LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043546.D
Acq On : 7 Nov 2019 19:30
Operator : JU
Sample : K5723-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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	3.173	8	14	27	rVB	103901	187763	8.68%	1.517%
2	5.112	337	344	352	rBV	100677	158377	7.32%	1.280%
3	5.606	421	428	440	rBV	474280	833352	38.53%	6.734%
4	7.216	694	702	722	rBV	501907	973792	45.03%	7.869%
5	7.556	751	760	776	rBV	540276	957188	44.26%	7.735%
6	8.009	829	837	845	rBV	102525	182535	8.44%	1.475%
7	8.332	884	892	904	rBV	414629	728028	33.66%	5.883%
8	9.172	1027	1035	1049	rBV	273946	562220	26.00%	4.543%
9	10.811	1306	1314	1325	rBV	111558	228653	10.57%	1.848%
10	13.261	1722	1731	1747	rBV	761211	1299675	60.09%	10.502%
11	14.090	1866	1872	1886	rBV	78389	142256	6.58%	1.150%
12	14.542	1942	1949	1956	rBV4	37711	64418	2.98%	0.521%
13	14.636	1958	1965	1977	rVV2	217769	358936	16.60%	2.900%
14	15.018	2025	2030	2038	rVB2	27166	44414	2.05%	0.359%
15	16.129	2212	2219	2232	rBV	758092	1272364	58.83%	10.281%
16	17.386	2426	2433	2444	rBV	256785	457414	21.15%	3.696%
17	17.503	2449	2453	2459	rVB5	19823	31033	1.43%	0.251%
18	17.562	2459	2463	2468	rBV7	25122	35826	1.66%	0.289%
19	18.273	2579	2584	2590	rBV2	44879	77185	3.57%	0.624%
20	19.190	2736	2740	2744	rBV6	16385	28203	1.30%	0.228%
21	19.413	2773	2778	2781	rBV6	16065	30935	1.43%	0.250%
22	19.760	2834	2837	2841	rBV2	20560	24957	1.15%	0.202%
23	19.995	2868	2877	2887	rBV	1600423	2162740	100.00%	17.476%
24	20.288	2924	2927	2931	rBV4	28486	42767	1.98%	0.346%
25	20.471	2955	2958	2964	rBV4	39270	71120	3.29%	0.575%
26	20.747	3001	3005	3008	rBV	197520	240951	11.14%	1.947%
27	21.652	3154	3159	3168	rVB2	283258	526769	24.36%	4.257%
28	24.848	3697	3703	3716	rVB3	230542	651453	30.12%	5.264%

Sum of corrected areas: 12375324

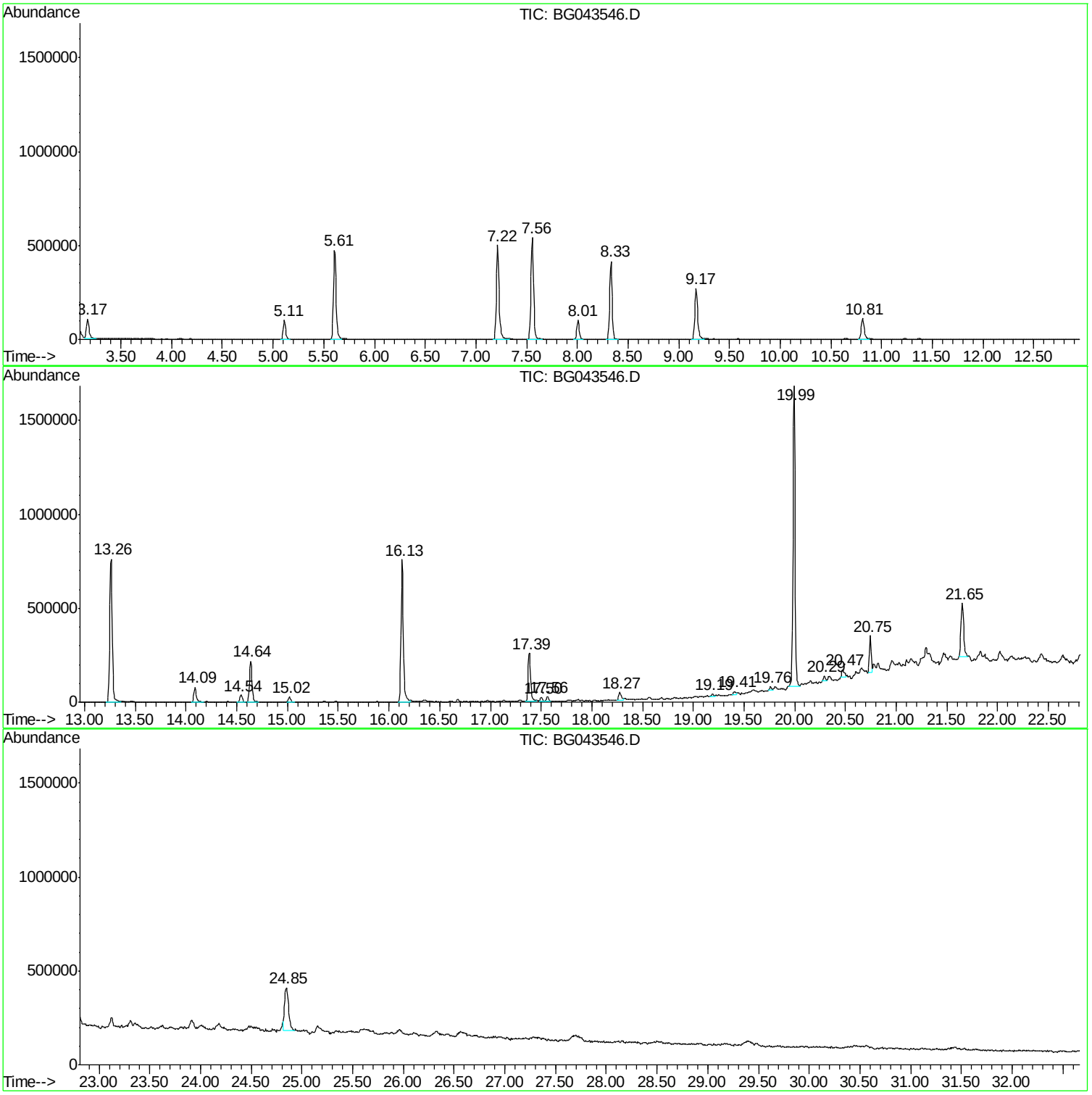
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043546.D
Acq On : 7 Nov 2019 19:30
Operator : JU
Sample : K5723-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043546.D
Acq On : 7 Nov 2019 19:30
Operator : JU
Sample : K5723-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

