LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050719\
Data File : BG040775.D
Acq On : 7 May 2019 18:30
Operator : HP/JU
Sample : K2697-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-4-20190502

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-BG042319.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	3.153	5	11	19	rBV	287517	518972	8.70%	2.037%
2	3.229	19	24	42	rVB	808187	1144783	19.18%	4.493%
3	5.674	433	440	448	rBV	557910	884398	14.82%	3.471%
4	7.278	706	713	722	rBV	423798	704185	11.80%	2.764%
5	7.665	769	779	791	rBV	1003420	1719528	28.81%	6.748%
6	8.141	853	860	872	rBV	172656	309664	5.19%	1.215%
7	8.464	908	915	923	rBV	772483	1348637	22.60%	5.293%
8	9.322	1053	1061	1071	rBV	799284	1448450	24.27%	5.684%
9	10.967	1333	1341	1349	rBV	226707	412147	6.91%	1.617%
10	13.400	1744	1755	1762	rBV	2054203	3260398	54.63%	12.795%
11	14.775	1982	1989	1998	rBV2	394405	639587	10.72%	2.510%
12	16.255	2234	2241	2258	rBV	1688142	2614581	43.81%	10.261%
13	17.513	2448	2455	2462	rBV	595967	907320	15.20%	3.561%
14	20.110	2891	2897	2909	rBV	4518257	5967952	100.00%	23.421%
15	21.796	3178	3184	3197	rBV	577990	1005319	16.85%	3.945%
16	21.955	3206	3211	3216	rVB	68518	88302	1.48%	0.347%
17	22.583	3312	3318	3326	rVB	120229	181579	3.04%	0.713%
18	23.300	3434	3440	3447	rVB2	163662	303475	5.09%	1.191%
19	24.134	3575	3582	3591	rVB3	163633	362732	6.08%	1.424%
20	25.139	3743	3753	3774	rBV4	304064	1168871	19.59%	4.587%
21	26.308	3943	3952	3962	rVB2	100373	309087	5.18%	1.213%
22	27.724	4183	4193	4207	rBV5	49175	181207	3.04%	0.711%

Sum of corrected areas: 25481174

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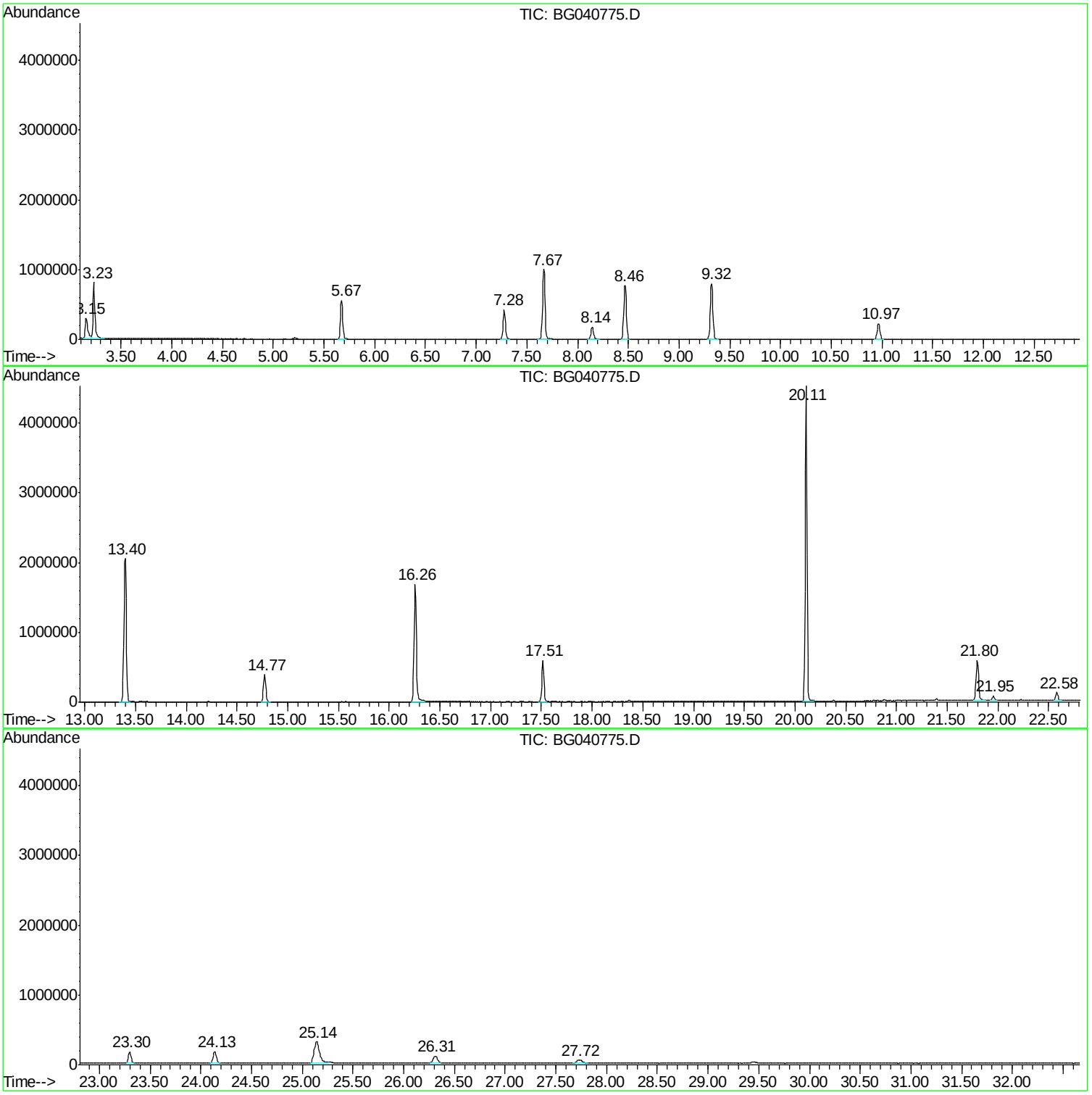
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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 : BG040775.D
Acq On : 7 May 2019 18:30
Operator : HP/JU
Sample : K2697-04
Misc :
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Instrument : BNA_G
ClientSampleId : MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

