LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053351.D
Acq On : 27 Apr 2022 17:27
Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1R

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: BG053351.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.554	191	198	209	rBV	56026	95298	3.15%	0.865%
2	5.195	302	307	314	rVB2	20688	32848	1.09%	0.298%
3	5.671	382	388	397	rBV	285861	465651	15.40%	4.225%
4	7.262	653	659	670	rBV	177138	320398	10.60%	2.907%
5	7.633	716	722	726	rBV	27340	42749	1.41%	0.388%
6	7.680	726	730	738	rVB2	27165	43578	1.44%	0.395%
7	7.868	755	762	771	rBV	41001	72495	2.40%	0.658%
8	8.103	795	802	807	rBV	103010	177118	5.86%	1.607%
9	8.161	807	812	818	rVB	64559	106704	3.53%	0.968%
10	9.266	993	1000	1011	rBV	393260	710354	23.50%	6.445%
11	10.916	1273	1281	1287	rBV	132355	241741	8.00%	2.193%
12	13.084	1645	1650	1659	rBV	50407	86357	2.86%	0.784%
13	13.354	1685	1696	1704	rBV	1006344	1735701	57.41%	15.748%
14	13.566	1726	1732	1738	rBV	218341	331829	10.98%	3.011%
15	14.729	1923	1930	1937	rVB	213775	353667	11.70%	3.209%
16	15.528	2059	2066	2072	rVB	47722	70154	2.32%	0.637%
17	16.062	2152	2157	2168	rVB	48201	74441	2.46%	0.675%
18	16.215	2176	2183	2197	rBV	858559	1391924	46.04%	12.629%
19	17.472	2390	2397	2403	rBV	305205	466487	15.43%	4.232%
20	18.130	2503	2509	2514	rBV	40610	51715	1.71%	0.469%
21	20.075	2834	2840	2846	rBV	2204655	3023342	100.00%	27.431%
22	21.755	3119	3126	3135	rBV2	326866	562349	18.60%	5.102%
23	25.050	3676	3687	3698	rBV2	187043	564788	18.68%	5.124%

