LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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	3.196	13	18	40	rVB	432443	748039	10.43%	1.742%
2	5.611	421	429	439	rBV	1903403	3037336	42.35%	7.073%
3	7.197	691	699	714	rBV	1960722	3423112	47.73%	7.972%
4	7.579	756	764	777	rBV	1943811	3297854	45.98%	7.680%
5	8.049	836	844	851	rBV	375874	633118	8.83%	1.474%
6	8.372	890	899	910	rVB	1448208	2485821	34.66%	5.789%
7	9.201	1031	1040	1051	rBV	1168449	2053750	28.63%	4.783%
8	10.852	1314	1321	1329	rVB	488963	874404	12.19%	2.036%
9	13.296	1729	1737	1747	rBV	2806509	4512662	62.92%	10.509%
10	14.112	1870	1876	1887	rBV	495231	715291	9.97%	1.666%
11	14.665	1958	1970	1980	rVB2	764753	1292384	18.02%	3.010%
12	16.145	2214	2222	2235	rBV	2388482	3935510	54.87%	9.165%
13	17.397	2428	2435	2446	rBV2	1102790	1668796	23.27%	3.886%
14	20.006	2872	2879	2886	rBV	5161636	7172438	100.00%	16.703%
15	21.116	3064	3068	3075	rVB	74340	100199	1.40%	0.233%
16	21.322	3097	3103	3128	rBV	188295	692186	9.65%	1.612%
17	21.651	3152	3159	3166	rVB	1201432	1966383	27.42%	4.579%
18	21.868	3192	3196	3202	rBV	95919	140384	1.96%	0.327%
19	22.479	3295	3300	3309	rBV	146165	253730	3.54%	0.591%
20	23.178	3412	3419	3429	rVB2	209475	392105	5.47%	0.913%
21	23.989	3550	3557	3567	rVB	213318	461537	6.43%	1.075%
22	24.847	3692	3703	3711	rBV2	711306	2013728	28.08%	4.690%
23	24.947	3713	3720	3731	rVB3	179983	469396	6.54%	1.093%
24	26.081	3906	3913	3925	rVB2	135652	400043	5.58%	0.932%
25	27.456	4141	4147	4157	rVB4	61107	199771	2.79%	0.465%

Sum of corrected areas: 42939977

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
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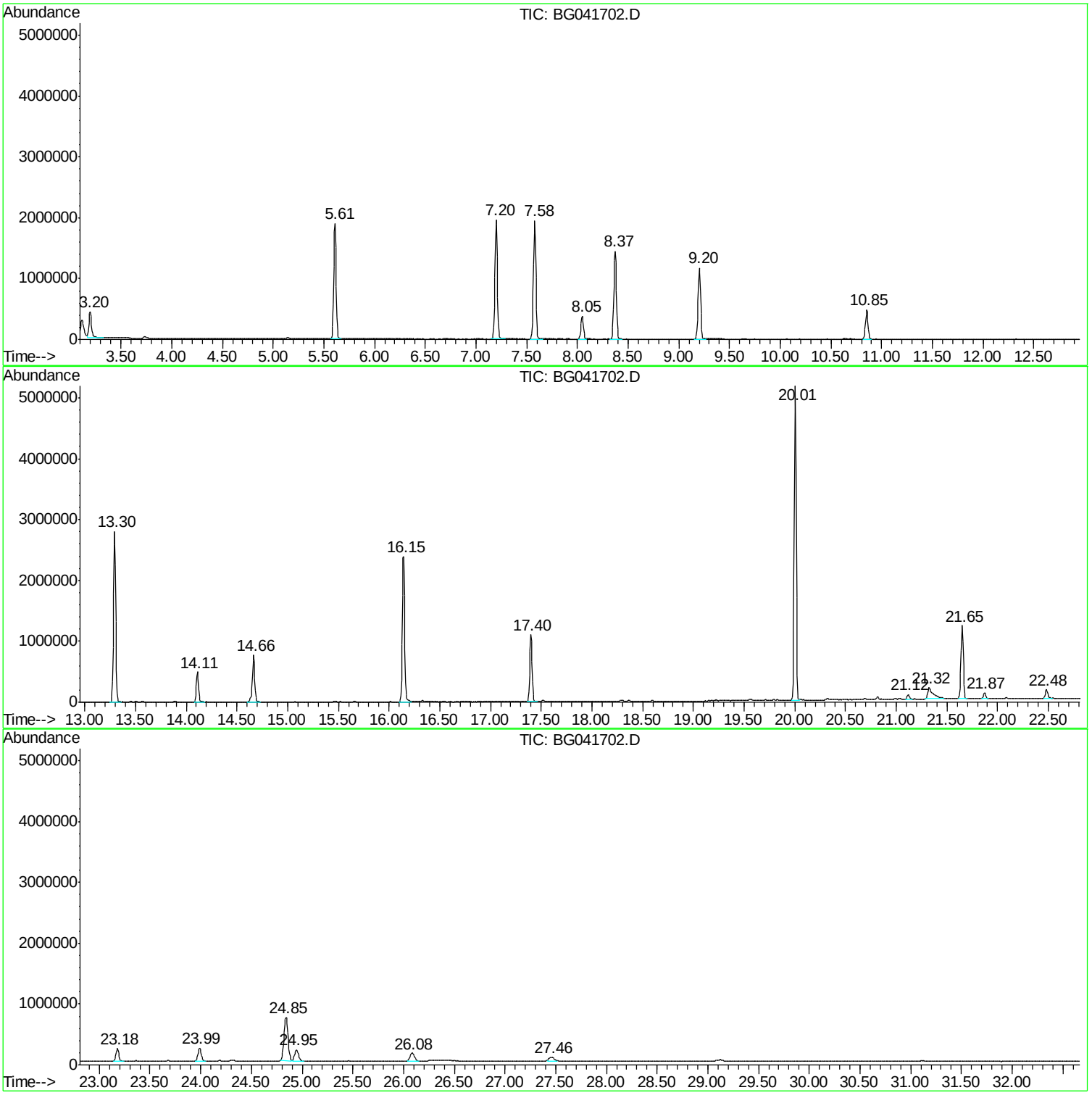
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-12(6-8)

