LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
Data File : BG044784.D
Acq On : 14 Mar 2020 4:52
Operator : CG/JU
Sample : PB127427BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB127427BL

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-BG031020.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	3.154	4	11	19	rBV2	268094	656790	8.09%	1.641%
2	3.231	19	24	39	rVB	655659	1205333	14.84%	3.011%
3	5.158	347	352	362	rVB	67938	120069	1.48%	0.300%
4	5.622	423	431	443	rBV	941121	1588776	19.57%	3.968%
5	7.202	693	700	711	rVB	591687	1046375	12.89%	2.614%
6	8.054	836	845	852	rBV	468670	810952	9.99%	2.026%
7	8.378	891	900	908	rBV	1852012	3324333	40.94%	8.303%
8	9.212	1033	1042	1051	rBV	1536098	2875361	35.41%	7.182%
9	10.863	1314	1323	1331	rVB	617271	1142295	14.07%	2.853%
10	13.313	1732	1740	1752	rVB	3952456	6320841	77.85%	15.788%
11	14.130	1874	1879	1885	rBV	135205	200316	2.47%	0.500%
12	14.688	1967	1974	1984	rBV	971453	1579601	19.45%	3.945%
13	16.168	2219	2226	2235	rBV	2893161	4716248	58.09%	11.780%
14	17.432	2433	2441	2450	rBV	1173772	1790849	22.06%	4.473%
15	18.331	2589	2594	2602	rBV2	145449	210692	2.59%	0.526%
16	19.752	2832	2836	2842	rVB	95146	108908	1.34%	0.272%
17	20.046	2879	2886	2892	rBV	6006820	8119516	100.00%	20.281%
18	21.362	3106	3110	3123	rVB3	193802	352718	4.34%	0.881%
19	21.703	3161	3168	3176	rVB	995425	1719745	21.18%	4.296%
20	23.254	3428	3432	3438	rVB4	56877	104394	1.29%	0.261%
21	23.442	3459	3464	3472	rVB2	109687	230795	2.84%	0.576%
22	24.065	3567	3570	3577	rVB5	53296	99742	1.23%	0.249%
23	24.923	3705	3716	3728	rBV2	606058	1711162	21.07%	4.274%

