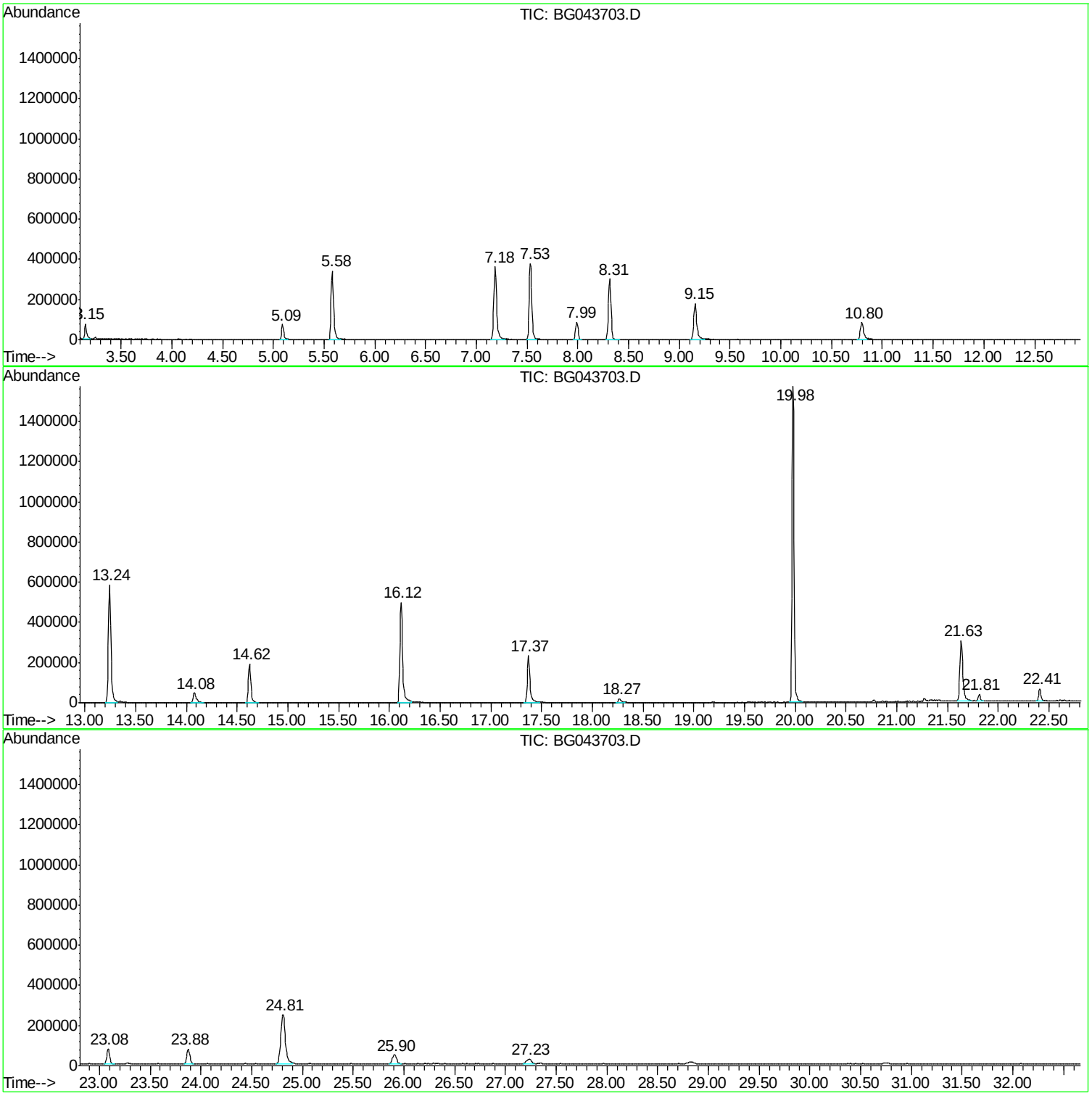
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111919\
Data File : BG043703.D
Acq On : 19 Nov 2019 18:16
Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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\BG111919\
Data File : BG043703.D
Acq On : 19 Nov 2019 18:16
Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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

