LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041709.D
Acq On : 18 Jul 2019 14:35
Operator : HP/JU
Sample : K3835-44
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-6(8-10)

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	3.198	14	19	31	rVB	424290	784097	10.80%	1.907%
2	5.607	422	429	449	rBV	1882000	3077848	42.40%	7.484%
3	7.200	690	700	718	rBV	1995678	3466833	47.76%	8.430%
4	7.576	757	764	774	rBV	1917539	3293703	45.37%	8.009%
5	8.046	837	844	852	rBV	377432	633690	8.73%	1.541%
6	8.369	891	899	911	rBV	1423694	2508689	34.56%	6.100%
7	9.203	1032	1041	1051	rBV	1147788	2058735	28.36%	5.006%
8	10.854	1314	1322	1330	rBV	465454	858874	11.83%	2.088%
9	13.292	1729	1737	1749	rBV	2938862	4699376	64.74%	11.426%
10	14.109	1870	1876	1882	rBV	228828	335417	4.62%	0.816%
11	14.661	1959	1970	1978	rBV2	719885	1200529	16.54%	2.919%
12	16.142	2215	2222	2235	rBV	2545896	3920478	54.01%	9.533%
13	17.399	2428	2436	2446	rBV2	997788	1615299	22.25%	3.928%
14	20.002	2873	2879	2893	rBV	5349808	7259290	100.00%	17.651%
15	21.312	3097	3102	3112	rBV2	169687	468711	6.46%	1.140%
16	21.647	3152	3159	3166	rBV	1131864	1855203	25.56%	4.511%
17	21.865	3192	3196	3203	rBV	61243	100964	1.39%	0.245%
18	22.476	3296	3300	3310	rVB	84024	147224	2.03%	0.358%
19	23.175	3413	3419	3427	rVB	105682	204334	2.81%	0.497%
20	23.986	3550	3557	3564	rBV2	101221	213203	2.94%	0.518%