Sum of corrected areas: 40035811

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Misc :
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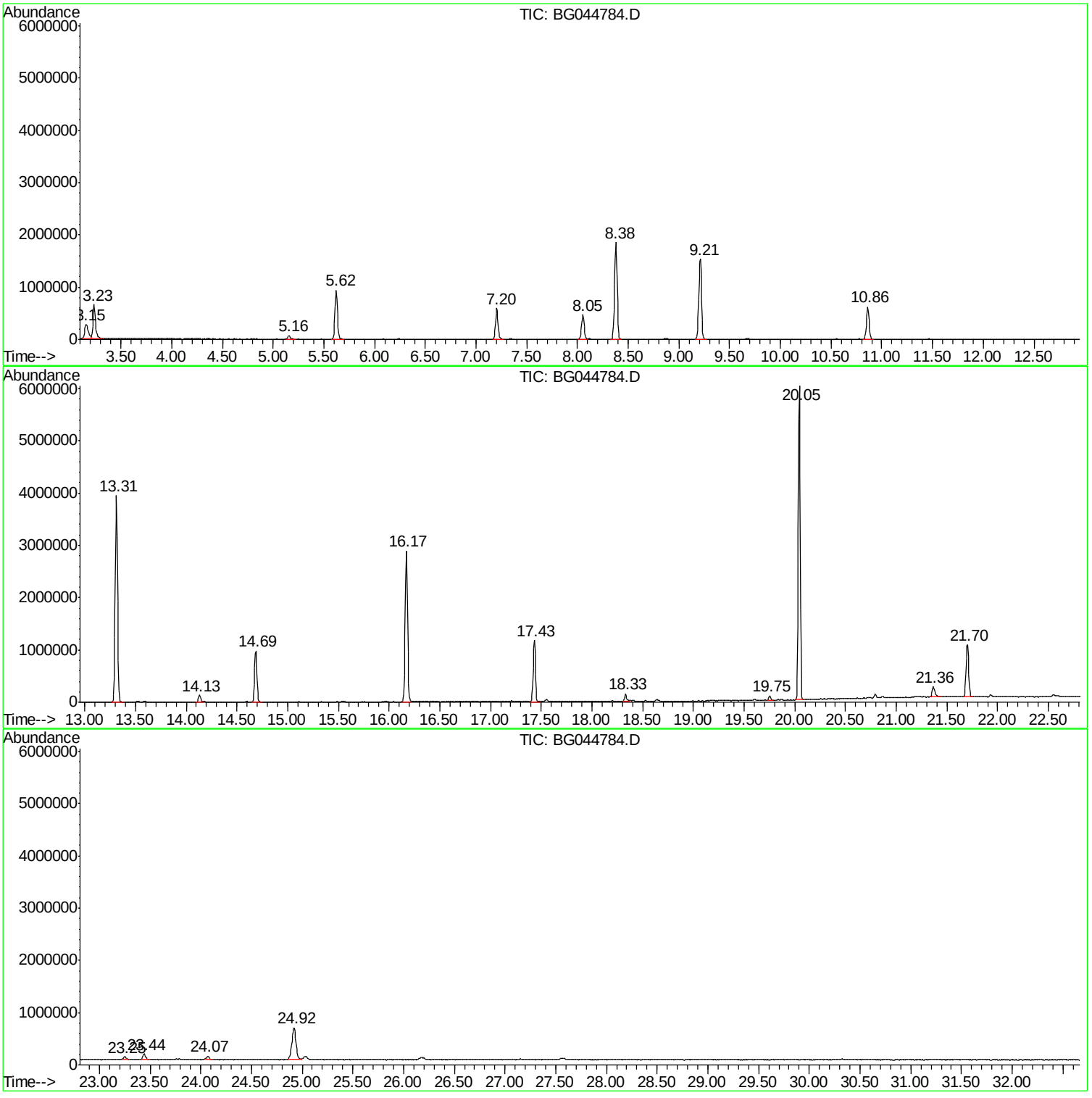
Instrument :
BNA_G
ClientSampleId :
PB127427BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.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\BG031320\
Data File : BG044784.D
Acq On : 14 Mar 2020 4:52
Operator : CG/JU
Sample : PB127427BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB127427BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

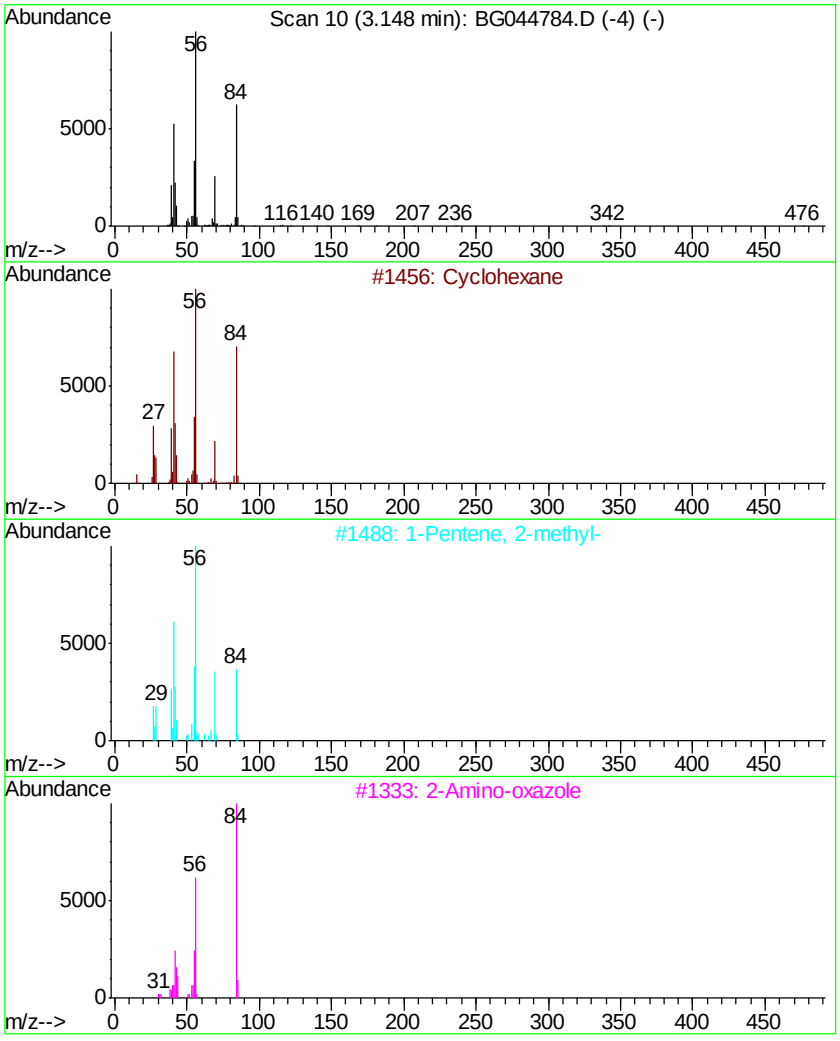
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

