LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054886.D
Acq On : 8 Sep 2022 16:28
Operator : CG/JU
Sample : N4537-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW6

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054886.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.654	56	62	71	rVB	40042	59052	2.47%	0.591%
2	4.594	214	222	236	rVB	124905	198498	8.32%	1.986%
3	5.211	319	327	334	rBV	24095	38001	1.59%	0.380%
4	5.687	402	408	419	rBV	230834	382564	16.03%	3.828%
5	7.303	676	683	695	rVB	123135	219377	9.19%	2.195%
6	8.149	820	827	834	rBV	122501	209674	8.78%	2.098%
7	9.324	1019	1027	1041	rBV	380949	702552	29.43%	7.029%
8	10.975	1300	1308	1315	rBV	171527	321117	13.45%	3.213%
9	12.091	1493	1498	1505	rVB5	15700	34888	1.46%	0.349%
10	12.520	1564	1571	1578	rBV	51513	94672	3.97%	0.947%
11	13.296	1699	1703	1712	rVB5	15669	31683	1.33%	0.317%
12	13.407	1715	1722	1728	rVB	1111112	1743516	73.04%	17.444%
13	13.566	1745	1749	1755	rVB8	15219	28769	1.21%	0.288%
14	13.630	1756	1760	1765	rVV	16603	25172	1.05%	0.252%
15	13.959	1813	1816	1822	rBV4	12600	25999	1.09%	0.260%
16	14.195	1851	1856	1859	rBV3	23676	44656	1.87%	0.447%
17	14.488	1902	1906	1915	rBV5	25580	65913	2.76%	0.659%
18	14.606	1923	1926	1930	rVB4	20373	28799	1.21%	0.288%
19	14.782	1951	1956	1963	rVB	236780	364061	15.25%	3.642%
20	15.223	2027	2031	2035	rBV2	48059	72745	3.05%	0.728%
21	15.364	2051	2055	2061	rBV5	28544	55011	2.30%	0.550%
22	15.663	2102	2106	2111	rVB3	36263	50725	2.12%	0.508%
23	16.210	2196	2199	2203	rBV3	31979	51651	2.16%	0.517%
24	16.274	2204	2210	2219	rVB	830603	1304789	54.66%	13.054%
25	16.774	2291	2295	2299	rBV2	76143	122165	5.12%	1.222%
26	17.314	2383	2387	2395	rVB6	63763	122496	5.13%	1.226%
27	17.532	2419	2424	2435	rVB	375572	601691	25.20%	6.020%
28	20.129	2861	2866	2873	rVB	1761910	2387210	100.00%	23.884%
29	21.827	3149	3155	3169	rVB	339356	607497	25.45%	6.078%

