LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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	3.165	9	13	27	rVB	172968	302898	10.37%	1.974%
2	5.110	338	344	356	rBV	130882	205587	7.04%	1.339%
3	5.609	421	429	442	rBV	614650	1075042	36.79%	7.004%
4	7.213	692	702	717	rBV	654395	1247078	42.67%	8.125%
5	7.560	752	761	772	rBV	669875	1221698	41.81%	7.960%
6	8.006	829	837	846	rBV	108032	184944	6.33%	1.205%
7	8.329	885	892	905	rBV	539840	955401	32.69%	6.225%
8	9.170	1026	1035	1048	rBV	350302	722643	24.73%	4.708%
9	10.650	1279	1287	1297	rBV5	16170	47470	1.62%	0.309%
10	10.815	1306	1315	1327	rBV	114160	231552	7.92%	1.509%
11	13.259	1724	1731	1743	rBV	1077143	1769741	60.56%	11.531%
12	14.087	1866	1872	1885	rBV	97278	164907	5.64%	1.074%
13	14.546	1941	1950	1956	rBV2	75396	132343	4.53%	0.862%
14	14.640	1959	1966	1978	rVB	213351	367332	12.57%	2.393%
15	15.022	2025	2031	2038	rBV2	50944	79216	2.71%	0.516%
16	16.132	2212	2220	2233	rBV	1011025	1699868	58.17%	11.075%
17	16.678	2307	2313	2318	rBV	47146	68982	2.36%	0.449%
18	17.131	2384	2390	2395	rBV4	20993	37264	1.28%	0.243%
19	17.295	2412	2418	2427	rBV4	23845	57797	1.98%	0.377%
20	17.383	2427	2433	2444	rVV	277215	477181	16.33%	3.109%
21	17.501	2448	2453	2459	rBV4	32315	52410	1.79%	0.341%
22	17.566	2459	2464	2469	rBV3	79630	112031	3.83%	0.730%
23	18.277	2581	2585	2589	rBV2	45716	63882	2.19%	0.416%
24	19.998	2872	2878	2886	rVB	2150606	2922315	100.00%	19.040%
25	20.744	3001	3005	3009	rBV	565704	675259	23.11%	4.400%
26	21.655	3156	3160	3167	rVB	300285	473285	16.20%	3.084%

Sum of corrected areas: 15348126

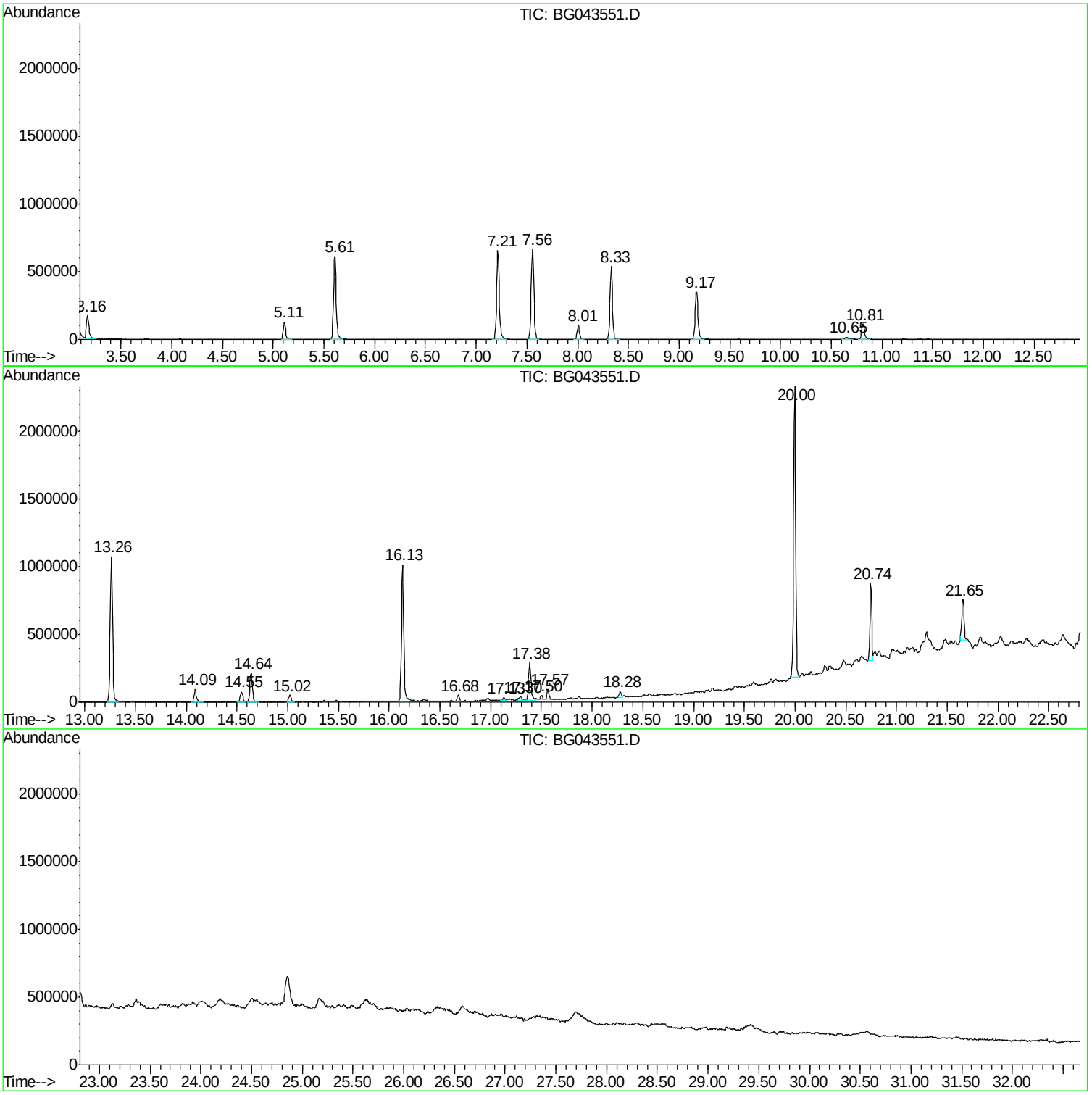
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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



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Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

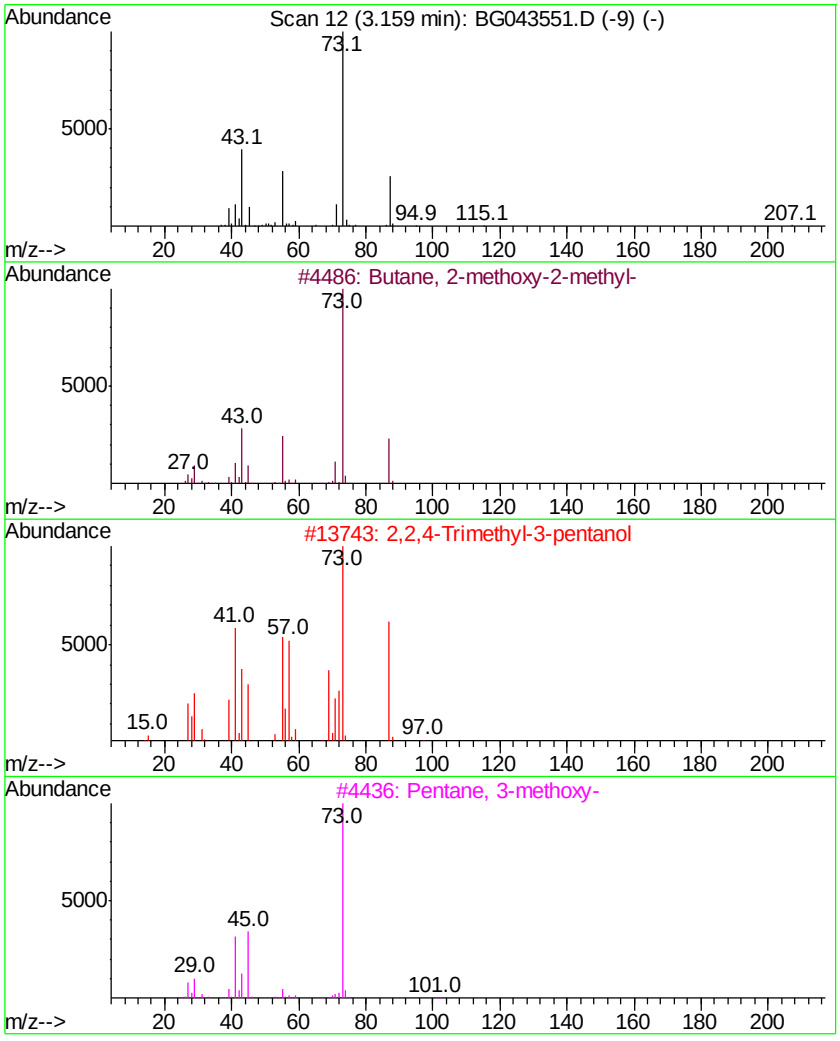
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