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 : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
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Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

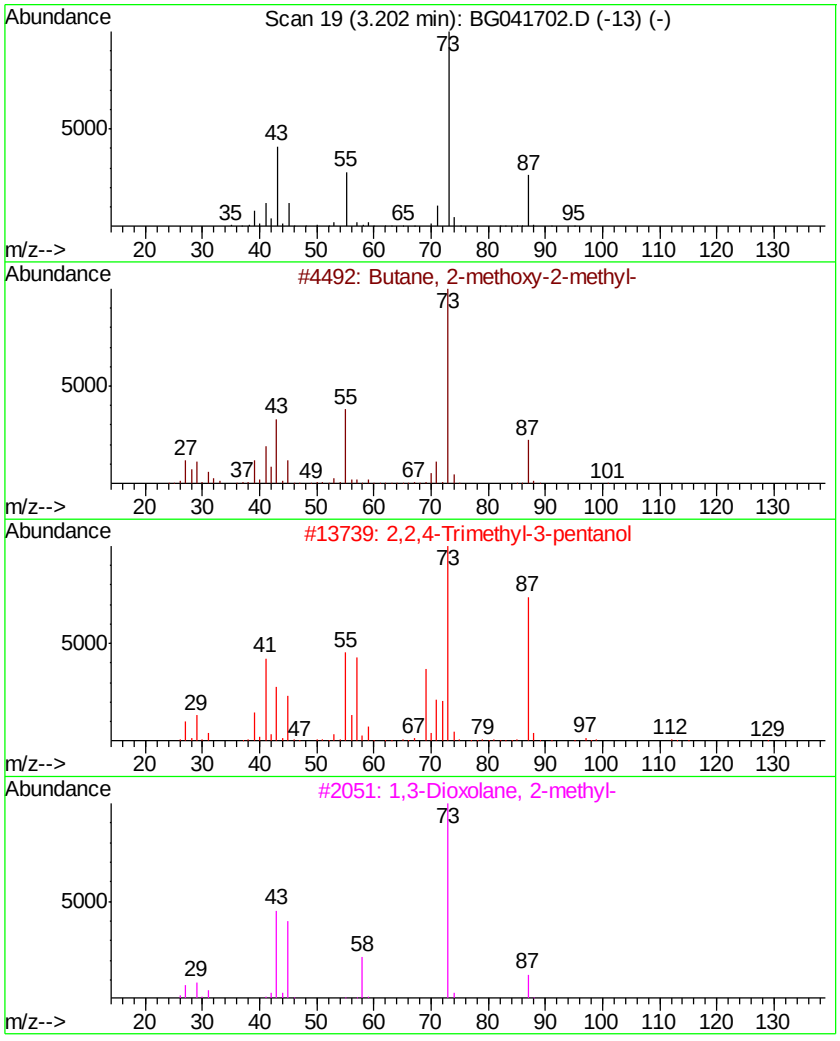
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

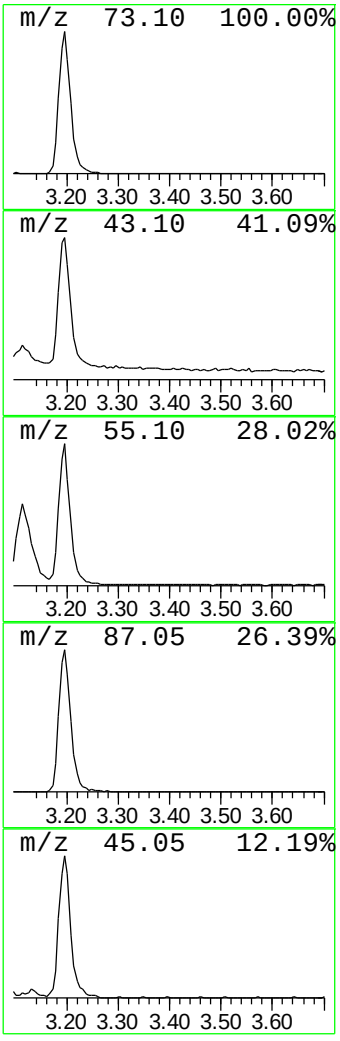
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	23.63 ng	748039	1,4-Dichlorobenzene-d4	8.05

