LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-21A

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	3.187	13	17	29	rVB	111610	176507	6.26%	1.212%
2	5.126	342	347	357	rBV	99247	157501	5.59%	1.081%
3	5.608	422	429	443	rBV	473160	825187	29.29%	5.665%
4	7.206	693	701	719	rBV	510660	969937	34.43%	6.659%
5	7.564	754	762	773	rBV	523146	950183	33.73%	6.523%
6	8.023	833	840	852	rBV	131697	244234	8.67%	1.677%
7	8.346	888	895	905	rBV	405287	727991	25.84%	4.998%
8	9.186	1030	1038	1054	rBV	255333	562482	19.96%	3.862%
9	10.831	1308	1318	1328	rBV	145940	313175	11.12%	2.150%
10	13.269	1726	1733	1750	rBV	884732	1539610	54.65%	10.570%
11	14.098	1868	1874	1886	rBV	63570	129967	4.61%	0.892%
12	14.650	1959	1968	1980	rBV	302124	533014	18.92%	3.659%
13	16.137	2214	2221	2242	rBV	807586	1404320	49.85%	9.641%
14	17.394	2428	2435	2452	rBV2	402207	689768	24.48%	4.735%
15	17.512	2452	2455	2462	rVB6	18929	29799	1.06%	0.205%
16	18.281	2582	2586	2595	rBV4	28588	61630	2.19%	0.423%
17	20.003	2873	2879	2895	rBV	2094999	2817370	100.00%	19.342%
18	21.301	3096	3100	3109	rBV5	28101	60007	2.13%	0.412%
19	21.384	3110	3114	3122	rVB	26756	48777	1.73%	0.335%
20	21.660	3154	3161	3179	rBV	481554	869722	30.87%	5.971%
21	21.842	3188	3192	3199	rVB3	25077	35130	1.25%	0.241%
22	22.447	3290	3295	3300	rBV3	32873	50736	1.80%	0.348%
23	23.129	3405	3411	3419	rBV	47161	94822	3.37%	0.651%
24	23.933	3539	3548	3555	rVB4	47323	112160	3.98%	0.770%
25	24.850	3694	3704	3716	rBV2	326559	1004804	35.66%	6.898%
26	25.978	3887	3896	3905	rBV4	32734	93641	3.32%	0.643%
27	27.318	4116	4124	4134	rVB7	19597	63581	2.26%	0.437%