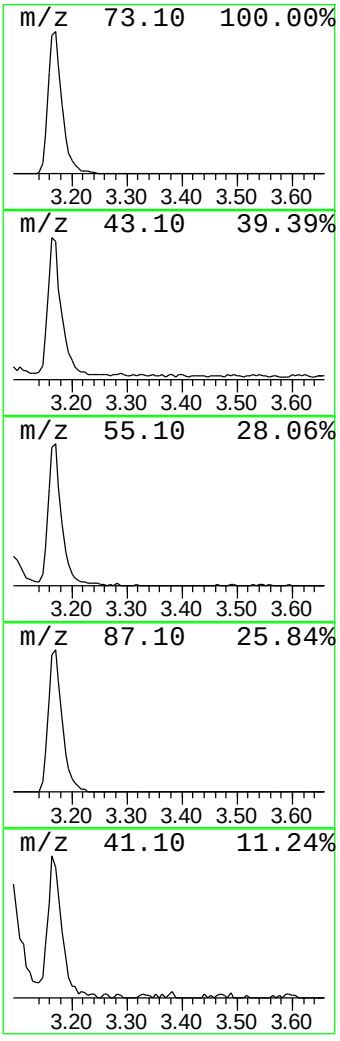
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	32.76 ng	302898	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

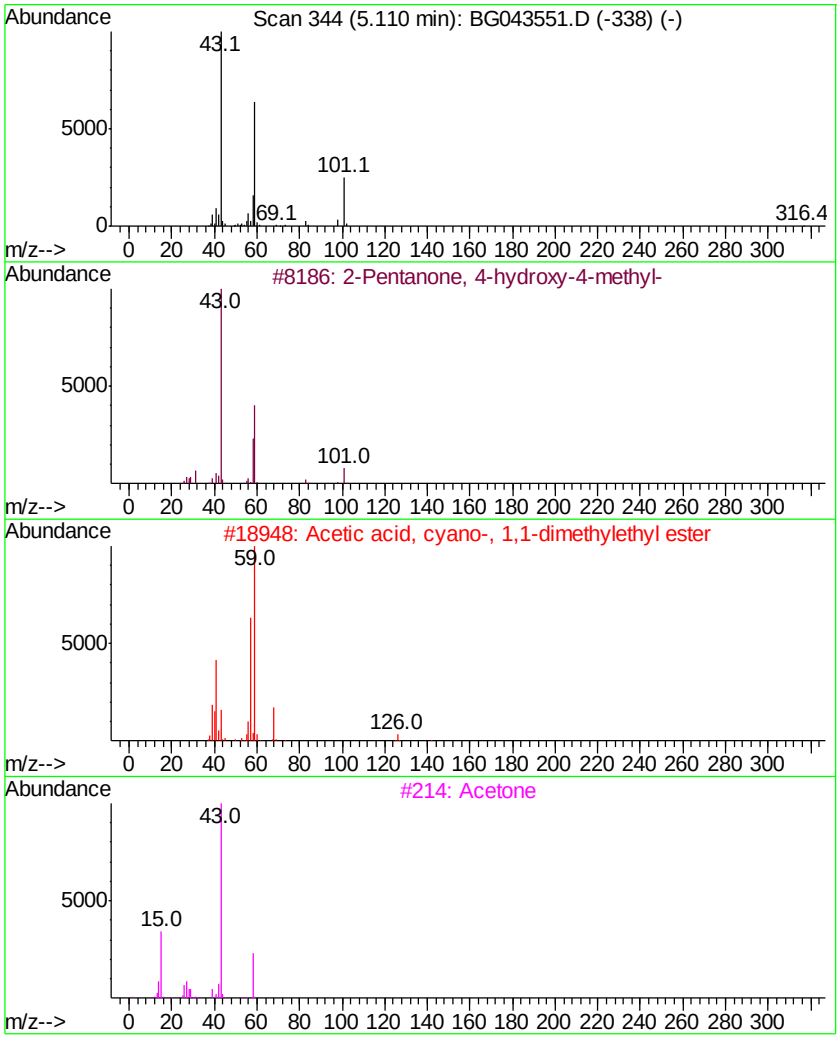
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

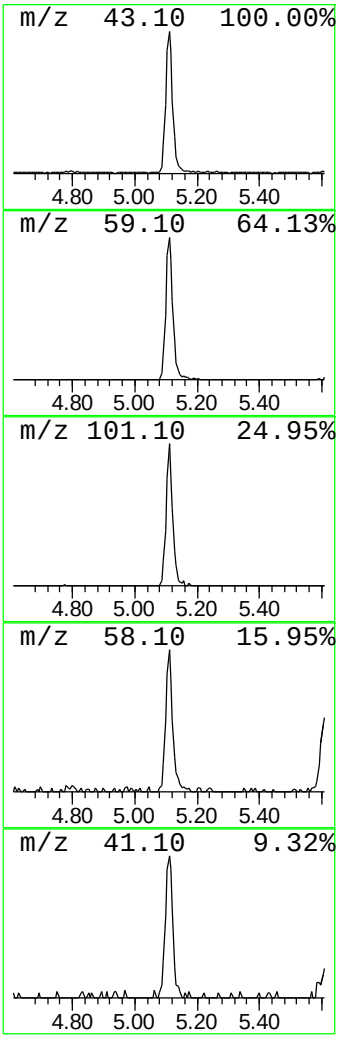
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	22.23 ng	205587	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Acetone	58	C3H6O	000067-64-1	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