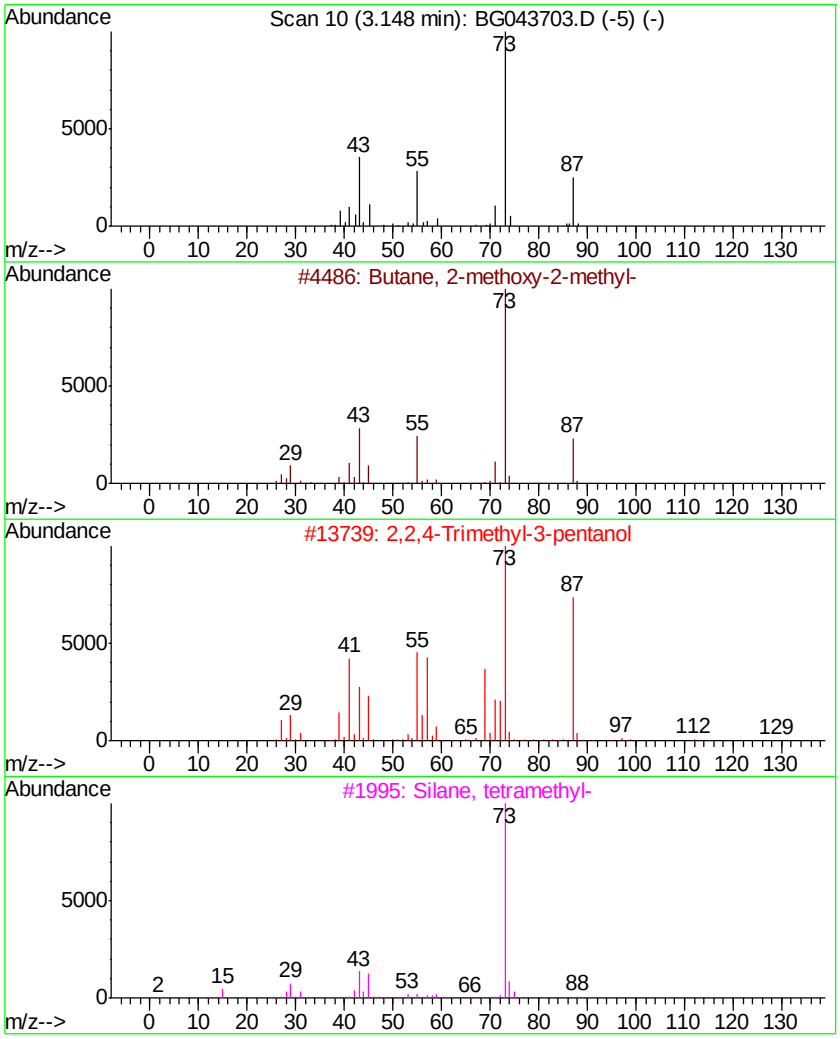
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

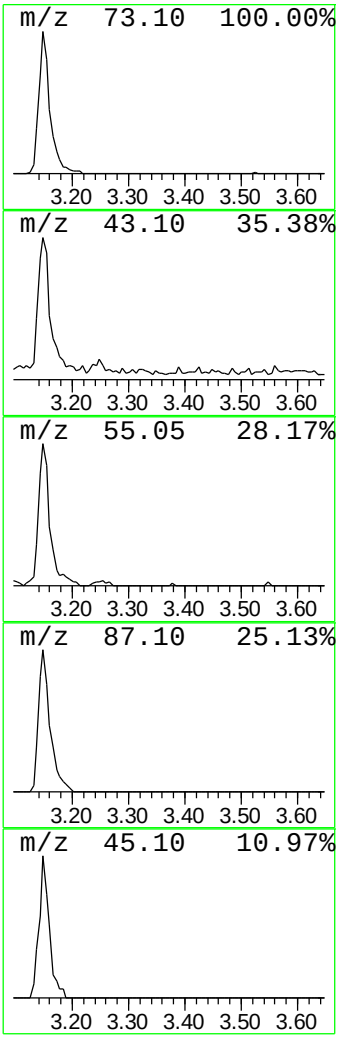
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	13.09 ng	103865	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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Data File : BG043703.D
Acq On : 19 Nov 2019 18:16
Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