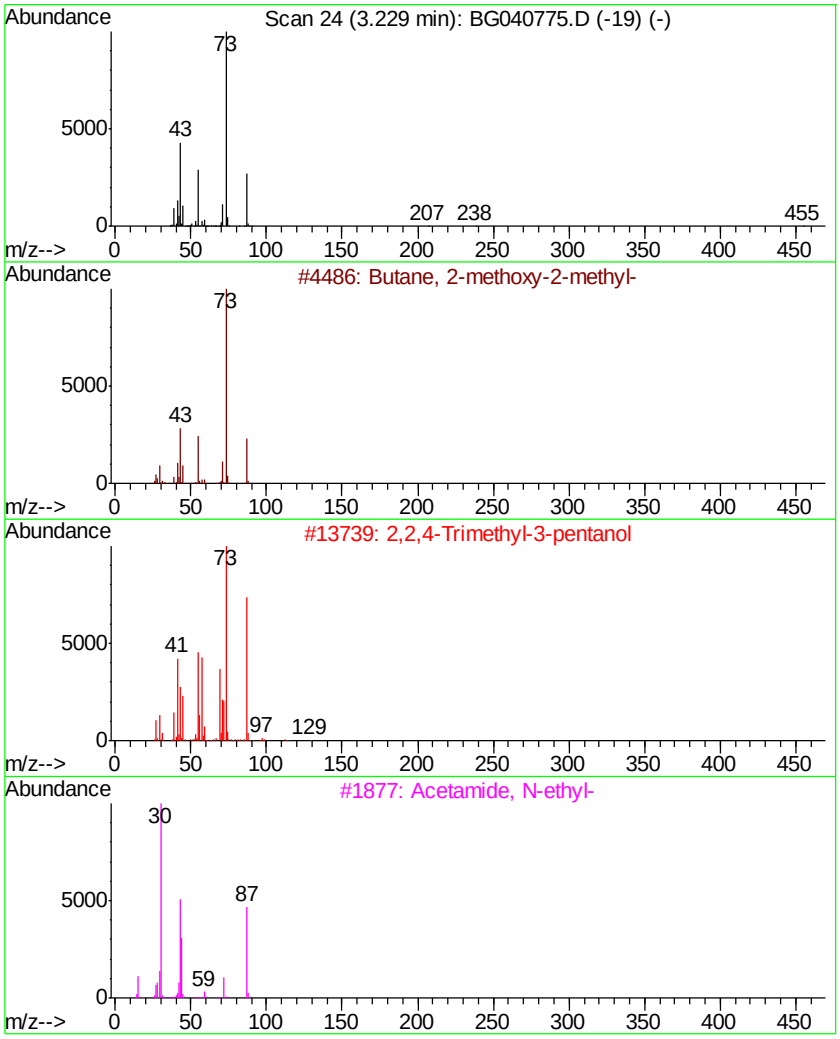
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