21	24.838	3691	3702	3712	rBV2	678803	1911744	26.34%	4.648%
22	24.938	3713	3719	3729	rVB2	90617	220312	3.03%	0.536%
23	26.077	3906	3913	3924	rVB4	56018	172750	2.38%	0.420%
24	27.441	4139	4145	4156	rVB3	35935	119957	1.65%	0.292%

Sum of corrected areas: 41127260

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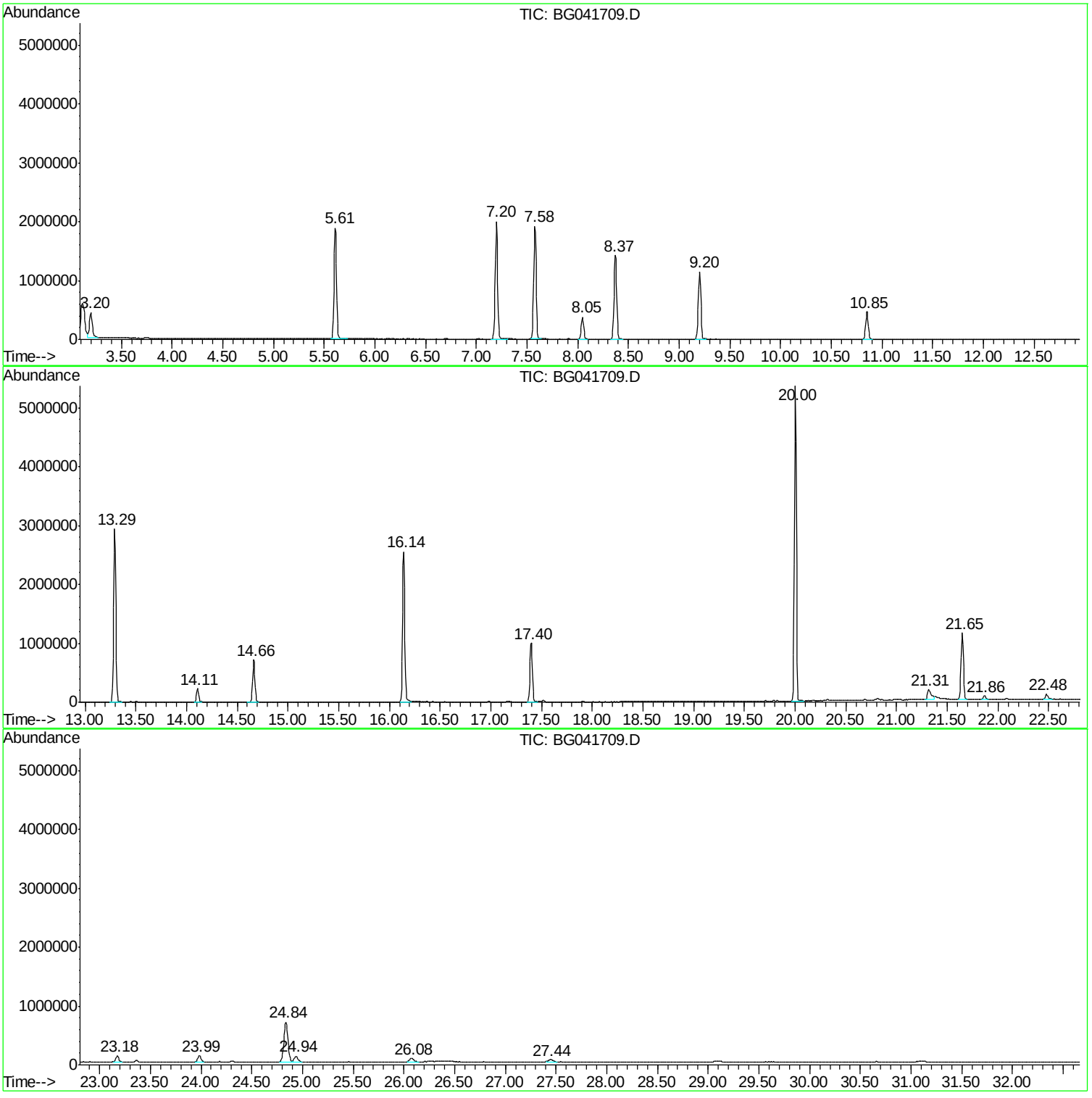
Instrument :
BNA_G
ClientSampleId :
SB-6(8-10)

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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Instrument : BNA_G
ClientSampleId : SB-6(8-10)

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

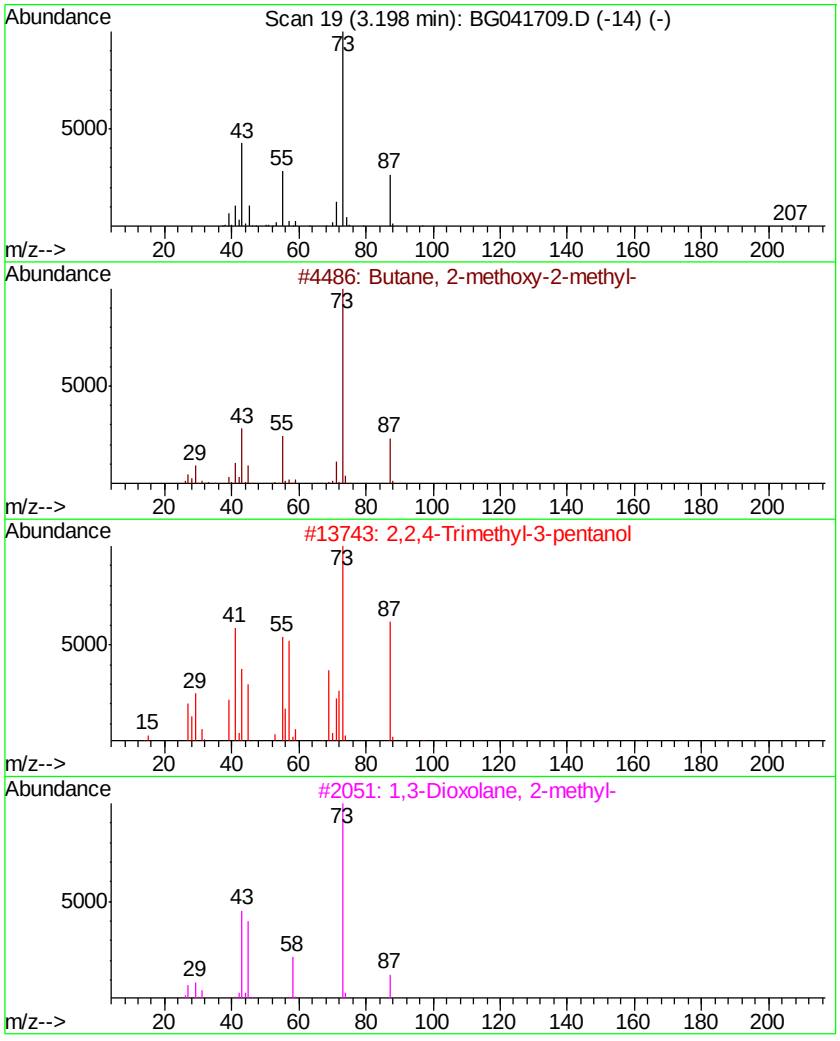
