LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG032018\
Data File : BG033269.D
Acq On : 20 Mar 2018 16:04
Operator : SJ/JU
Sample : J1979-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A3960

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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	3.499	29	36	47	rBV2	133592	273562	7.48%	1.545%
2	3.587	47	51	61	rVB	97399	153905	4.21%	0.869%
3	5.802	420	428	434	rBV	31362	52419	1.43%	0.296%
4	6.313	506	515	536	rBV	246326	554846	15.18%	3.133%
5	7.999	794	802	826	rBV	150150	443756	12.14%	2.506%
6	8.405	863	871	885	rBV	486843	1074642	29.40%	6.068%
7	8.892	947	954	963	rBV2	111066	249469	6.83%	1.409%
8	9.227	1003	1011	1030	rBV	457582	978570	26.77%	5.526%
9	10.091	1151	1158	1180	rBV	390837	920878	25.20%	5.200%
10	11.777	1438	1445	1461	rBV2	172762	390594	10.69%	2.206%
11	14.139	1839	1847	1859	rBV	1266253	2160167	59.10%	12.198%
12	14.927	1973	1981	1987	rBV	87558	150317	4.11%	0.849%
13	15.338	2046	2051	2056	rBV	50367	69959	1.91%	0.395%
14	15.508	2074	2080	2087	rBV2	344005	595557	16.29%	3.363%
15	15.573	2087	2091	2097	rVB	38380	63779	1.75%	0.360%
16	16.272	2206	2210	2217	rVB	89738	116961	3.20%	0.660%
17	16.677	2272	2279	2282	rBV3	24759	45322	1.24%	0.256%
18	16.983	2324	2331	2342	rBV	1146339	1940688	53.10%	10.959%
19	17.130	2352	2356	2365	rVB	75045	121950	3.34%	0.689%
20	17.917	2486	2490	2496	rVB	41269	56402	1.54%	0.318%
21	18.240	2539	2545	2553	rBV	476728	791983	21.67%	4.472%
22	18.652	2611	2615	2622	rVB4	23378	38262	1.05%	0.216%
23	19.039	2676	2681	2692	rBV	318757	502876	13.76%	2.840%
24	20.273	2887	2891	2898	rBV	137129	195961	5.36%	1.107%
25	20.761	2968	2974	2988	rBV	2729307	3654850	100.00%	20.639%
26	22.112	3200	3204	3216	rVB3	145127	278995	7.63%	1.575%
27	22.600	3280	3287	3299	rVB	459600	923937	25.28%	5.217%
28	24.486	3603	3608	3616	rVB9	15447	36912	1.01%	0.208%
29	26.395	3922	3933	3948	rBV2	258821	871140	23.84%	4.919%

Sum of corrected areas: 17708659

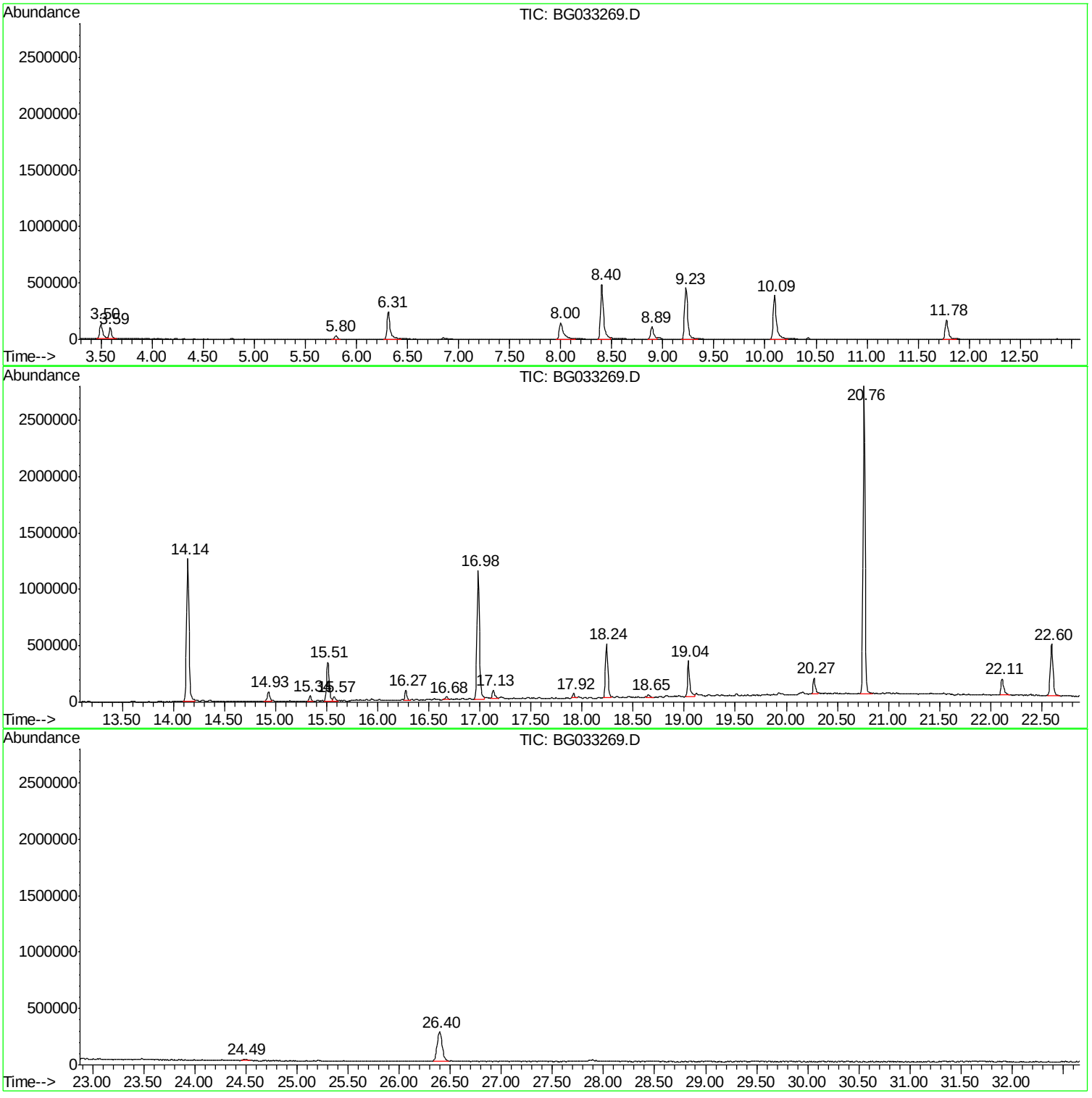
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG032018\
Data File : BG033269.D
Acq On : 20 Mar 2018 16:04
Operator : SJ/JU
Sample : J1979-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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 : BG033269.D
Acq On : 20 Mar 2018 16:04
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Sample : J1979-05
Misc :
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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

