LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033257.D
Acq On : 20 Mar 2018 1:59
Operator : SJ/JU
Sample : J1953-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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	30	36	47	rBV	131909	267666	6.55%	1.512%
2	3.587	47	51	60	rVB	73458	118689	2.91%	0.670%
3	6.313	508	515	529	rBV	143830	333263	8.16%	1.882%
4	7.999	794	802	817	rBV	82414	250410	6.13%	1.414%
5	8.405	863	871	894	rBV	326037	757526	18.55%	4.278%
6	8.893	948	954	968	rBV2	96114	221579	5.43%	1.251%
7	9.227	1003	1011	1025	rBV	480853	986393	24.15%	5.571%
8	10.091	1150	1158	1166	rBV	404158	873795	21.40%	4.935%
9	10.226	1168	1181	1195	rVB2	247714	930375	22.78%	5.254%
10	11.002	1303	1313	1328	rBV2	45291	170905	4.19%	0.965%
11	11.777	1438	1445	1458	rBV	147486	320887	7.86%	1.812%
12	12.629	1582	1590	1602	rBV6	20920	70229	1.72%	0.397%
13	14.139	1838	1847	1868	rBV	1367596	2346877	57.47%	13.254%
14	14.927	1974	1981	1987	rBV	34087	56688	1.39%	0.320%
15	15.279	2032	2041	2047	rBV	215318	424991	10.41%	2.400%
16	15.338	2047	2051	2057	rVB3	36410	58428	1.43%	0.330%
17	15.508	2074	2080	2091	rVB3	306547	534096	13.08%	3.016%
18	15.767	2118	2124	2132	rBV7	15104	41712	1.02%	0.236%
19	16.190	2189	2196	2200	rBV4	20166	48170	1.18%	0.272%
20	16.272	2207	2210	2215	rVB	49609	64111	1.57%	0.362%
21	16.983	2324	2331	2341	rBV	928266	1576469	38.60%	8.903%
22	17.130	2352	2356	2367	rVB2	45336	79223	1.94%	0.447%
23	17.917	2486	2490	2496	rVB2	32583	41244	1.01%	0.233%
24	18.240	2536	2545	2558	rBV	467125	809401	19.82%	4.571%
25	19.034	2676	2680	2687	rBV	115524	185843	4.55%	1.050%
26	20.267	2884	2890	2897	rBV7	29839	60698	1.49%	0.343%
27	20.761	2967	2974	2985	rBV	2970809	4083673	100.00%	23.063%
28	22.106	3198	3203	3218	rBV3	110941	230902	5.65%	1.304%
29	22.594	3279	3286	3299	rVB2	461648	899401	22.02%	5.079%
30	26.390	3920	3932	3946	rBV3	254052	862900	21.13%	4.873%

Sum of corrected areas: 17706544

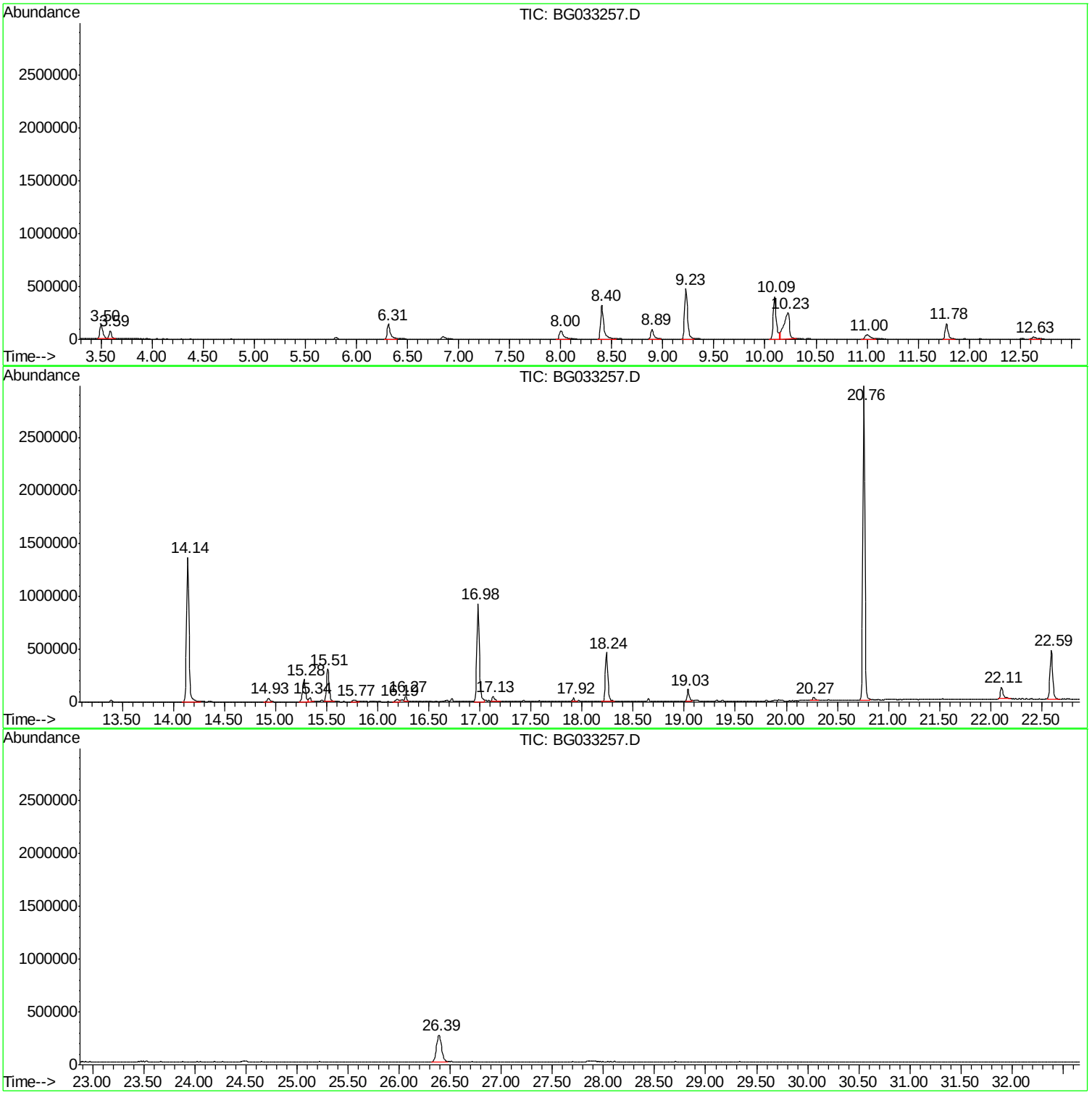
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033257.D
Acq On : 20 Mar 2018 1:59
Operator : SJ/JU
Sample : J1953-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