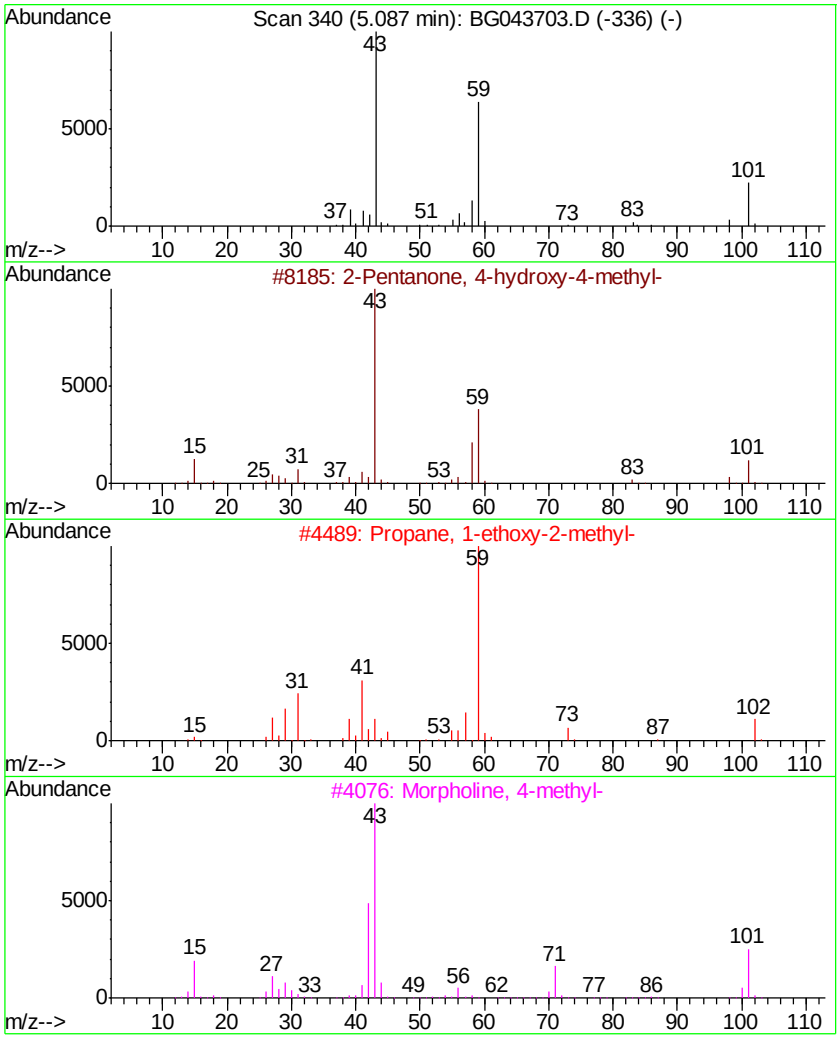
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

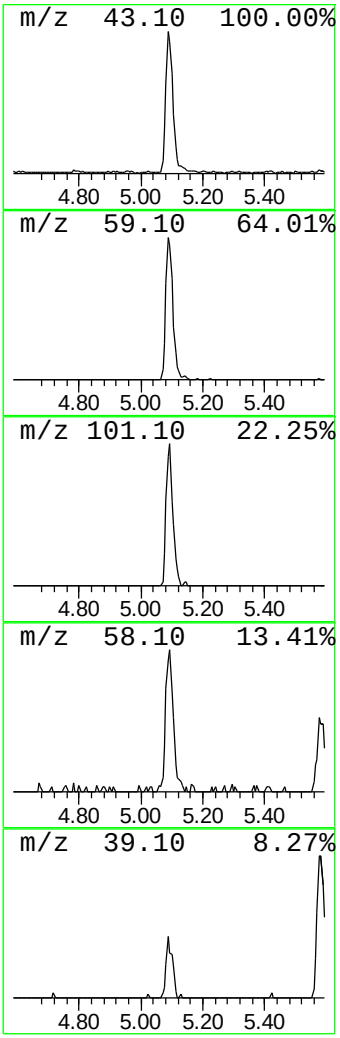
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	14.93 ng	118467	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	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111919\
Data File : BG043703.D
Acq On : 19 Nov 2019 18:16
Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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