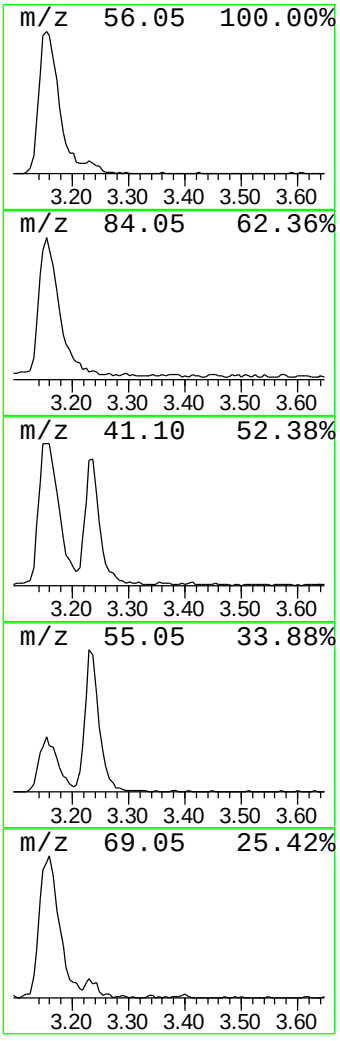
****

Peak Number 1 Cyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	16.20 ng	656790	1,4-Dichlorobenzene-d4	8.05

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	56
3	2-Amino-oxazole	84	C3H4N2O	004570-45-0	47
4	2-Pentene, 2-methyl-	84	C6H12	000625-27-4	43
5	Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
Data File : BG044784.D
Acq On : 14 Mar 2020 4:52
Operator : CG/JU
Sample : PB127427BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB127427BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

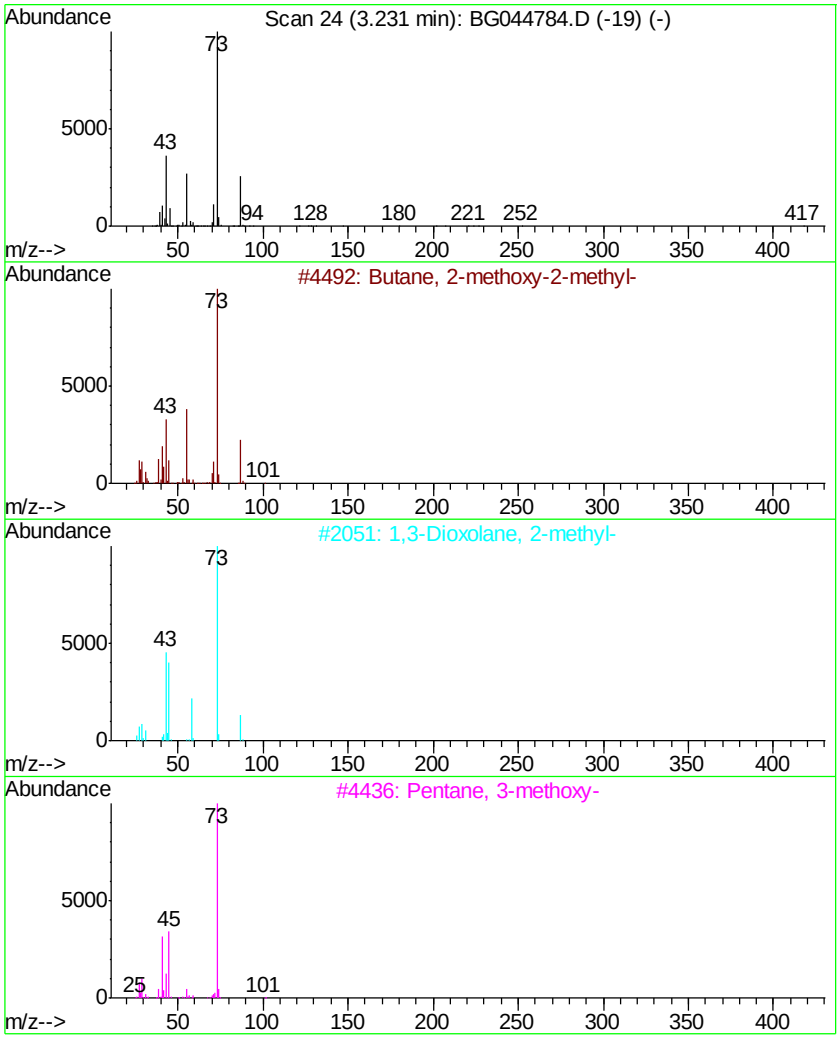
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

