LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043468.D
Acq On : 1 Nov 2019 16:40
Operator : JU
Sample : K5603-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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	3.181	11	16	24	rVB	108908	174755	3.36%	1.268%
2	5.143	339	350	362	rBV	2634286	5207478	100.00%	37.798%
3	5.602	422	428	438	rBV	33319	60301	1.16%	0.438%
4	7.194	691	699	712	rBV	98054	222964	4.28%	1.618%
5	7.311	713	719	727	rVB	72722	129927	2.50%	0.943%
6	7.552	754	760	770	rVB	64235	116456	2.24%	0.845%
7	8.011	832	838	846	rBV	129249	236874	4.55%	1.719%
8	8.334	886	893	908	rBV	284369	526373	10.11%	3.821%
9	9.174	1029	1036	1048	rBV	156907	335802	6.45%	2.437%
10	10.819	1307	1316	1325	rBV	157205	320541	6.16%	2.327%
11	13.263	1724	1732	1747	rBV	489111	836560	16.06%	6.072%
12	14.092	1864	1873	1882	rBV	95087	167759	3.22%	1.218%
13	14.638	1959	1966	1974	rBV	320868	513179	9.85%	3.725%
14	16.136	2215	2221	2227	rBV2	29025	57842	1.11%	0.420%
15	17.141	2386	2392	2397	rBV5	37148	66500	1.28%	0.483%
16	17.388	2426	2434	2446	rBV	387871	665595	12.78%	4.831%
17	19.997	2872	2878	2893	rBV	1318297	1795318	34.48%	13.031%
18	21.289	3094	3098	3105	rBV2	74288	137091	2.63%	0.995%
19	21.653	3153	3160	3171	rBV	436361	805820	15.47%	5.849%
20	22.447	3289	3295	3299	rBV5	34443	69002	1.33%	0.501%
21	23.921	3540	3546	3553	rVB2	81423	167617	3.22%	1.217%
22	24.844	3692	3703	3717	rBV3	298636	936816	17.99%	6.800%
23	25.860	3870	3876	3886	rVB3	29682	77484	1.49%	0.562%
24	25.972	3887	3895	3906	rVB4	50028	149153	2.86%	1.083%

Sum of corrected areas: 13777207

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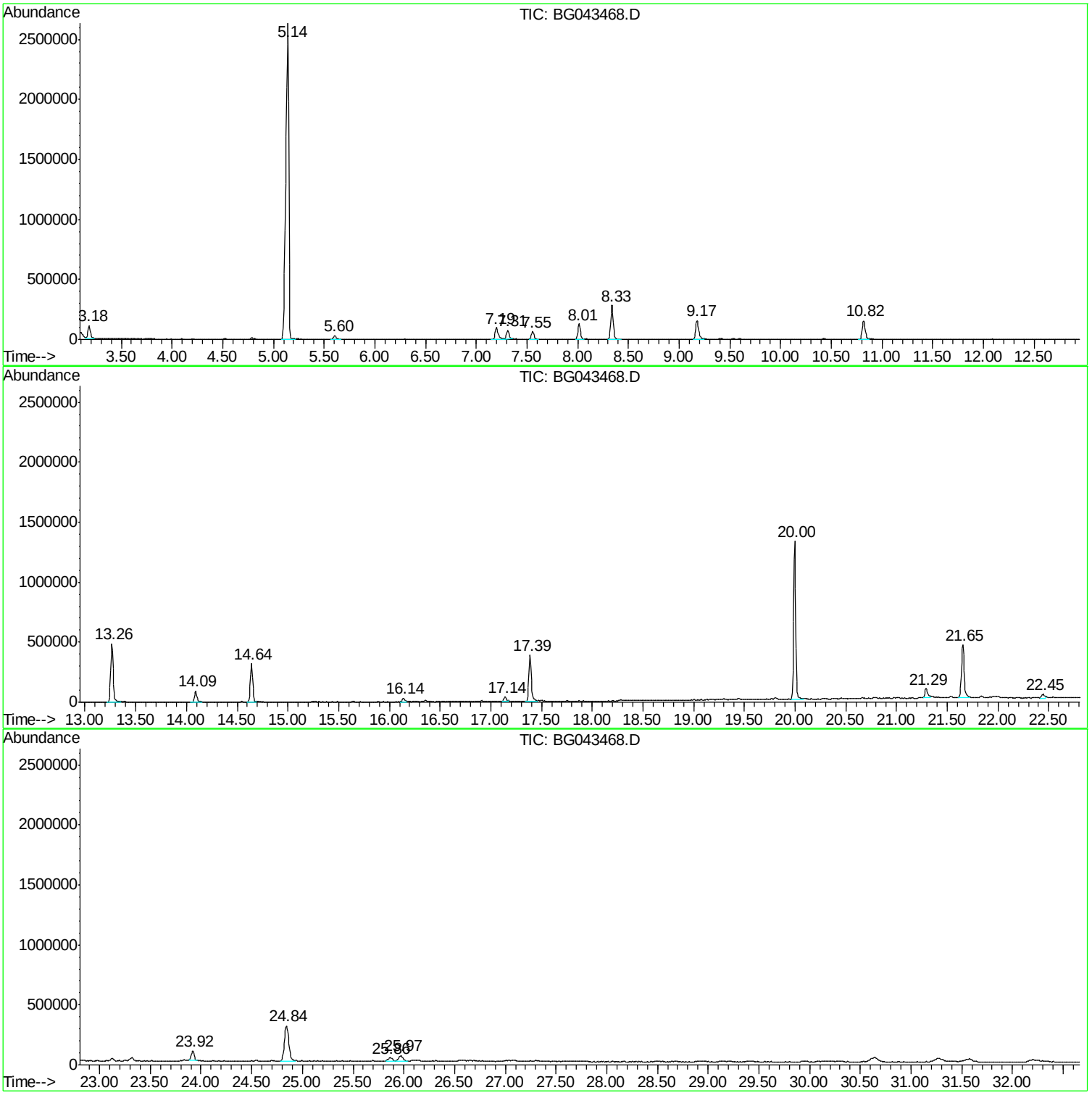
Instrument :
BNA_G
ClientSampleId :
20190949-AMENDED-COMPOSITE-

