LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053348.D
Acq On : 27 Apr 2022 15:31
Operator : CG/JU
Sample : N2481-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-24

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-BG040822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053348.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.550	193	198	204	rBV2	31209	50474	1.70%	0.461%
2	5.191	302	307	315	rVB2	19994	32438	1.10%	0.296%
3	5.666	382	388	399	rVB	259370	437423	14.77%	3.995%
4	7.264	654	660	670	rBV	168537	305248	10.31%	2.788%
5	7.628	717	722	727	rBV	23618	36674	1.24%	0.335%
6	7.681	727	731	738	rVB2	22561	36235	1.22%	0.331%
7	7.869	756	763	771	rBV	37032	66147	2.23%	0.604%
8	8.104	796	803	808	rBV	96942	165096	5.58%	1.508%
9	9.267	993	1001	1009	rBV	380951	699740	23.63%	6.390%
10	10.912	1274	1281	1288	rBV	124199	231879	7.83%	2.118%
11	11.265	1334	1341	1351	rBV3	13344	30918	1.04%	0.282%
12	13.086	1645	1651	1658	rBV	62820	97895	3.31%	0.894%
13	13.350	1685	1696	1706	rBV	1038632	1765976	59.63%	16.128%
14	13.567	1726	1733	1746	rBV	320922	485171	16.38%	4.431%
15	14.725	1924	1930	1937	rVB	218385	342457	11.56%	3.128%
16	15.453	2050	2054	2061	rVB	22820	33912	1.15%	0.310%
17	15.529	2061	2067	2073	rVB	42191	62132	2.10%	0.567%
18	16.064	2153	2158	2166	rBV2	38055	56296	1.90%	0.514%
19	16.217	2177	2184	2197	rBV	884037	1412815	47.71%	12.903%
20	17.474	2391	2398	2410	rBV	307953	475519	16.06%	4.343%
21	18.126	2502	2509	2514	rVB2	26236	32279	1.09%	0.295%
22	18.431	2555	2561	2567	rVB3	27473	41476	1.40%	0.379%
23	20.076	2834	2841	2847	rBV	2231752	2961312	100.00%	27.045%
24	21.756	3120	3127	3136	rVB	319080	545130	18.41%	4.978%
25	25.052	3678	3688	3698	rVB	187620	545085	18.41%	4.978%

Sum of corrected areas: 10949727

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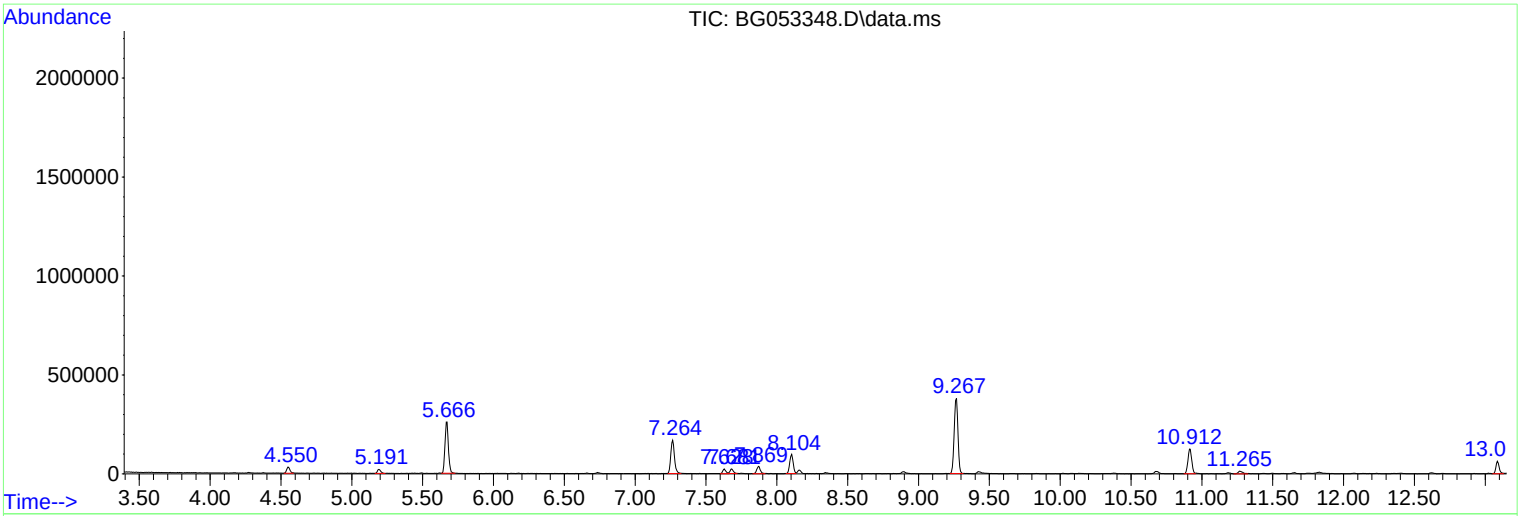
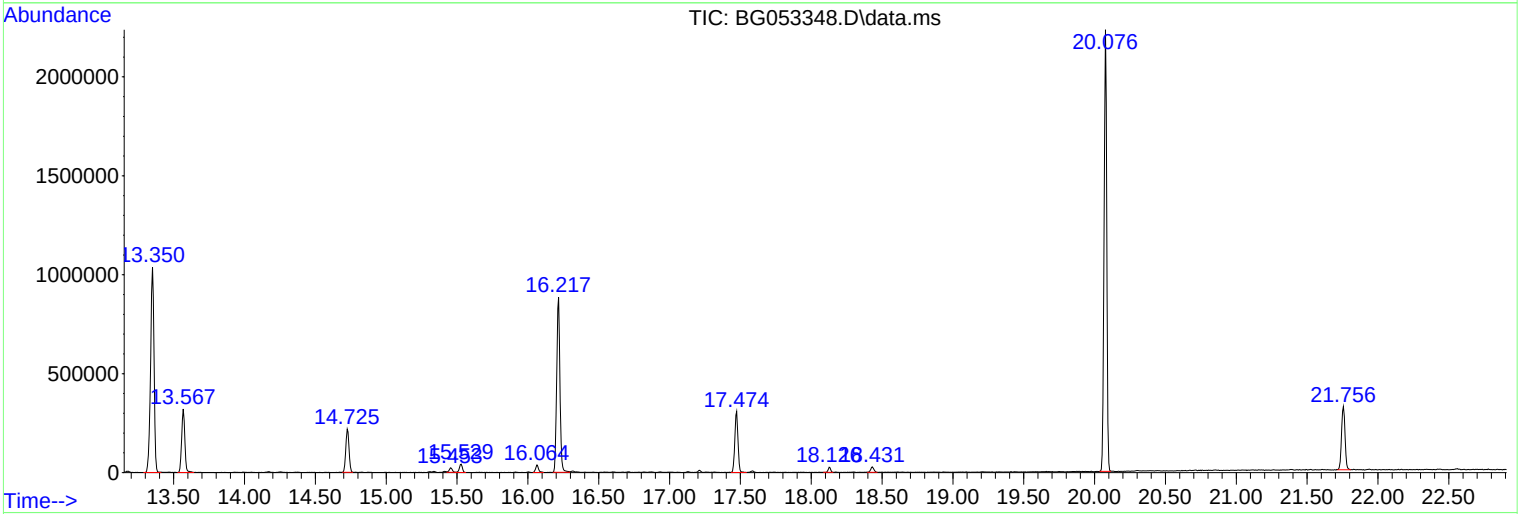
ALS Vial : 10 Sample Multiplier: 1

