LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040424\
Data File : BG060786.D
Acq On : 4 Apr 2024 20:18
Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR21145

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-BG032924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060786.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.178	27	32	47	rVB	428809	850090	10.91%	1.808%
2	5.540	426	434	445	rBV	1101714	1802142	23.13%	3.833%
3	6.610	606	616	621	rBV	458725	706144	9.07%	1.502%
4	7.115	695	702	711	rBV	1091522	1835893	23.57%	3.905%
5	7.955	837	845	852	rBV	352041	604576	7.76%	1.286%
6	9.107	1025	1041	1048	rBV	681283	1335140	17.14%	2.840%
7	10.528	1276	1283	1292	rBV3	175421	463222	5.95%	0.985%
8	10.622	1294	1299	1304	rBV4	159746	278761	3.58%	0.593%
9	10.746	1311	1320	1333	rBV	543619	1389156	17.83%	2.955%
10	11.339	1411	1421	1425	rBV6	135442	385947	4.95%	0.821%
11	11.533	1448	1454	1459	rBV4	200552	457168	5.87%	0.972%
12	11.674	1474	1478	1483	rBV7	156997	287126	3.69%	0.611%
13	11.809	1496	1501	1507	rBV5	279501	835383	10.72%	1.777%
14	11.950	1520	1525	1532	rBV4	295621	502295	6.45%	1.068%
15	12.503	1614	1619	1624	rBV5	461743	931962	11.96%	1.982%
16	12.561	1625	1629	1632	rBV3	312921	482765	6.20%	1.027%
17	12.673	1644	1648	1652	rBV2	516893	801405	10.29%	1.705%
18	13.155	1727	1730	1733	rBV2	567139	656419	8.43%	1.396%
19	13.214	1734	1740	1745	rBV2	1815325	3190627	40.96%	6.787%
20	13.877	1850	1853	1858	rBV4	1220034	1776457	22.81%	3.779%
21	14.030	1875	1879	1884	rBV	2500243	4216211	54.13%	8.968%
22	14.113	1890	1893	1896	rBV3	1488542	2140576	27.48%	4.553%
23	14.447	1946	1950	1958	rVB3	3235947	6394196	82.08%	13.601%
24	14.588	1969	1974	1980	rBV6	2441253	6899405	88.57%	14.676%
25	14.647	1980	1984	1989	rVB	5272872	7789763	100.00%	16.569%

Sum of corrected areas: 47012829

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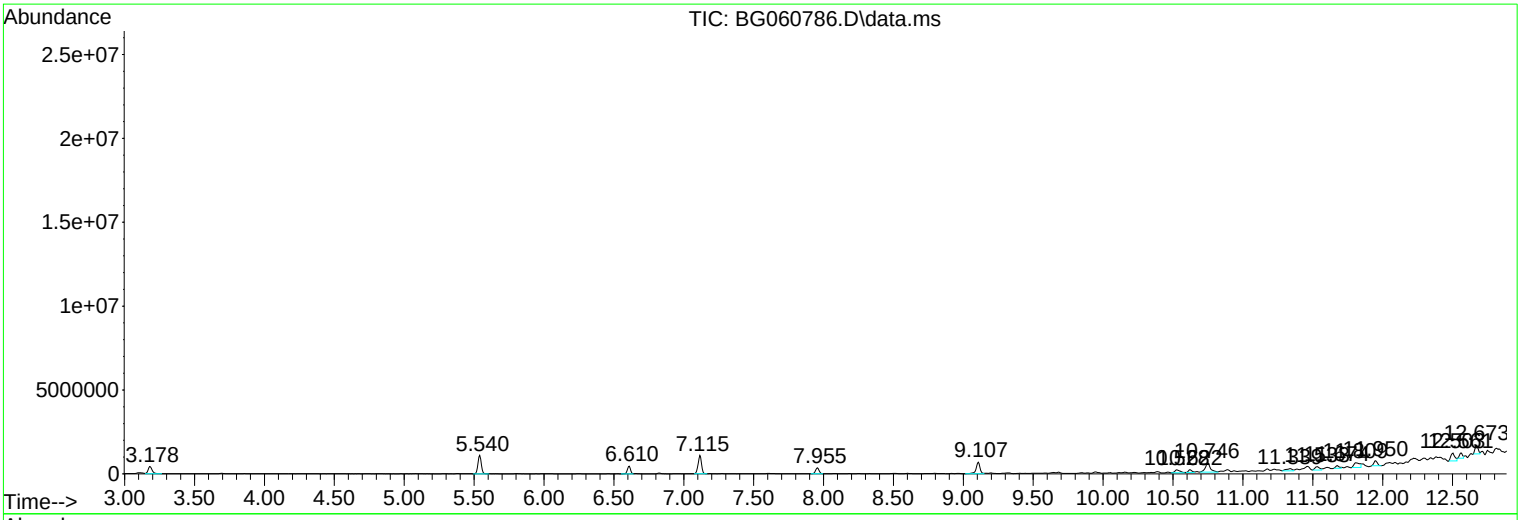
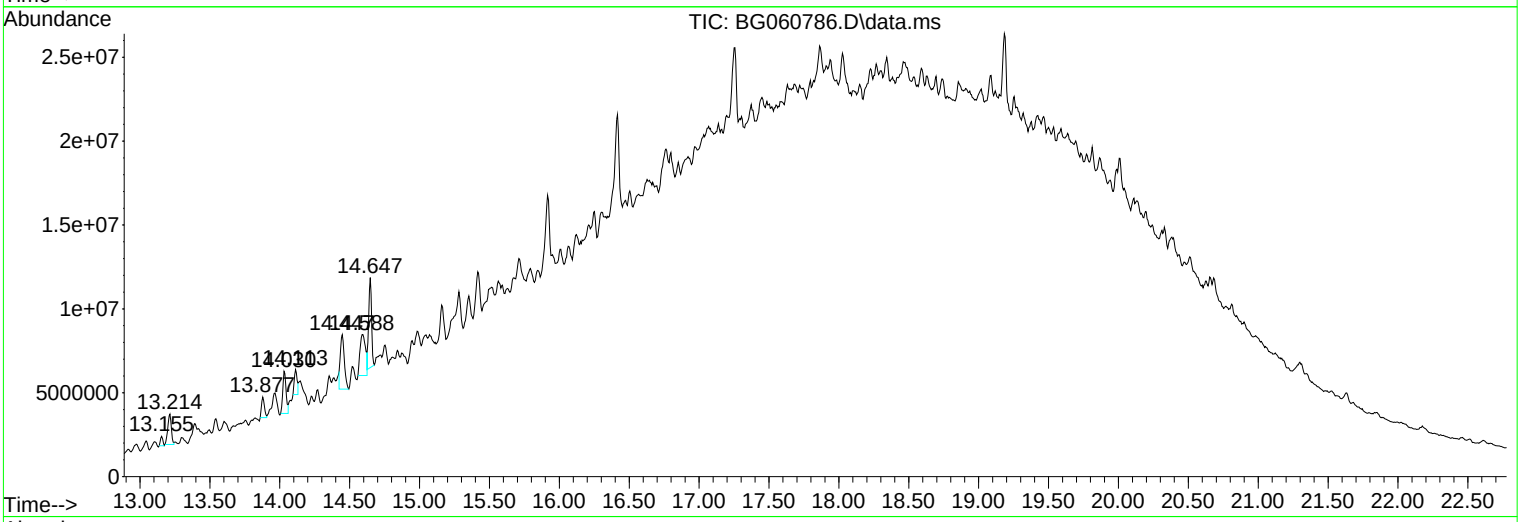
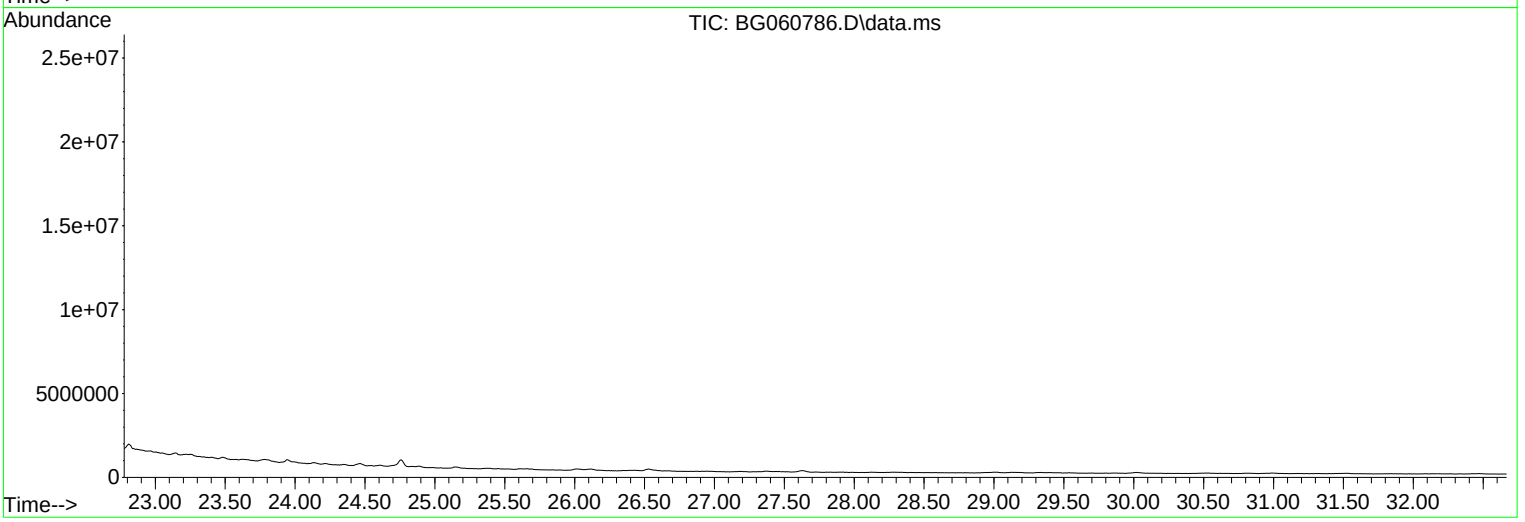
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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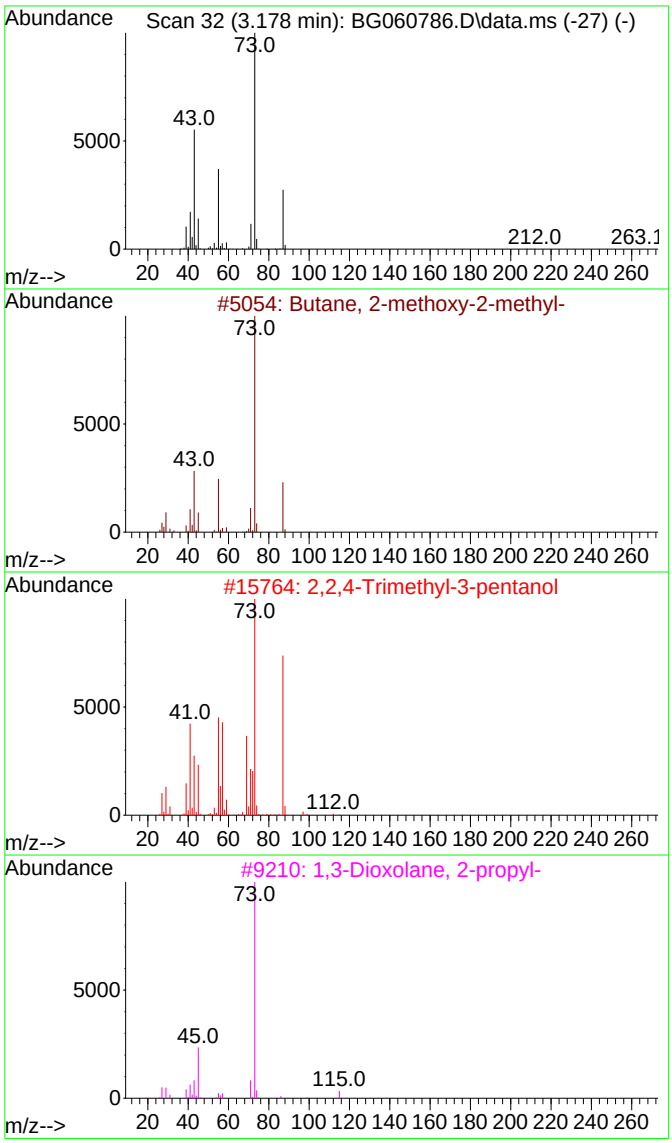
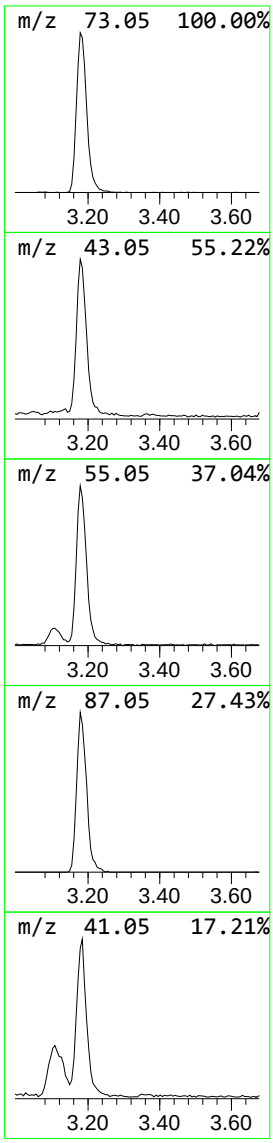
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.178	28.12 ng	850090	1,4-Dichlorobenzene-d4	7.955

