LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053355.D
Acq On : 28 Apr 2022 1:18
Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 17 Sample Multiplier: 2

Instrument :
BNA_G
ClientSampleId :
MW-7R

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: BG053355.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.551	191	198	209	rVB	68183	116227	4.76%	1.047%
2	5.191	302	307	316	rVB2	25093	38541	1.58%	0.347%
3	5.667	382	388	400	rVB	248692	416477	17.05%	3.752%
4	7.265	653	660	670	rBV	178938	318078	13.02%	2.865%
5	7.629	715	722	726	rBV	42102	66168	2.71%	0.596%
6	7.682	726	731	738	rVB	44763	71365	2.92%	0.643%
7	7.870	756	763	771	rBV	73459	123264	5.05%	1.110%
8	8.105	793	803	808	rBV	161892	287938	11.79%	2.594%
9	8.158	808	812	819	rVB	48258	75832	3.10%	0.683%
10	9.262	993	1000	1009	rBV	286427	522836	21.40%	4.710%
11	10.913	1273	1281	1288	rBV	212270	386718	15.83%	3.484%
12	11.817	1428	1435	1446	rBV4	13797	31805	1.30%	0.287%
13	13.086	1645	1651	1657	rBV	56593	90698	3.71%	0.817%
14	13.351	1687	1696	1705	rBV	752903	1304163	53.38%	11.749%
15	13.568	1726	1733	1739	rBV	230655	347128	14.21%	3.127%
16	14.725	1923	1930	1937	rVB	352888	563381	23.06%	5.075%
17	15.524	2060	2066	2071	rVB	36743	54051	2.21%	0.487%
18	16.065	2153	2158	2167	rBV2	40776	58917	2.41%	0.531%
19	16.211	2176	2183	2197	rBV	639393	1057733	43.30%	9.529%
20	17.474	2391	2398	2404	rBV	494815	769944	31.52%	6.936%
21	18.126	2505	2509	2514	rVB2	24792	28529	1.17%	0.257%
22	20.077	2835	2841	2849	rVB	1873016	2443080	100.00%	22.009%
23	21.757	3120	3127	3137	rBV	581687	962961	39.42%	8.675%
24	25.058	3677	3689	3702	rVB2	327418	964781	39.49%	8.691%

Sum of corrected areas: 11100615

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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Misc :
ALS Vial : 17 Sample Multiplier: 2