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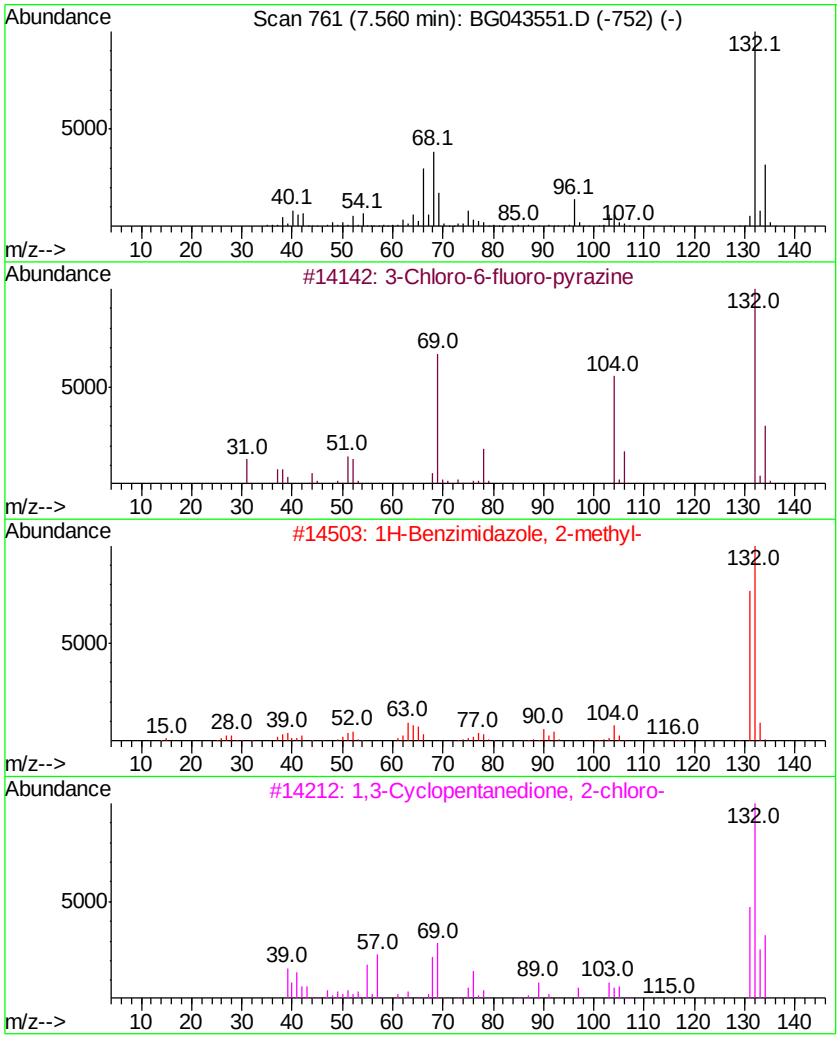
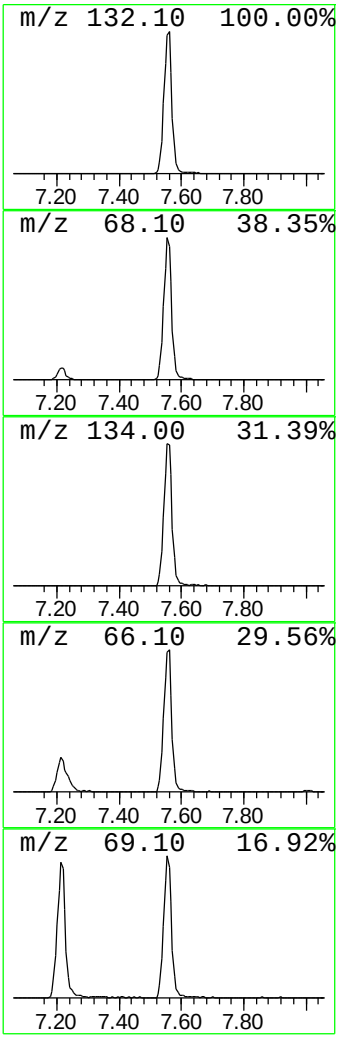
Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	132.12 ng	1221700	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

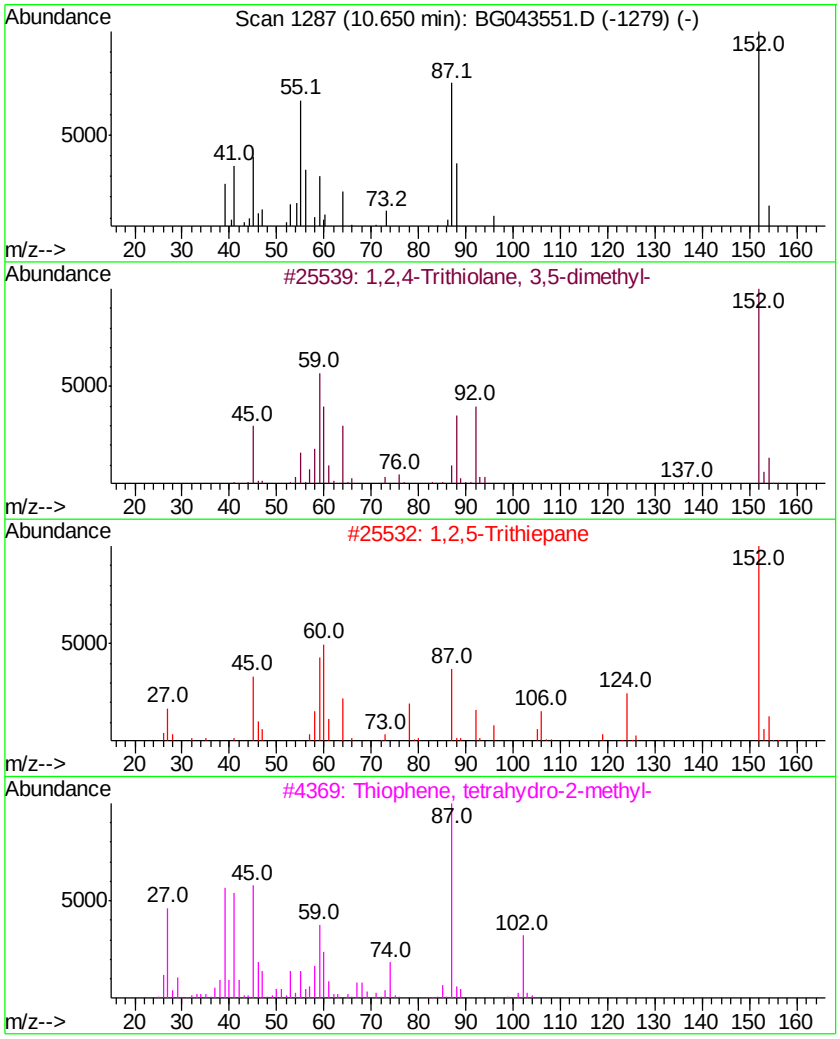
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

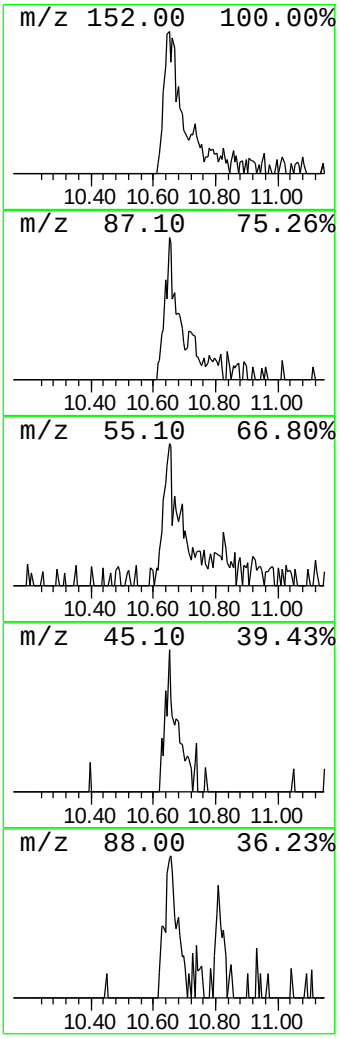
****

Peak Number 5 unknown10.65 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.10 ng	47470	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	43
2	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	38
3	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	38
4	6-(Methylthio)hexa-1,5-dien-3-ol	144	C7H12OS	1000191-74-3	23
5	1-Butanamine, 4-(methylthio)-	119	C5H13NS	055021-77-7	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