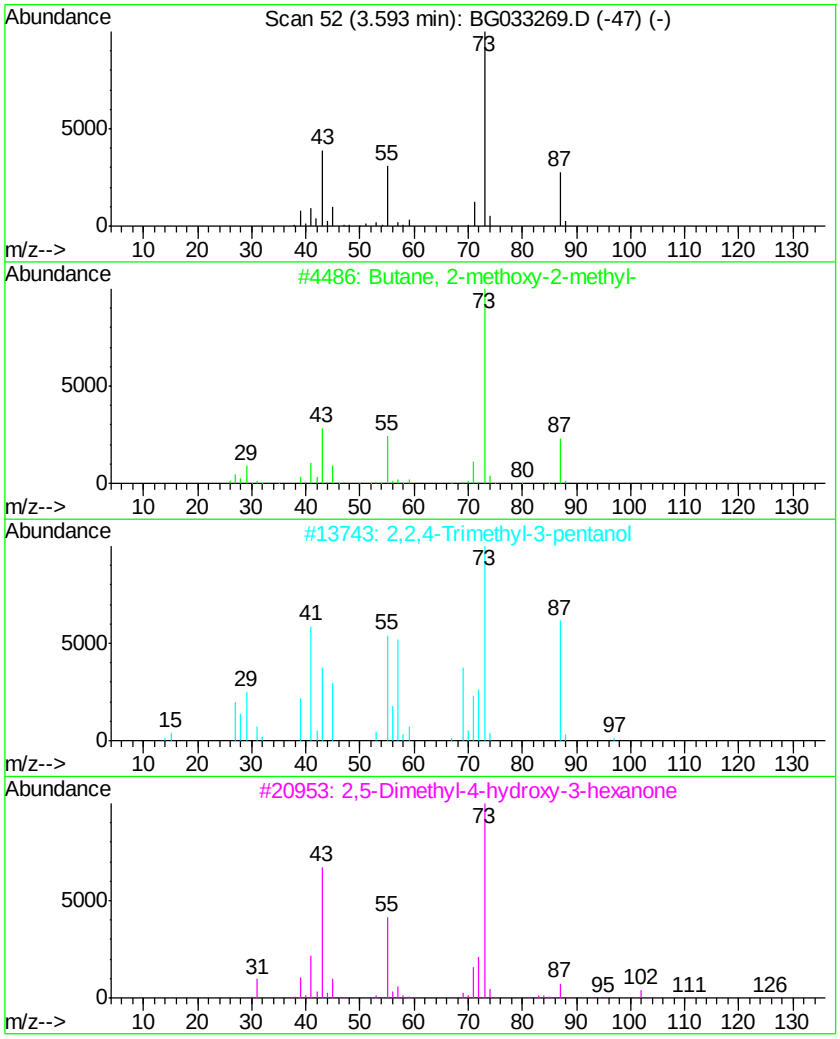
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

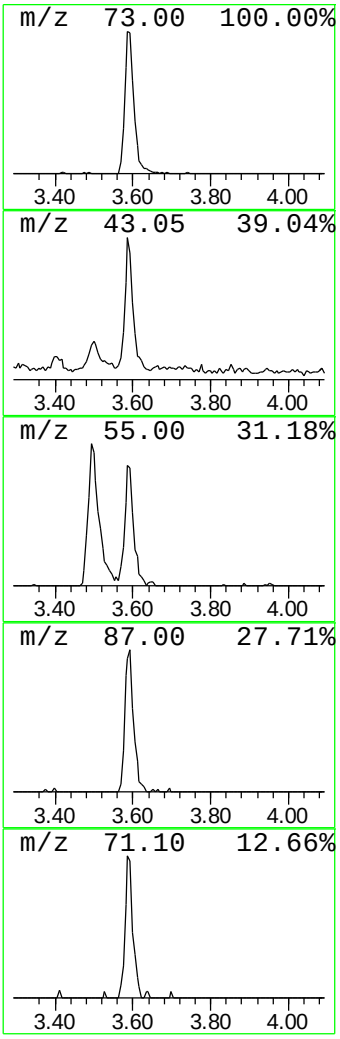
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	12.34 ng	153905	1,4-Dichlorobenzene-d4	8.89