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

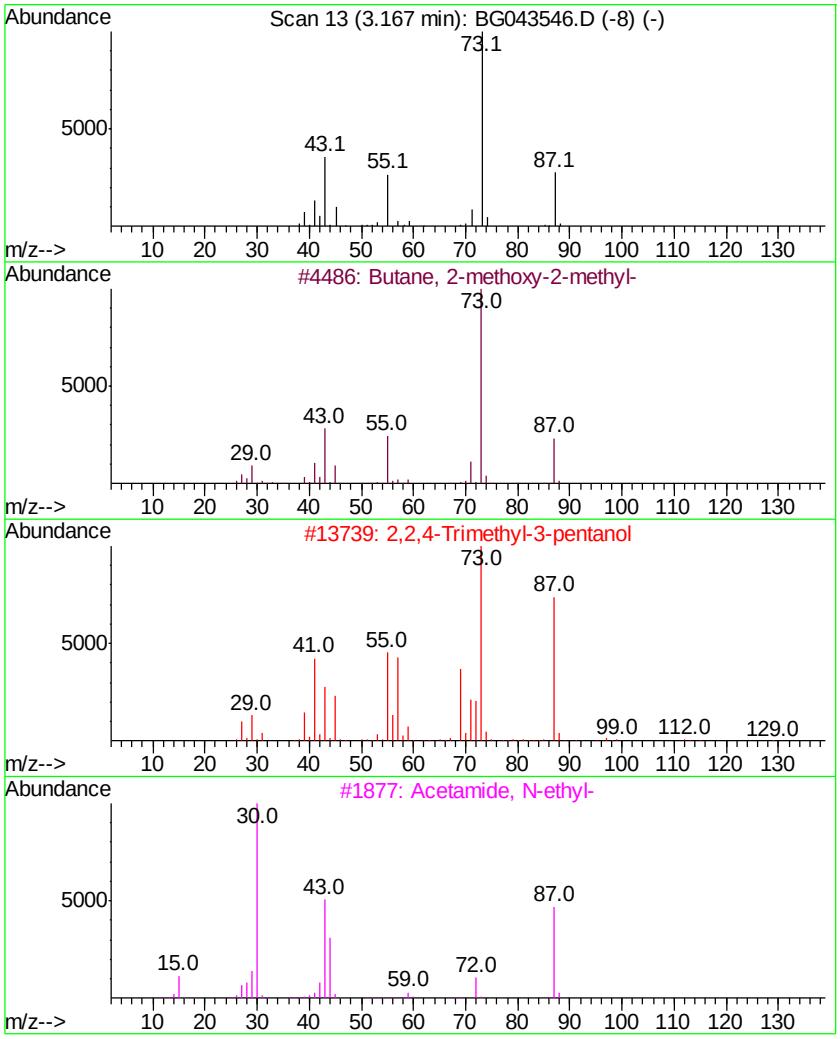
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

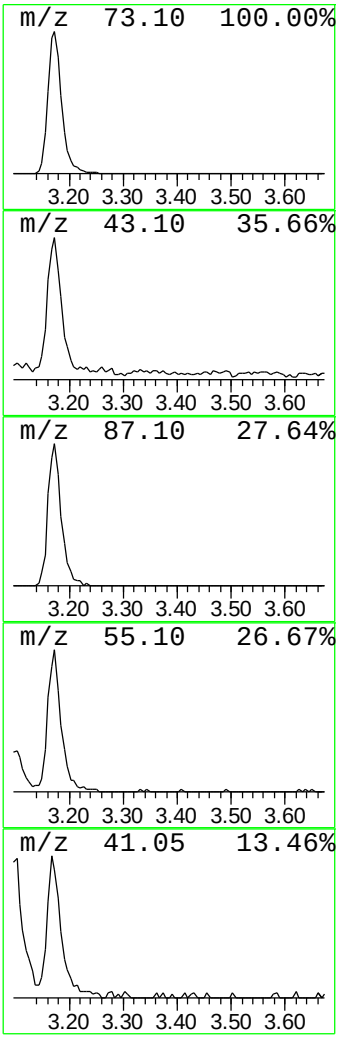
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	20.57 ng	187763	1,4-Dichlorobenzene-d4	8.01