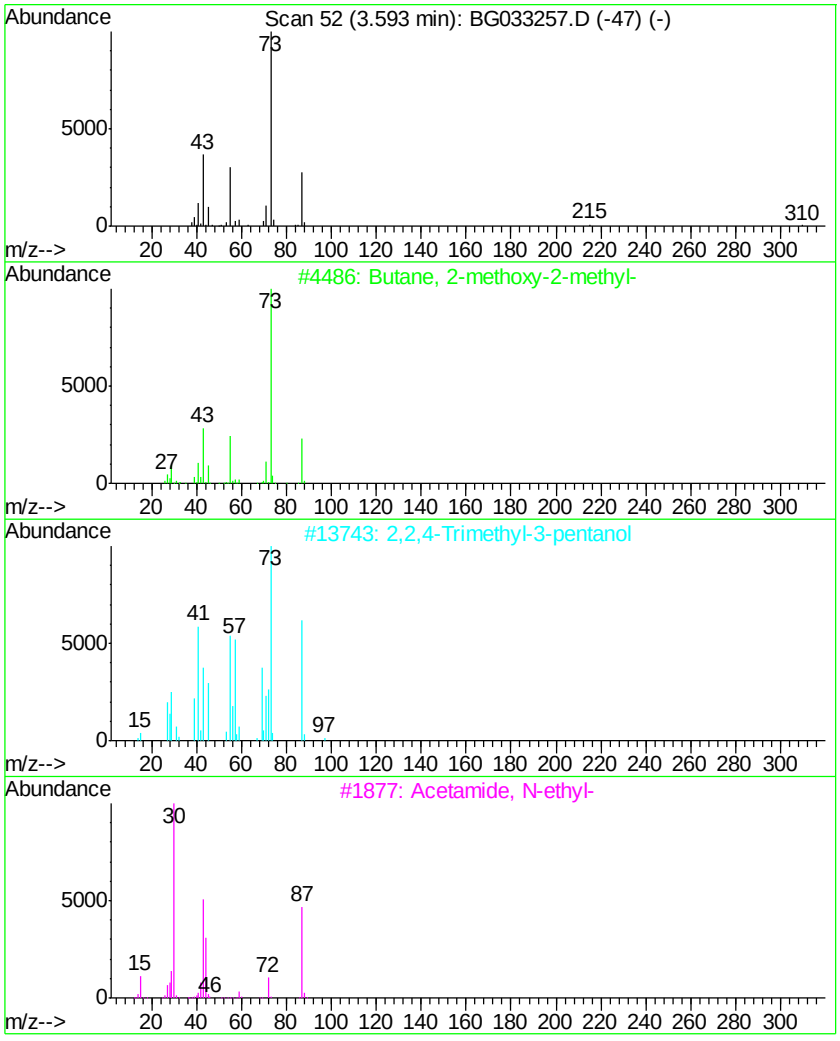
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

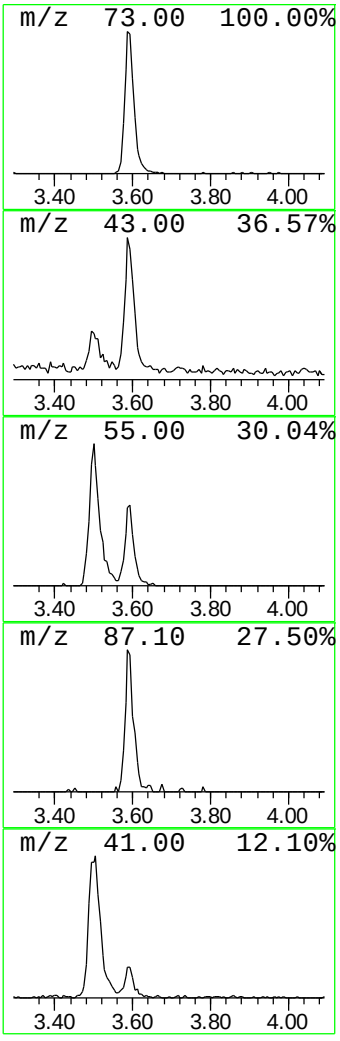
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	10.71 ng	118689	1,4-Dichlorobenzene-d4	8.90

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





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Sample : J1953-08
Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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