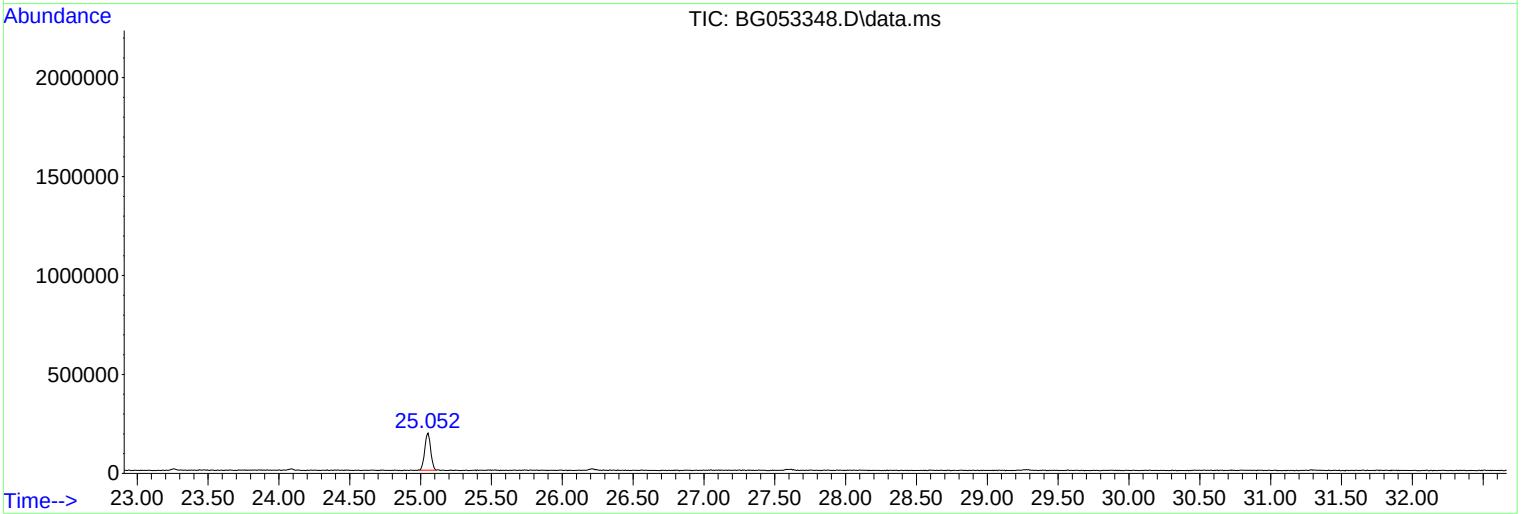
Instrument :
BNA_G
ClientSampleId :
MW-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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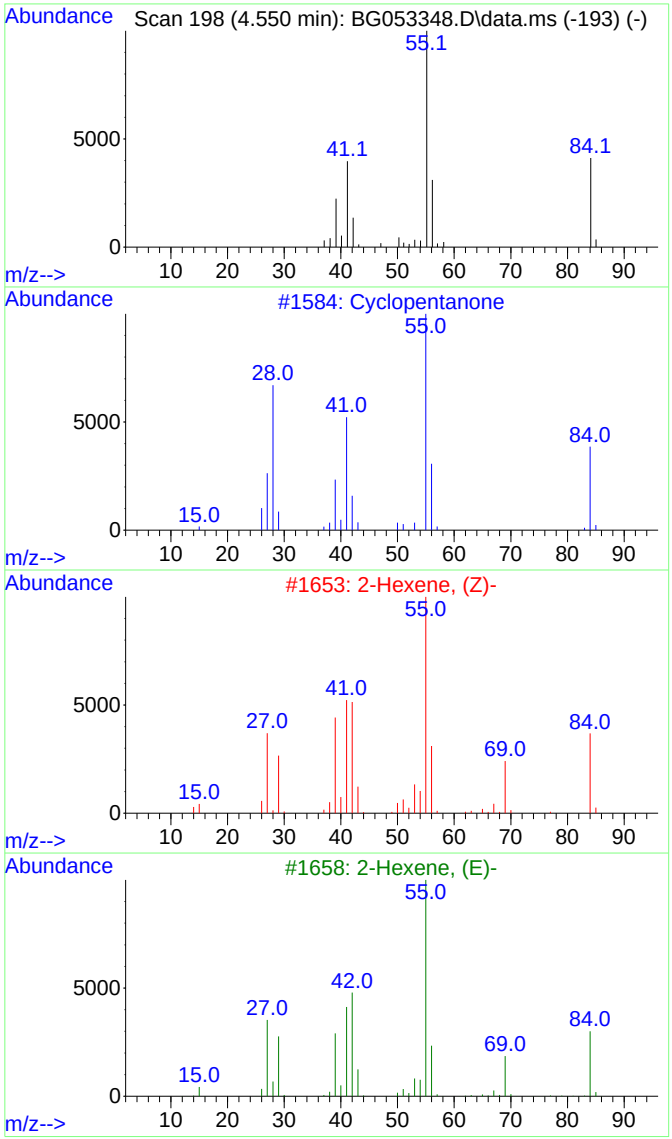
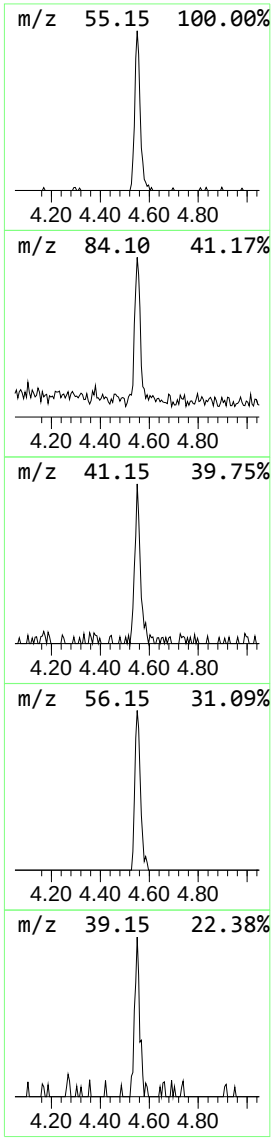
****