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	40
3	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	33
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Data File : BG033269.D
Acq On : 20 Mar 2018 16:04
Operator : SJ/JU
Sample : J1979-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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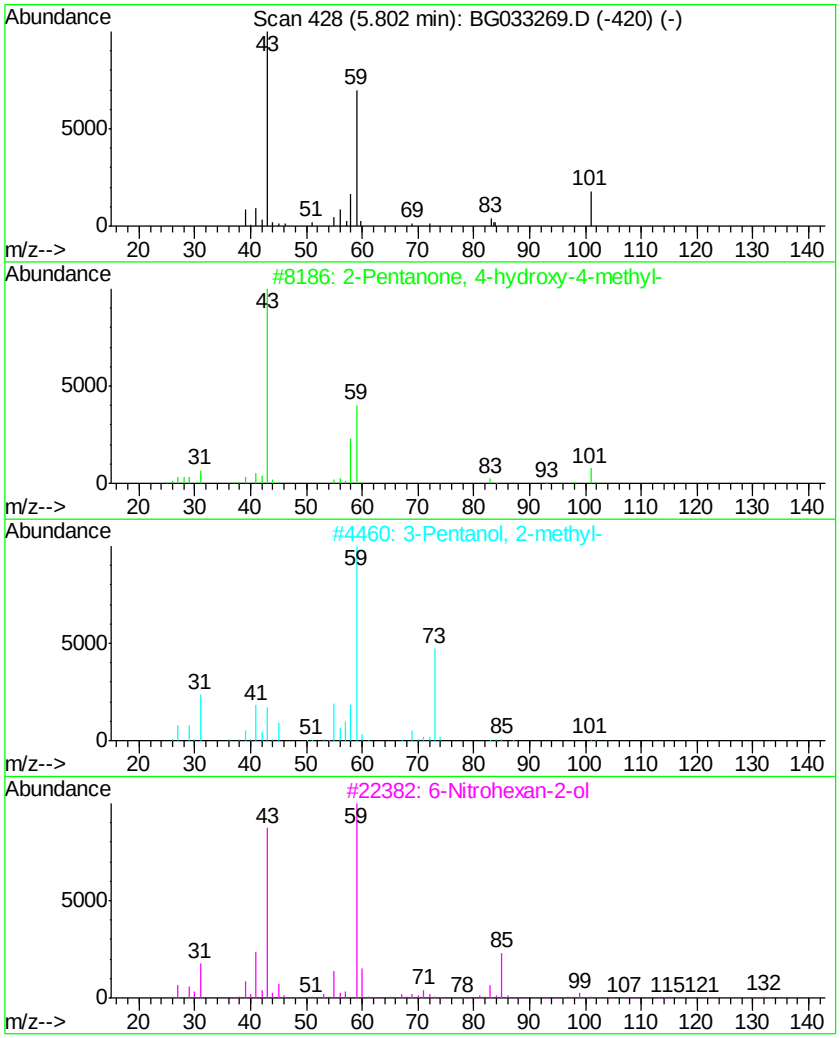
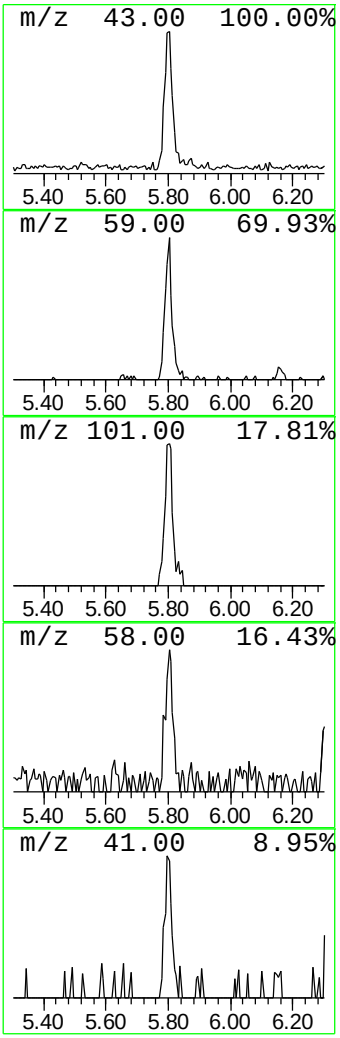
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	4.20 ng	52419	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	37
3	6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	33
4	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	33
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25





