LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

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-BG061520.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	3.311	29	38	57	rVB	171844	495385	1.79%	0.824%
2	4.192	180	188	201	rVB3	358379	807571	2.93%	1.344%
3	5.538	409	417	428	rBV	292433	670549	2.43%	1.116%
4	7.194	693	699	709	rVB	187077	405468	1.47%	0.675%
5	7.306	712	718	727	rVB	288164	504980	1.83%	0.840%
6	7.811	795	804	815	rVV	597639	1159251	4.20%	1.929%
7	7.958	815	829	837	rVV	2277480	4434333	16.07%	7.378%
8	8.304	869	888	894	rBV	11395437	27598129	100.00%	45.919%
9	8.569	929	933	939	rVB2	406578	670747	2.43%	1.116%
10	9.039	1003	1013	1016	rBV2	496619	941713	3.41%	1.567%
11	9.086	1016	1021	1037	rVB3	615466	1479739	5.36%	2.462%
12	9.221	1037	1044	1051	rBV4	161050	380170	1.38%	0.633%
13	9.350	1059	1066	1067	rBV	417296	722279	2.62%	1.202%
14	9.515	1089	1094	1106	rVB4	205137	505949	1.83%	0.842%
15	9.732	1125	1131	1138	rVB	259968	476037	1.72%	0.792%
16	10.143	1186	1201	1209	rBV3	316277	852908	3.09%	1.419%
17	10.402	1233	1245	1254	rVV4	146240	422853	1.53%	0.704%
18	10.513	1254	1264	1268	rVV2	498980	973106	3.53%	1.619%
19	10.560	1268	1272	1281	rVB4	175413	446518	1.62%	0.743%
20	10.725	1292	1300	1305	rBV	274953	560213	2.03%	0.932%
21	11.835	1483	1489	1495	rVB3	158079	301189	1.09%	0.501%
22	12.364	1575	1579	1587	rVB	206396	335868	1.22%	0.559%
23	13.186	1713	1719	1726	rVB	1687051	2653005	9.61%	4.414%
24	13.368	1744	1750	1755	rBV	337171	597109	2.16%	0.993%
25	13.533	1773	1778	1784	rBV2	161591	286890	1.04%	0.477%
26	13.644	1790	1797	1809	rVB2	325014	947294	3.43%	1.576%
27	14.396	1916	1925	1936	rVB6	139827	389940	1.41%	0.649%
28	14.567	1945	1954	1962	rBV2	427255	833102	3.02%	1.386%
29	16.070	2204	2210	2217	rVB	1451093	2337228	8.47%	3.889%
30	16.300	2244	2249	2260	rVB	212426	402612	1.46%	0.670%
31	17.316	2417	2422	2429	rVB	497039	796191	2.88%	1.325%
32	18.232	2574	2578	2584	rBV	234836	316937	1.15%	0.527%
33	19.936	2863	2868	2874	rVB	2964208	3824848	13.86%	6.364%
34	21.575	3142	3147	3153	rVB	467197	751709	2.72%	1.251%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

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-BG061520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	24.706	3672	3680	3692	rVB	290781	819826	2.97%	1.364%

Sum of corrected areas: 60101646

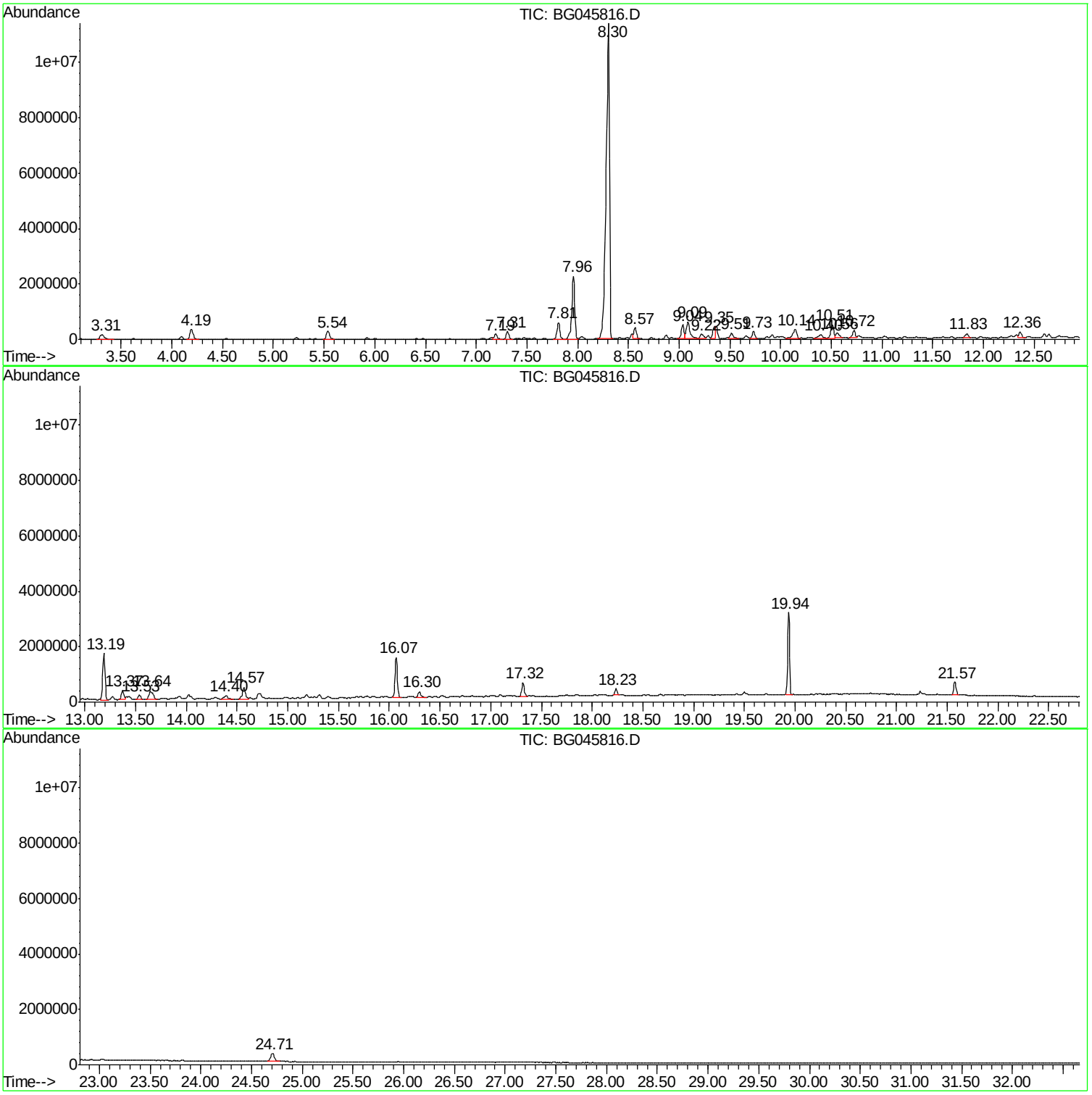
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.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\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

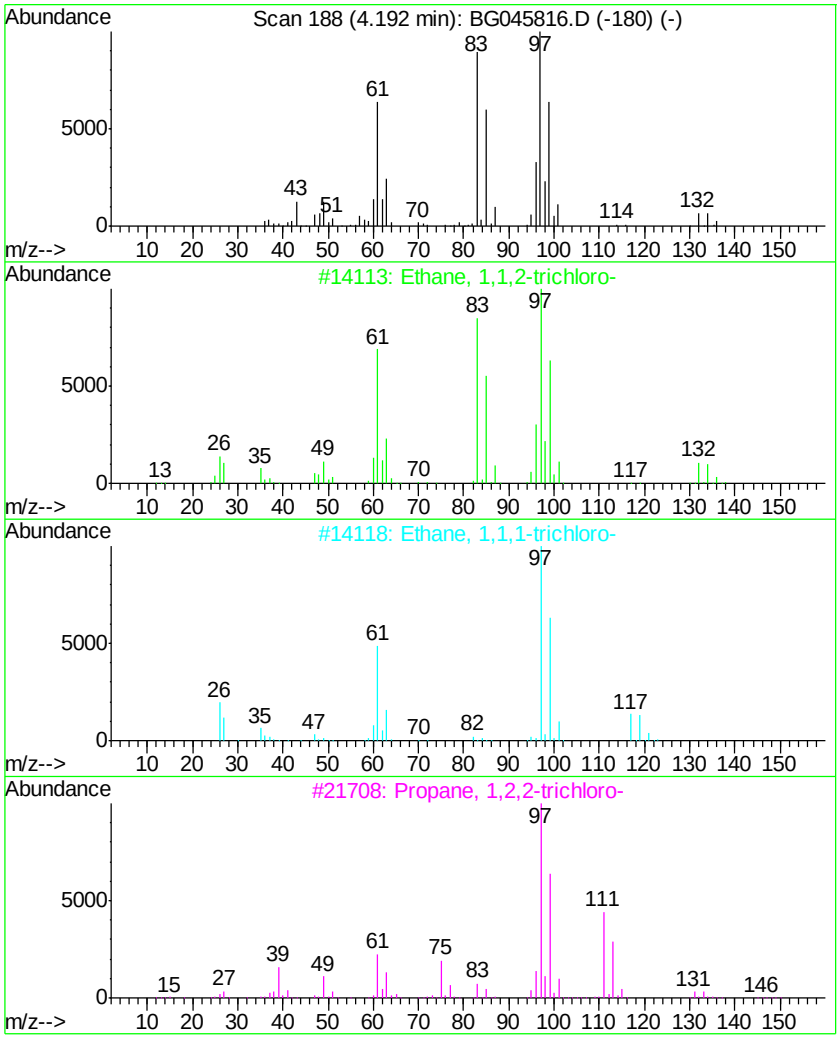
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