Sum of corrected areas: 9994943

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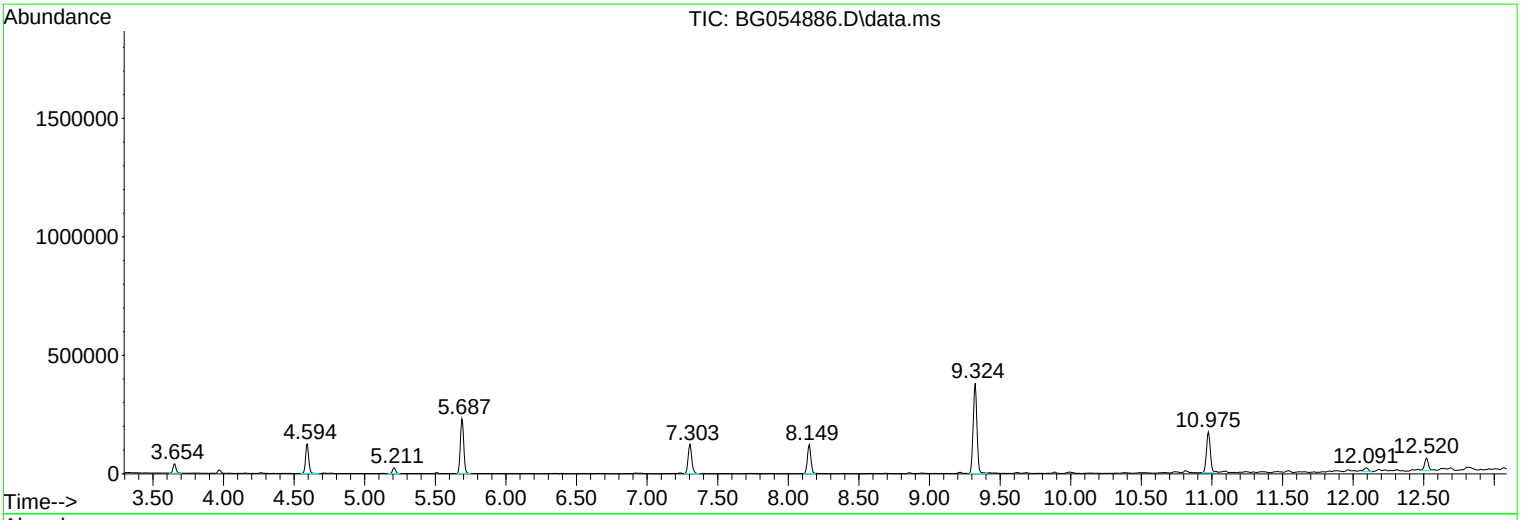
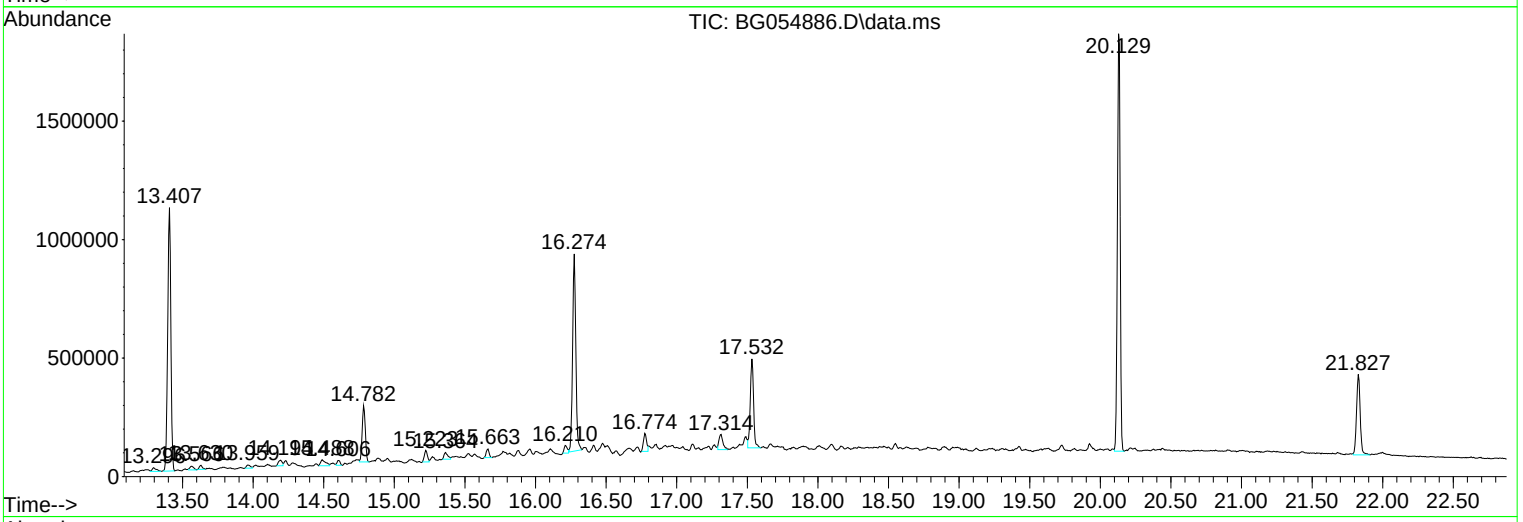
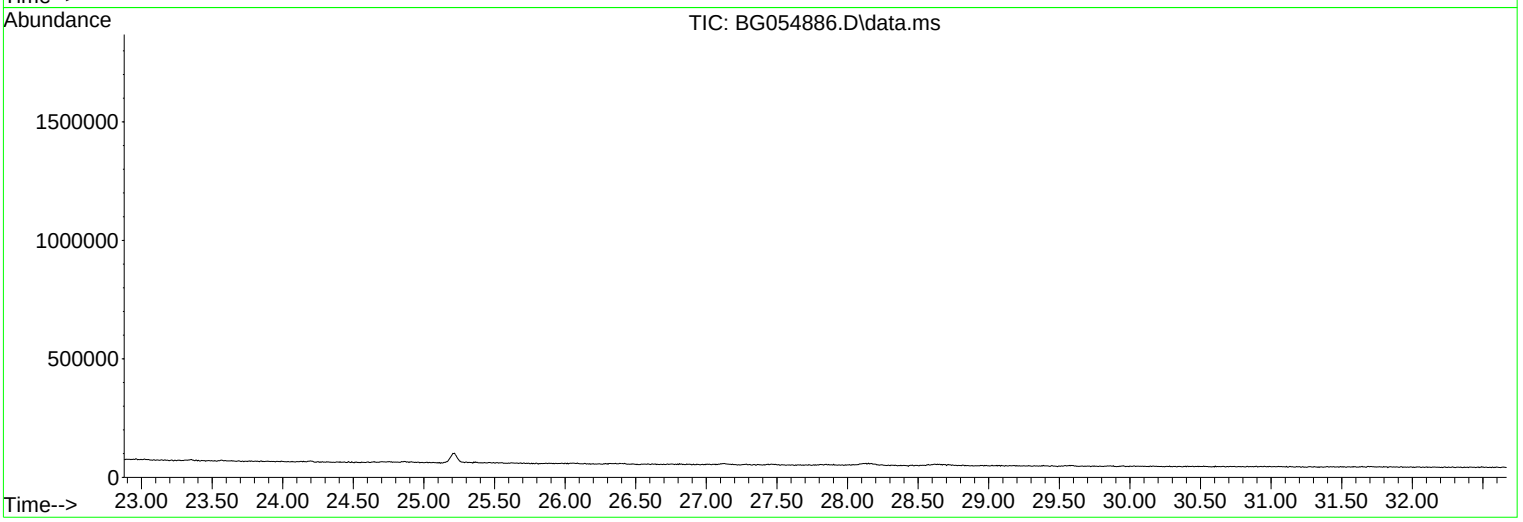
MW6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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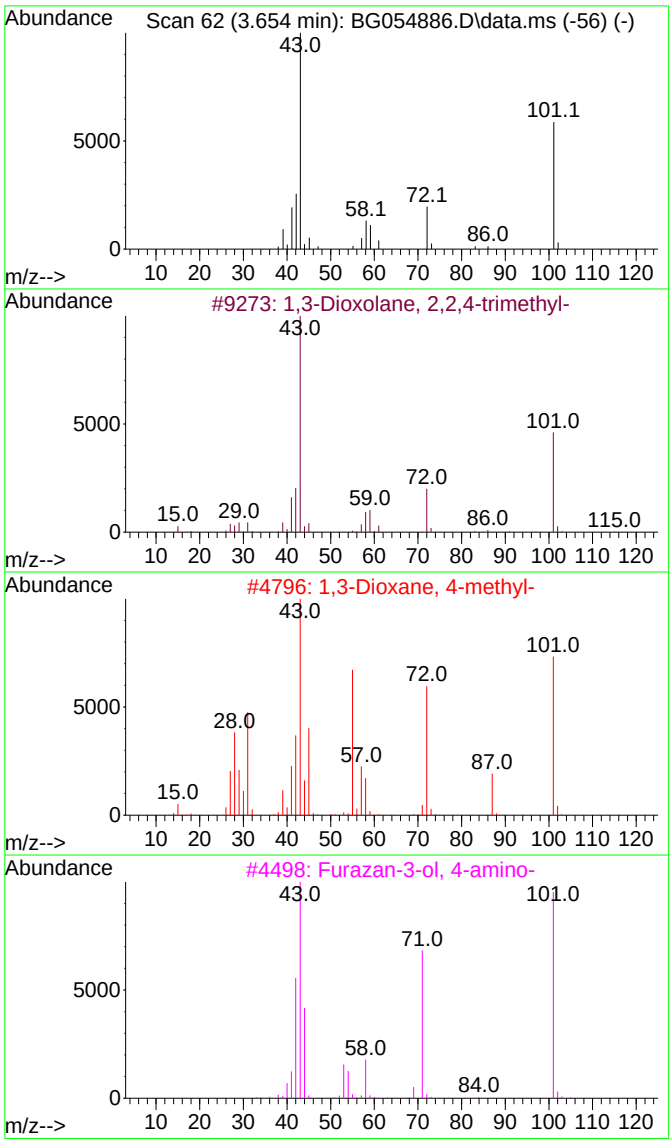
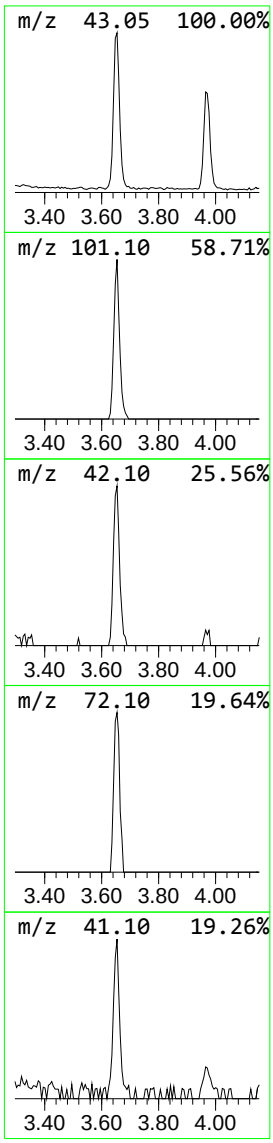
****
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.654	5.63 ng	59052	1,4-Dichlorobenzene-d4	8.149

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	42
3	Furazan-3-ol, 4-amino-	101	C2H3N3O2	159013-90-8	9
4	Butane	58	C4H10	000106-97-8	9
5	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	9