Instrument :
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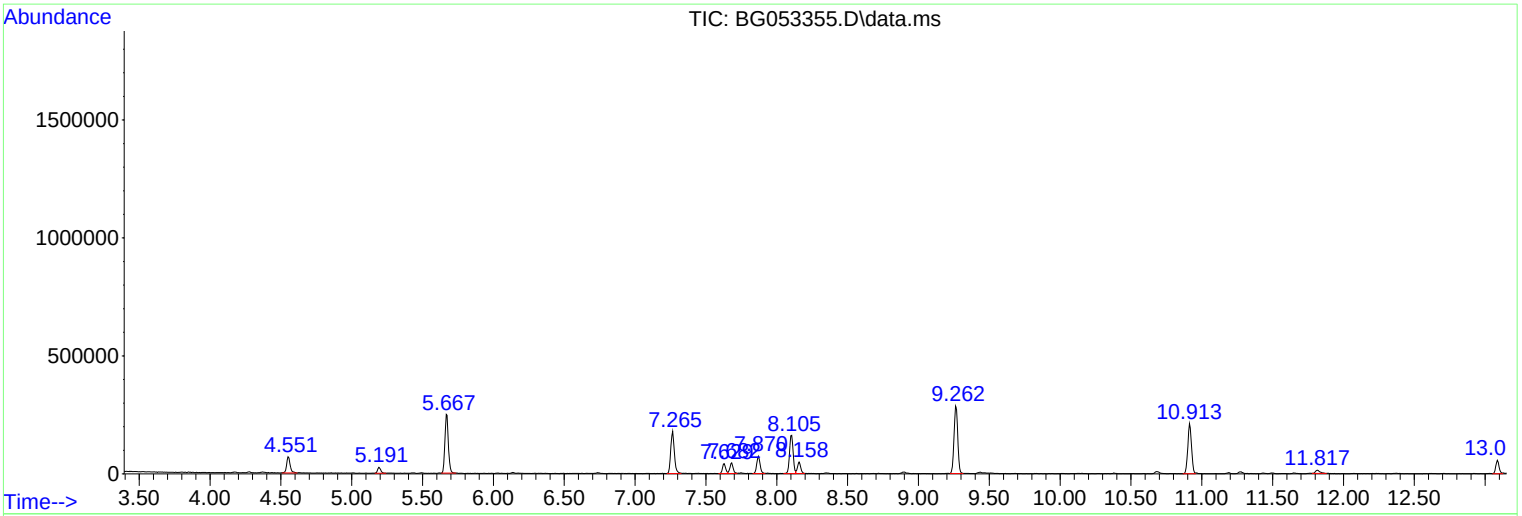
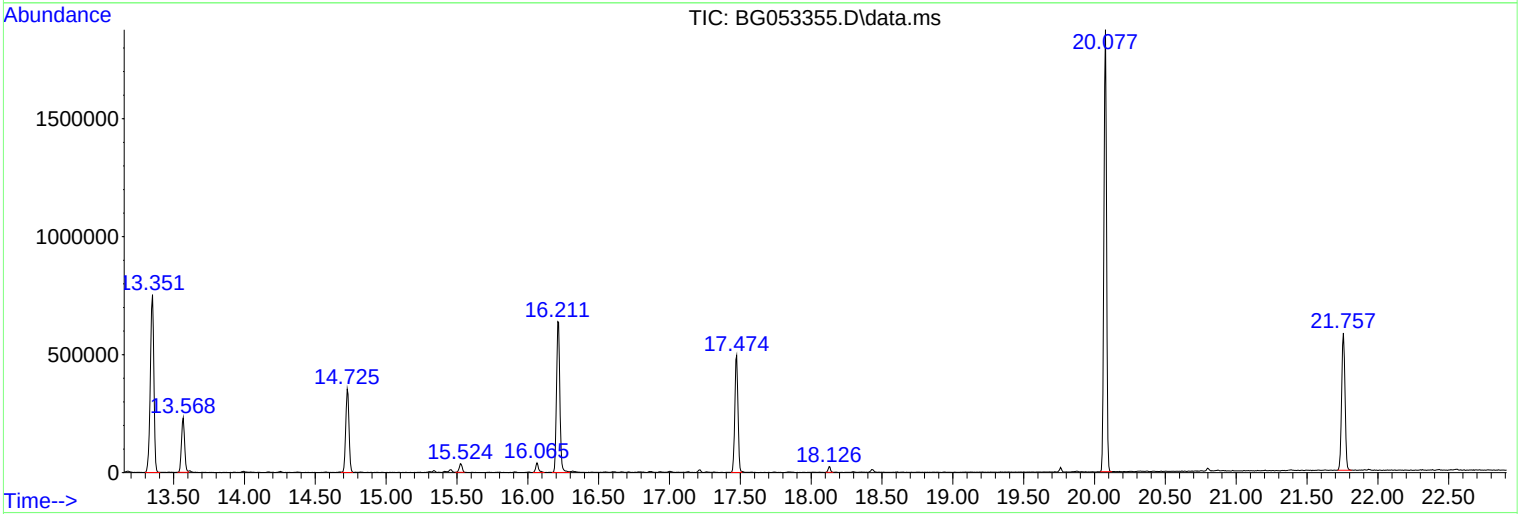
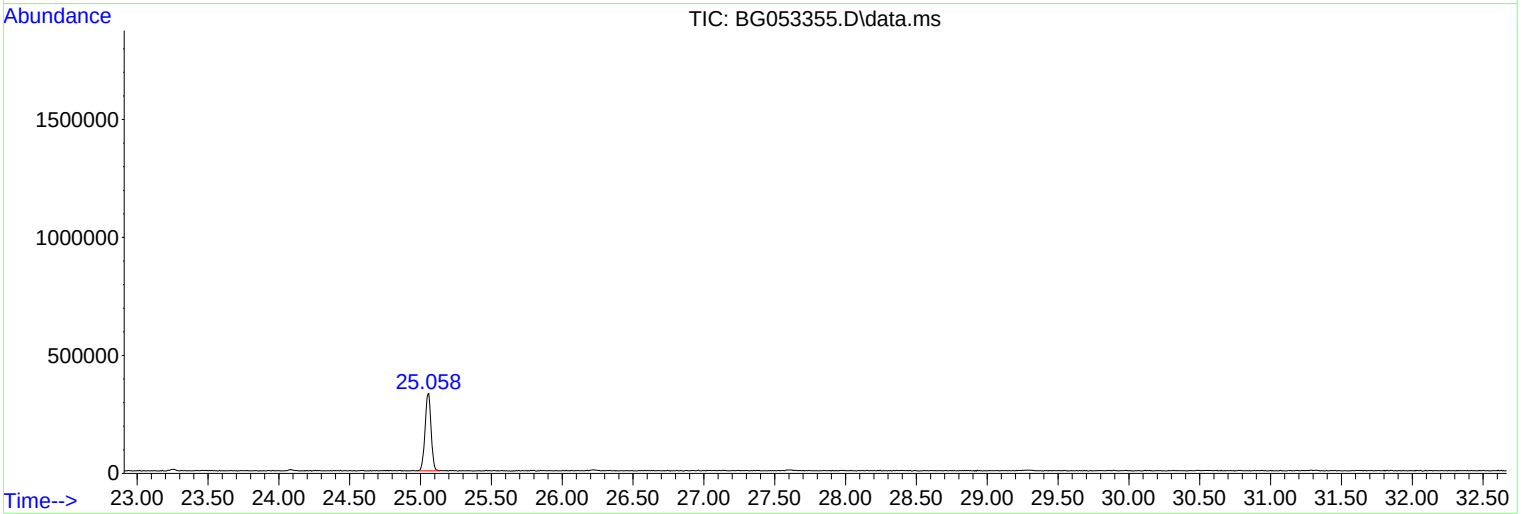
ClientSampleId :
MW-7R

