LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG030519\
Data File : BG039776.D
Acq On : 5 Mar 2019 22:44
Operator : JU/SJ
Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

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-BG030419.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	3.211	15	21	29	rBV	172092	318972	8.77%	1.826%
2	3.282	29	33	41	rVB	121300	166804	4.58%	0.955%
3	5.696	438	444	454	rBV	347123	557776	15.33%	3.193%
4	7.300	709	717	727	rBV	238925	456918	12.56%	2.615%
5	7.682	775	782	799	rBV	651953	1136229	31.23%	6.504%
6	8.157	856	863	874	rBV	146009	258896	7.11%	1.482%
7	8.480	910	918	927	rBV	530403	891406	24.50%	5.102%
8	9.332	1054	1063	1072	rBV	514178	928622	25.52%	5.315%
9	10.977	1336	1343	1351	rBV	216819	387508	10.65%	2.218%
10	13.403	1746	1756	1764	rBV	1416353	2229203	61.26%	12.759%
11	14.220	1889	1895	1902	rBV	72158	107619	2.96%	0.616%
12	14.784	1984	1991	1998	rVB2	363134	603887	16.60%	3.457%
13	16.270	2236	2244	2257	rBV	1250065	1955499	53.74%	11.193%
14	17.527	2451	2458	2468	rBV	544524	810312	22.27%	4.638%
15	18.373	2597	2602	2607	rBV3	71338	106858	2.94%	0.612%
16	20.118	2893	2899	2905	rBV	2726704	3638762	100.00%	20.828%
17	21.404	3113	3118	3128	rBV2	89206	169091	4.65%	0.968%
18	21.815	3180	3188	3196	rBV	523695	892575	24.53%	5.109%
19	21.962	3208	3213	3218	rBV	48372	68085	1.87%	0.390%
20	22.585	3314	3319	3326	rVB	77161	120726	3.32%	0.691%
21	23.302	3434	3441	3450	rBV	92835	186986	5.14%	1.070%
22	24.142	3577	3584	3594	rVB	99370	199881	5.49%	1.144%
23	25.187	3744	3762	3773	rVB3	279080	1036967	28.50%	5.935%
24	26.309	3944	3953	3965	rVB4	51860	159309	4.38%	0.912%
25	27.737	4187	4196	4207	rVB6	25182	82053	2.25%	0.470%

Sum of corrected areas: 17470944

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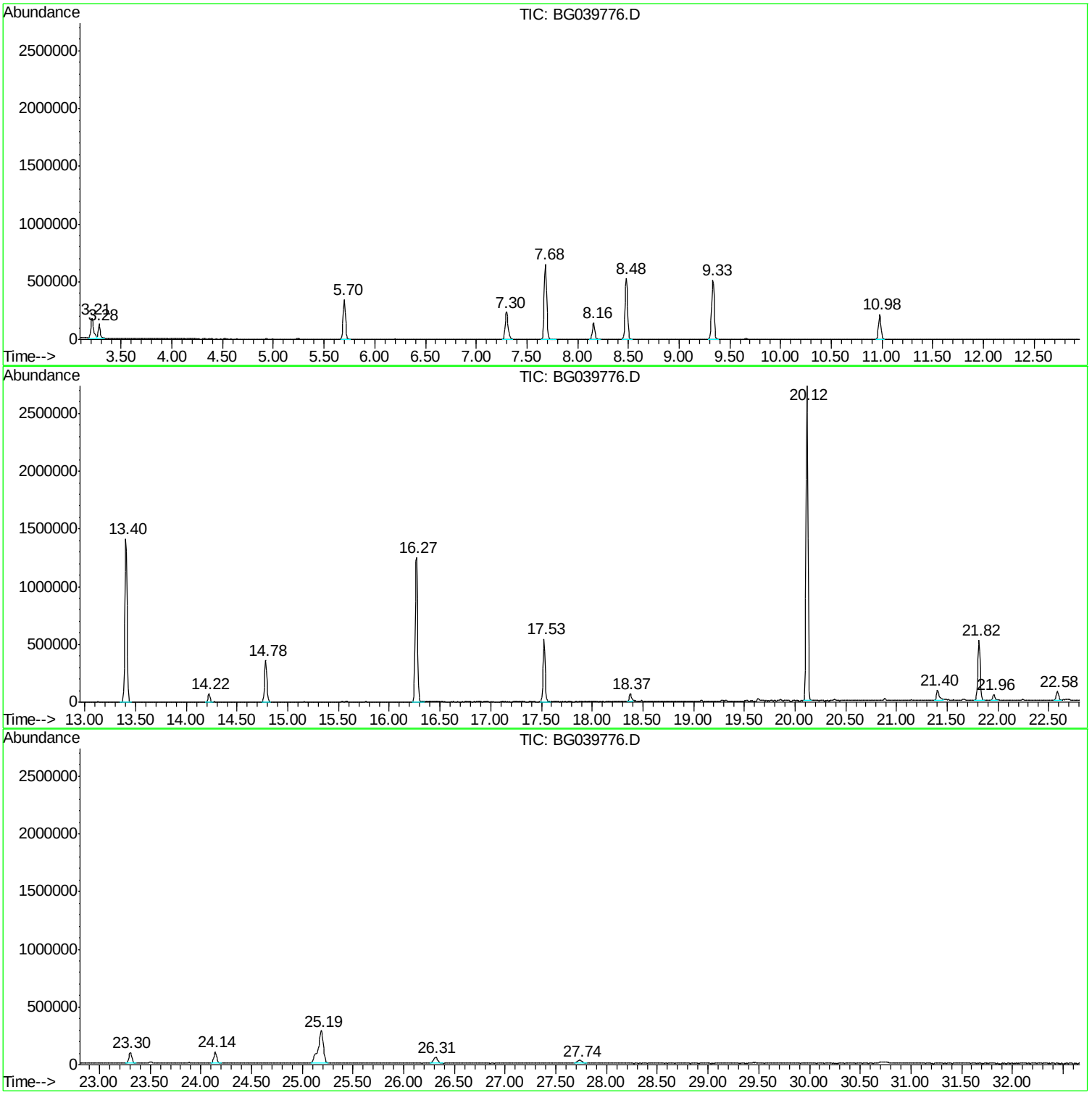
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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 : BG039776.D
Acq On : 5 Mar 2019 22:44
Operator : JU/SJ
Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

