LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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	3.193	13	18	31	rVB	142404	236447	8.61%	1.447%
2	5.608	422	429	440	rBV	583992	1008193	36.70%	6.168%
3	7.206	693	701	715	rBV	619053	1183957	43.10%	7.244%
4	7.565	753	762	774	rBV	649187	1157661	42.14%	7.083%
5	8.023	833	840	850	rBV	140612	256335	9.33%	1.568%
6	8.346	887	895	911	rBV	471753	853522	31.07%	5.222%
7	9.186	1030	1038	1058	rBV2	320295	689506	25.10%	4.219%
8	10.826	1309	1317	1330	rBV	142624	312729	11.38%	1.913%
9	13.276	1726	1734	1747	rBV	886367	1559222	56.76%	9.540%
10	14.098	1867	1874	1887	rBV	57416	127234	4.63%	0.778%
11	14.651	1960	1968	1984	rBV	313730	538461	19.60%	3.294%
12	16.137	2214	2221	2244	rBV	951178	1701831	61.95%	10.412%
13	17.394	2429	2435	2450	rBV2	382100	731880	26.64%	4.478%
14	17.518	2452	2456	2465	rVB5	23031	42718	1.56%	0.261%
15	18.288	2581	2587	2598	rBV4	49694	109114	3.97%	0.668%
16	19.445	2778	2784	2795	rBV	60731	101135	3.68%	0.619%
17	19.809	2836	2846	2855	rBV	52959	110635	4.03%	0.677%
18	20.003	2873	2879	2896	rBV	2035386	2746946	100.00%	16.807%
19	21.308	3095	3101	3111	rBV4	79913	226790	8.26%	1.388%
20	21.660	3152	3161	3176	rBV2	501260	1037025	37.75%	6.345%
21	21.848	3189	3193	3198	rBV3	35590	51590	1.88%	0.316%
22	22.453	3290	3296	3301	rBV2	38819	65967	2.40%	0.404%
23	22.665	3327	3332	3337	rVB5	16133	27649	1.01%	0.169%
24	23.135	3406	3412	3418	rBV2	48482	81560	2.97%	0.499%
25	23.329	3439	3445	3452	rVB2	56825	110981	4.04%	0.679%
26	23.852	3527	3534	3536	rBV4	21489	43867	1.60%	0.268%
27	23.928	3541	3547	3556	rVB4	47275	121522	4.42%	0.744%
28	24.862	3694	3706	3723	rBV2	338231	1052245	38.31%	6.438%
29	25.979	3891	3896	3903	rBV6	23461	57803	2.10%	0.354%