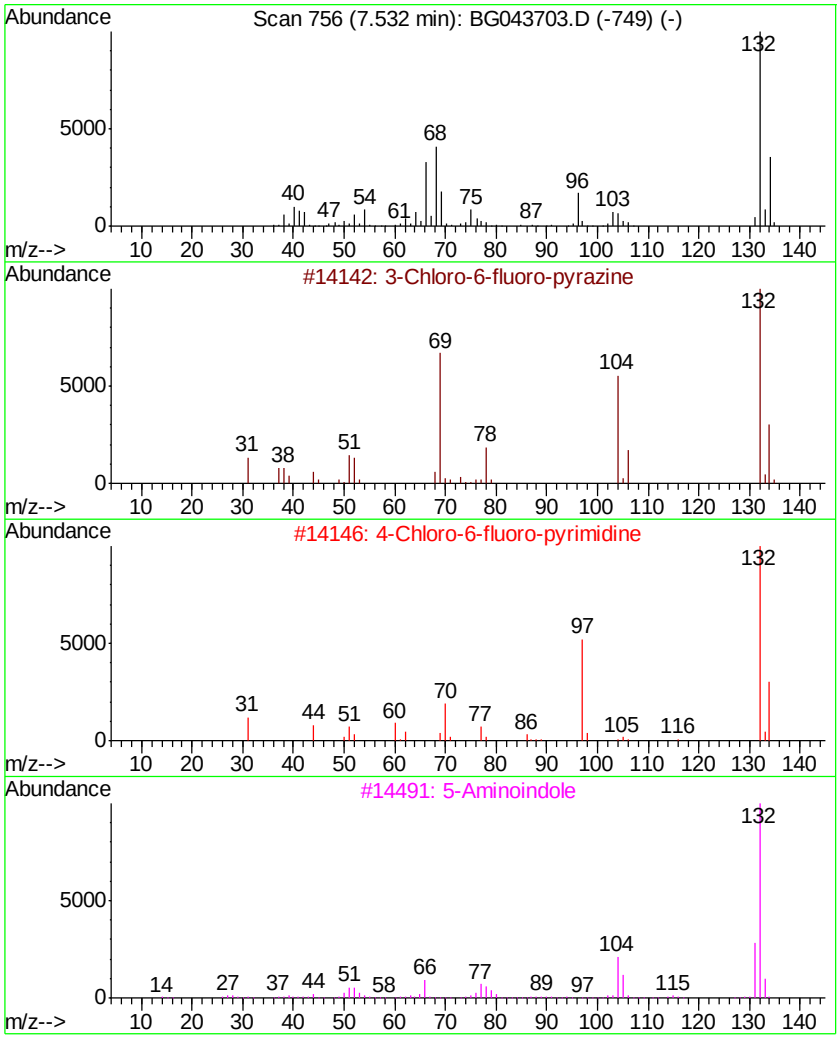
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

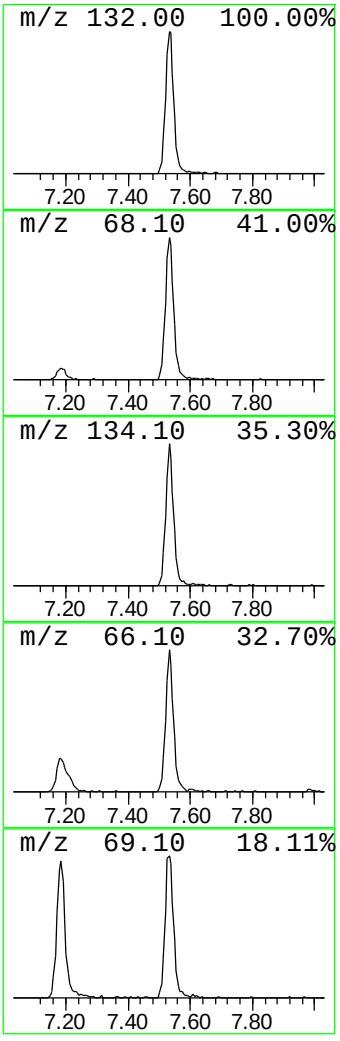
****

Peak Number 3 unknown7.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	86.56 ng	686932	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	5-Aminoindole	132	C8H8N2	005192-03-0	27
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111919\
Data File : BG043703.D
Acq On : 19 Nov 2019 18:16
Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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