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Data File : BG033269.D
Acq On : 20 Mar 2018 16:04
Operator : SJ/JU
Sample : J1979-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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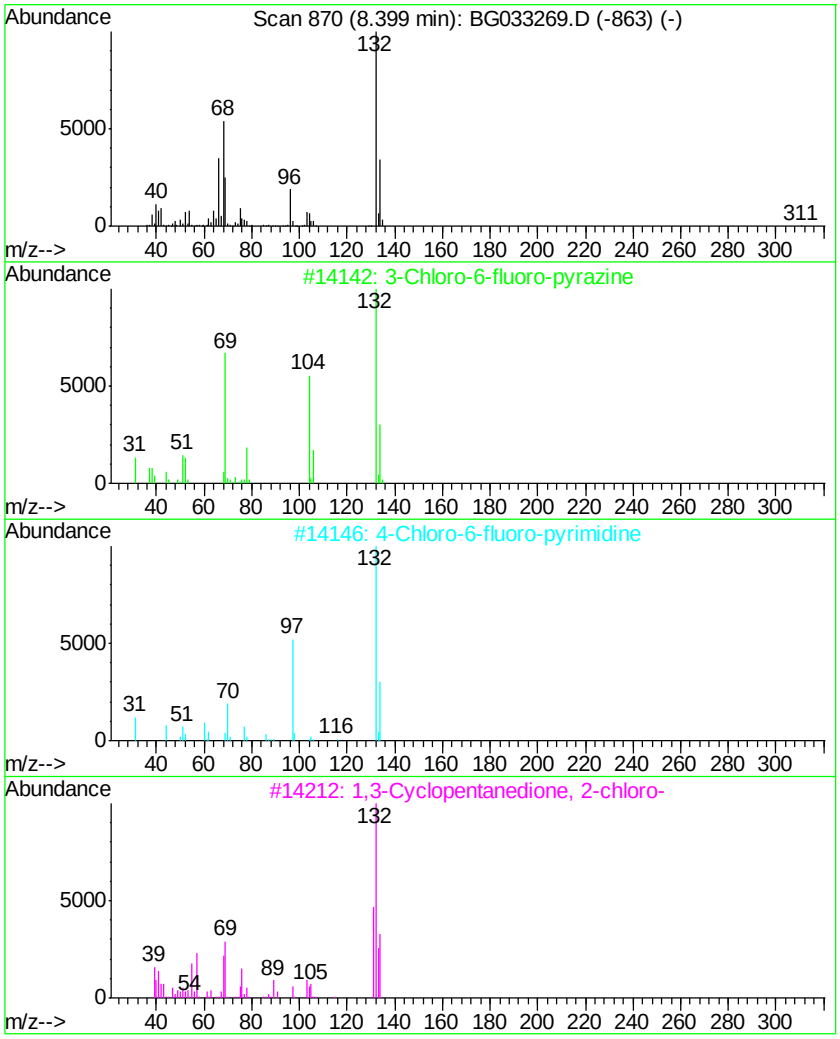
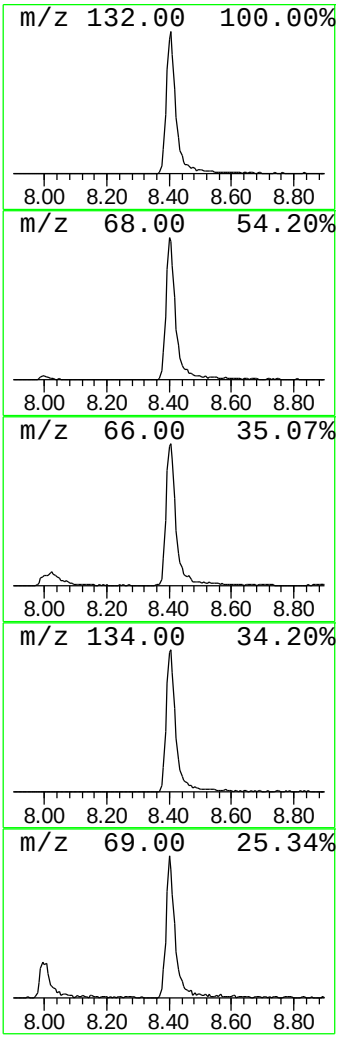
Peak Number 4 unknown8.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	86.15 ng	1074640	1,4-Dichlorobenzene-d4	8.89

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	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22





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Acq On : 20 Mar 2018 16:04
Operator : SJ/JU
Sample : J1979-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

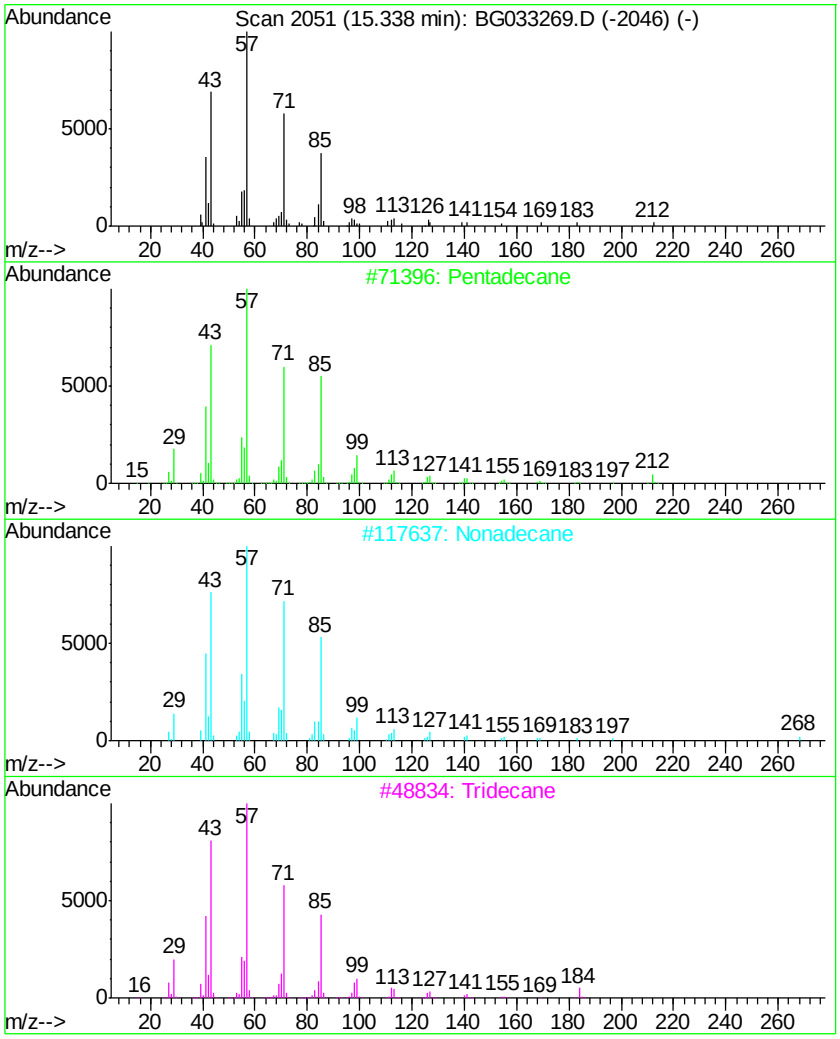
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