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9





Library Search Compound Report

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Data File : BG043546.D
Acq On : 7 Nov 2019 19:30
Operator : JU
Sample : K5723-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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

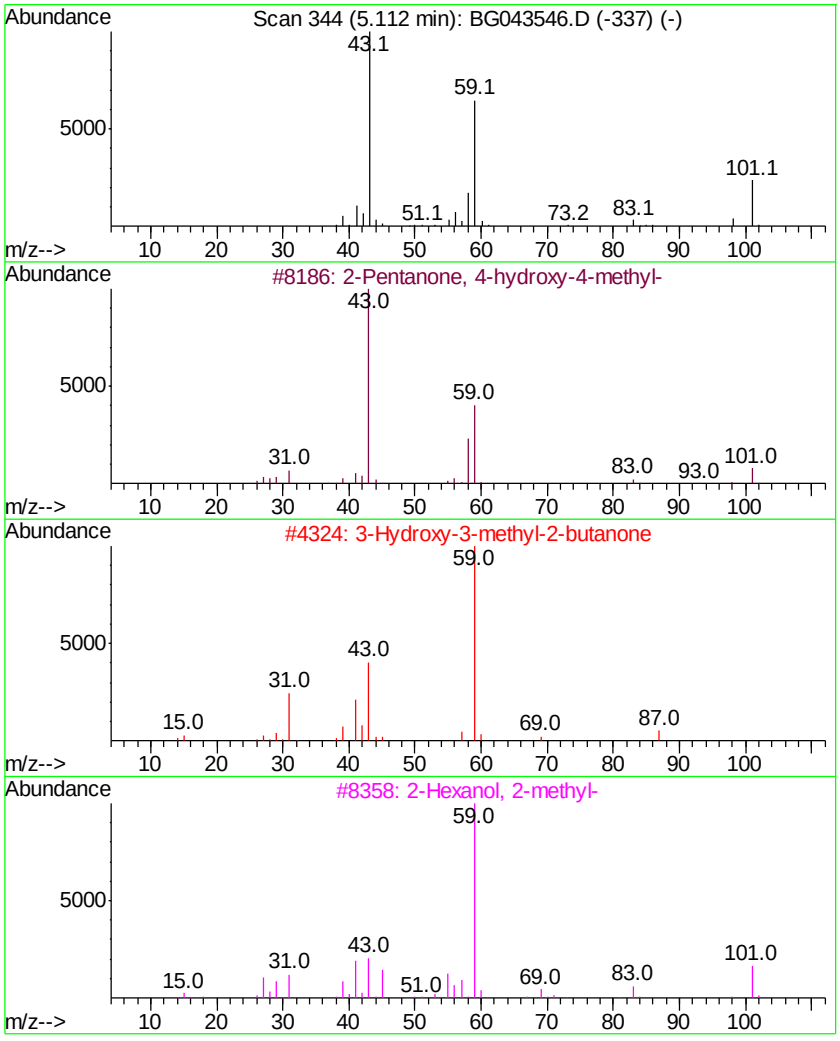
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

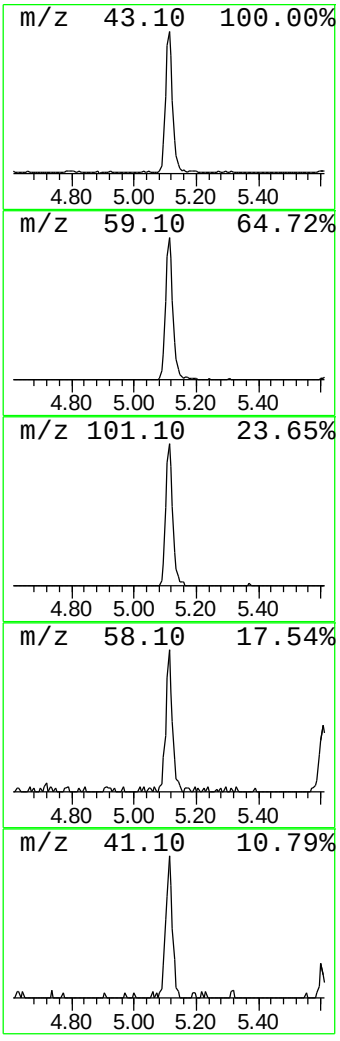
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	17.35 ng	158377	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043546.D
Acq On : 7 Nov 2019 19:30
Operator : JU
Sample : K5723-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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