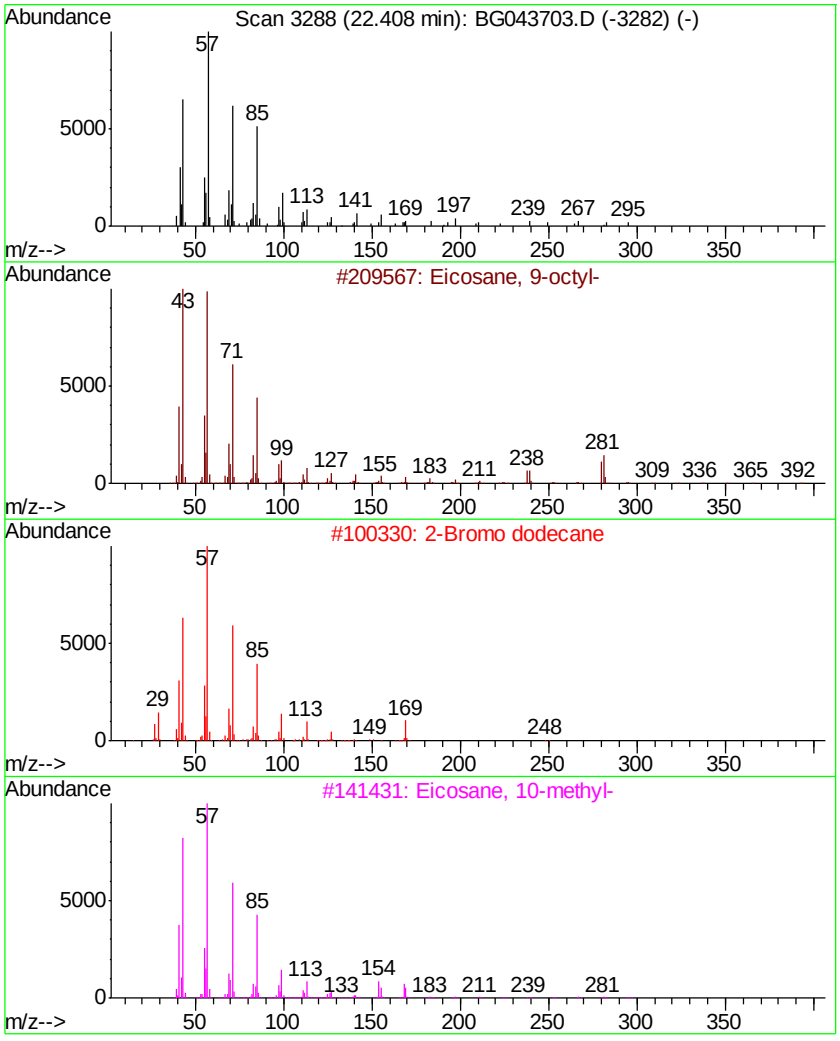
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

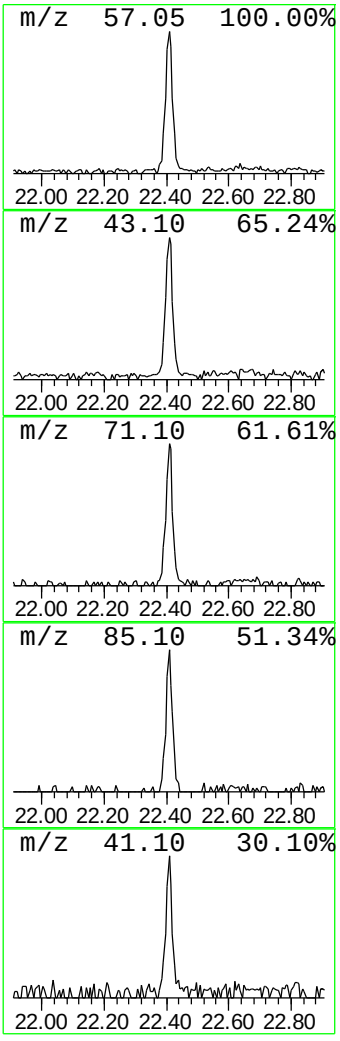
****

Peak Number 5 Eicosane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.98 ng	91158	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 9-octyl-	394	C28H58	013475-77-9	80
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111919\
Data File : BG043703.D
Acq On : 19 Nov 2019 18:16
Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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