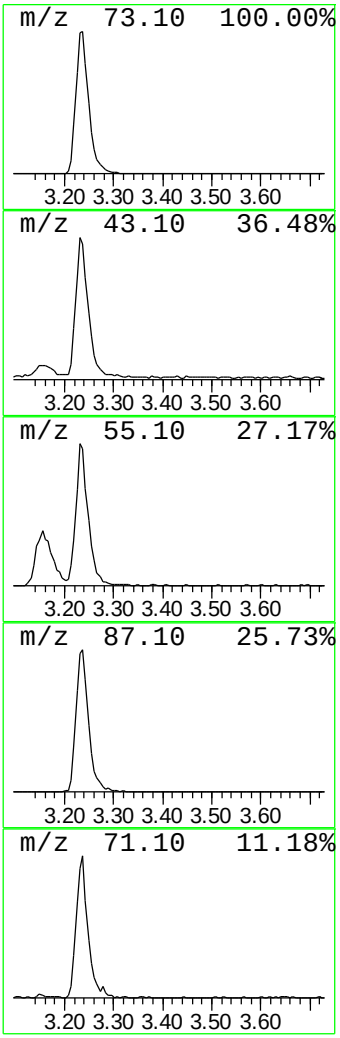
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	29.73 ng	1205330	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	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
Data File : BG044784.D
Acq On : 14 Mar 2020 4:52
Operator : CG/JU
Sample : PB127427BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB127427BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.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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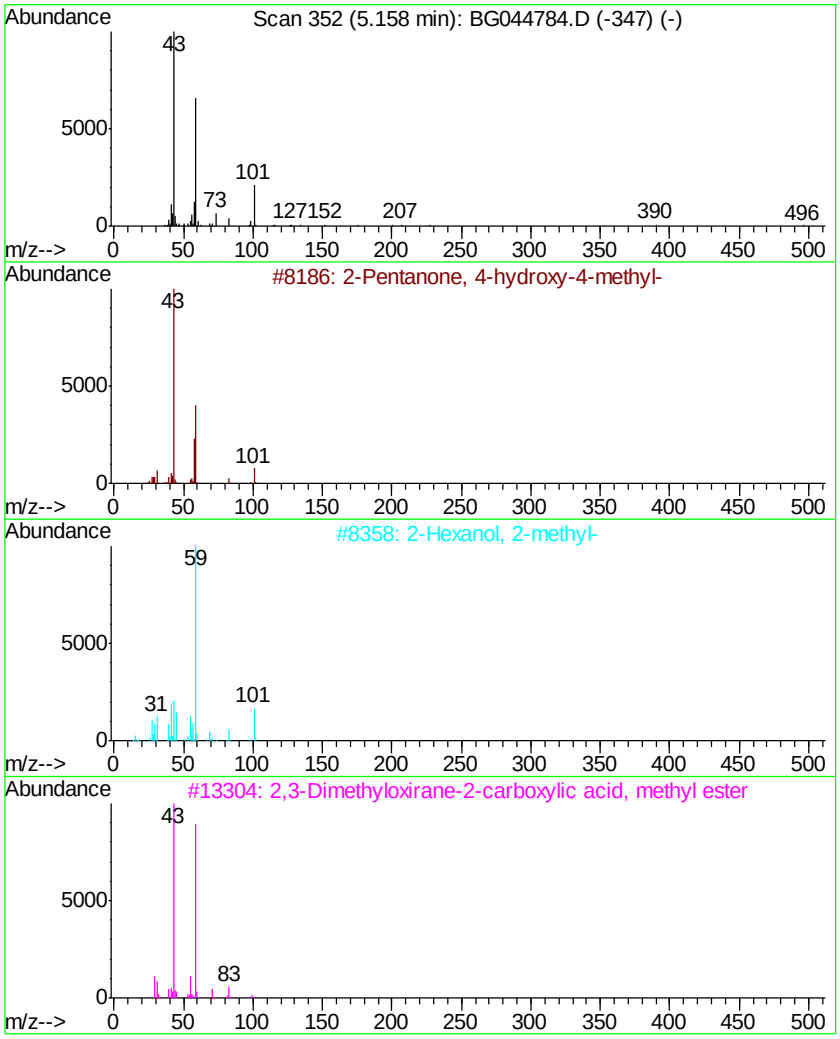
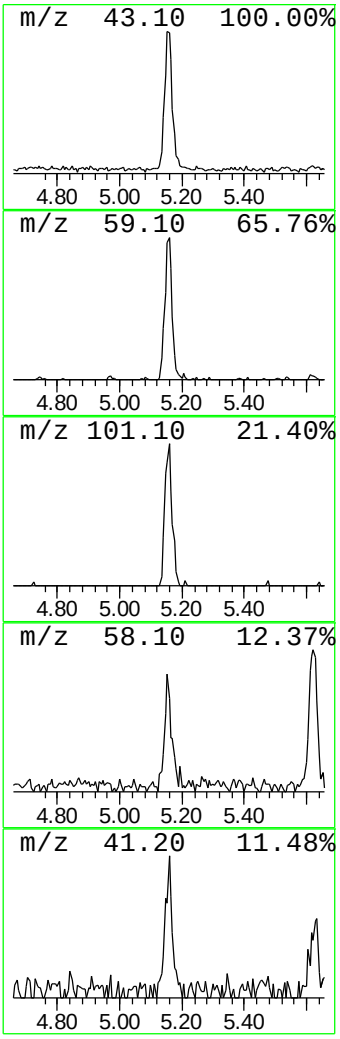
Peak Number 3 unknown5.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	2.96 ng	120069	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Acetaldehyde N-formyl-N-methylhy...	100	C4H8N2O	016568-02-8	25