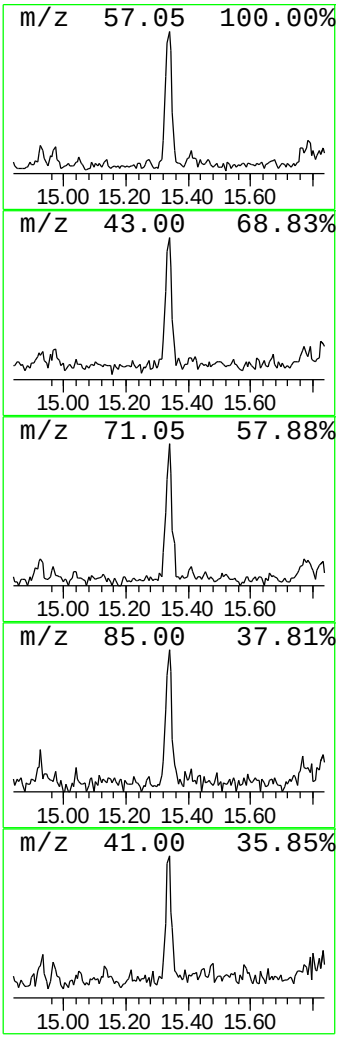
****

Peak Number 6 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.35 ng	69959	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Nonadecane	268	C19H40	000629-92-5	83
3	Tridecane	184	C13H28	000629-50-5	78
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	72
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG032018\
Data File : BG033269.D
Acq On : 20 Mar 2018 16:04
Operator : SJ/JU
Sample : J1979-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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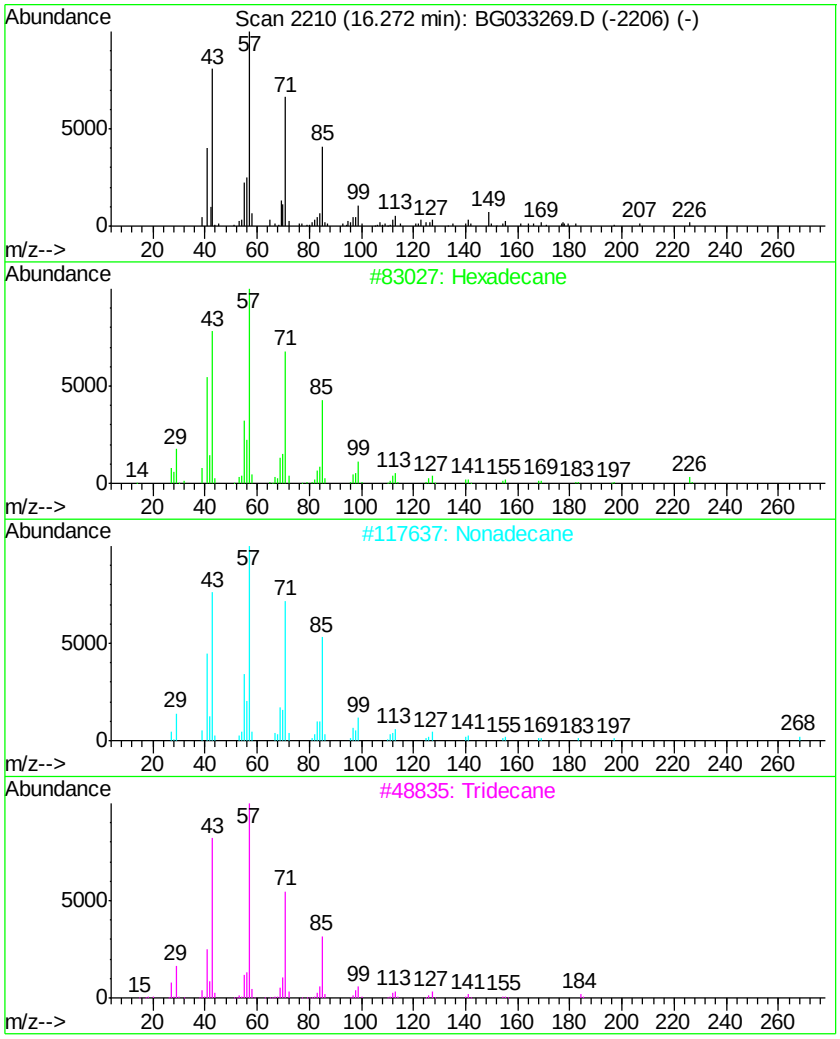
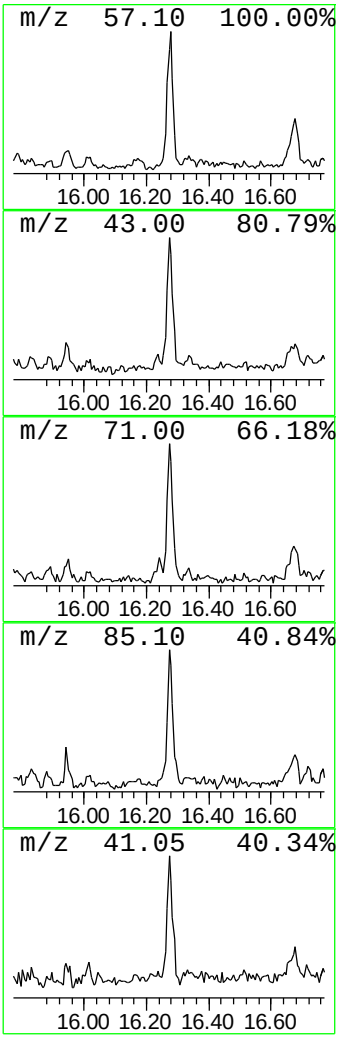
****

Peak Number 8 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	3.93 ng	116961	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Nonadecane	268	C19H40	000629-92-5	83
3	Tridecane	184	C13H28	000629-50-5	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Pentadecane	212	C15H32	000629-62-9	74