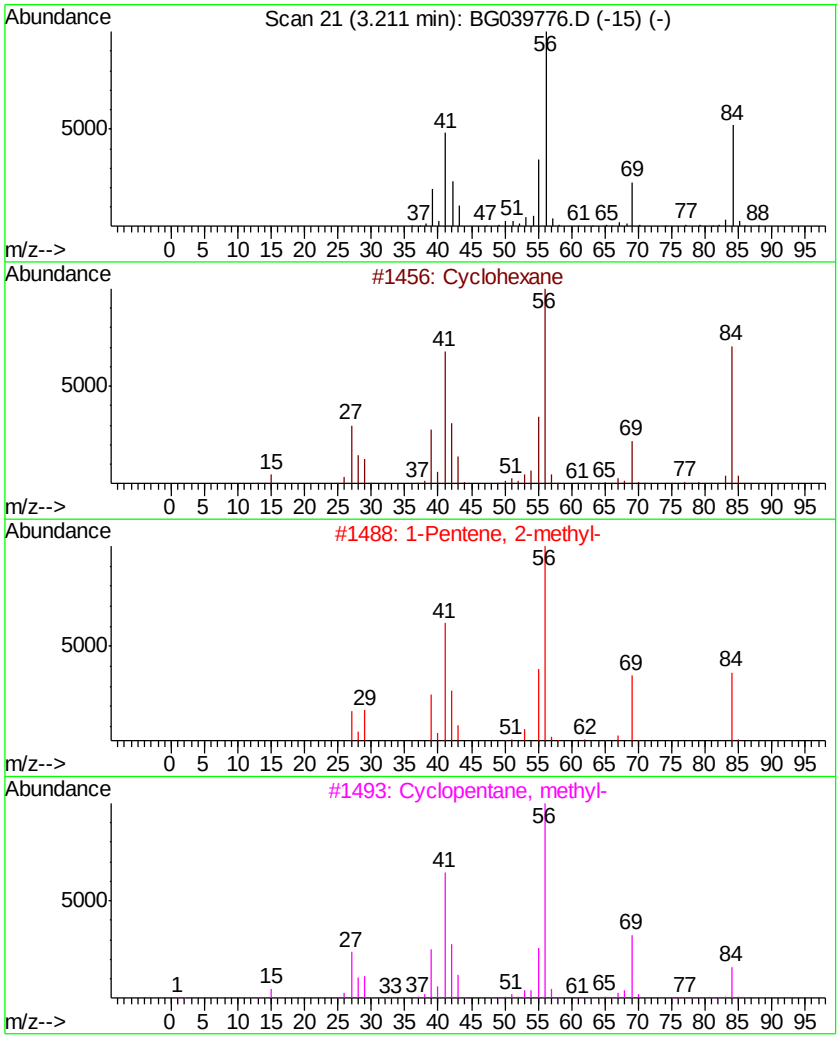
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

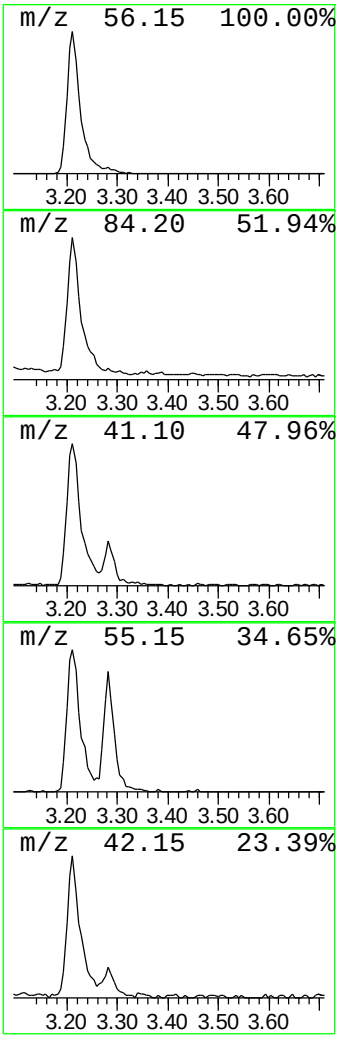
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	24.64 ng	318972	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	59
4	2,2-Dimethylglutaric anhydride	142	C7H10O3	002938-48-9	50
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	47





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Data File : BG039776.D
Acq On : 5 Mar 2019 22:44
Operator : JU/SJ
Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