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

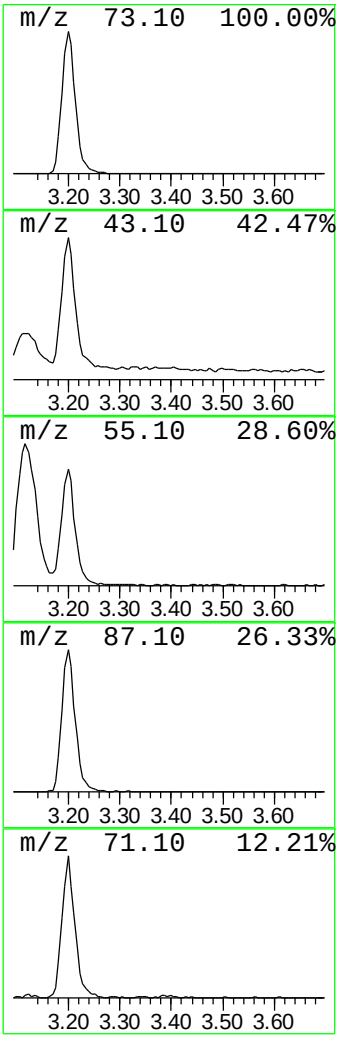
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	24.75 ng	784097	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Data File : BG041709.D
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Operator : HP/JU
Sample : K3835-44
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-6(8-10)

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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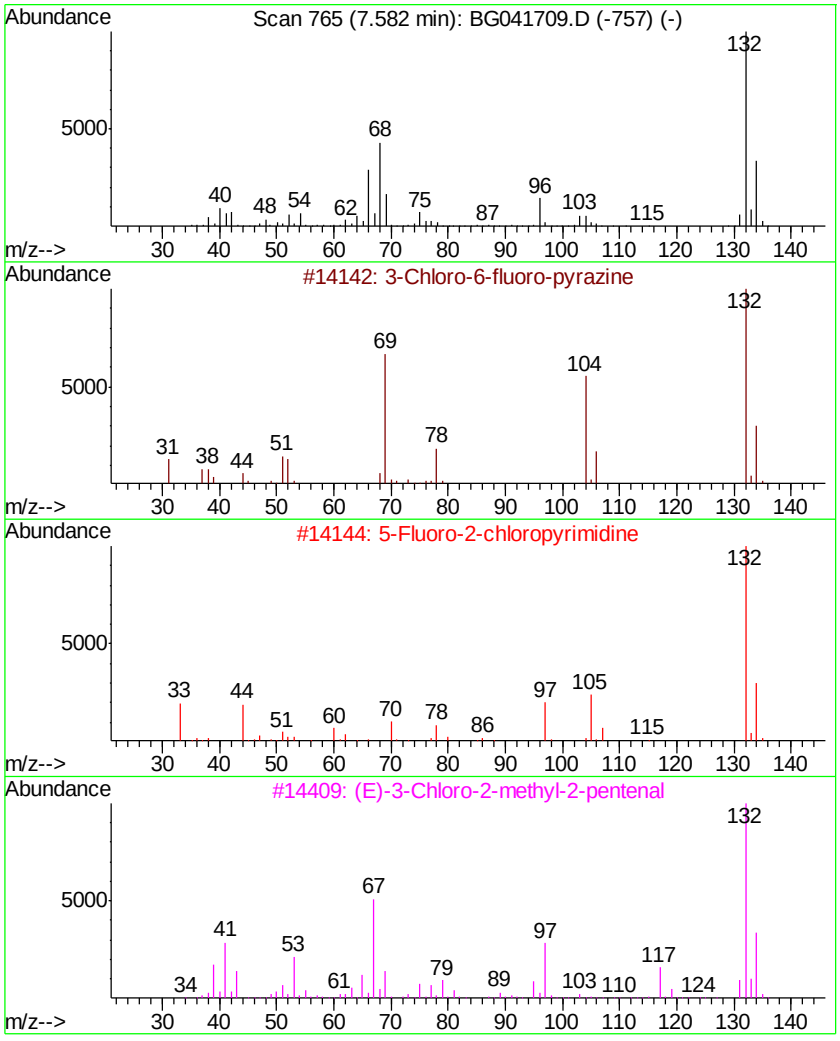
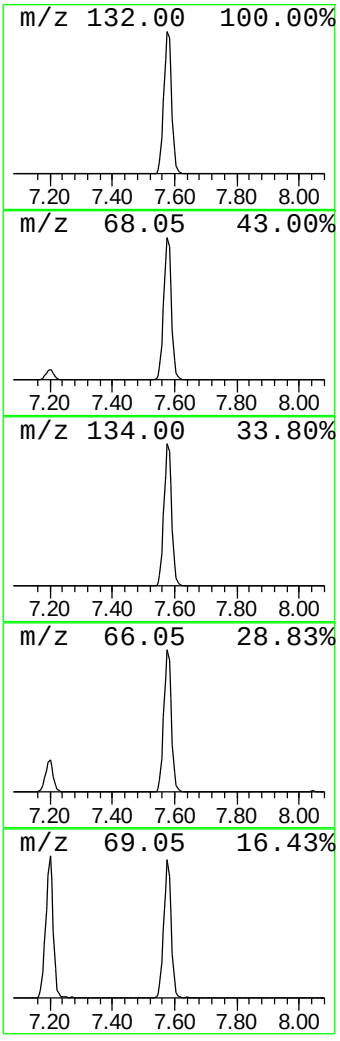
Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	103.95 ng	3293700	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Amphetaminil	250	C17H18N2	017590-01-1	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
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Acq On : 18 Jul 2019 14:35
Operator : HP/JU
Sample : K3835-44
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-6(8-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
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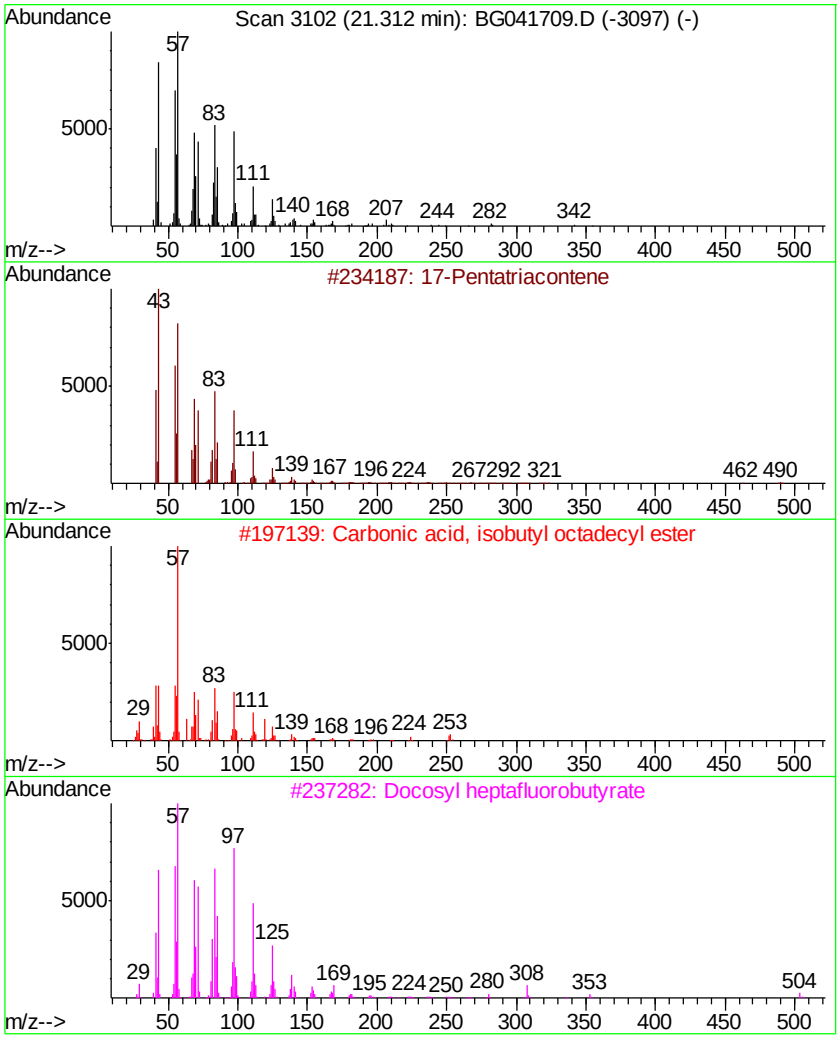
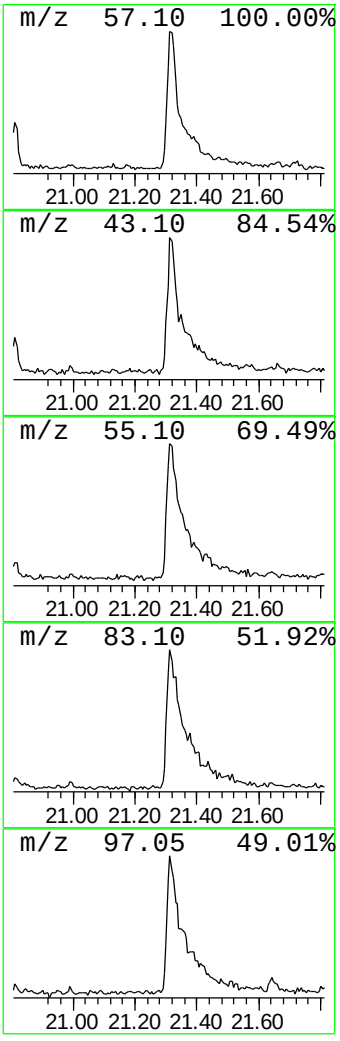
Peak Number 4 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	5.05 ng	468711	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
3	Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	86