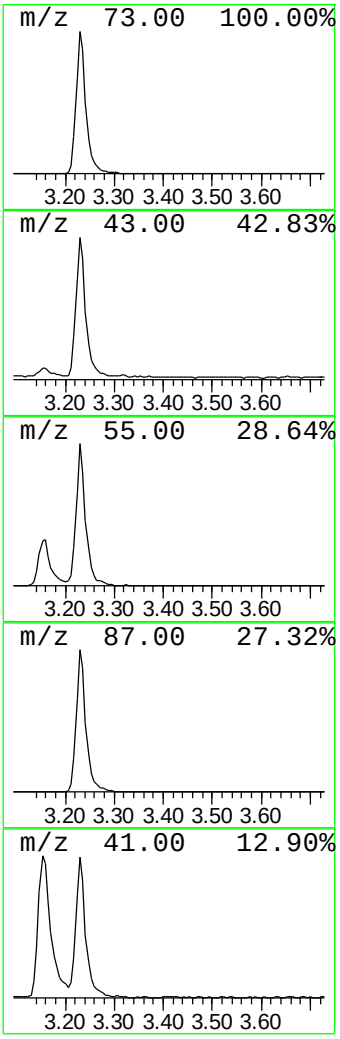
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	73.94 ng	1144780	1,4-Dichlorobenzene-d4	8.15

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	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050719\
Data File : BG040775.D
Acq On : 7 May 2019 18:30
Operator : HP/JU
Sample : K2697-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

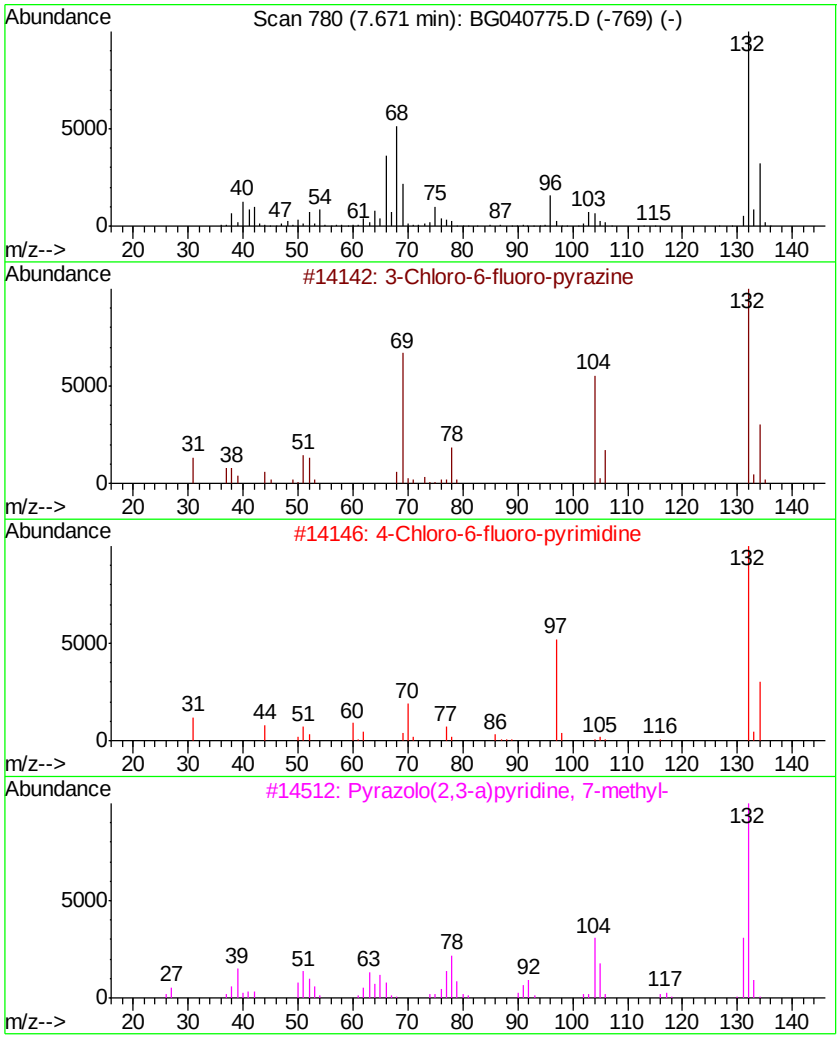
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