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

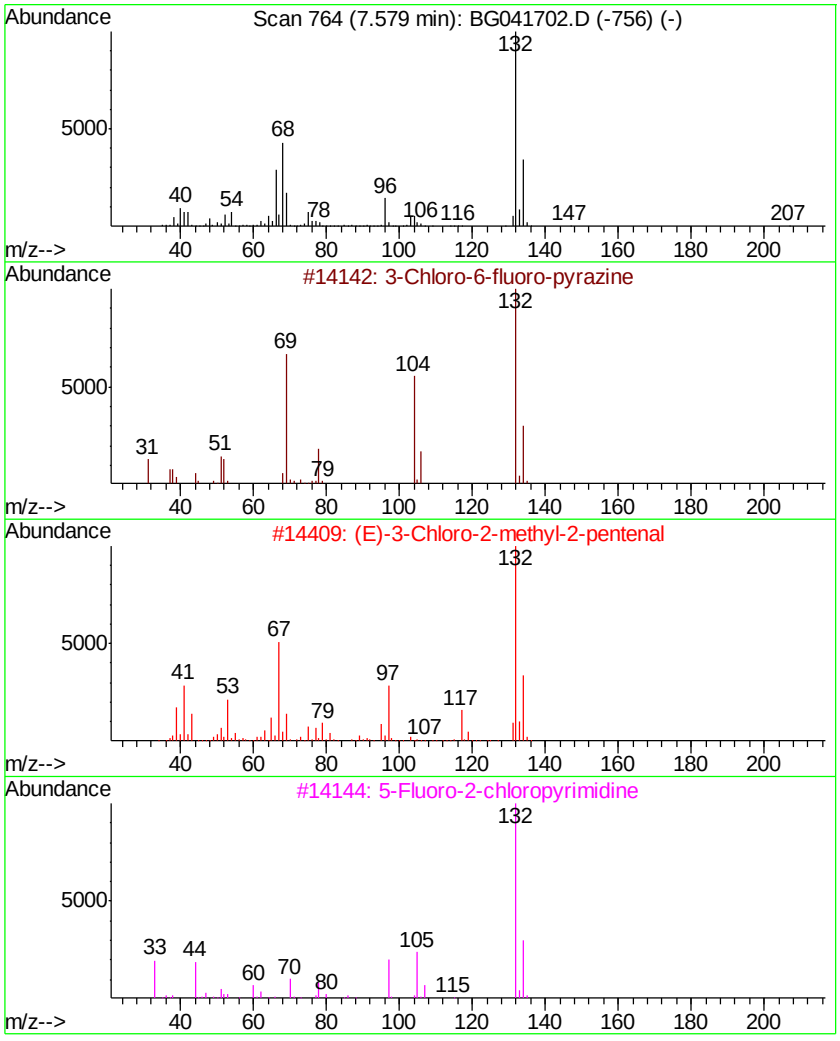
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

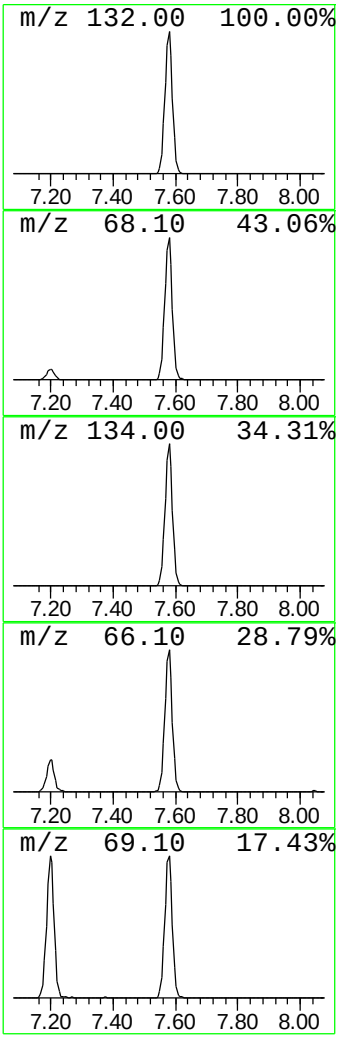
****

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	104.18 ng	3297850	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