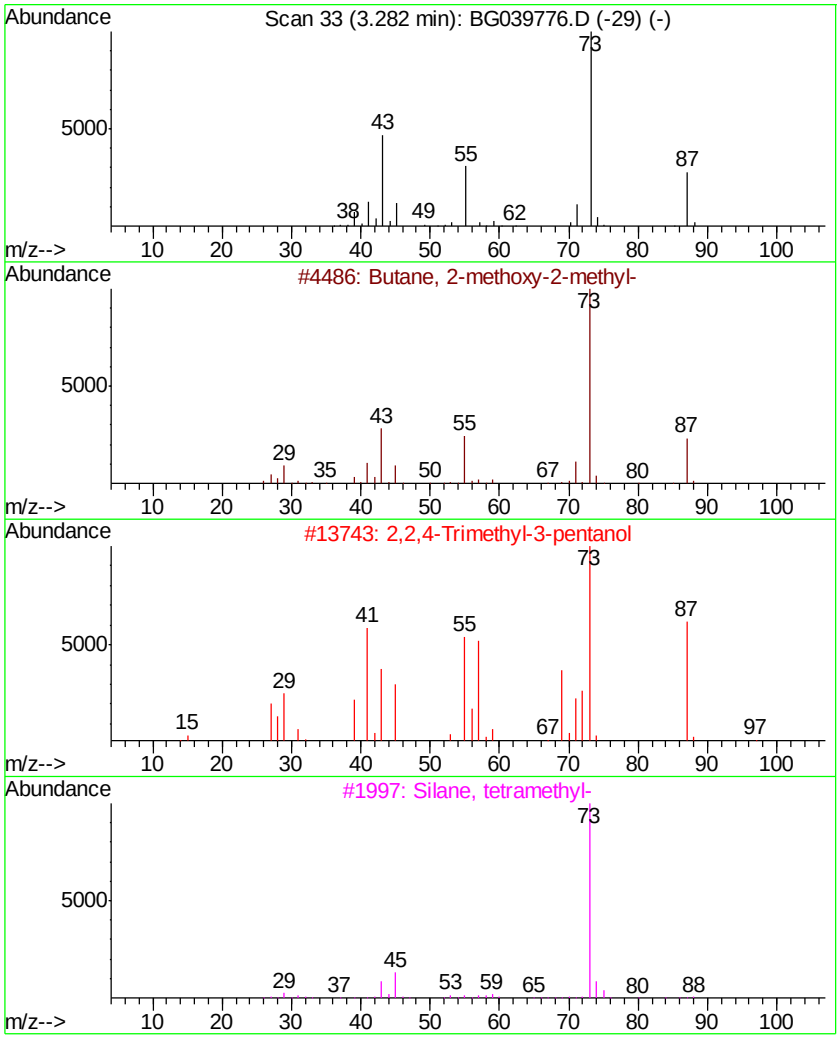
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

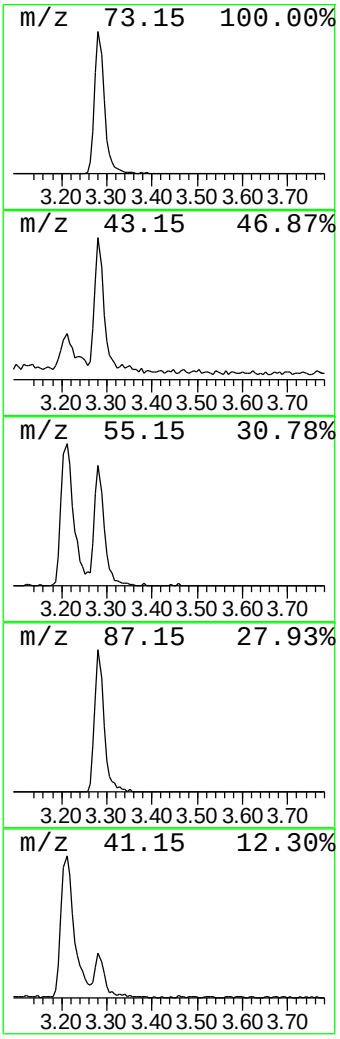
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	12.89 ng	166804	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG030519\
Data File : BG039776.D
Acq On : 5 Mar 2019 22:44
Operator : JU/SJ
Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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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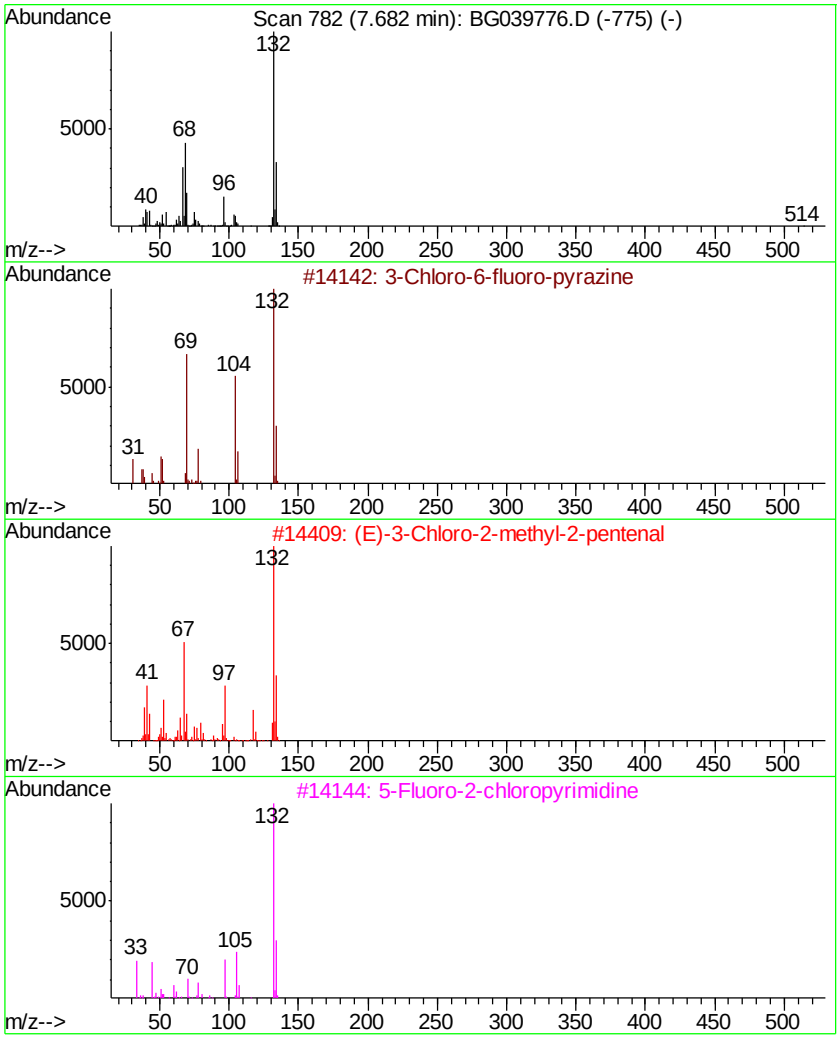
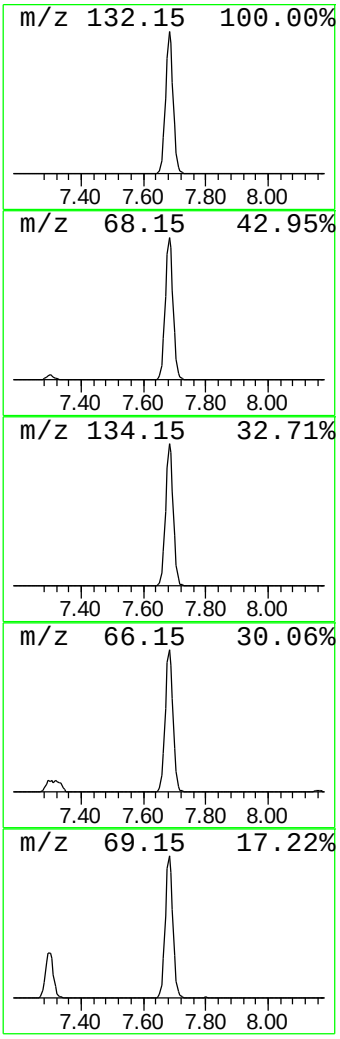
Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	87.77 ng	1136230	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	(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	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