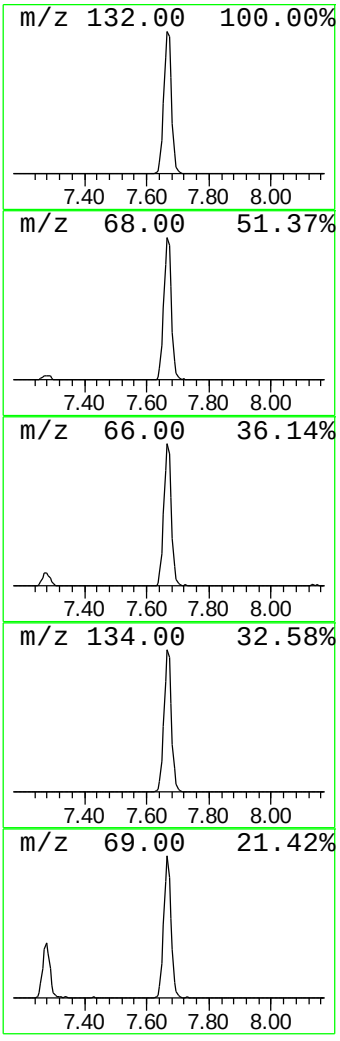
****

Peak Number 3 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	111.06 ng	1719530	1,4-Dichlorobenzene-d4	8.15

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





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050719\
Data File : BG040775.D
Acq On : 7 May 2019 18:30
Operator : HP/JU
Sample : K2697-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

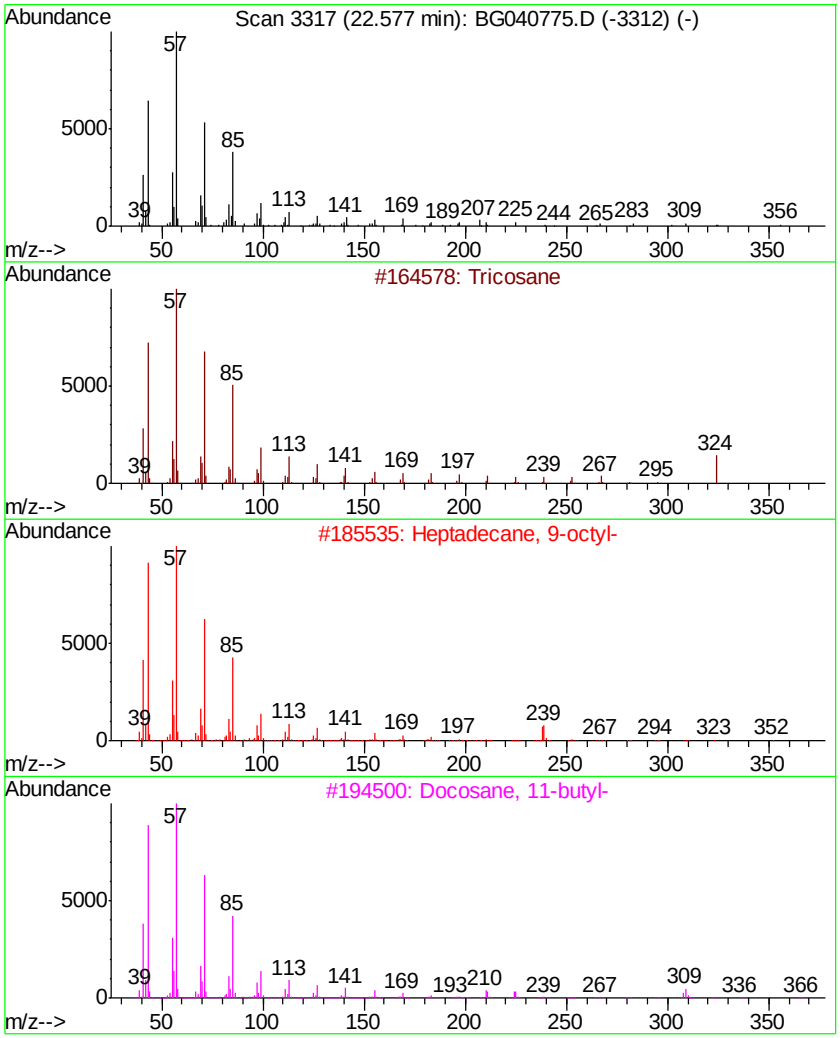
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