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Data File : BG044784.D
Acq On : 14 Mar 2020 4:52
Operator : CG/JU
Sample : PB127427BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB127427BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.M
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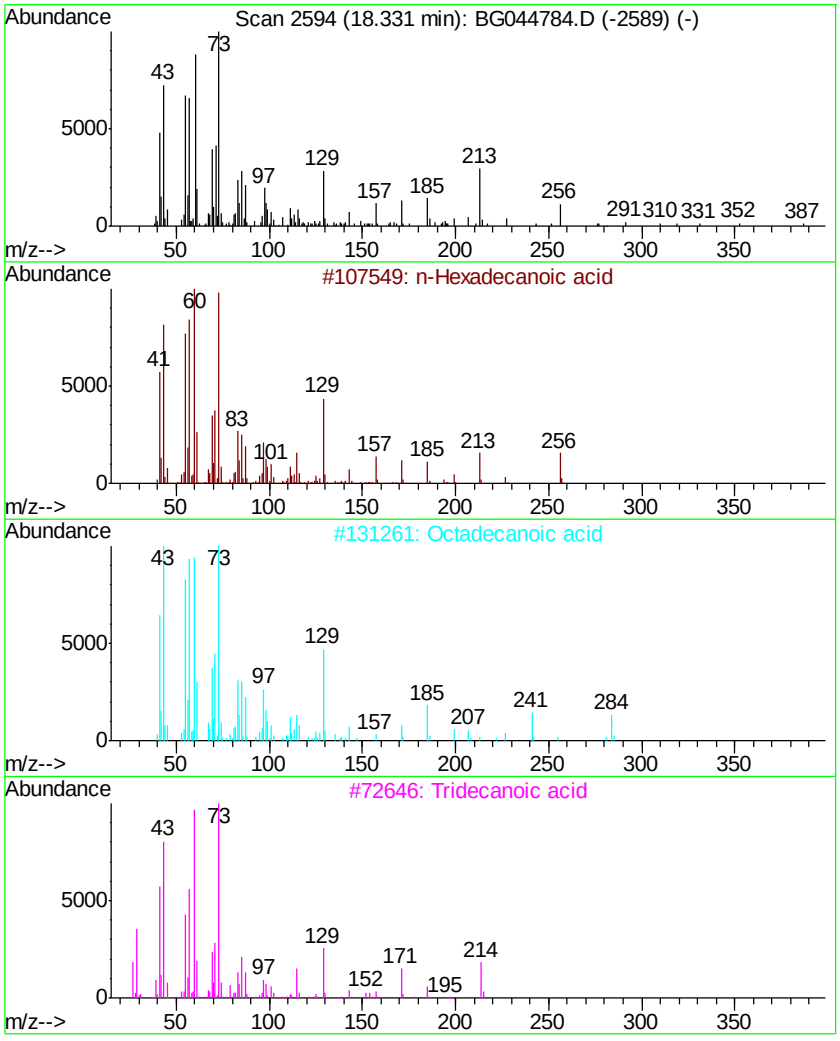
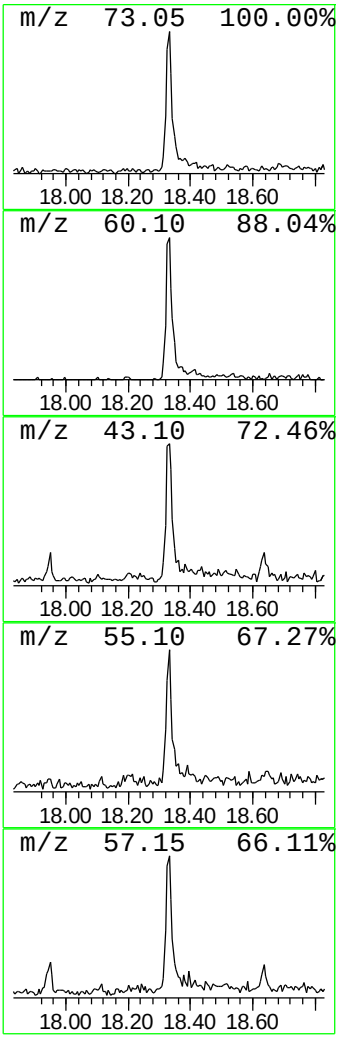
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.35 ng	210692	Phenanthrene-d10	17.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031320\
Data File : BG044784.D
Acq On : 14 Mar 2020 4:52
Operator : CG/JU
Sample : PB127427BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB127427BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