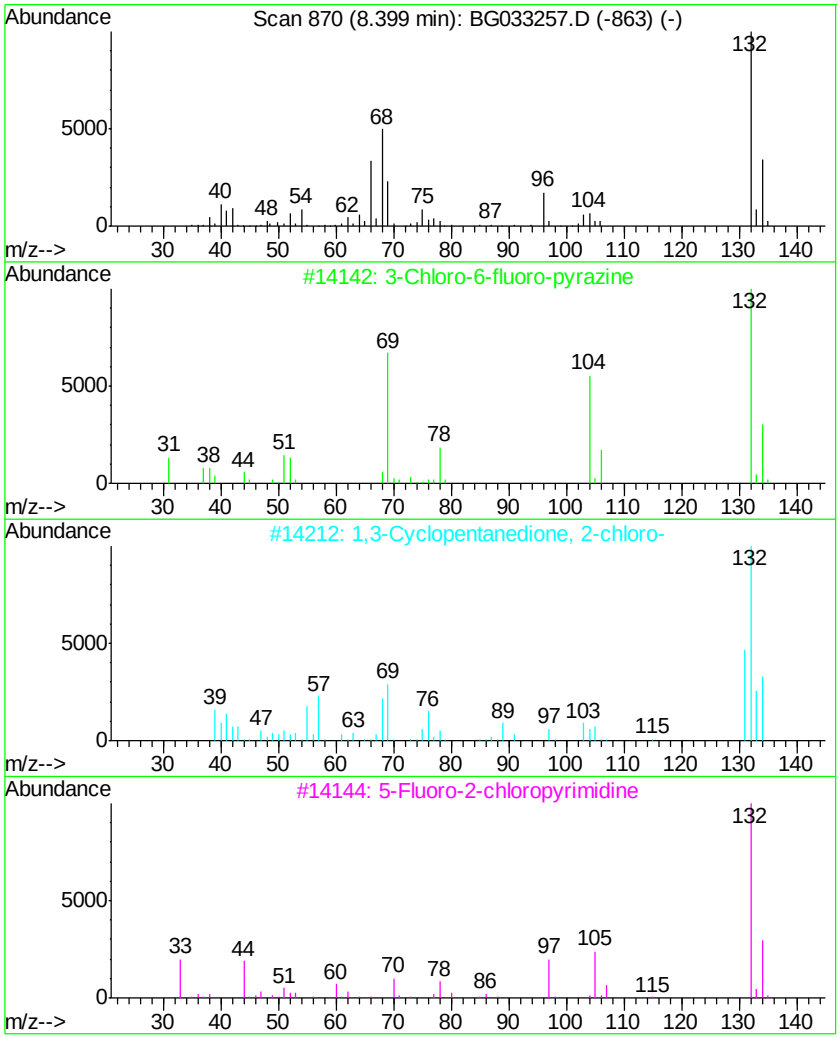
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

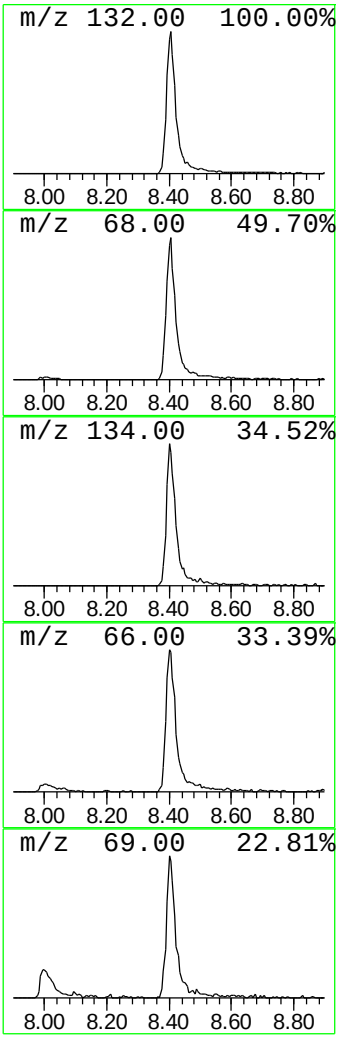
****

Peak Number 3 unknown8.40 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	68.38 ng	757526	1,4-Dichlorobenzene-d4	8.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





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Operator : SJ/JU
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Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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

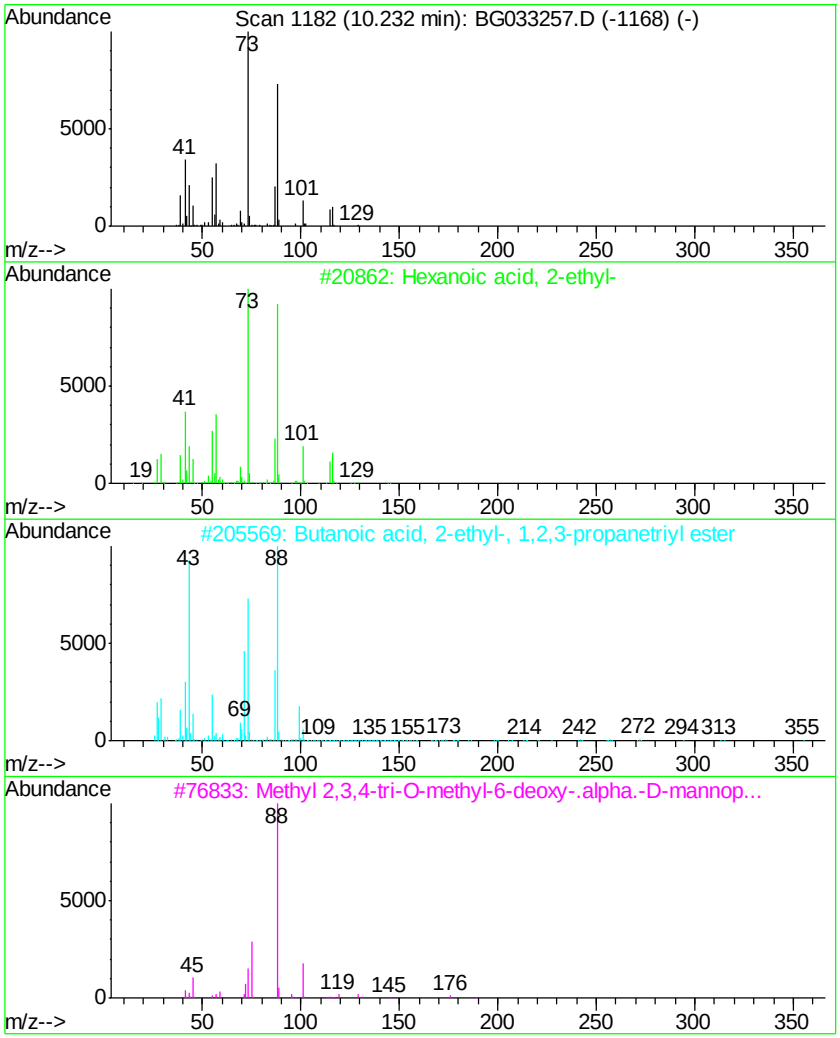
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