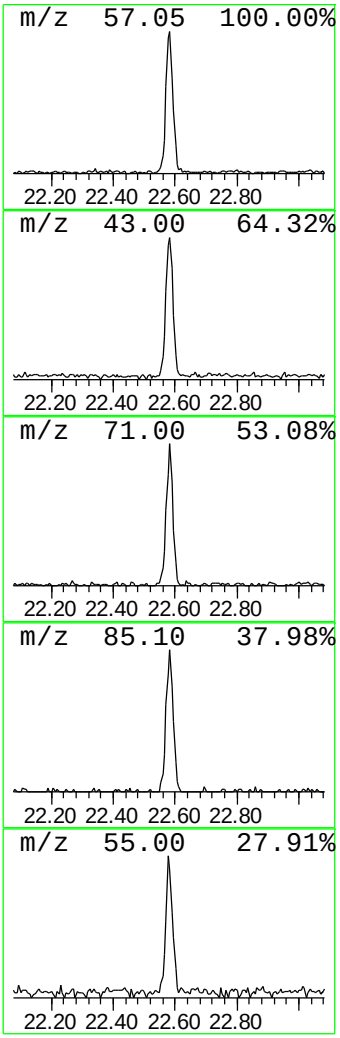
****

Peak Number 5 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	3.61 ng	181579	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Docosane	310	C22H46	000629-97-0	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050719\
Data File : BG040775.D
Acq On : 7 May 2019 18:30
Operator : HP/JU
Sample : K2697-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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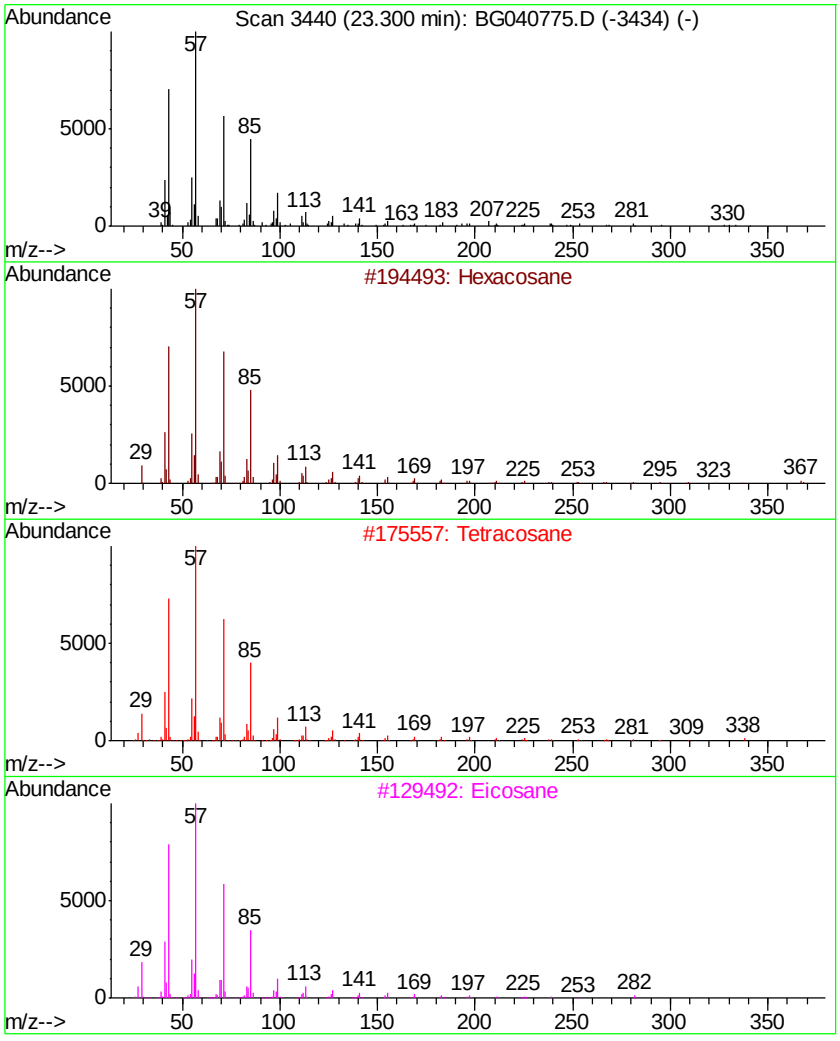
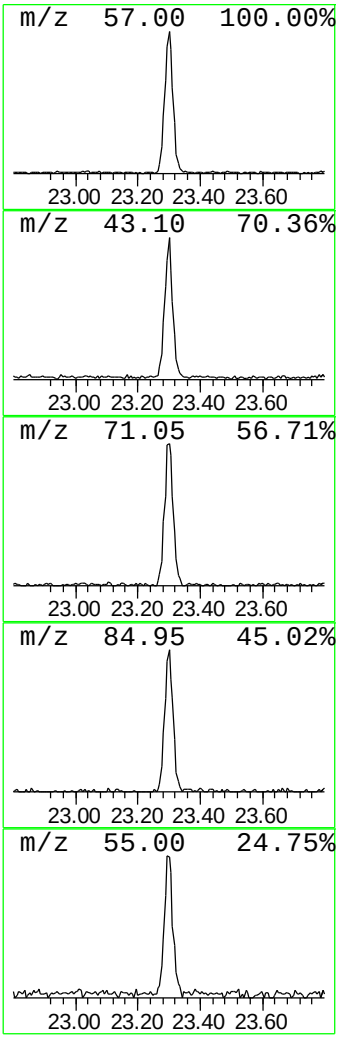
Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	6.04 ng	303475	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	87
5	1-Iodoundecane	282	C11H23I	004282-44-4	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050719\
Data File : BG040775.D
Acq On : 7 May 2019 18:30
Operator : HP/JU
Sample : K2697-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