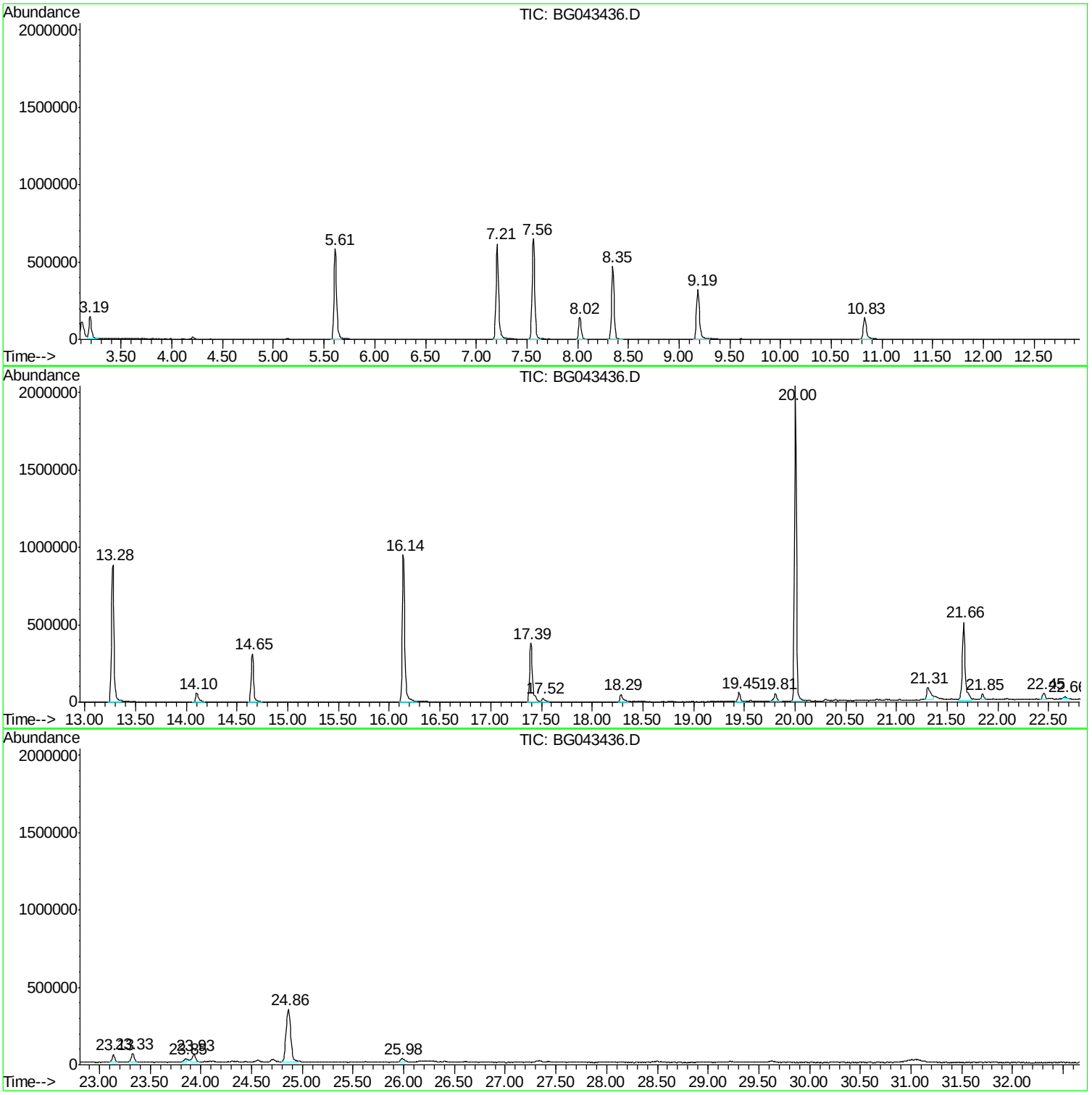
Sum of corrected areas: 16344525

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
169-32-(0-1)

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\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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

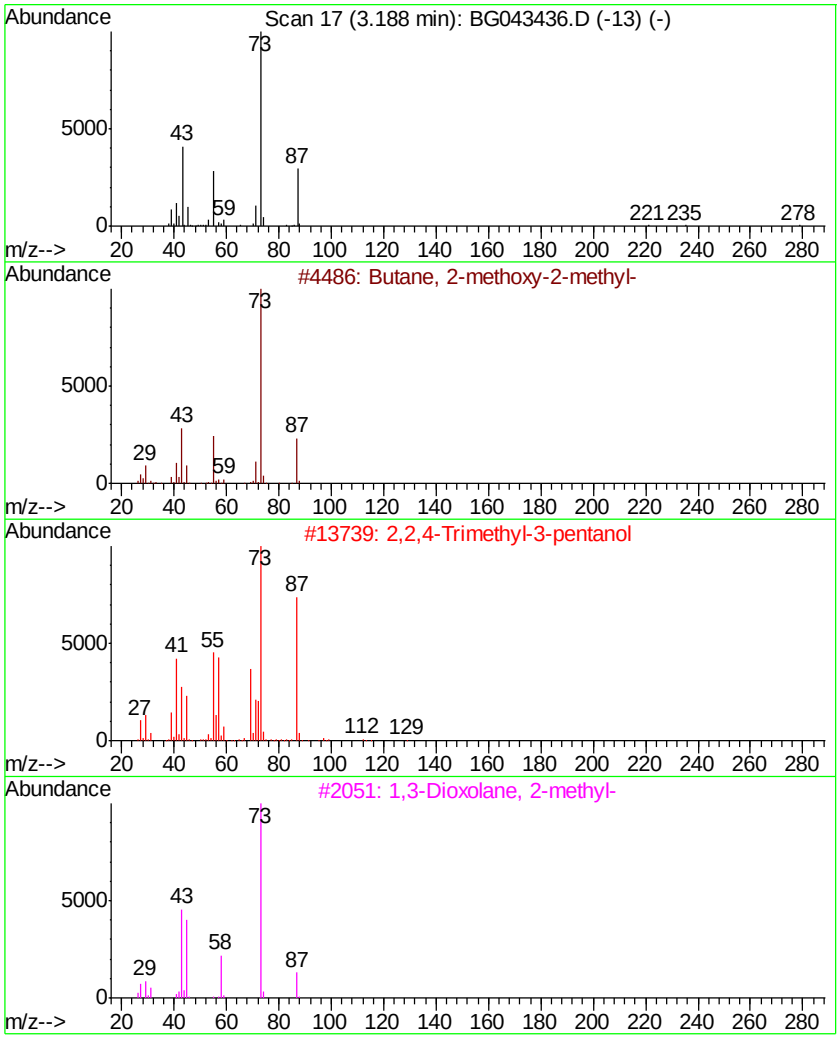
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