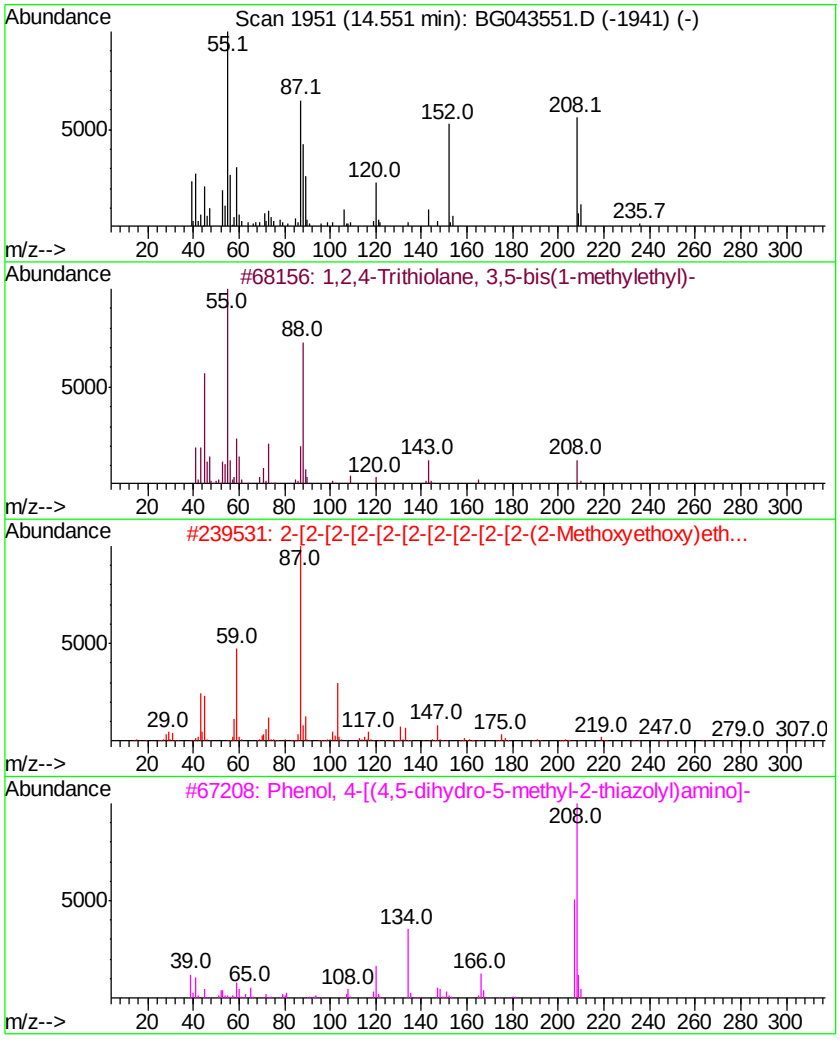
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

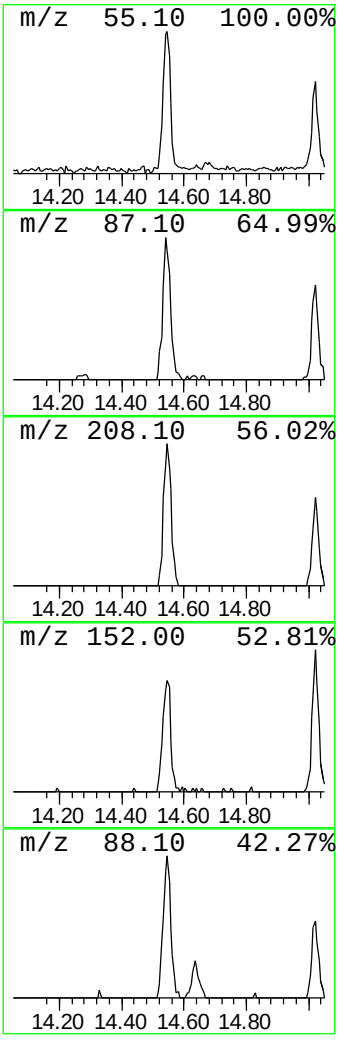
****

Peak Number 6 unknown14.55 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	7.21 ng	132343	Acenaphthene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane, 3,5-bis(1-met...	208	C8H16S3	054934-99-5	12
2	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	558	C25H50O13	1000351-91-9	10
3	Phenol, 4-[(4,5-dihydro-5-methyl...	208	C10H12N2OS	1000362-46-0	10
4	2-Propenenitrile, 2-chloro-	87	C3H2ClN	000920-37-6	10
5	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Met...	514	C23H46O12	1000351-89-8	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
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Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

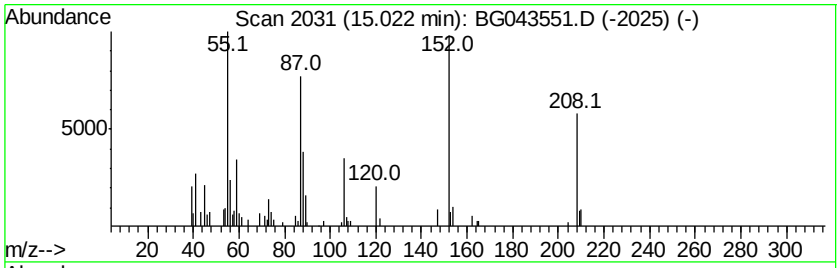
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

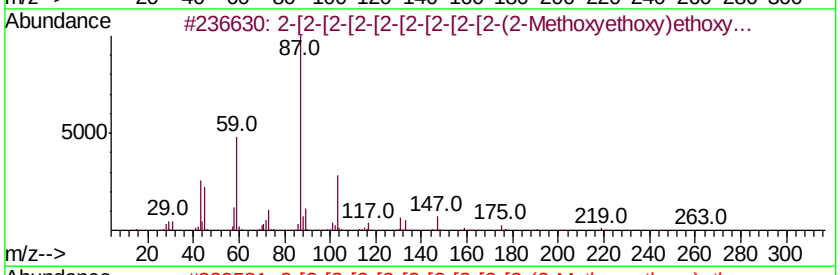
****

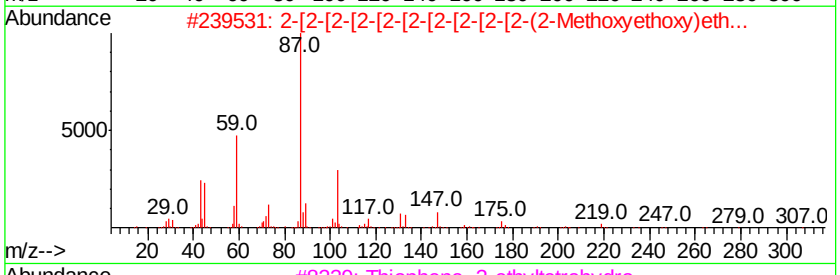
Peak Number 7 unknown15.02 Concentration Rank 8

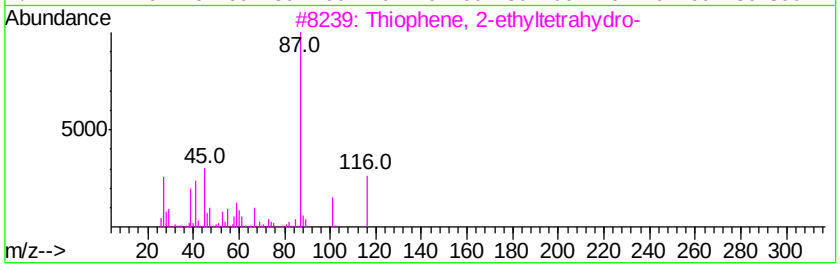
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	4.31 ng	79216	Acenaphthene-d10	14.64