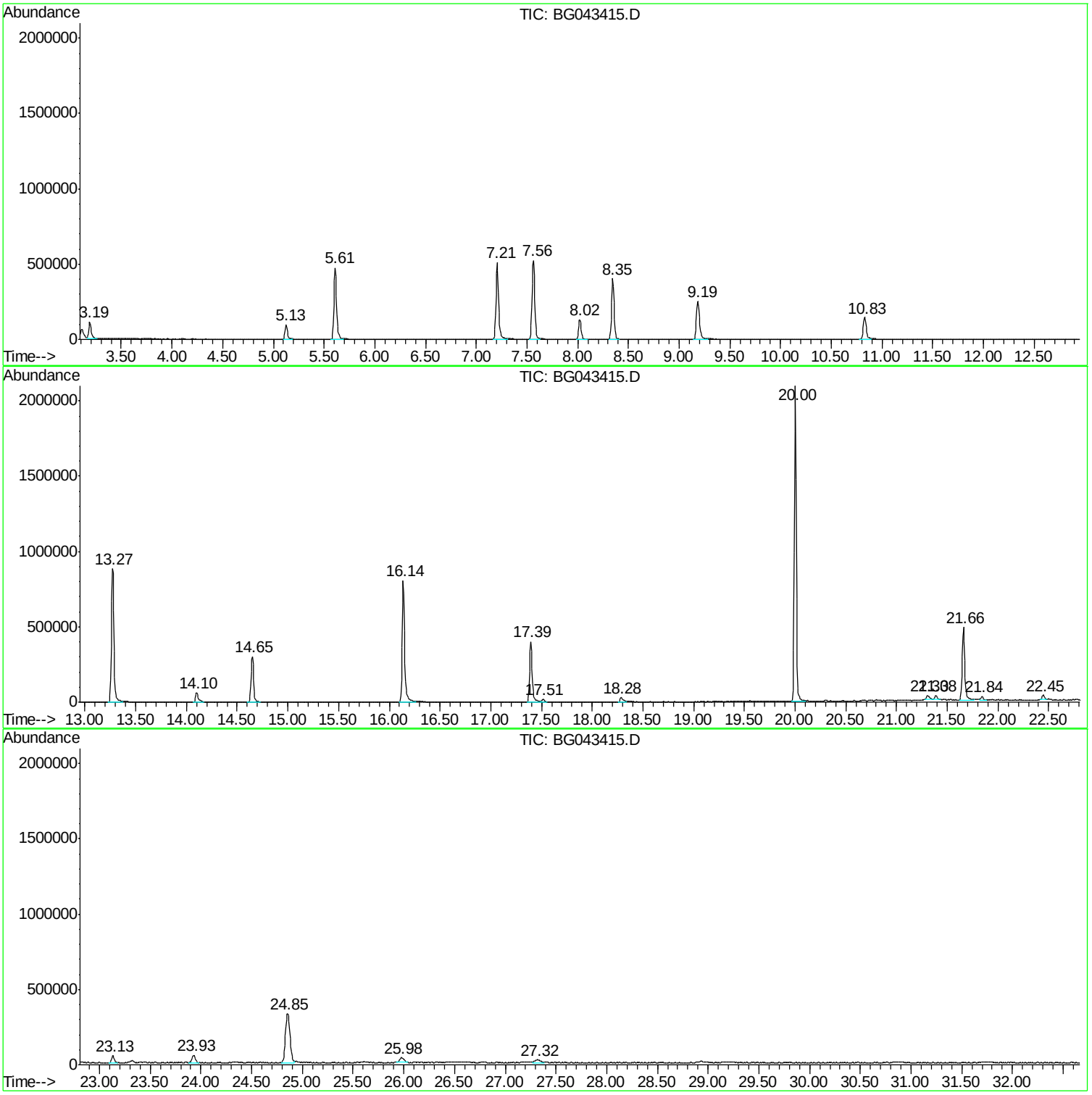
Sum of corrected areas: 14566055

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
Z3-21A

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-21A

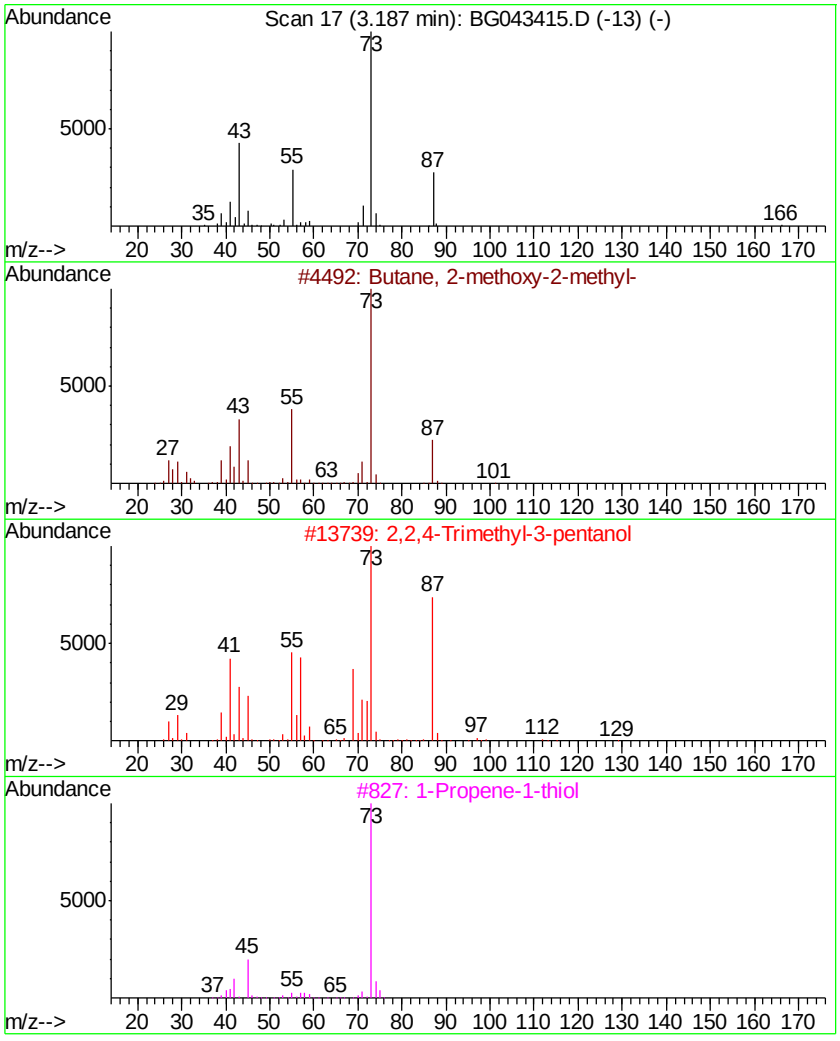
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