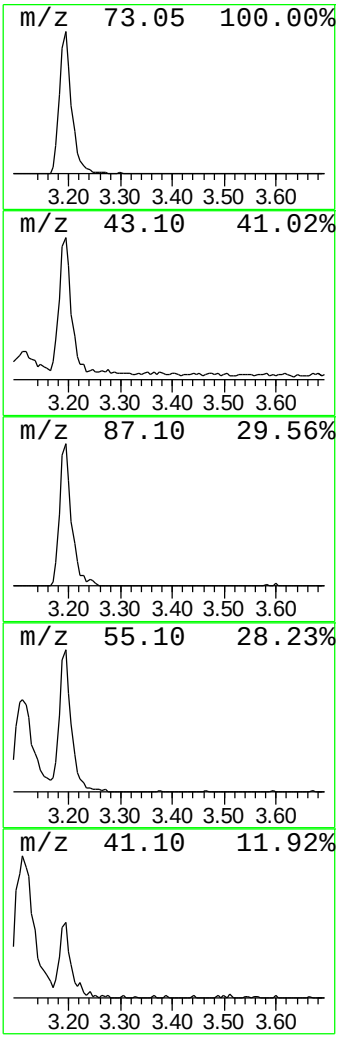
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	18.45 ng	236447	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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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

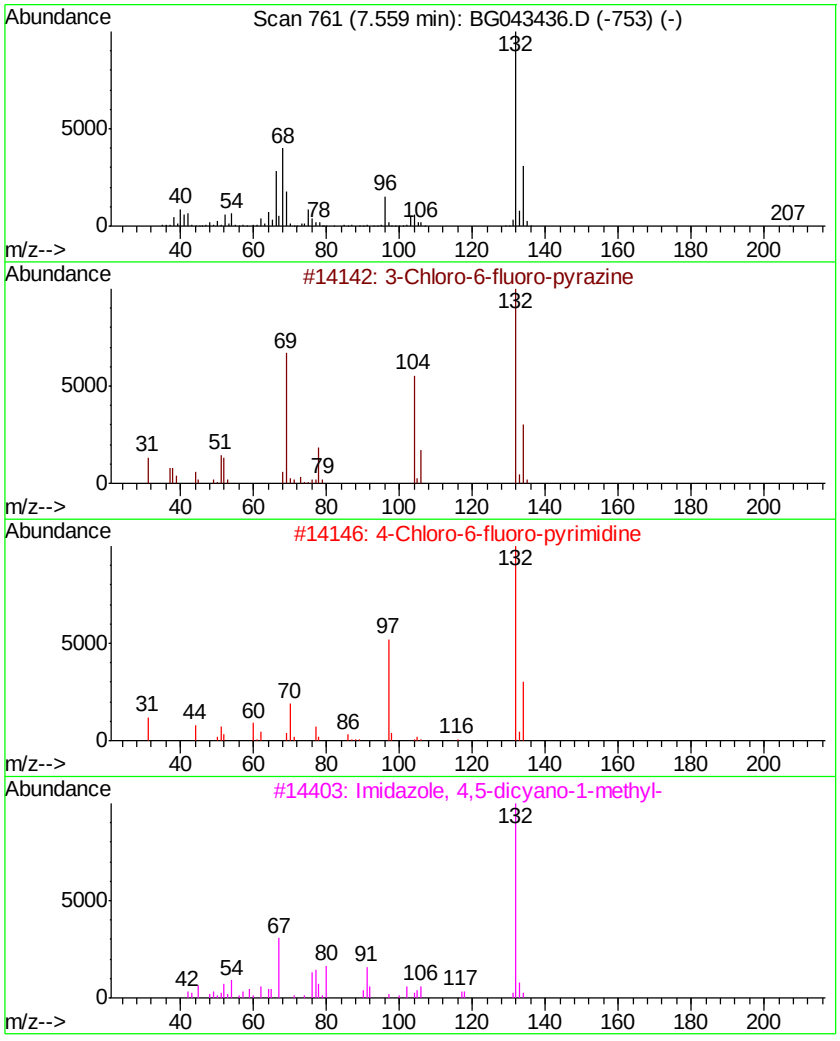
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