Sum of corrected areas: 11021688

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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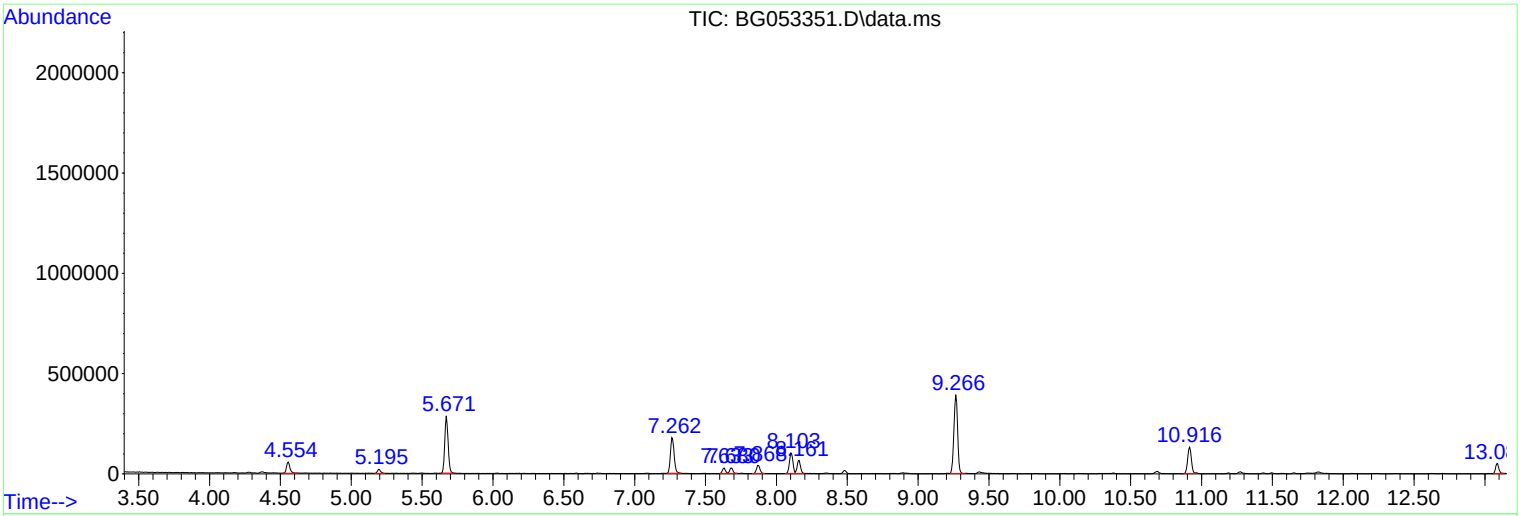
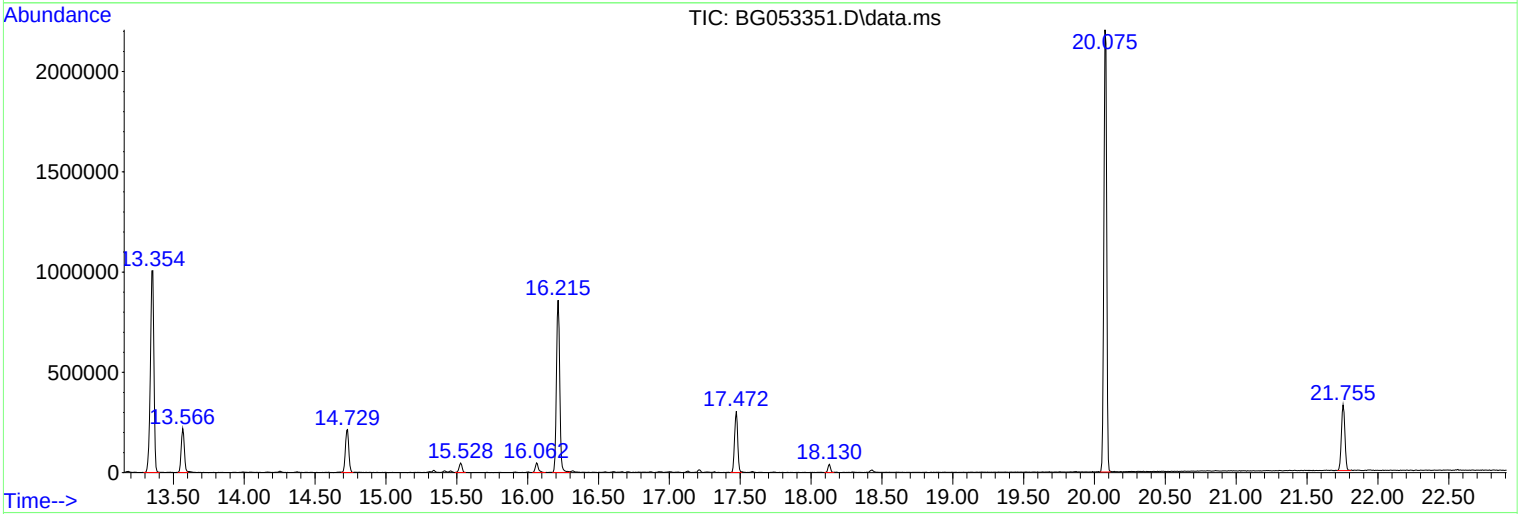
Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

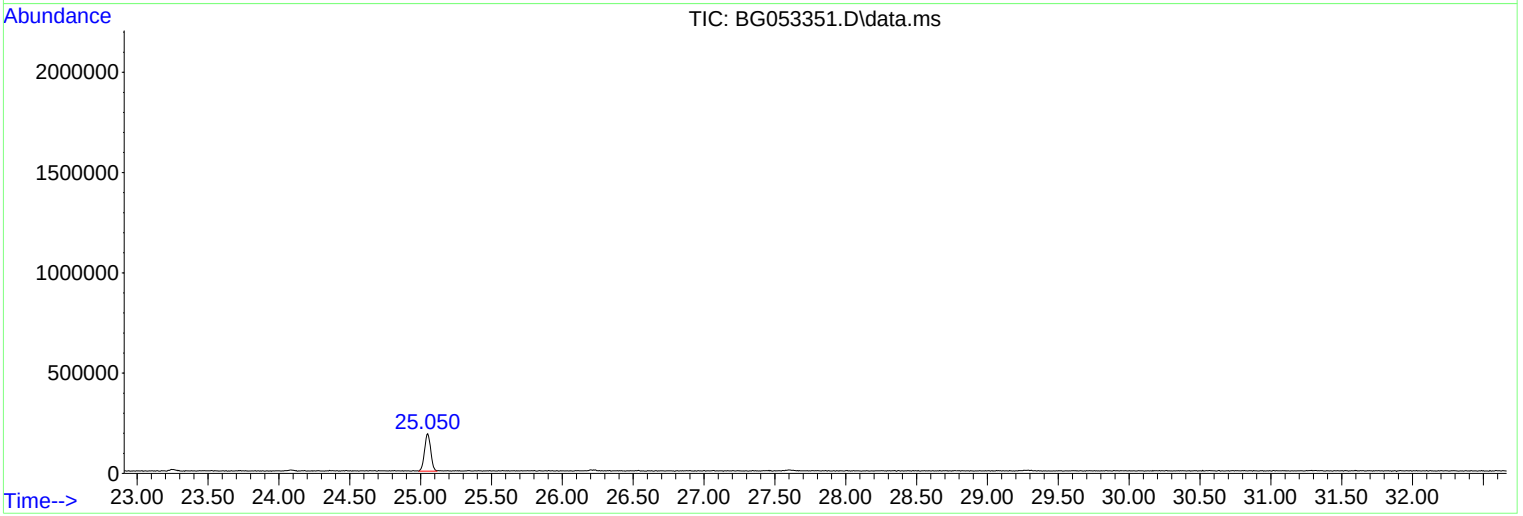
Instrument :
BNA_G
ClientSampleId :
MW-1R