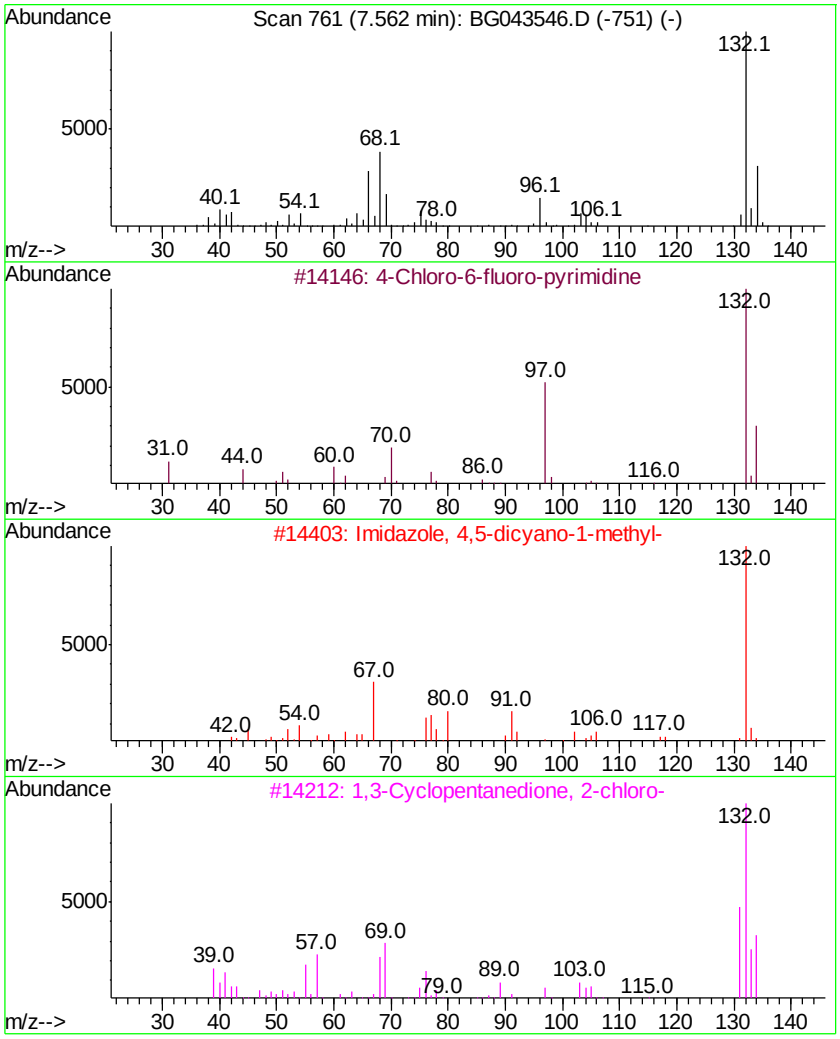
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

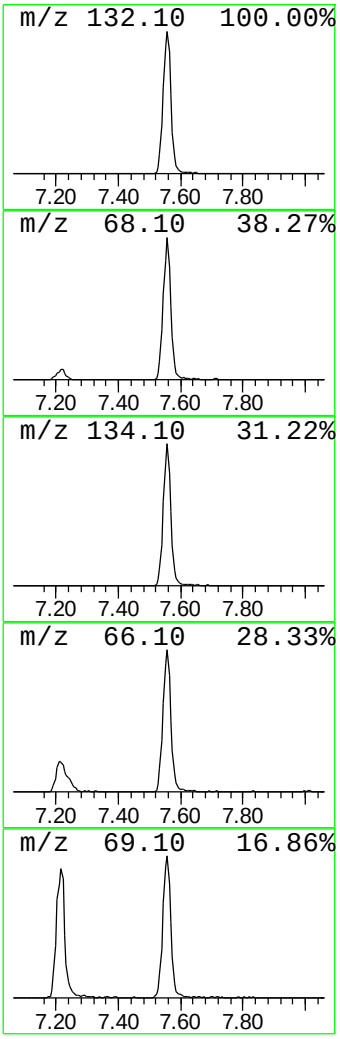
****

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	104.88 ng	957188	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043546.D
Acq On : 7 Nov 2019 19:30
Operator : JU
Sample : K5723-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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

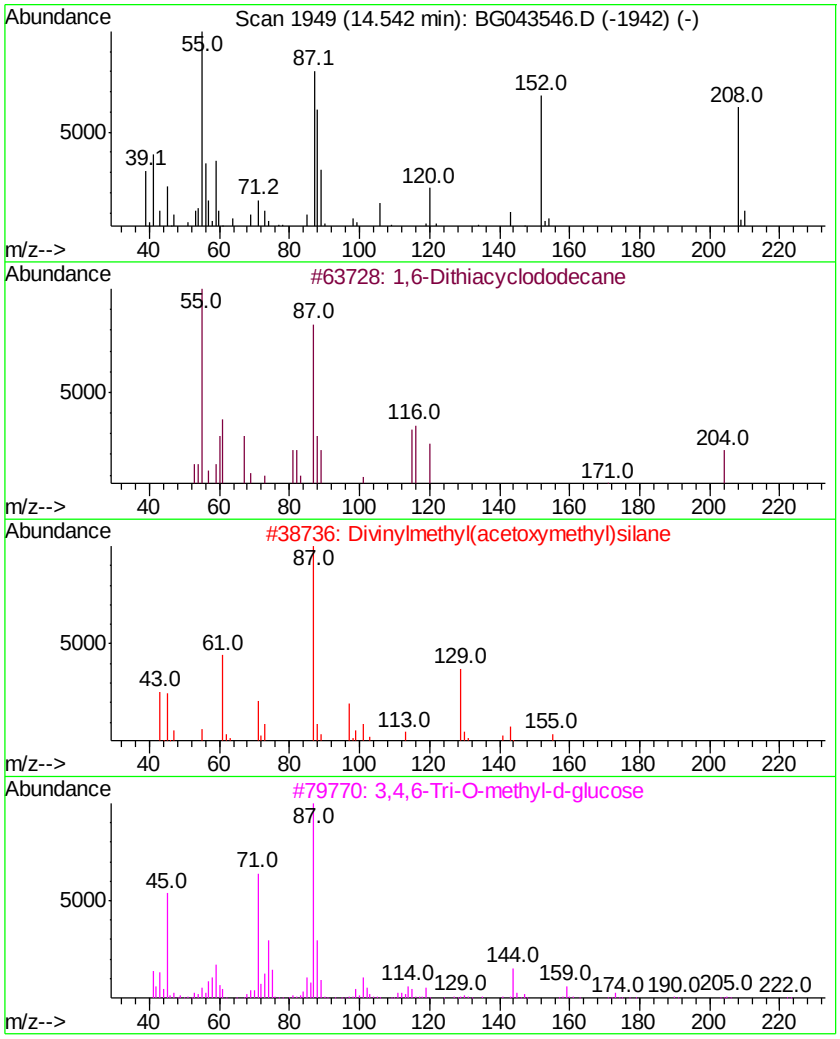
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