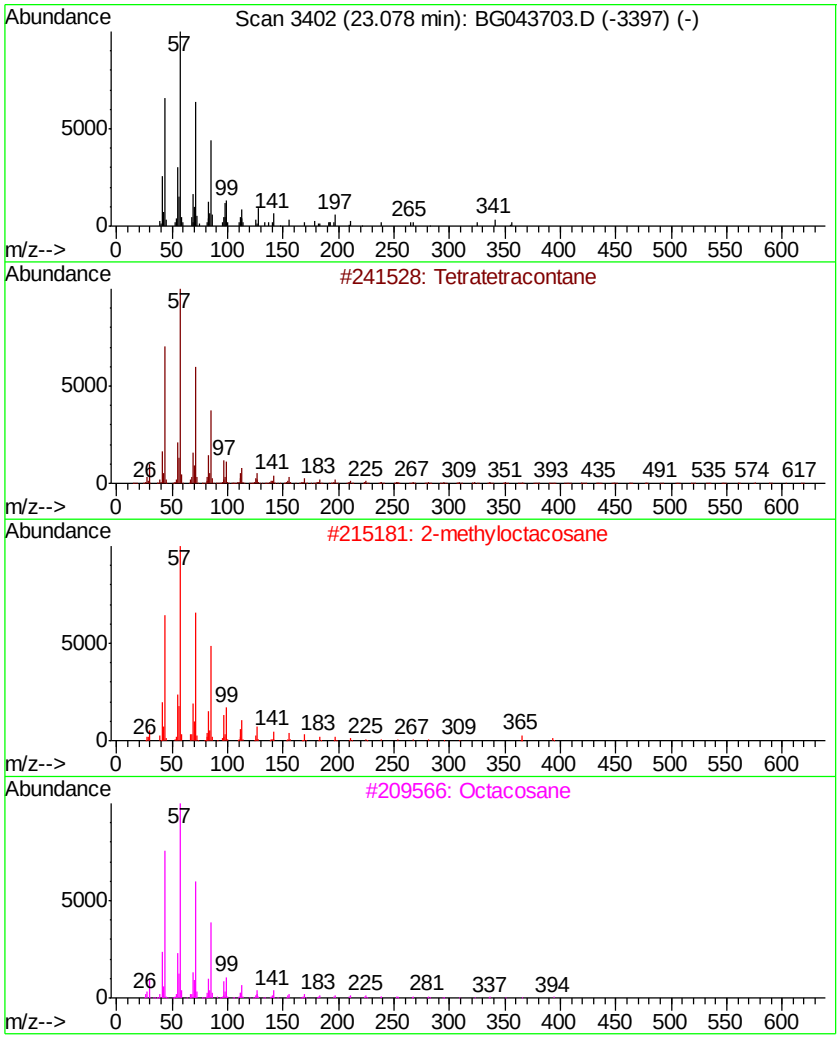
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

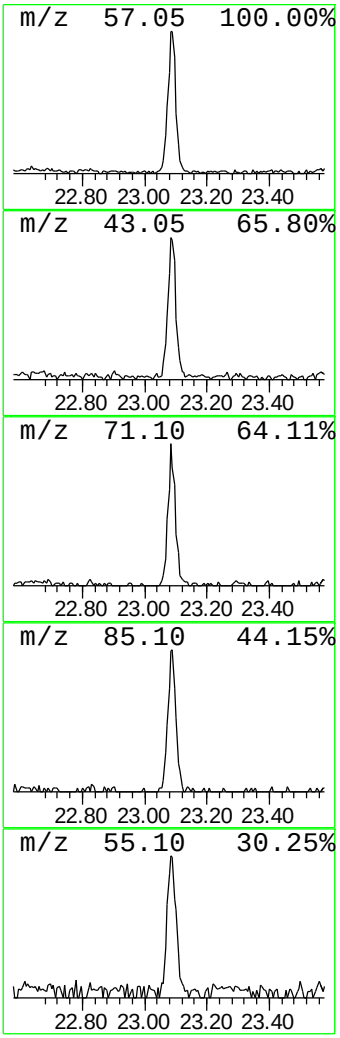
****

Peak Number 6 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.08	4.73 ng	144409	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Data File : BG043703.D
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Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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