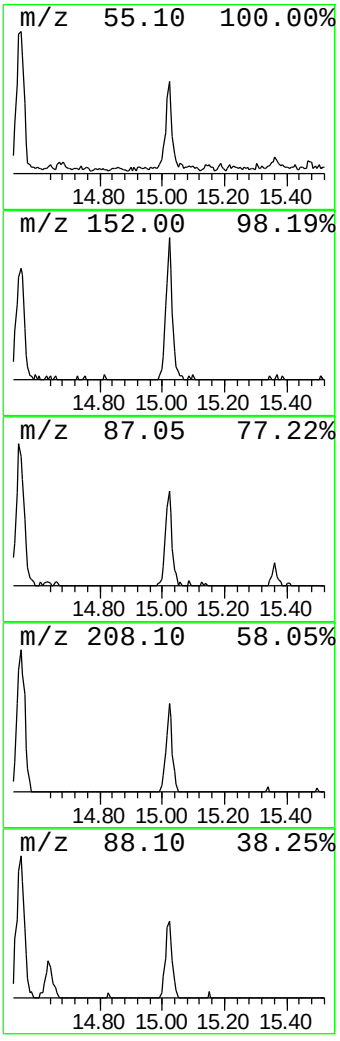
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Met...	514	C23H46O12	1000351-89-8	22
2	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	558	C25H50O13	1000351-91-9	22
3	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	14
4	2-Methyl-6-nitroaniline	152	C7H8N2O2	000570-24-1	14
5	5-Methyl-2-nitroaniline	152	C7H8N2O2	000578-46-1	14











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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

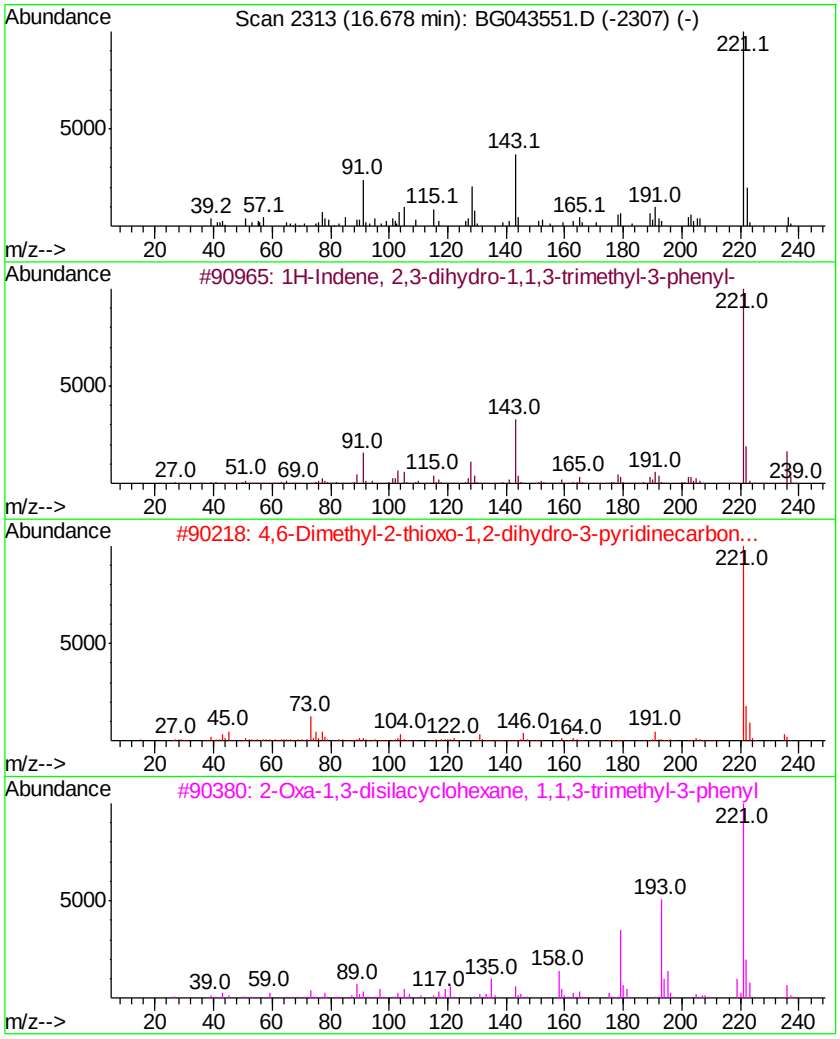
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

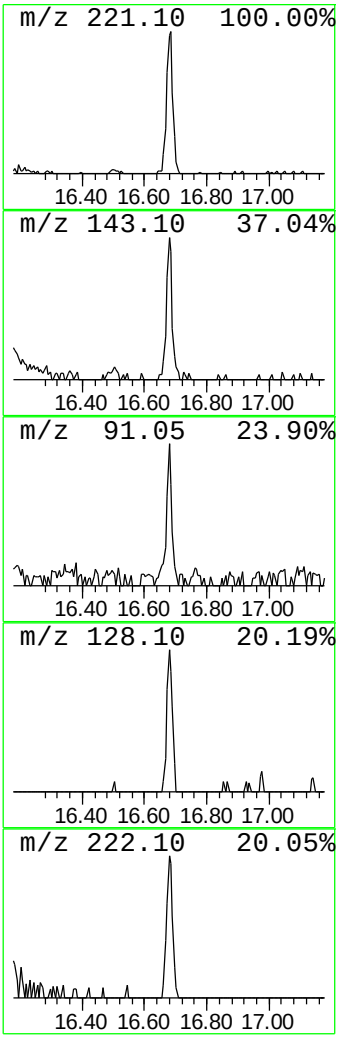
****

Peak Number 8 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.68	2.89 ng	68982	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	80
2	4,6-Dimethyl-2-thioxo-1,2-dihydr...	236	C11H16N2SSi	1000332-43-1	50
3	2-Oxa-1,3-disilacyclohexane, 1,1...	236	C12H20OSi2	1000308-85-9	47
4	Benz[j]isoquinoline, 3,6,8-trime...	221	C16H15N	061171-16-2	47
5	Benzo[h]quinoline, 2,3,4-trimethyl-	221	C16H15N	063042-66-0	47





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Acq On : 7 Nov 2019 22:44
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