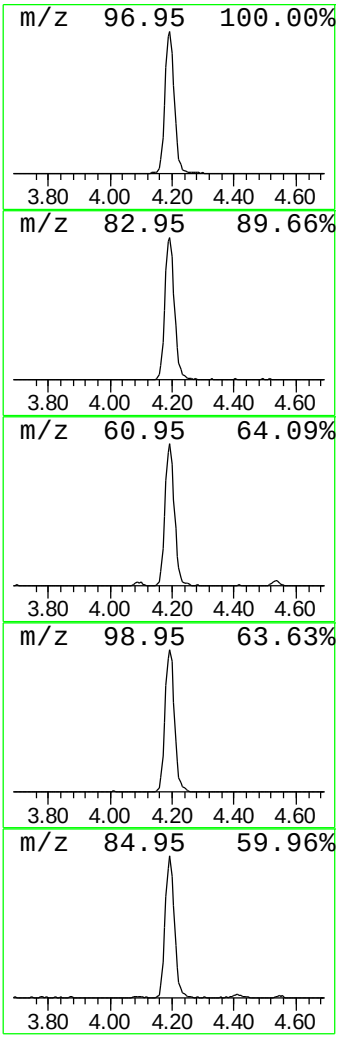
****

Peak Number 2 Ethane, 1,1,2-trichloro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	3.64 ng	807571	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1,2-trichloro-	132	C2H3Cl3	000079-00-5	96
2	Ethane, 1,1,1-trichloro-	132	C2H3Cl3	000071-55-6	43
3	Propane, 1,2,2-trichloro-	146	C3H5Cl3	003175-23-3	38
4	Ethane, 1,1-dichloro-1-nitro-	143	C2H3Cl2NO2	000594-72-9	38
5	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

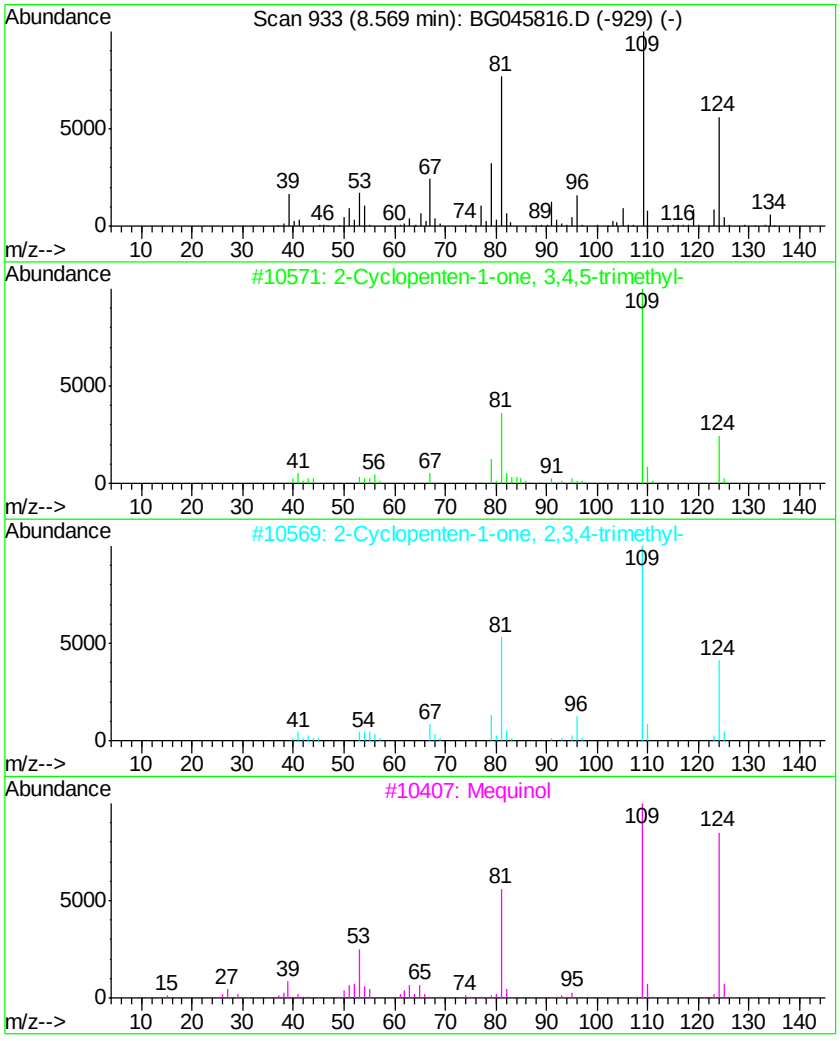
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

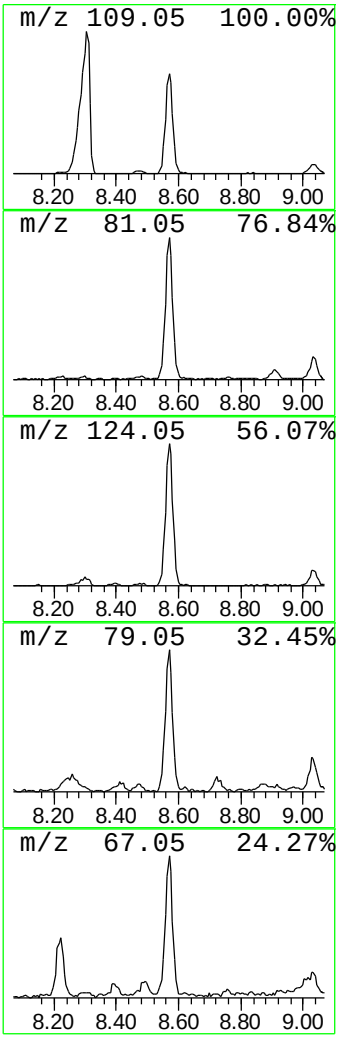
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Cyclopenten-1-one, 3,4,5-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	3.03 ng	670747	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	86
2	2-Cyclopenten-1-one, 2,3,4-trime...	124	C8H12O	028790-86-5	83
3	Mequinol	124	C7H8O2	000150-76-5	76
4	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	76
5	2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

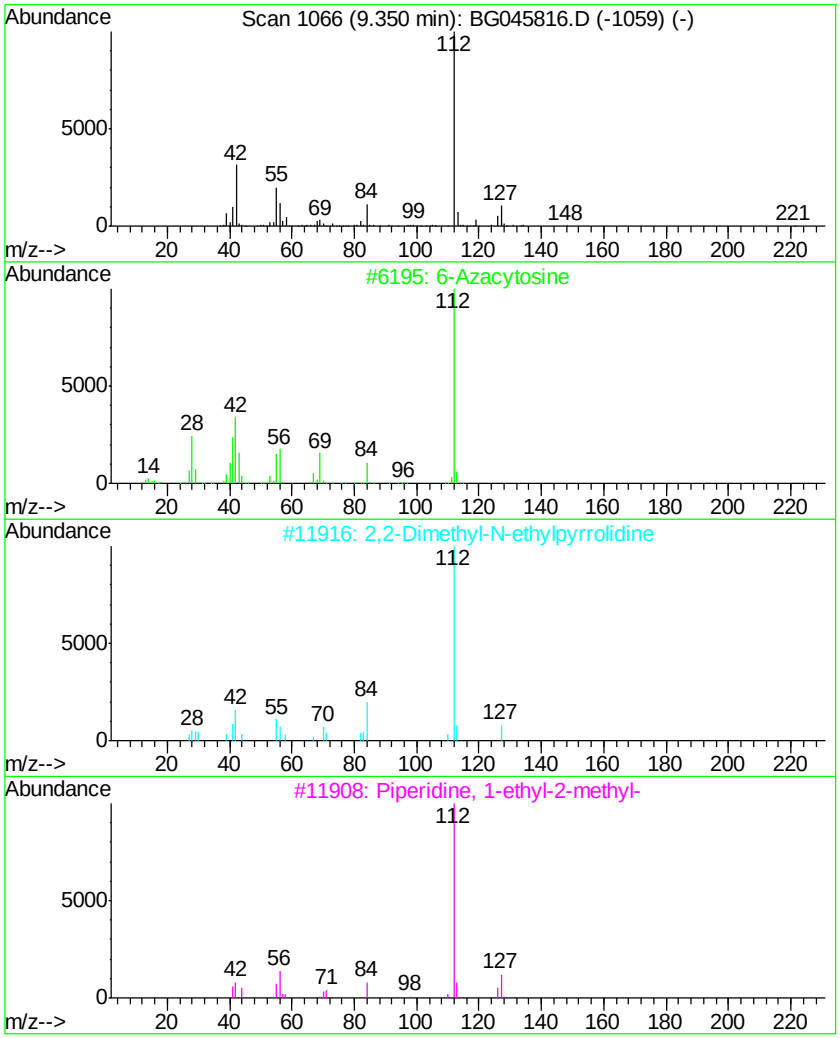
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