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



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Data File : BG043468.D
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Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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

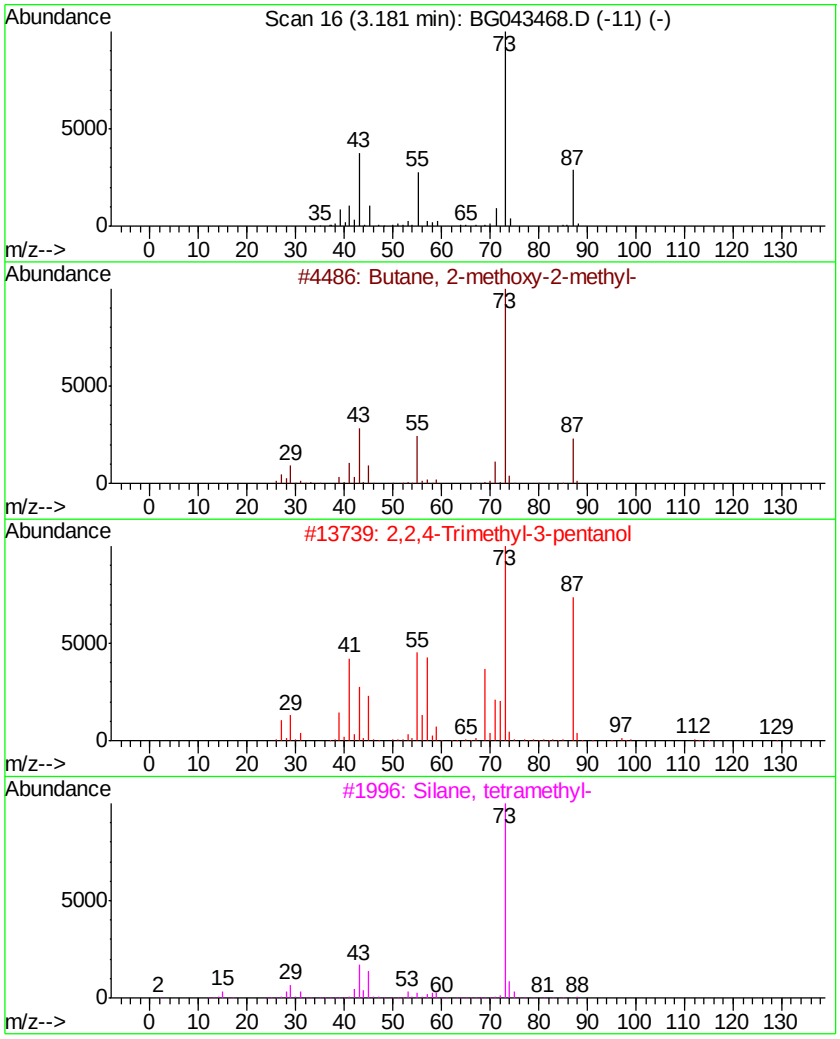
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