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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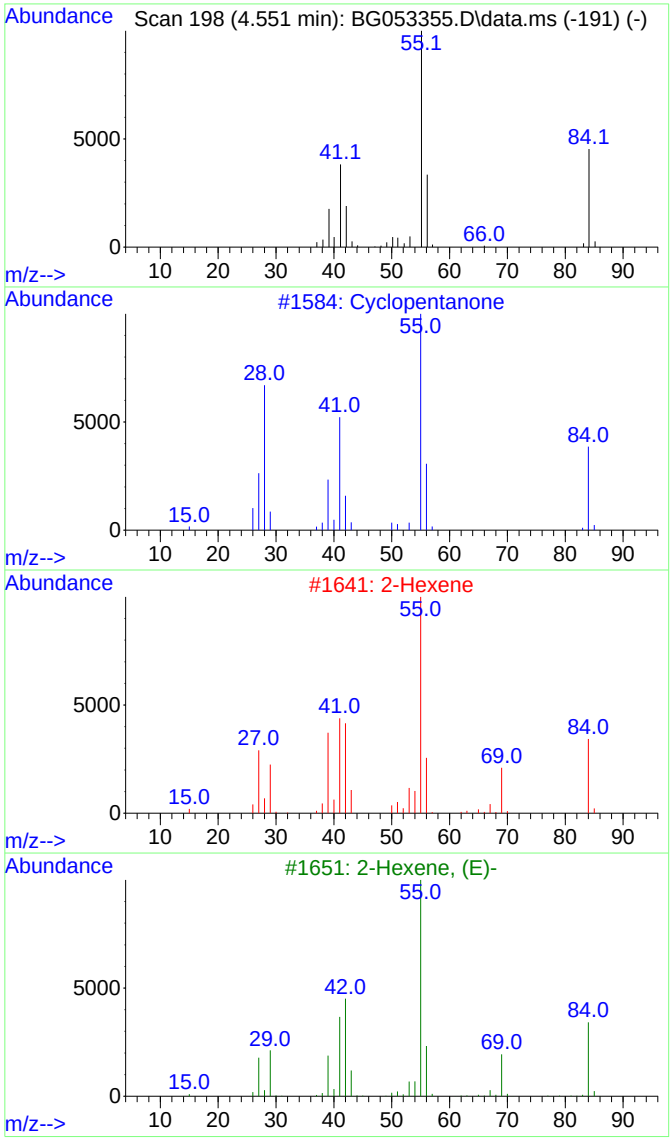
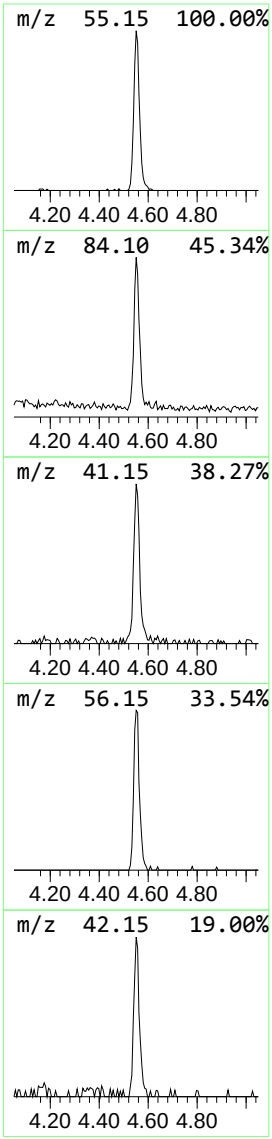
****

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.551	8.07 ng	116227	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene	84	C6H12	000592-43-8	64
3	2-Hexene, (E)-	84	C6H12	004050-45-7	64
4	2-Hexene, (Z)-	84	C6H12	007688-21-3	59
5	3-Hexene	84	C6H12	000592-47-2	59





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Data File : BG053355.D
Acq On : 28 Apr 2022 1:18
Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 17 Sample Multiplier: 2

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

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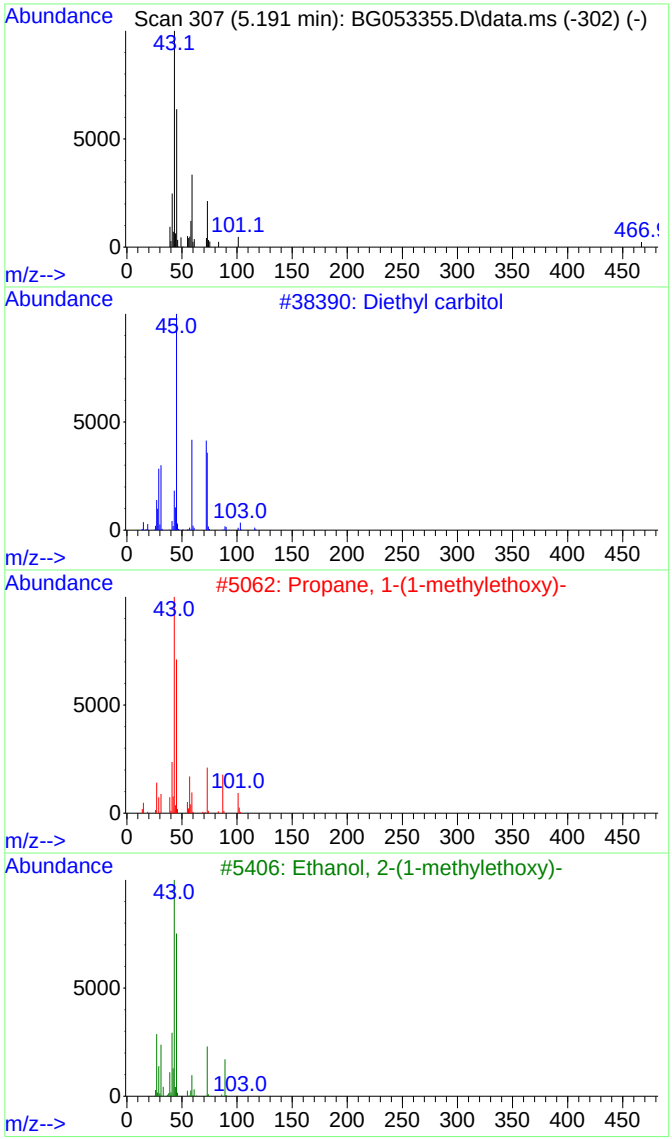
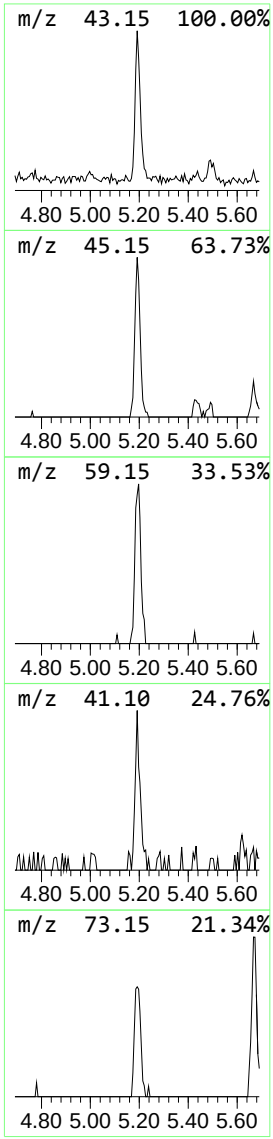
Peak Number 2 unknown5.191 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	2.68 ng	38541	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl carbitol	162	C8H18O3	000112-36-7	42
2	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40
3	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	40
4	Acetamide, 2-(2-hydroxyethoxy)-	119	C4H9NO3	000123-85-3	38
5	1-(Methoxymethoxy)-3-methyl-3-hy...	148	C7H16O3	037587-78-3	36