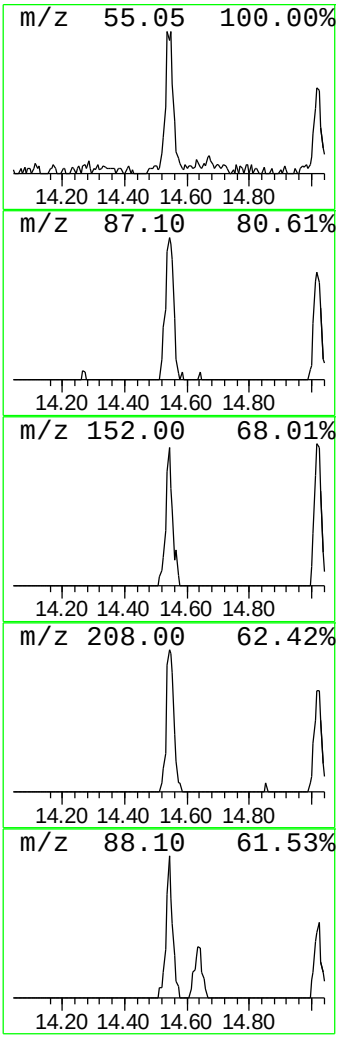
****

Peak Number 5 unknown14.54 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.59 ng	64418	Acenaphthene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Dithiacyclododecane	204	C10H20S2	038241-91-7	23
2	Divinylmethyl(acetoxymethyl)silane	170	C8H14O2Si	116065-60-2	22
3	3,4,6-Tri-O-methyl-d-glucose	222	C9H18O6	1000127-03-2	16
4	Allyl dithioisobutyrate	160	C7H12S2	063881-54-9	14
5	Uridine, 2'-O-methyl-	258	C10H14N2O6	002140-76-3	14





Library Search Compound Report

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Sample : K5723-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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
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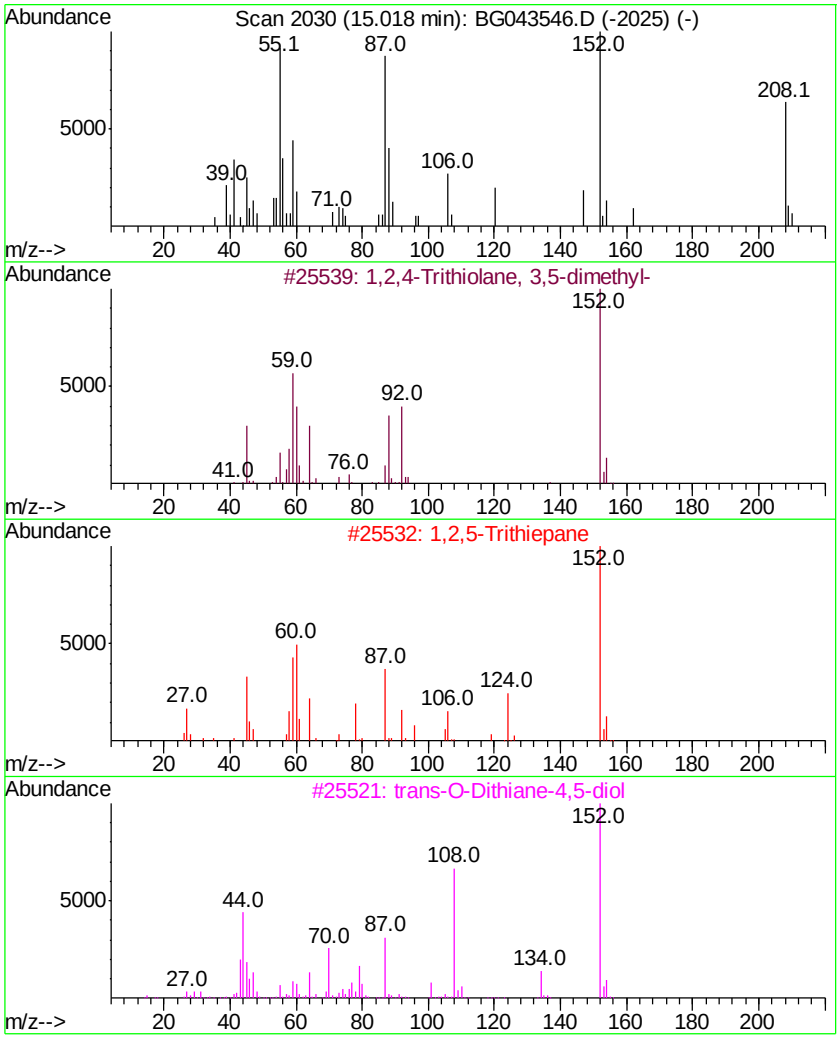
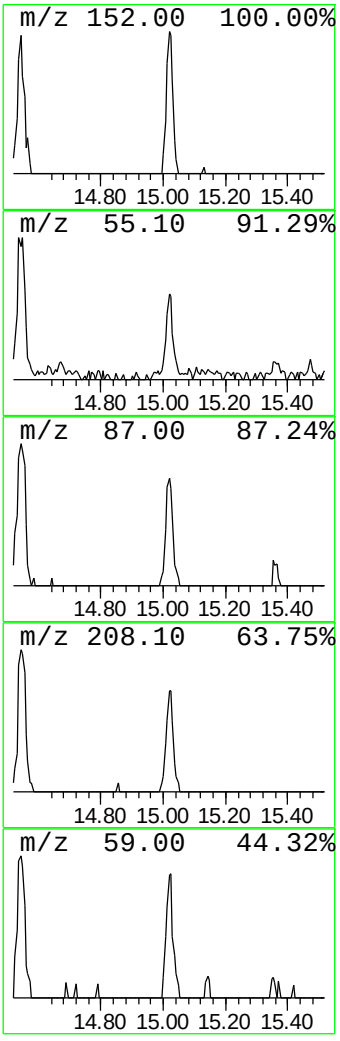
****

