LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-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:\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	3.172	8	14	25	rVB	145222	252966	8.09%	1.611%
2	5.111	338	344	353	rBV	136015	210606	6.74%	1.341%
3	5.605	421	428	443	rBV	634438	1123253	35.92%	7.153%
4	7.215	694	702	719	rBV	676091	1289494	41.24%	8.211%
5	7.555	752	760	770	rBV	697314	1259195	40.27%	8.019%
6	8.008	830	837	845	rBV2	106011	191781	6.13%	1.221%
7	8.331	883	892	902	rBV	578506	1007068	32.21%	6.413%
8	9.171	1027	1035	1051	rBV	385239	758094	24.24%	4.828%
9	10.646	1279	1286	1294	rBV5	12136	35080	1.12%	0.223%
10	10.816	1306	1315	1327	rBV	114346	239788	7.67%	1.527%
11	13.260	1724	1731	1745	rBV	1134299	1887453	60.36%	12.019%
12	14.089	1865	1872	1883	rBV	89312	161359	5.16%	1.028%
13	14.541	1941	1949	1956	rBV3	43882	80438	2.57%	0.512%
14	14.635	1959	1965	1977	rVV	210466	370213	11.84%	2.358%
15	15.017	2024	2030	2036	rBV3	28318	46491	1.49%	0.296%
16	16.134	2212	2220	2235	rBV	1069414	1798168	57.51%	11.451%
17	16.680	2308	2313	2318	rBV	36551	50005	1.60%	0.318%
18	17.285	2411	2416	2422	rBV4	20457	41861	1.34%	0.267%
19	17.385	2427	2433	2441	rBV	279892	470270	15.04%	2.995%
20	17.561	2458	2463	2470	rBV3	60967	94519	3.02%	0.602%
21	18.278	2581	2585	2593	rBV2	69492	115432	3.69%	0.735%
22	18.560	2629	2633	2638	rBV4	18125	36337	1.16%	0.231%
23	19.994	2872	2877	2886	rVB	2246182	3126929	100.00%	19.912%
24	20.746	3001	3005	3009	rBV	507364	594764	19.02%	3.787%
25	21.651	3155	3159	3165	rVB2	280479	462018	14.78%	2.942%

Sum of corrected areas: 15703582

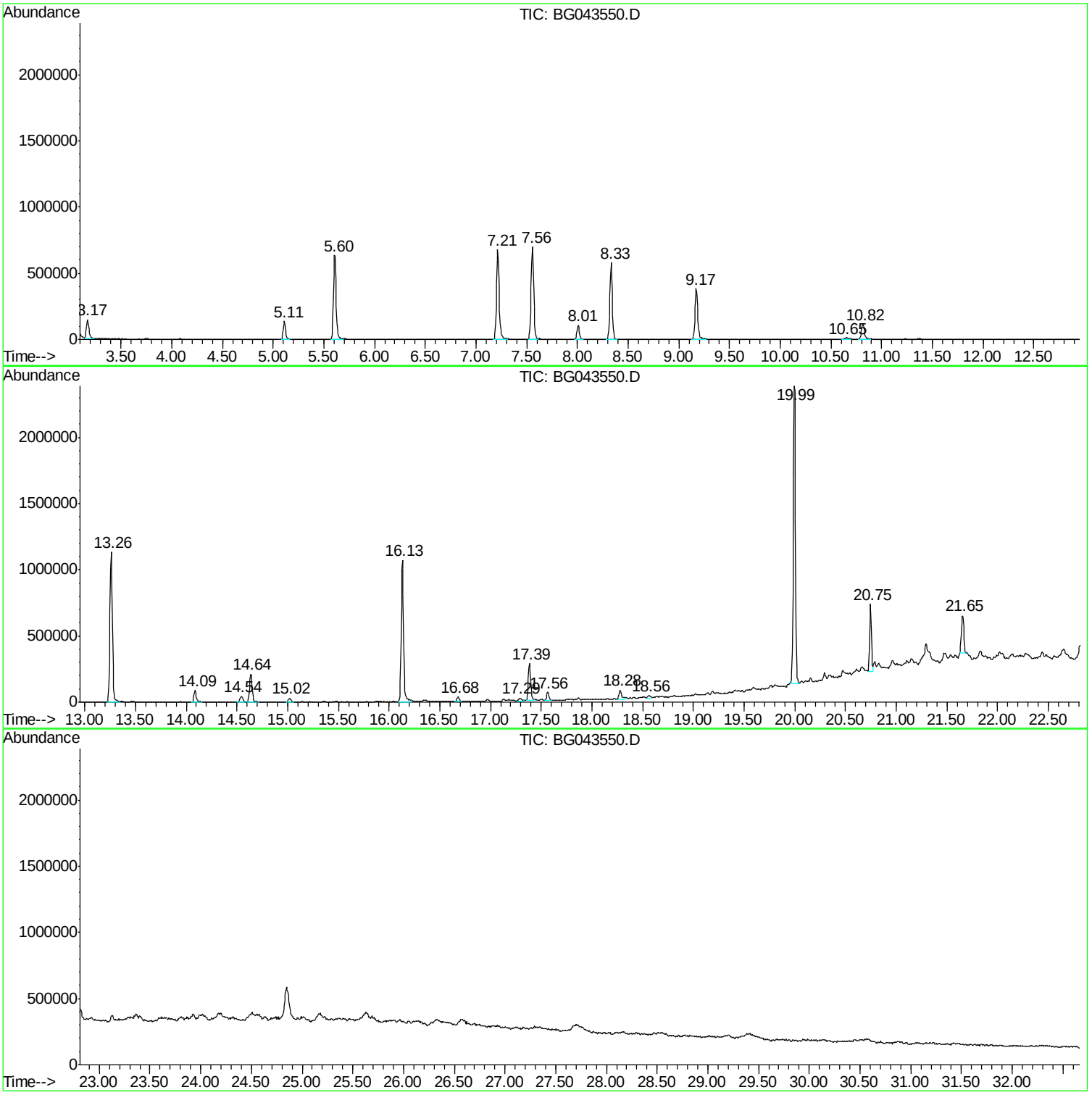
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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