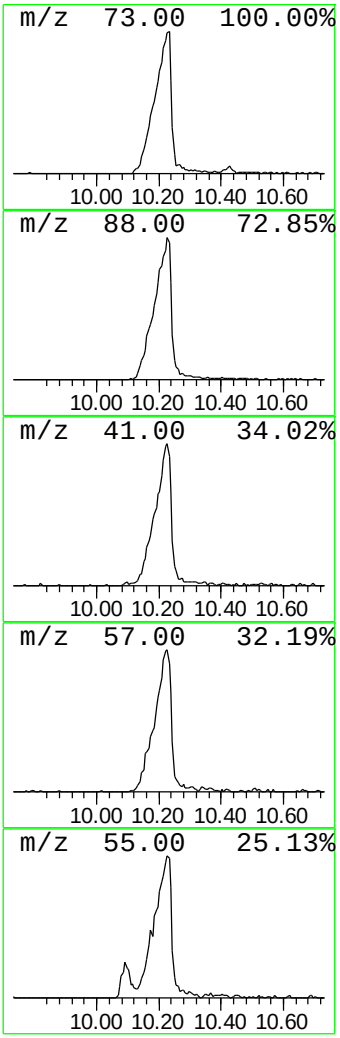
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	83.98 ng	930375	1,4-Dichlorobenzene-d4	8.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	56
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	53
4	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	42
5	1,4-Dioxane	88	C4H8O2	000123-91-1	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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Operator : SJ/JU
Sample : J1953-08
Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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

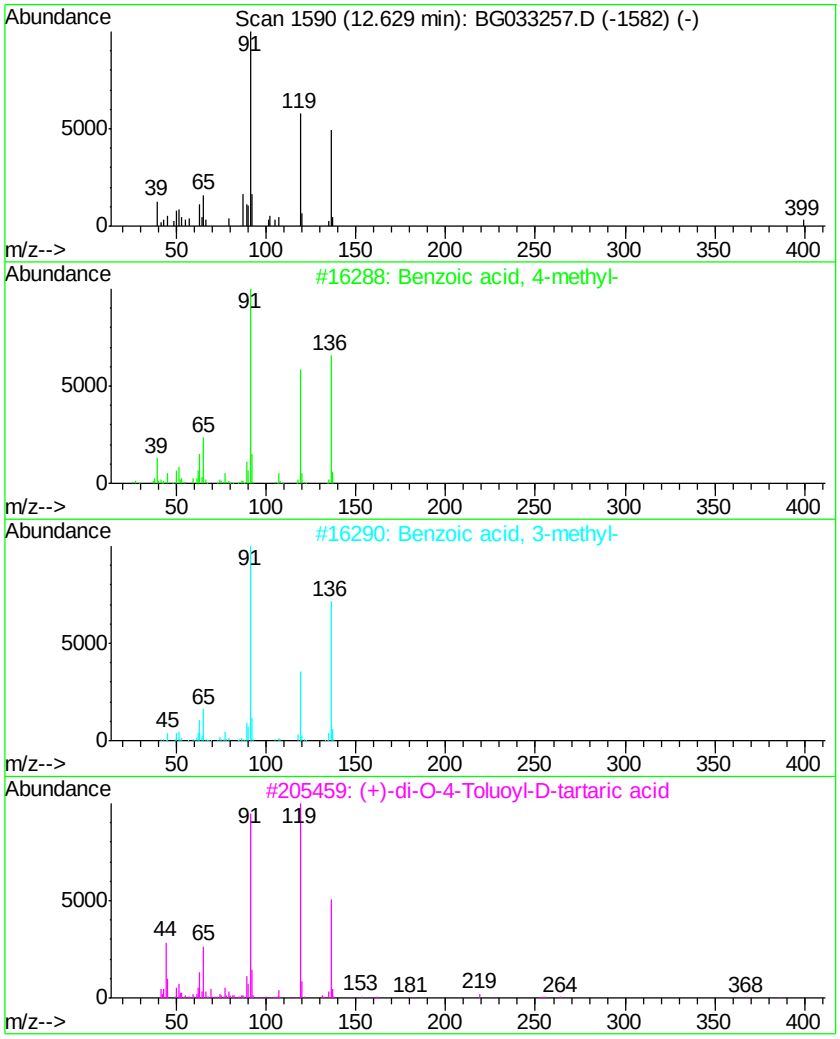
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