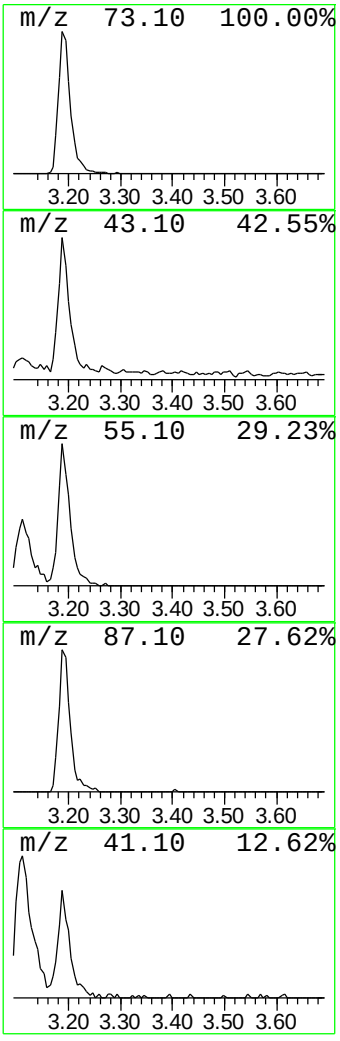
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	14.45 ng	176507	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	39
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	38
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-21A

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

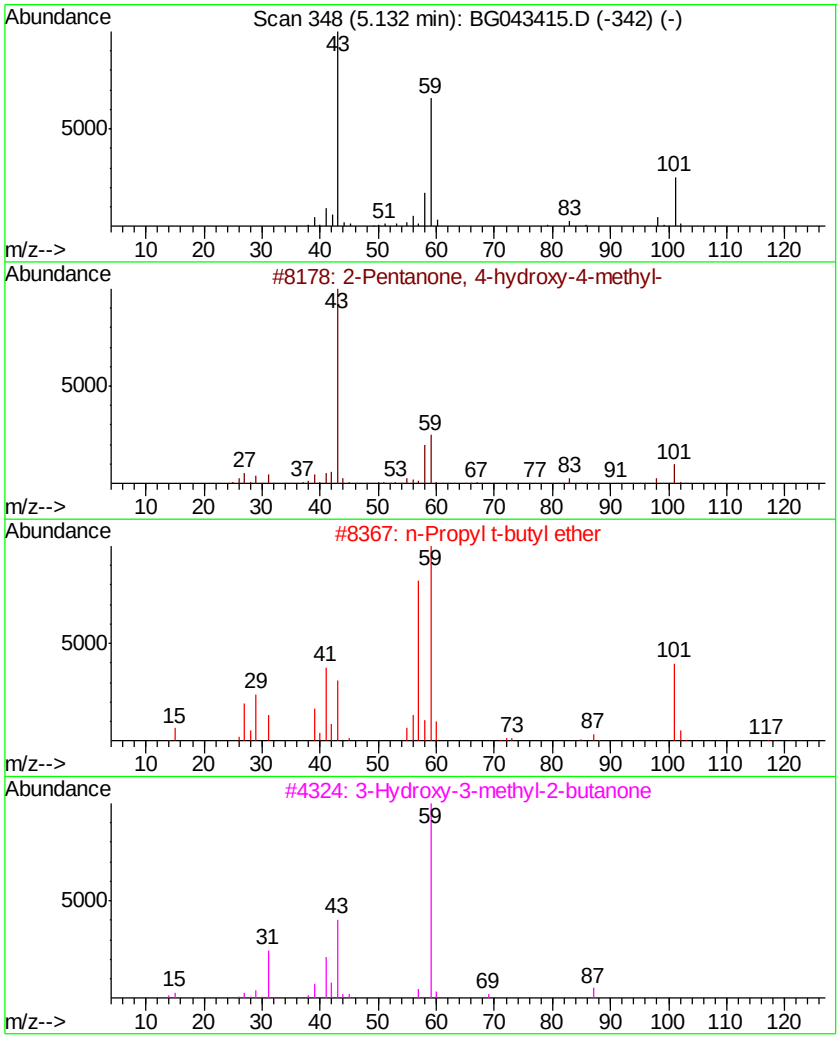
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