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.550	6.11 ng	50474	1,4-Dichlorobenzene-d4	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene, (Z)-	84	C6H12	007688-21-3	72
3	2-Hexene, (E)-	84	C6H12	004050-45-7	64
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	64
5	3-Hexene, (E)-	84	C6H12	013269-52-8	64





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Data File : BG053348.D
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Operator : CG/JU
Sample : N2481-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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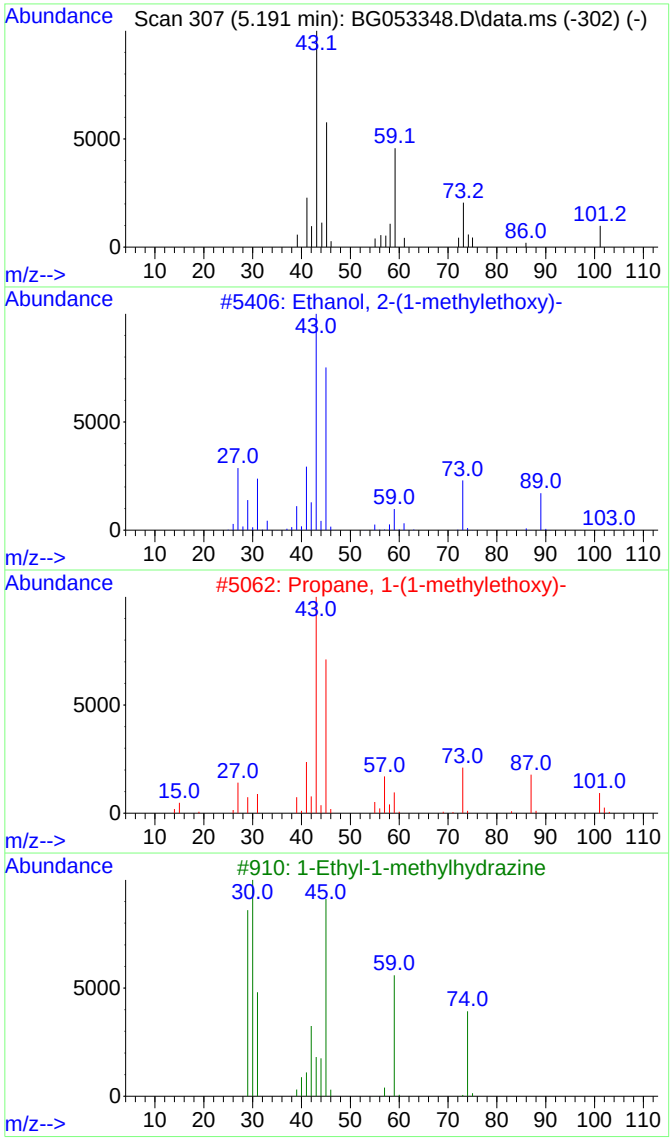
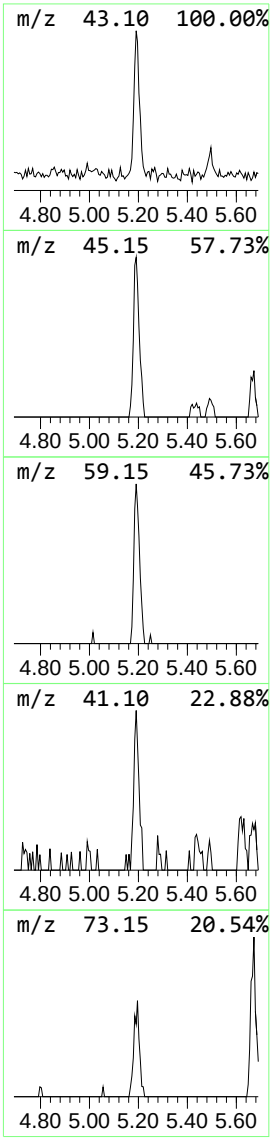
Peak Number 2 unknown5.191 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	3.93 ng	32438	1,4-Dichlorobenzene-d4	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	47
2	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38
3	1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	37
4	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	28
5	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	28