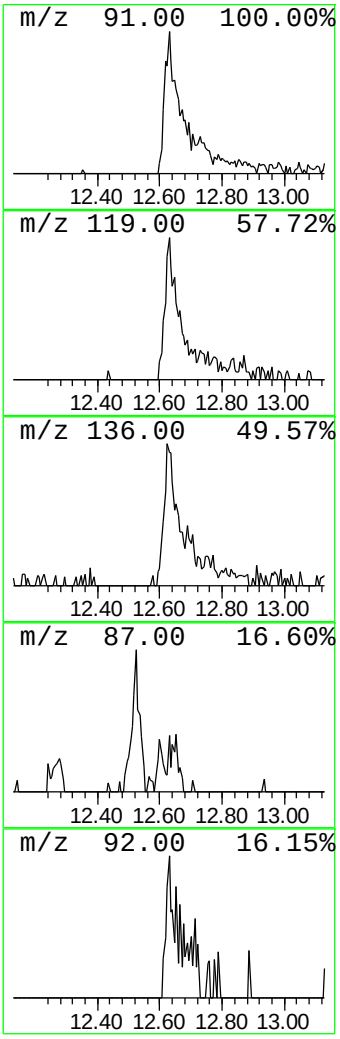
****

Peak Number 6 Benzoic acid, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	4.38 ng	70229	Naphthalene-d8	11.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	90
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	68
3	(+)-di-O-4-Toluoyl-D-tartaric acid	386	C20H18O8	032634-68-7	50
4	o-Toluic acid, 4-methylpentyl ester	220	C14H20O2	1000293-42-2	50
5	Ethyl 4-methylbenzoate	164	C10H12O2	000094-08-6	47





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Sample : J1953-08
Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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

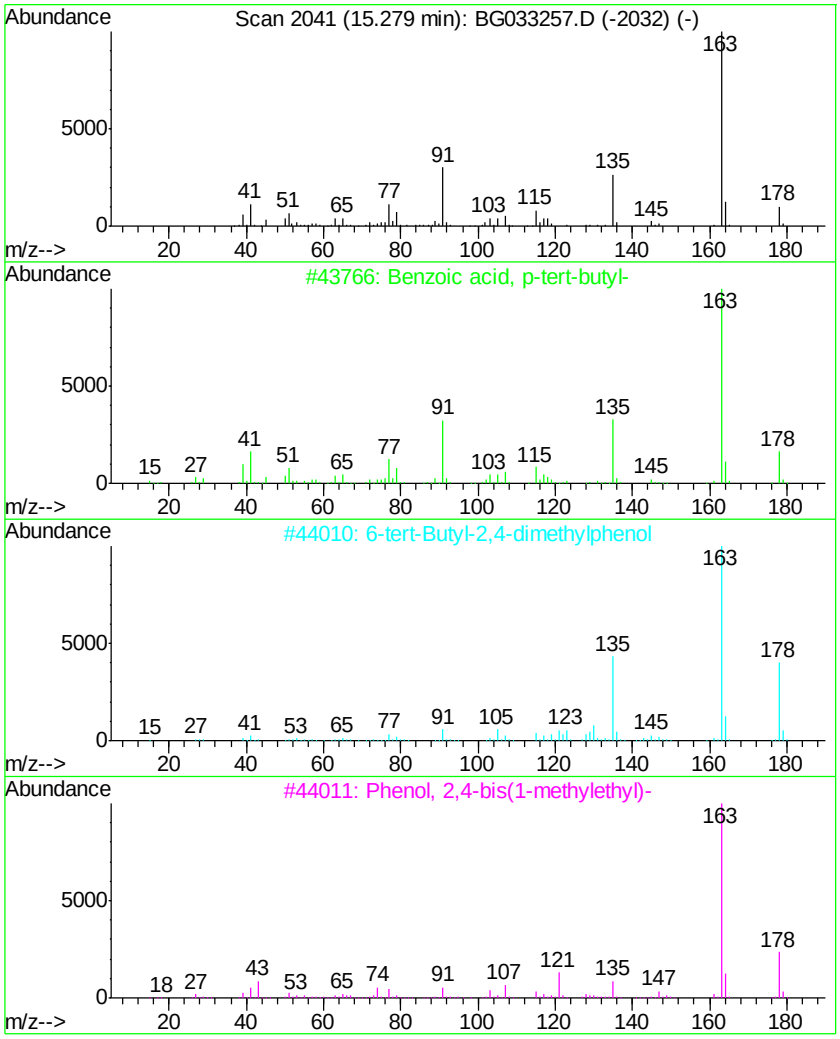
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

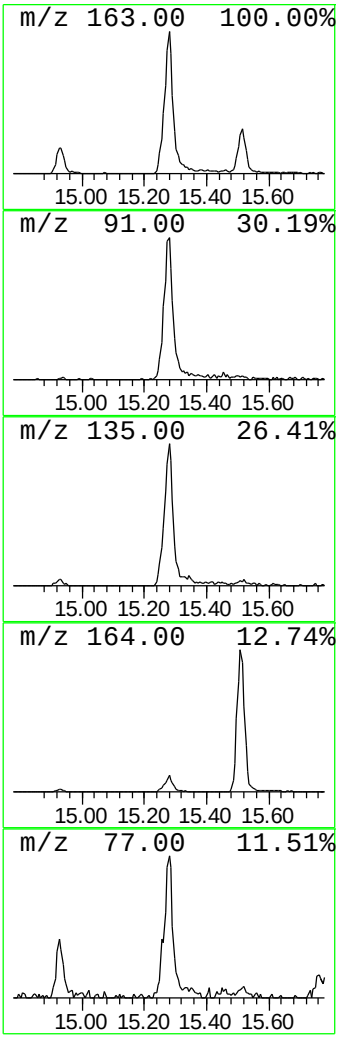
****

Peak Number 7 Benzoic acid, p-tert-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	15.91 ng	424991	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	93
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	64
3	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	59
4	Silane, (4-ethylphenyl)trimethyl-	178	C11H18Si	017988-50-0	53
5	Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	53





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Sample : J1953-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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