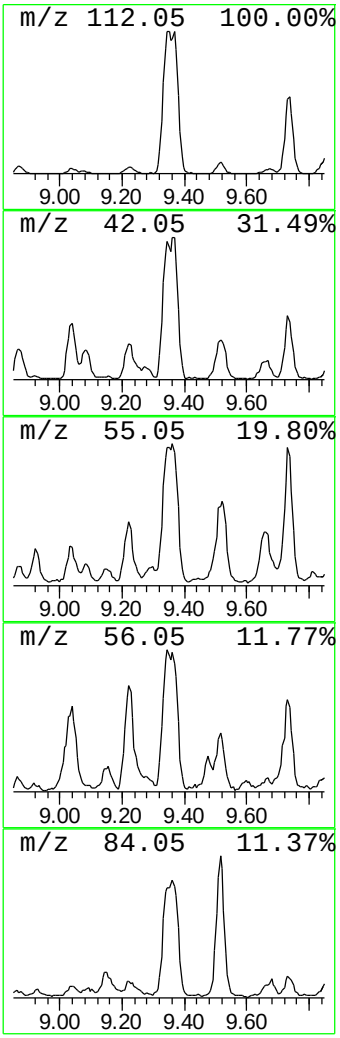
****

Peak Number 4 6-Azacytosine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.35	25.79 ng	722279	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Azacytosine	112	C3H4N4O	000931-85-1	80
2	2,2-Dimethyl-N-ethylpyrrolidine	127	C8H17N	089214-93-7	78
3	Piperidine, 1-ethyl-2-methyl-	127	C8H17N	000766-52-9	72
4	1-Ethyl-4-piperidone	127	C7H13NO	003612-18-8	50
5	Piperidine, 5-ethyl-2-methyl-	127	C8H17N	000104-89-2	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

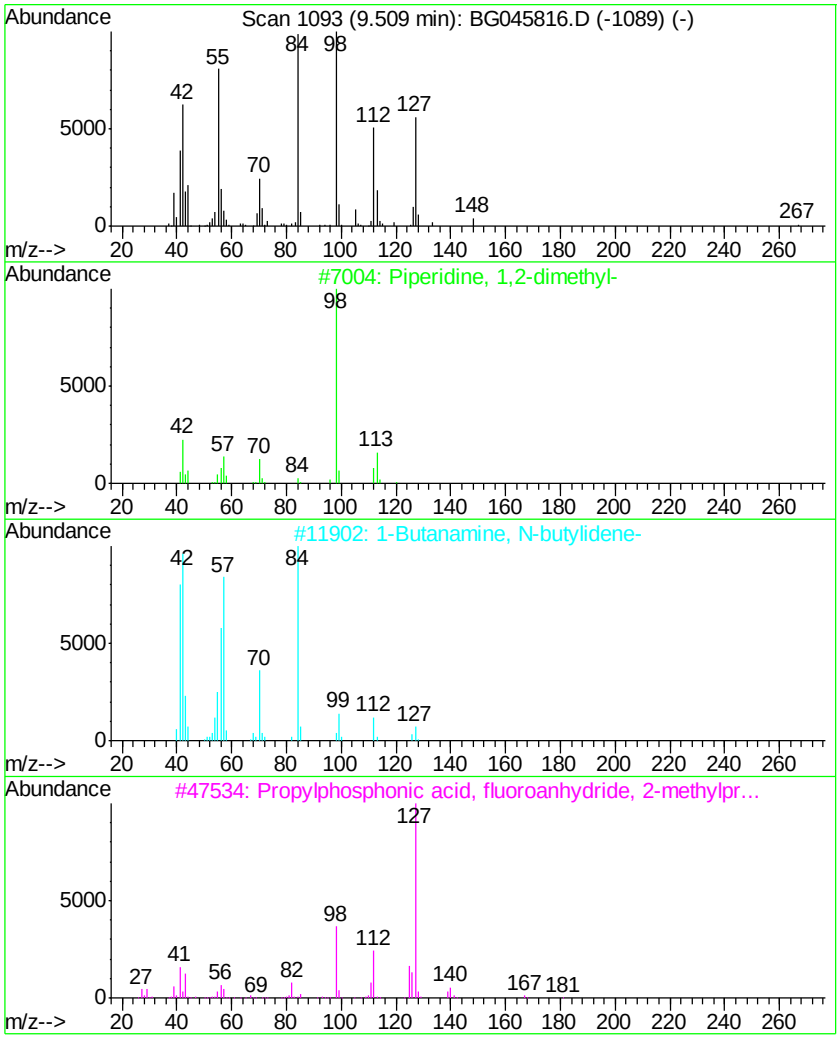
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

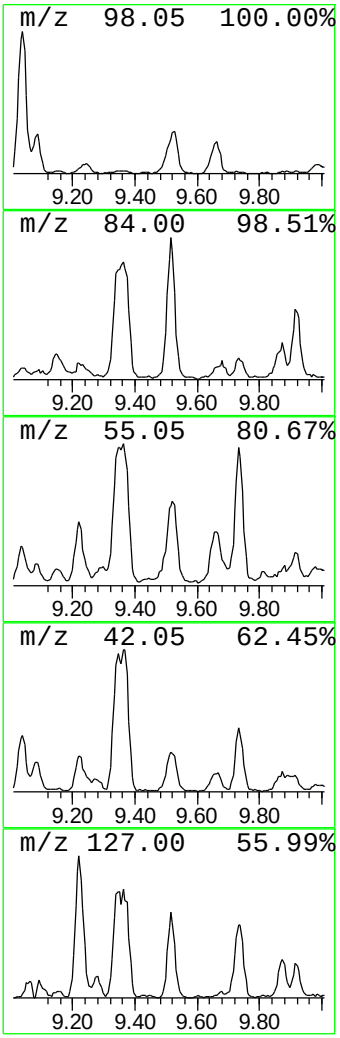
****

Peak Number 5 unknown9.51 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	18.06 ng	505949	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidine, 1,2-dimethyl-	113	C7H15N	000671-36-3	49
2	1-Butanamine, N-butylidene-	127	C8H17N	004853-56-9	47
3	Propylphosphonic acid, fluoroanh...	182	C7H16FO2P	333416-26-5	43
4	Piperidine, 1-ethyl-	113	C7H15N	000766-09-6	38
5	3-Piperidinone, 1,6-dimethyl-	127	C7H13NO	043152-92-7	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

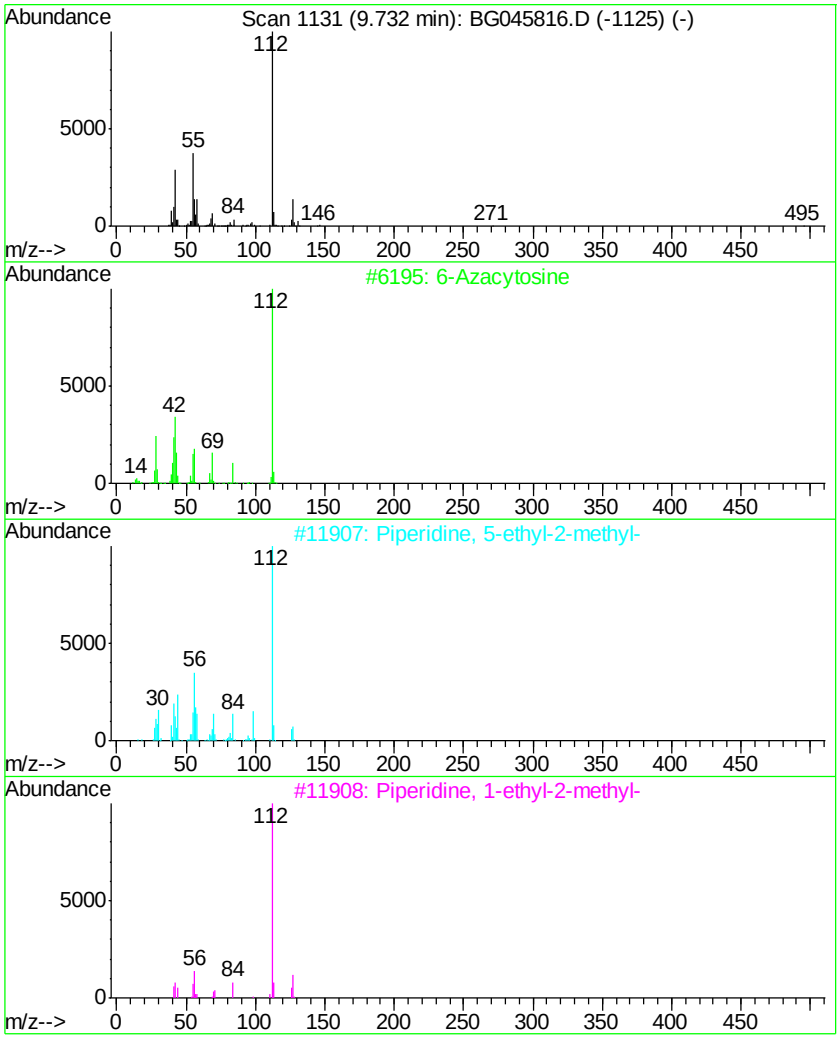
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