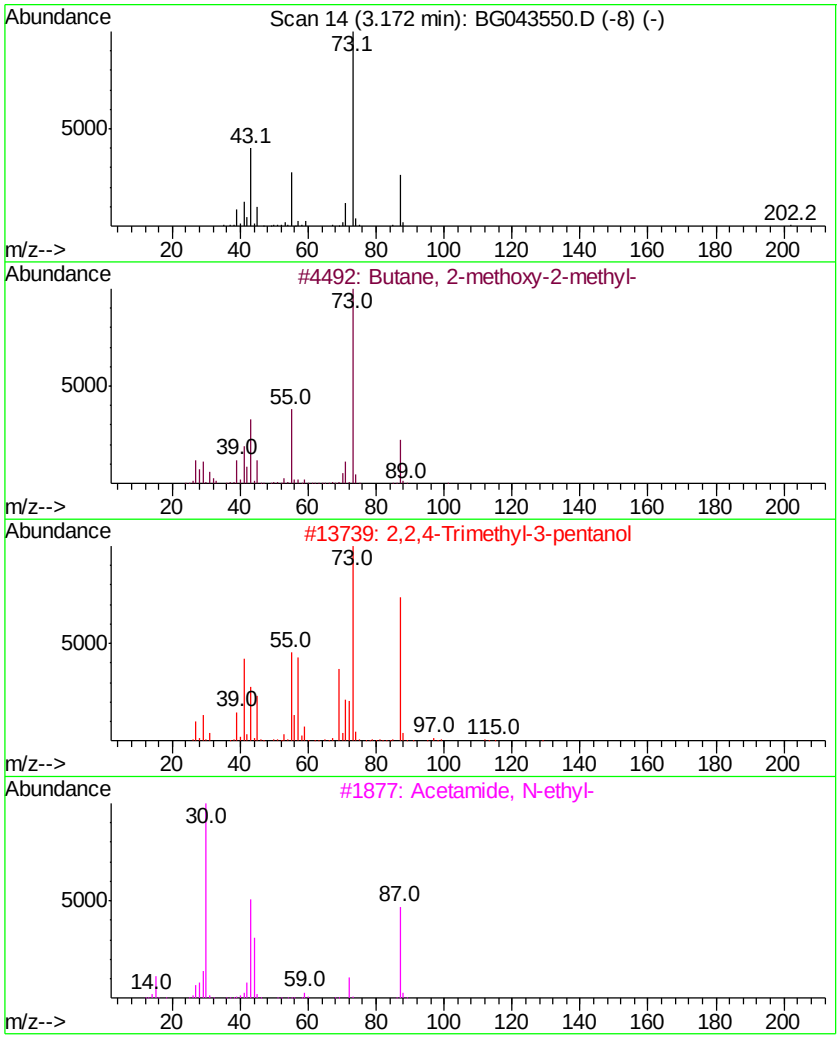
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

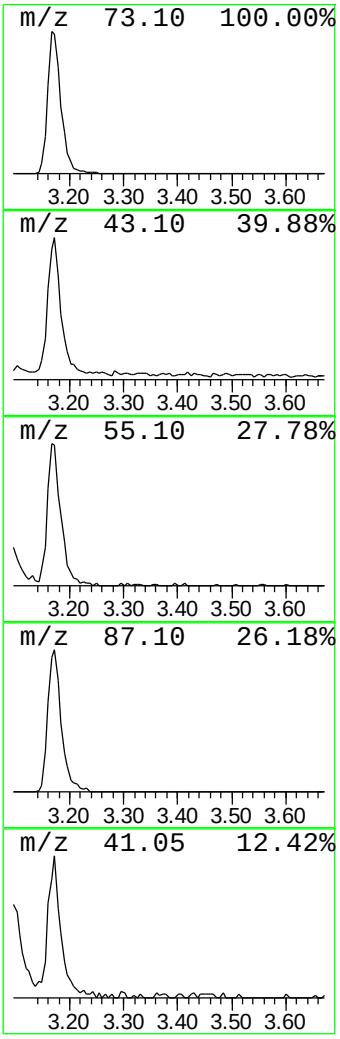
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	26.38 ng	252966	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	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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

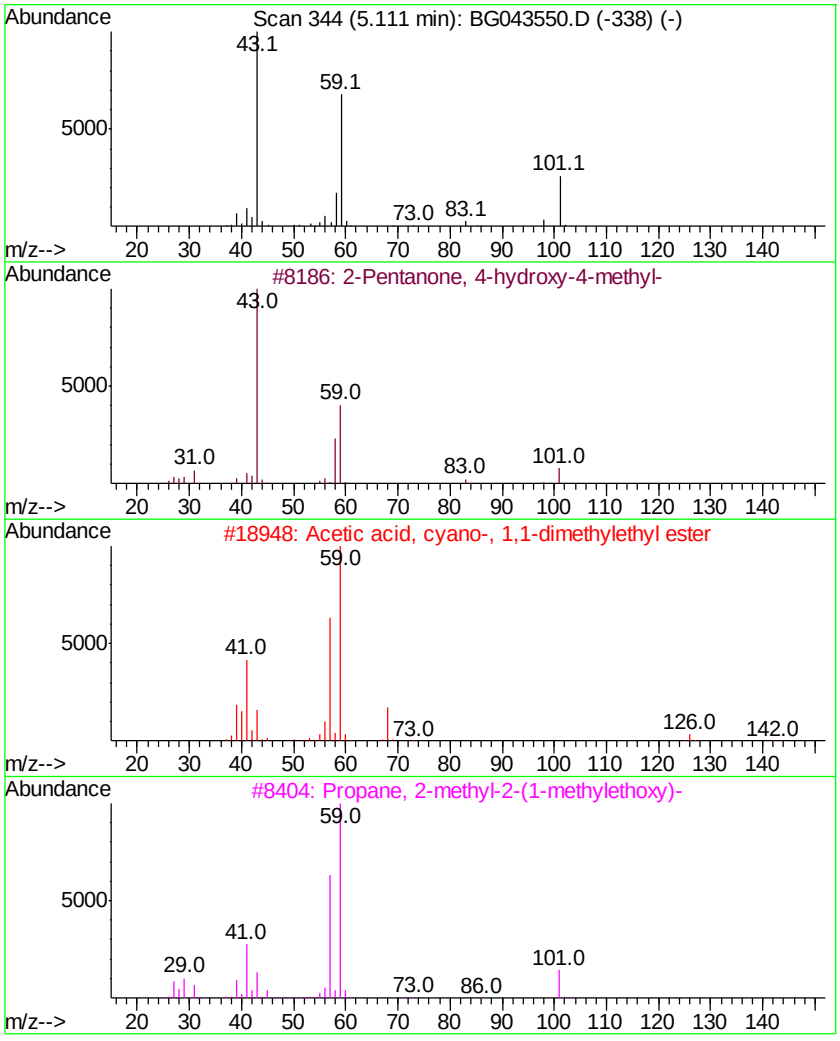
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