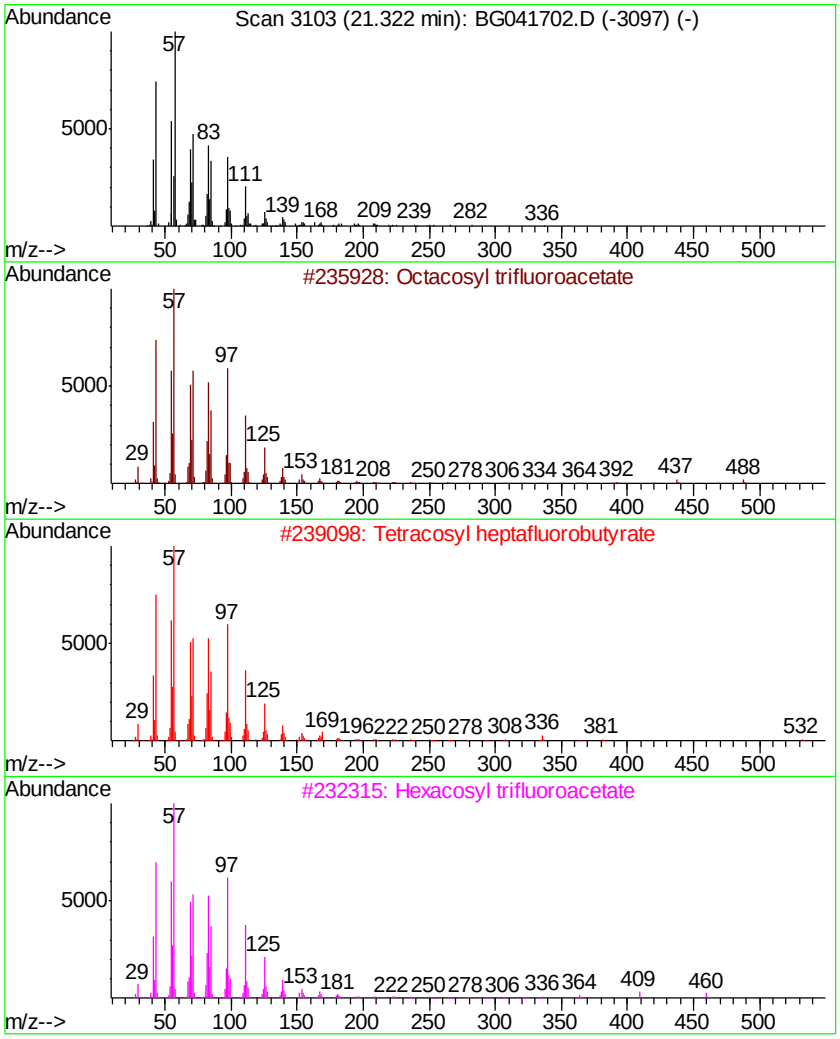
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

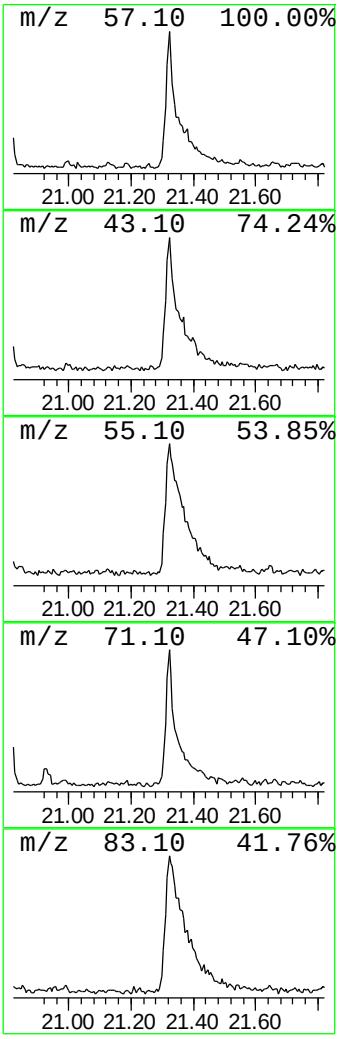
****

Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	7.04 ng	692186	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
4	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

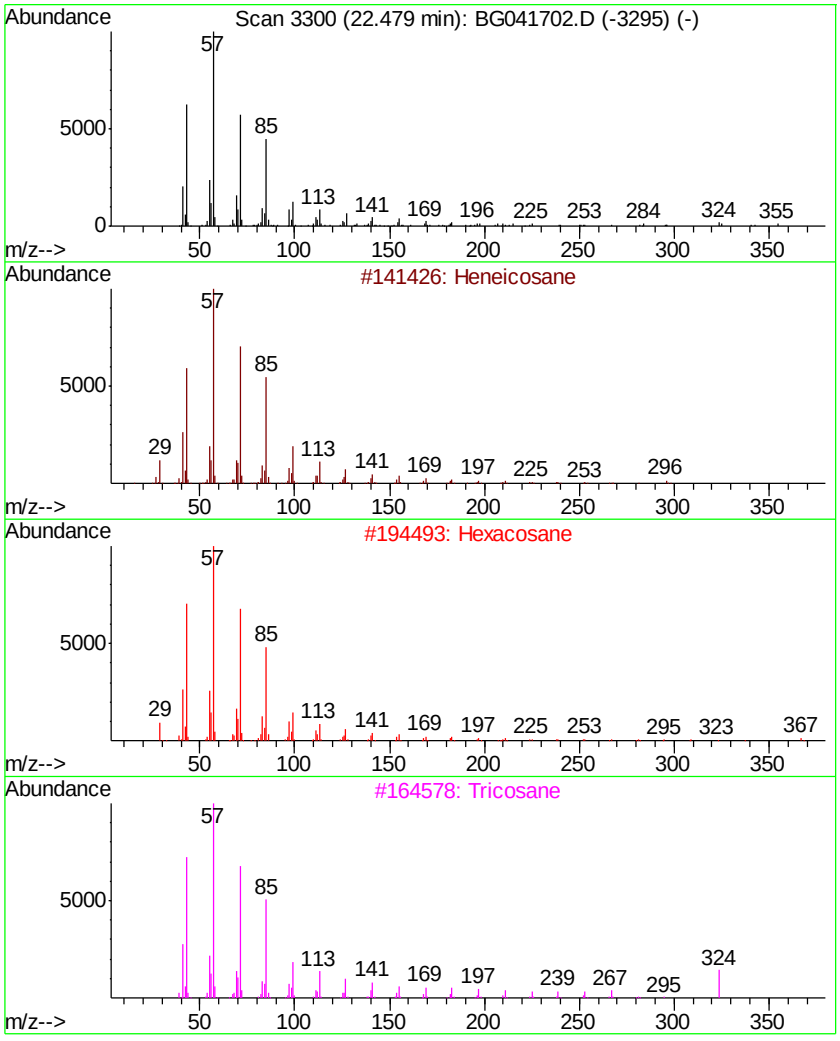
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