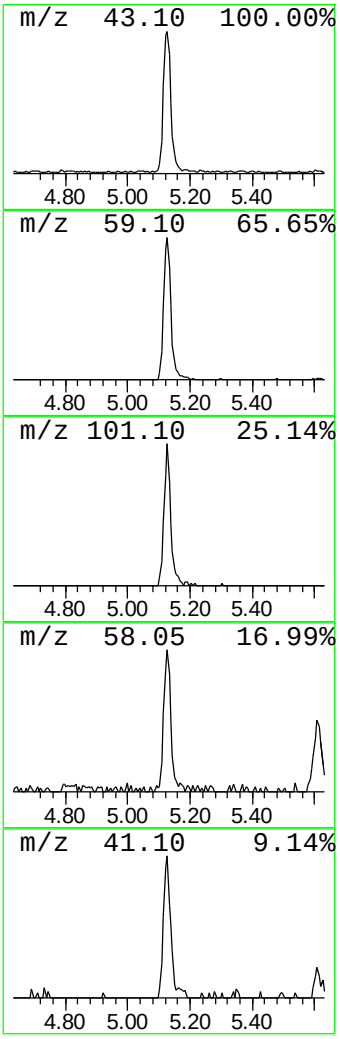
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	12.90 ng	157501	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-21A