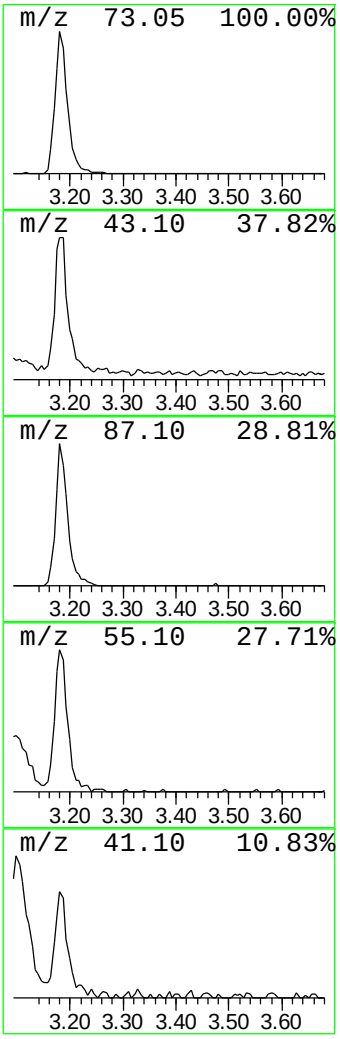
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	14.76 ng	174755	1,4-Dichlorobenzene-d4	8.02

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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BG043468.D
Acq On : 1 Nov 2019 16:40
Operator : JU
Sample : K5603-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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

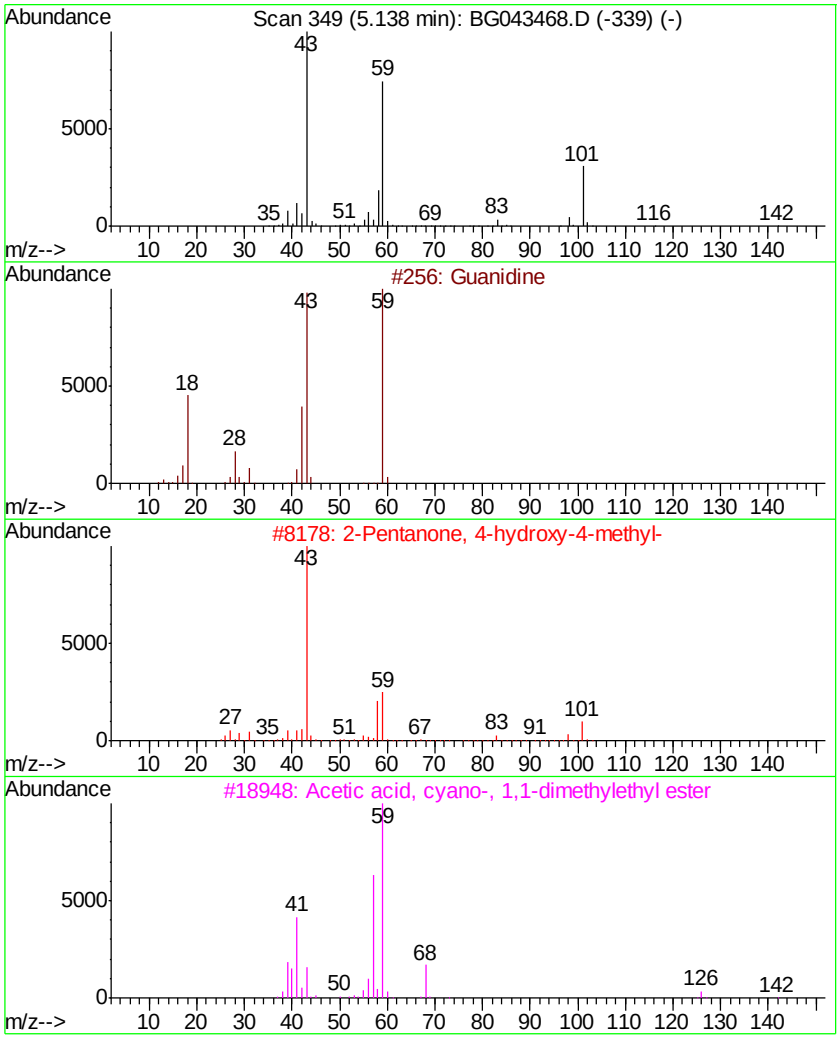
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

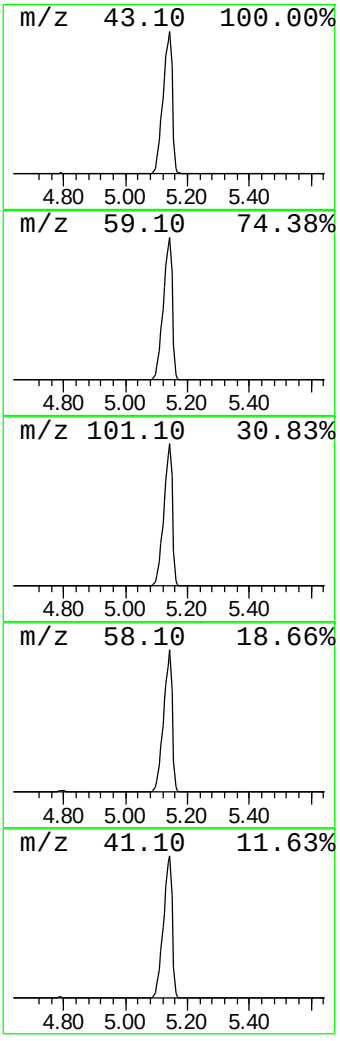
****

Peak Number 2 unknown5.14 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	439.68 ng	5207480	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	47
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32