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Misc :
ALS Vial : 10 Sample Multiplier: 1

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

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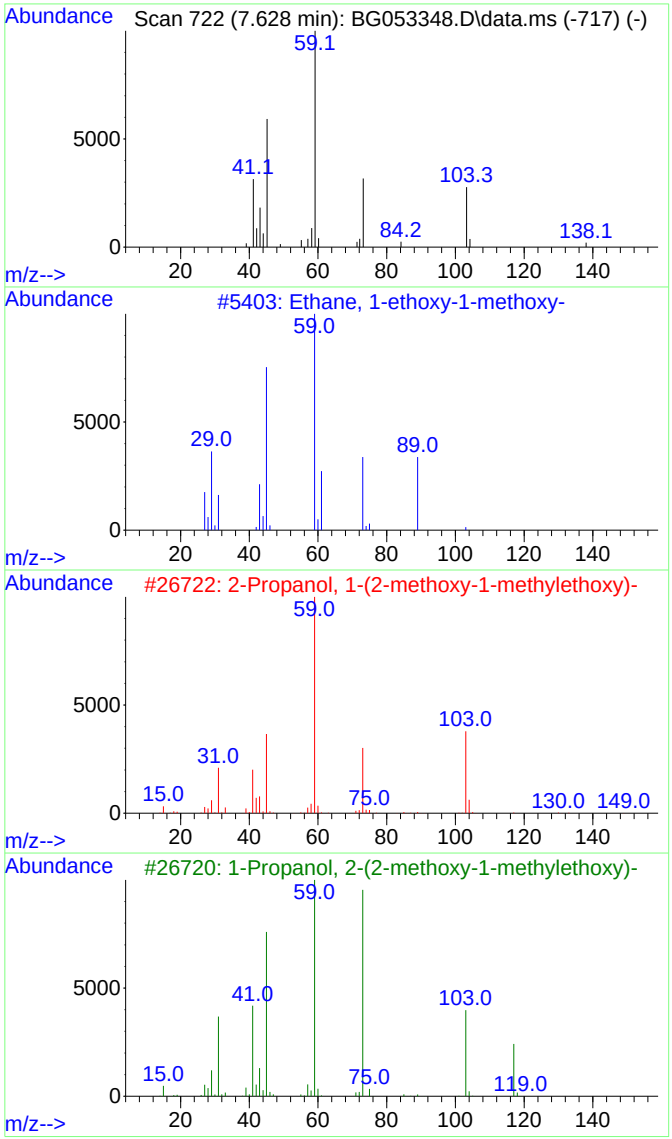
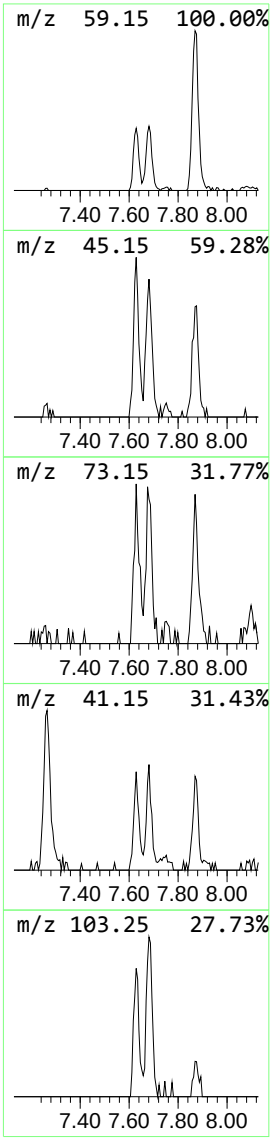
****

Peak Number 3 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.628	4.44 ng	36674	1,4-Dichlorobenzene-d4	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	64
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
3	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	50
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	42