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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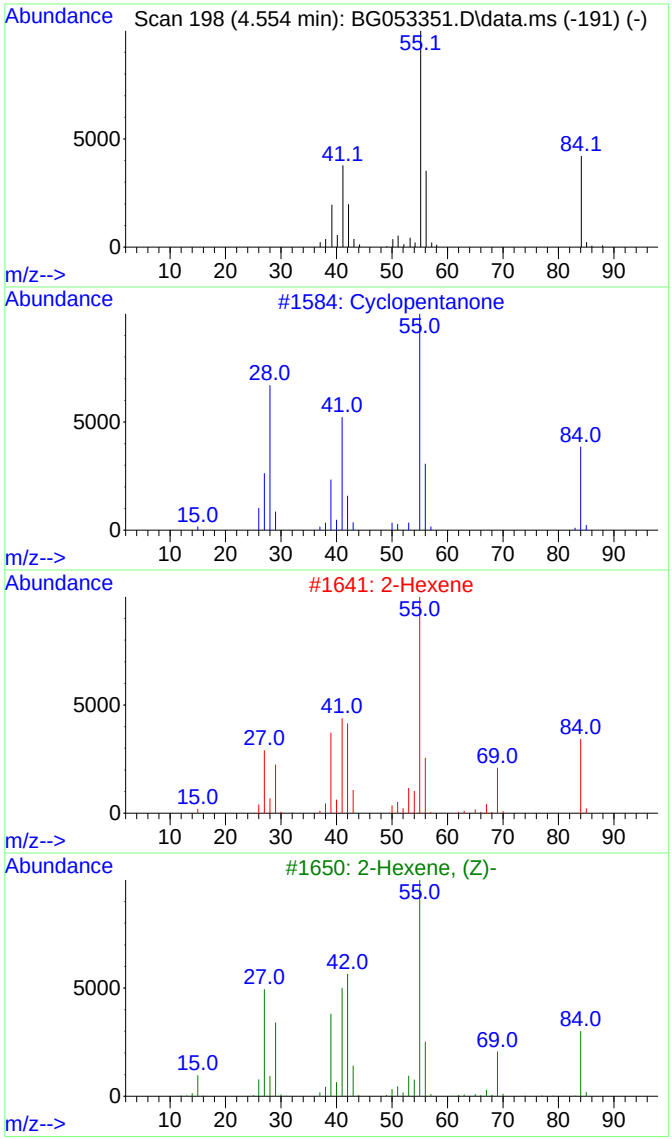
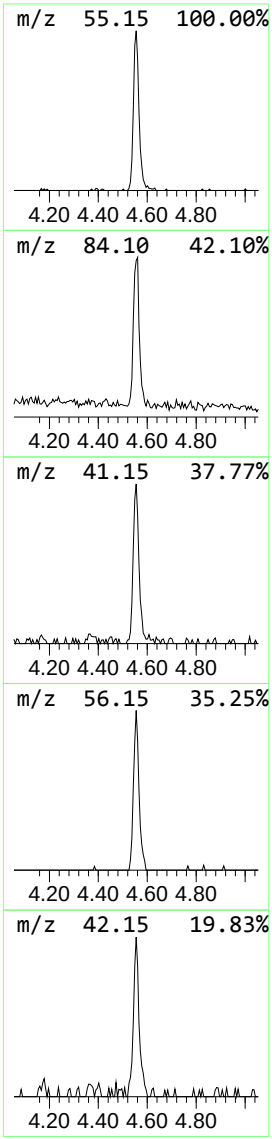
****