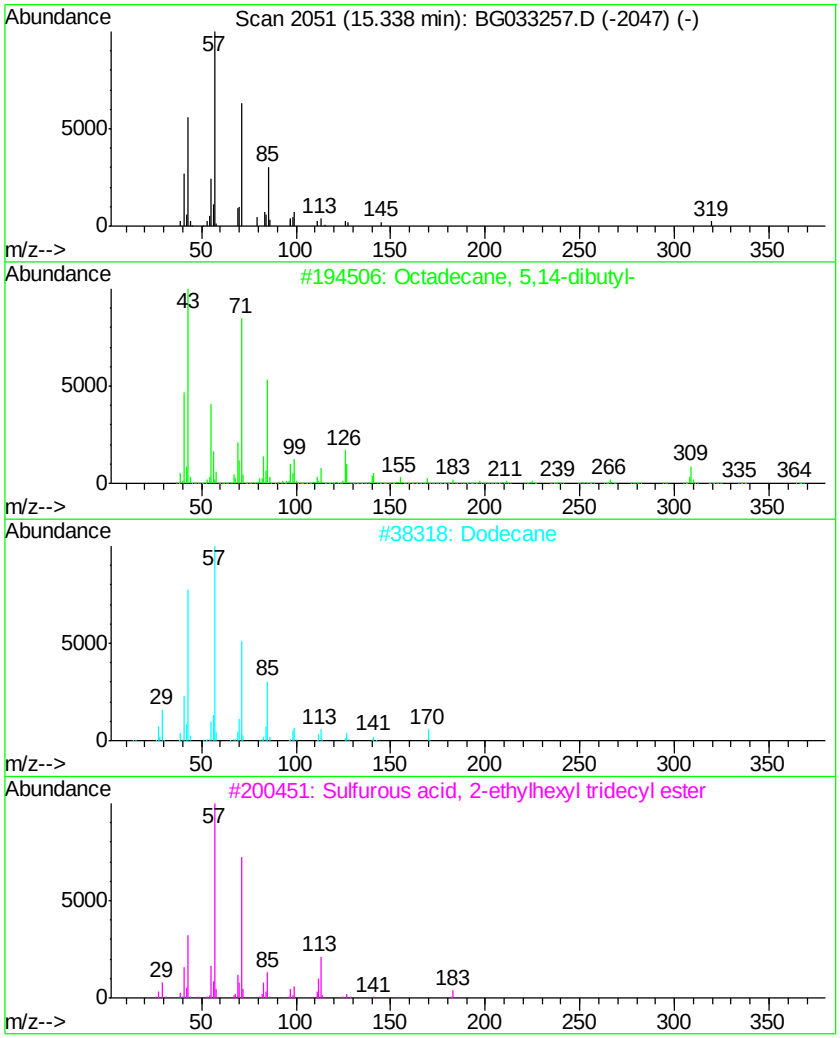
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

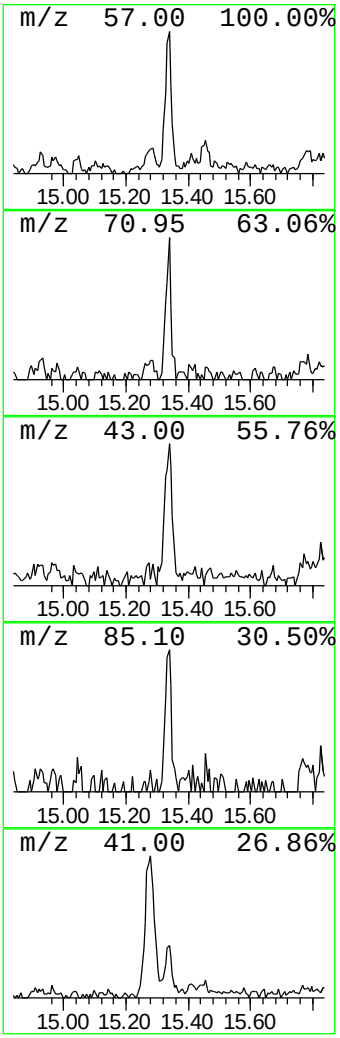
****

Peak Number 8 Octadecane, 5,14-dibutyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.19 ng	58428	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	72
2	Dodecane	170	C12H26	000112-40-3	72
3	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	64
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	59
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	59





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Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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

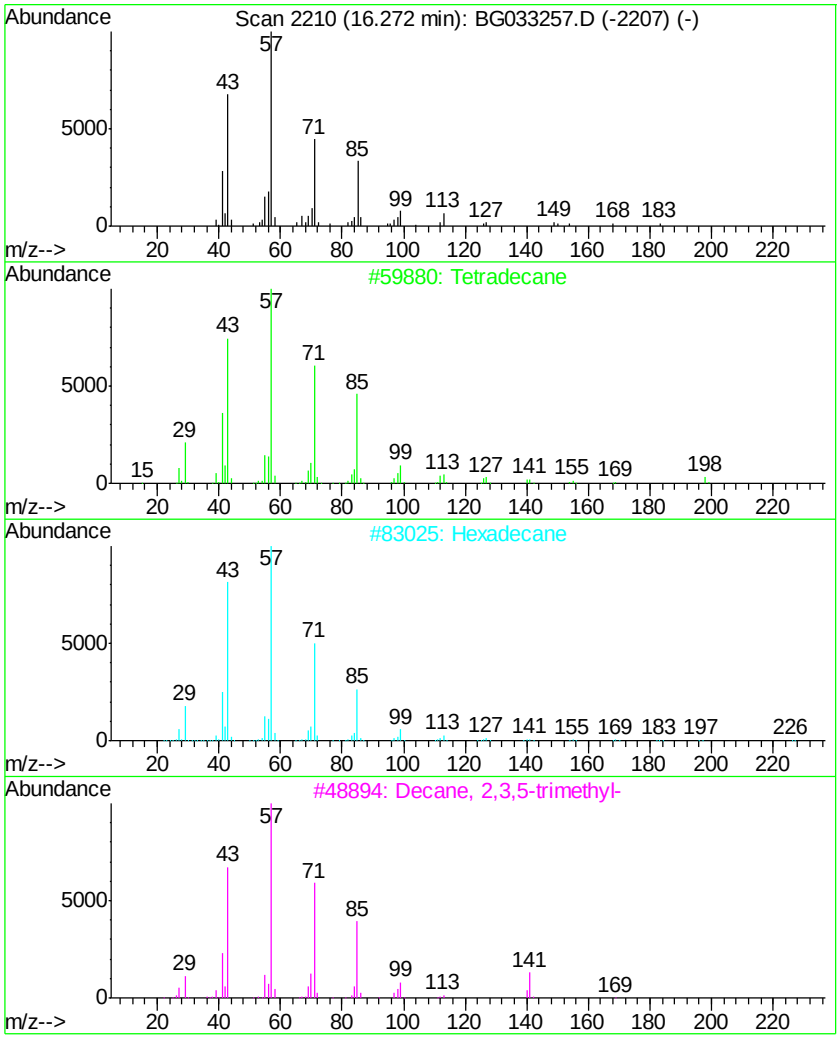
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