Library Search Compound Report

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Data File : BG041709.D
Acq On : 18 Jul 2019 14:35
Operator : HP/JU
Sample : K3835-44
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-6(8-10)

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
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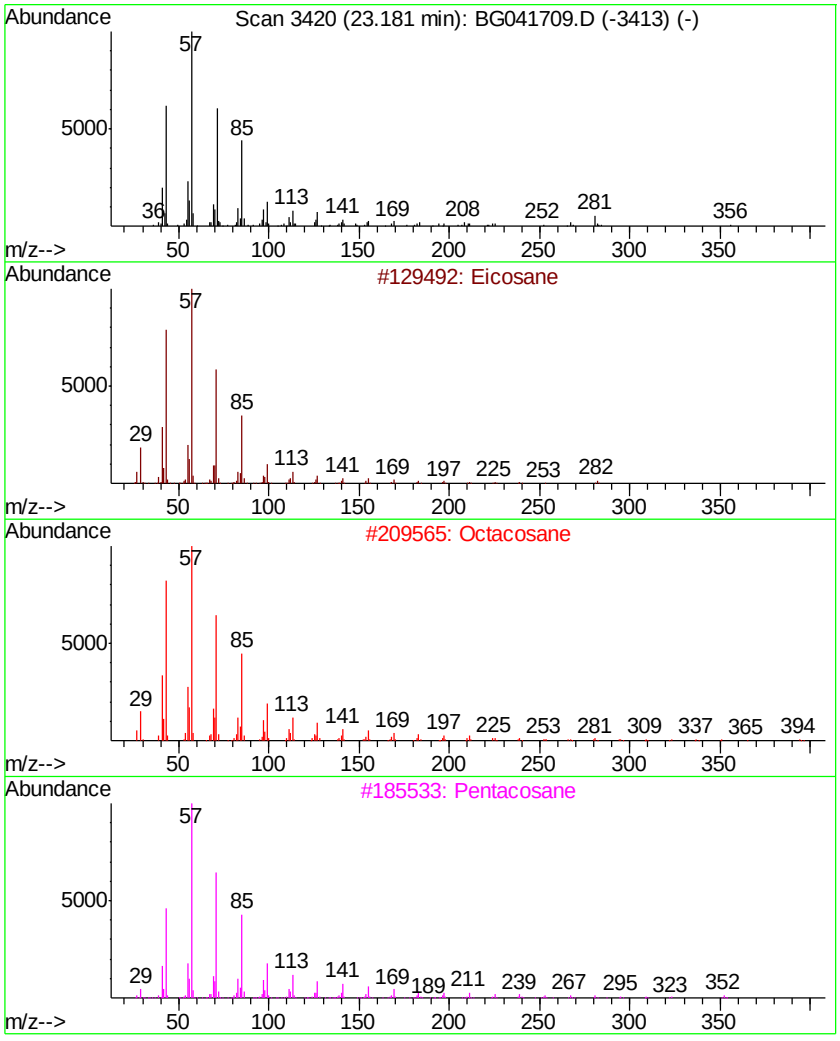
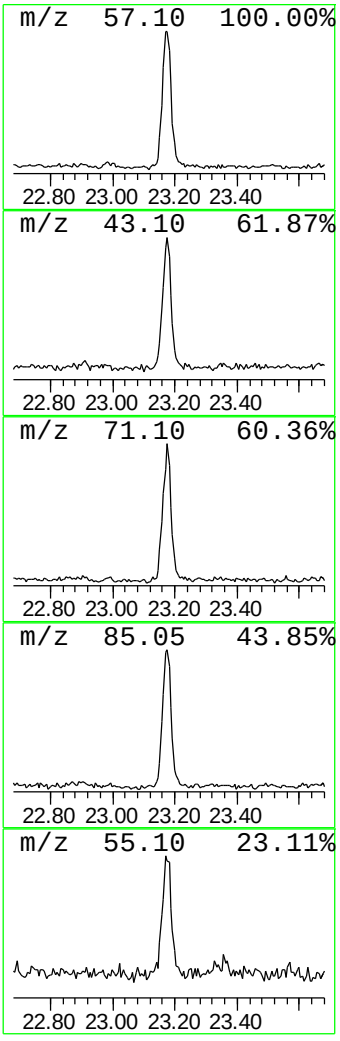
Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	2.20 ng	204334	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentacosane	352	C25H52	000629-99-2	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