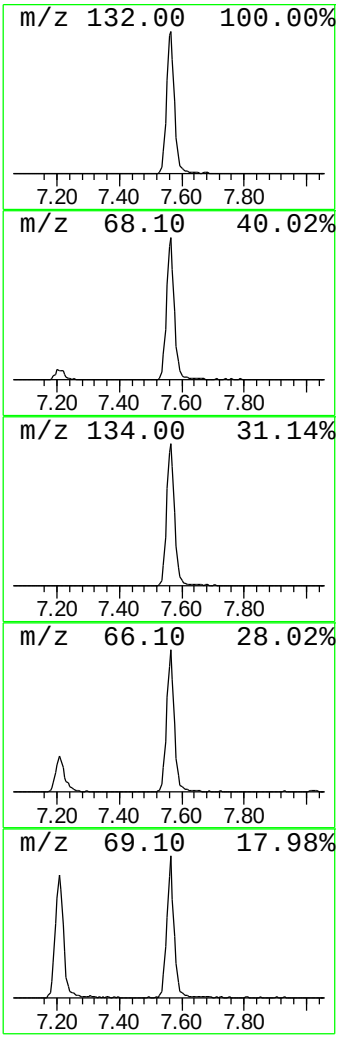
****

Peak Number 2 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	90.32 ng	1157660	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	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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