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	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4	Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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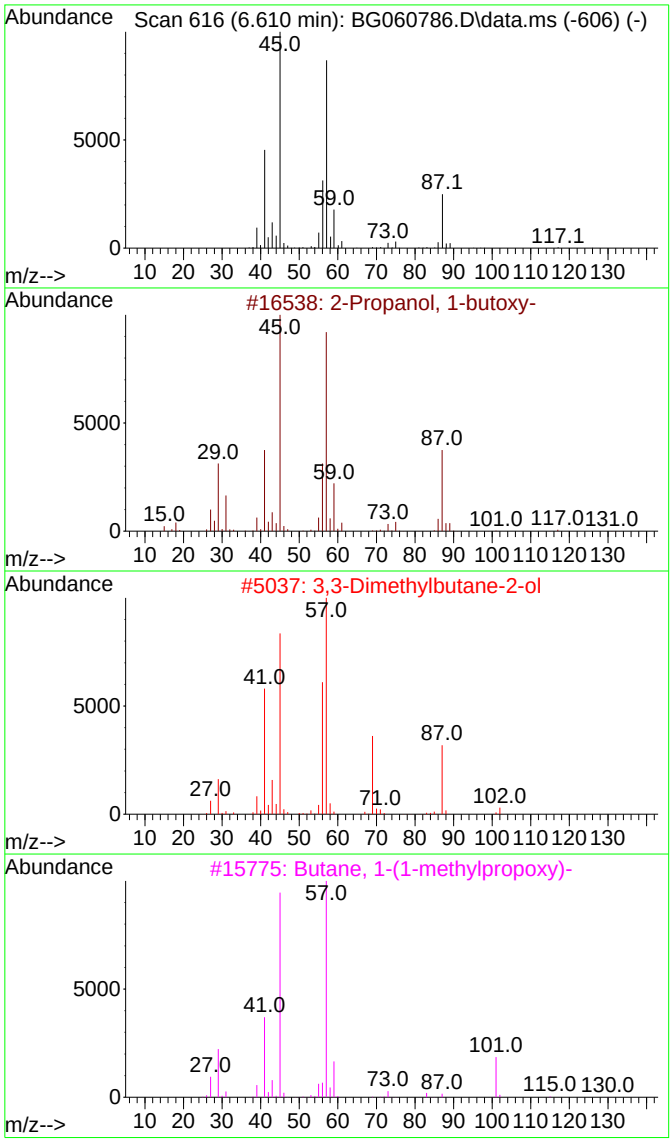
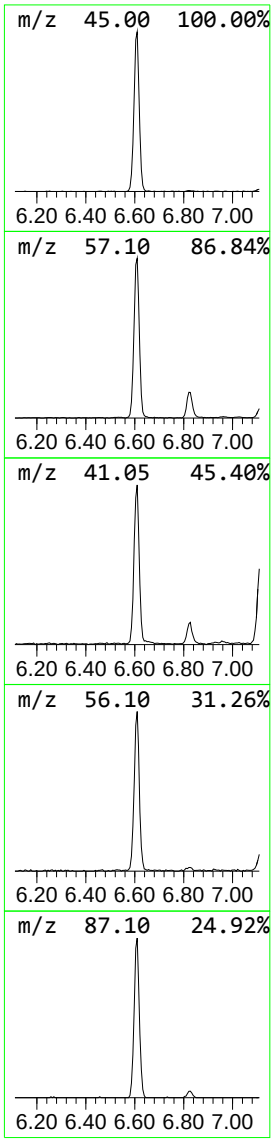
****
Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.610	23.36 ng	706144	1,4-Dichlorobenzene-d4	7.955

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	59
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Diisopropyl ether	102	C6H14O	000108-20-3	53
5	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	53