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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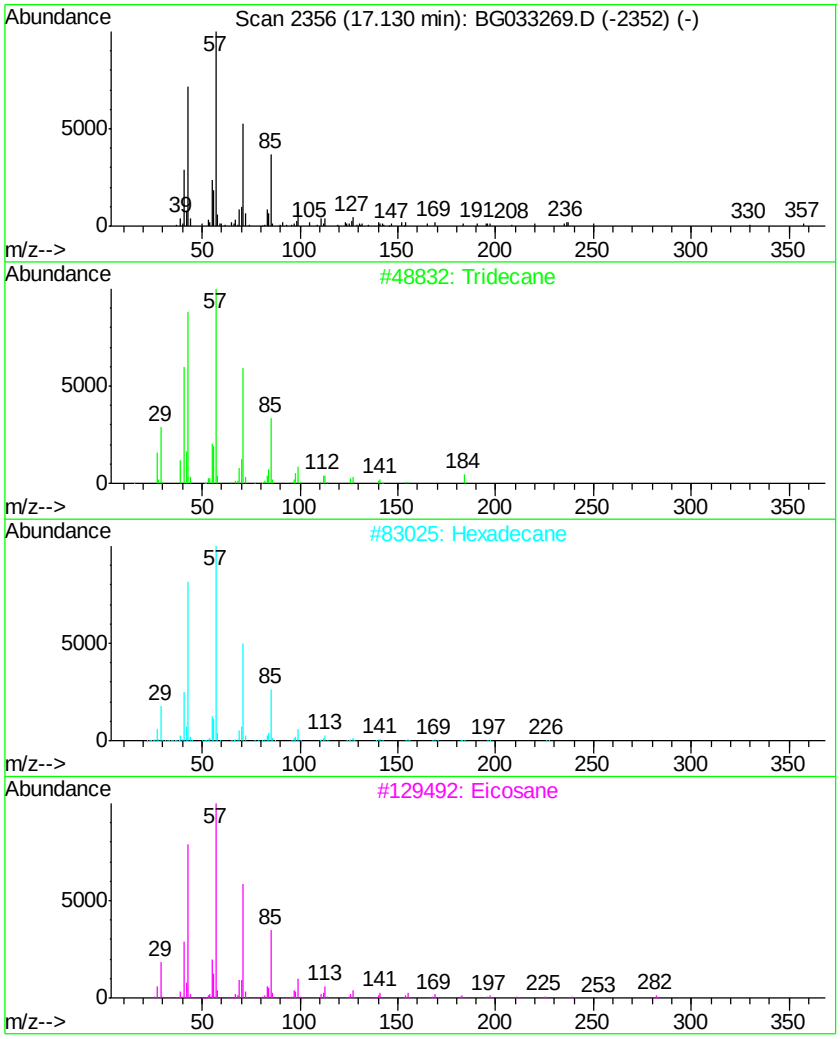
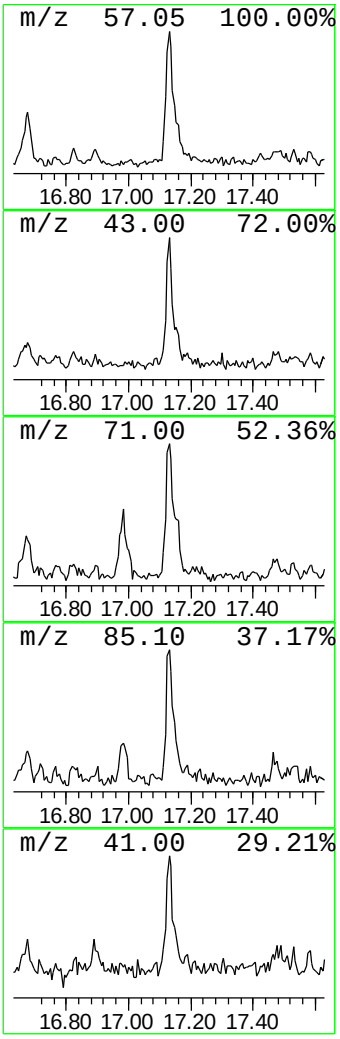
Peak Number 9 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	3.08 ng	121950	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	80
2	Hexadecane	226	C16H34	000544-76-3	80
3	Eicosane	282	C20H42	000112-95-8	80
4	Heptacosane	380	C27H56	000593-49-7	72
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	62





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Misc :
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Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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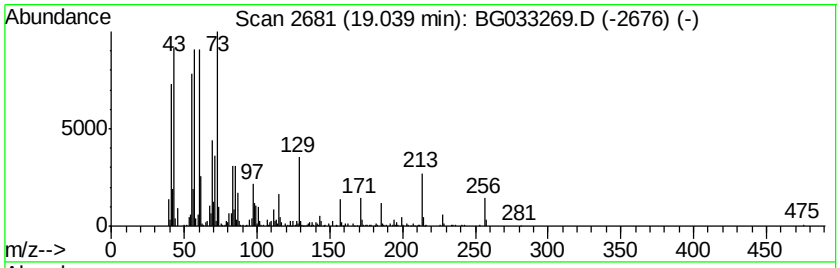
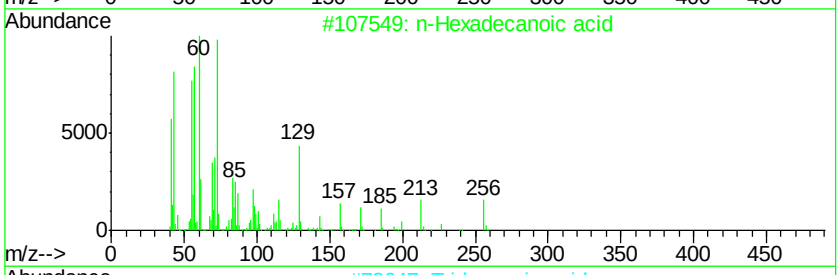
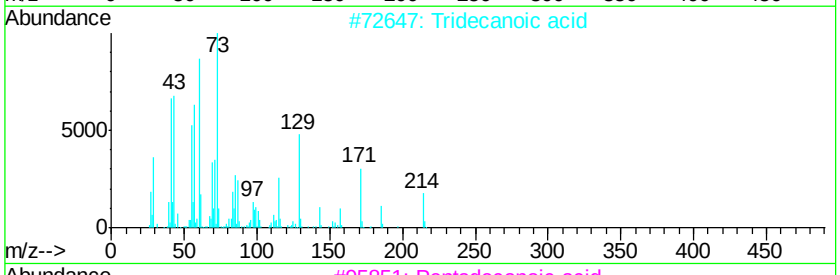
Peak Number 10 n-Hexadecanoic acid Concentration Rank 4