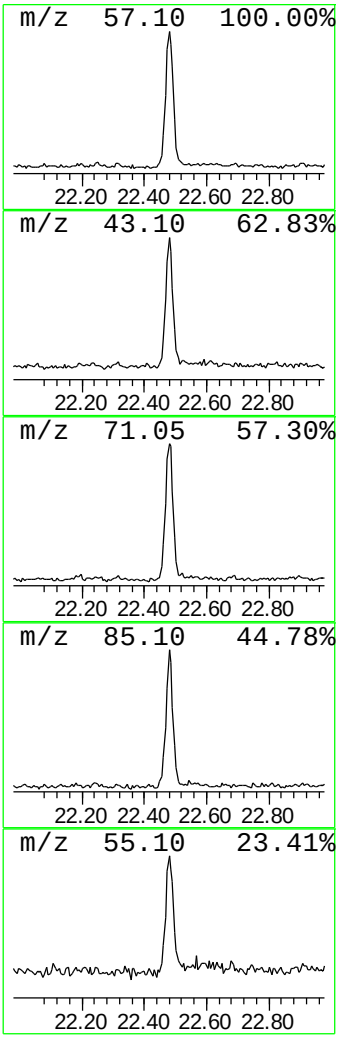
****

Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	2.58 ng	253730	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Hexacosane	366	C26H54	000630-01-3	93
3	Tricosane	324	C23H48	000638-67-5	93
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Octacosane	394	C28H58	000630-02-4	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

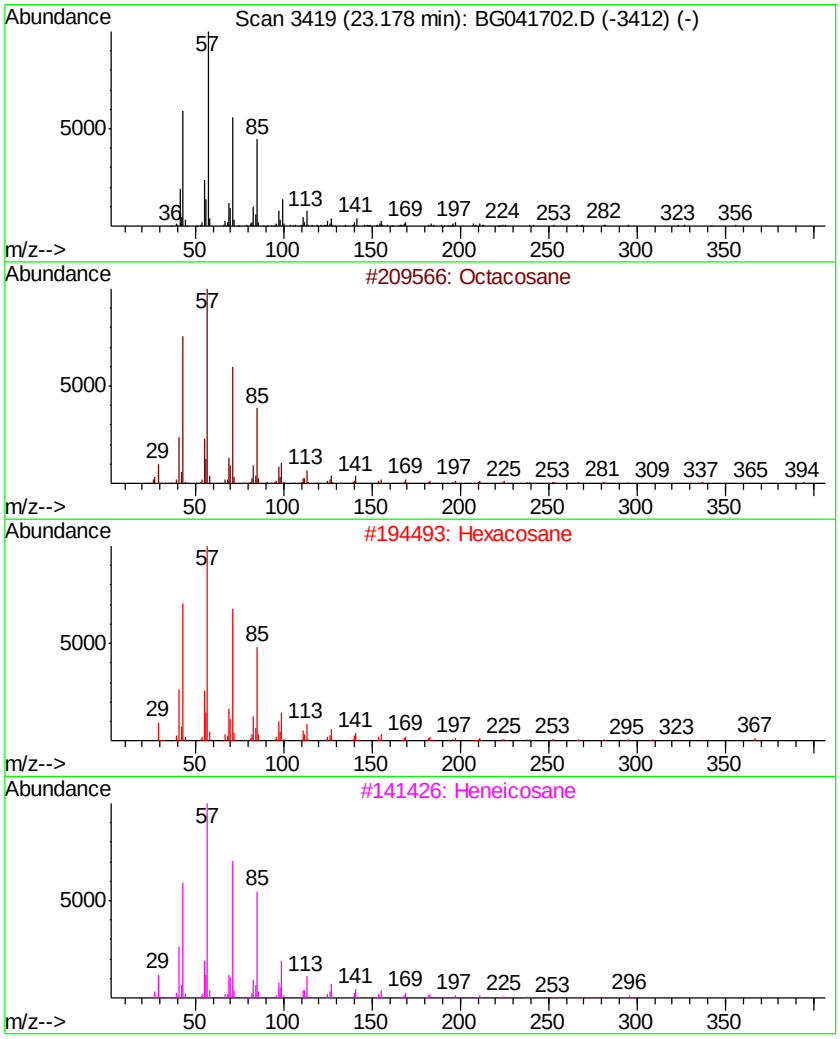
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