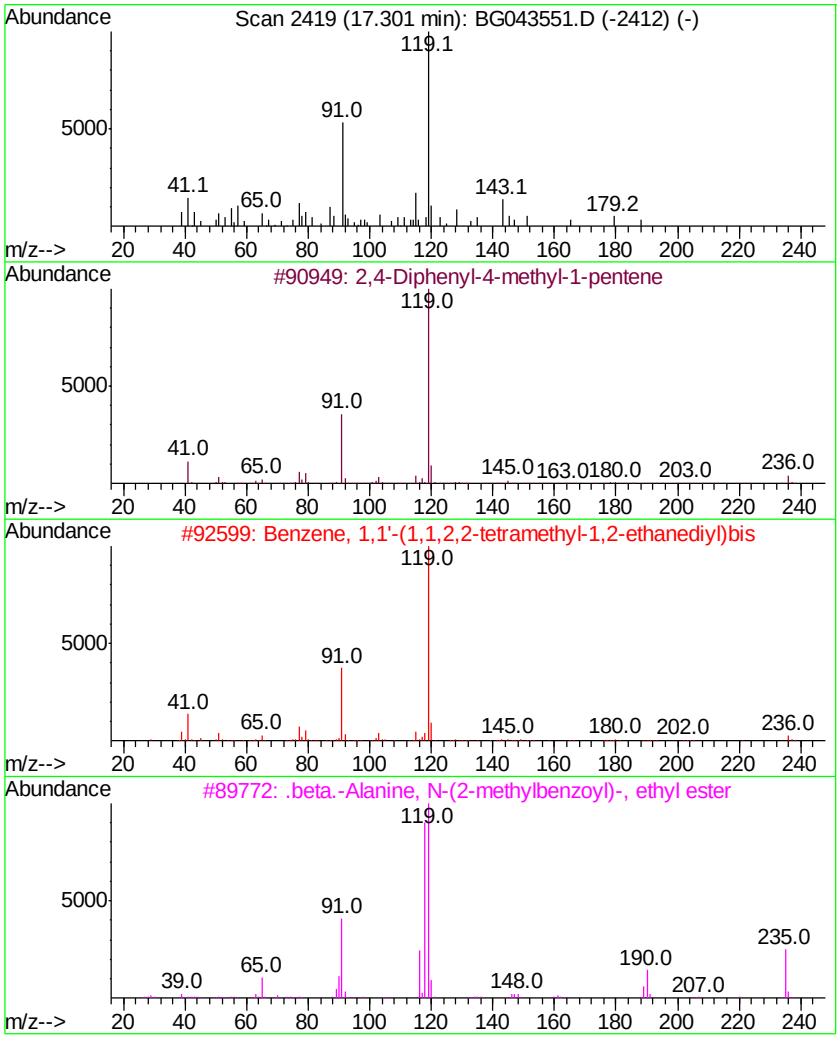
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

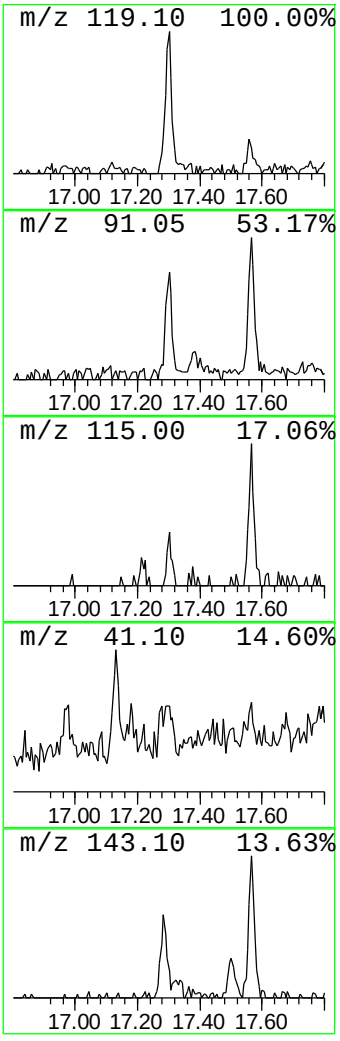
****

Peak Number 9 unknown17.30 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.42 ng	57797	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Diphenyl-4-methyl-1-pentene	236	C18H20	1000111-58-0	49
2	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	47
3	.beta.-Alanine, N-(2-methylbenzo...	235	C13H17NO3	1000321-61-2	47
4	Benzene, isocyanato-	119	C7H5NO	000103-71-9	46
5	Benzene, tert-butyl-	134	C10H14	000098-06-6	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

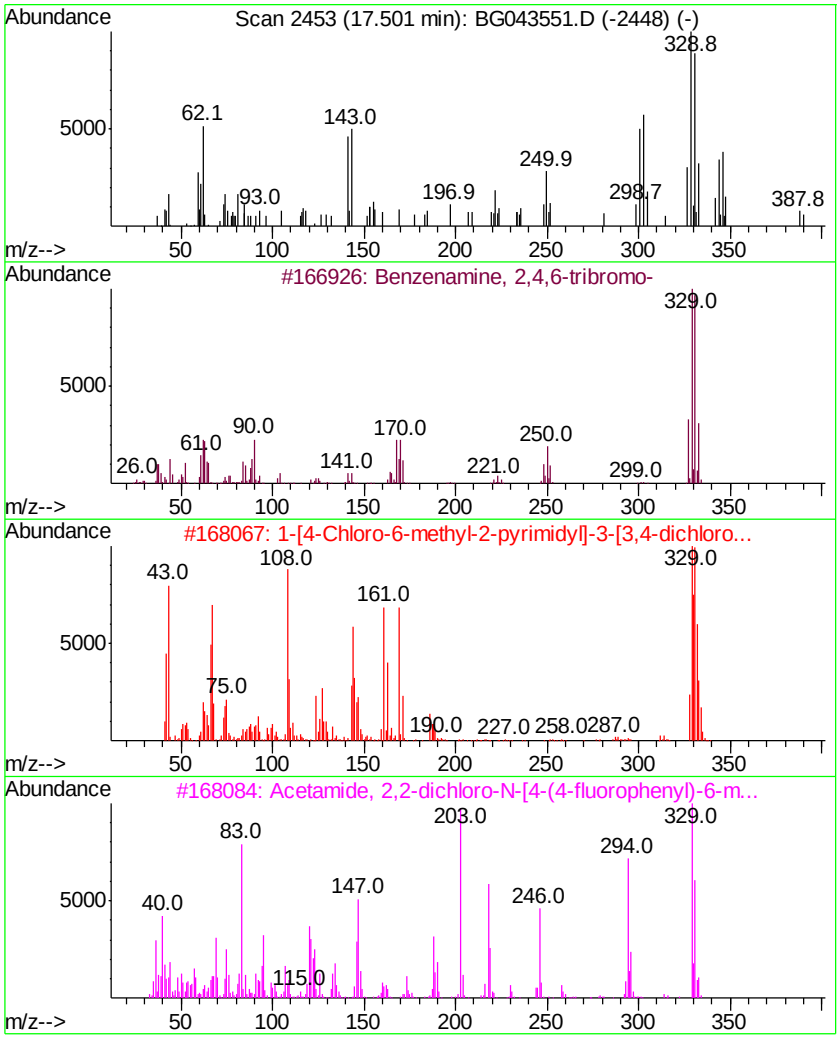
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

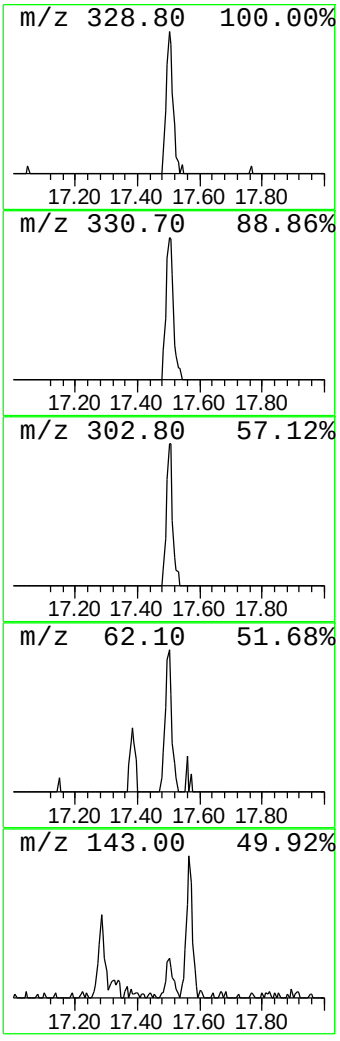
****

Peak Number 10 Benzenamine, 2,4,6-tribromo- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.50	2.20 ng	52410	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	55
2	1-[4-Chloro-6-methyl-2-pyrimidyl...	329	C12H10Cl3N5	051387-79-2	35
3	Acetamide, 2,2-dichloro-N-[4-(4-...	329	C13H10Cl2FN3O2	1000267-98-1	18
4	2,5-Di(trifluoroacetyloxy)acetop...	344	C12H6F6O5	1000365-30-5	11
5	2H-1,4-Benzodiazepin-2-one, 7-br...	364	C15H10BrClN2O2	070030-09-0	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