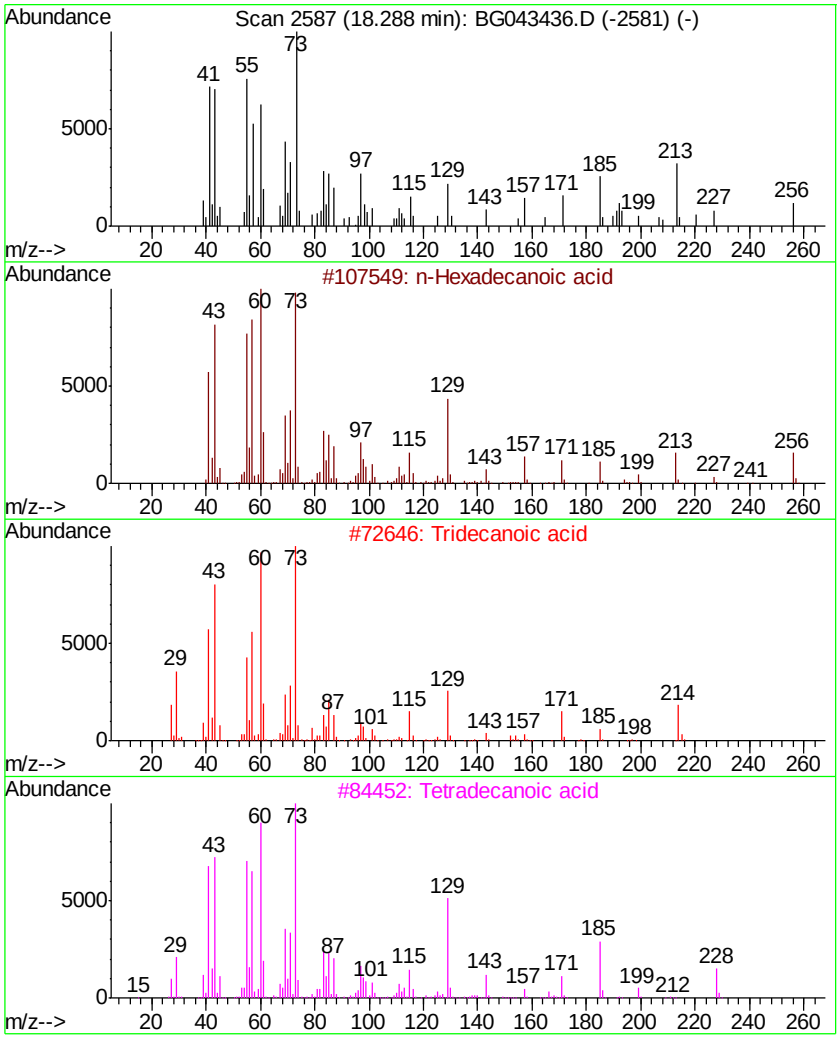
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

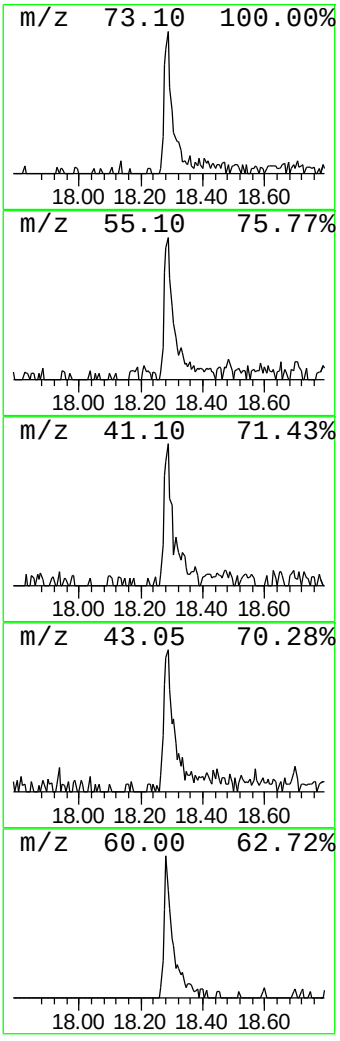
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	2.98 ng	109114	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
2	Tridecanoic acid	214	C13H26O2	000638-53-9	49
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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