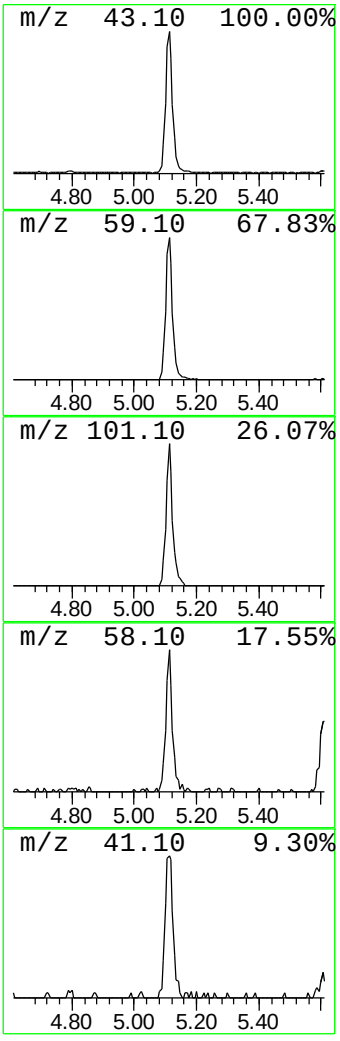
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	21.96 ng	210606	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	23
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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

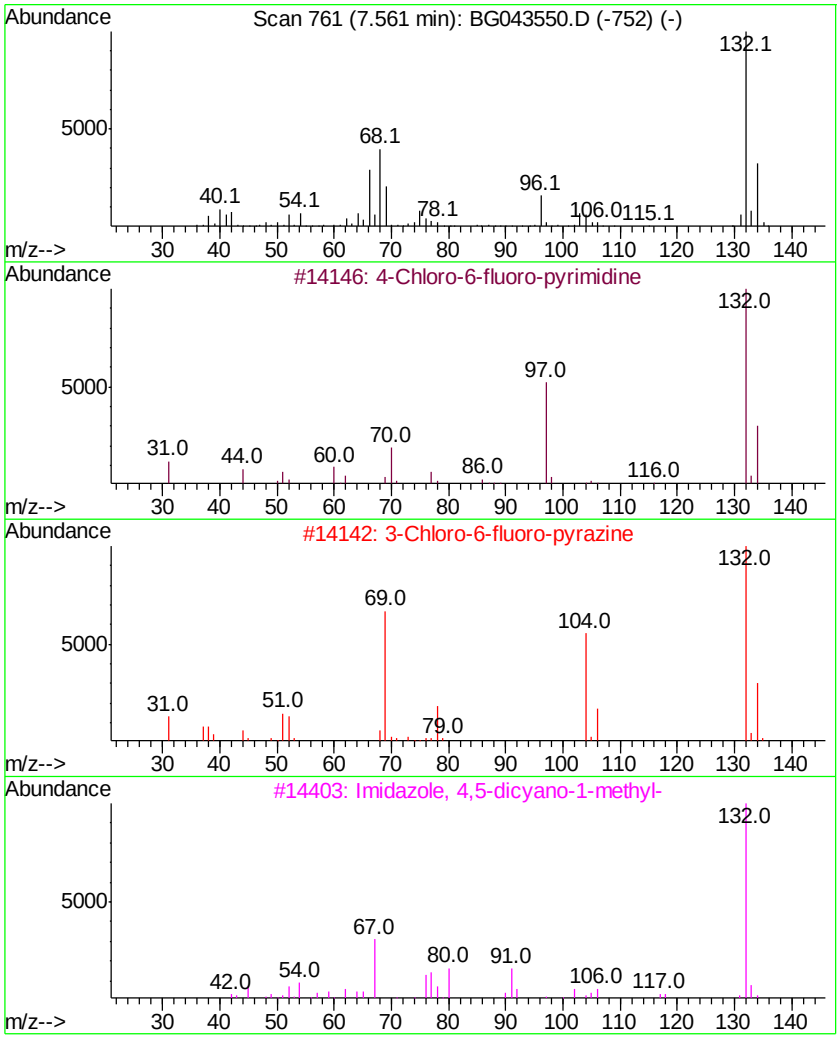
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

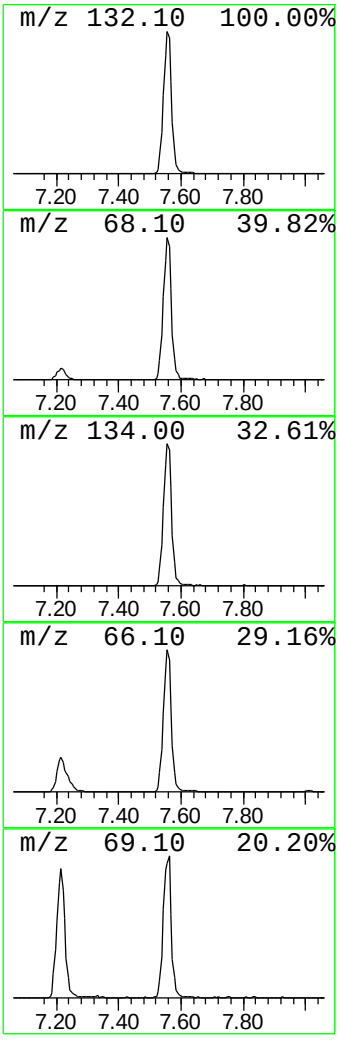
****

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	131.32 ng	1259200	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	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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