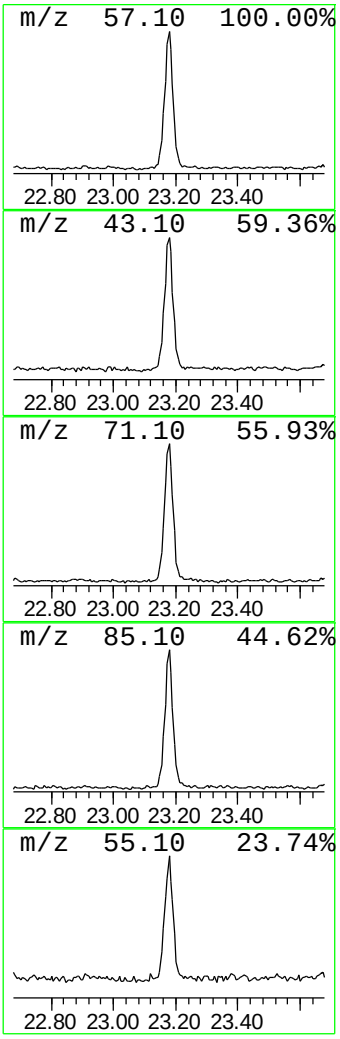
****

Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	3.99 ng	392105	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

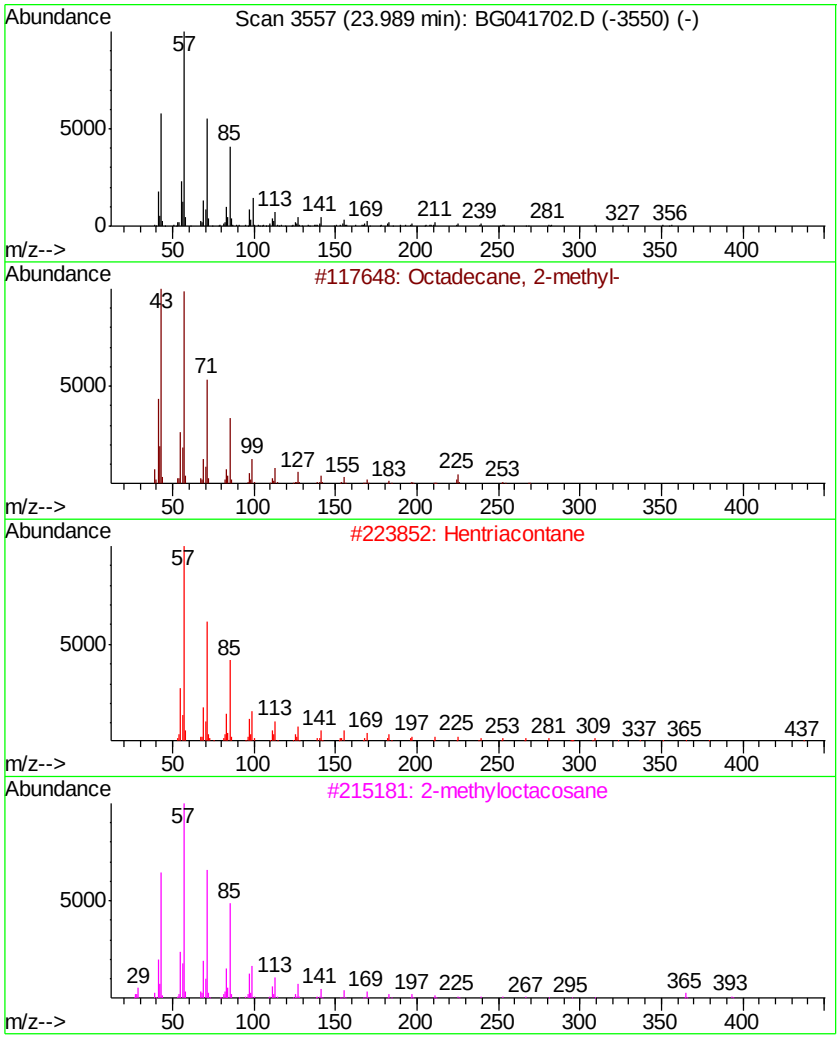
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