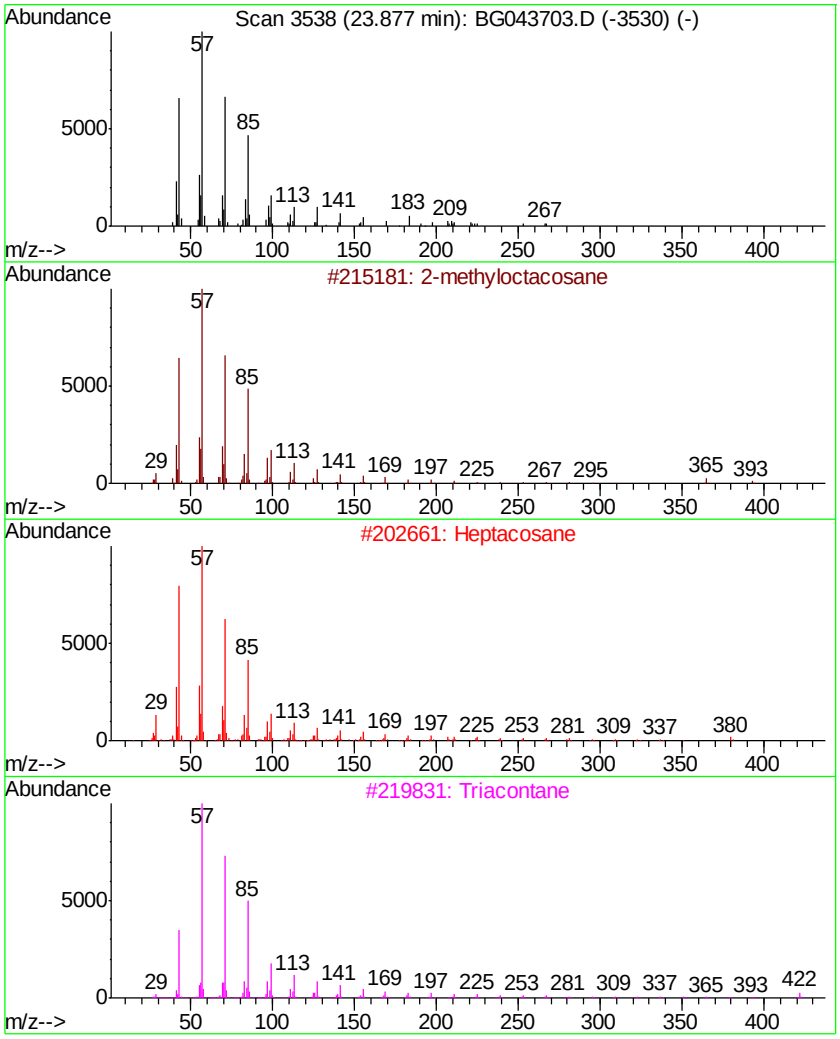
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

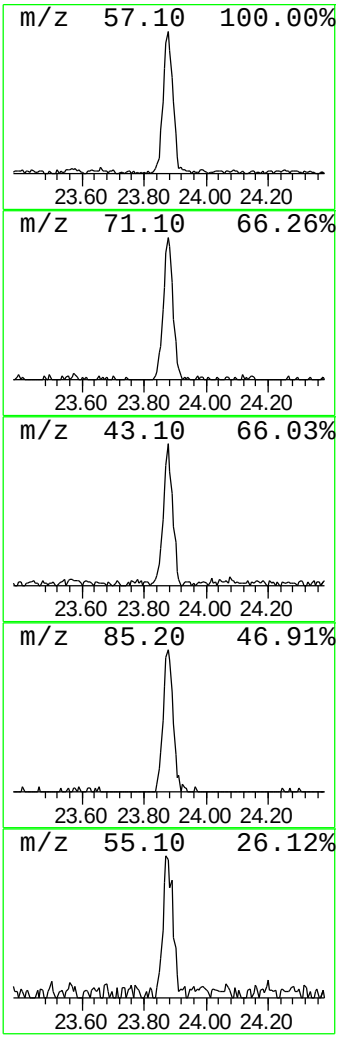
****

Peak Number 7 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.88	4.05 ng	159495	Perylene-d12	24.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexatriacontane	507	C36H74	000630-06-8	91





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Operator : JU
Sample : K5865-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2-(16-19)