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Sample : N2482-03
Misc :
ALS Vial : 17 Sample Multiplier: 2

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
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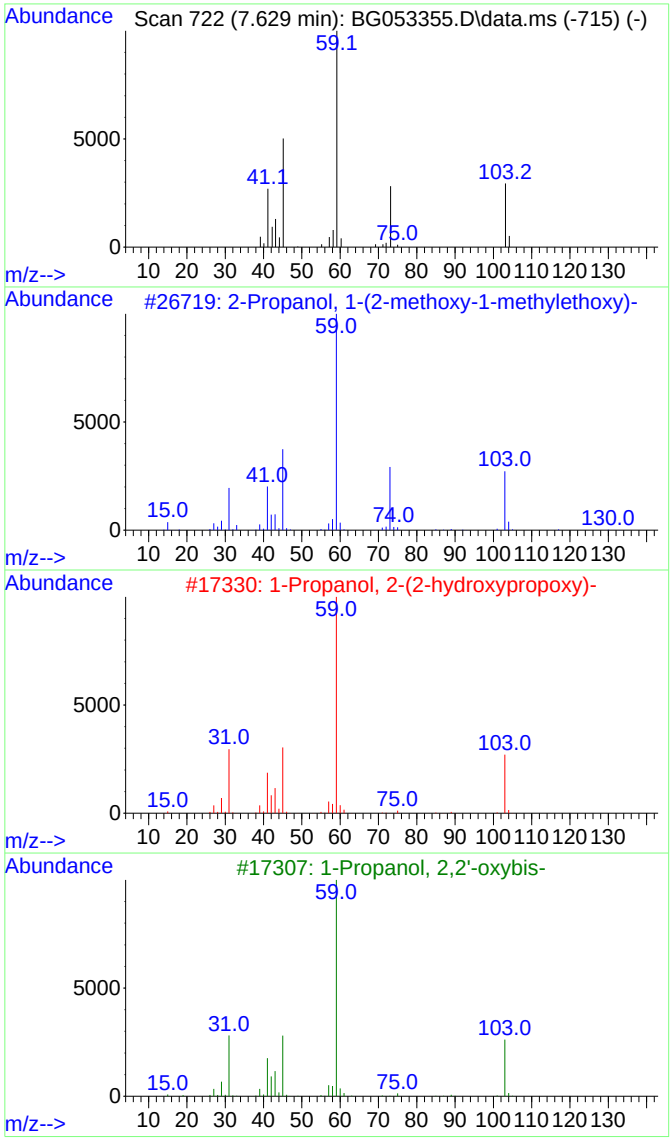
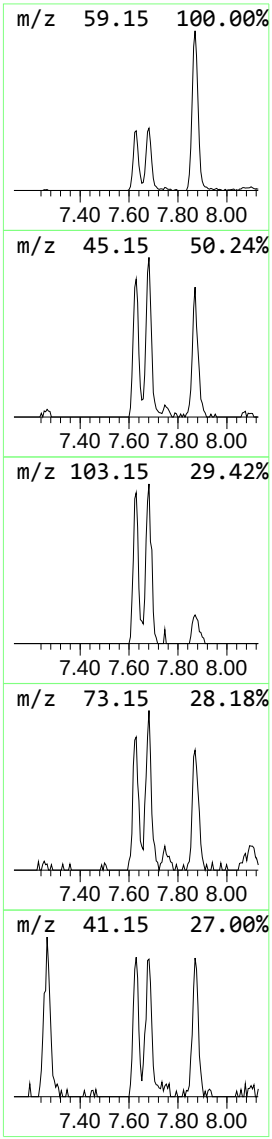
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.629	4.60 ng	66168	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	45
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	45





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Operator : CG/JU
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Misc :
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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