Peak Number 6 unknown15.02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.47 ng	44414	Acenaphthene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	35
2	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	35
3	trans-O-Dithiane-4,5-diol	152	C4H8O2S2	014193-38-5	22
4	2-[2-[2-[2-[2-[2-[2-(2-Methox...	470	C21H42O11	1000351-91-8	12
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Met...	514	C23H46O12	1000351-89-8	12





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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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

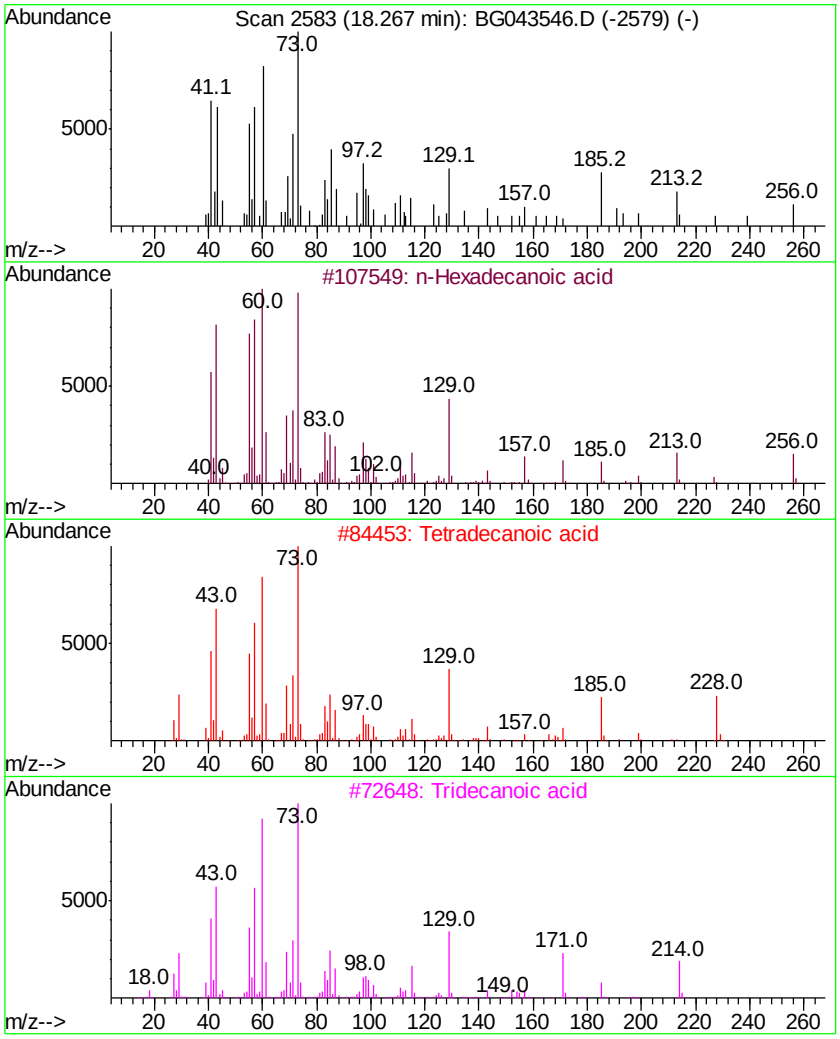
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