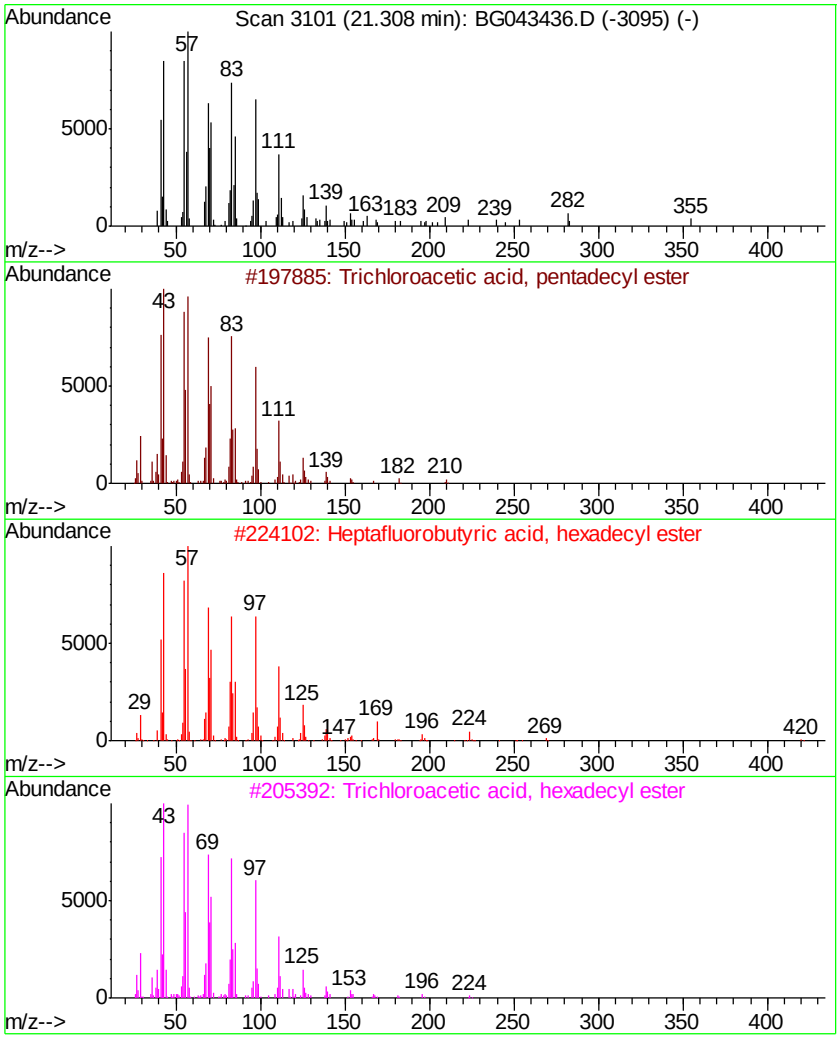
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

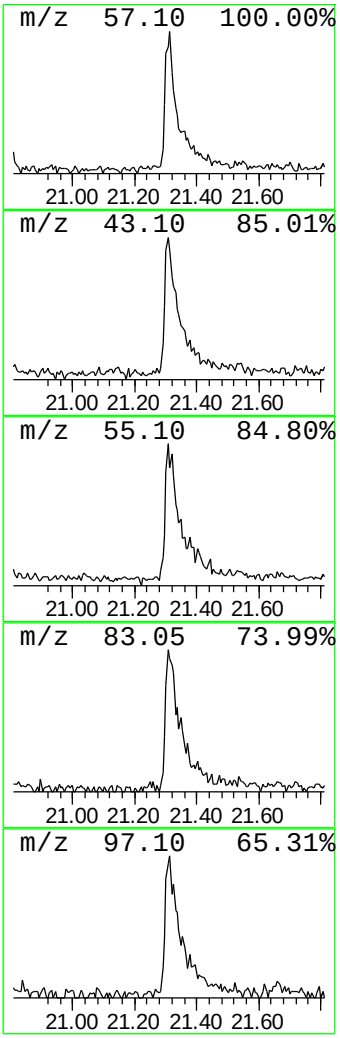
****

Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	4.37 ng	226790	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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