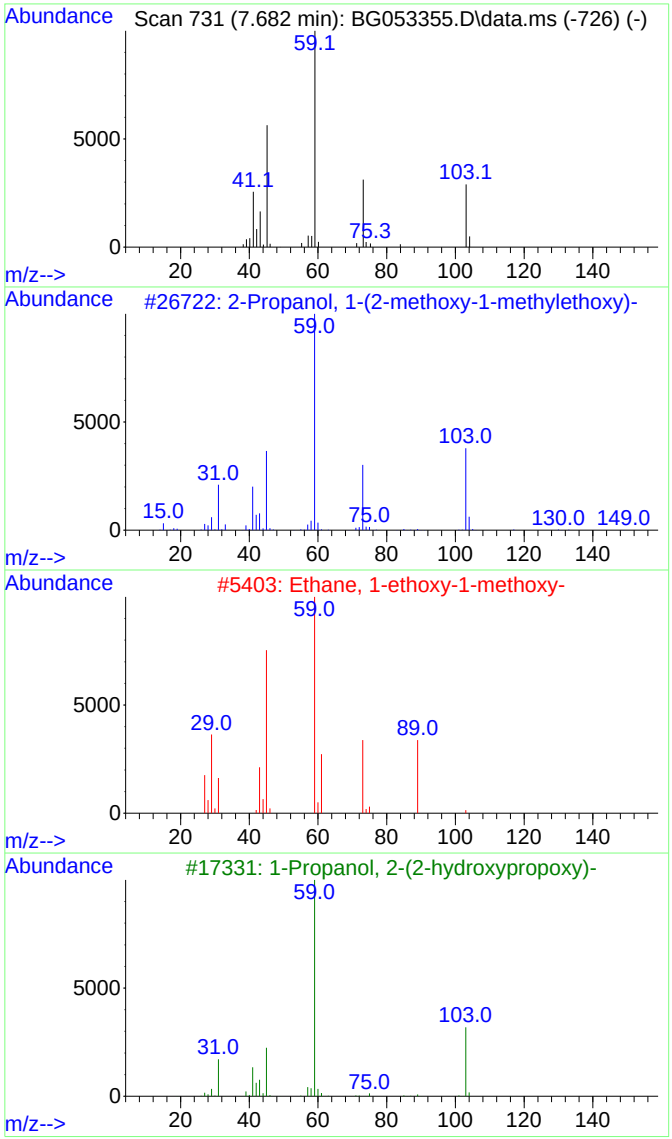
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

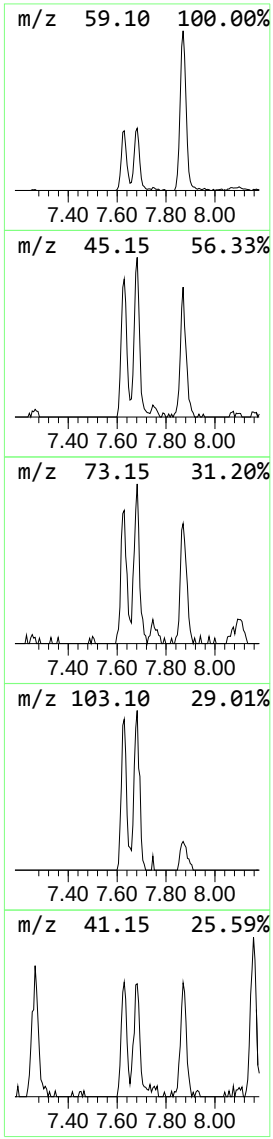
****

Peak Number 4 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.682	4.96 ng	71365	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	40
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	36





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Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 17 Sample Multiplier: 2

Instrument :
BNA_G
ClientSampleId :
MW-7R

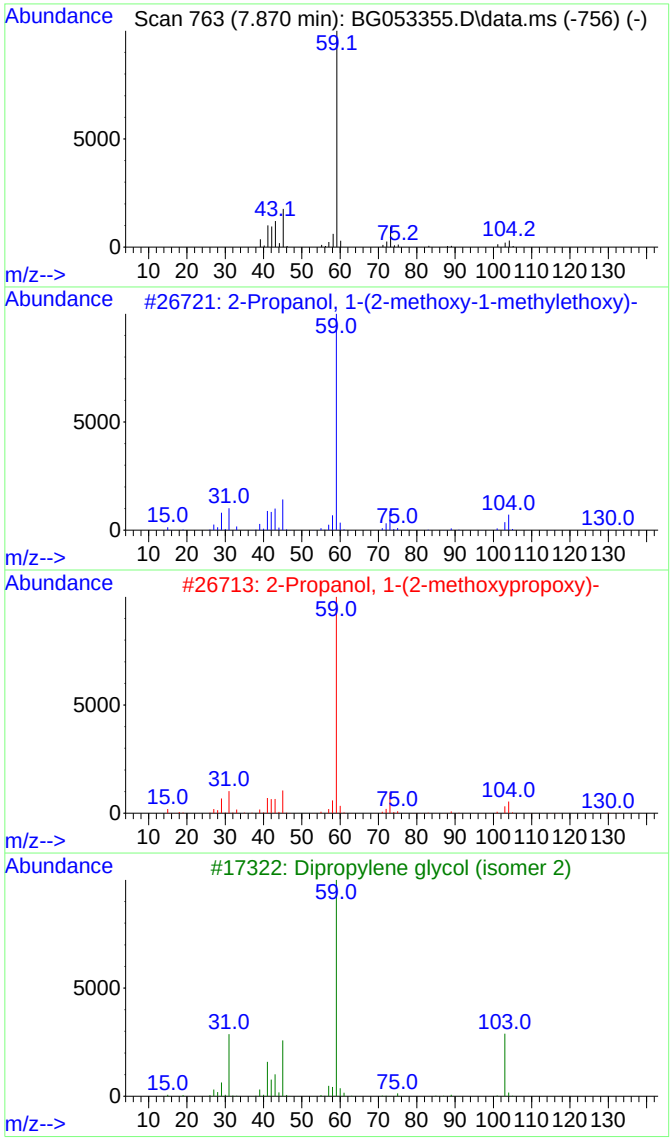
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