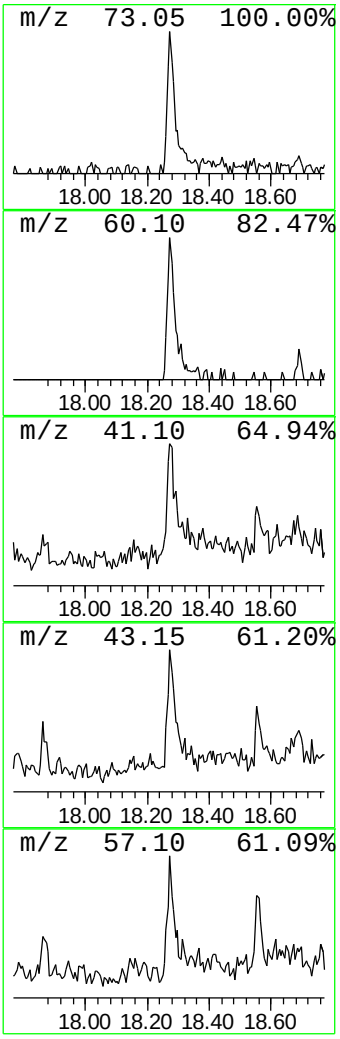
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	3.37 ng	77185	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





Library Search Compound Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9-A

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

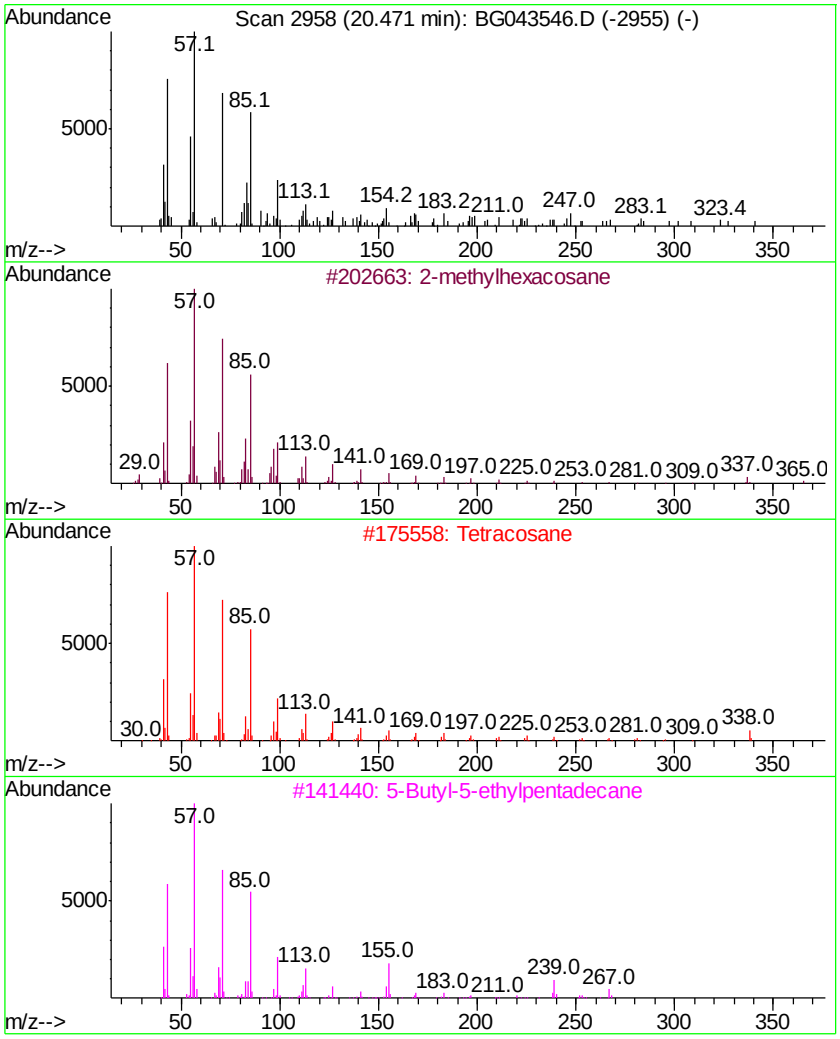
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

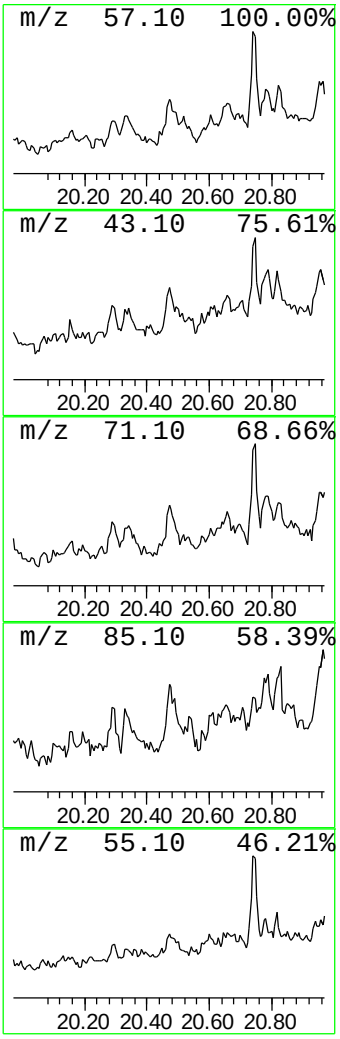
****

Peak Number 8 2-methylhexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	2.70 ng	71120	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methylhexacosane	380	C27H56	1000376-72-7	59
2	Tetracosane	338	C24H50	000646-31-1	59
3	5-Butyl-5-ethylpentadecane	296	C21H44	1000360-42-8	59
4	Tetradecane	198	C14H30	000629-59-4	53
5	Tricosane	324	C23H48	000638-67-5	53