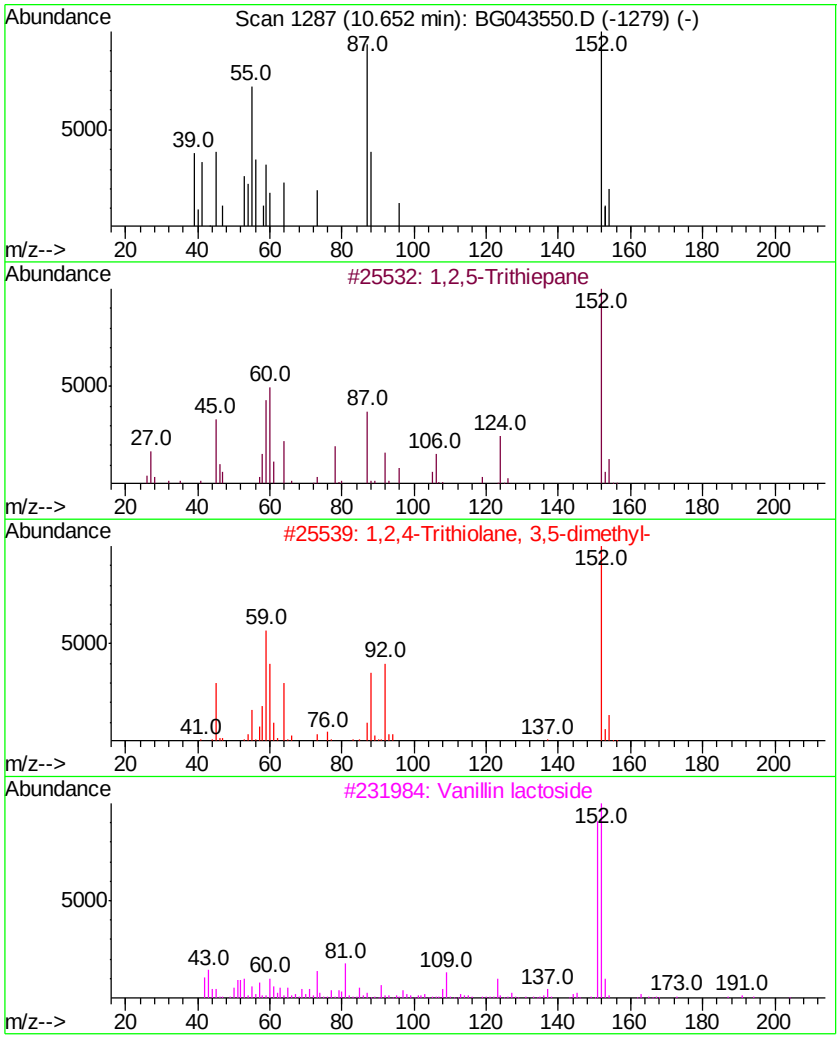
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

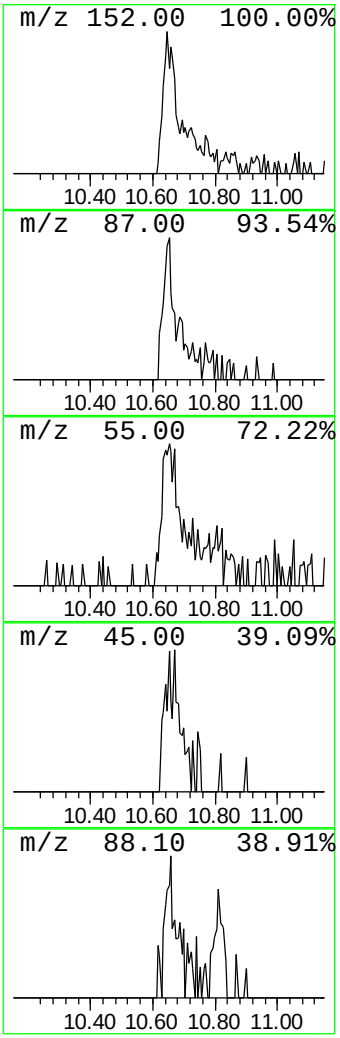
****

Peak Number 5 unknown10.65 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.93 ng	35080	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	47
2	1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	40
3	Vanillin lactoside	476	C20H28O13	1000129-94-7	27
4	6-Mercaptopurine	152	C5H4N4S	000050-44-2	25
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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

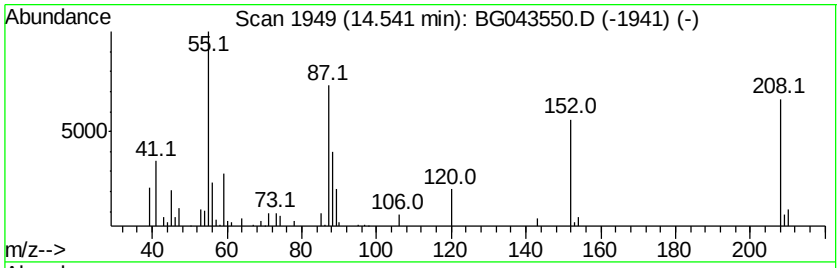
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

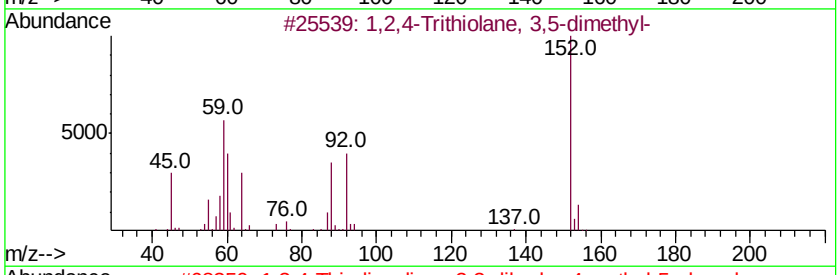
****

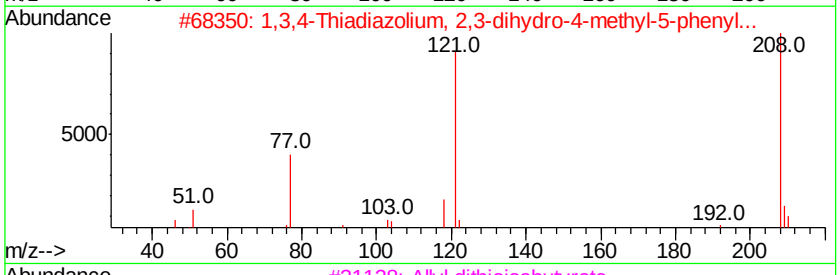
Peak Number 6 unknown14.54 Concentration Rank 7