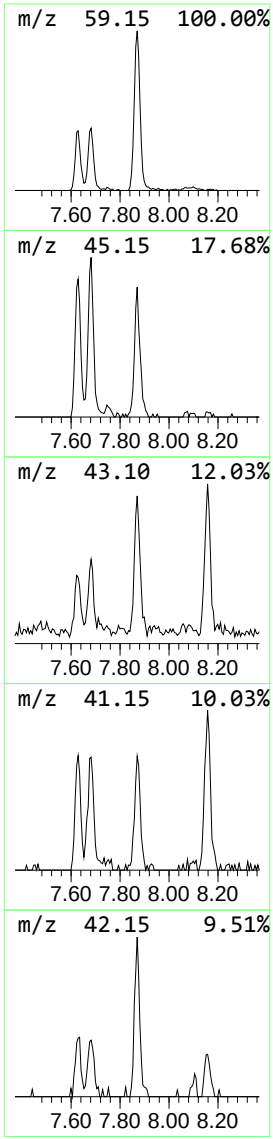
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.870	8.56 ng	123264	1,4-Dichlorobenzene-d4	8.105

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	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64





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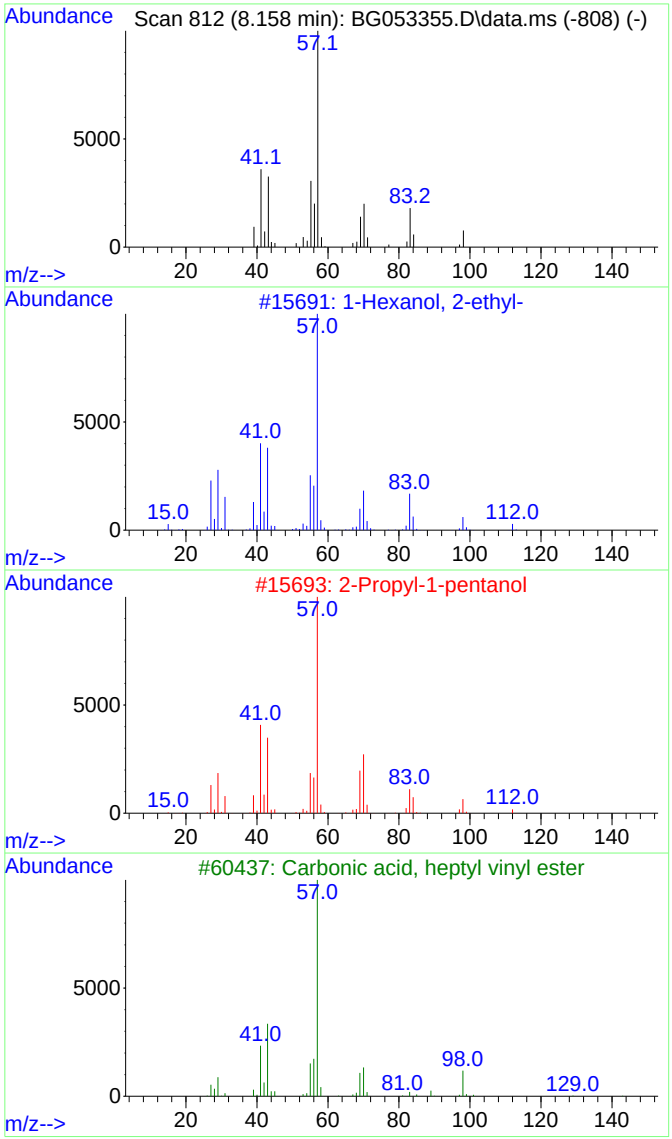
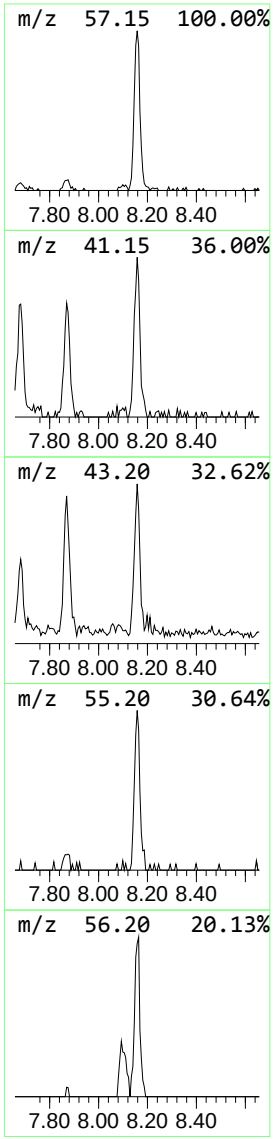
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	5.27 ng	75832	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53
4	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	38
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	38