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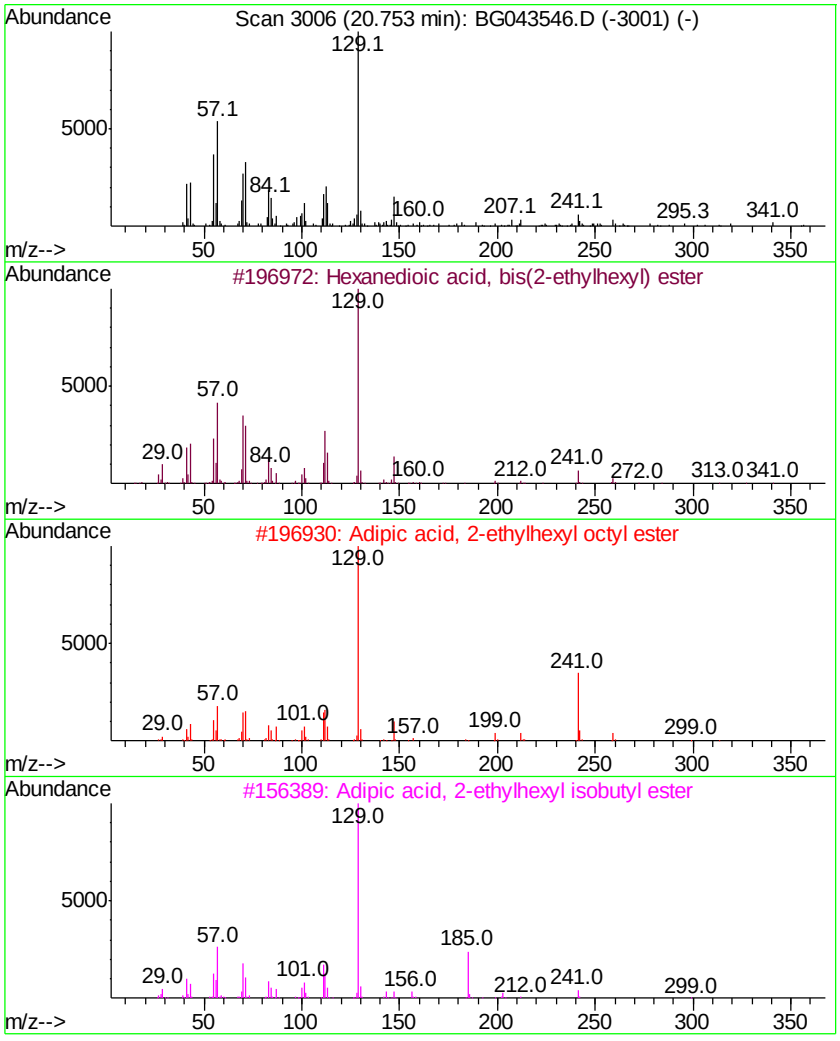
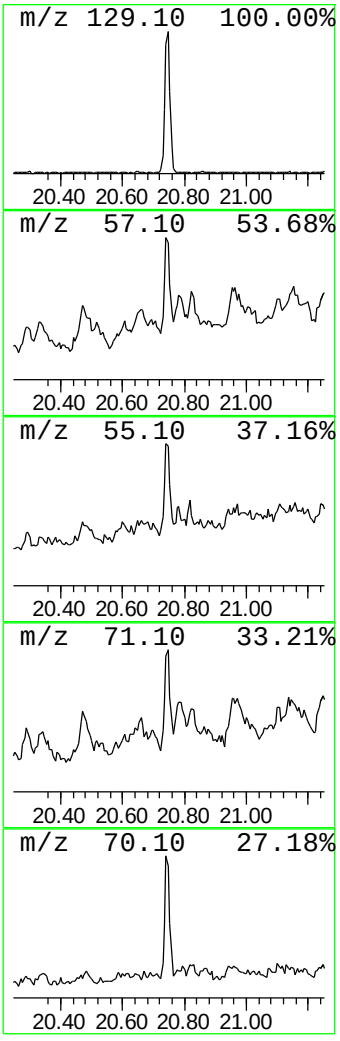
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	9.15 ng	240951	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	59
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	58
5	Diisooctyl adipate	370	C22H42O4	001330-86-5	52





Tentatively Identified Compound (LSC) summary

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Data File : BG043546.D
Acq On : 7 Nov 2019 19:30
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Instrument : BNA_G
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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...	3.17	20.6	ng	187763	1	8.01	182535	20.0
2-Pentanone, 4-hy...	5.11	17.4	ng	158377	1	8.01	182535	20.0
unknown7.56	7.56	104.9	ng	957188	1	8.01	182535	20.0
unknown14.54	14.54	3.6	ng	64418	3	14.64	358936	20.0
unknown15.02	15.02	2.5	ng	44414	3	14.64	358936	20.0
n-Hexadecanoic acid	18.27	3.4	ng	77185	4	17.38	457414	20.0
2-methylhexacosane	20.47	2.7	ng	71120	5	21.65	526769	20.0
Hexanedioic acid,...	20.75	9.2	ng	240951	5	21.65	526769	20.0