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Operator : JU/SJ
Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

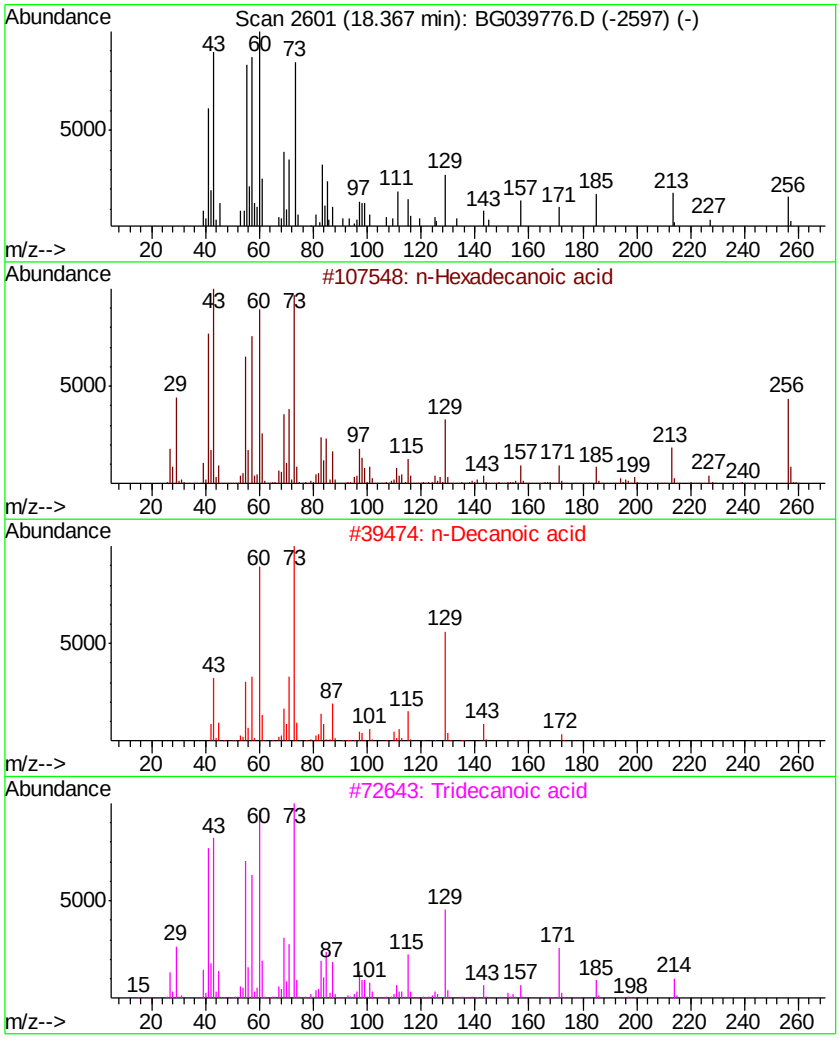
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

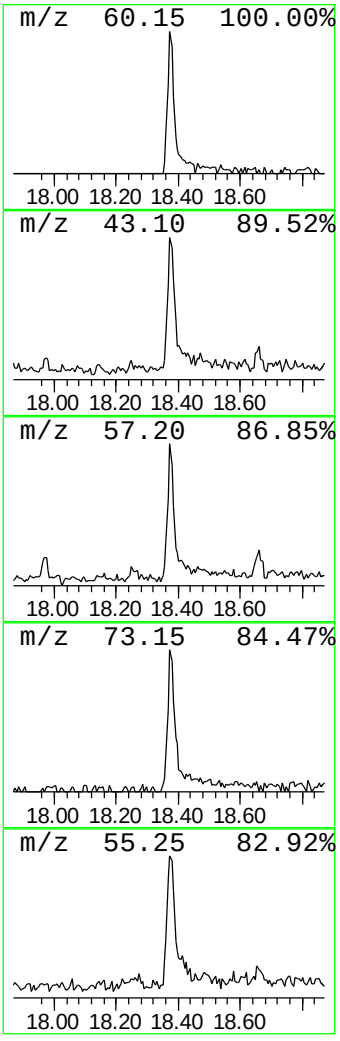
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	2.64 ng	106858	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	n-Decanoic acid	172	C10H20O2	000334-48-5	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG030519\
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Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