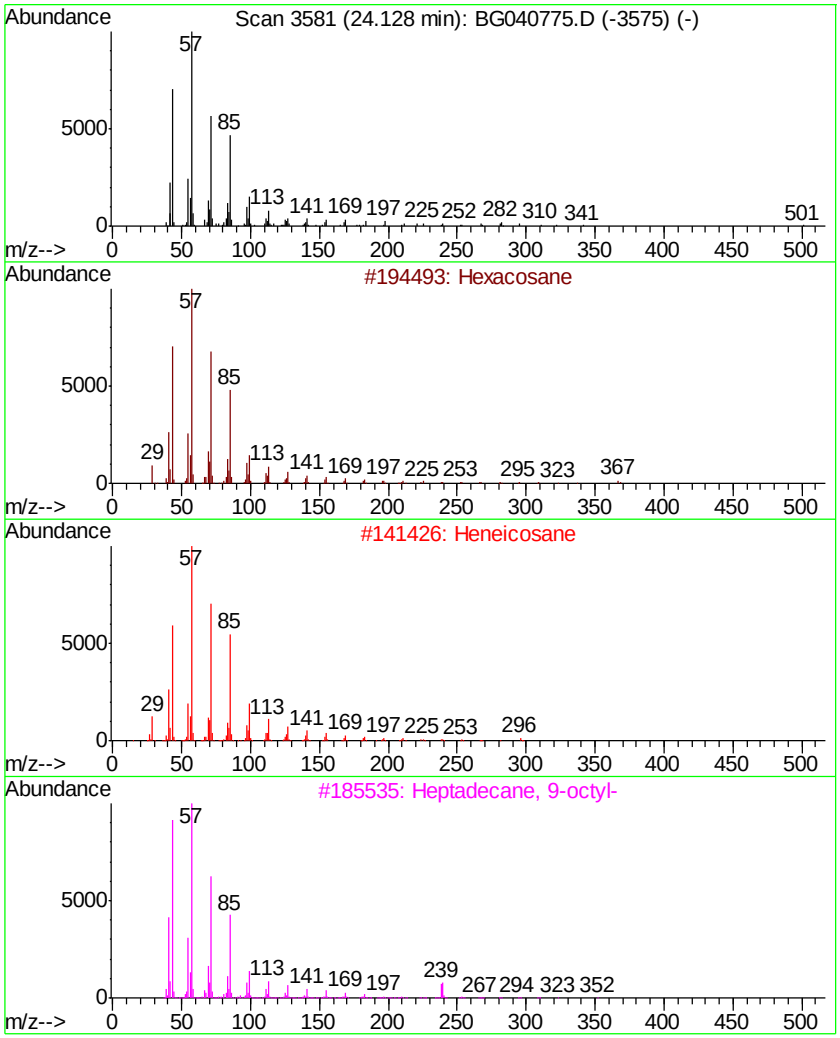
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

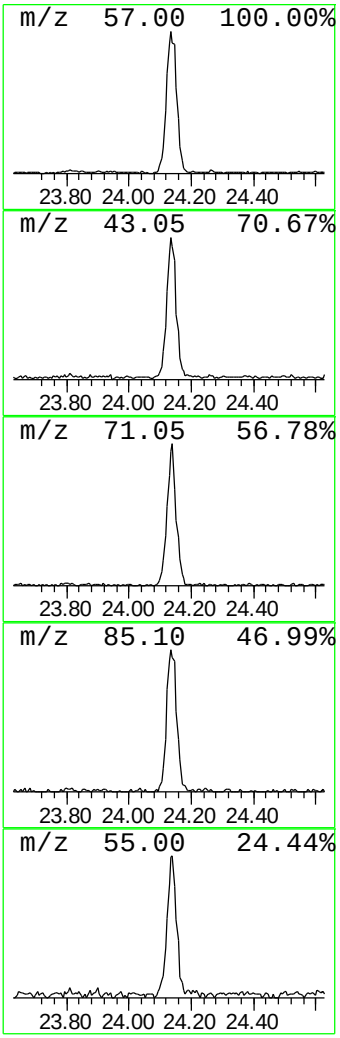
****

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	6.21 ng	362732	Perylene-d12	25.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Tetracosane	338	C24H50	000646-31-1	90





Library Search Compound Report

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Operator : HP/JU
Sample : K2697-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