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.554	10.76 ng	95298	1,4-Dichlorobenzene-d4	8.103

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	59
3	2-Hexene, (Z)-	84	C6H12	007688-21-3	53
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	53
5	1H-Tetrazole, 1-methyl-	84	C2H4N4	016681-77-9	53





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Data File : BG053351.D
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Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 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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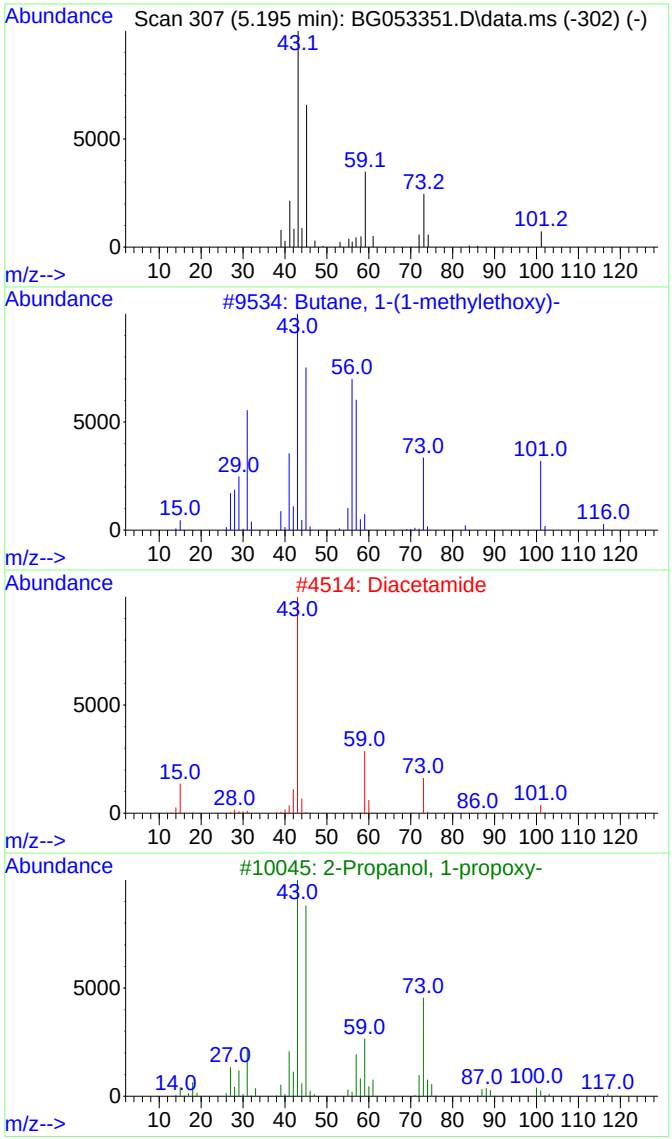
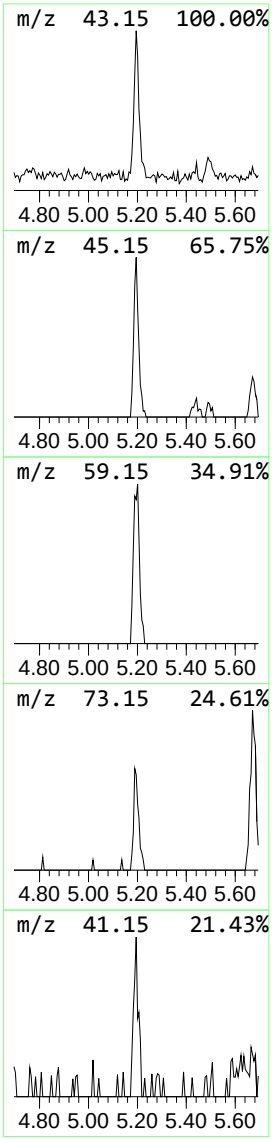
****

Peak Number 2 unknown5.195 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.195	3.71 ng	32848	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	42
2	Diacetamide	101	C4H7NO2	000625-77-4	38
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	36
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	33
5	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	32





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Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1R