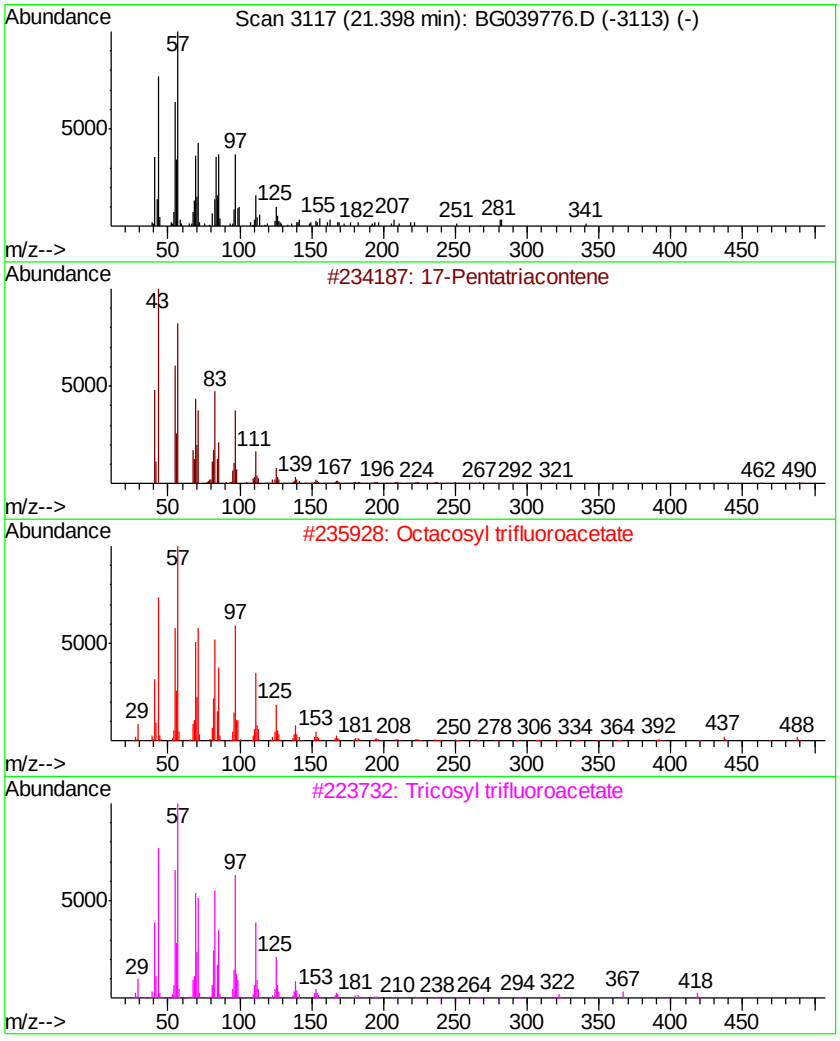
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

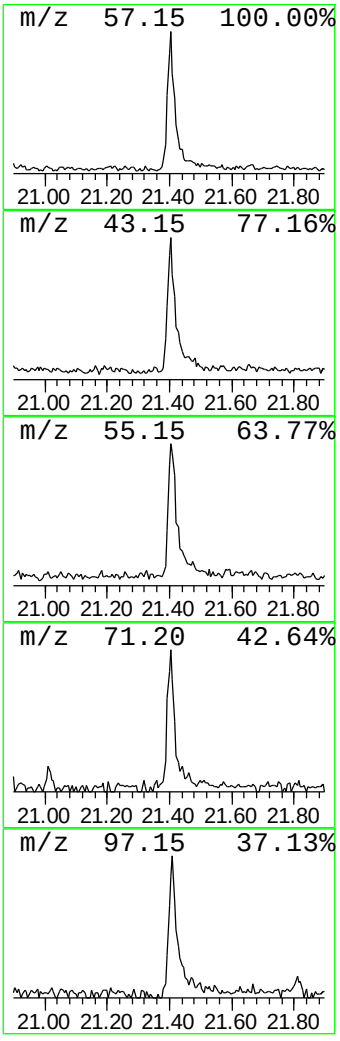
****

Peak Number 6 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	3.79 ng	169091	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Cyclotetradecane	196	C14H28	000295-17-0	86
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81





Library Search Compound Report

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Operator : JU/SJ
Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