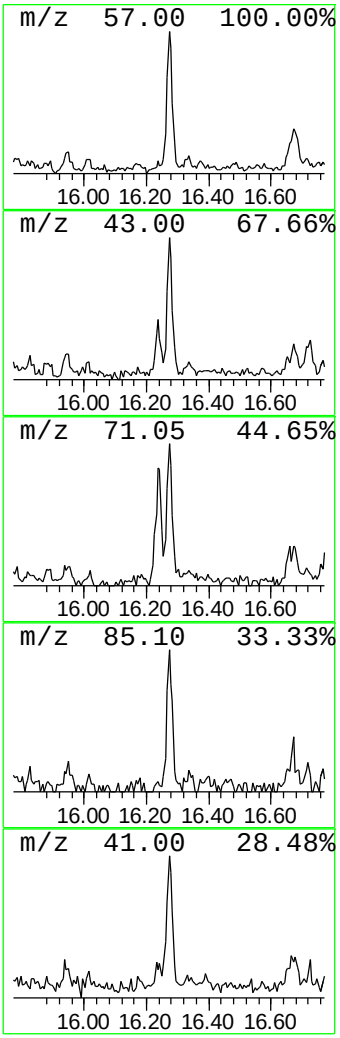
****

Peak Number 9 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	2.40 ng	64111	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	78
2	Hexadecane	226	C16H34	000544-76-3	78
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	78
5	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	72





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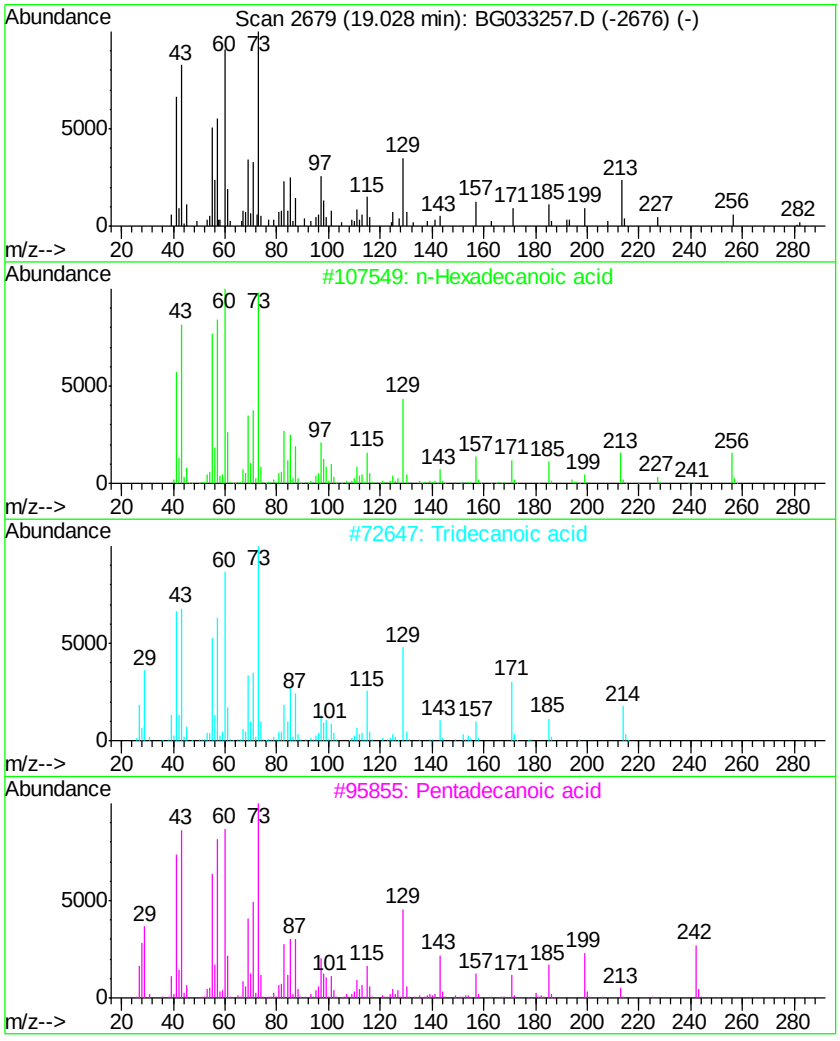
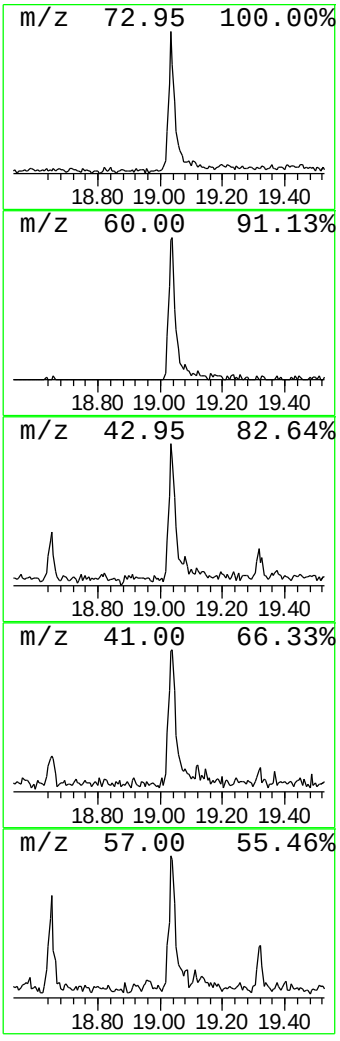
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	4.59 ng	185843	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70