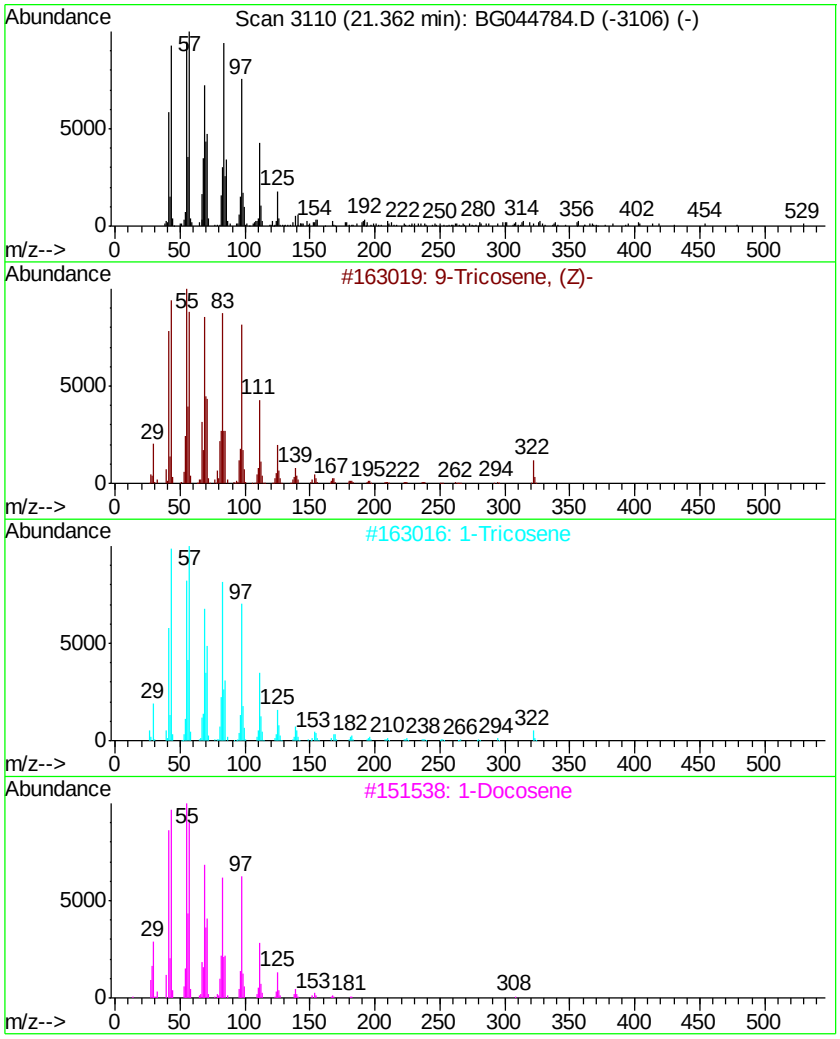
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