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Sample : K3835-44
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-6(8-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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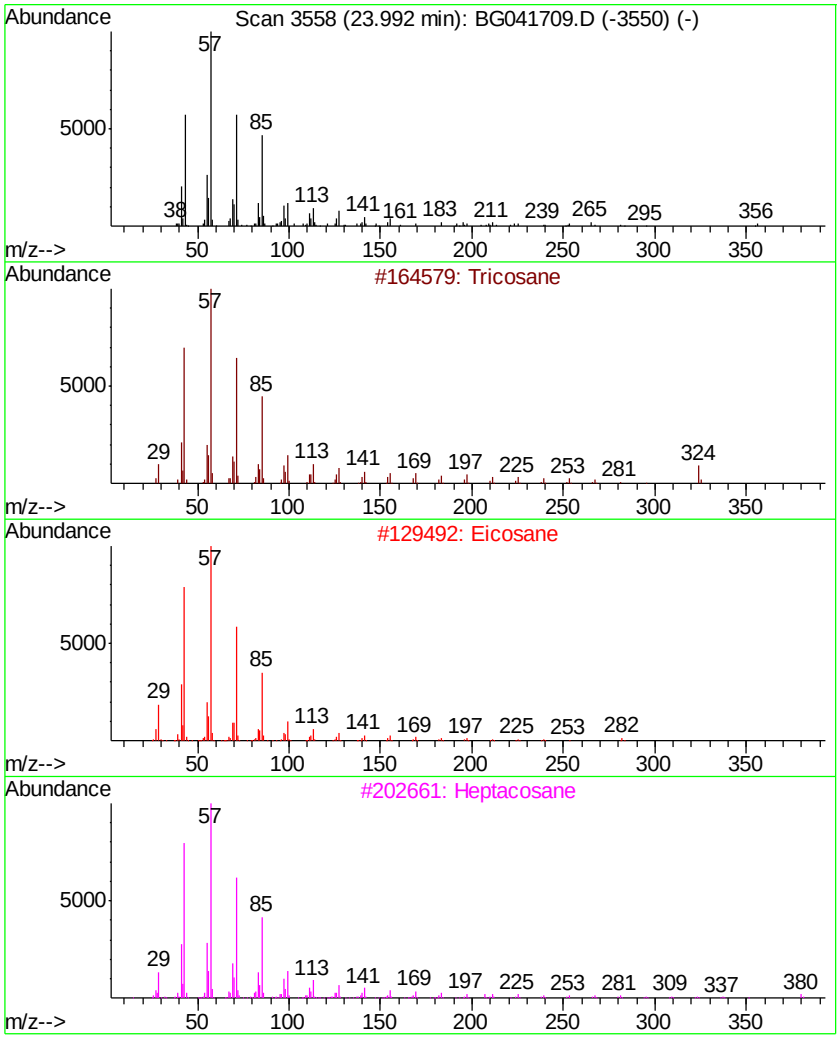
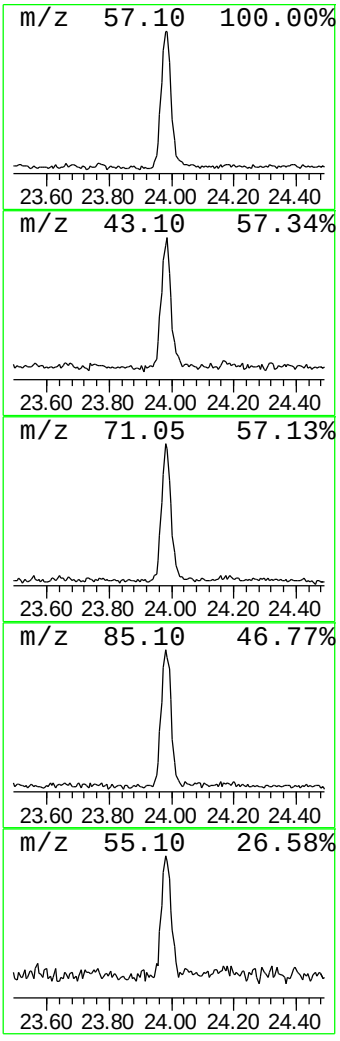
Peak Number 6 Tricosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.23 ng	213203	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	95
2	Eicosane	282	C20H42	000112-95-8	95
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Sample : K3835-44
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-6(8-10)