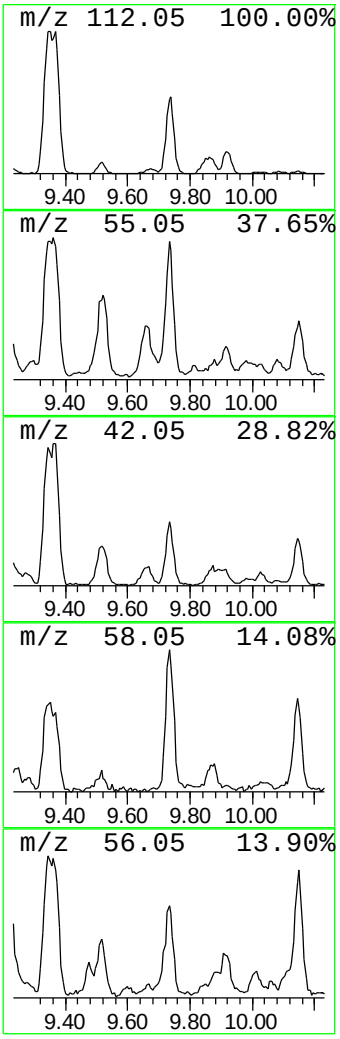
****

Peak Number 6 Piperidine, 5-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.73	16.99 ng	476037	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Azacytosine	112	C3H4N4O	000931-85-1	64
2	Piperidine, 5-ethyl-2-methyl-	127	C8H17N	000104-89-2	64
3	Piperidine, 1-ethyl-2-methyl-	127	C8H17N	000766-52-9	59
4	3H-Pyrazol-3-one, 2,4-dihydro-2,...	112	C5H8N2O	002749-59-9	53
5	2-Hydroxymethyl-2-methyl-pyrroli...	143	C7H13NO2	1000189-82-1	42





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Operator : CG/JU
Sample : L3033-08
Misc :
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Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

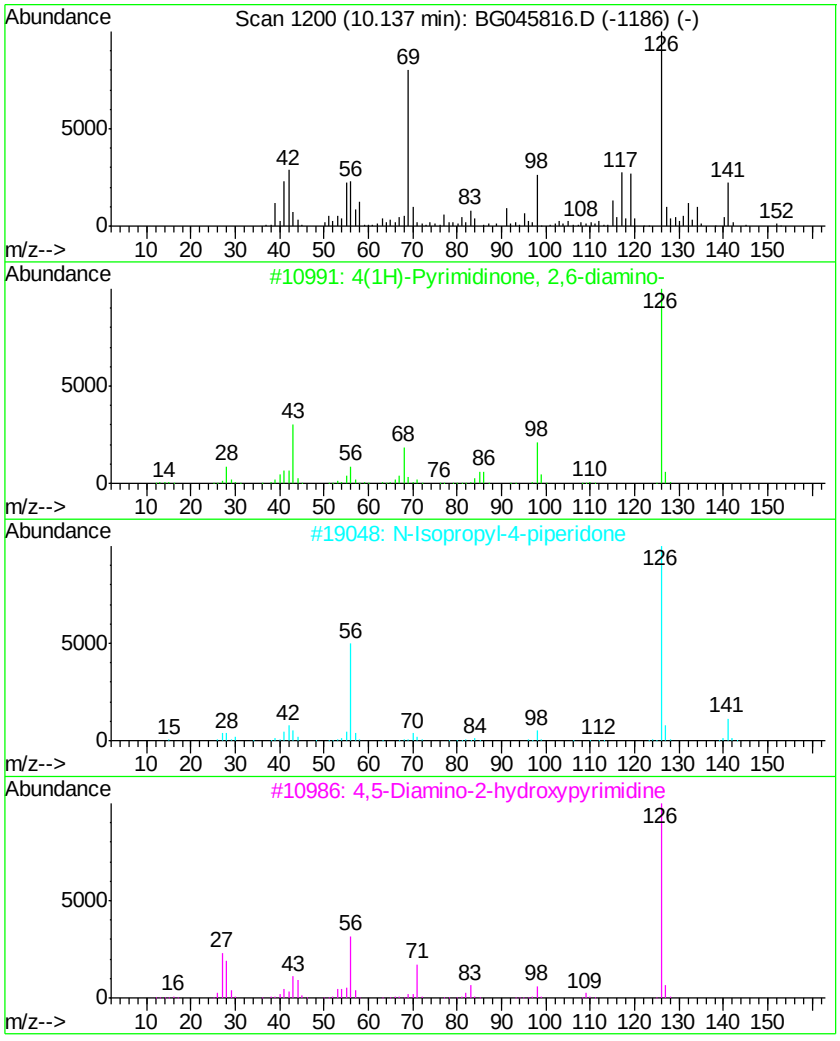
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

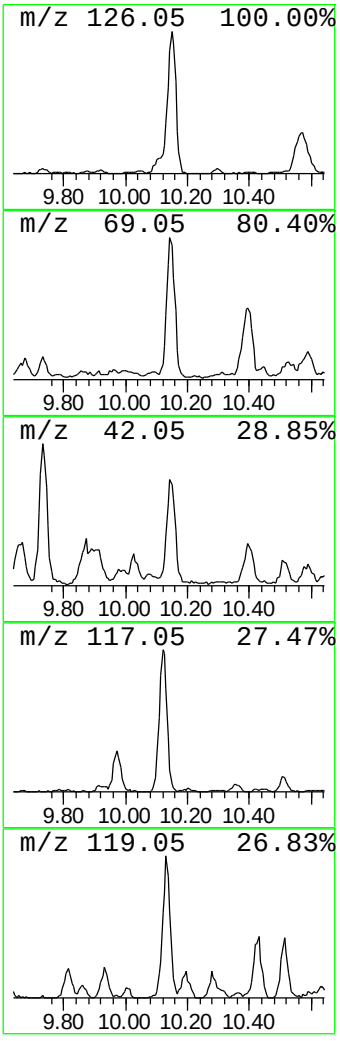
****

Peak Number 7 4(1H)-Pyrimidinone, 2,6-dia... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	30.45 ng	852908	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4(1H)-Pyrimidinone, 2,6-diamino-	126	C4H6N4O	000056-06-4	59
2	N-Isopropyl-4-piperidone	141	C8H15NO	005355-68-0	58
3	4,5-Diamino-2-hydroxypyrimidine	126	C4H6N4O	023899-73-2	47
4	Fumaric acid, monoamide, N,N-dim...	287	C12H11Cl2NO3	1000357-45-6	43
5	(2S,5S)-2-Butyl-5-pentylpyrrolidine	197	C13H27N	103833-64-3	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
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Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

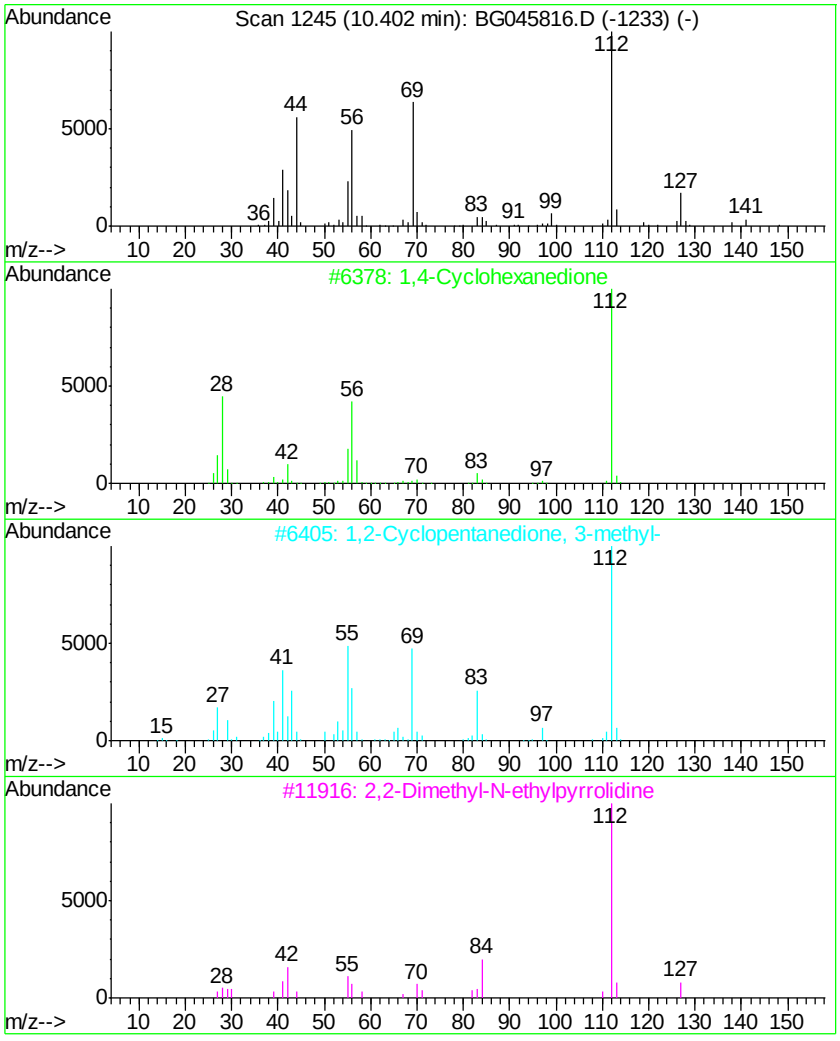
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