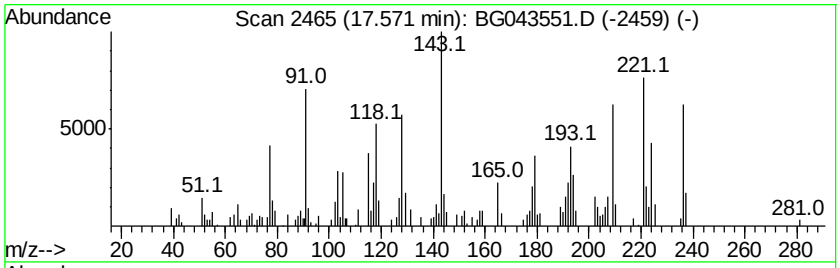
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

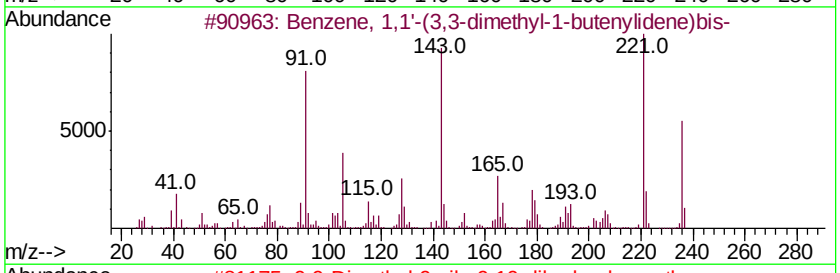
****

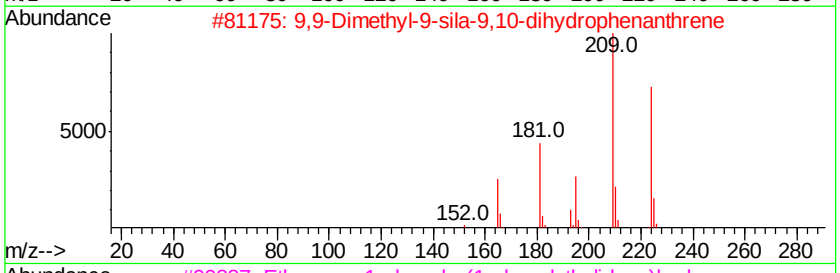
Peak Number 11 Benzene, 1,1'-(3,3-dimethyl... Concentration Rank 7

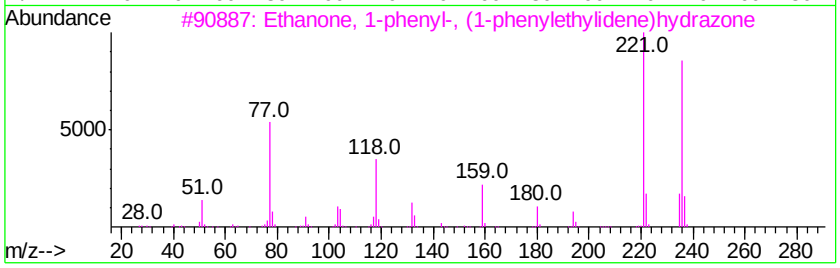
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	4.70 ng	112031	Phenanthrene-d10	17.38

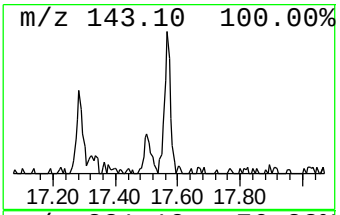
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(3,3-dimethyl-1-bu...	236	C18H20	023586-64-3	50
2	9,9-Dimethyl-9-sila-9,10-dihydro...	224	C15H16Si	187328-55-8	30
3	Ethanone, 1-phenyl-, (1-phenylet...	236	C16H16N2	000729-43-1	18
4	Carbazole, 2,4,7-trimethyl-	209	C15H15N	078787-89-0	15
5	3,5-di-tert-Butyl-4-hydroxybenzy...	236	C15H24O2	000088-26-6	11

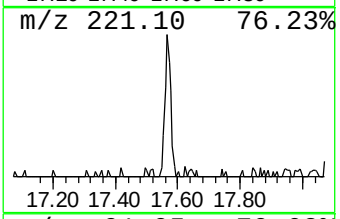


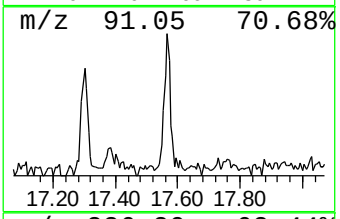


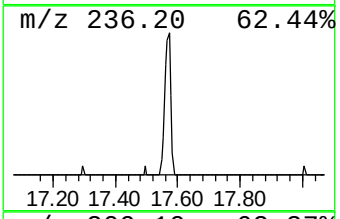


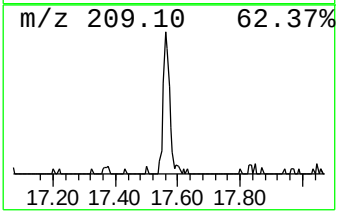












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Acq On : 7 Nov 2019 22:44
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Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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

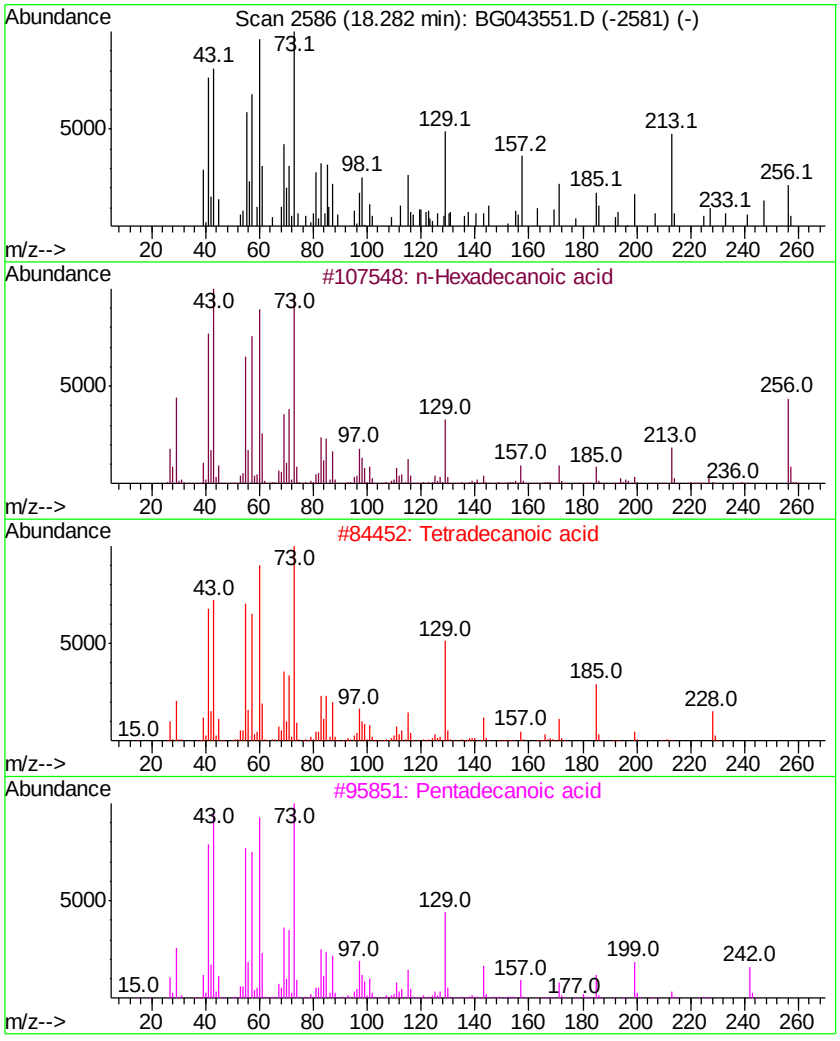
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