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

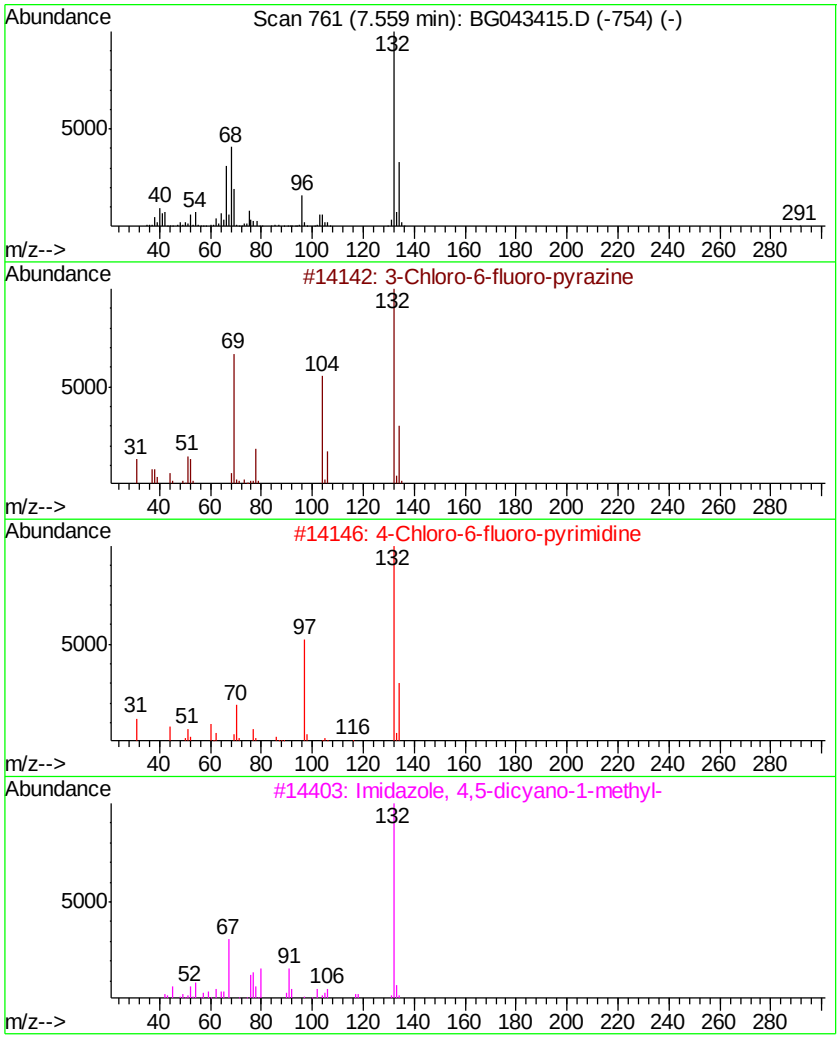
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

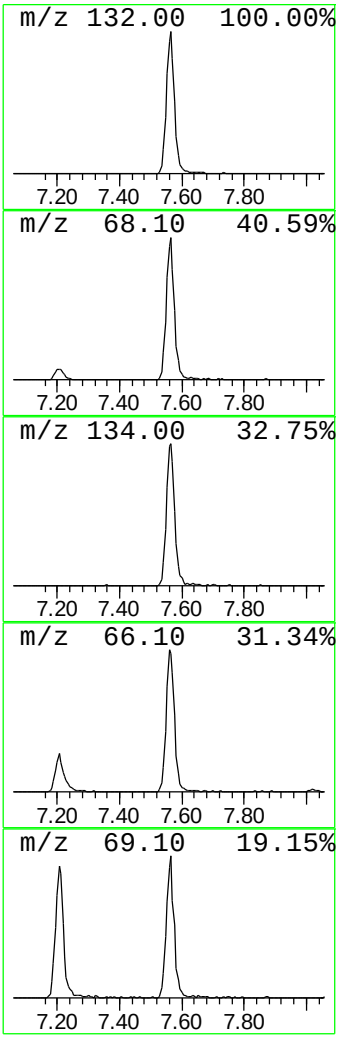
****

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	77.81 ng	950183	1,4-Dichlorobenzene-d4	8.02

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	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-21A