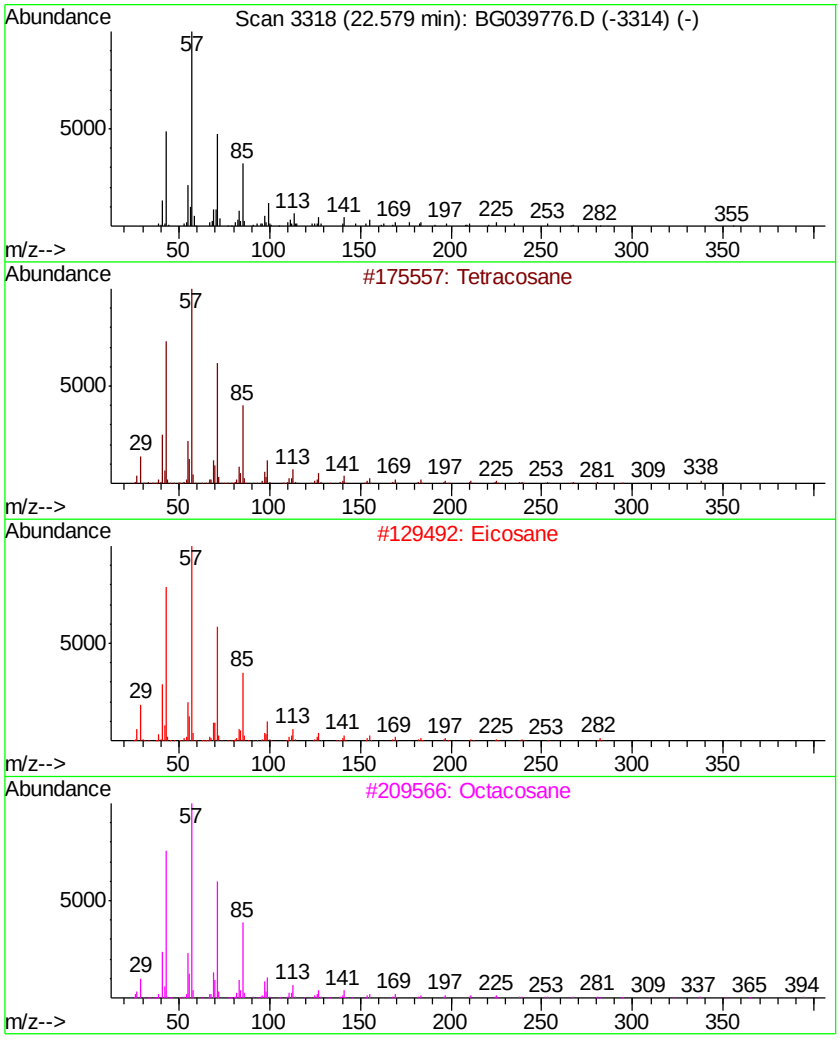
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

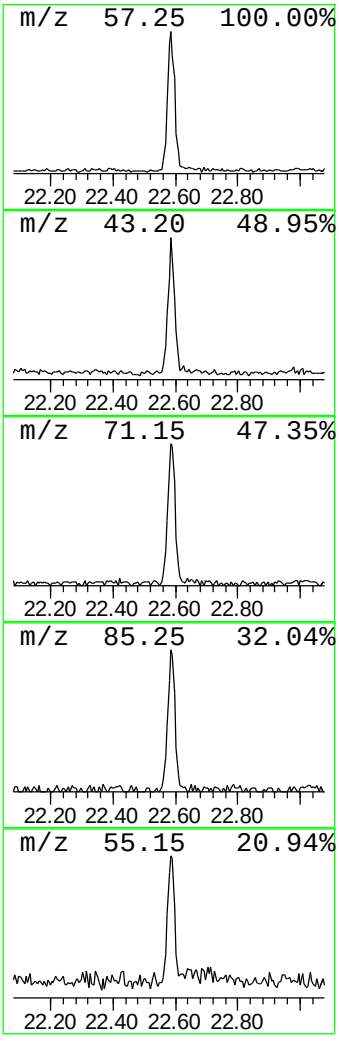
****

Peak Number 7 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	2.71 ng	120726	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentacosane	352	C25H52	000629-99-2	87





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Instrument : BNA_G
ClientSampleId : DSN001

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

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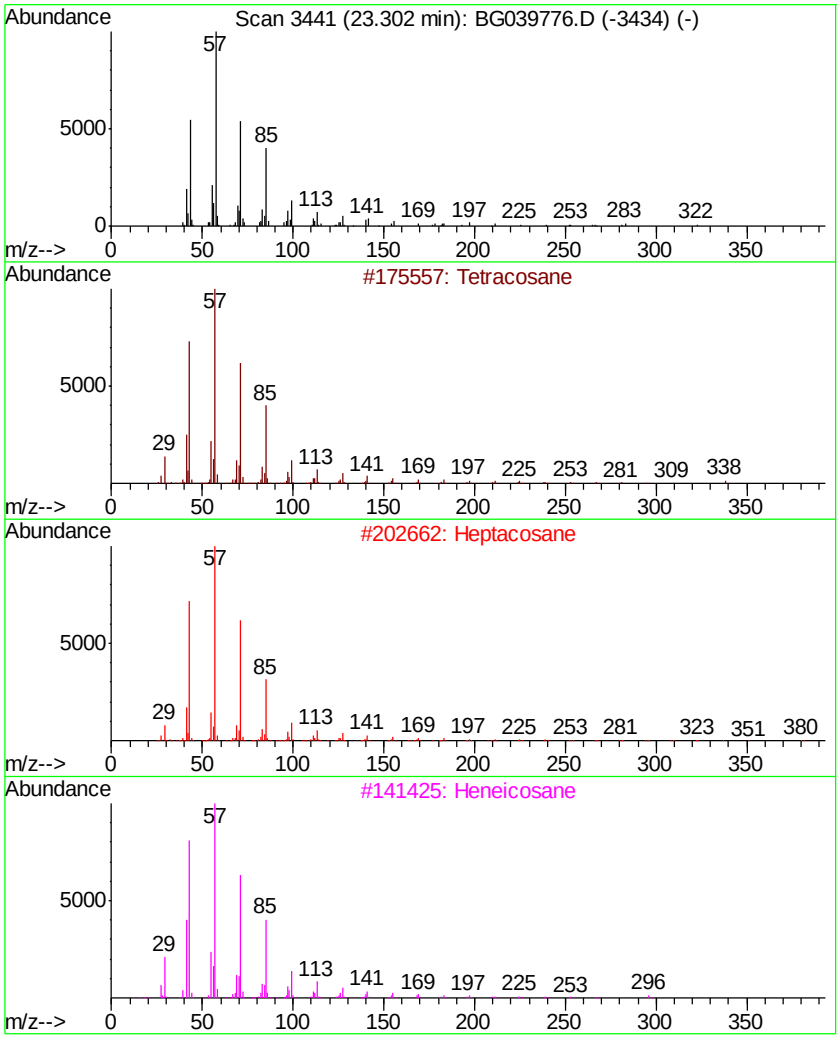
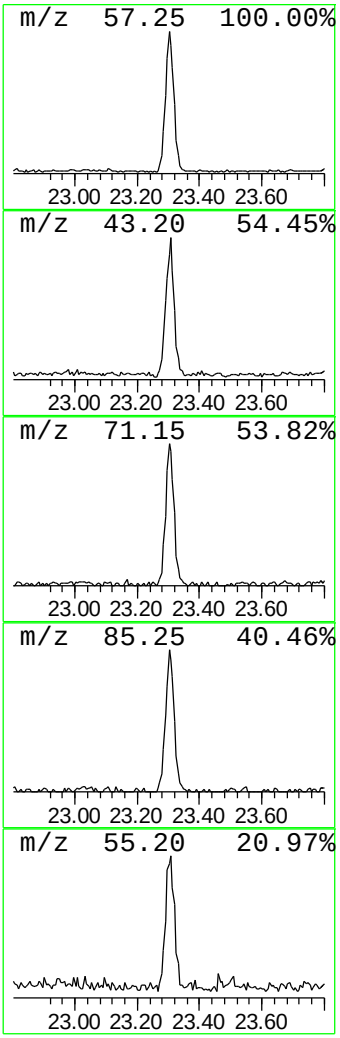
Peak Number 8 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	4.19 ng	186986	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Eicosane	282	C20H42	000112-95-8	91