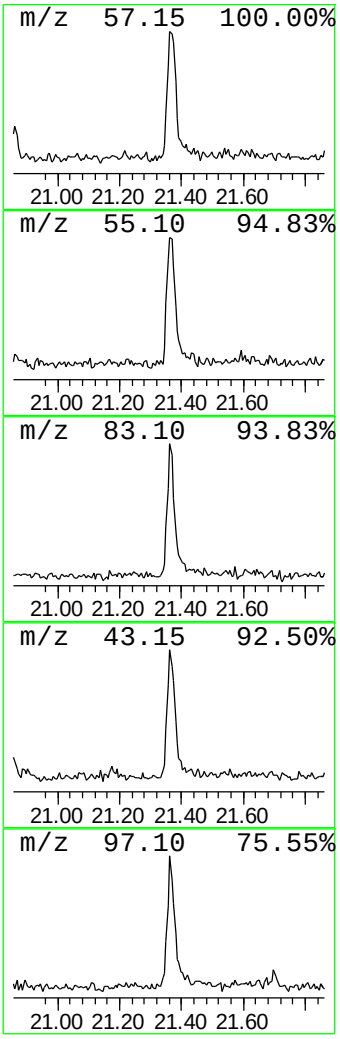
****

Peak Number 6 9-Tricosene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.36	4.10 ng	352718	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
2	1-Tricosene	322	C23H46	018835-32-0	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	93