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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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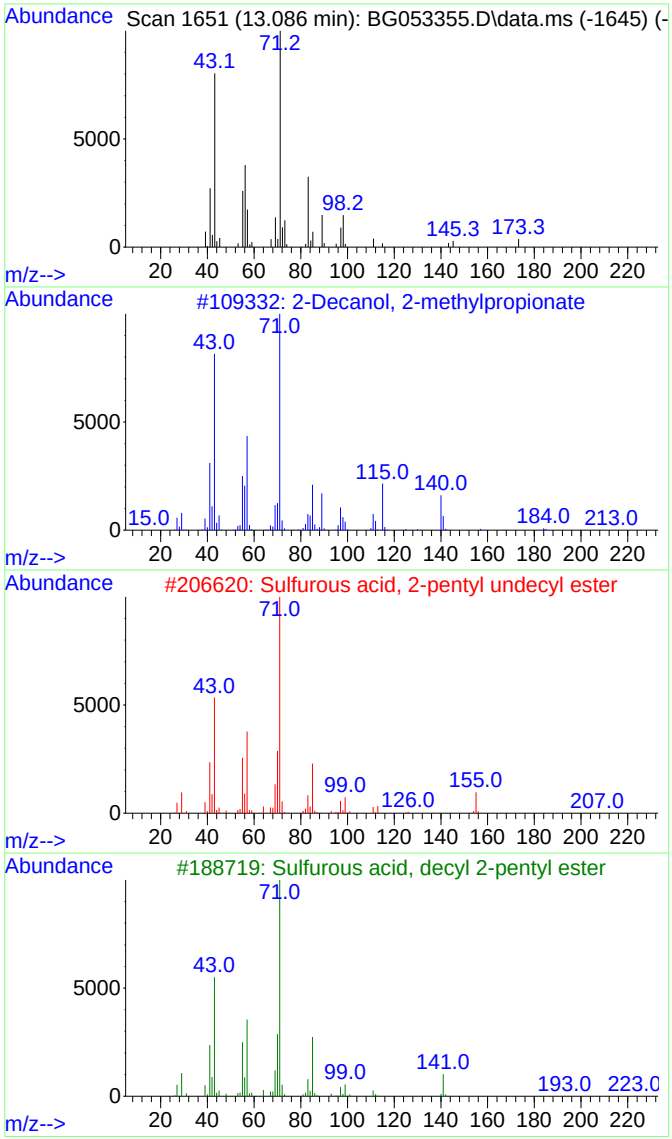
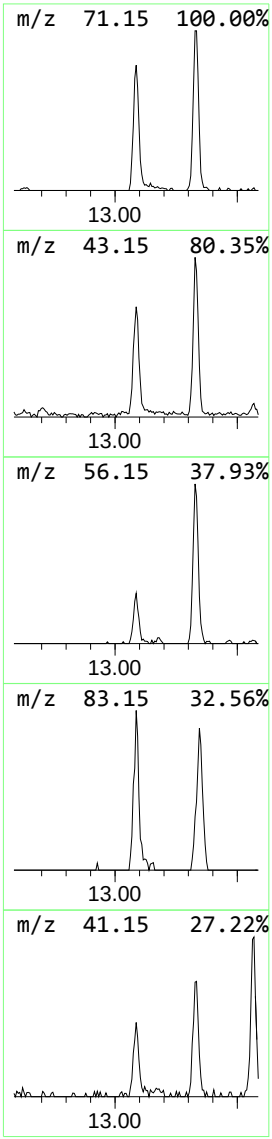
****
Peak Number 7 2-Decanol, 2-methylpropionate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	3.22 ng	90698	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decanol, 2-methylpropionate	228	C14H28O2	1000447-30-4	59
2	Sulfurous acid, 2-pentyl undecyl...	306	C16H34O3S	1000309-16-0	50
3	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	50
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
5	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	47





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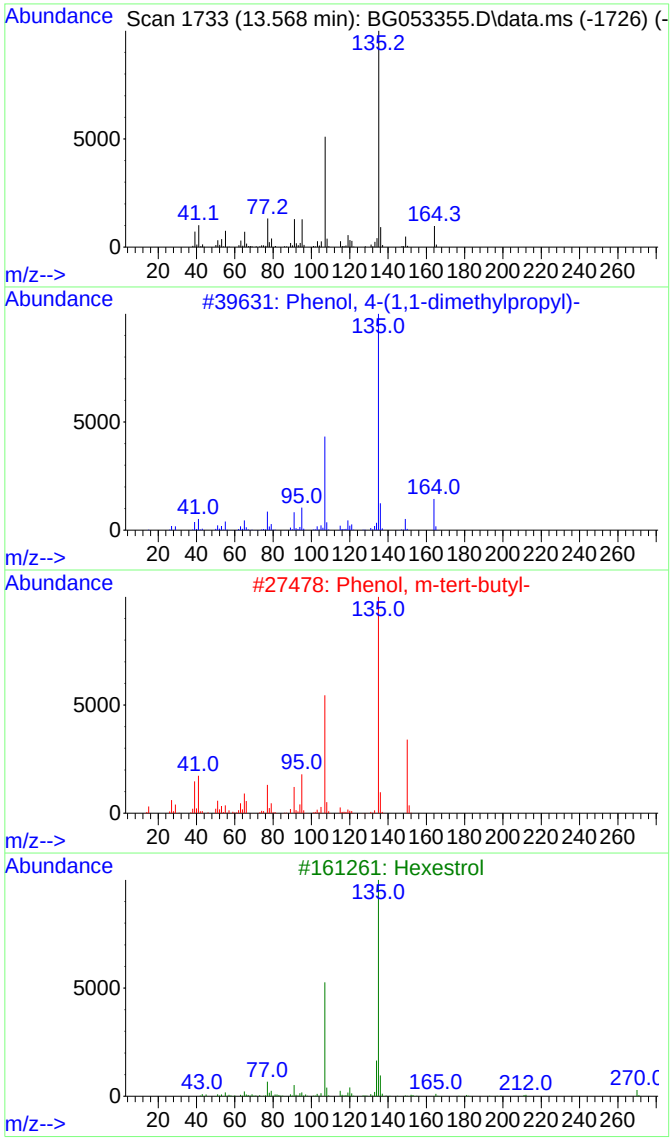
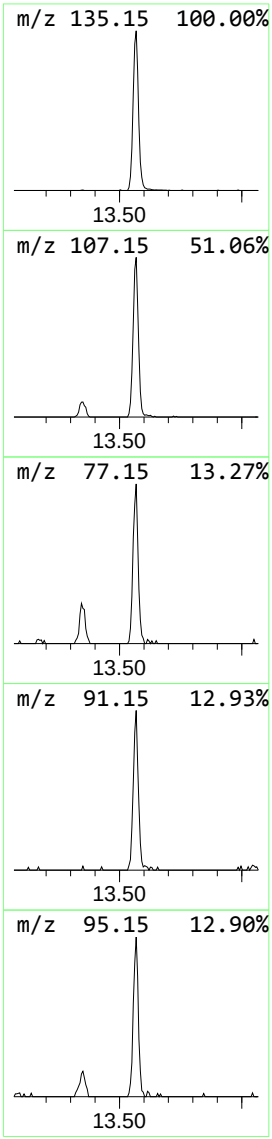
****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	12.32 ng	347128	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
3	Hexestrol	270	C18H22O2	000084-16-2	64
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64