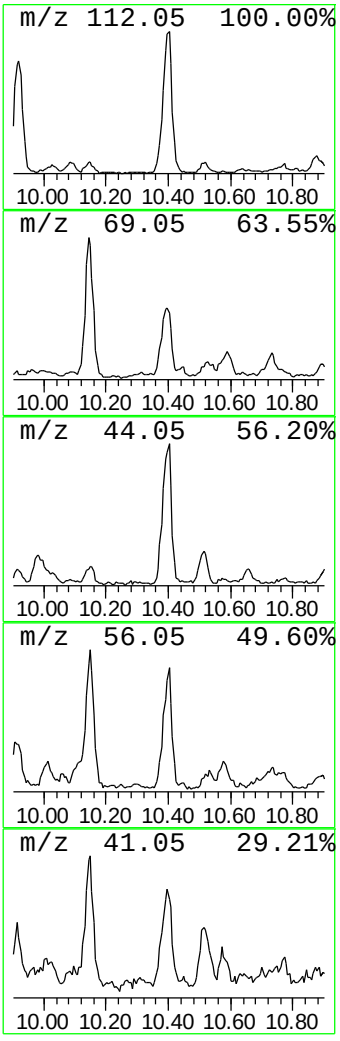
****

Peak Number 8 1,4-Cyclohexanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	15.10 ng	422853	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Cyclohexanedione	112	C6H8O2	000637-88-7	50
2	1,2-Cyclopentanedione, 3-methyl-	112	C6H8O2	000765-70-8	47
3	2,2-Dimethyl-N-ethylpyrrolidine	127	C8H17N	089214-93-7	43
4	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	43
5	Uracil	112	C4H4N2O2	000066-22-8	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

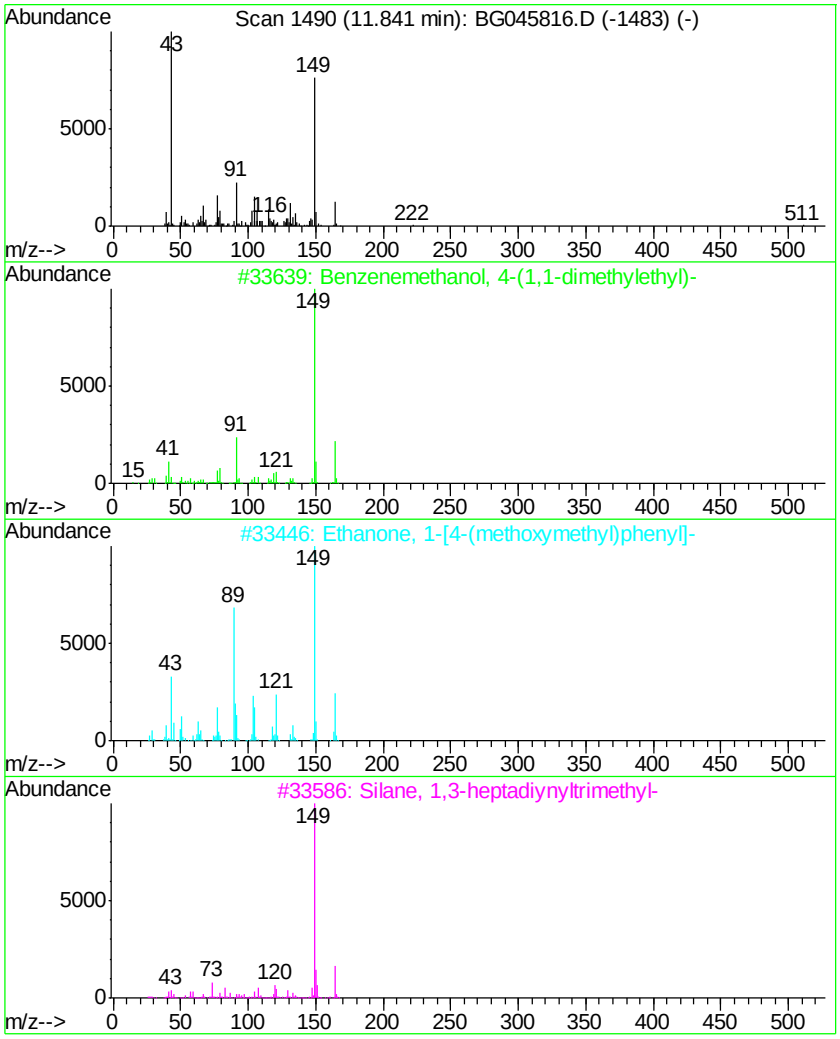
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