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Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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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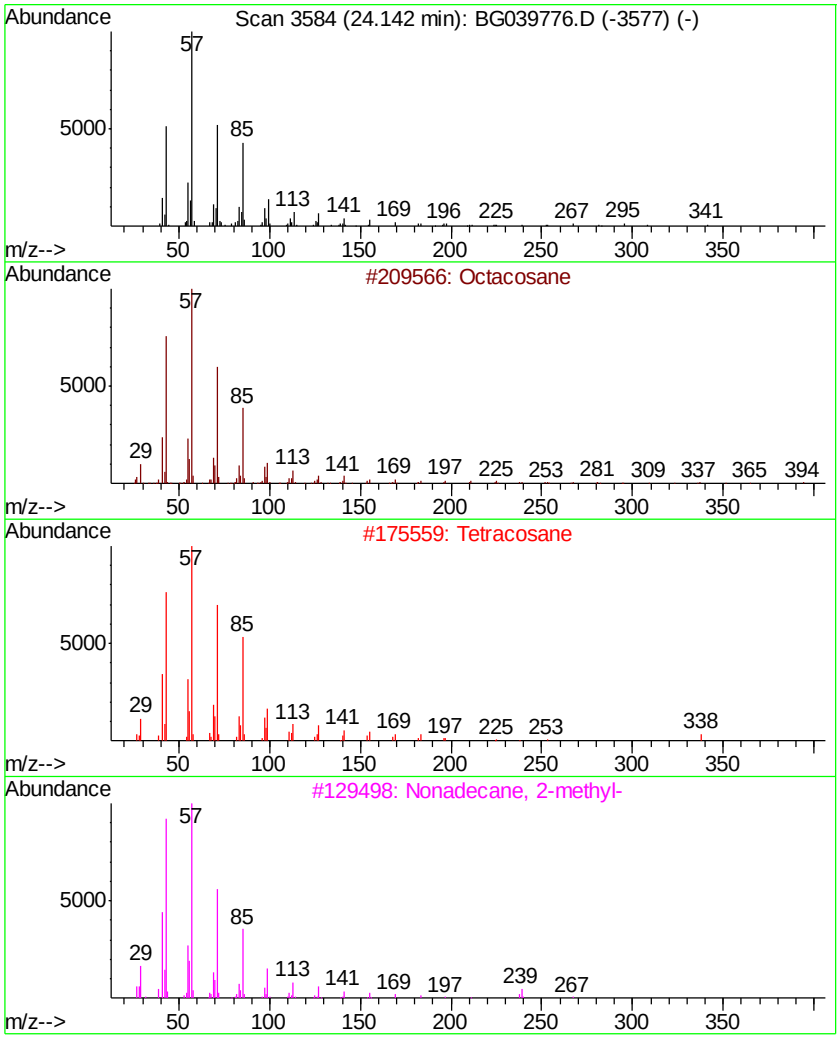
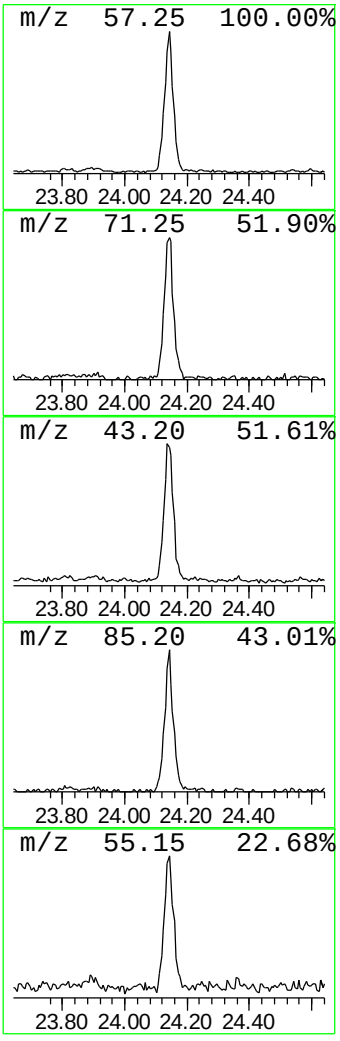
Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.14	3.86 ng	199881	Perylene-d12	25.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Hexacosane	366	C26H54	000630-01-3	87