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Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
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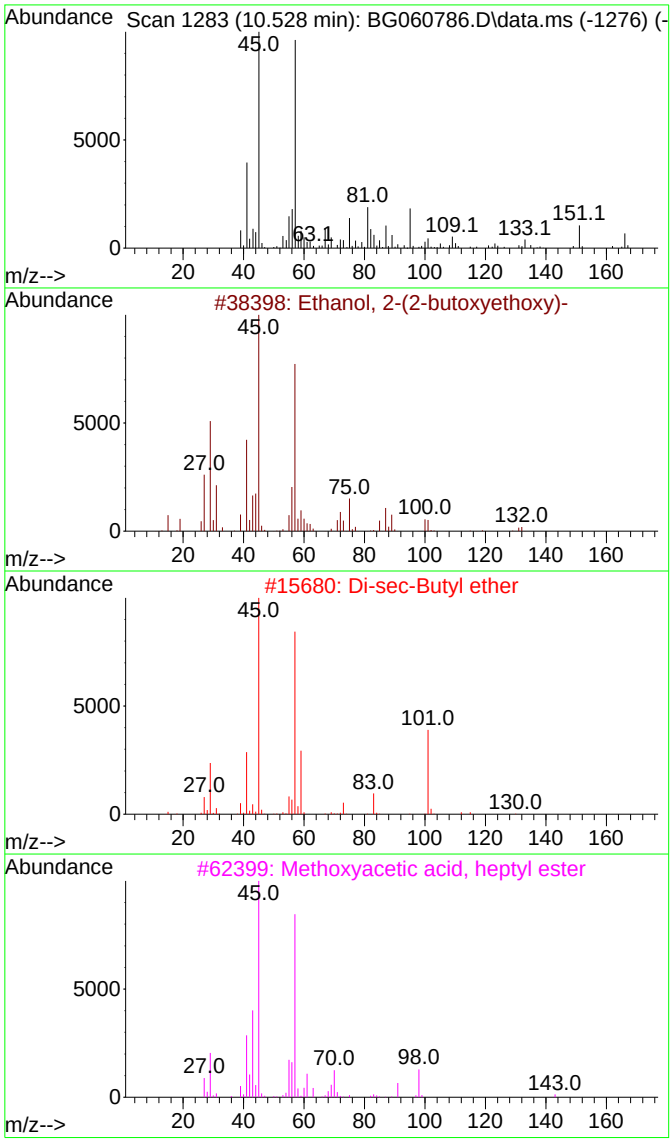
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

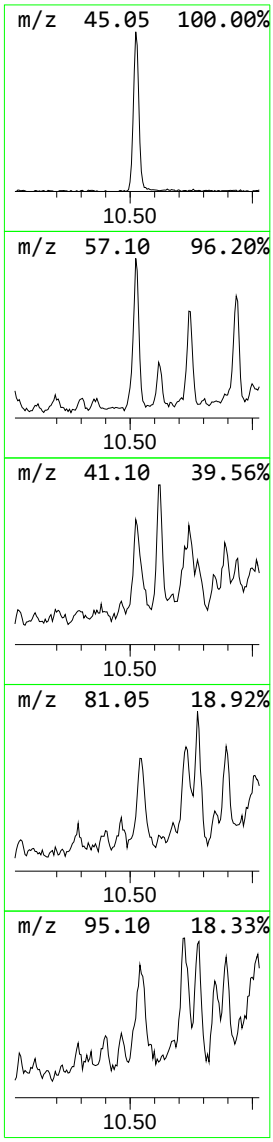
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.528	6.67 ng	463222	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	53
2	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
3	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	50





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Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

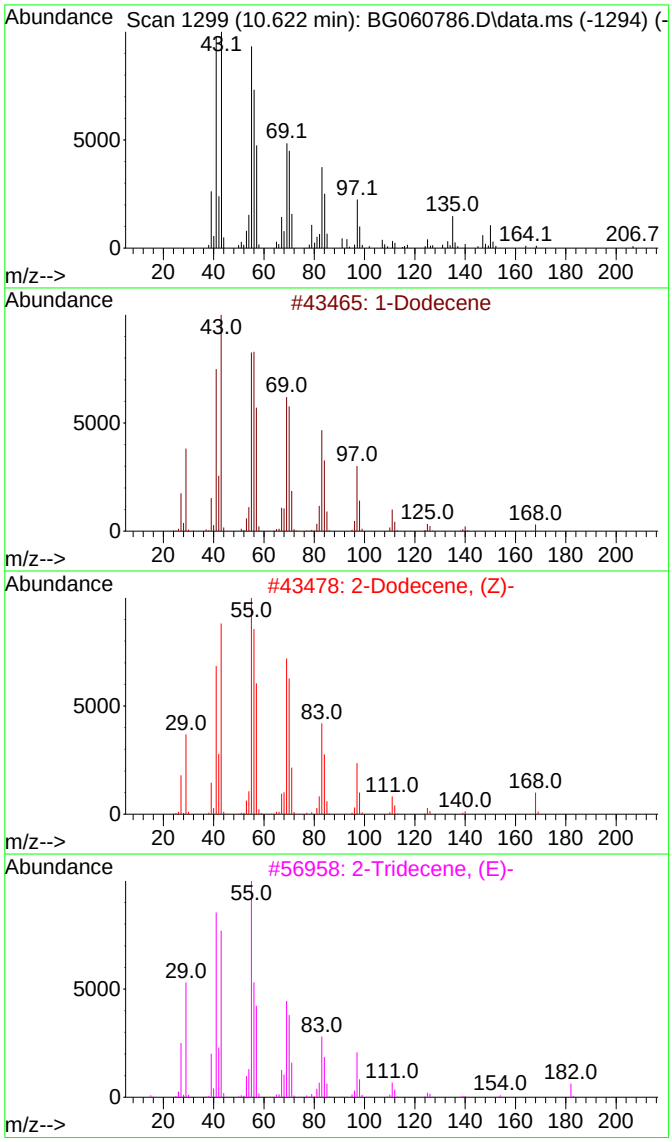
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

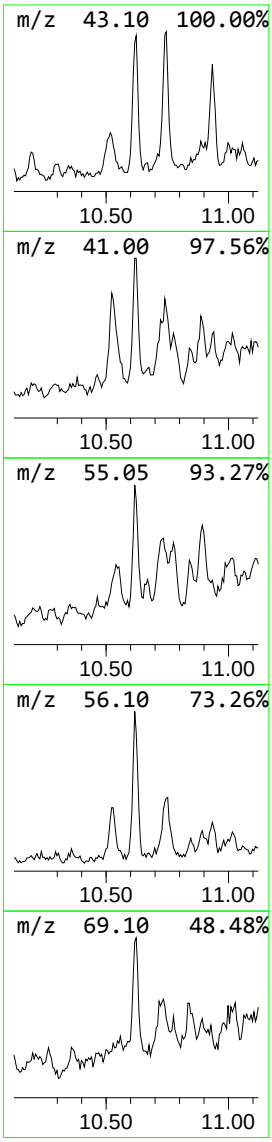
****

Peak Number 4 1-Dodecene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.623	4.01 ng	278761	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecene	168	C12H24	000112-41-4	93
2	2-Dodecene, (Z)-	168	C12H24	007206-26-0	86
3	2-Tridecene, (E)-	182	C13H26	041446-58-6	86
4	2-Dodecene, (E)-	168	C12H24	007206-13-5	86
5	1-Decene	140	C10H20	000872-05-9	80





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Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
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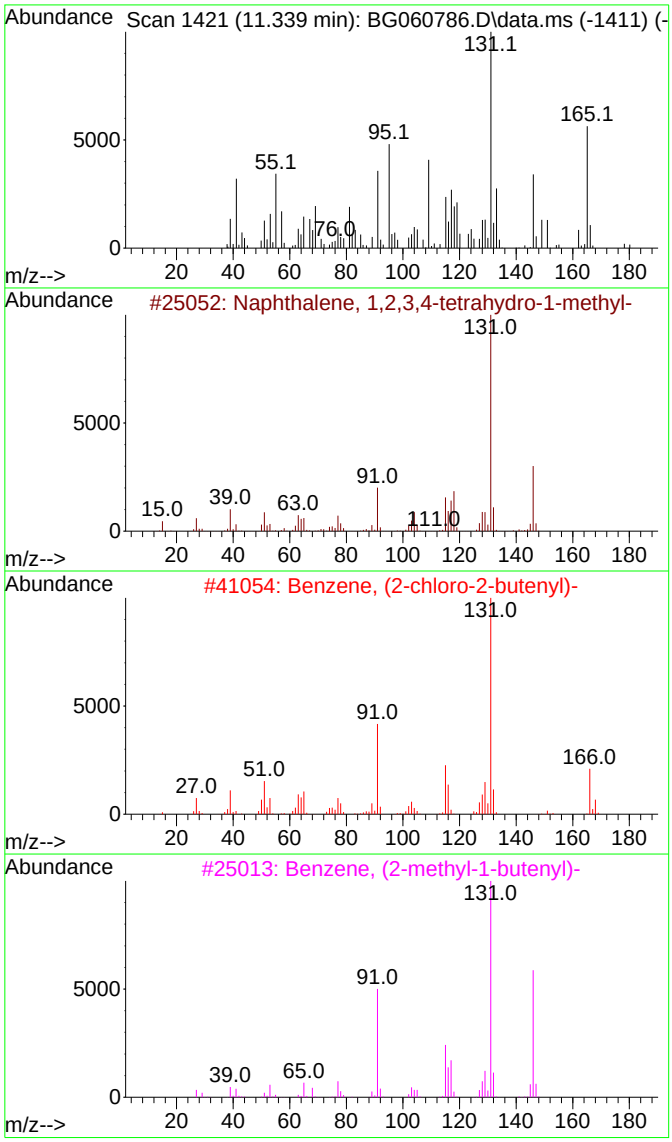
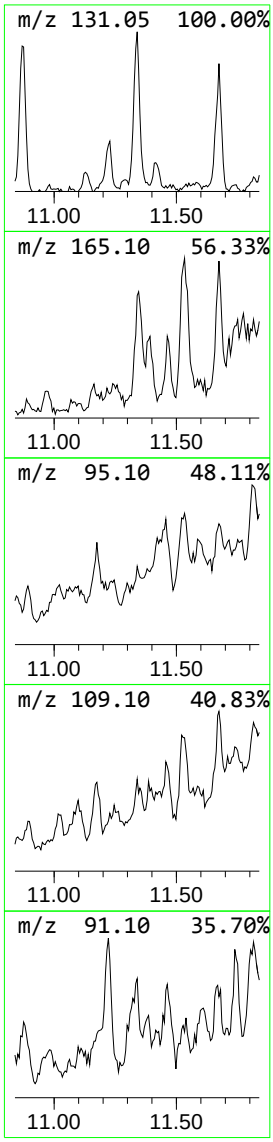
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.339	5.56 ng	385947	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	83
2	Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	62
3	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	52
4	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	47
5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	43