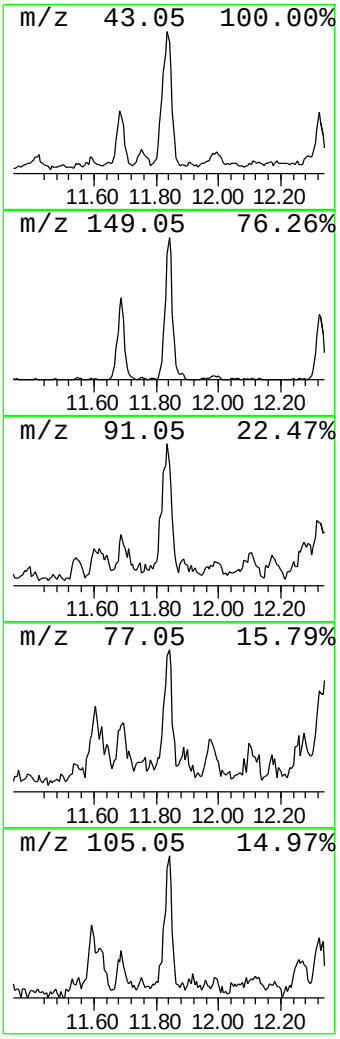
****

Peak Number 9 Benzenemethanol, 4-(1,1-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	10.75 ng	301189	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, 4-(1,1-dimethyl...	164	C11H16O	000877-65-6	50
2	Ethanone, 1-[4-(methoxymethyl)ph...	164	C10H12O2	022072-50-0	47
3	Silane, 1,3-heptadiynyltrimethyl-	164	C10H16Si	019024-47-6	43
4	Benzene, 2-methoxy-4-methyl-1-(1...	164	C11H16O	001076-56-8	38
5	Phthalic acid, octyl tridec-2-yn...	456	C29H44O4	1000315-44-1	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045816.D
Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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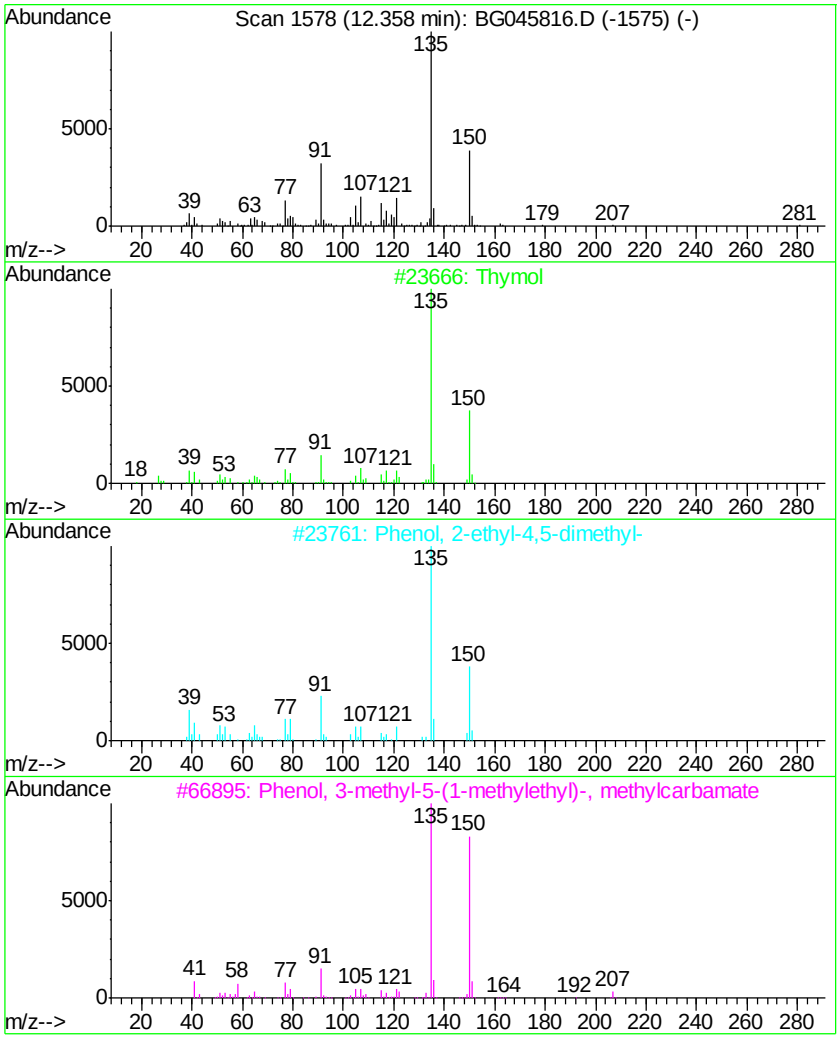
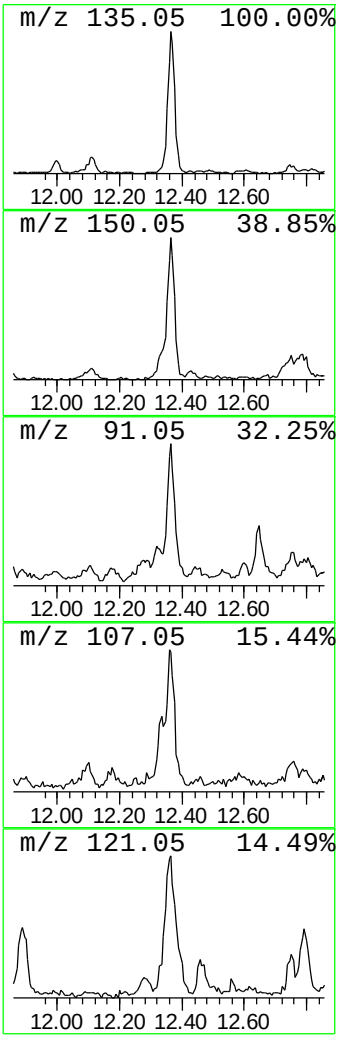
****

Peak Number 10 Thymol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	11.99 ng	335868	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thymol	150	C10H14O	000089-83-8	87
2	Phenol, 2-ethyl-4,5-dimethyl-	150	C10H14O	002219-78-5	83
3	Phenol, 3-methyl-5-(1-methylethy...	207	C12H17NO2	002631-37-0	78
4	Benzene, 2-methoxy-1,3,5-trimethyl-	150	C10H14O	004028-66-4	74
5	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	72





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Acq On : 19 Jun 2020 15:26
Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.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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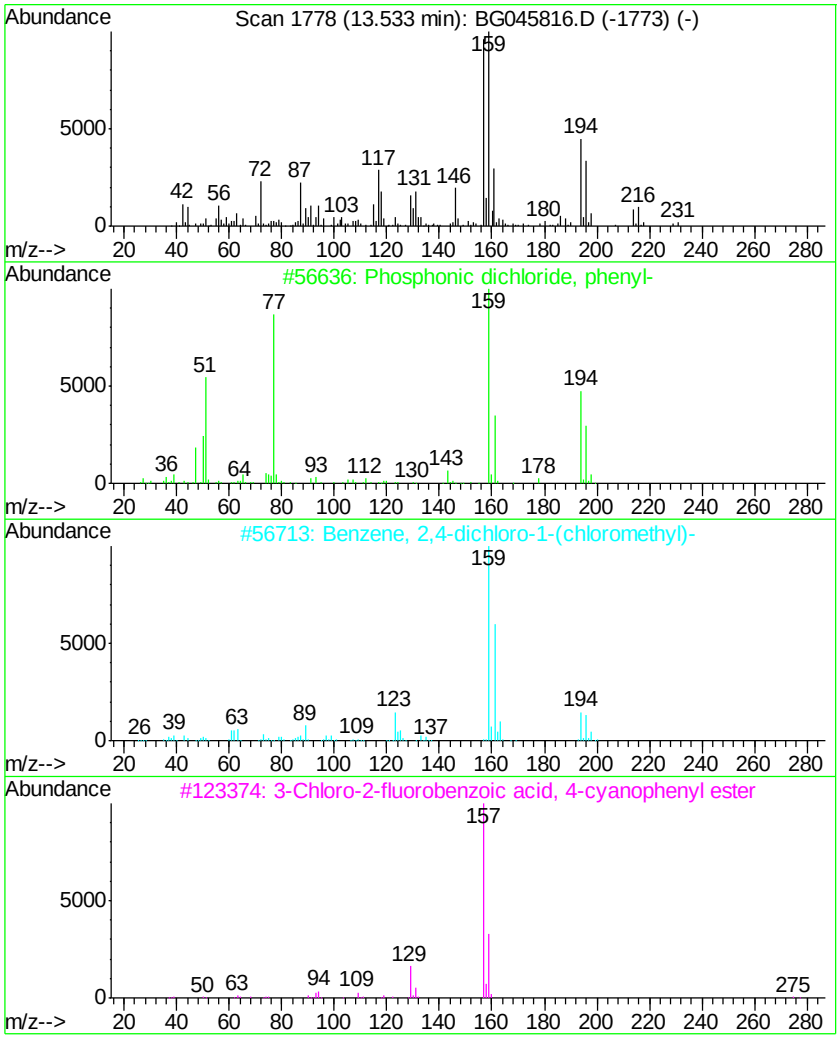
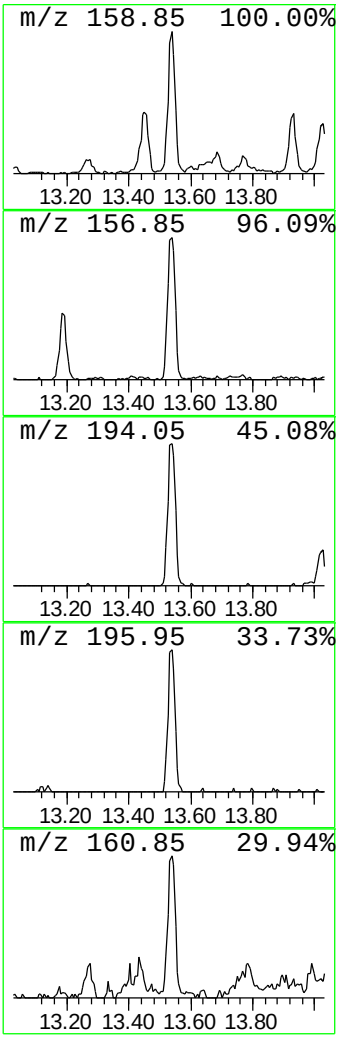
Peak Number 11 unknown13.53 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	6.89 ng	286890	Acenaphthene-d10	14.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphonic dichloride, phenyl-	194	C6H5Cl2OP	000824-72-6	41
2	Benzene, 2,4-dichloro-1-(chlorom...	194	C7H5Cl3	000094-99-5	27
3	3-Chloro-2-fluorobenzoic acid, 4...	275	C14H7ClFNO2	1000357-73-2	14
4	3-Chloro-2-fluorobenzoic acid, 2...	346	C14H6Cl3FO3	1000357-33-8	14
5	3-Chlorobicyclo(2.2.1)heptan-2-o...	159	C7H10ClNO	010499-35-1	11





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Instrument : BNA_G
ClientSampleId : SS043MW009-200616