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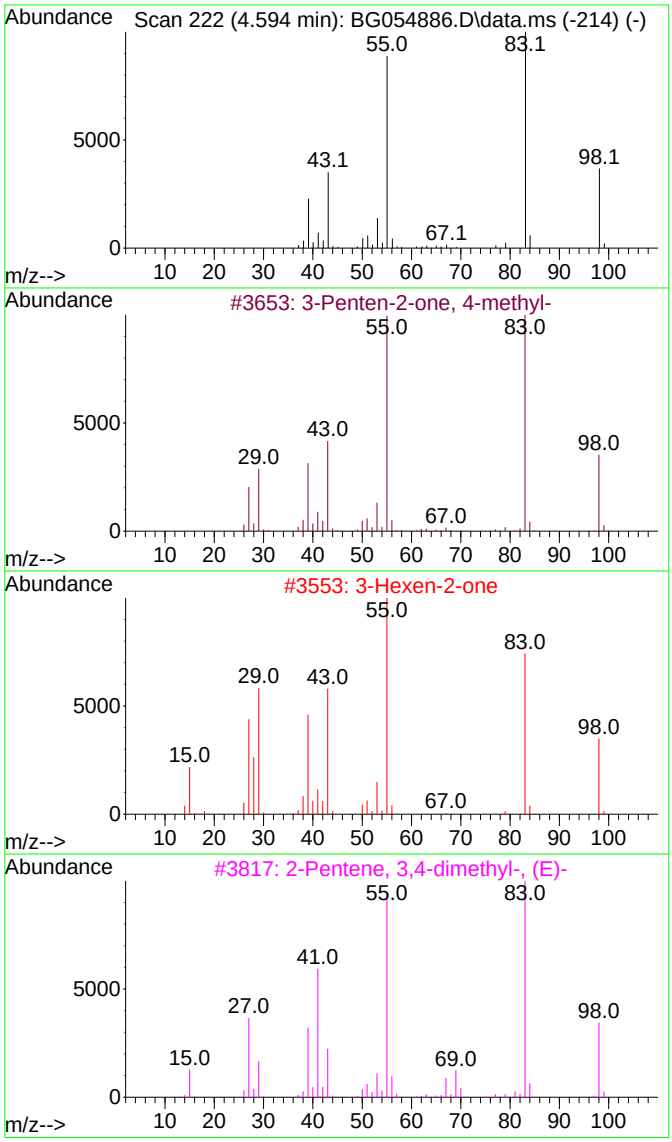
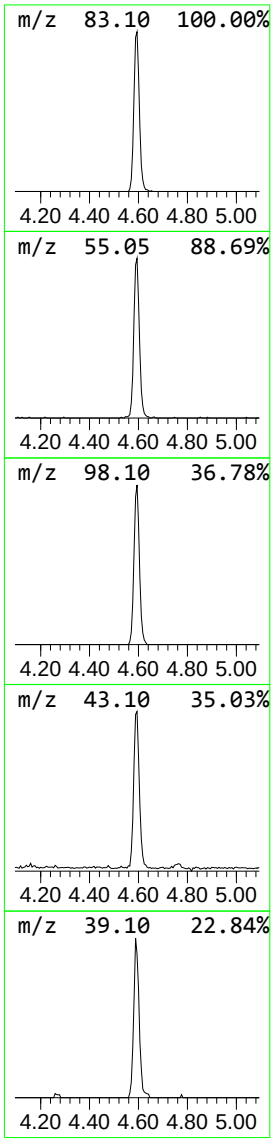
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.594	18.93 ng	198498	1,4-Dichlorobenzene-d4	8.149

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
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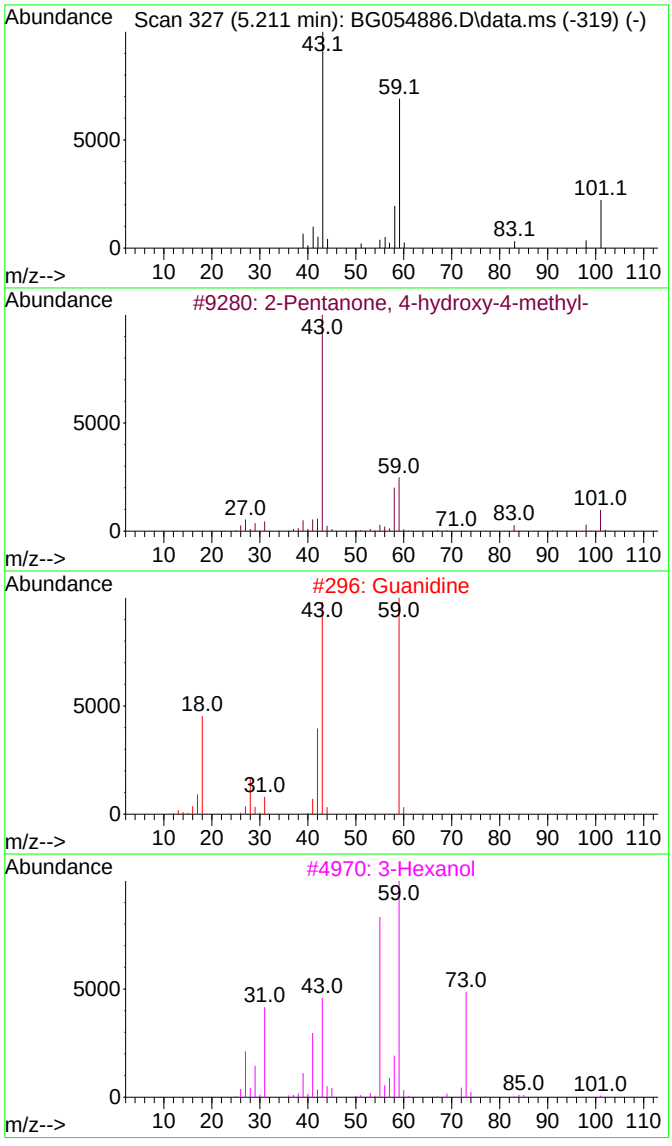
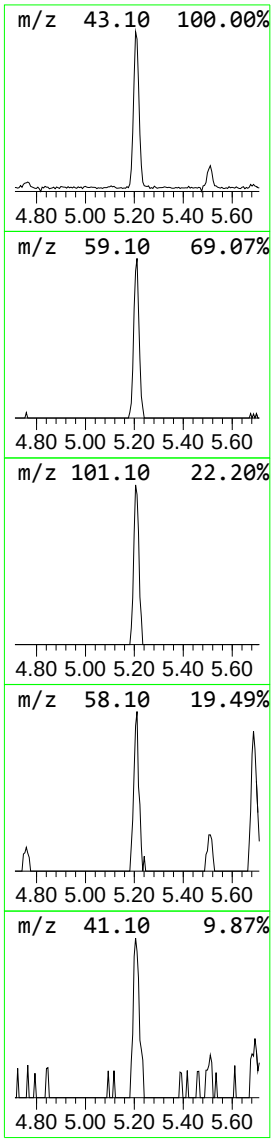
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.211	3.62 ng	38001	1,4-Dichlorobenzene-d4	8.149