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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-B

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

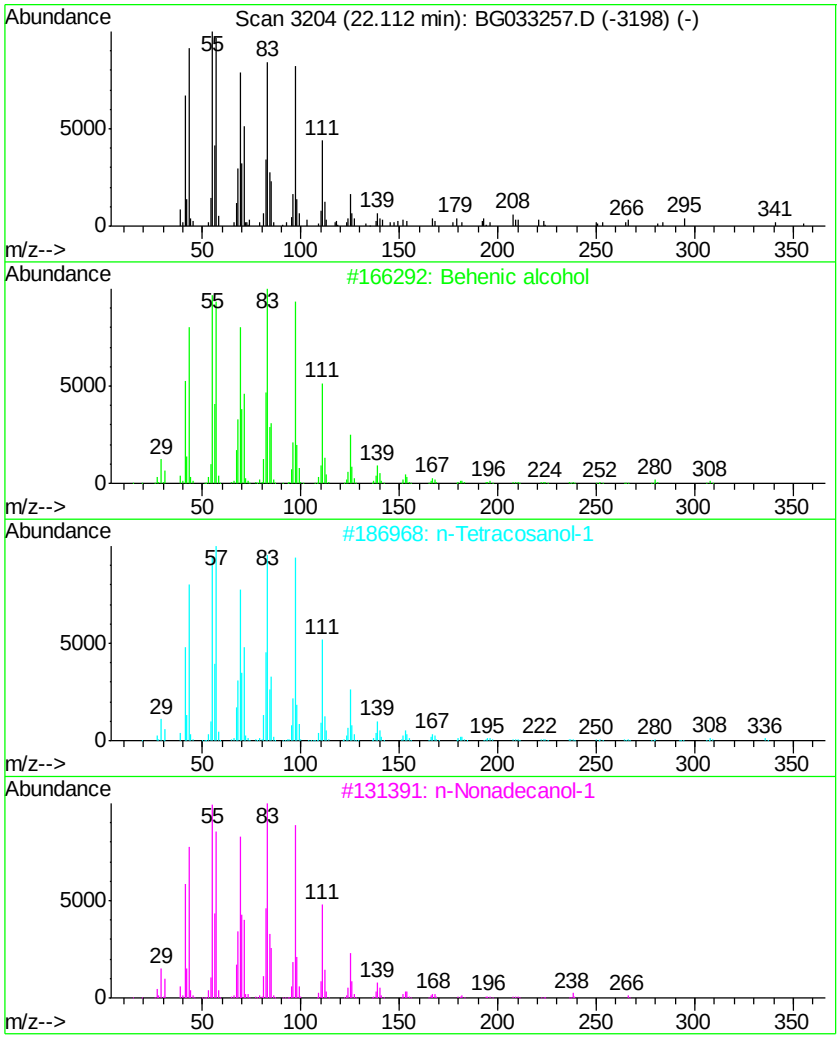
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

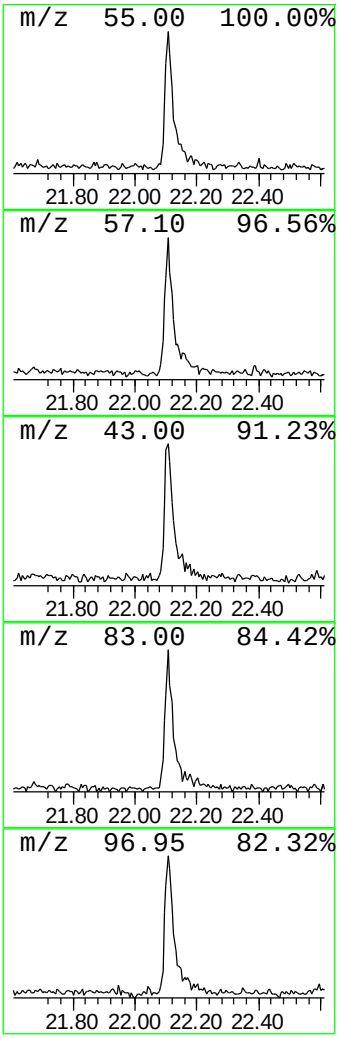
****

Peak Number 11 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	5.13 ng	230902	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
4	1-Heneicosanol	312	C21H44O	015594-90-8	87
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.59	10.7	ng	118689	1	8.90	221579	20.0
unknown8.40	8.40	68.4	ng	757526	1	8.90	221579	20.0
Hexanoic acid, 2-...	10.23	84.0	ng	930375	1	8.90	221579	20.0
Benzoic acid, 4-m...	12.63	4.4	ng	70229	2	11.78	320887	20.0
Benzoic acid, p-t...	15.28	15.9	ng	424991	3	15.51	534096	20.0
Octadecane, 5,14-...	15.34	2.2	ng	58428	3	15.51	534096	20.0
Tetradecane	16.27	2.4	ng	64111	3	15.51	534096	20.0
n-Hexadecanoic acid	19.03	4.6	ng	185843	4	18.24	809401	20.0
Behenic alcohol	22.11	5.1	ng	230902	5	22.59	899401	20.0