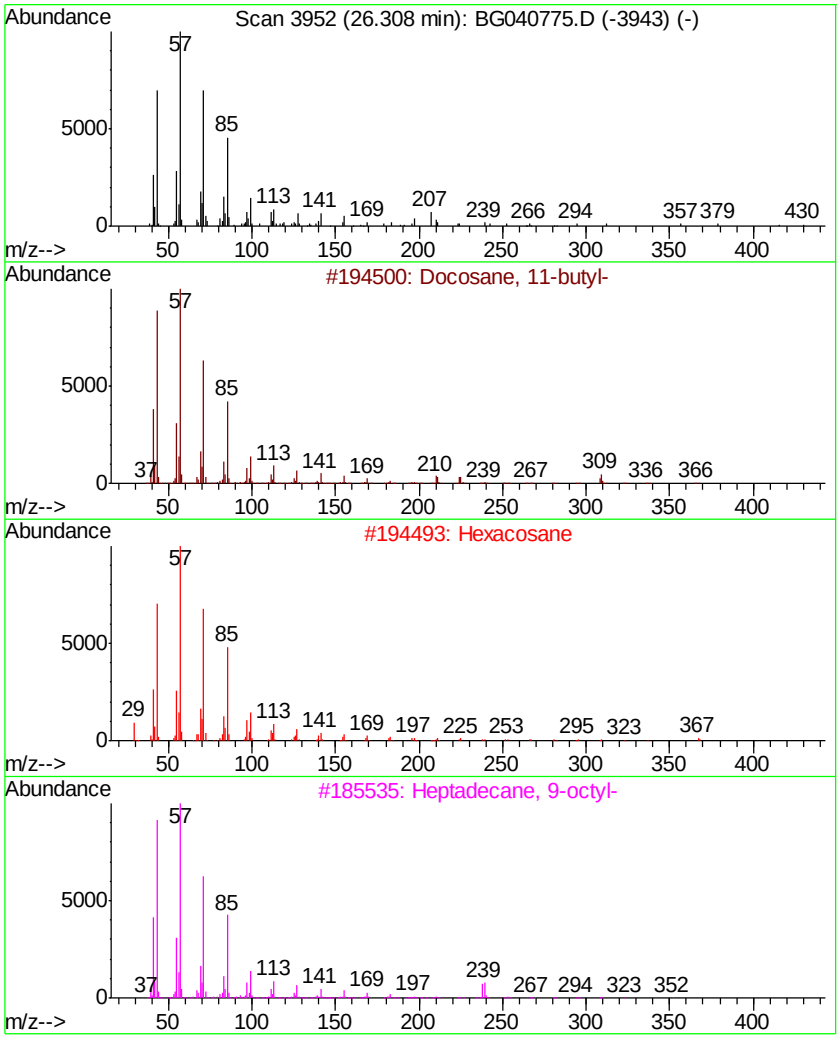
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

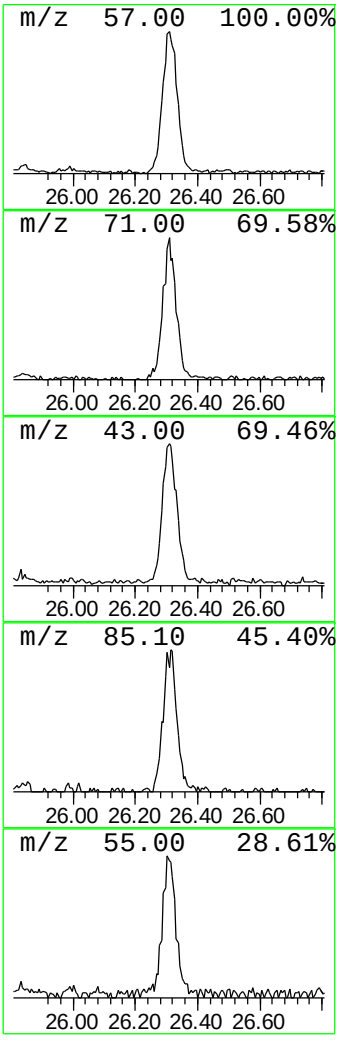
****

Peak Number 8 Docosane, 11-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.31	5.29 ng	309087	Perylene-d12	25.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86