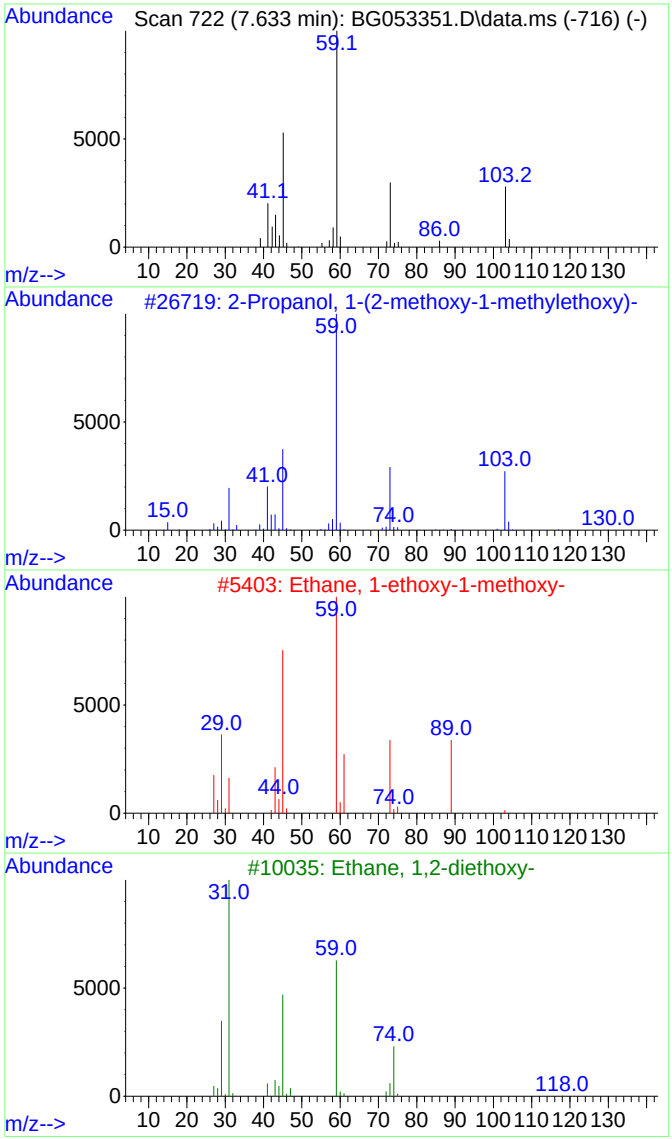
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

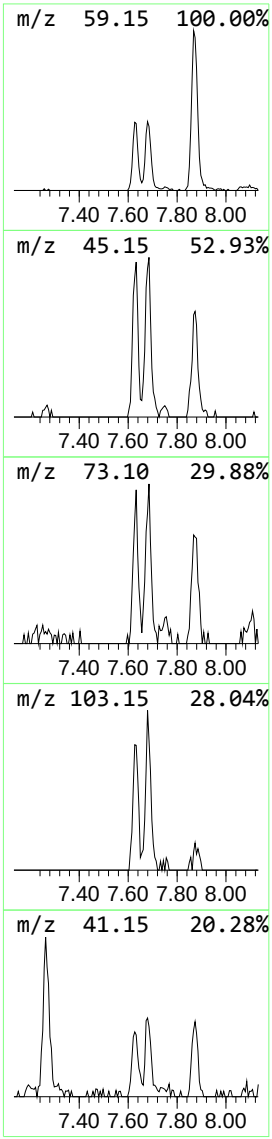
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.633	4.83 ng	42749	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	50
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	49
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	45





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Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1R

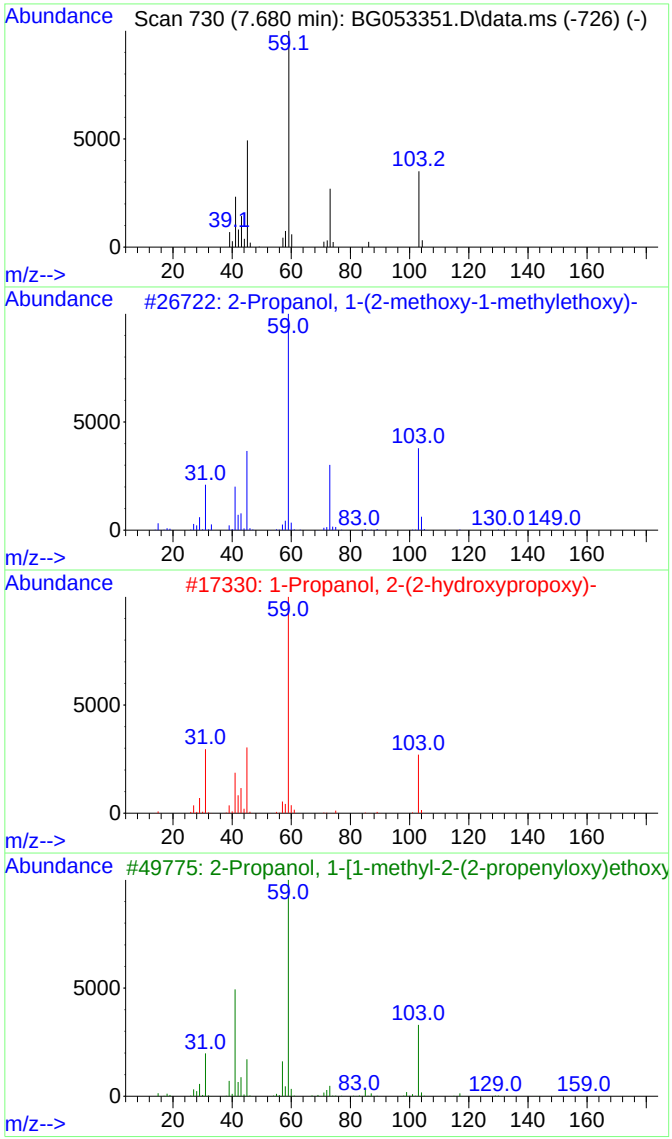
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