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Sample : N2481-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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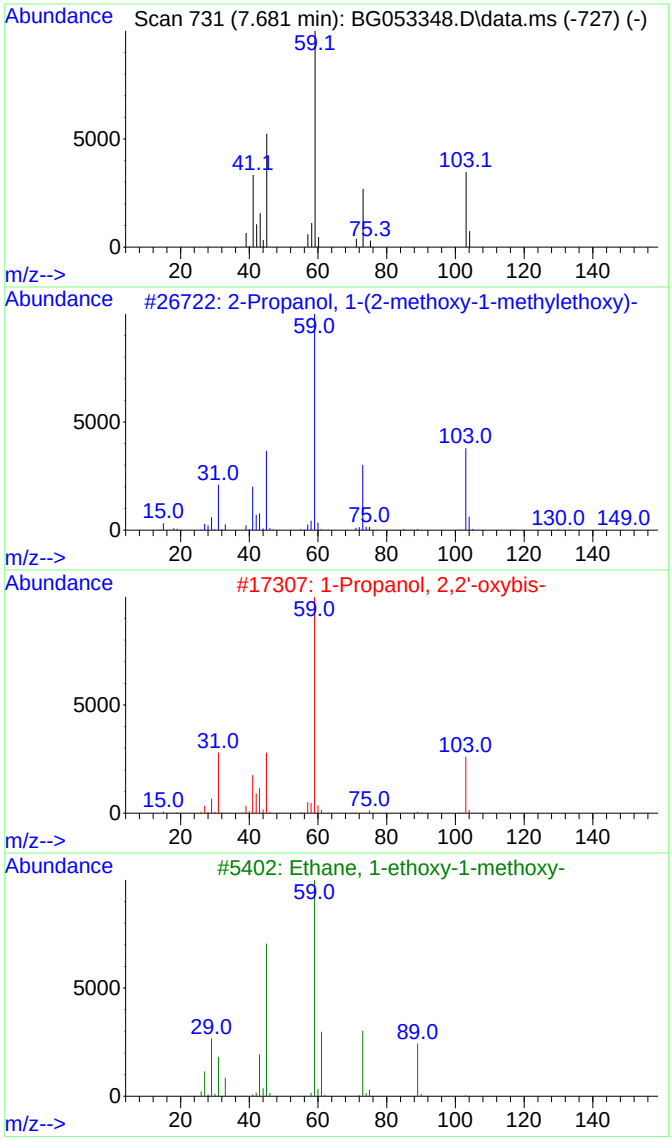
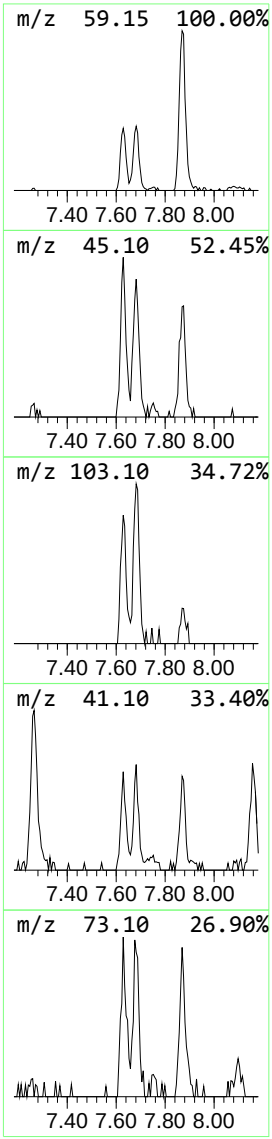
****

Peak Number 4 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.681	4.39 ng	36235	1,4-Dichlorobenzene-d4	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	42
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	42
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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Operator : CG/JU
Sample : N2481-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
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TIC Library : C:\Database\NIST20.L
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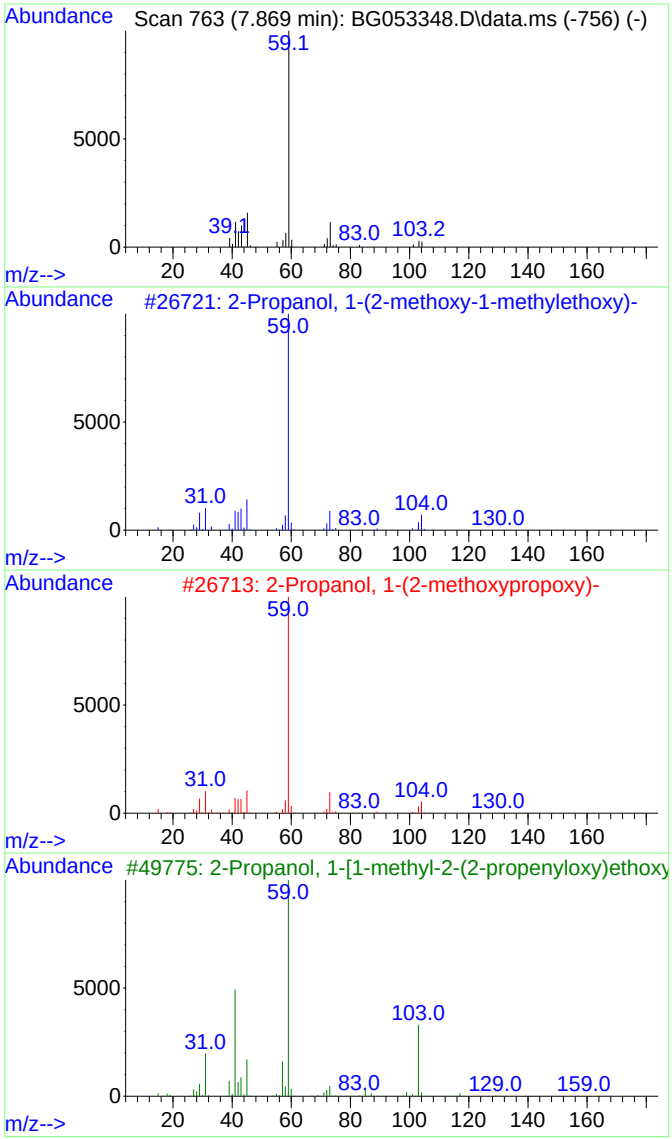
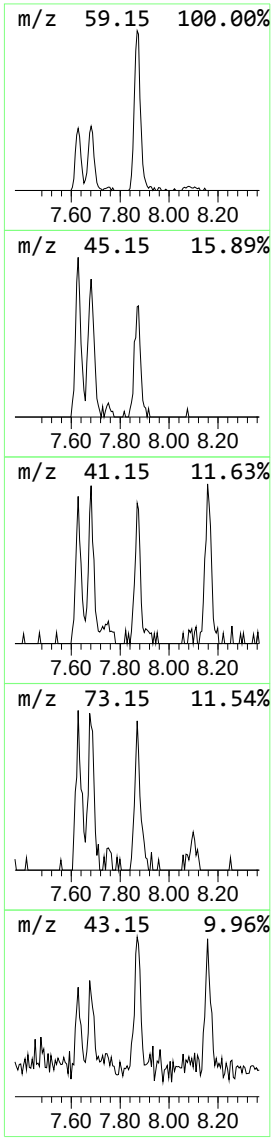
****

Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.869	8.01 ng	66147	1,4-Dichlorobenzene-d4	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	64
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64





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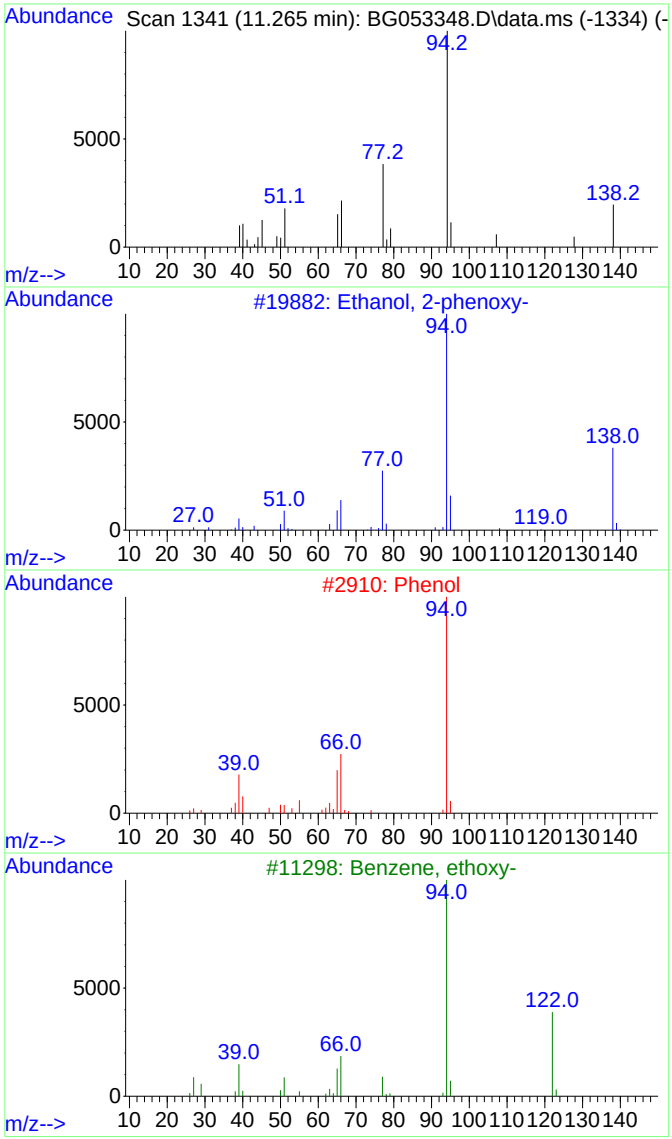
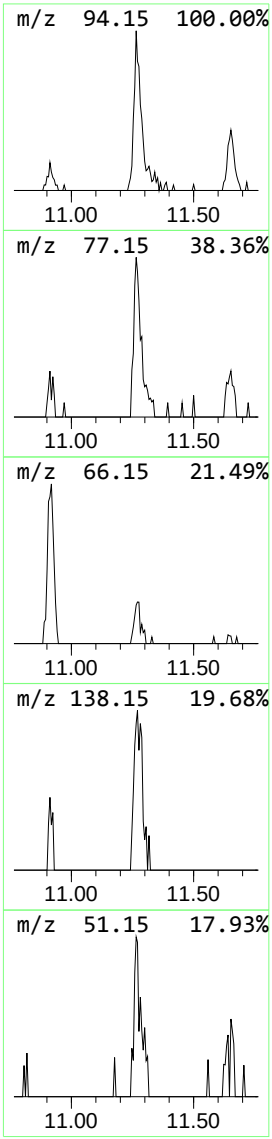
****

Peak Number 6 Ethanol, 2-phenoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.265	2.67 ng	30918	Naphthalene-d8	10.912

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	91
2	Phenol	94	C6H6O	000108-95-2	50
3	Benzene, ethoxy-	122	C8H10O	000103-73-1	45
4	Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	42
5	Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	37