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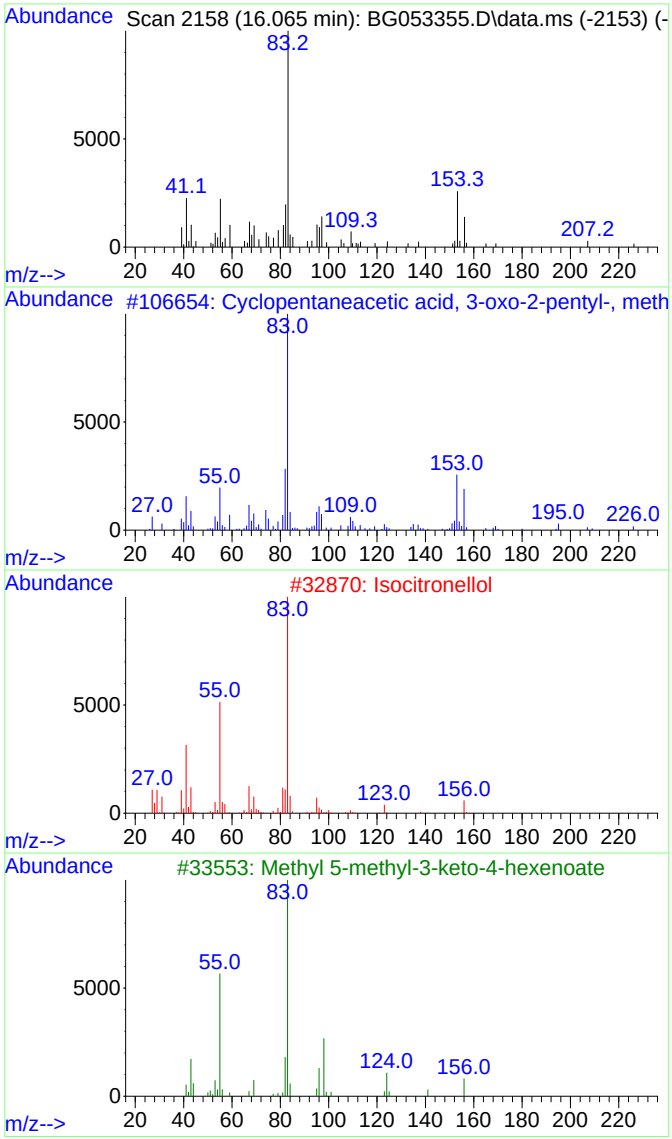
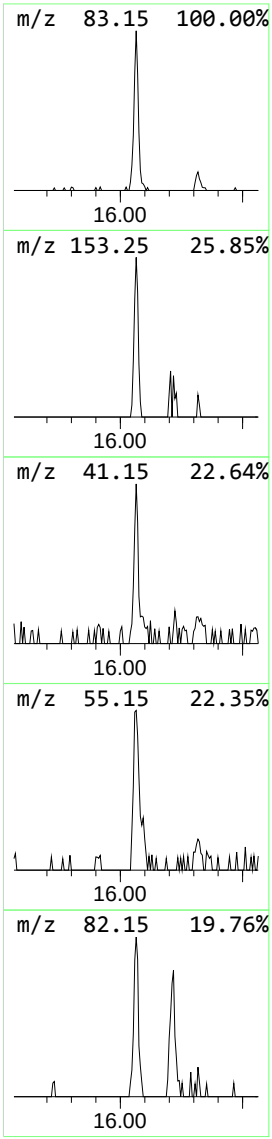
****
Peak Number 9 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.064	2.09 ng	58917	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	94
2	Isocitronellol	156	C10H20O	018479-52-2	47
3	Methyl 5-methyl-3-keto-4-hexenoate	156	C8H12O3	1000427-08-8	47
4	Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	47
5	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053355.D
Acq On : 28 Apr 2022 1:18
Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 17 Sample Multiplier: 2

Instrument :
BNA_G
ClientSampleId :
MW-7R

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	4.551	8.1	ng	116227	1	8.105	287938	20.0
unknown5.191	5.191	2.7	ng	38541	1	8.105	287938	20.0
2-Propanol, 1-(...	7.629	4.6	ng	66168	1	8.105	287938	20.0
Ethane, 1-ethox...	7.682	5.0	ng	71365	1	8.105	287938	20.0
2-Propanol, 1-(...	7.870	8.6	ng	123264	1	8.105	287938	20.0
1-Hexanol, 2-et...	8.158	5.3	ng	75832	1	8.105	287938	20.0
2-Decanol, 2-me...	13.086	3.2	ng	90698	3	14.725	563381	20.0
Phenol, 4-(1,1-...	13.568	12.3	ng	347128	3	14.725	563381	20.0
Cyclopentaneace...	16.064	2.1	ng	58917	3	14.725	563381	20.0