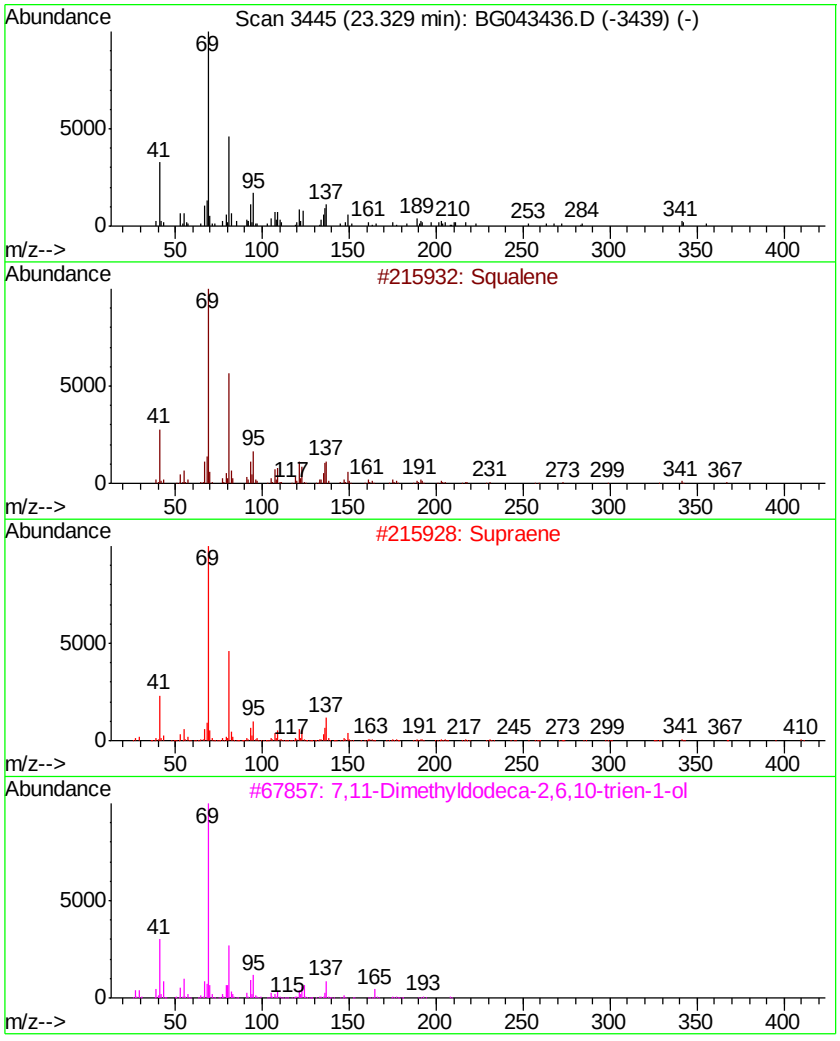
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

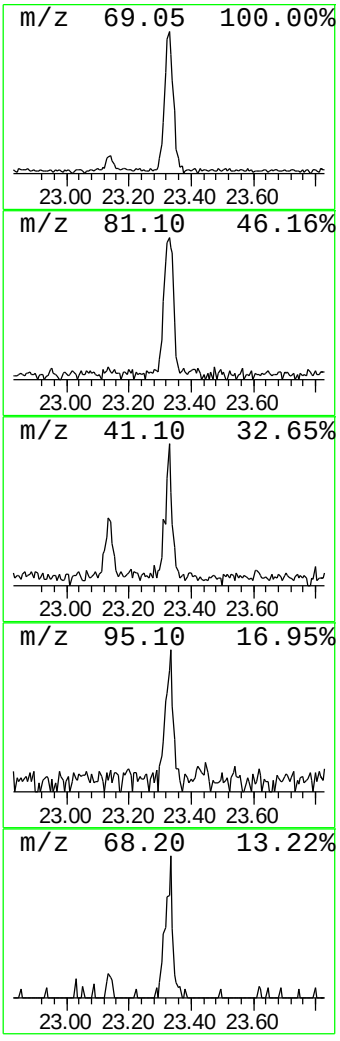
****

Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.33	2.11 ng	110981	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	80
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72
5	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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