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

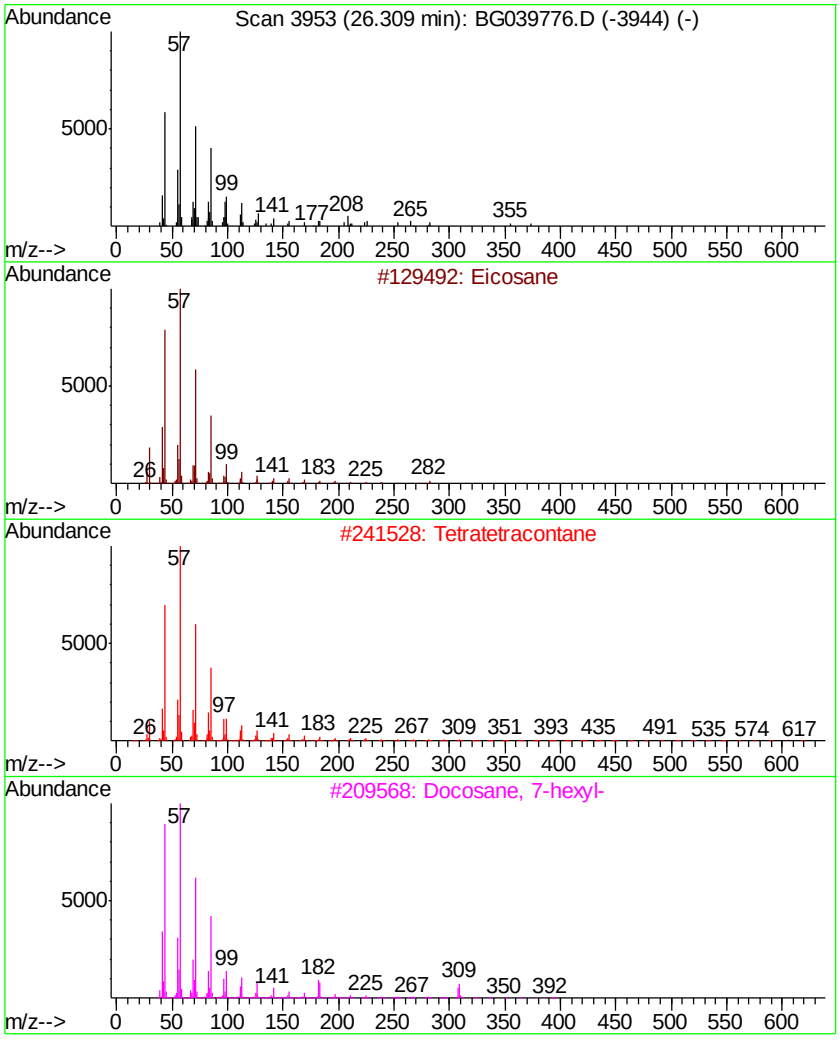
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

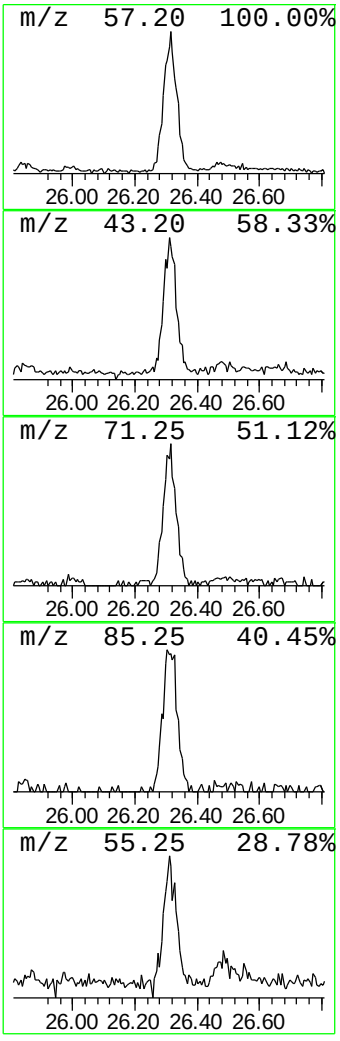
****

Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.31	3.07 ng	159309	Perylene-d12	25.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	87
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG030519\
Data File : BG039776.D
Acq On : 5 Mar 2019 22:44
Operator : JU/SJ
Sample : K1726-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DSN001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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
1-Pentene, 2-methyl-	3.21	24.6	ng	318972	1	8.15	258896	20.0
Butane, 2-methoxy...	3.28	12.9	ng	166804	1	8.15	258896	20.0
unknown7.68	7.68	87.8	ng	1136230	1	8.15	258896	20.0
n-Hexadecanoic acid	18.37	2.6	ng	106858	4	17.53	810312	20.0
17-Pentatriacontene	21.40	3.8	ng	169091	5	21.82	892575	20.0
Tetracosane	22.58	2.7	ng	120726	5	21.82	892575	20.0
Heptacosane	23.30	4.2	ng	186986	5	21.82	892575	20.0
Octacosane	24.14	3.9	ng	199881	6	25.19	1036970	20.0
Eicosane	26.31	3.1	ng	159309	6	25.19	1036970	20.0