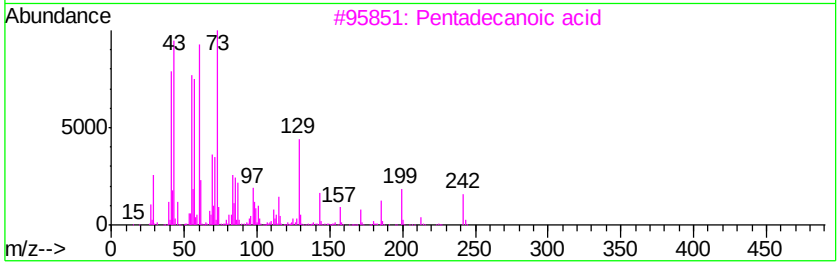
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	12.70 ng	502876	Phenanthrene-d10	18.24

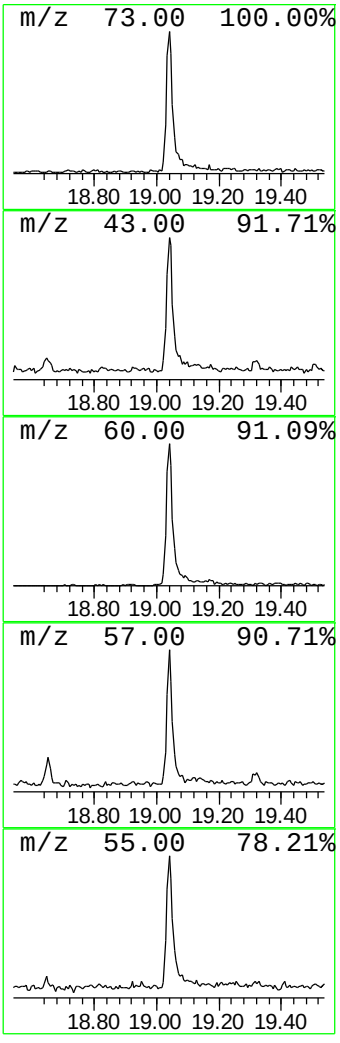
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59











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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

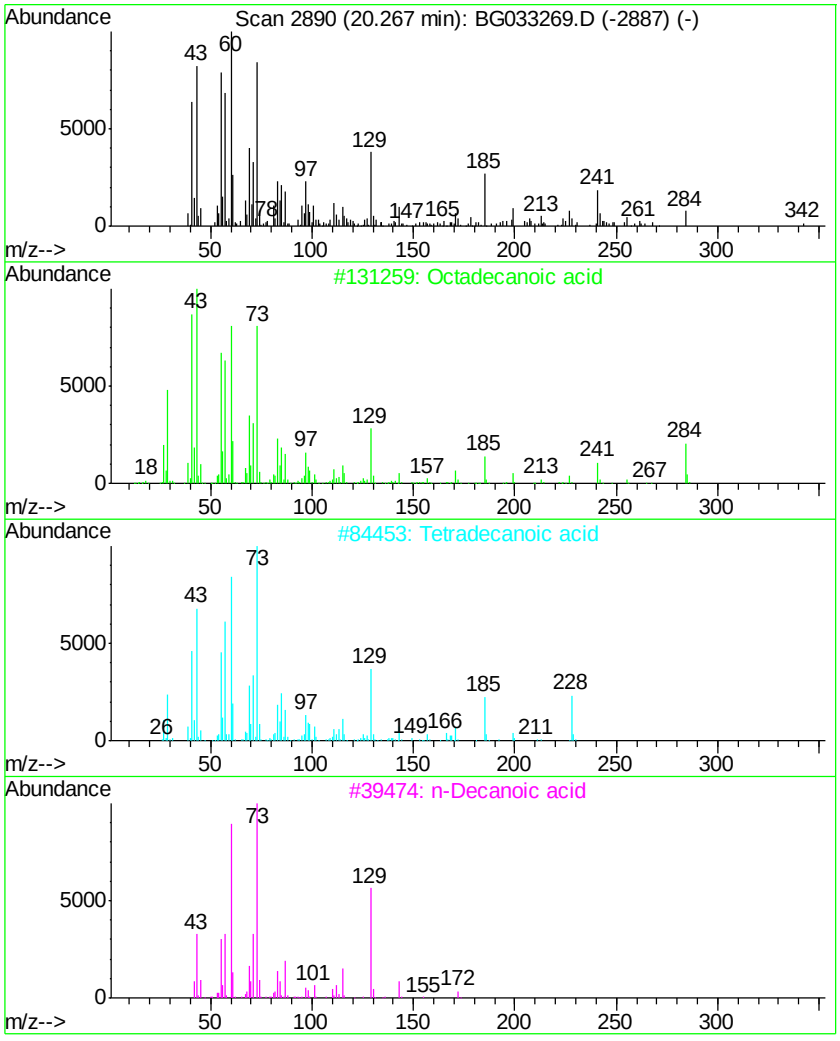
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