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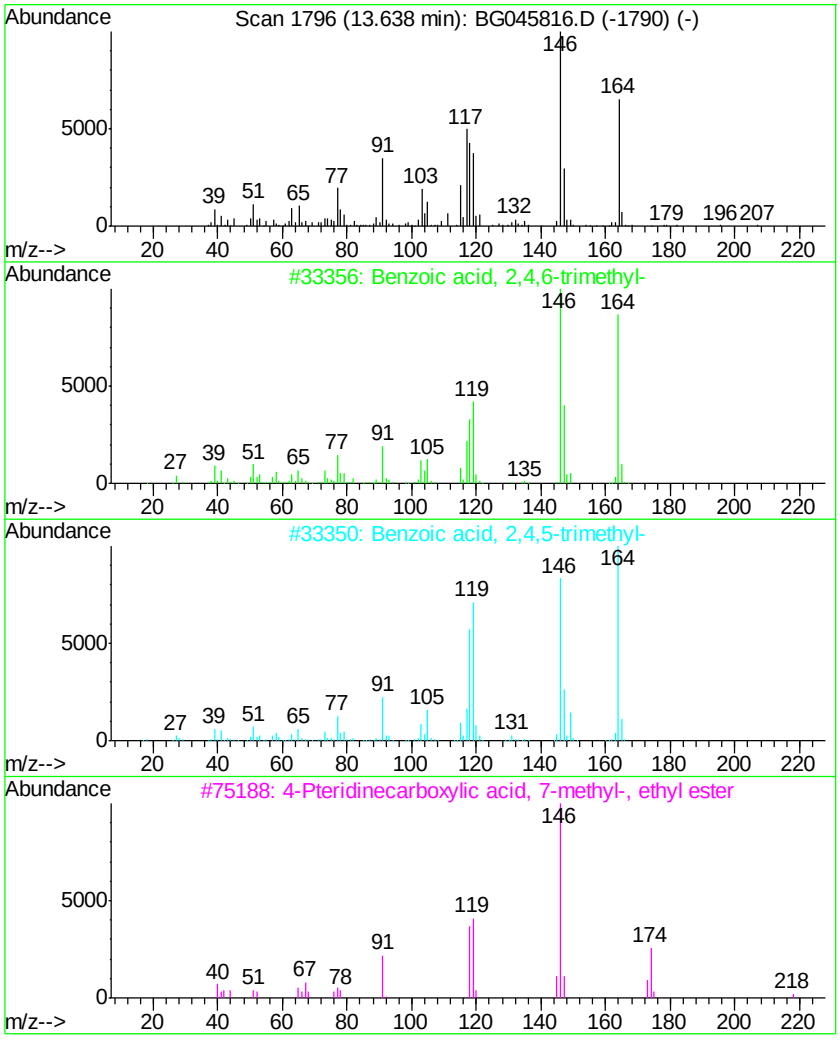
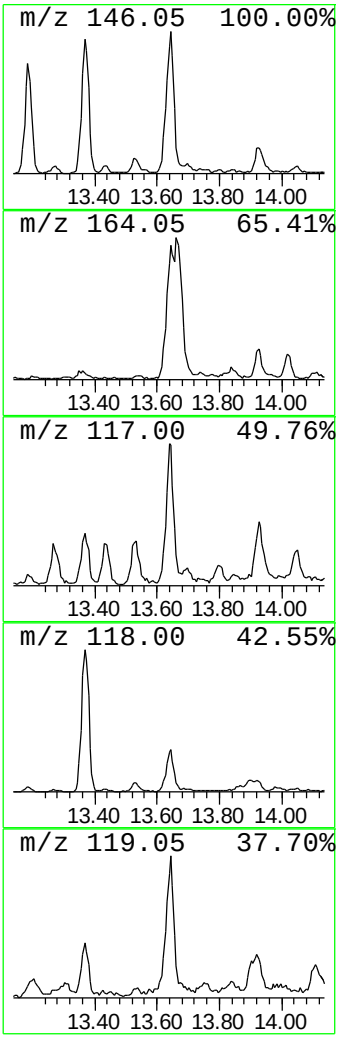
Peak Number 12 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	22.74 ng	947294	Acenaphthene-d10	14.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	93
2	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	47
3	4-Pteridinecarboxylic acid, 7-me...	218	C10H10N4O2	016008-52-9	43
4	2-Hydroxy-1,7-naphthyridine	146	C8H6N2O	054920-82-0	35
5	1H-Indole, 2,3-dihydro-5-nitro-	164	C8H8N2O2	032692-19-6	30





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Operator : CG/JU
Sample : L3033-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
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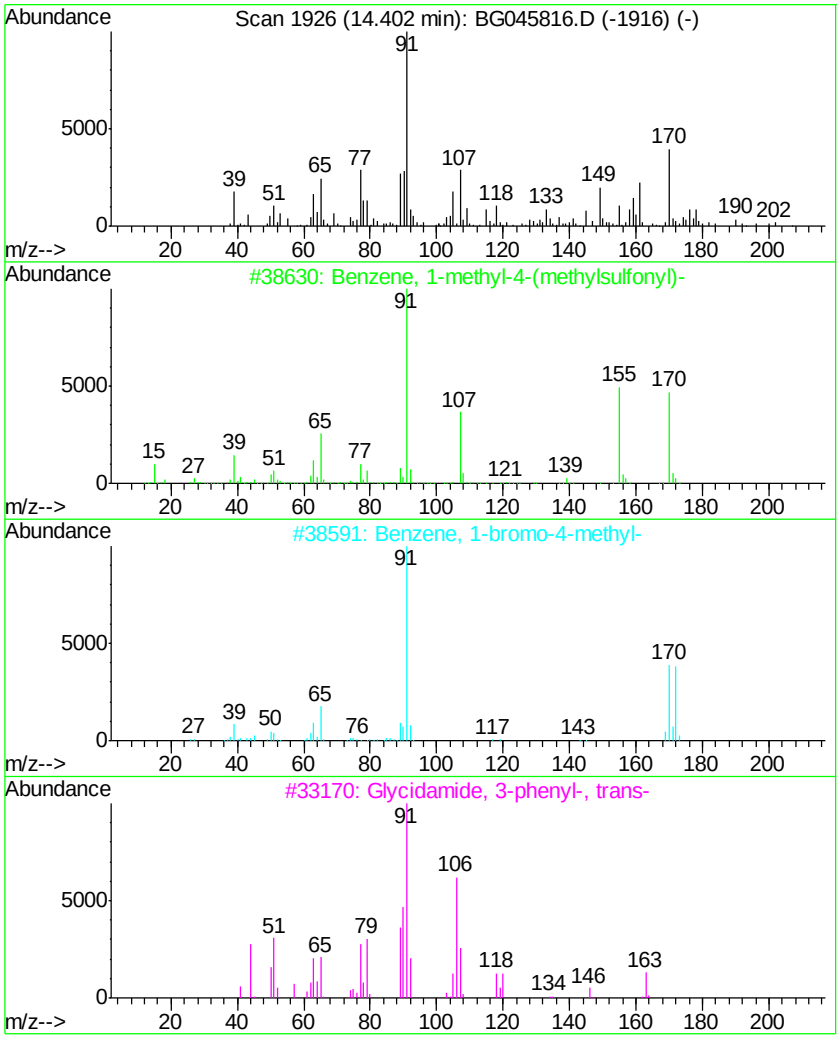
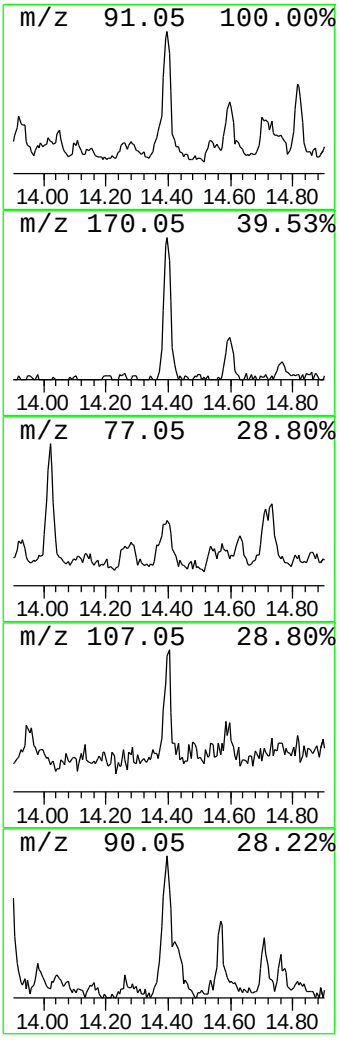
Peak Number 13 unknown14.40 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	9.36 ng	389940	Acenaphthene-d10	14.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(methylsulfo...	170	C8H10O2S	003185-99-7	16
2	Benzene, 1-bromo-4-methyl-	170	C7H7Br	000106-38-7	10
3	Glycidamide, 3-phenyl-, trans-	163	C9H9NO2	019464-96-1	10
4	Benzyl methacrylate	176	C11H12O2	002495-37-6	10
5	2-(3-Chlorophenyl)ethylamine	155	C8H10ClN	013078-79-0	9