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Guanidine	59	CH5N3	000113-00-8	38
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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TIC Library : C:\Database\NIST20.L
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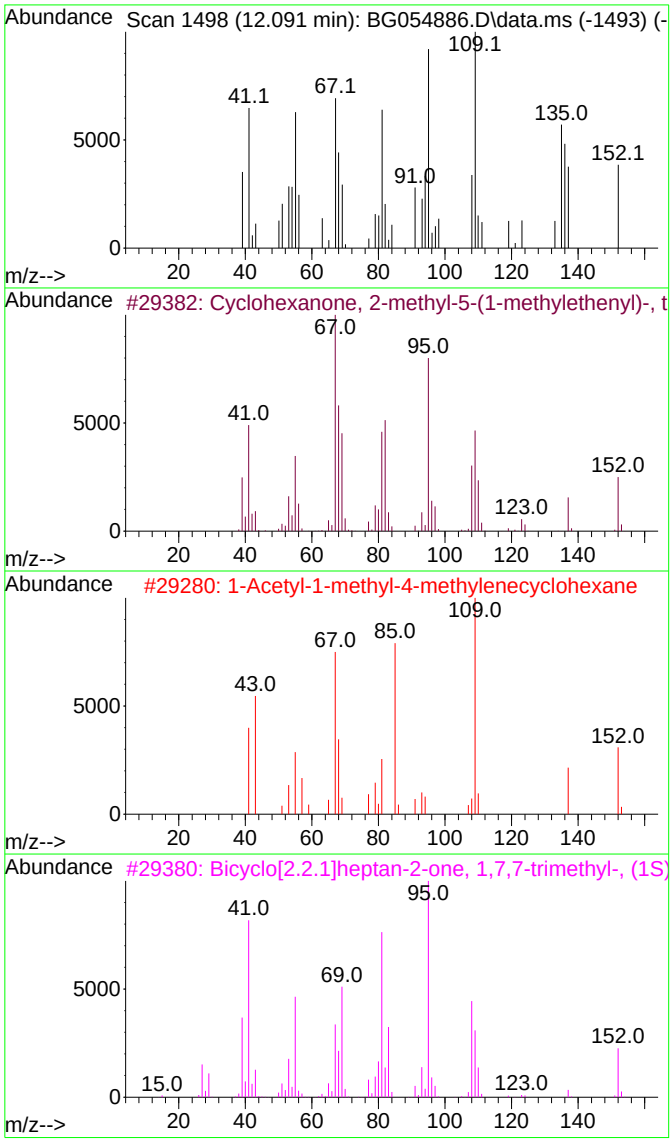
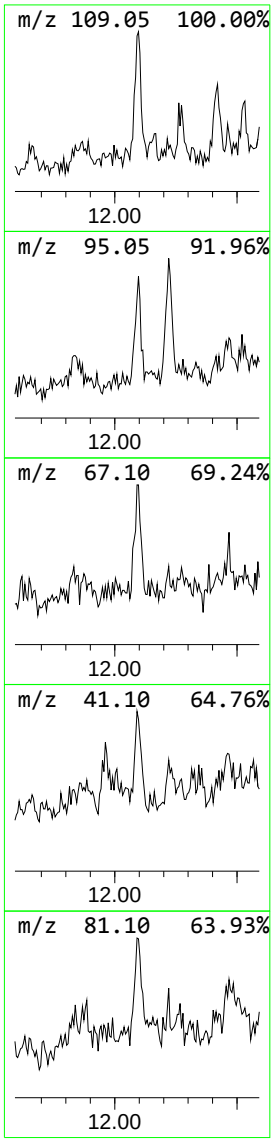
****
Peak Number 4 Cyclohexanone, 2-methyl-5-(... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	2.17 ng	34888	Naphthalene-d8	10.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	50
2	1-Acetyl-1-methyl-4-methylenecyc...	152	C10H16O	1000424-28-4	46
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	38
4	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	35
5	(+)-2-Bornanone	152	C10H16O	000464-49-3	27





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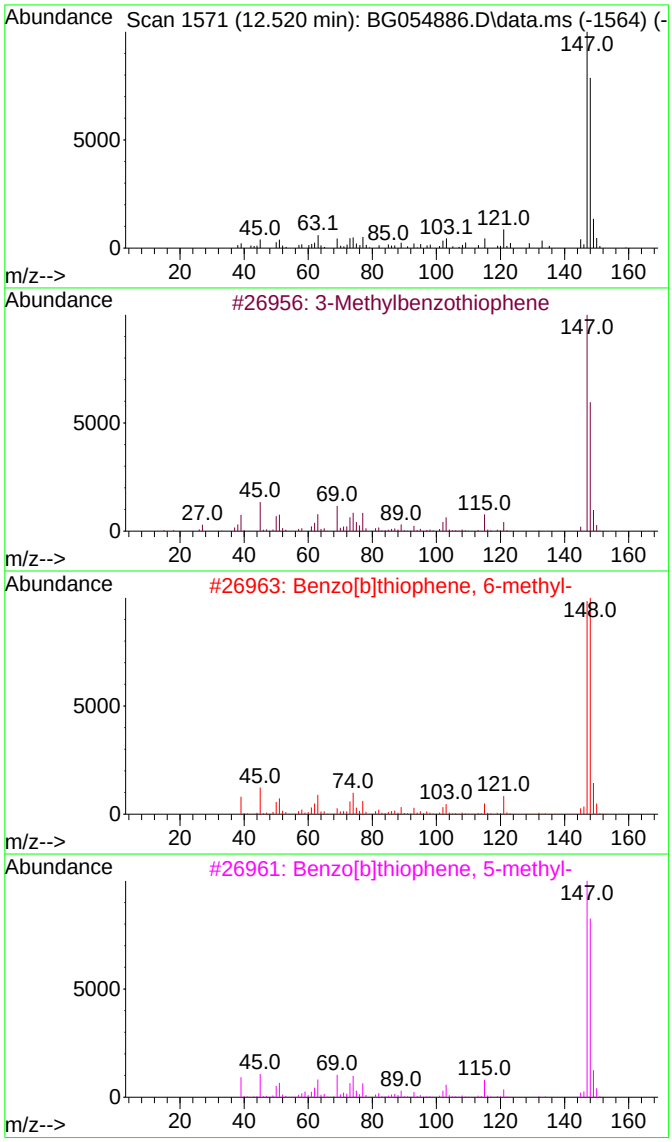
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

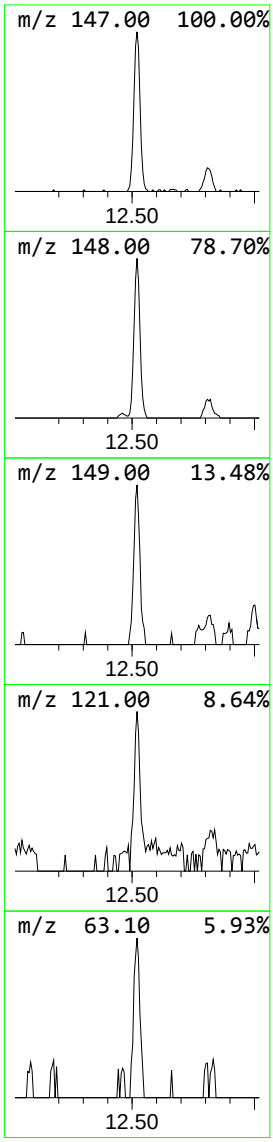
****

Peak Number 5 3-Methylbenzothiophene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.520	5.90 ng	94672	Naphthalene-d8	10.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methylbenzothiophene	148	C9H8S	001455-18-1	91
2	Benzo[b]thiophene, 6-methyl-	148	C9H8S	016587-47-6	91
3	Benzo[b]thiophene, 5-methyl-	148	C9H8S	014315-14-1	91
4	Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	90
5	Benzo[b]thiophene, 4-methyl-	148	C9H8S	014315-11-8	83