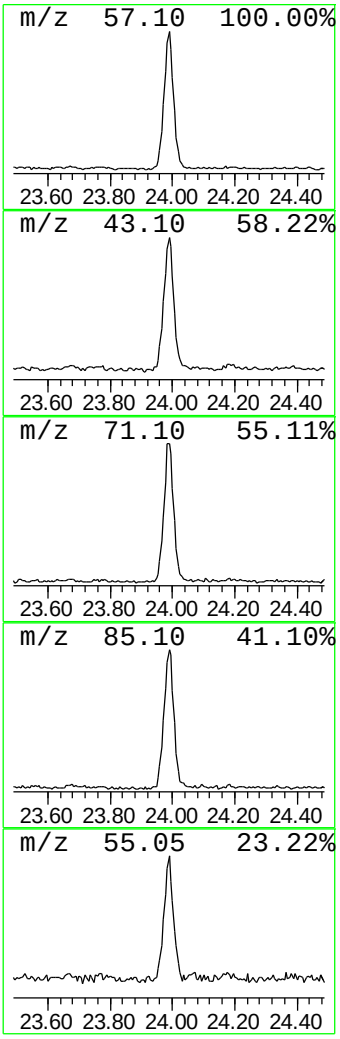
****

Peak Number 7 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	4.58 ng	461537	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Hentriacontane	437	C31H64	000630-04-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

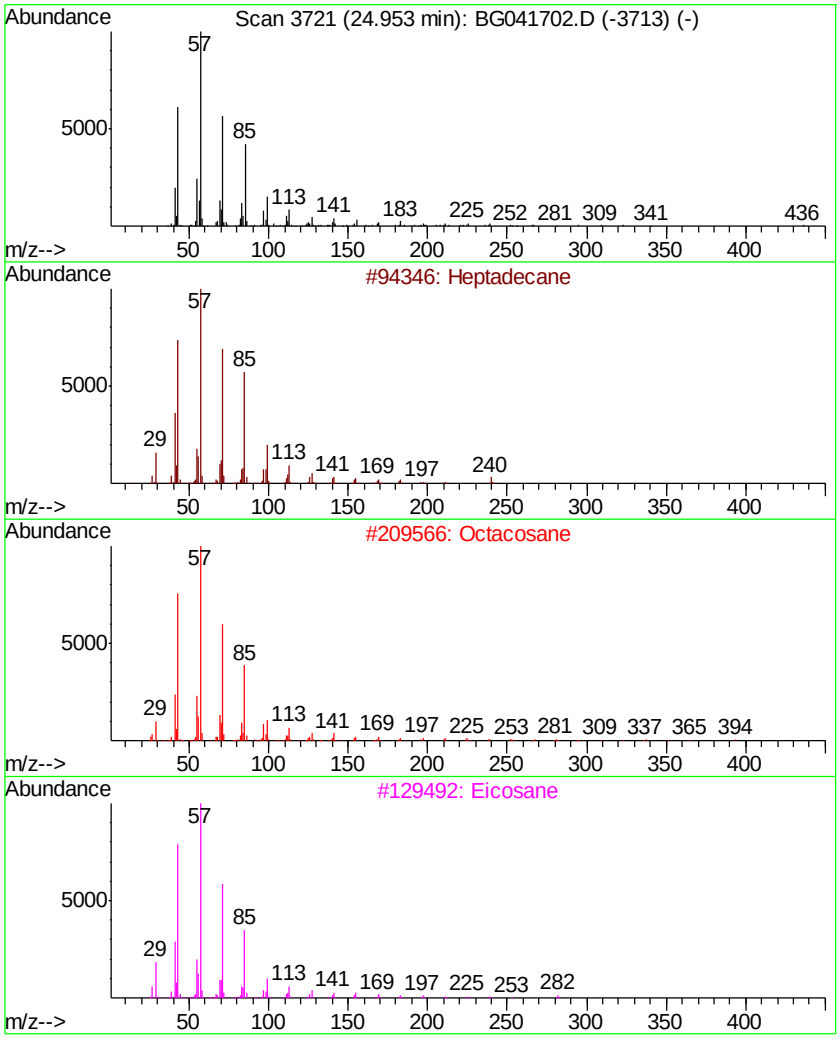
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

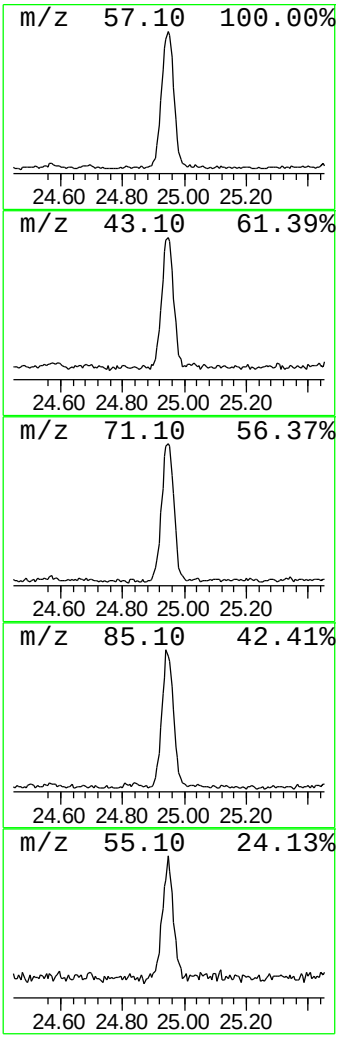
****

Peak Number 8 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.95	4.66 ng	469396	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Eicosane	282	C20H42	000112-95-8	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Nonadecane	268	C19H40	000629-92-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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