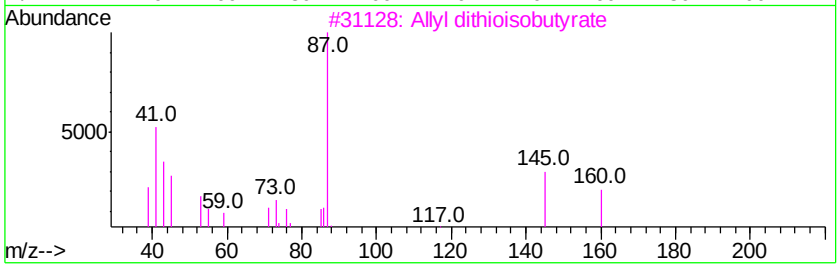
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	4.35 ng	80438	Acenaphthene-d10	14.64

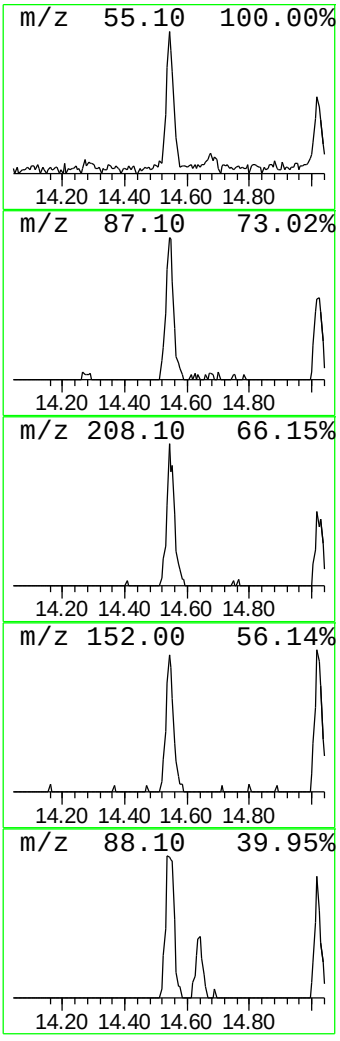
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	10
2	1,3,4-Thiadiazolium, 2,3-dihydro...	208	C9H8N2S2	019703-86-7	10
3	Allyl dithioisobutyrate	160	C7H12S2	063881-54-9	10
4	3-Hexanol, 3,4-diethyl-,	158	C10H22O	019398-78-8	10
5	Thiophane, propyl-	130	C7H14S	001551-34-4	10











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Data File : BG043550.D
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Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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

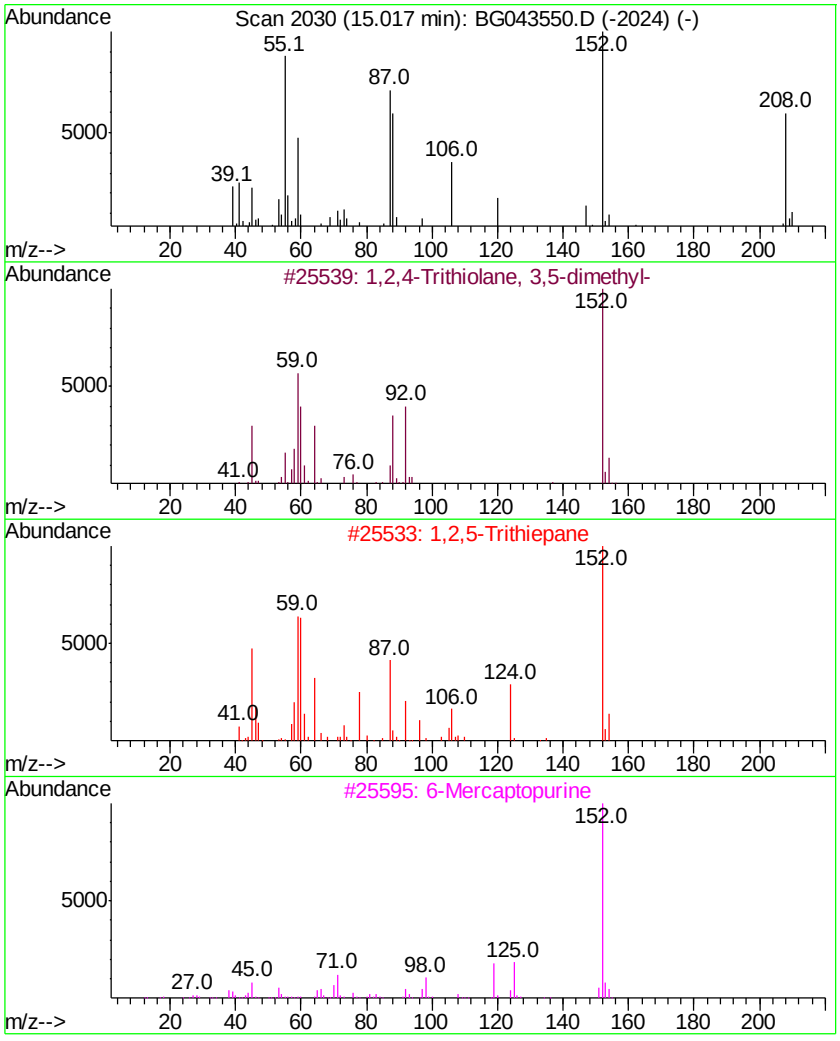
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

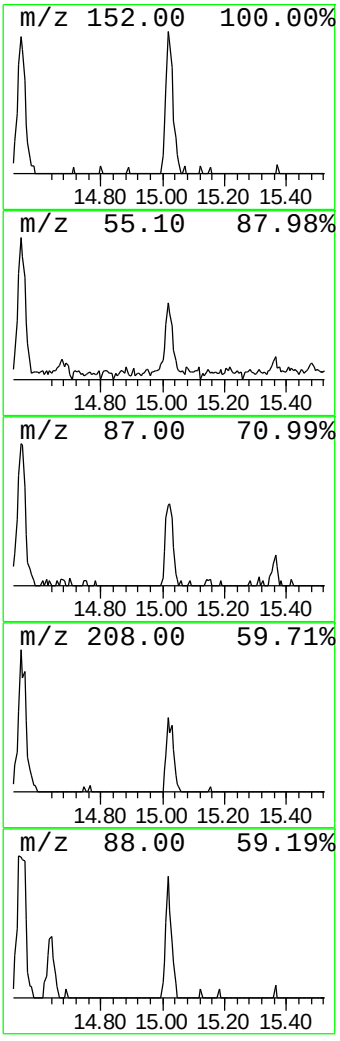
****

Peak Number 7 unknown15.02 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.51 ng	46491	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	32
2	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	32
3	6-Mercaptopurine	152	C5H4N4S	000050-44-2	14
4	Trimethyl thioborate	152	C3H9BS3	000997-49-9	12
5	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	558	C25H50O13	1000351-91-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