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

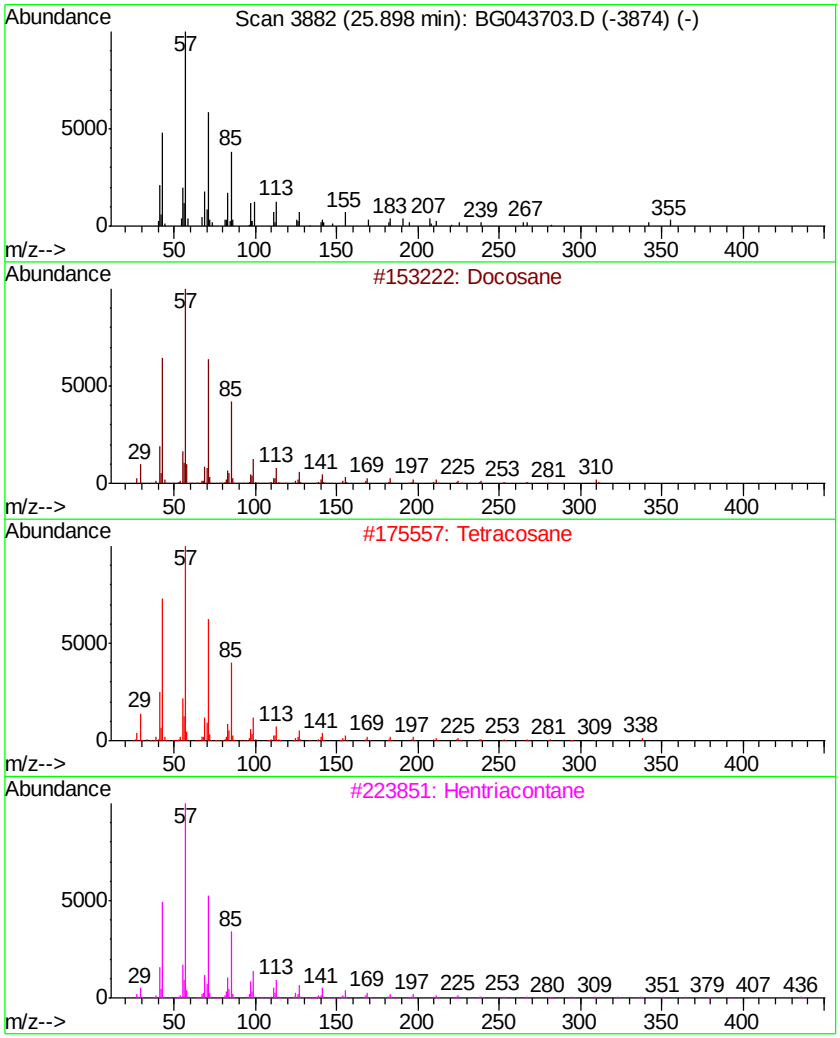
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

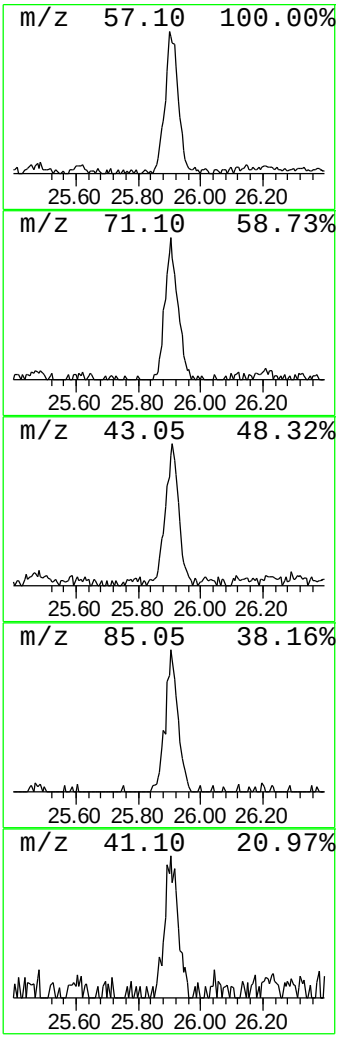
****

Peak Number 8 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.90	3.44 ng	135729	Perylene-d12	24.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111919\
Data File : BG043703.D
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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	13.1	ng	103865	1	7.99	158718	20.0
2-Pentanone, 4-hy...	5.09	14.9	ng	118467	1	7.99	158718	20.0
unknown7.53	7.53	86.6	ng	686932	1	7.99	158718	20.0
Eicosane, 9-octyl-	22.41	3.0	ng	91158	5	21.63	611149	20.0
Tetratetracontane	23.08	4.7	ng	144409	5	21.63	611149	20.0
2-methyloctacosane	23.88	4.0	ng	159495	6	24.81	788081	20.0
Docosane	25.90	3.4	ng	135729	6	24.81	788081	20.0