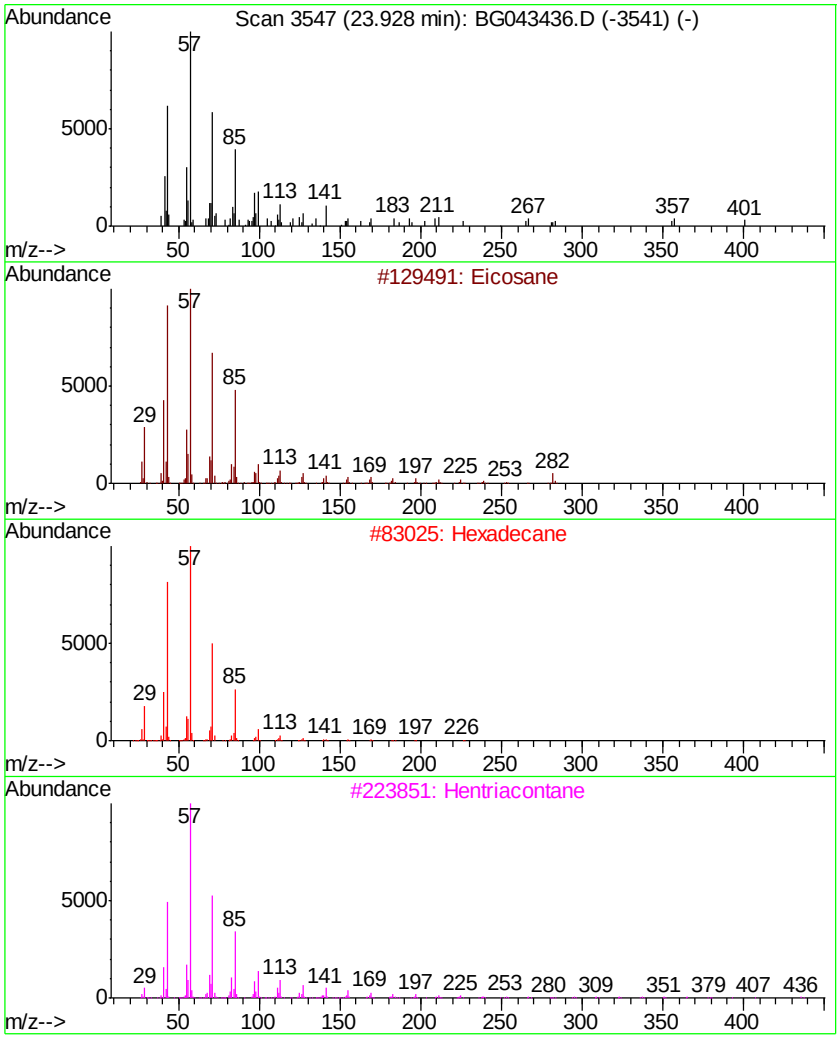
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

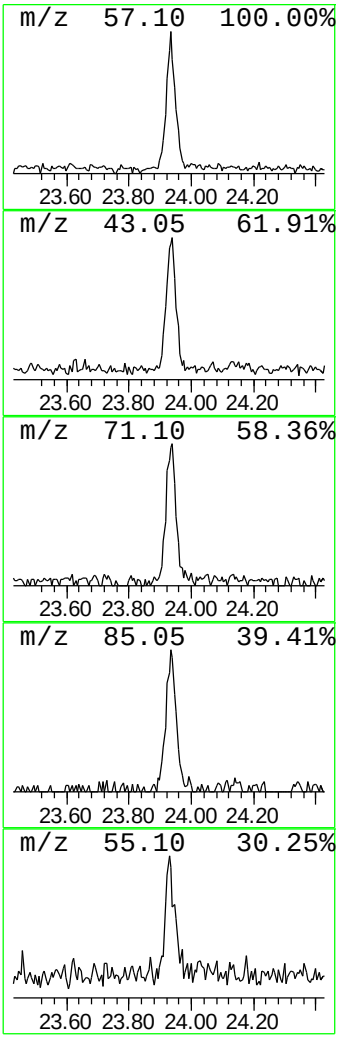
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.31 ng	121522	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hexadecane	226	C16H34	000544-76-3	93
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Docosane	310	C22H46	000629-97-0	87
5	Tetracosane	338	C24H50	000646-31-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG103119\
Data File : BG043436.D
Acq On : 31 Oct 2019 16:27
Operator : JU
Sample : K5497-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 169-32-(0-1)

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	18.4	ng	236447	1	8.02	256335	20.0
unknown7.56	7.56	90.3	ng	1157660	1	8.02	256335	20.0
n-Hexadecanoic acid	18.29	3.0	ng	109114	4	17.39	731880	20.0
Trichloroacetic a...	21.31	4.4	ng	226790	5	21.66	1037030	20.0
Squalene	23.33	2.1	ng	110981	6	24.86	1052250	20.0
Eicosane	23.93	2.3	ng	121522	6	24.86	1052250	20.0