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

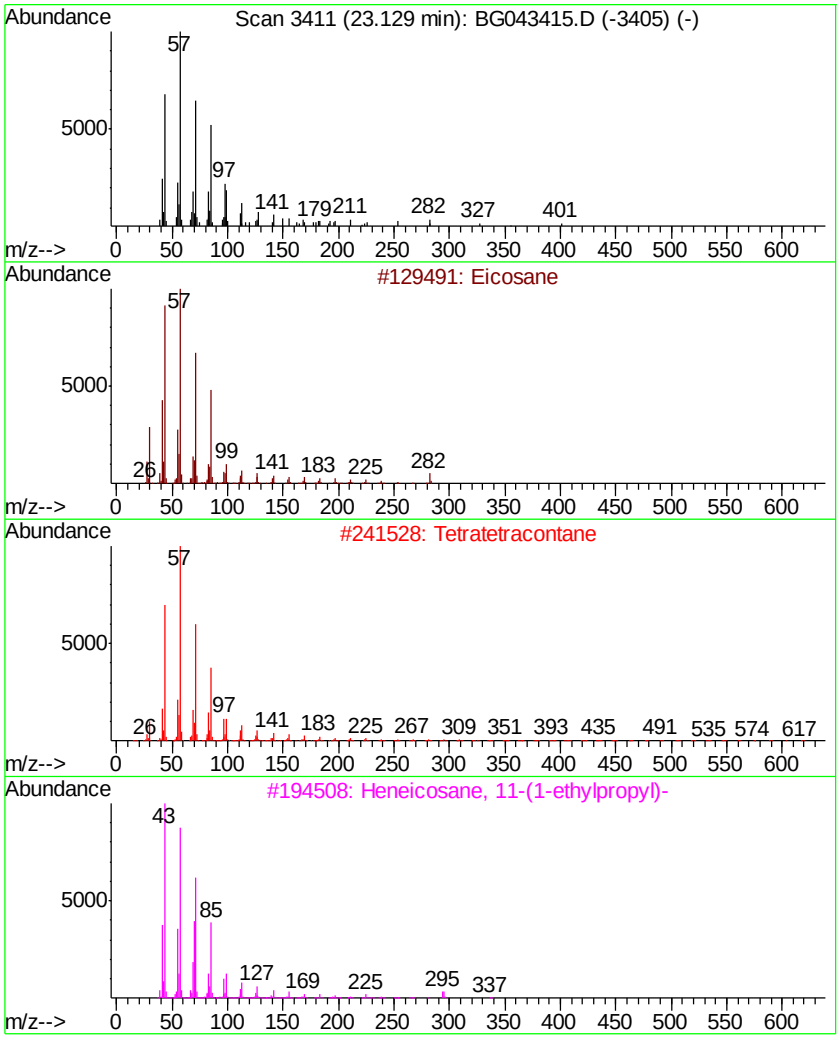
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

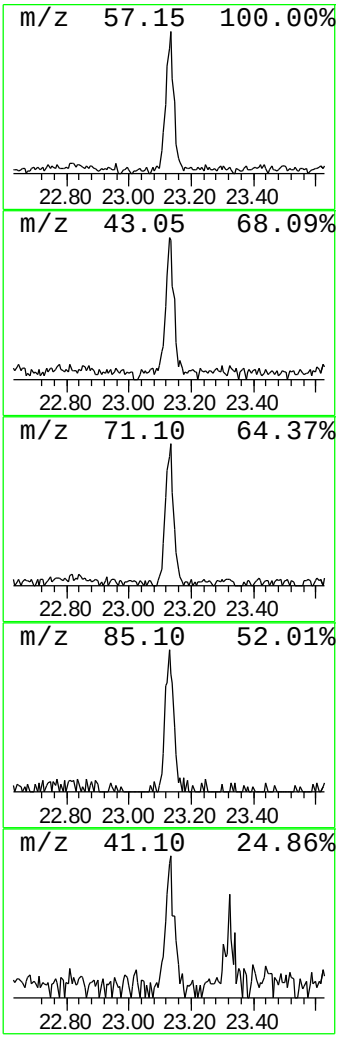
****

Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	2.18 ng	94822	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tetratetracontane	619	C44H90	007098-22-8	83
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80
5	2-methyloctacosane	408	C29H60	1000376-72-8	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-21A