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ClientSampleId : SS043MW009-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
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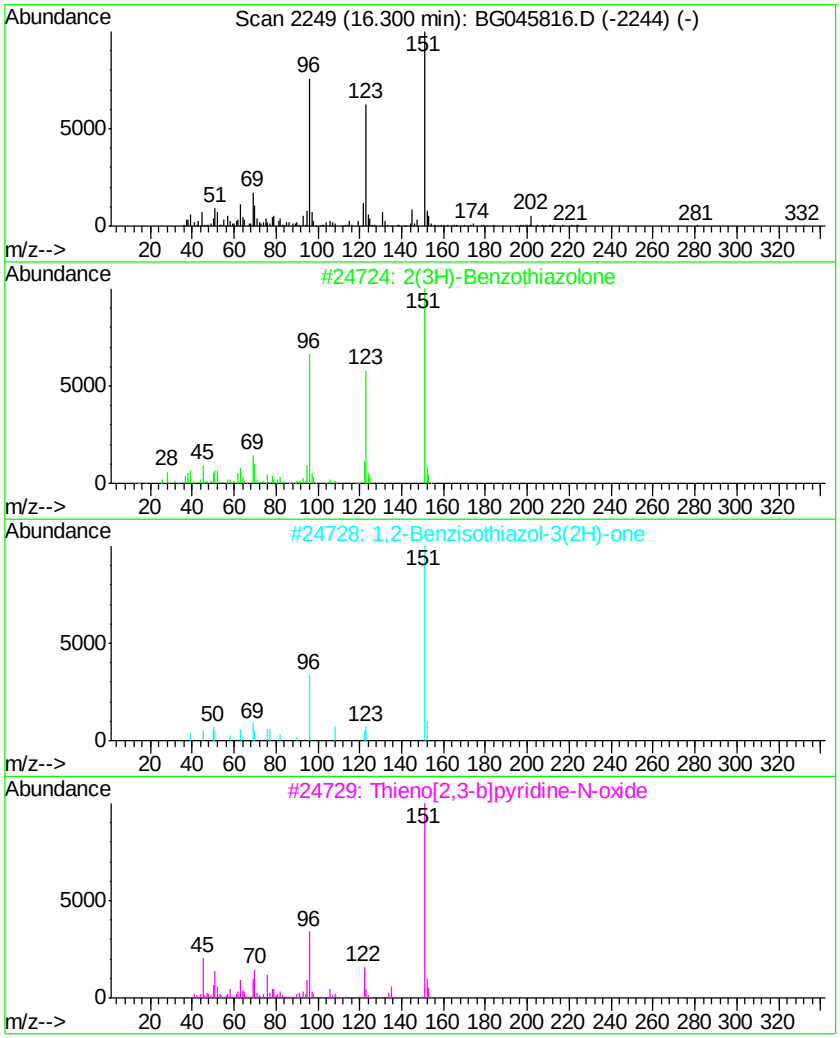
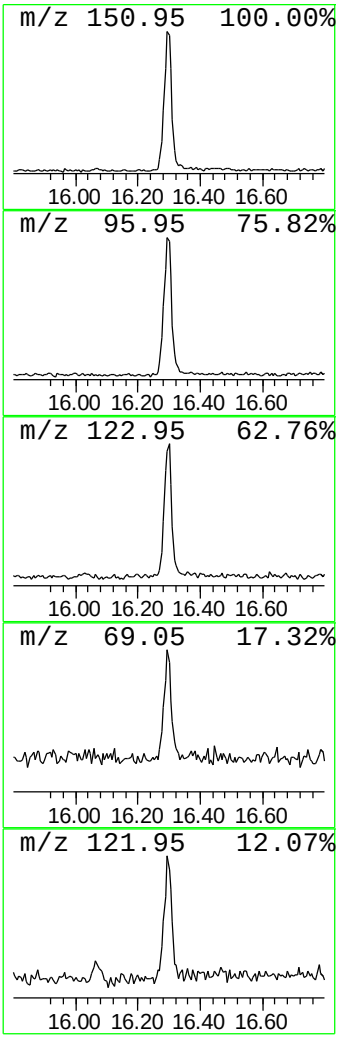
Peak Number 14 2(3H)-Benzothiazolone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	10.11 ng	402612	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	42
4	2-Ethylimino-4-methyl-pentanenit...	138	C8H14N2	1000189-21-4	38
5	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	38





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Sample : L3033-08
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW009-200616

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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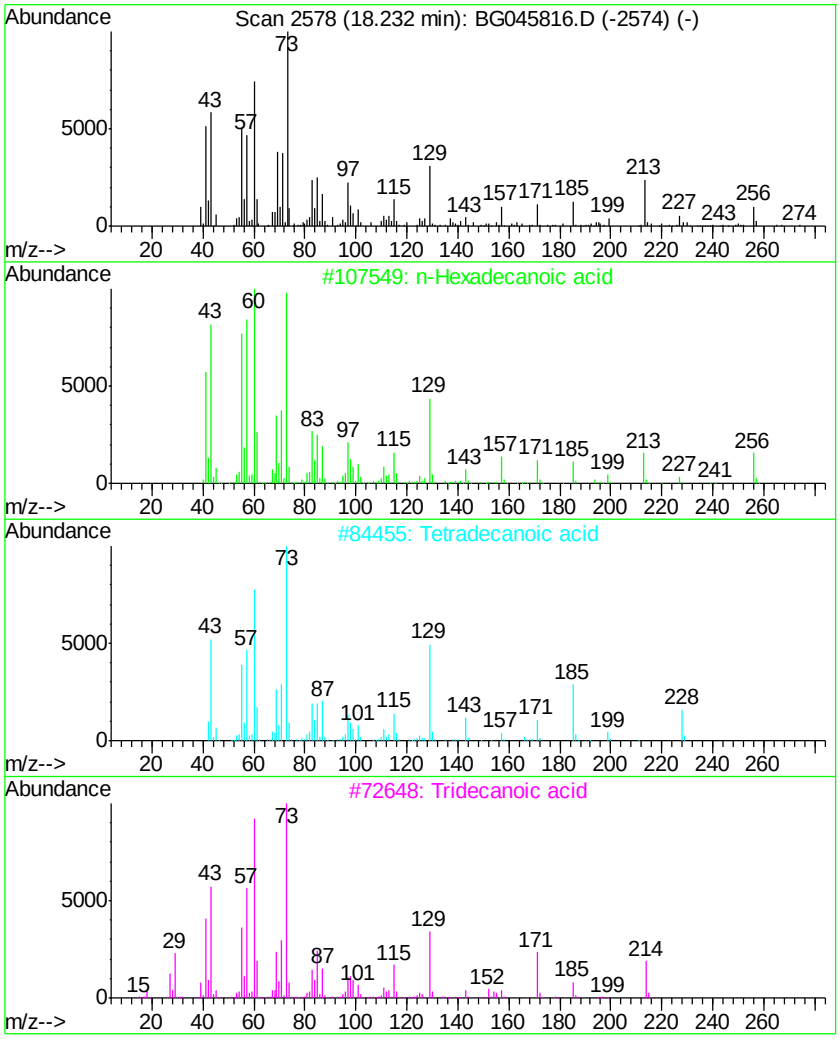
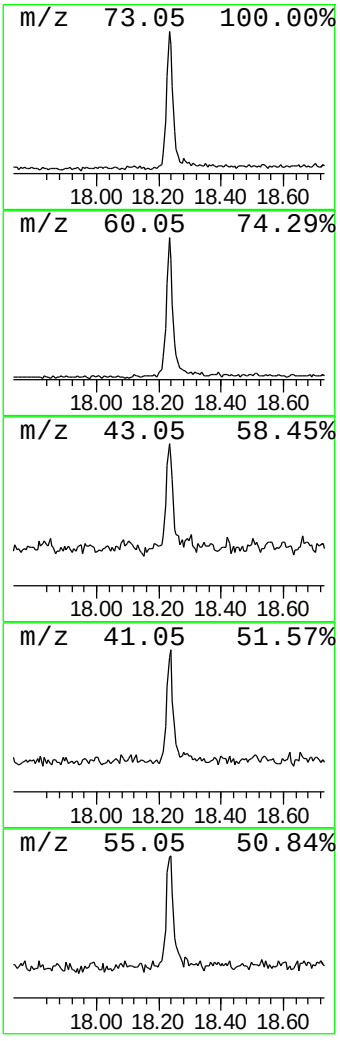
Peak Number 15 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.23	7.96 ng	316937	Phenanthrene-d10	17.32

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	70
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





Tentatively Identified Compound (LSC) summary

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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
Ethane, 1,1,2-tri...	4.19	3.6	ng	807571	1	7.92	4434330	20.0
2-Cyclopenten-1-o...	8.57	3.0	ng	670747	1	7.92	4434330	20.0
6-Azacytosine	9.35	25.8	ng	722279	2	10.72	560213	20.0
unknown9.51	9.51	18.1	ng	505949	2	10.72	560213	20.0
Piperidine, 5-eth...	9.73	17.0	ng	476037	2	10.72	560213	20.0
4(1H)-Pyrimidinon...	10.14	30.4	ng	852908	2	10.72	560213	20.0
1,4-Cyclohexanedione	10.40	15.1	ng	422853	2	10.72	560213	20.0
Benzenemethanol, ...	11.84	10.8	ng	301189	2	10.72	560213	20.0
Thymol	12.36	12.0	ng	335868	2	10.72	560213	20.0
unknown13.53	13.53	6.9	ng	286890	3	14.57	833102	20.0
Benzoic acid, 2,4...	13.64	22.7	ng	947294	3	14.57	833102	20.0
unknown14.40	14.40	9.4	ng	389940	3	14.57	833102	20.0
2(3H)-Benzothiazo...	16.30	10.1	ng	402612	4	17.32	796191	20.0
n-Hexadecanoic acid	18.23	8.0	ng	316937	4	17.32	796191	20.0