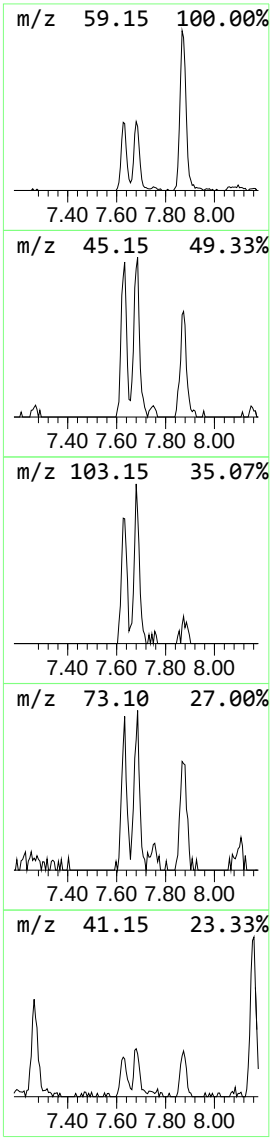
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.680	4.92 ng	43578	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	56
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	53
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	52
5	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1R

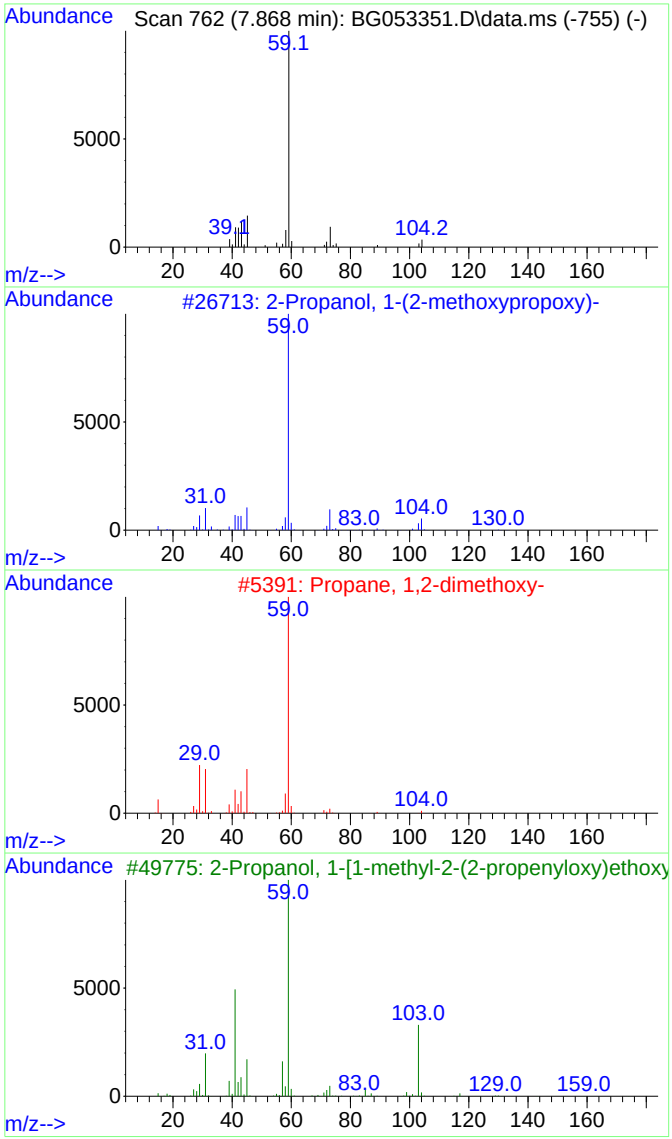
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