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

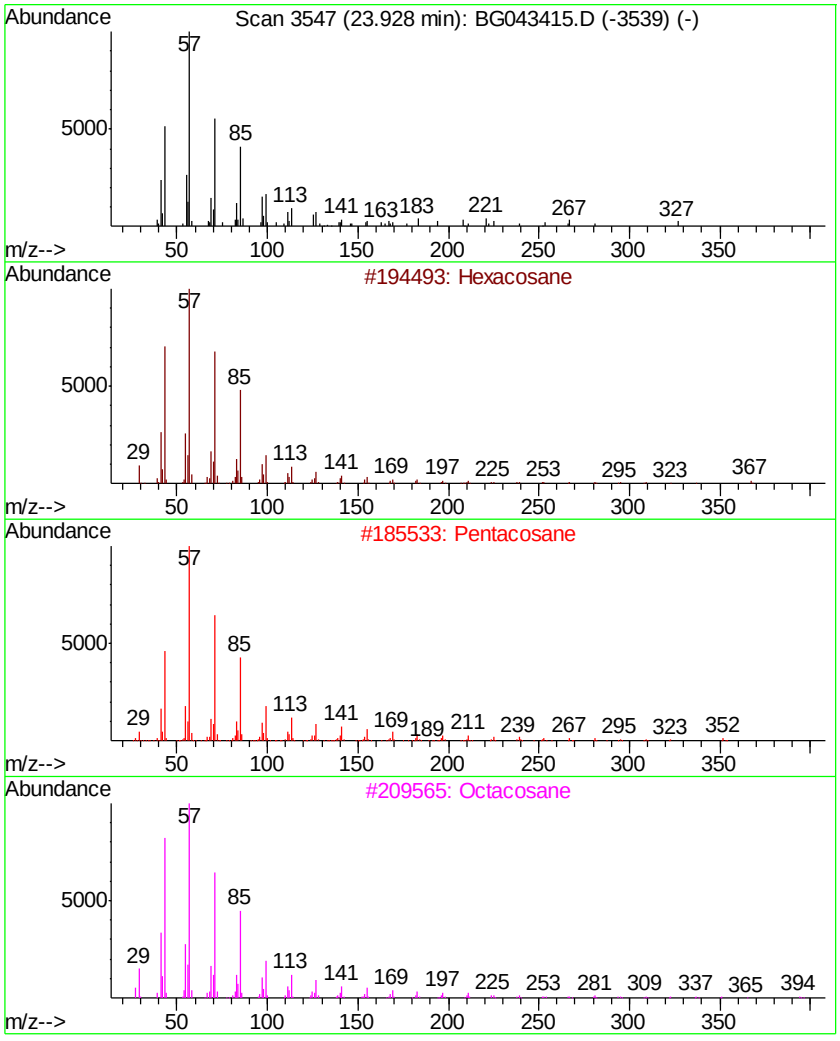
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

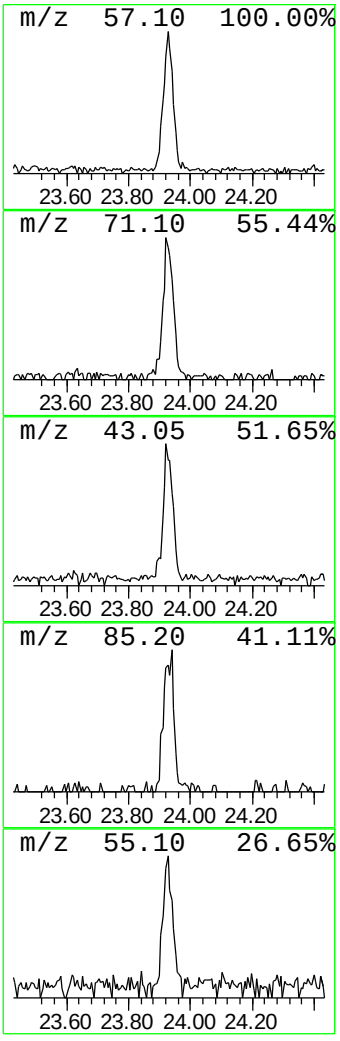
****

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.23 ng	112160	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hentriacontane	437	C31H64	000630-04-6	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG103019\
Data File : BG043415.D
Acq On : 31 Oct 2019 00:25
Operator : JU
Sample : K5599-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : Z3-21A

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.19	14.4	ng	176507	1	8.02	244234	20.0
2-Pentanone, 4-hy...	5.13	12.9	ng	157501	1	8.02	244234	20.0
unknown7.56	7.56	77.8	ng	950183	1	8.02	244234	20.0
Eicosane	23.13	2.2	ng	94822	5	21.66	869722	20.0
Hexacosane	23.93	2.2	ng	112160	6	24.85	1004800	20.0