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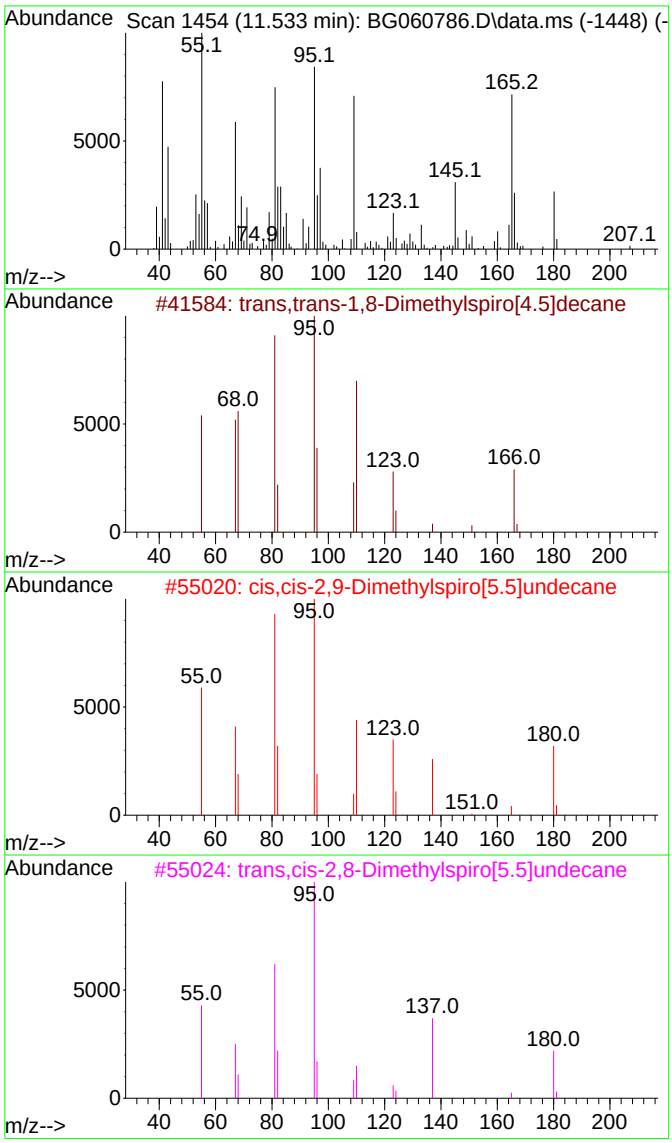
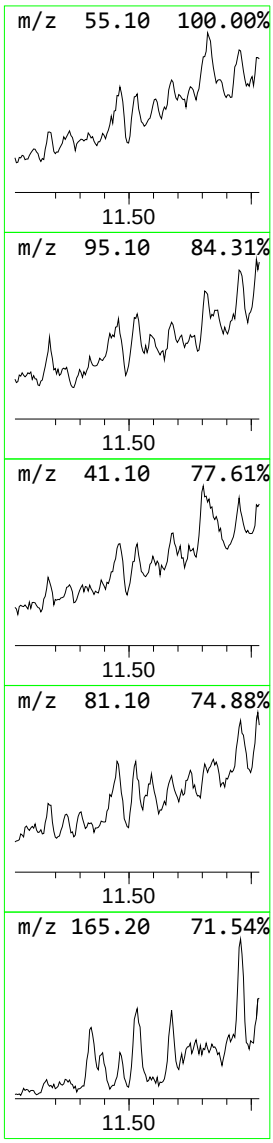
****
Peak Number 6 trans,trans-1,8-Dimethylspi... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.533	6.58 ng	457168	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans,trans-1,8-Dimethylspiro[4....	166	C12H22	1000111-72-8	52
2	cis,cis-2,9-Dimethylspiro[5.5]un...	180	C13H24	095472-51-8	49
3	trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	49
4	(4R*,5R*,9S*)-5,9-Dimethylspiro[...	166	C11H18O	063088-19-7	46
5	cis,cis-1,9-Dimethylspiro[5.5]un...	180	C13H24	1000111-73-4	46





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Sample : P1954-03
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ALS Vial : 16 Sample Multiplier: 1

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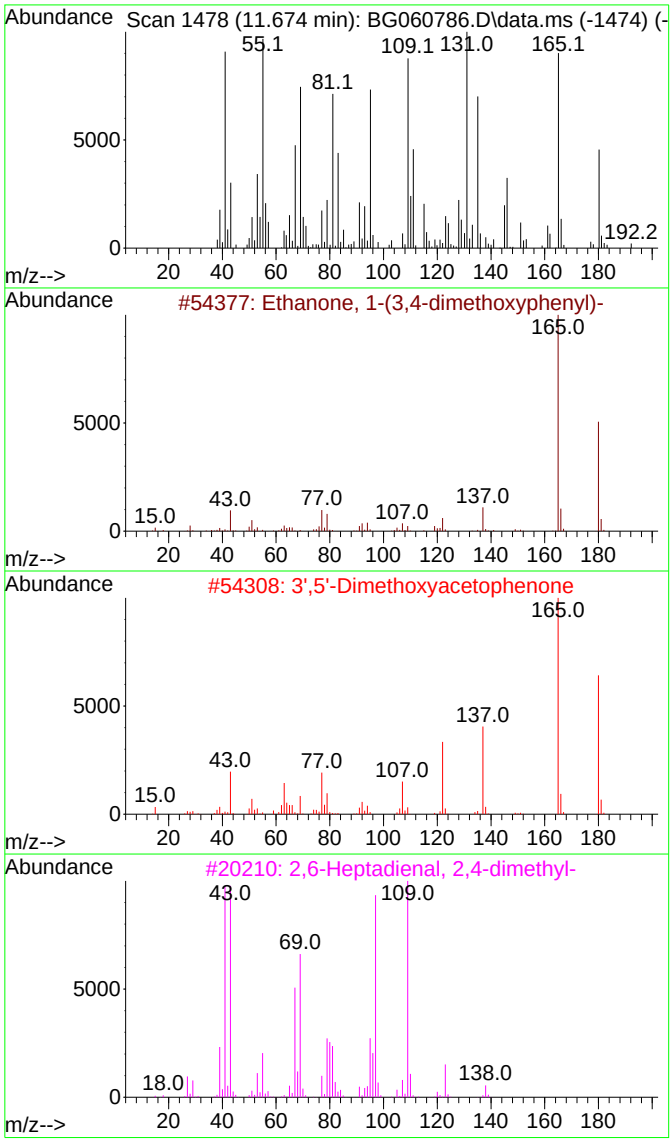
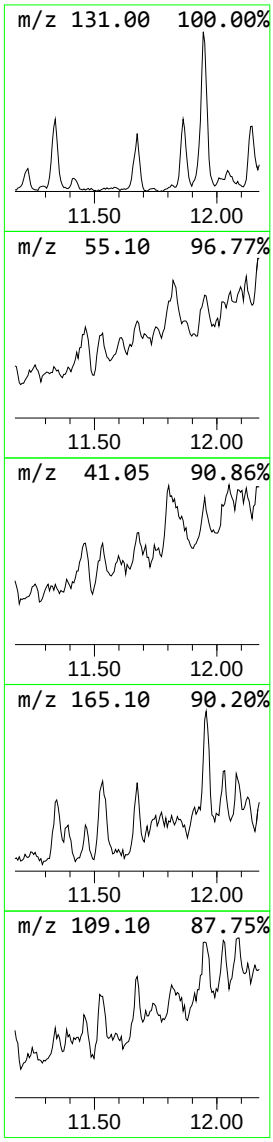
Peak Number 7 unknown11.674 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.674	4.13 ng	287126	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	25
2	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	25
3	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	18
4	p-Formophenetidide	165	C9H11NO2	061587-14-2	18
5	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	15