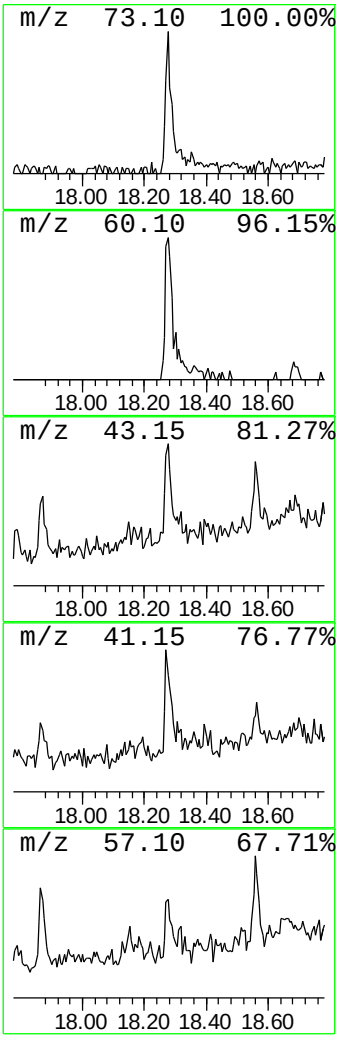
****

Peak Number 12 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.68 ng	63882	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	53
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	35
5	n-Decanoic acid	172	C10H20O2	000334-48-5	35





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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

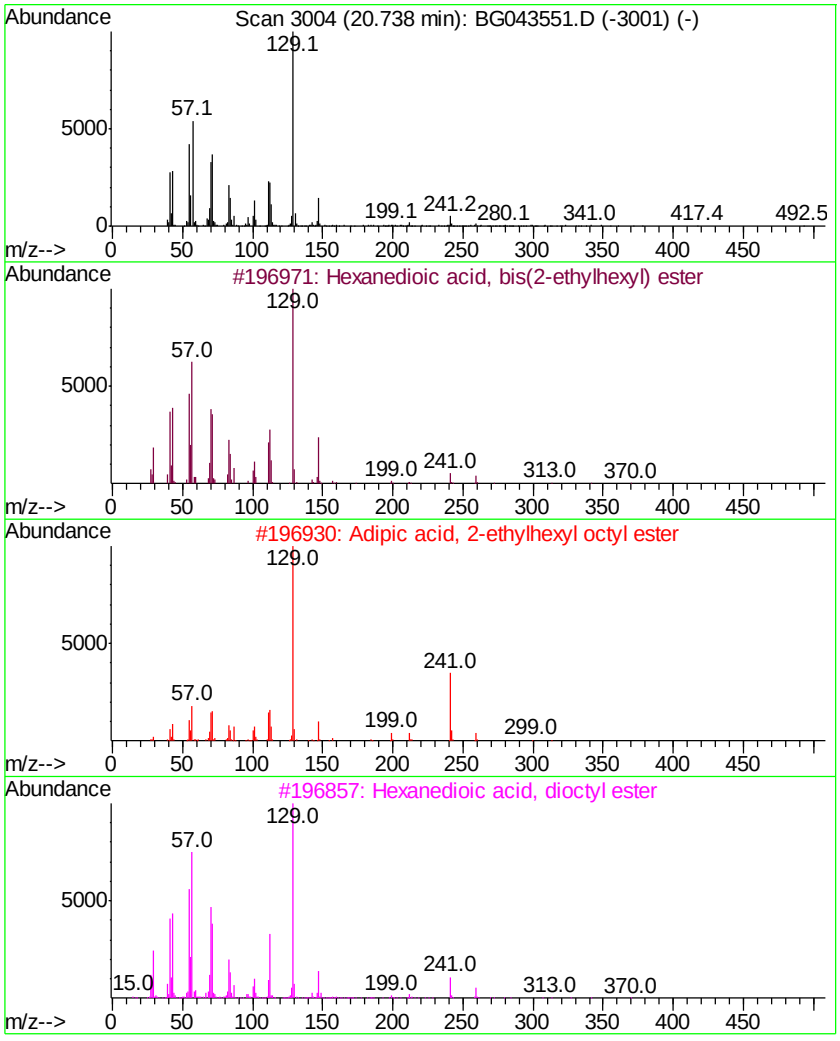
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

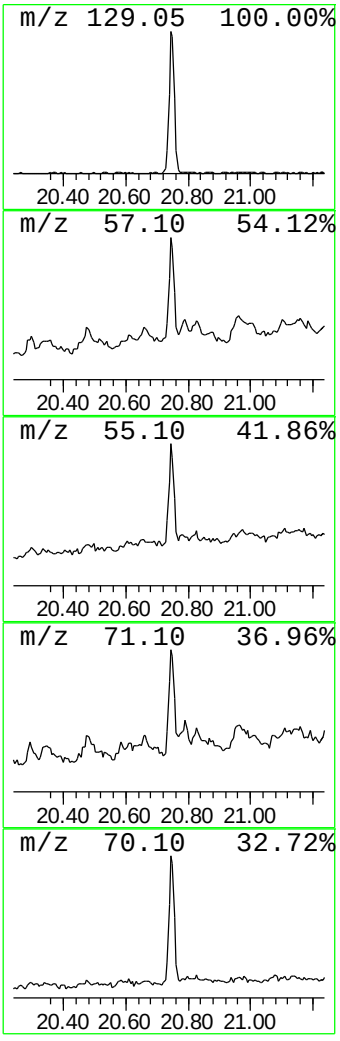
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Hexanedioic acid, bis(2-eth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.74	28.54 ng	675259	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	78
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	64
4	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	53
5	Diisooctyl adipate	370	C22H42O4	001330-86-5	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110719\
Data File : BG043551.D
Acq On : 7 Nov 2019 22:44
Operator : JU
Sample : K5723-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-C

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...	3.16	32.8	ng	302898	1	8.01	184944	20.0
2-Pentanone, 4-hy...	5.11	22.2	ng	205587	1	8.01	184944	20.0
unknown7.56	7.56	132.1	ng	1221700	1	8.01	184944	20.0
unknown10.65	10.65	4.1	ng	47470	2	10.81	231552	20.0
unknown14.55	14.55	7.2	ng	132343	3	14.64	367332	20.0
unknown15.02	15.02	4.3	ng	79216	3	14.64	367332	20.0
1H-Indene, 2,3-di...	16.68	2.9	ng	68982	4	17.38	477181	20.0
unknown17.30	17.30	2.4	ng	57797	4	17.38	477181	20.0
Benzenamine, 2,4,...	17.50	2.2	ng	52410	4	17.38	477181	20.0
Benzene, 1,1'-(3,...	17.57	4.7	ng	112031	4	17.38	477181	20.0
n-Hexadecanoic acid	18.28	2.7	ng	63882	4	17.38	477181	20.0
Hexanedioic acid,...	20.74	28.5	ng	675259	5	21.65	473285	20.0