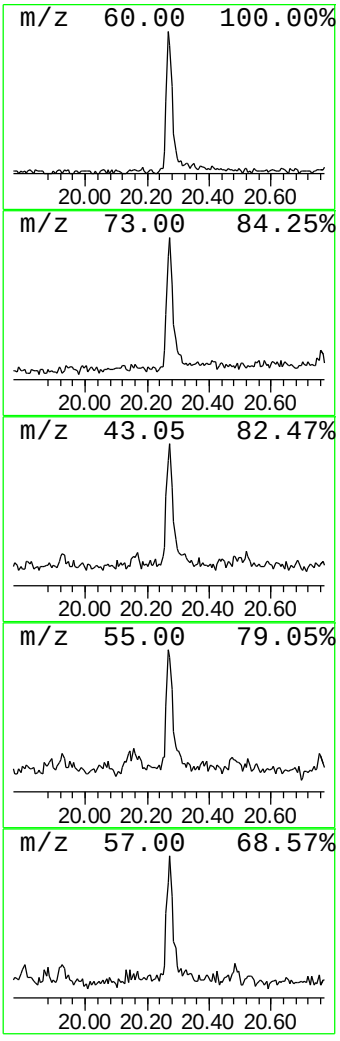
****

Peak Number 11 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	4.95 ng	195961	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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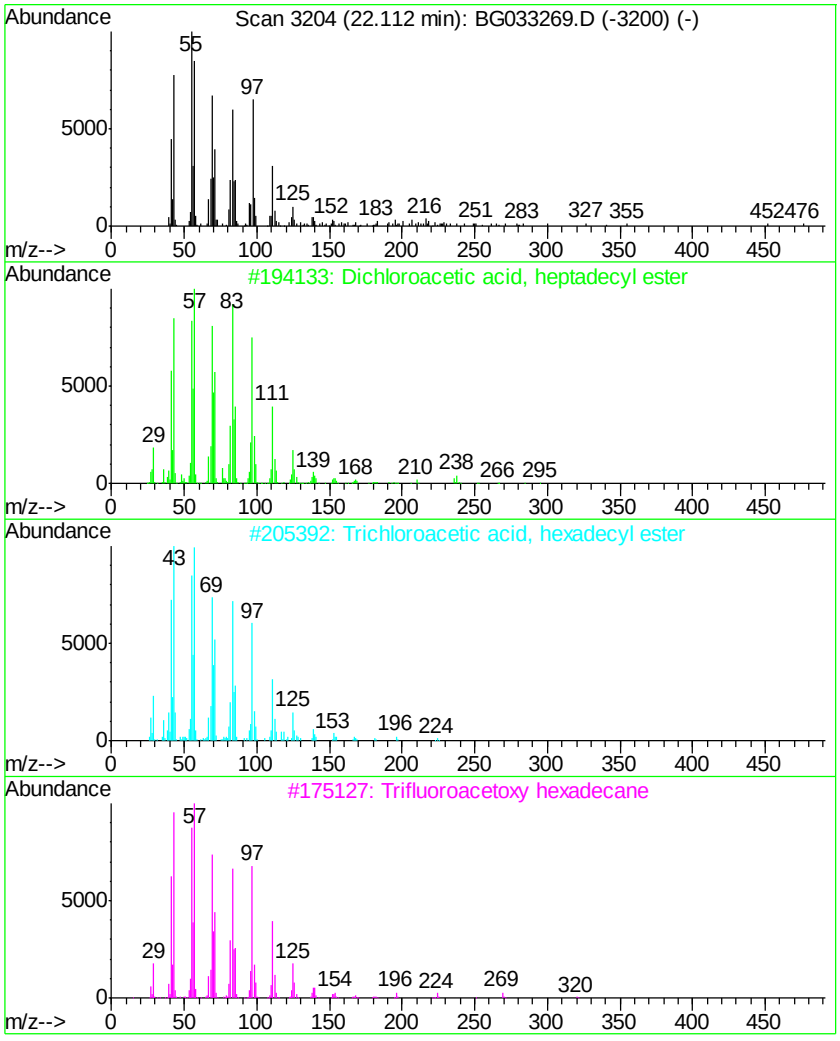
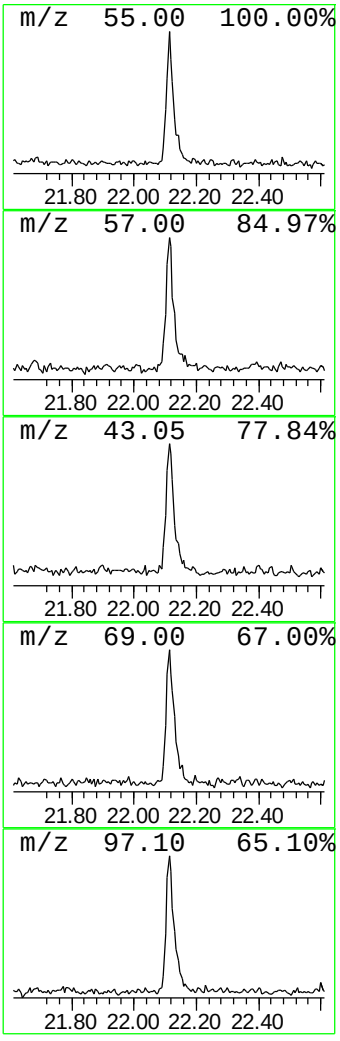
****

Peak Number 12 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	6.04 ng	278995	Chrysene-d12	22.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	1-Tricosene	322	C23H46	018835-32-0	91
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG032018\
Data File : BG033269.D
Acq On : 20 Mar 2018 16:04
Operator : SJ/JU
Sample : J1979-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A3960

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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...	3.59	12.3	ng	153905	1	8.89	249469	20.0
2-Pentanone, 4-hy...	5.80	4.2	ng	52419	1	8.89	249469	20.0
unknown8.40	8.40	86.2	ng	1074640	1	8.89	249469	20.0
Pentadecane	15.34	2.4	ng	69959	3	15.51	595557	20.0
Hexadecane	16.27	3.9	ng	116961	3	15.51	595557	20.0
Tridecane	17.13	3.1	ng	121950	4	18.24	791983	20.0
n-Hexadecanoic acid	19.04	12.7	ng	502876	4	18.24	791983	20.0
Octadecanoic acid	20.27	5.0	ng	195961	4	18.24	791983	20.0
Dichloroacetic ac...	22.11	6.0	ng	278995	5	22.60	923937	20.0