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TIC Library : C:\Database\NIST20.L
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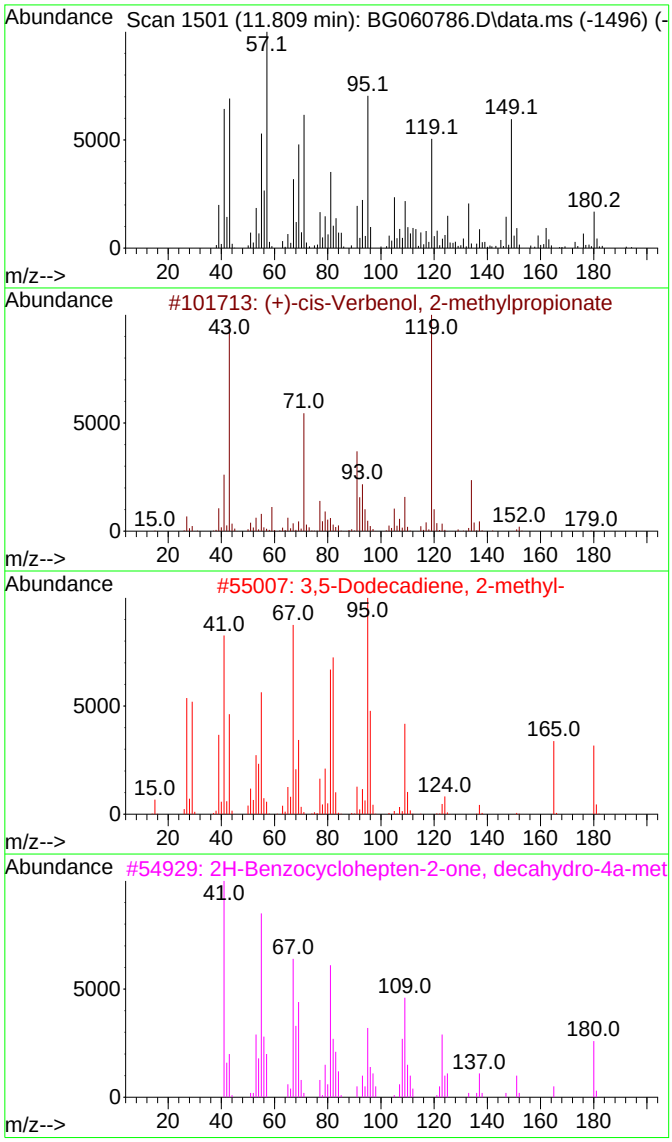
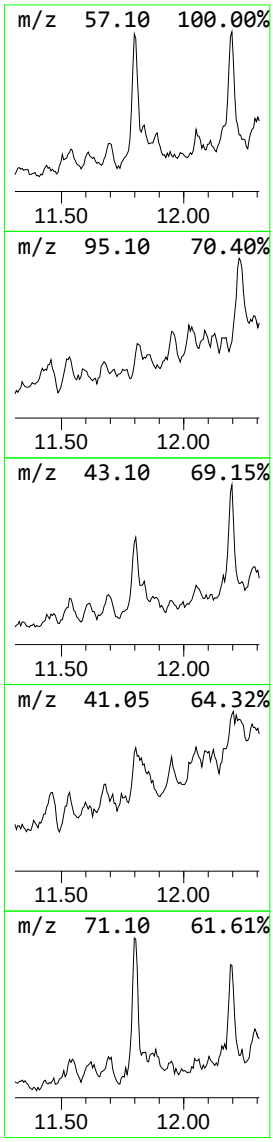
****

Peak Number 8 unknown11.809 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.809	12.03 ng	835383	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-cis-Verbenol, 2-methylpropio...	222	C14H22O2	1000462-96-7	27
2	3,5-Dodecadiene, 2-methyl-	180	C13H24	055638-51-2	20
3	2H-Benzocyclohepten-2-one, decah...	180	C12H20O	055103-64-5	15
4	Bicyclo[3.3.1]nonan-9-one, 1,2,4...	225	C12H19NO3	129967-65-3	14
5	Thiophenol, S-(2-methylpropionyl)-	180	C10H12OS	058443-71-3	14





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Instrument :
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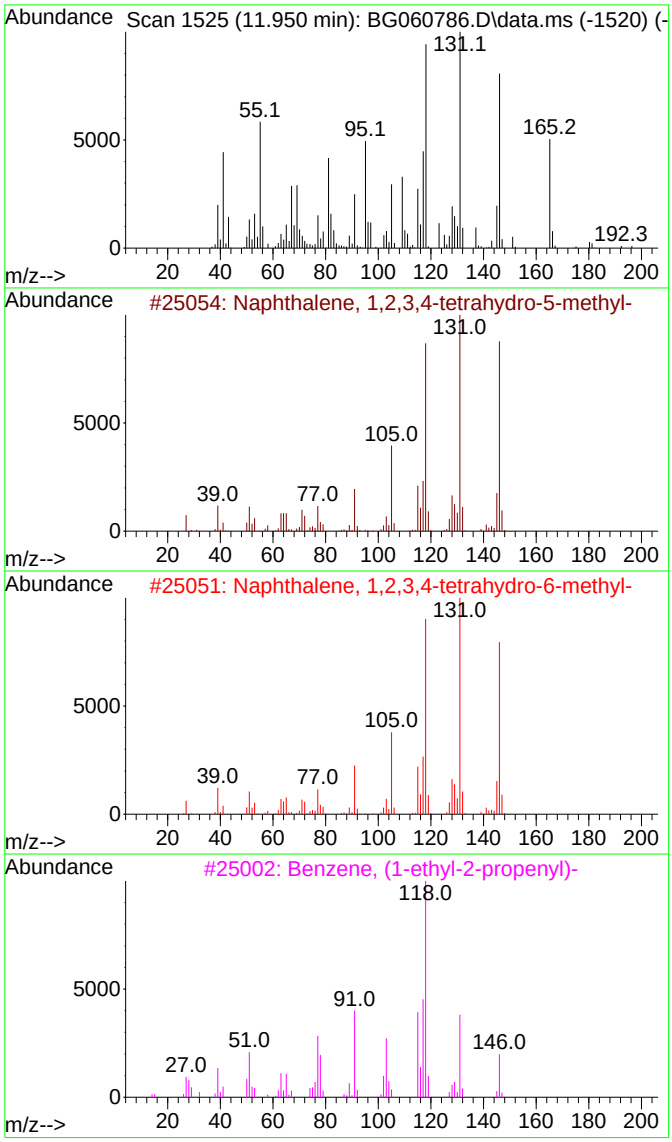
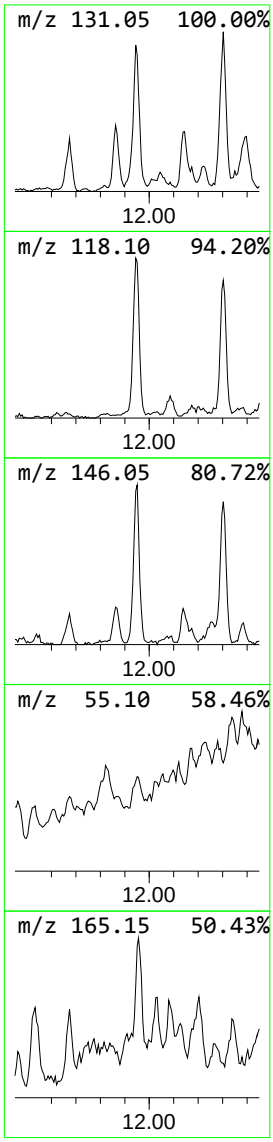
****

Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.950	7.23 ng	502295	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	86
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	86
3	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	64
4	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	49
5	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040424\
Data File : BG060786.D
Acq On : 4 Apr 2024 20:18
Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

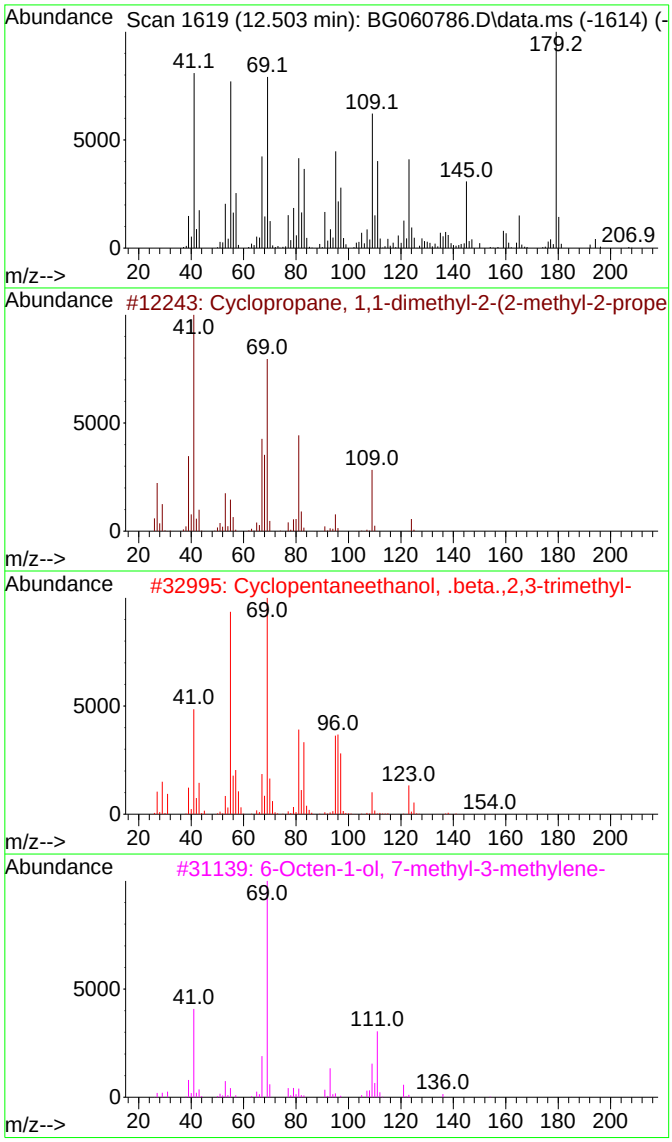
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