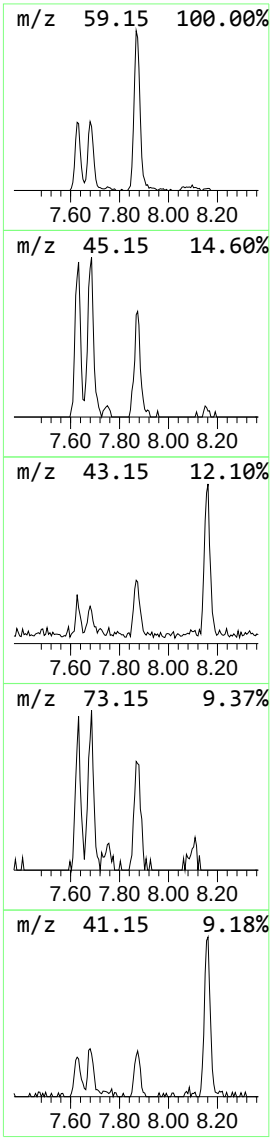
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.868	8.19 ng	72495	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	Propane, 1,2-dimethoxy-	104	C5H12O2	007778-85-0	45
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43
4	1-(1-Methoxypropan-2-yloxy)propa...	190	C9H18O4	1000367-08-6	39
5	Propane, 2-methoxy-	74	C4H10O	000598-53-8	39





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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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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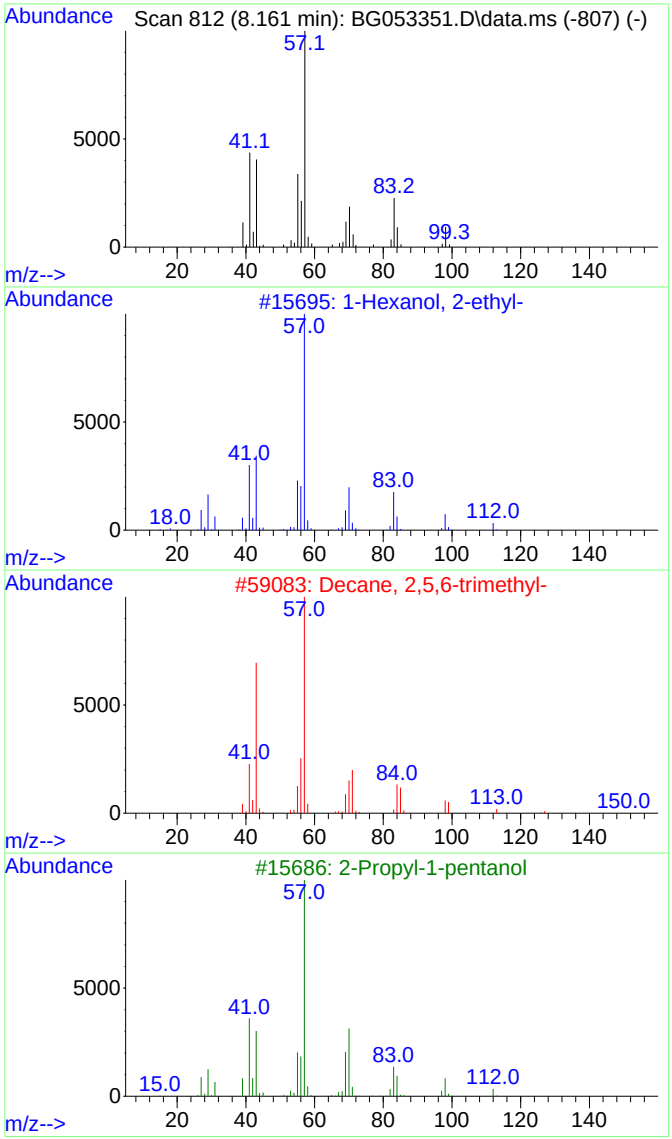
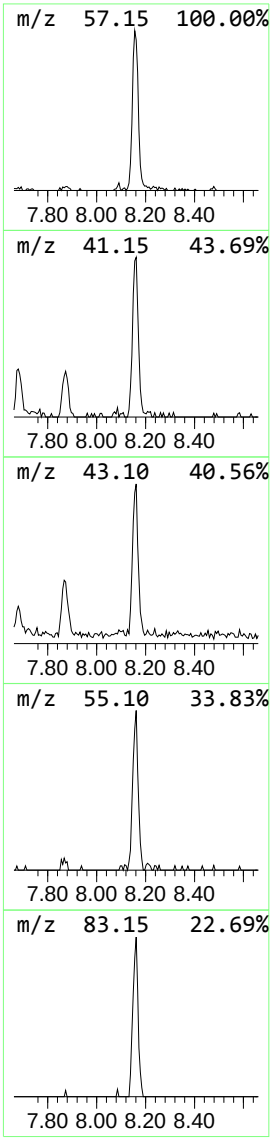
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	12.05 ng	106704	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	50
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	50
5	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	47