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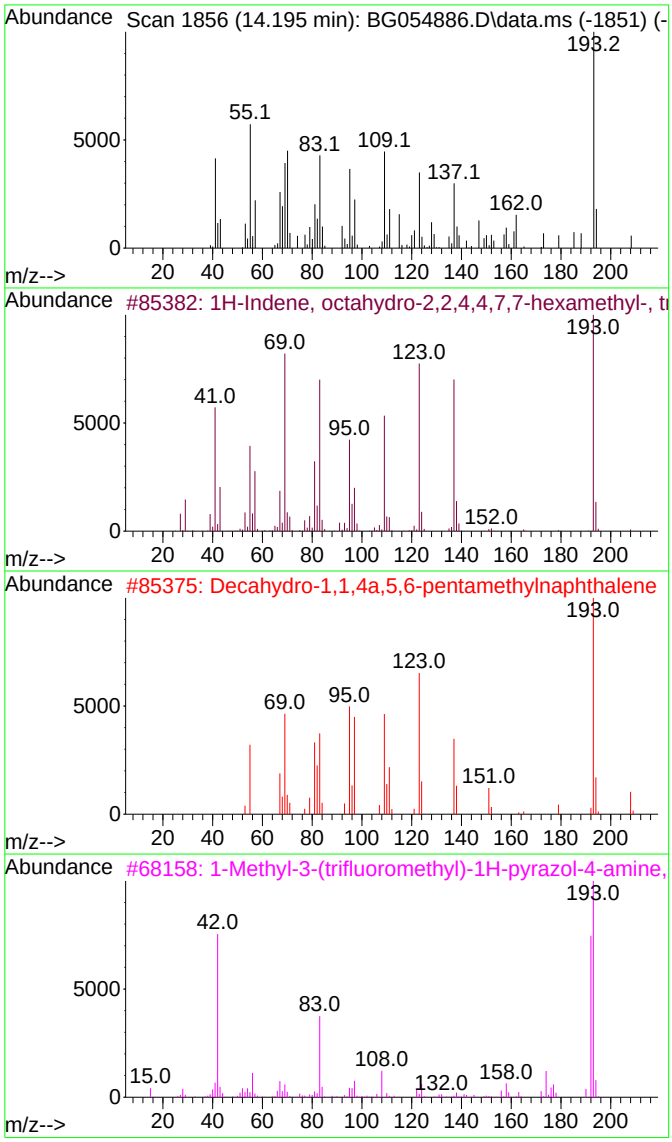
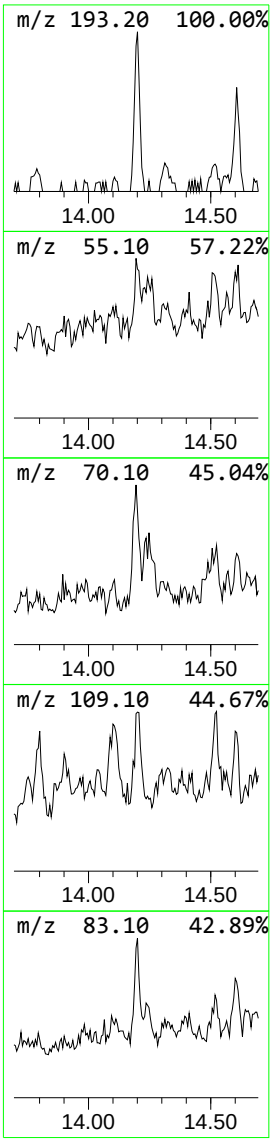
****

Peak Number 6 unknown14.195 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.195	2.45 ng	44656	Acenaphthene-d10	14.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	35
3	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	35
4	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	25
5	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	25





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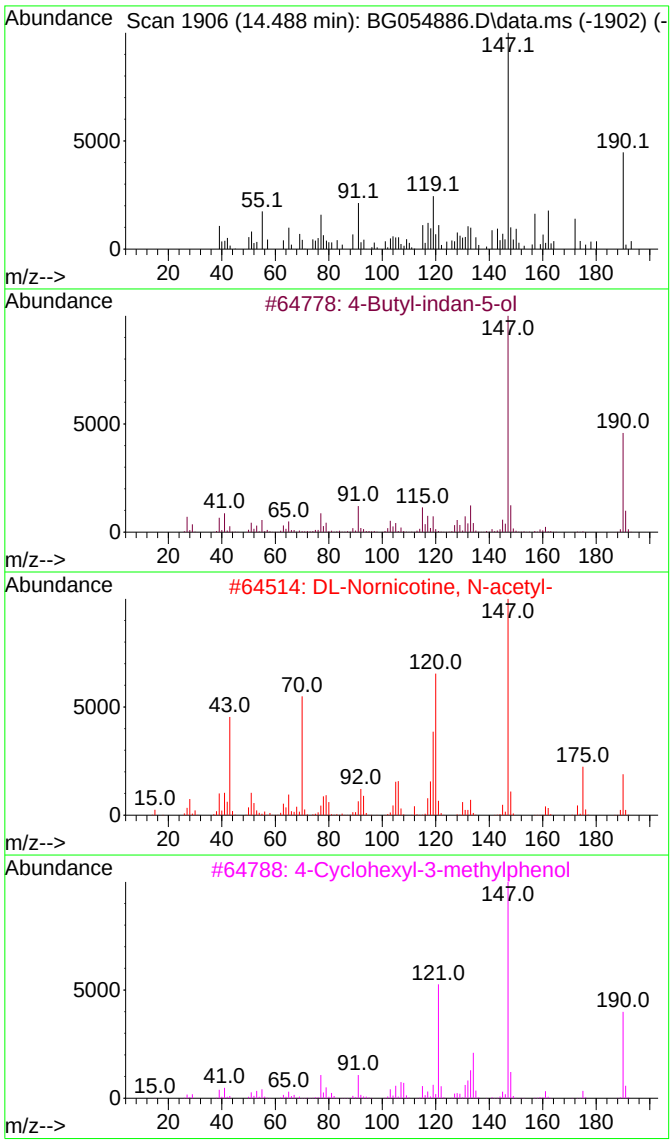
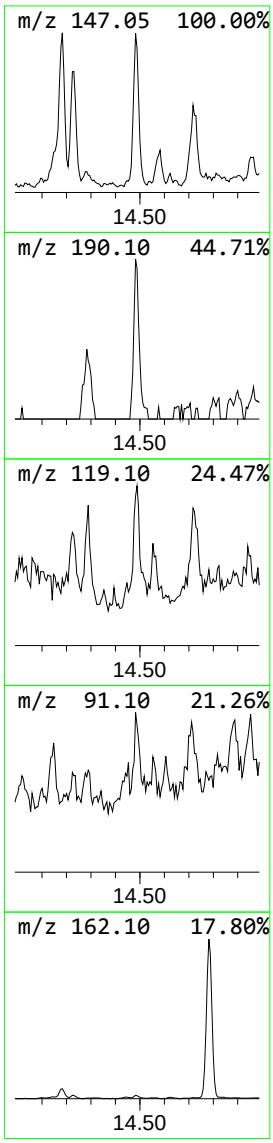
****