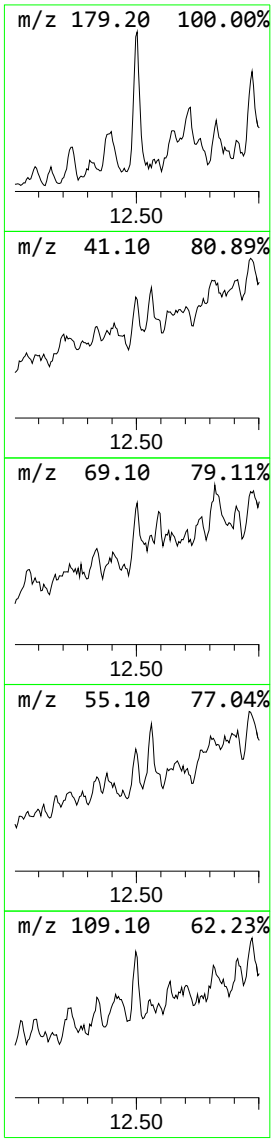
****

Peak Number 10 unknown12.503 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.503	13.42 ng	931962	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	25
2	Cyclopentaneethanol, .beta.,2,3-...	156	C10H20O	021721-18-6	22
3	6-Octen-1-ol, 7-methyl-3-methylene-	154	C10H18O	013066-51-8	22
4	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
5	Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	20





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Acq On : 4 Apr 2024 20:18
Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

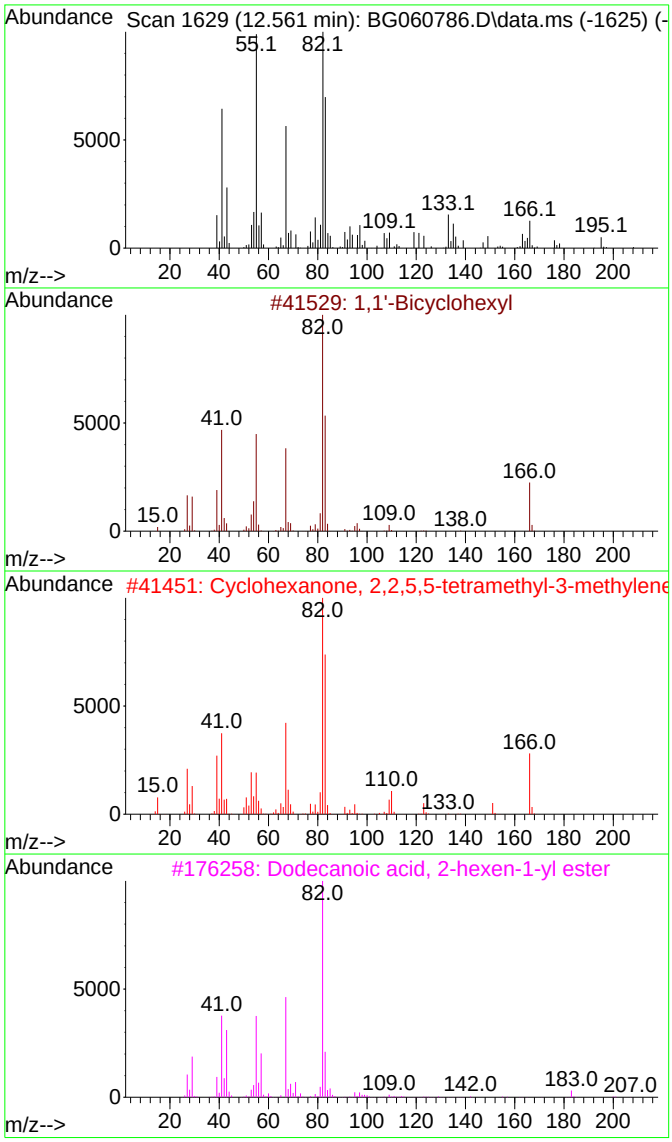
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

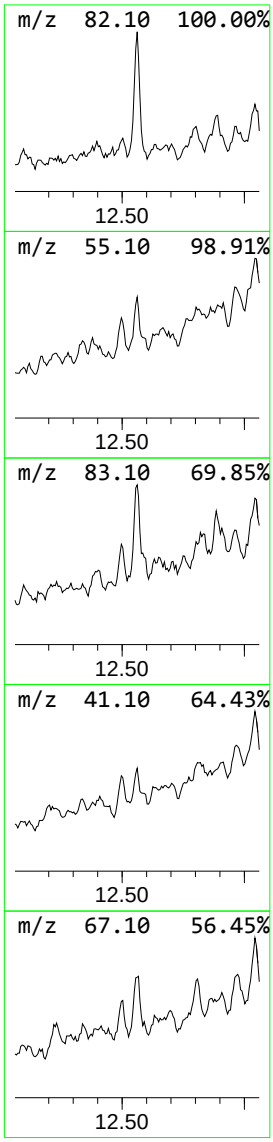
****

Peak Number 11 1,1'-Bicyclohexyl Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.561	6.95 ng	482765	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Bicyclohexyl	166	C12H22	000092-51-3	59
2	Cyclohexanone, 2,2,5,5-tetrameth...	166	C11H18O	035505-97-6	50
3	Dodecanoic acid, 2-hexen-1-yl ester	282	C18H34O2	1000159-97-0	47
4	Cyclopentane, 1-methyl-3-(1-meth...	126	C9H18	053771-88-3	47
5	1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	47





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Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

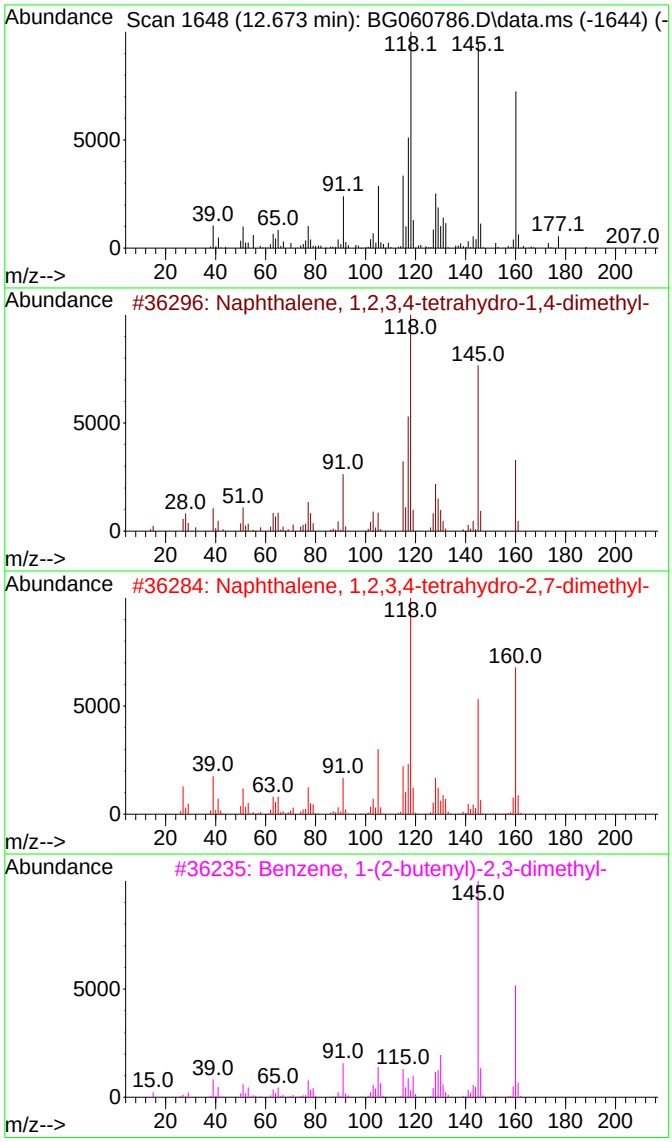
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