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Data File : BG043468.D
Acq On : 1 Nov 2019 16:40
Operator : JU
Sample : K5603-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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
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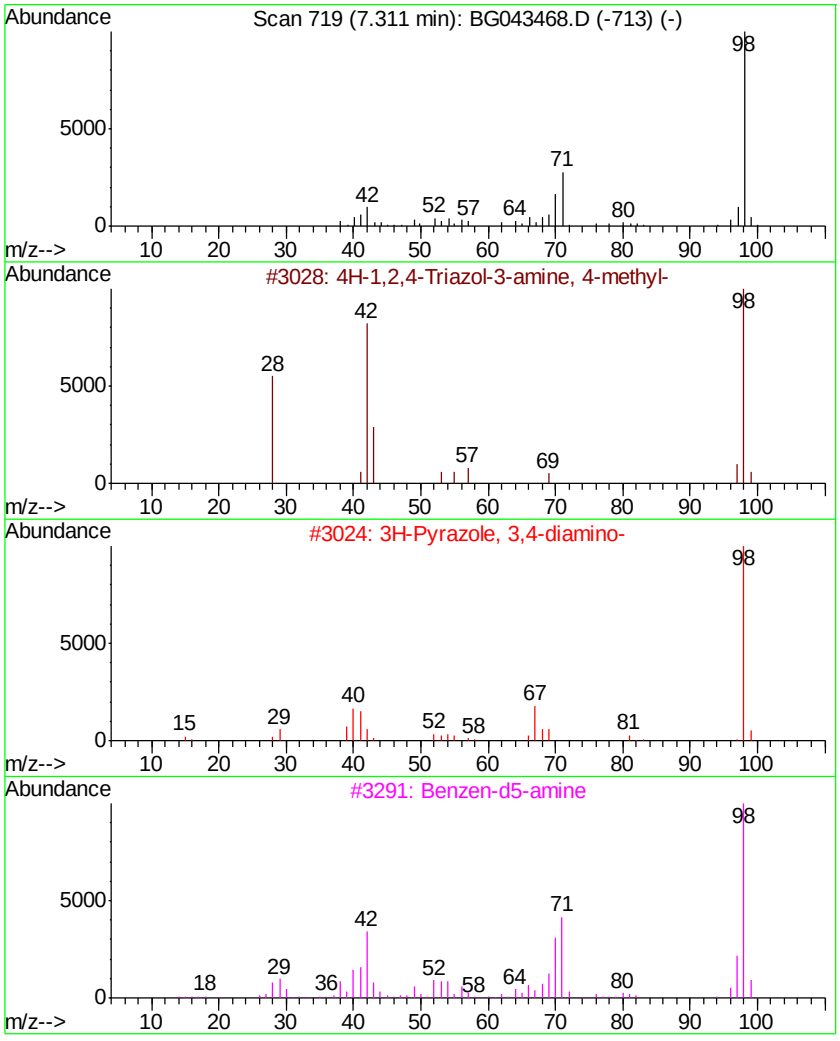
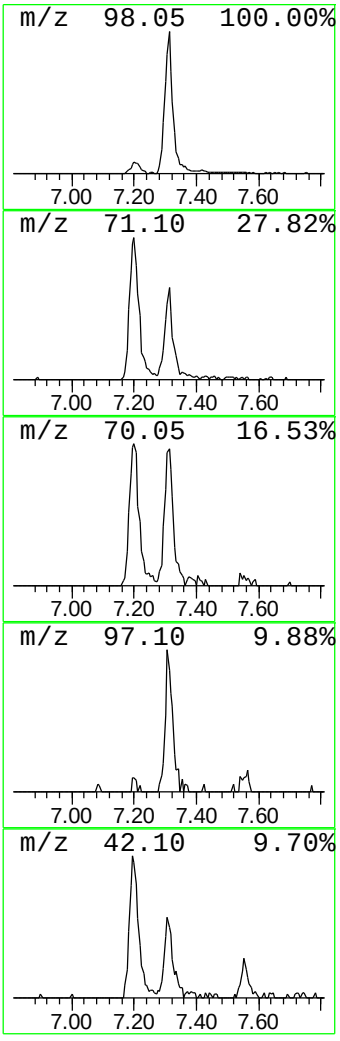
****