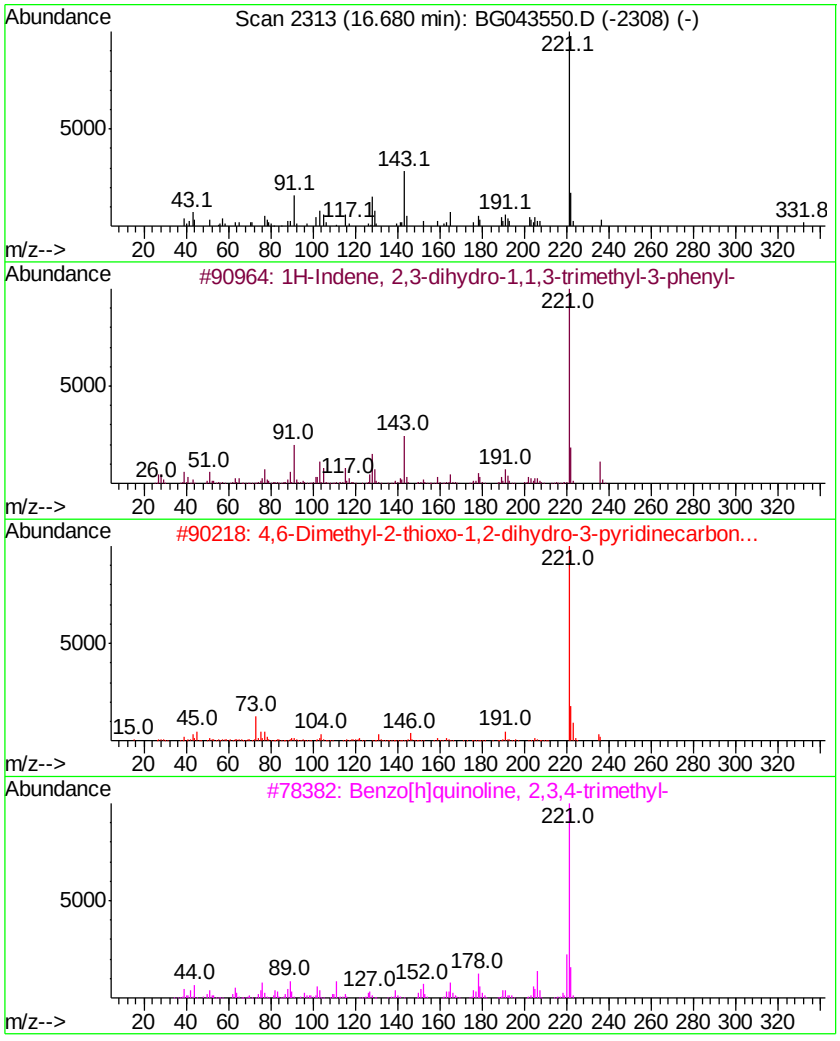
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

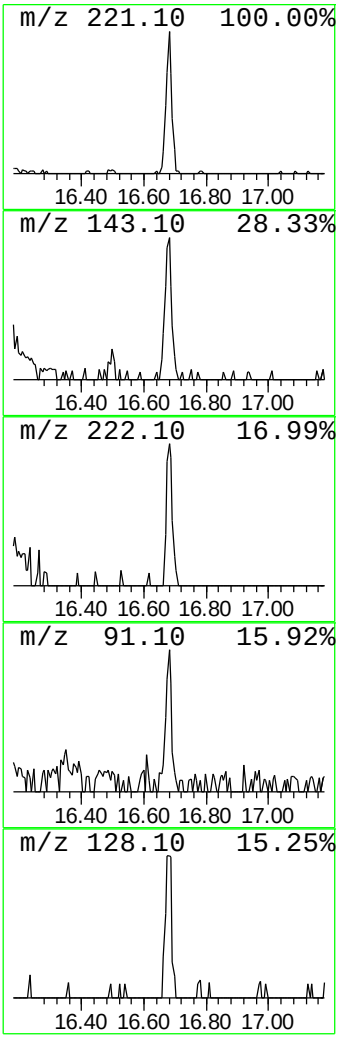
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.68	2.13 ng	50005	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	74
2	4,6-Dimethyl-2-thioxo-1,2-dihydr...	236	C11H16N2SSi	1000332-43-1	52
3	Benzo[h]quinoline, 2,3,4-trimethyl-	221	C16H15N	063042-66-0	52
4	1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	50
5	Benz[j]isoquinoline, 3,6,8-trime...	221	C16H15N	061171-16-2	50