Peak Number 7 4-Butyl-indan-5-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.488	3.62 ng	65913	Acenaphthene-d10	14.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butyl-indan-5-ol	190	C13H18O	1000194-67-3	70
2	DL-Nornicotine, N-acetyl-	190	C11H14N2O	1000448-47-2	68
3	4-Cyclohexyl-3-methylphenol	190	C13H18O	001596-16-3	62
4	2-Benzoxazolamine, N,N-diethyl-	190	C11H14N2O	020852-38-4	58
5	Benzene, 1,4-bis(1-methylethyl)-	162	C12H18	000100-18-5	55





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TIC Library : C:\Database\NIST20.L
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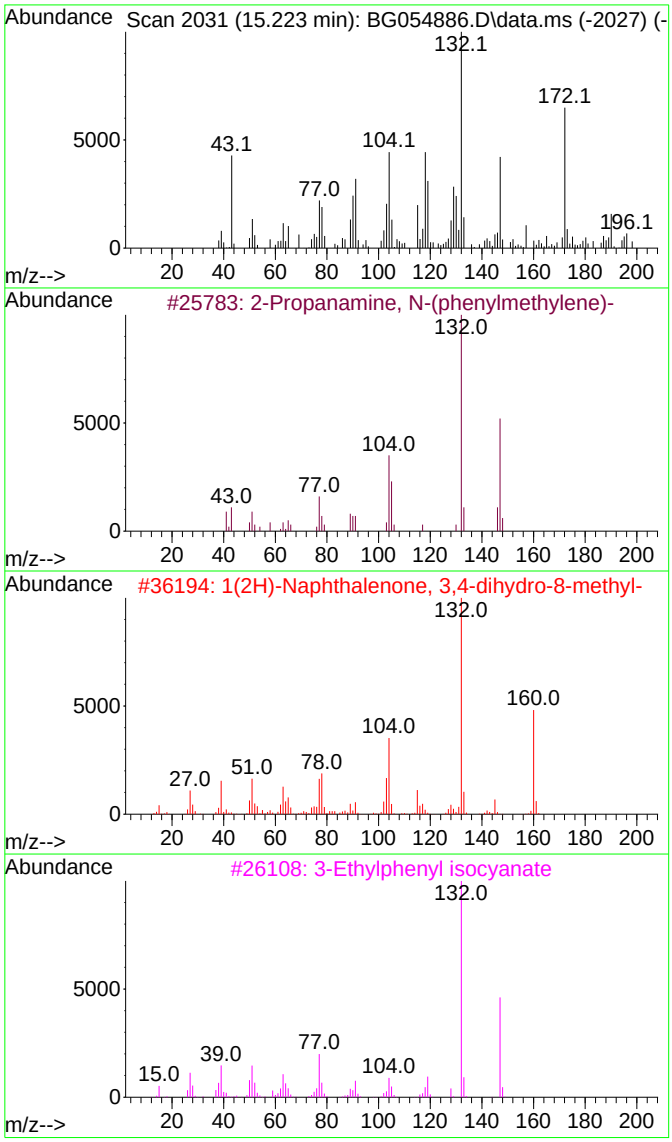
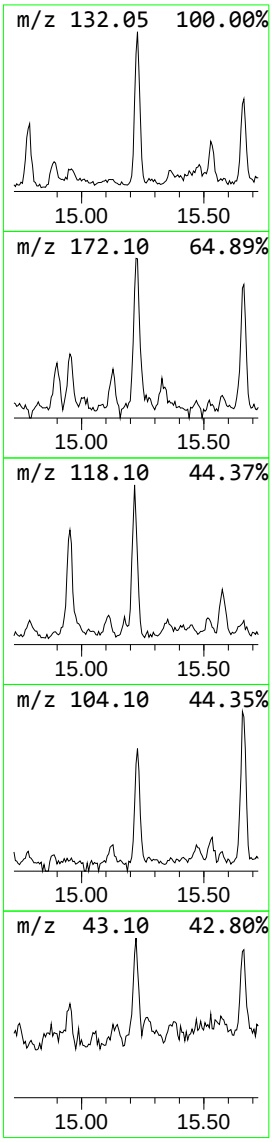
Peak Number 8 unknown15.223 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.223	4.00 ng	72745	Acenaphthene-d10	14.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanamine, N-(phenylmethylene)-	147	C10H13N	006852-56-8	45
2	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	051015-28-2	42
3	3-Ethylphenyl isocyanate	147	C9H9NO	023138-58-1	42
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	38
5	Quinoline, 1,2,3,4-tetrahydro-2-...	147	C10H13N	001780-19-4	35





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Sample : N4537-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
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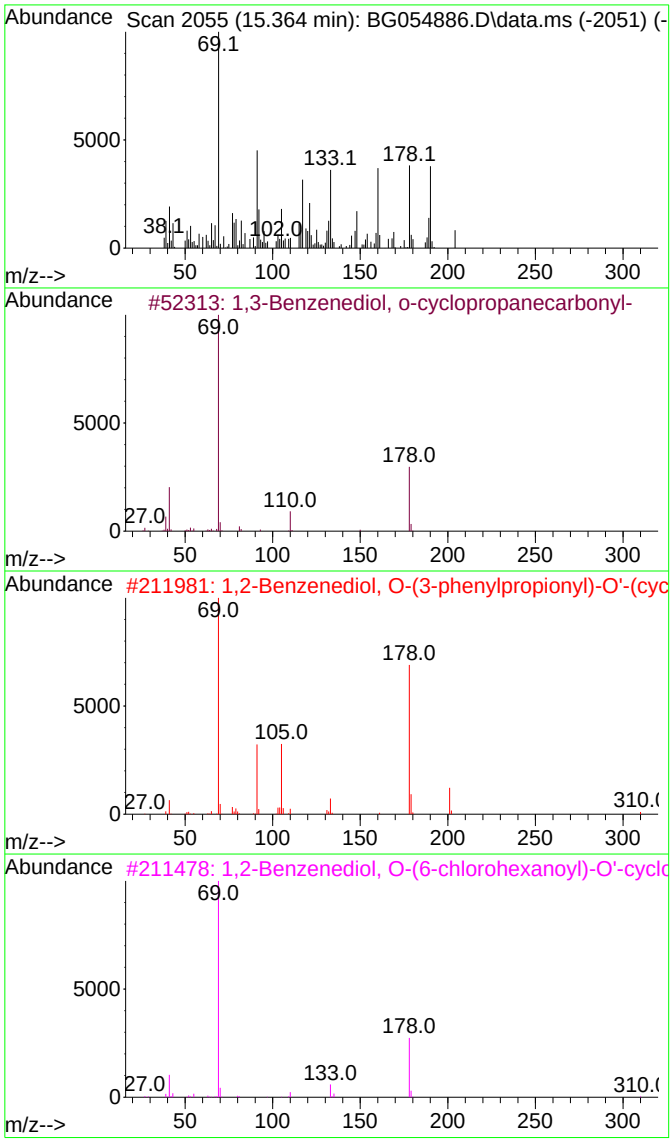
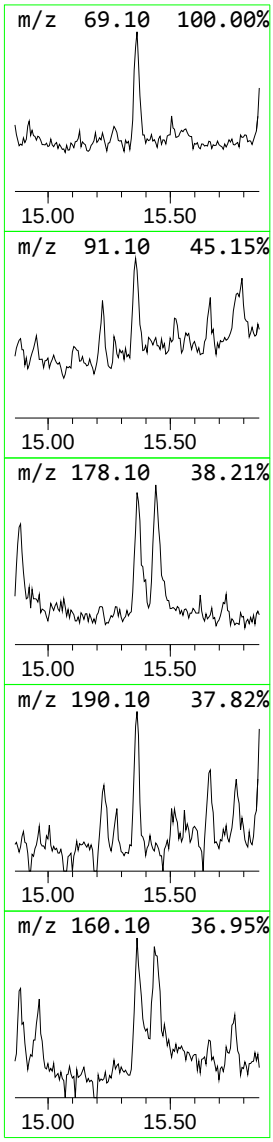
****