Peak Number 3 4H-1,2,4-Triazol-3-amine, 4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	10.97 ng	129927	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,2,4-Triazol-3-amine, 4-methyl-	98	C3H6N4	016681-76-8	58
2	3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	52
3	Benzen-d5-amine	98	C6H2D5N	004165-61-1	50
4	Propan-2-ol, 1-(2-methyl-4-nitro...	300	C12H20N4O3S	306326-24-9	42
5	1-Pyridineacetic acid, hexahydro-	143	C7H13NO2	1000362-53-3	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043468.D
Acq On : 1 Nov 2019 16:40
Operator : JU
Sample : K5603-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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
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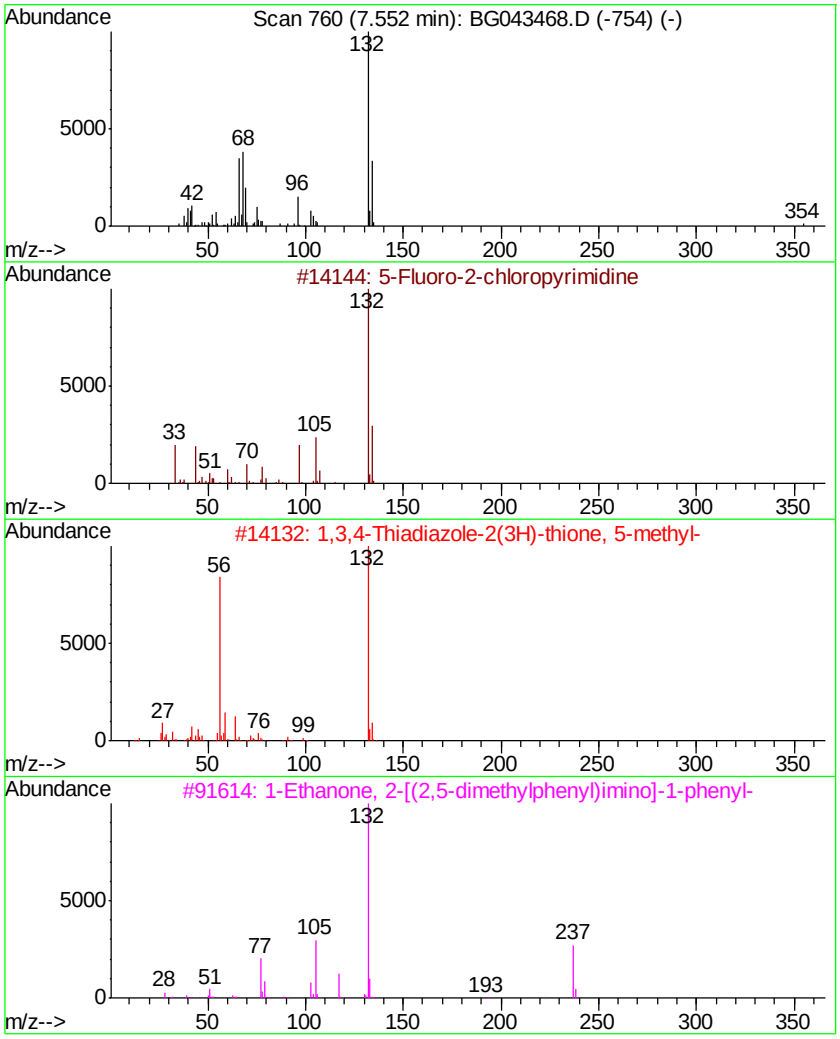
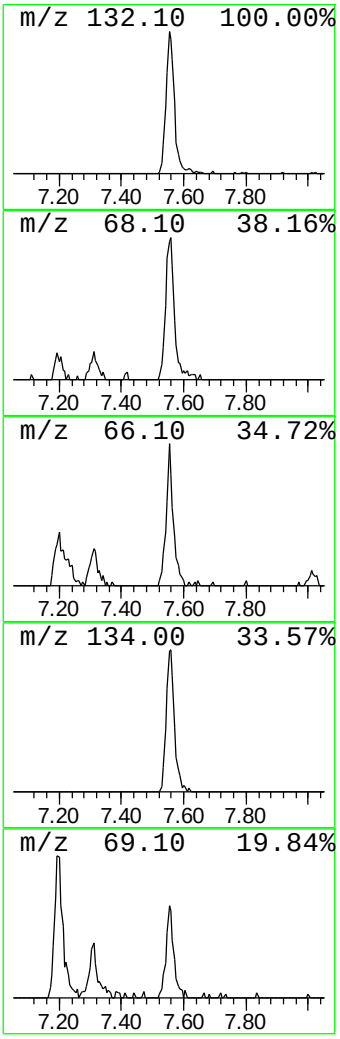
****