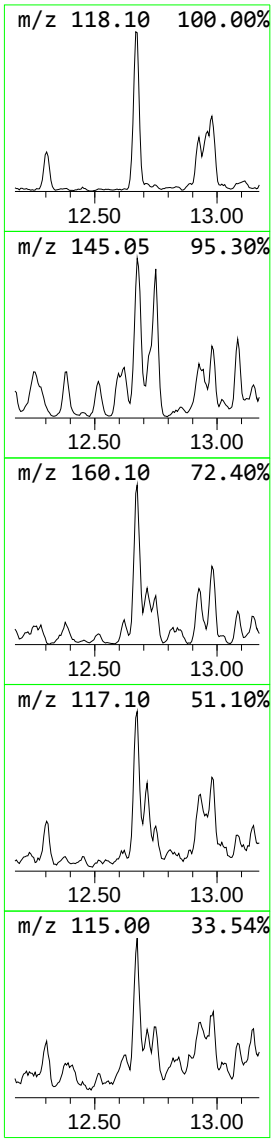
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.673	11.54 ng	801405	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	90
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	74
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	53
4	4-(1H-Imidazol-2-yl)pyridine	145	C8H7N3	021202-42-6	52
5	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	49





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Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

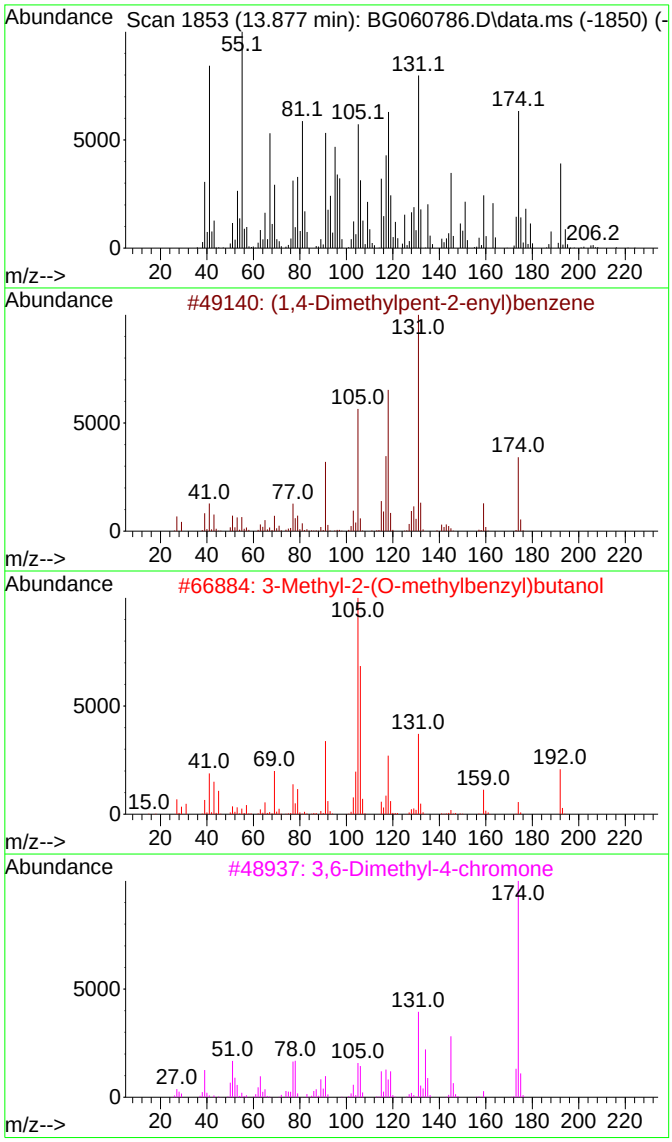
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

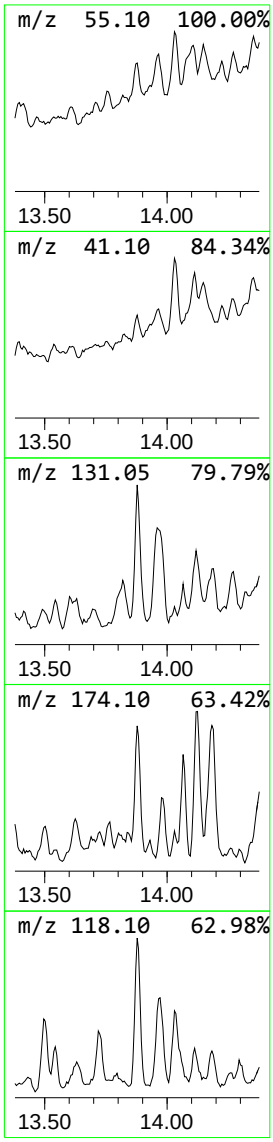
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 (1,4-Dimethylpent-2-enyl)be... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.878	5.15 ng	1776460	Acenaphthene-d10	14.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	55
2	3-Methyl-2-(O-methylbenzyl)butanol	192	C13H20O	029107-38-8	46
3	3,6-Dimethyl-4-chromone	174	C11H10O2	057646-01-2	43
4	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	43
5	1-Ethanone, 1-[3,6-dihydroxy-2-(...	192	C11H12O3	1000319-33-7	38





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Acq On : 4 Apr 2024 20:18
Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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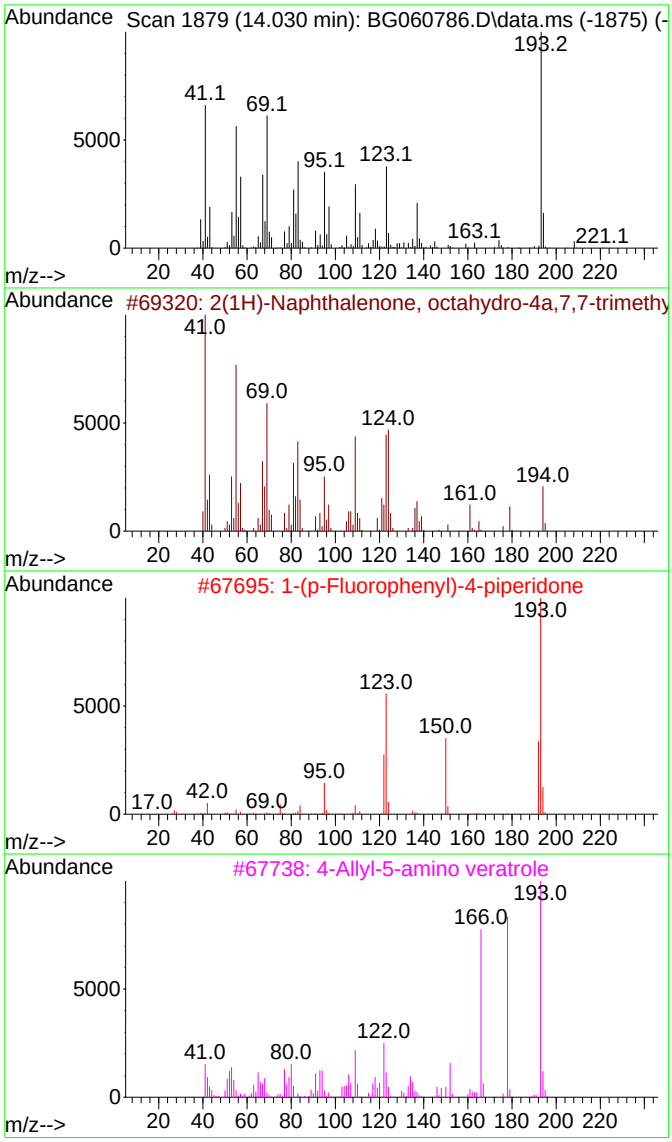
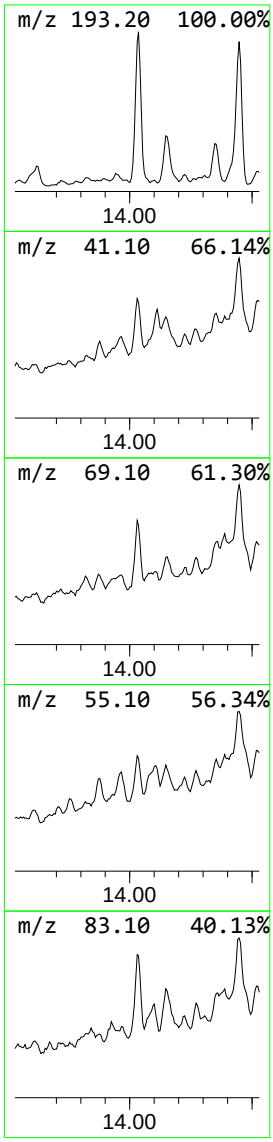
Peak Number 14 unknown14.030 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.030	12.22 ng	4216210	Acenaphthene-d10	14.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	35
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
3	4-Allyl-5-amino veratrole	193	C11H15NO2	030058-51-6	35
4	2-Anthracenamine	193	C14H11N	000613-13-8	27
5	3-Methyl-2-oxo-2,3-dihydro-1,3-b...	193	C9H7NO4	154780-52-6	25