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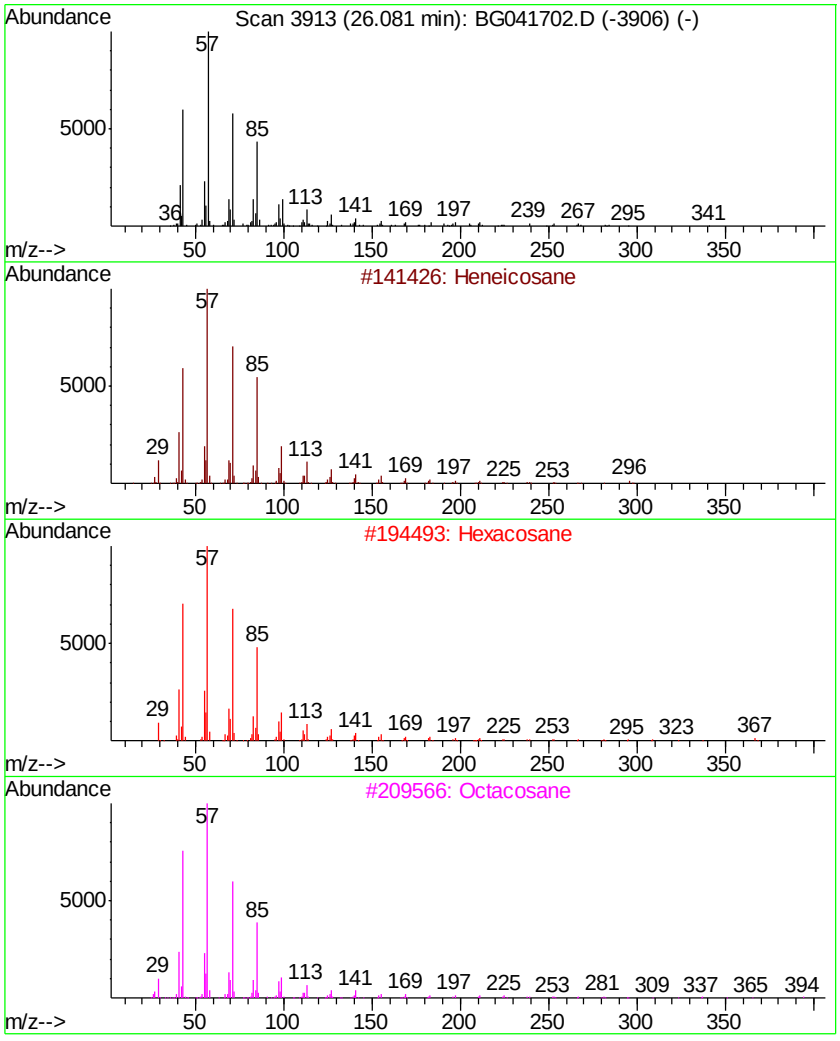
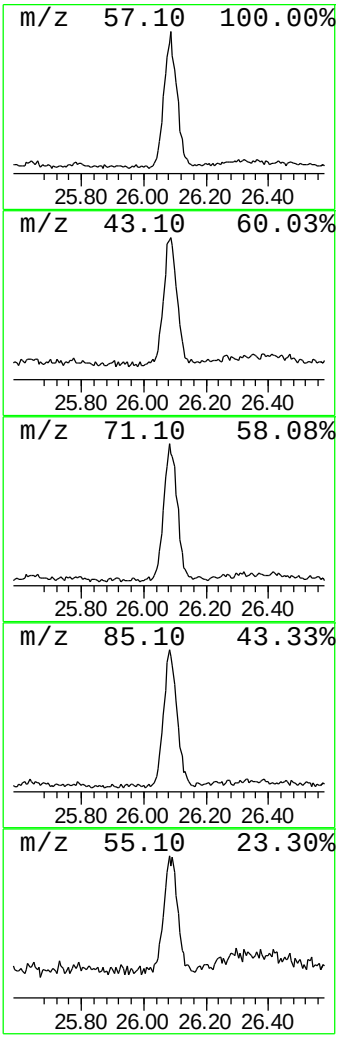
Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.08	3.97 ng	400043	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Eicosane	282	C20H42	000112-95-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071719\
Data File : BG041702.D
Acq On : 18 Jul 2019 00:12
Operator : HP/JU
Sample : K3835-24
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12(6-8)

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	23.6	ng	748039	1	8.05	633118	20.0
unknown7.58	7.58	104.2	ng	3297850	1	8.05	633118	20.0
Octacosyl trifluo...	21.32	7.0	ng	692186	5	21.65	1966380	20.0
Heneicosane	22.48	2.6	ng	253730	5	21.65	1966380	20.0
Octacosane	23.18	4.0	ng	392105	5	21.65	1966380	20.0
Octadecane, 2-met...	23.99	4.6	ng	461537	6	24.85	2013730	20.0
Heptadecane	24.95	4.7	ng	469396	6	24.85	2013730	20.0
Heptadecane, 9-oc...	26.08	4.0	ng	400043	6	24.85	2013730	20.0