Peak Number 4 unknown7.55 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	9.83 ng	116456	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	12
3	1-Ethanone, 2-[(2,5-dimethylphen...	237	C16H15NO	1000319-31-2	12
4	Benzimidazole, 2-heptyl-	216	C14H20N2	005851-49-0	10
5	4-Ethylphenyl isocyanate	147	C9H9NO	023138-50-3	10





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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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

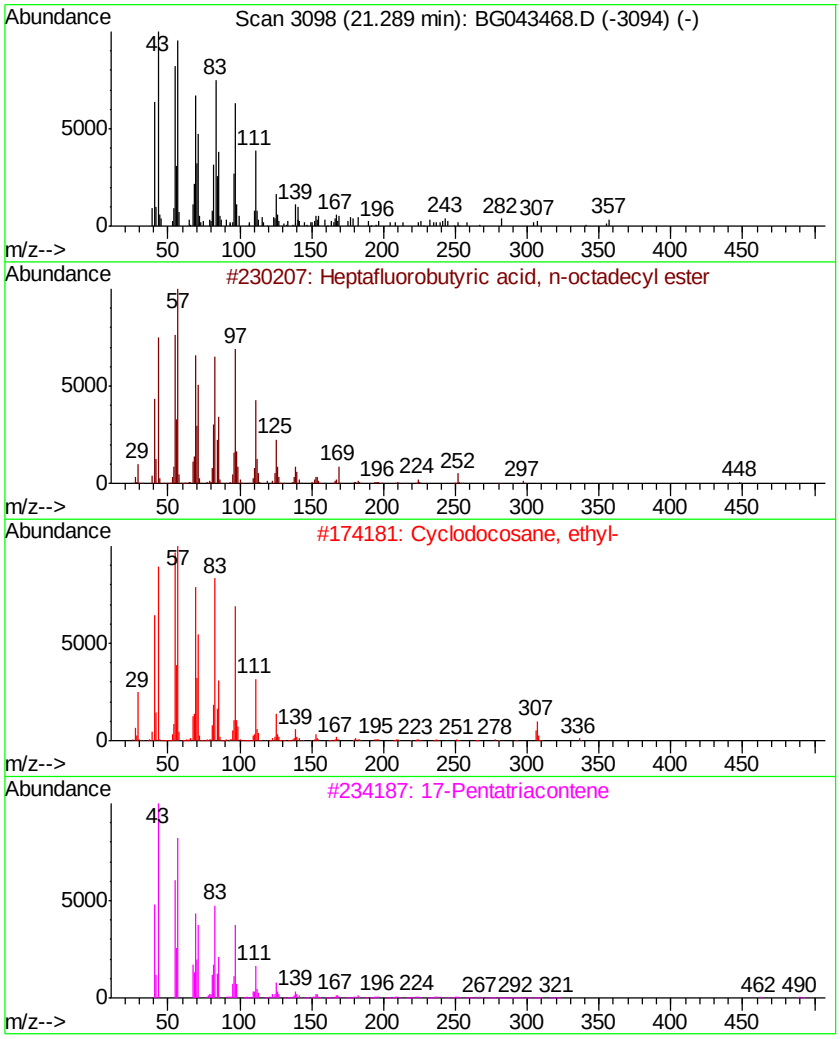
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

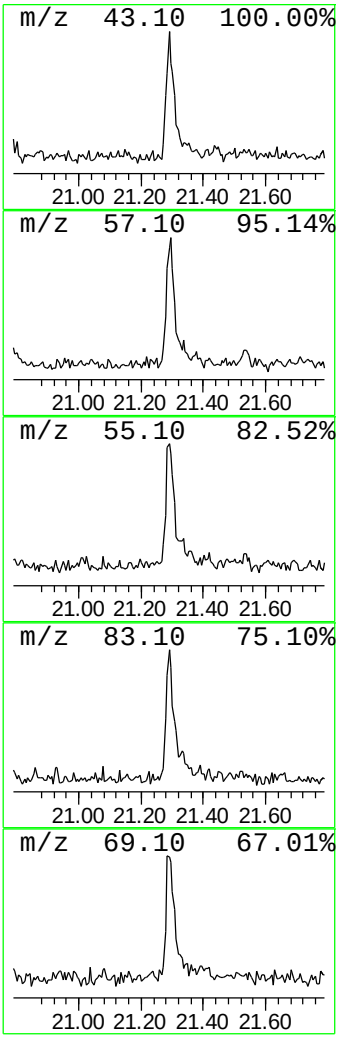
****

Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	3.40 ng	137091	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
2	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	87
3	17-Pentatriacontene	491	C35H70	006971-40-0	83
4	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	83
5	Octacosanol	410	C28H58O	000557-61-9	81