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB127427BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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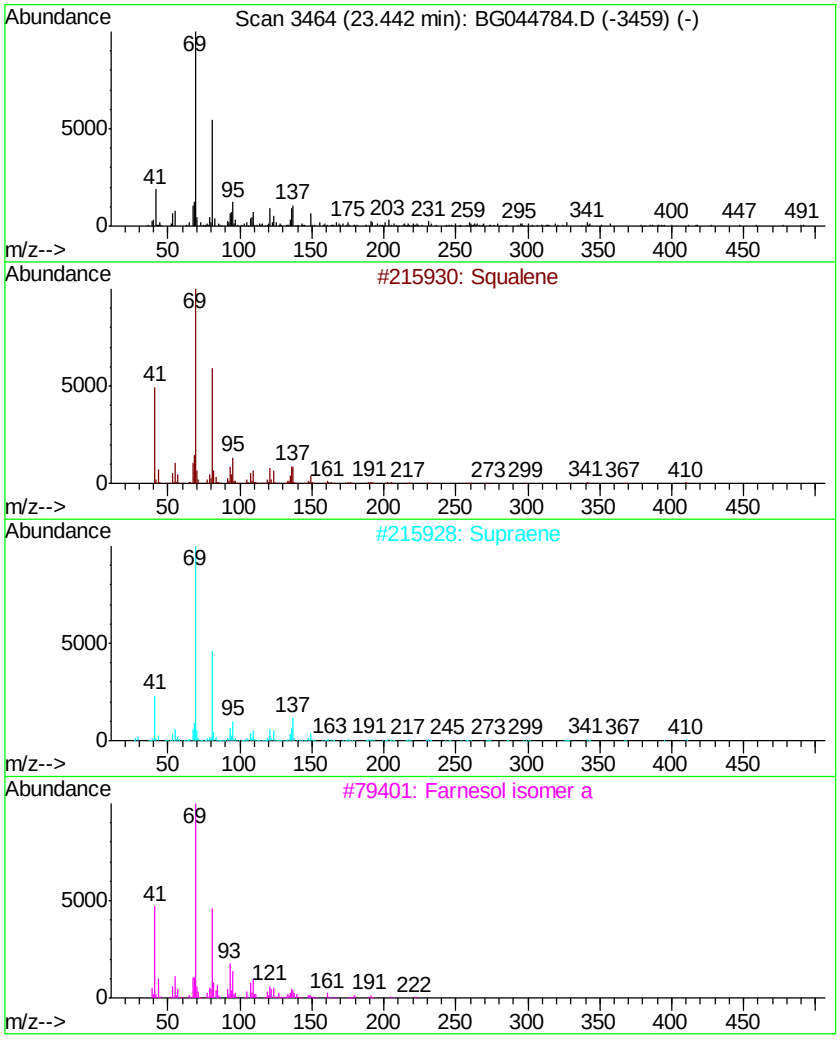
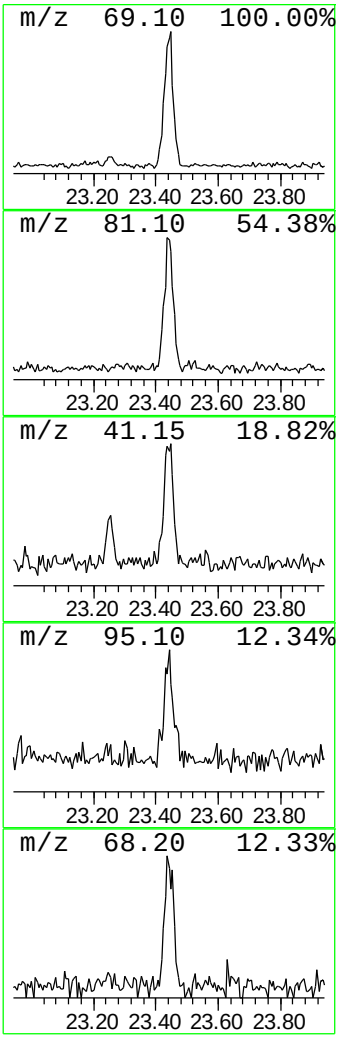
Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.44	2.70 ng	230795	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	86
3	Farnesol isomer a	222	C15H26O	1000108-92-4	74
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64





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
Cyclohexane	3.15	16.2	ng	656790	1	8.05	810952	20.0
Butane, 2-methoxy...	3.23	29.7	ng	1205330	1	8.05	810952	20.0
unknown5.16	5.16	3.0	ng	120069	1	8.05	810952	20.0
n-Hexadecanoic acid	18.33	2.4	ng	210692	4	17.43	1790850	20.0
9-Tricosene, (Z)-	21.36	4.1	ng	352718	5	21.70	1719750	20.0
Squalene	23.44	2.7	ng	230795	6	24.92	1711160	20.0