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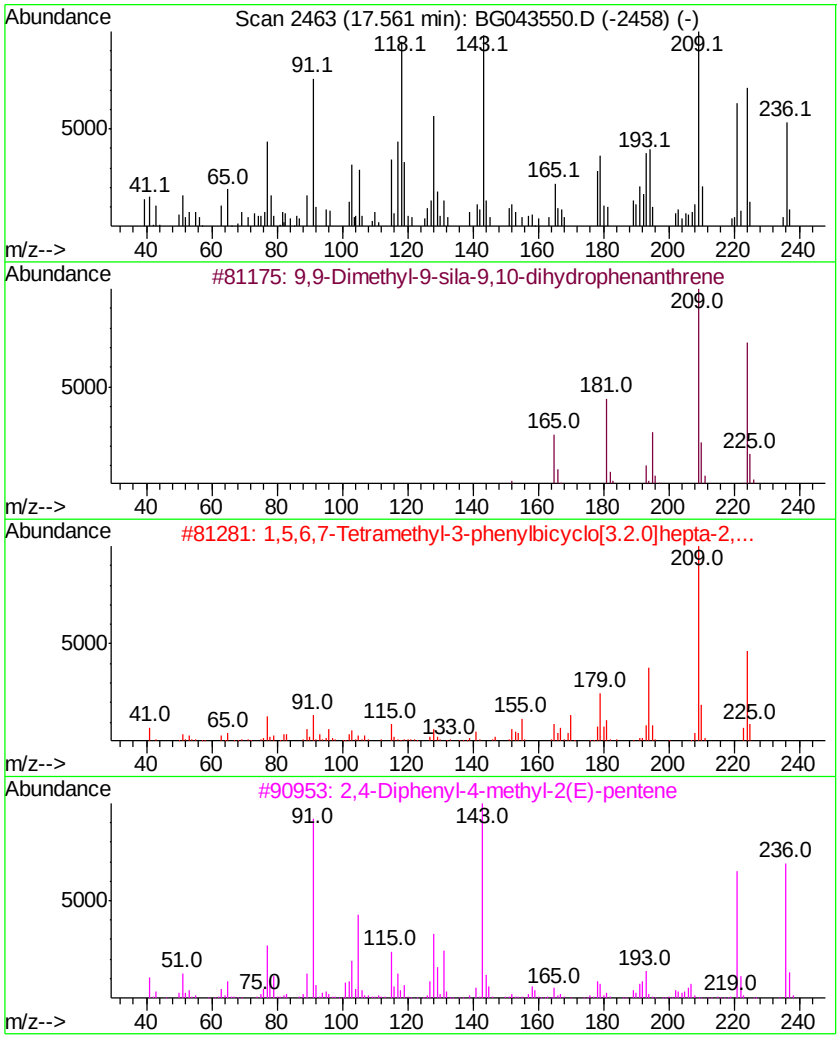
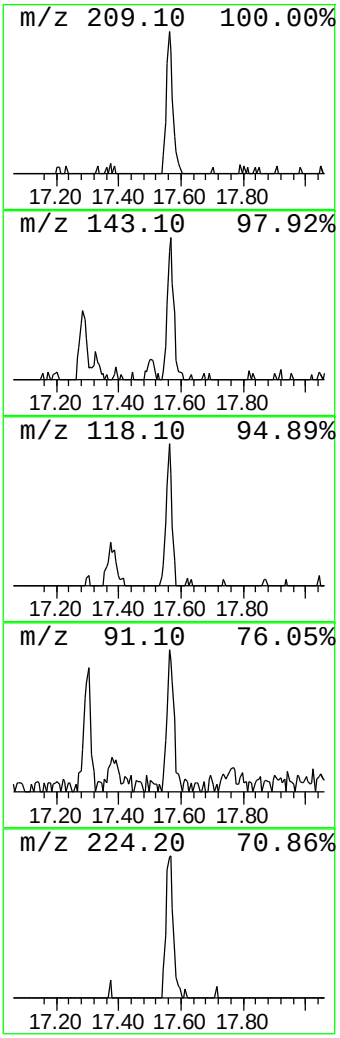
****

Peak Number 9 unknown17.56 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.56	4.02 ng	94519	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,9-Dimethyl-9-sila-9,10-dihydro...	224	C15H16Si	187328-55-8	46
2	1,5,6,7-Tetramethyl-3-phenylbicy...	224	C17H20	126584-00-7	38
3	2,4-Diphenyl-4-methyl-2(E)-pentene	236	C18H20	022768-22-5	38
4	2-Amino-5-isopropyl-8-methyl-1-a...	224	C15H16N2	093946-48-6	38
5	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	25





Library Search Compound Report

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Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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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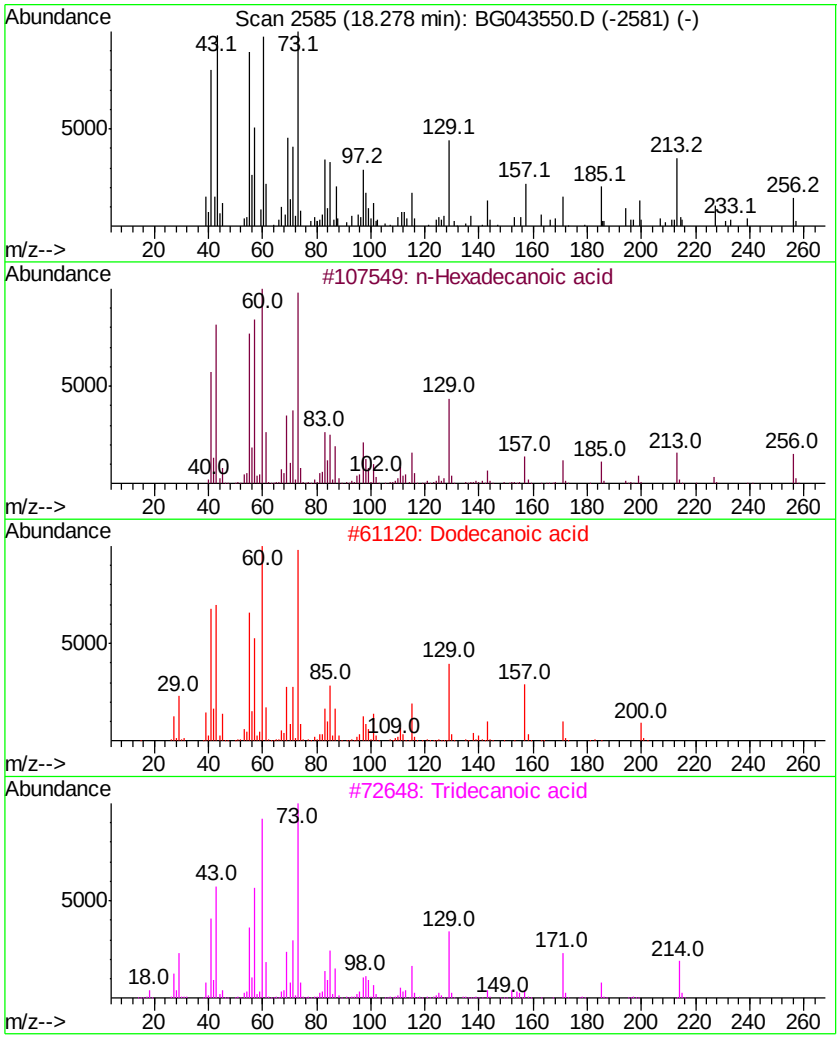
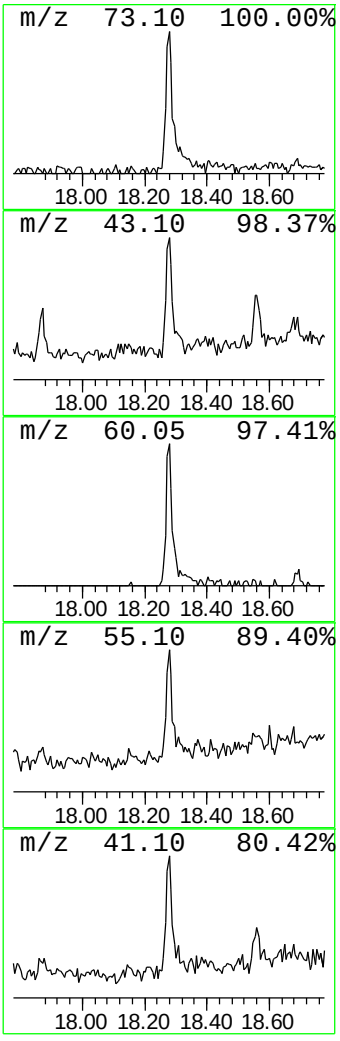
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	4.91 ng	115432	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Dodecanoic acid	200	C12H24O2	000143-07-7	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