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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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

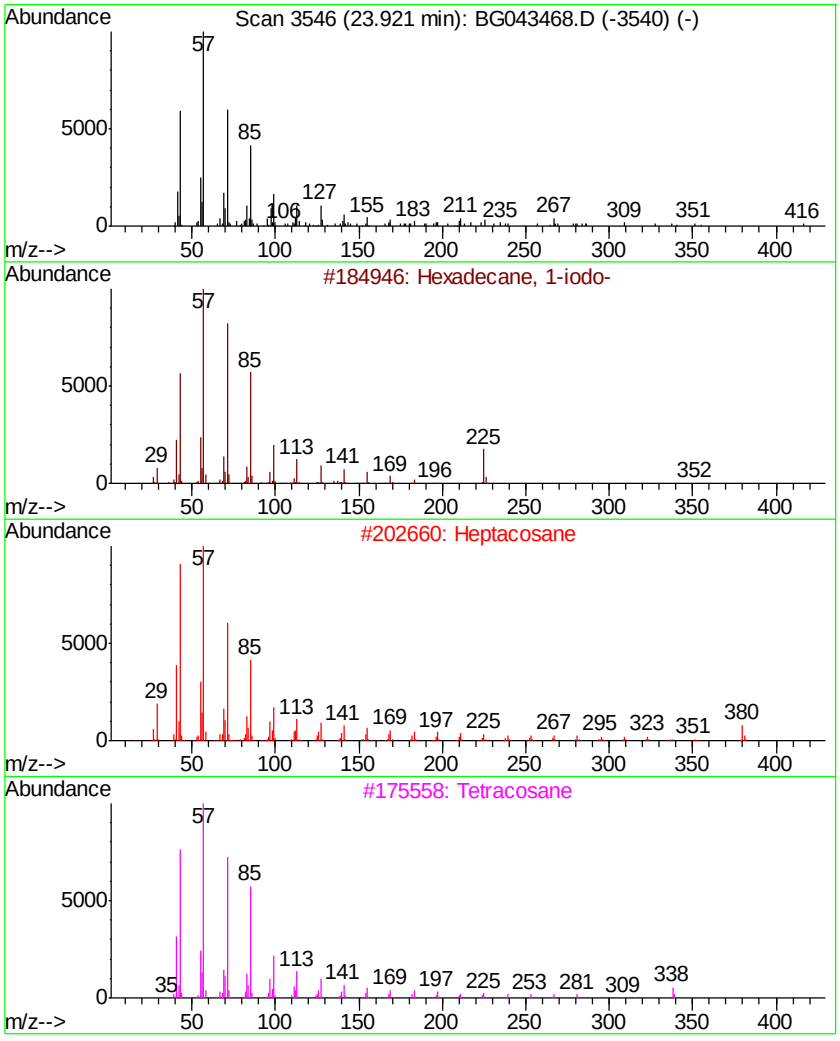
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

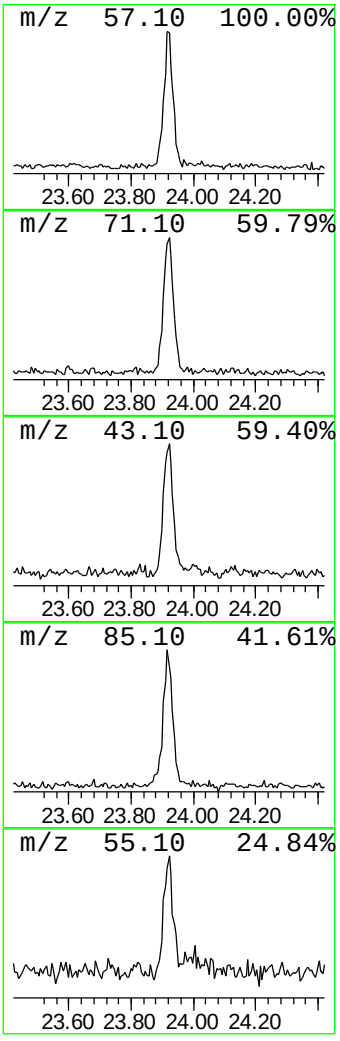
****

Peak Number 7 Hexadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	3.58 ng	167617	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
2	Heptacosane	380	C27H56	000593-49-7	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Octacosane	394	C28H58	000630-02-4	90





Library Search Compound Report

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Acq On : 1 Nov 2019 16:40
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Misc :
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Instrument : BNA_G
ClientSampleId : 20190949-AMENDED-COMPOSITE-