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Sample : N2481-13
Misc :
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Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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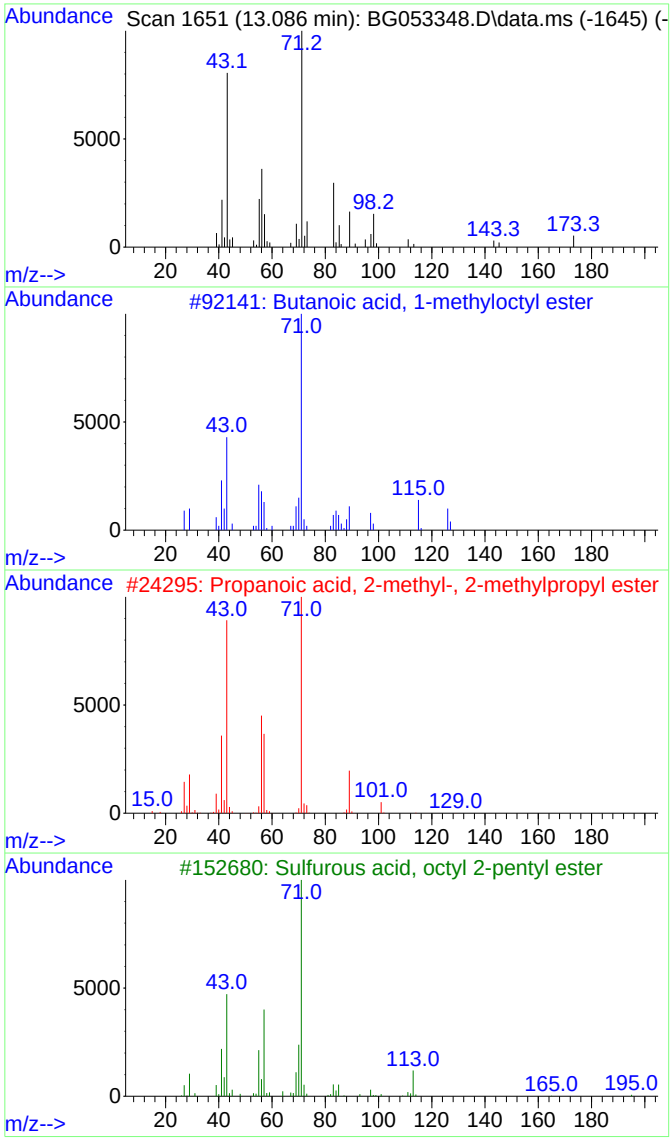
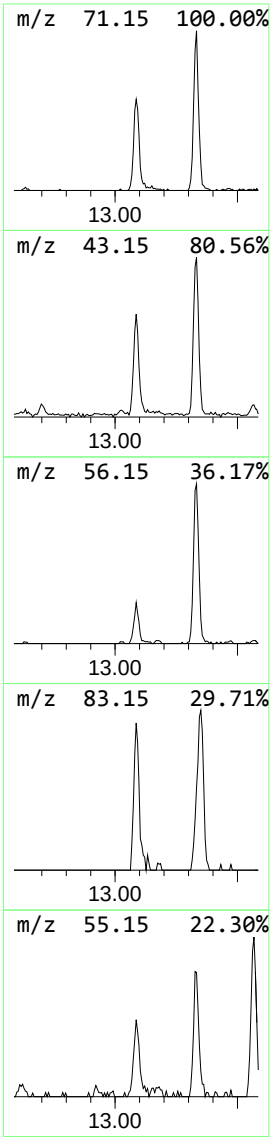
****
Peak Number 7 Butanoic acid, 1-methylocty... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	5.72 ng	97895	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	53
2	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
3	Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	50
4	Butanoic acid, decyl ester	228	C14H28O2	005454-09-1	50
5	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43