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Instrument : BNA_G
ClientSampleId : MW-4-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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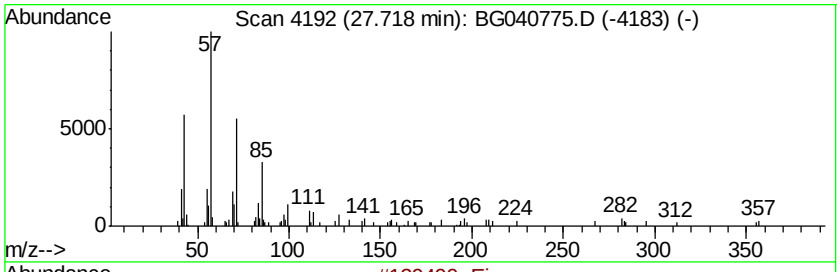
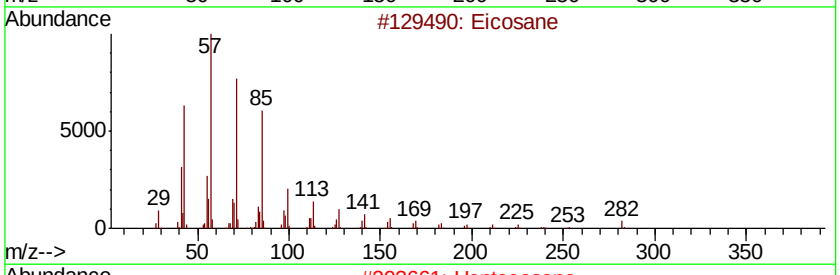
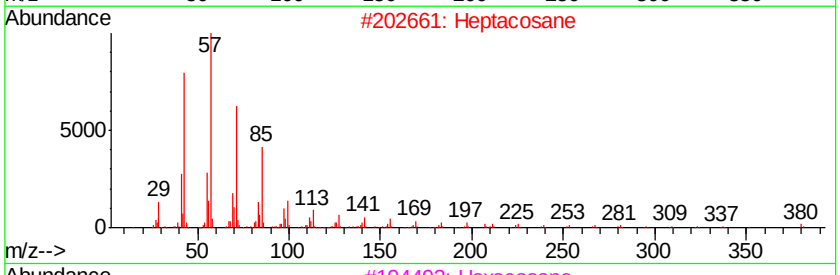
Peak Number 9 Eicosane Concentration Rank 9

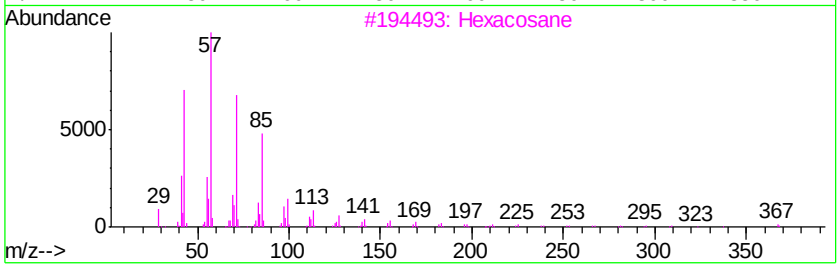
R.T.	EstConc	Area	Relative to ISTD	R.T.
27.72	3.10 ng	181207	Perylene-d12	25.14

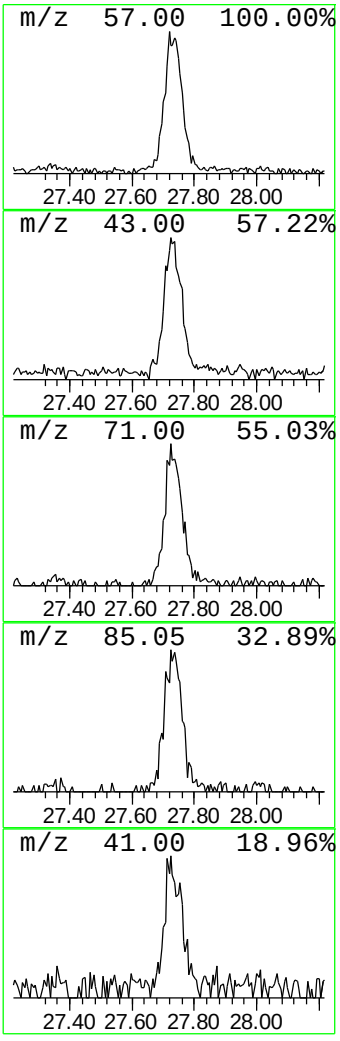
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heptacosane	380	C27H56	000593-49-7	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	87
5	Tetracosane	338	C24H50	000646-31-1	87











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...	3.23	73.9	ng	1144780	1	8.15	309664	20.0
unknown7.67	7.67	111.1	ng	1719530	1	8.15	309664	20.0
Tricosane	22.58	3.6	ng	181579	5	21.80	1005320	20.0
Hexacosane	23.30	6.0	ng	303475	5	21.80	1005320	20.0
Heneicosane	24.13	6.2	ng	362732	6	25.14	1168870	20.0
Docosane, 11-butyl-	26.31	5.3	ng	309087	6	25.14	1168870	20.0
Eicosane	27.72	3.1	ng	181207	6	25.14	1168870	20.0