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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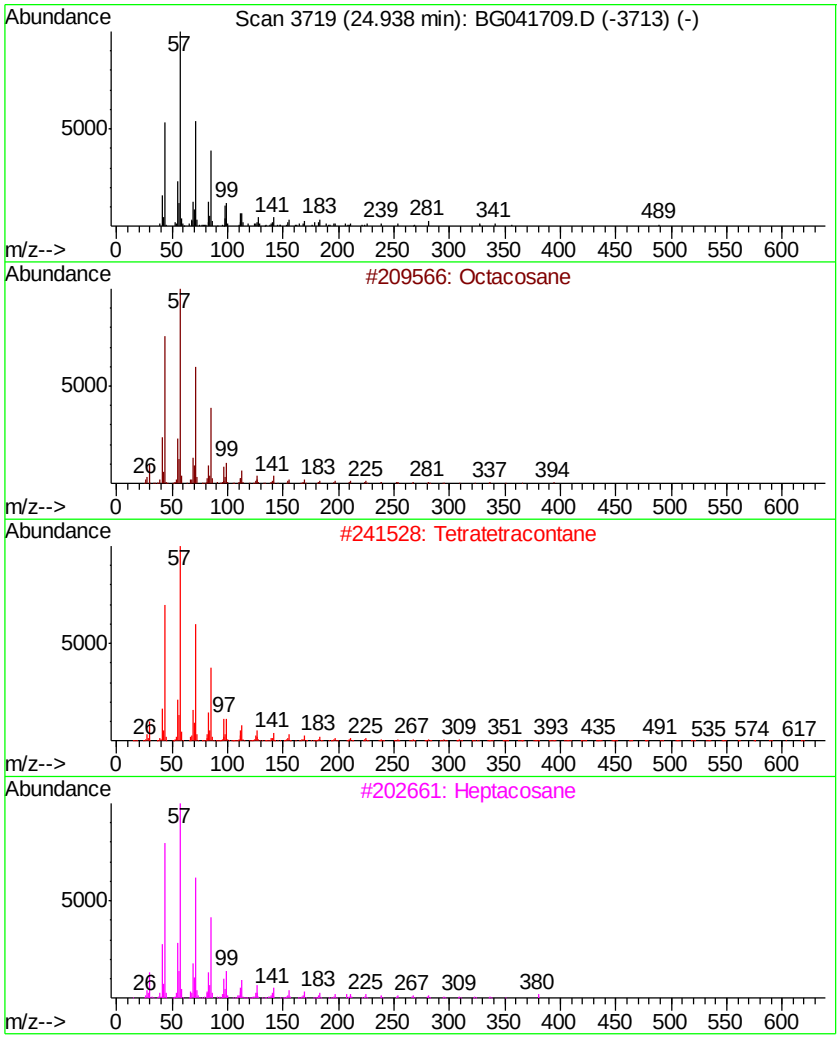
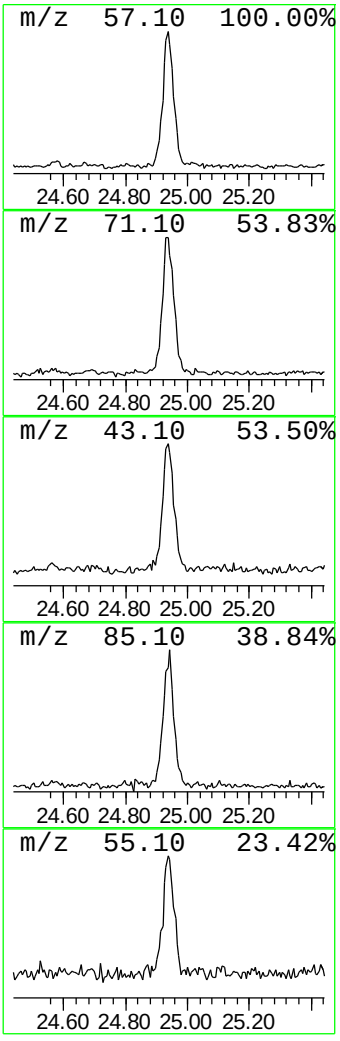
Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.94	2.30 ng	220312	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Eicosane	282	C20H42	000112-95-8	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...	3.20	24.8	ng	784097	1	8.05	633690	20.0
unknown7.58	7.58	104.0	ng	3293700	1	8.05	633690	20.0
17-Pentatriacontene	21.31	5.0	ng	468711	5	21.65	1855200	20.0
Eicosane	23.18	2.2	ng	204334	5	21.65	1855200	20.0
Tricosane	23.99	2.2	ng	213203	6	24.84	1911740	20.0
Octacosane	24.94	2.3	ng	220312	6	24.84	1911740	20.0