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TIC Library : C:\Database\NIST20.L
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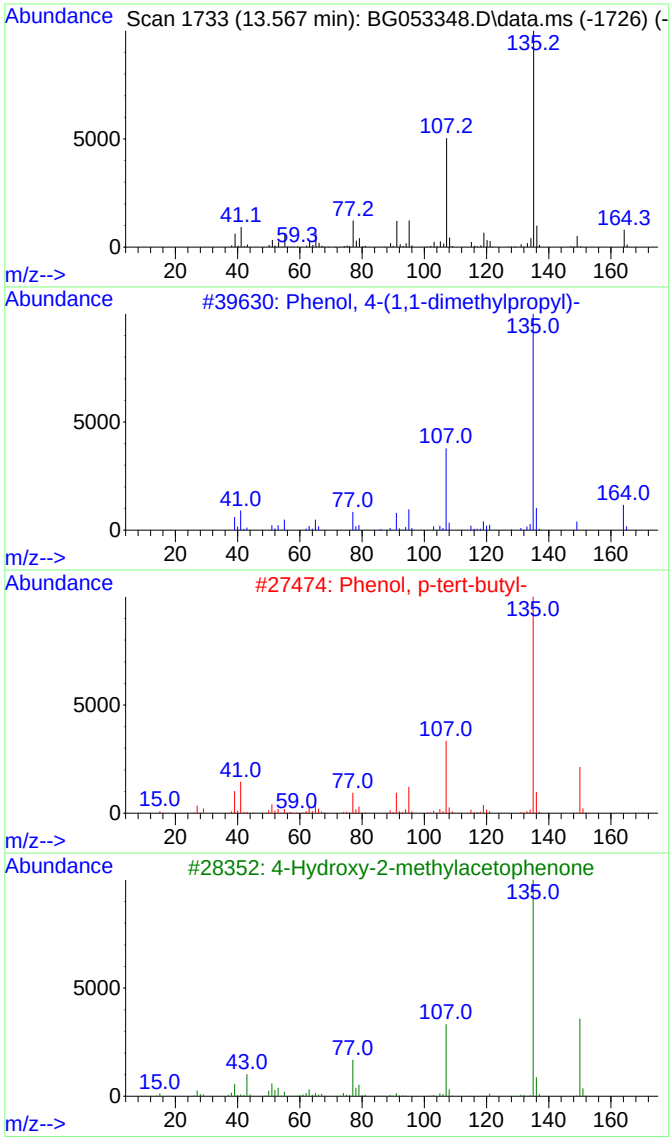
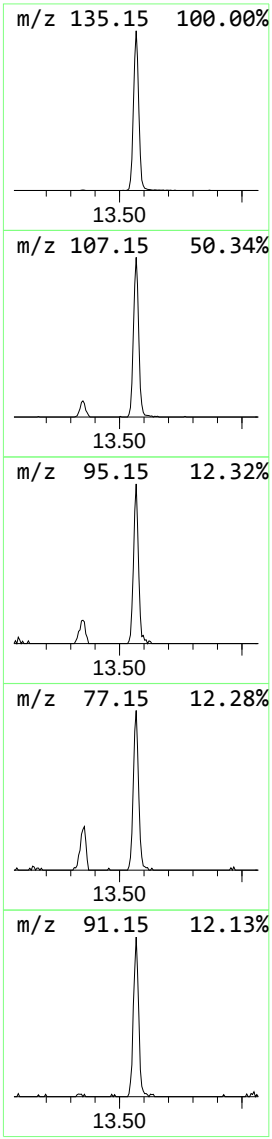
****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.567	28.33 ng	485171	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	68
4	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64
5	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
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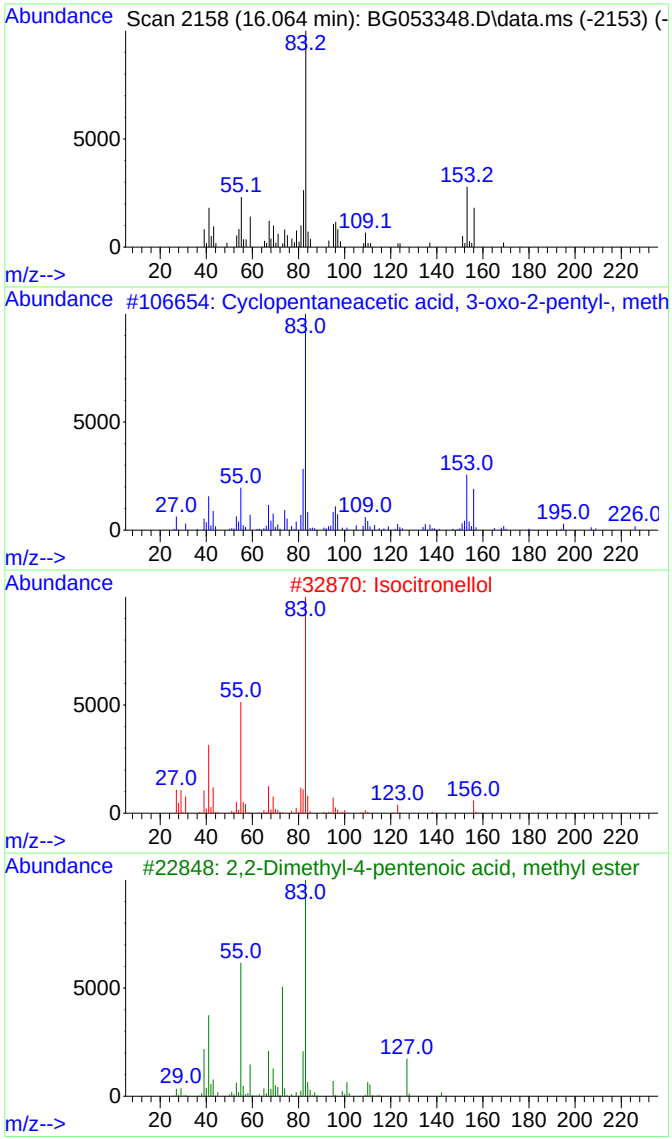
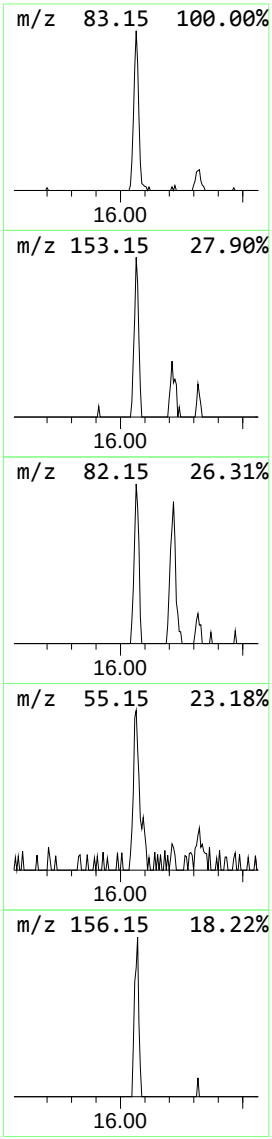
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopentaneacetic acid, 3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.064	3.29 ng	56296	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	90
2	Isocitronellol	156	C10H20O	018479-52-2	50
3	2,2-Dimethyl-4-pentenoic acid, m...	142	C8H14O2	076352-72-2	50
4	Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	47
5	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053348.D
Acq On : 27 Apr 2022 15:31
Operator : CG/JU
Sample : N2481-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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
Cyclopentanone	4.550	6.1	ng	50474	1	8.104	165096	20.0
unknown5.191	5.191	3.9	ng	32438	1	8.104	165096	20.0
Ethane, 1-ethox...	7.628	4.4	ng	36674	1	8.104	165096	20.0
2-Propanol, 1-(...	7.681	4.4	ng	36235	1	8.104	165096	20.0
2-Propanol, 1-(...	7.869	8.0	ng	66147	1	8.104	165096	20.0
Ethanol, 2-phen...	11.265	2.7	ng	30918	2	10.912	231879	20.0
Butanoic acid, ...	13.086	5.7	ng	97895	3	14.725	342457	20.0
Phenol, 4-(1,1-...	13.567	28.3	ng	485171	3	14.725	342457	20.0
Cyclopentaneace...	16.064	3.3	ng	56296	3	14.725	342457	20.0