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Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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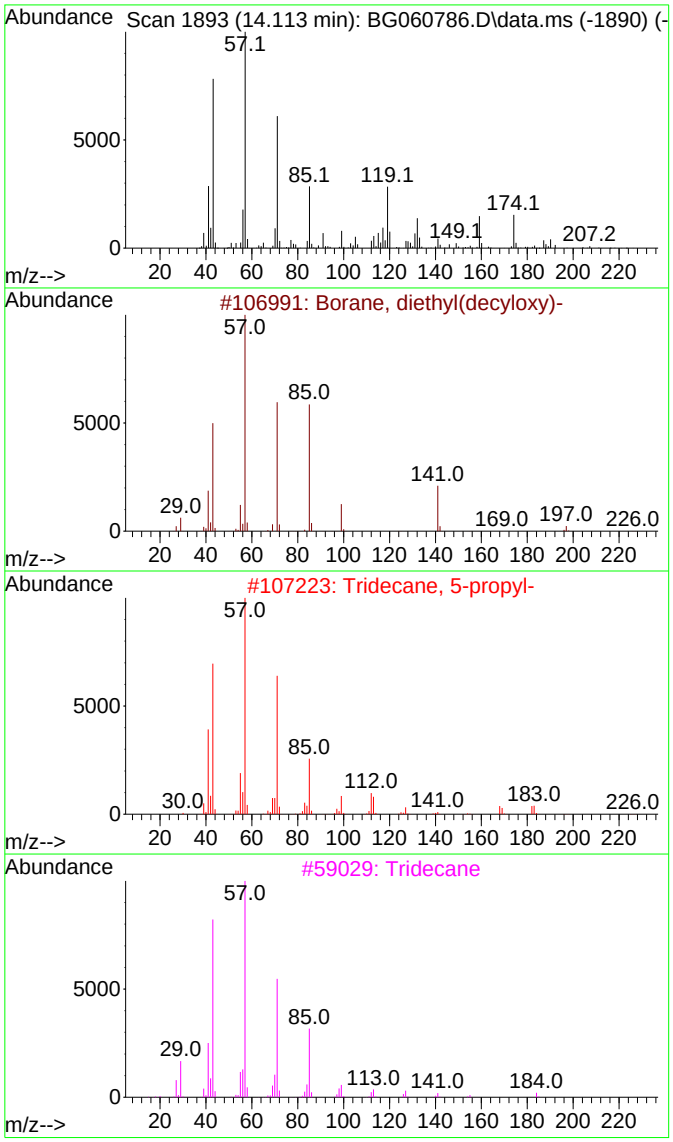
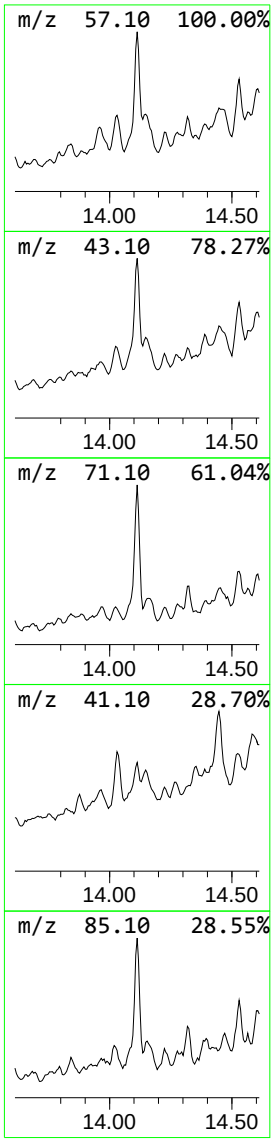
Peak Number 15 unknown14.113 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.113	6.21 ng	2140580	Acenaphthene-d10	14.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	49
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	49
3	Tridecane	184	C13H28	000629-50-5	46
4	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	43
5	Heptacosane	380	C27H56	000593-49-7	43





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Data File : BG060786.D
Acq On : 4 Apr 2024 20:18
Operator : MA/JU
Sample : P1954-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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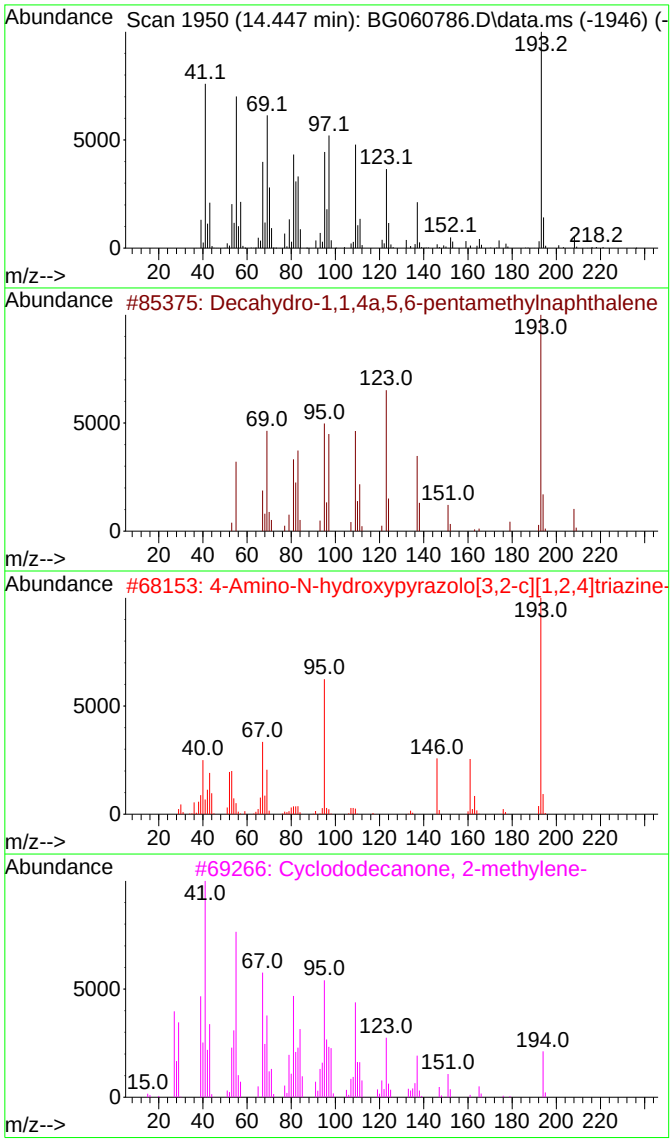
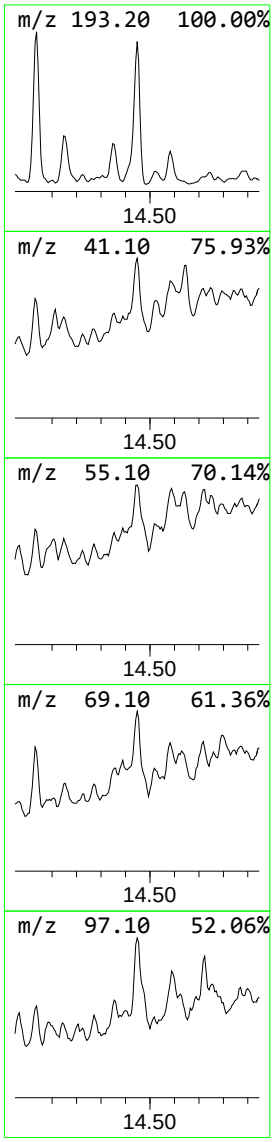
Peak Number 16 unknown14.447 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	18.54 ng	6394200	Acenaphthene-d10	14.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	38
3	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	38
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
5	Neopentylidenecyclohexane	152	C11H20	039546-80-0	18





Tentatively Identified Compound (LSC) summary

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Data File : BG060786.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.178	28.1	ng	850090	1	7.955	604576	20.0
2-Propanol, 1-b...	6.610	23.4	ng	706144	1	7.955	604576	20.0
Ethanol, 2-(2-b...	10.528	6.7	ng	463222	2	10.752	1389160	20.0
1-Dodecene	10.623	4.0	ng	278761	2	10.752	1389160	20.0
Naphthalene, 1,...	11.339	5.6	ng	385947	2	10.752	1389160	20.0
trans,trans-1,8...	11.533	6.6	ng	457168	2	10.752	1389160	20.0
unknown11.674	11.674	4.1	ng	287126	2	10.752	1389160	20.0
unknown11.809	11.809	12.0	ng	835383	2	10.752	1389160	20.0
Naphthalene, 1,...	11.950	7.2	ng	502295	2	10.752	1389160	20.0
unknown12.503	12.503	13.4	ng	931962	2	10.752	1389160	20.0
1,1'-Bicyclohexyl	12.561	7.0	ng	482765	2	10.752	1389160	20.0
Naphthalene, 1,...	12.673	11.5	ng	801405	2	10.752	1389160	20.0
(1,4-Dimethylpe...	13.878	5.2	ng	1776460	3	14.600	6899410	20.0
unknown14.030	14.030	12.2	ng	4216210	3	14.600	6899410	20.0
unknown14.113	14.113	6.2	ng	2140580	3	14.600	6899410	20.0
unknown14.447	14.447	18.5	ng	6394200	3	14.600	6899410	20.0