Peak Number 9 unknown15.364 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.364	3.02 ng	55011	Acenaphthene-d10	14.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenediol, o-cyclopropanec...	178	C10H10O3	1000330-78-1	43
2	1,2-Benzenediol, O-(3-phenylprop...	310	C19H18O4	1000329-80-3	37
3	1,2-Benzenediol, O-(6-chlorohexa...	310	C16H19ClO4	1000330-45-4	32
4	2-propenoic acid, 2-methyl-, 4-f...	190	C11H10O3	1000400-21-0	27
5	Cyclohexene, 3-(1,5-dimethyl-4-h...	204	C15H24	020307-83-9	25





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Data File : BG054886.D
Acq On : 8 Sep 2022 16:28
Operator : CG/JU
Sample : N4537-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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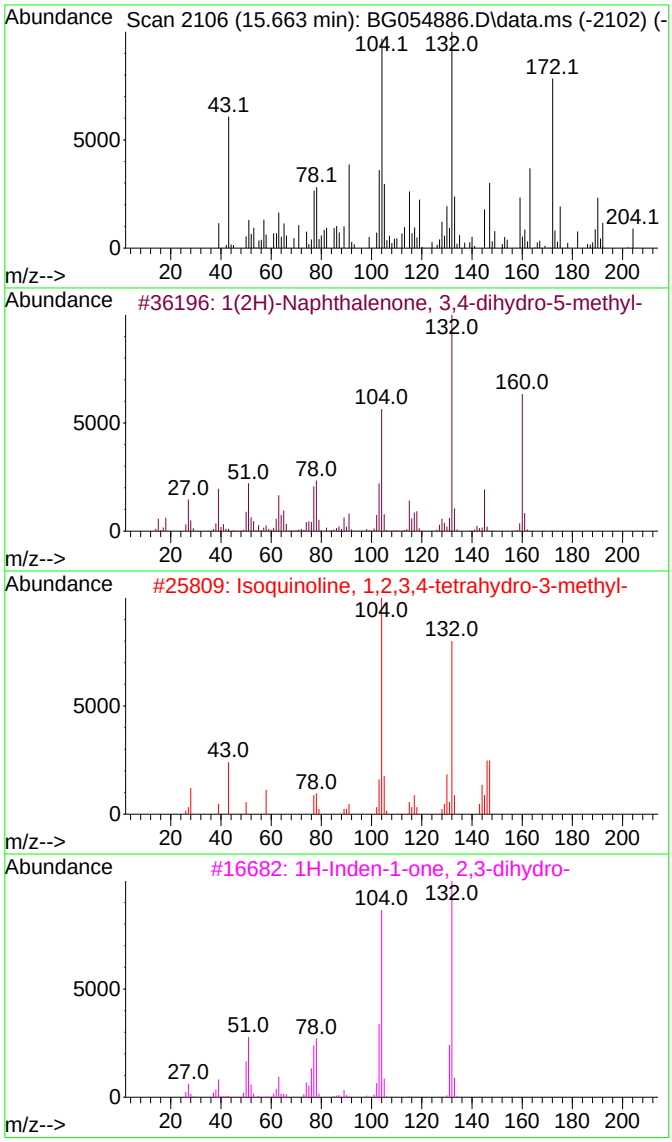
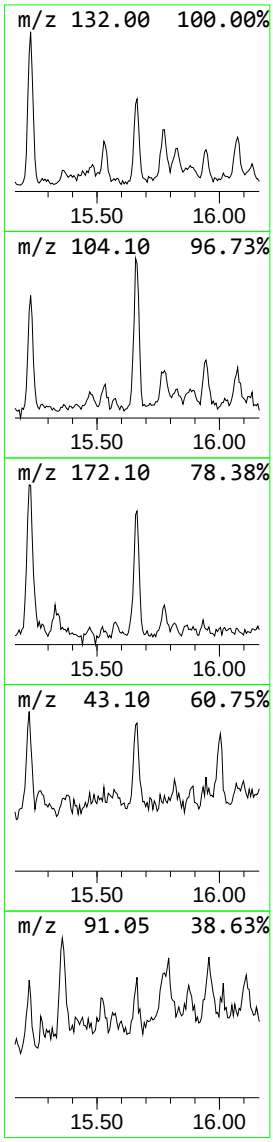
Peak Number 10 unknown15.663 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.663	2.79 ng	50725	Acenaphthene-d10	14.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	006939-35-1	46
2	Isoquinoline, 1,2,3,4-tetrahydro...	147	C10H13N	029726-60-1	45
3	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	38
4	5-Hydroxy-2-phenylpyrimidine	172	C10H8N2O	066739-85-3	30
5	Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054886.D
Acq On : 8 Sep 2022 16:28
Operator : CG/JU
Sample : N4537-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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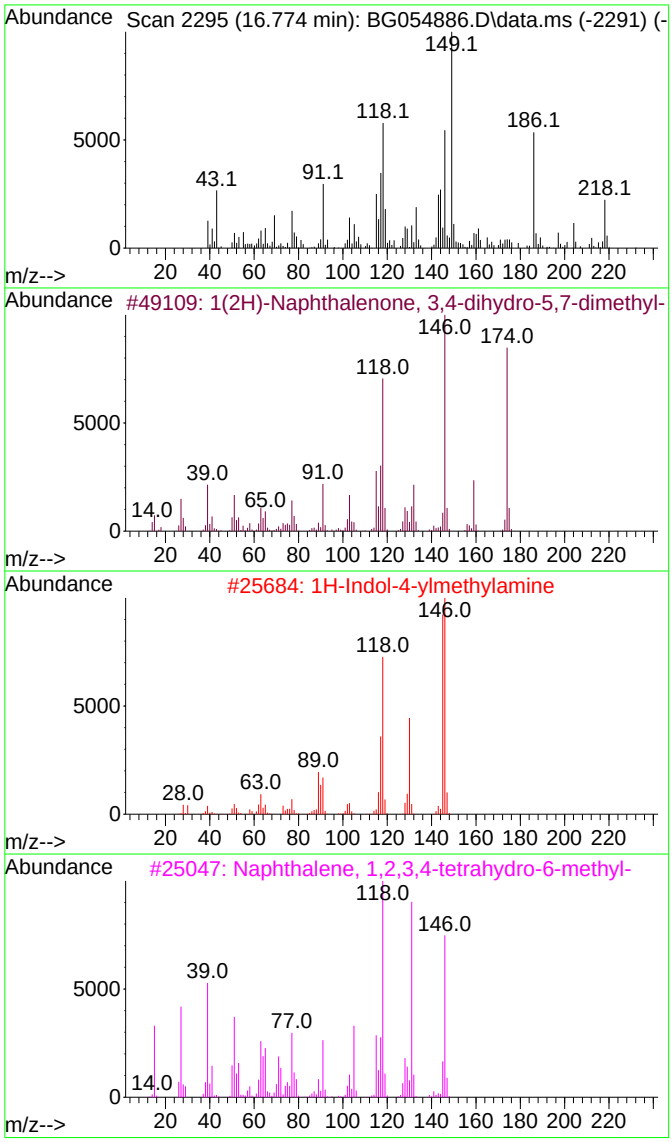
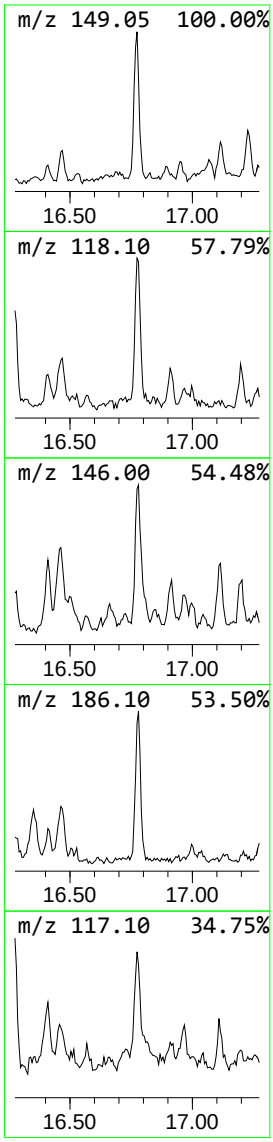
Peak Number 11 unknown16.774 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	4.06 ng	122165	Phenanthrene-d10	17.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Naphthalenone, 3,4-dihydro...	174	C12H14O	013621-25-5	35
2	1H-Indol-4-ylmethylamine	146	C9H10N2	003468-18-6	22
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	18