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

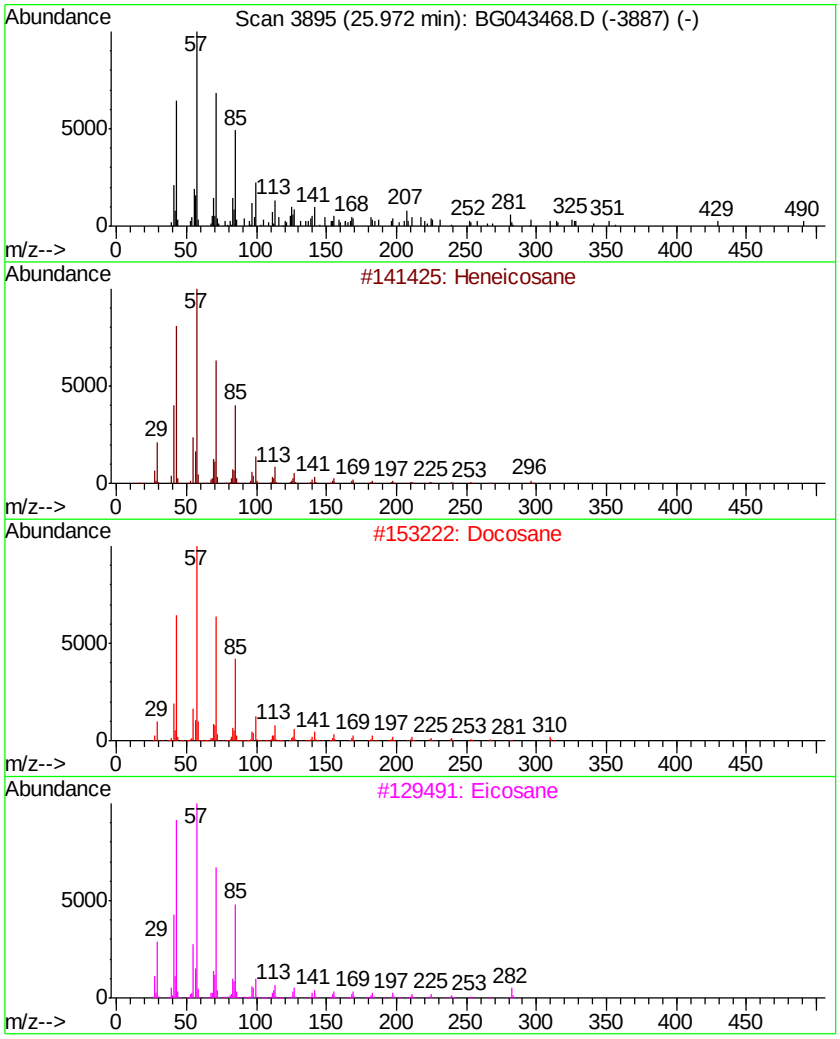
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

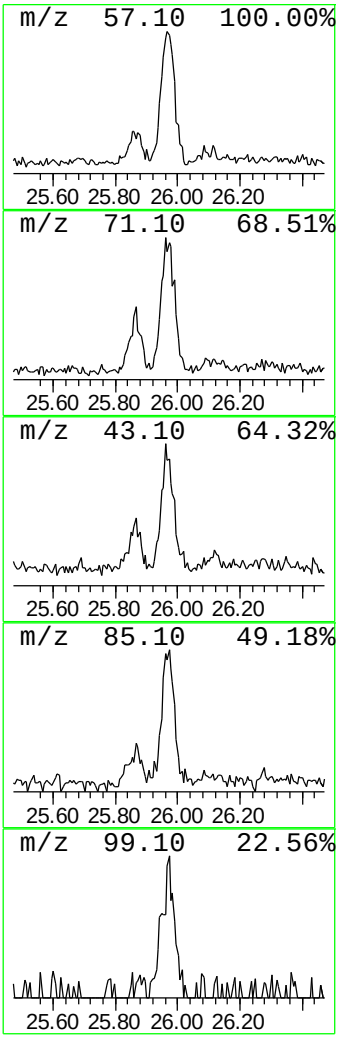
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	3.18 ng	149153	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Docosane	310	C22H46	000629-97-0	93
3	Eicosane	282	C20H42	000112-95-8	93
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

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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...	3.18	14.8	ng	174755	1	8.02	236874	20.0
unknown5.14	5.14	439.7	ng	5207480	1	8.02	236874	20.0
4H-1,2,4-Triazol-...	7.31	11.0	ng	129927	1	8.02	236874	20.0
unknown7.55	7.55	9.8	ng	116456	1	8.02	236874	20.0
Heptafluorobutyri...	21.29	3.4	ng	137091	5	21.65	805820	20.0
Hexadecane, 1-iodo-	23.92	3.6	ng	167617	6	24.84	936816	20.0
Heneicosane	25.97	3.2	ng	149153	6	24.84	936816	20.0