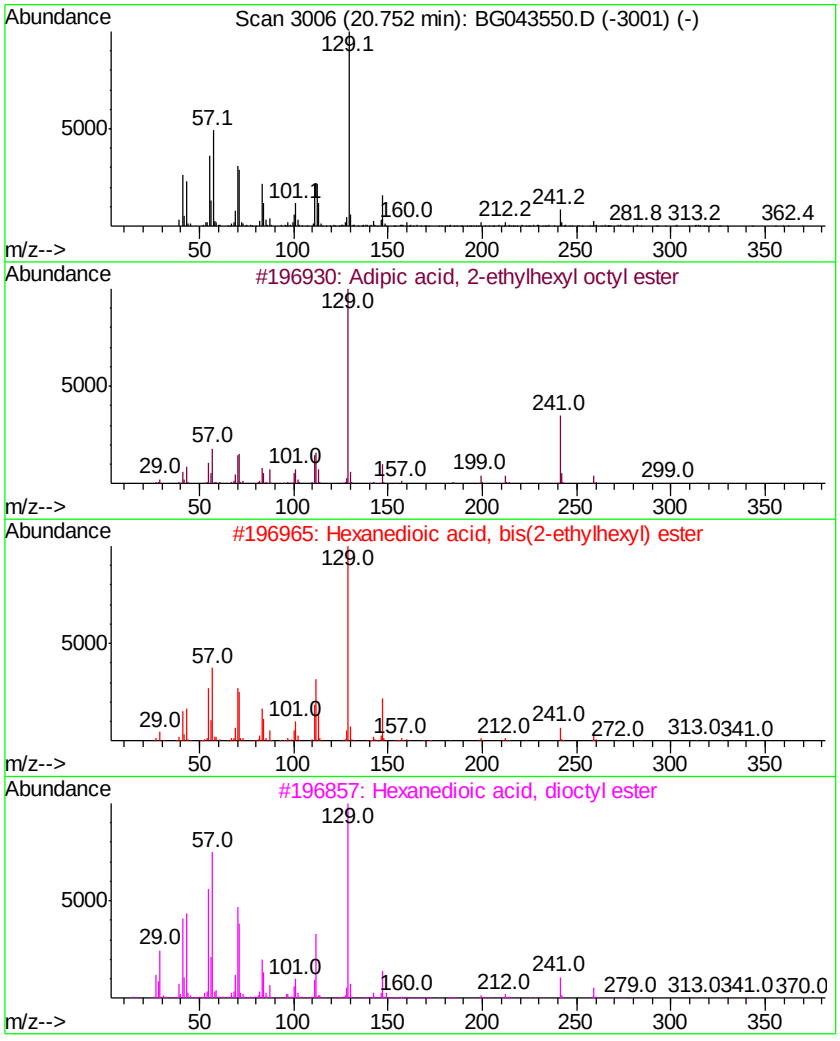
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

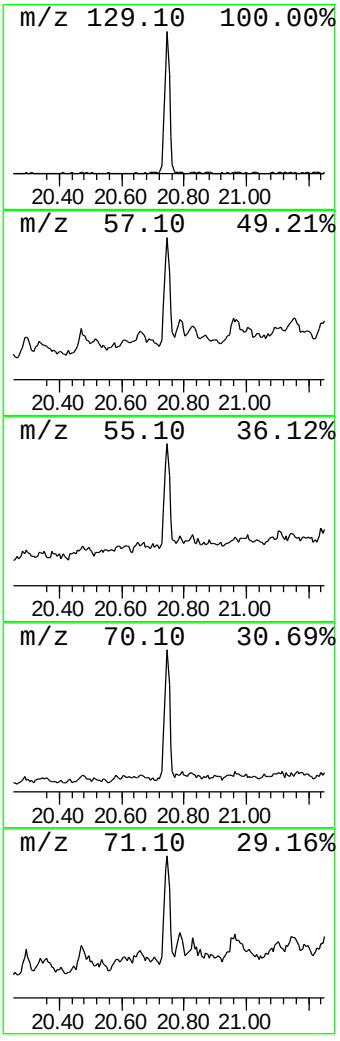
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Adipic acid, 2-ethylhexyl o... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	25.75 ng	594764	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	64
4	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	64
5	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110719\
Data File : BG043550.D
Acq On : 7 Nov 2019 22:05
Operator : JU
Sample : K5723-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 10-B

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	26.4	ng	252966	1	8.01	191781	20.0
2-Pentanone, 4-hy...	5.11	22.0	ng	210606	1	8.01	191781	20.0
unknown7.56	7.56	131.3	ng	1259200	1	8.01	191781	20.0
unknown10.65	10.65	2.9	ng	35080	2	10.81	239788	20.0
unknown14.54	14.54	4.3	ng	80438	3	14.64	370213	20.0
unknown15.02	15.02	2.5	ng	46491	3	14.64	370213	20.0
1H-Indene, 2,3-di...	16.68	2.1	ng	50005	4	17.39	470270	20.0
unknown17.56	17.56	4.0	ng	94519	4	17.39	470270	20.0
n-Hexadecanoic acid	18.28	4.9	ng	115432	4	17.39	470270	20.0
Adipic acid, 2-et...	20.75	25.8	ng	594764	5	21.65	462018	20.0