4	3-[5-(2-Cyano-ethyl)-pyrazin-2-y...	186	C10H10N4	1000186-64-9	15
5	1(2H)-Naphthalenone, 3,4-dihydro...	174	C12H14O	005037-63-8	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054886.D
Acq On : 8 Sep 2022 16:28
Operator : CG/JU
Sample : N4537-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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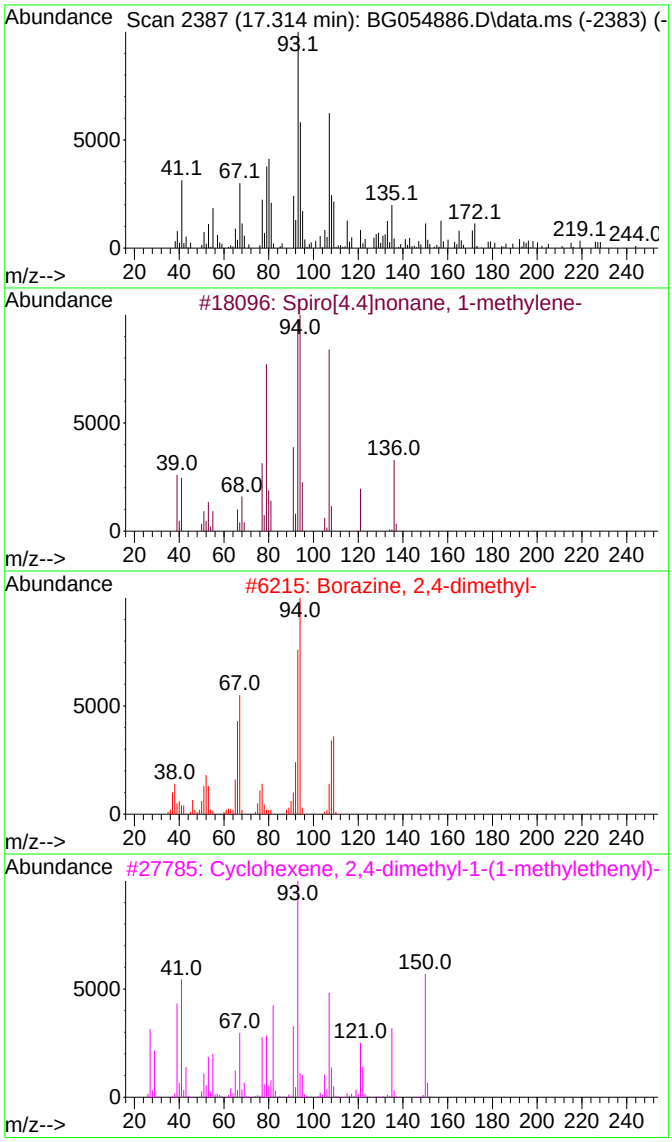
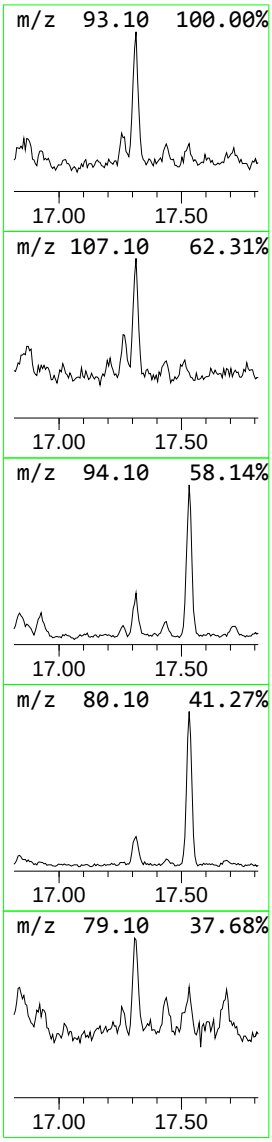
Peak Number 12 unknown17.314 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.314	4.07 ng	122496	Phenanthrene-d10	17.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[4.4]nonane, 1-methylene-	136	C10H16	019144-06-0	41
2	Borazine, 2,4-dimethyl-	109	C2H10B3N3	023208-27-7	38
3	Cyclohexene, 2,4-dimethyl-1-(1-m...	150	C11H18	056763-60-1	35
4	4-Butyl pyridine	135	C9H13N	005335-75-1	30
5	Cyclohexanemethanol, 4-methylene-	126	C8H14O	001004-24-6	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054886.D
Acq On : 8 Sep 2022 16:28
Operator : CG/JU
Sample : N4537-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
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
1,3-Dioxolane, ...	3.654	5.6	ng	59052	1	8.149	209674	20.0
3-Penten-2-one,...	4.594	18.9	ng	198498	1	8.149	209674	20.0
2-Pentanone, 4-...	5.211	3.6	ng	38001	1	8.149	209674	20.0
Cyclohexanone, ...	12.091	2.2	ng	34888	2	10.975	321117	20.0
3-Methylbenzoth...	12.520	5.9	ng	94672	2	10.975	321117	20.0
unknown14.195	14.195	2.5	ng	44656	3	14.782	364061	20.0
4-Butyl-indan-5-ol	14.488	3.6	ng	65913	3	14.782	364061	20.0
unknown15.223	15.223	4.0	ng	72745	3	14.782	364061	20.0
unknown15.364	15.364	3.0	ng	55011	3	14.782	364061	20.0
unknown15.663	15.663	2.8	ng	50725	3	14.782	364061	20.0
unknown16.774	16.774	4.1	ng	122165	4	17.532	601691	20.0
unknown17.314	17.314	4.1	ng	122496	4	17.532	601691	20.0