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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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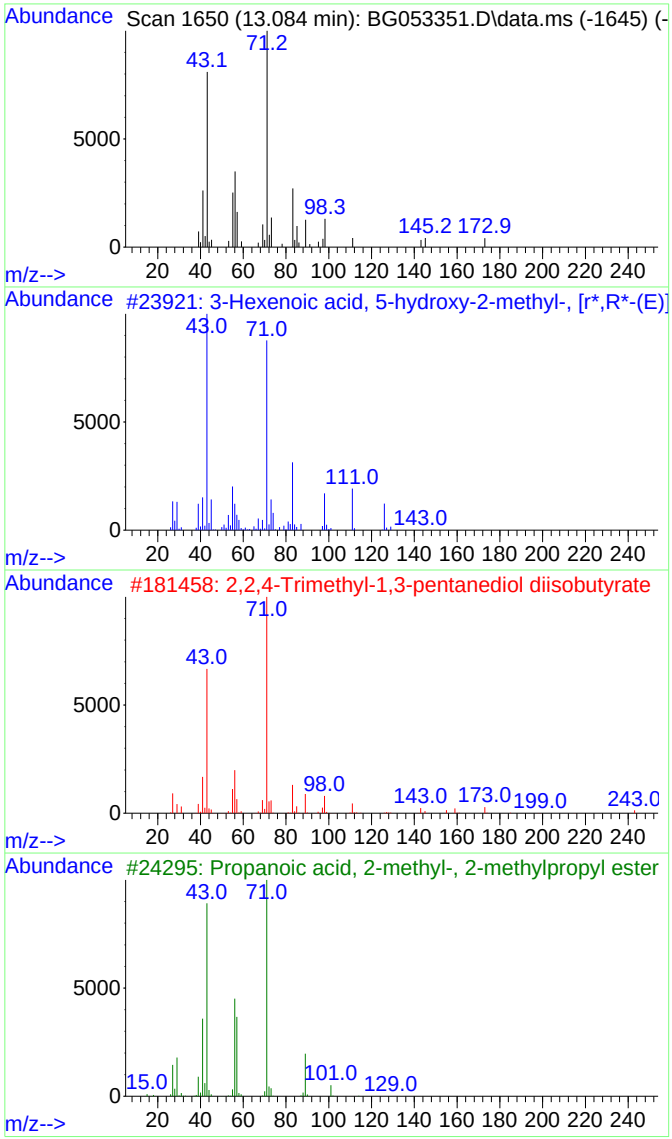
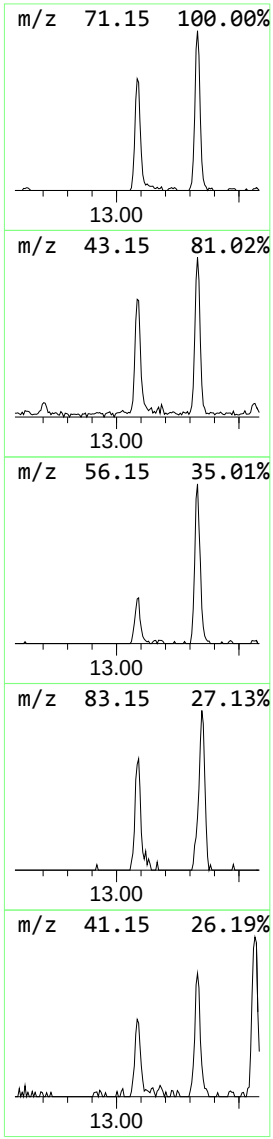
****
Peak Number 7 3-Hexenoic acid, 5-hydroxy-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.084	4.88 ng	86357	Acenaphthene-d10	14.729

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	59
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	59
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
4	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50
5	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	40





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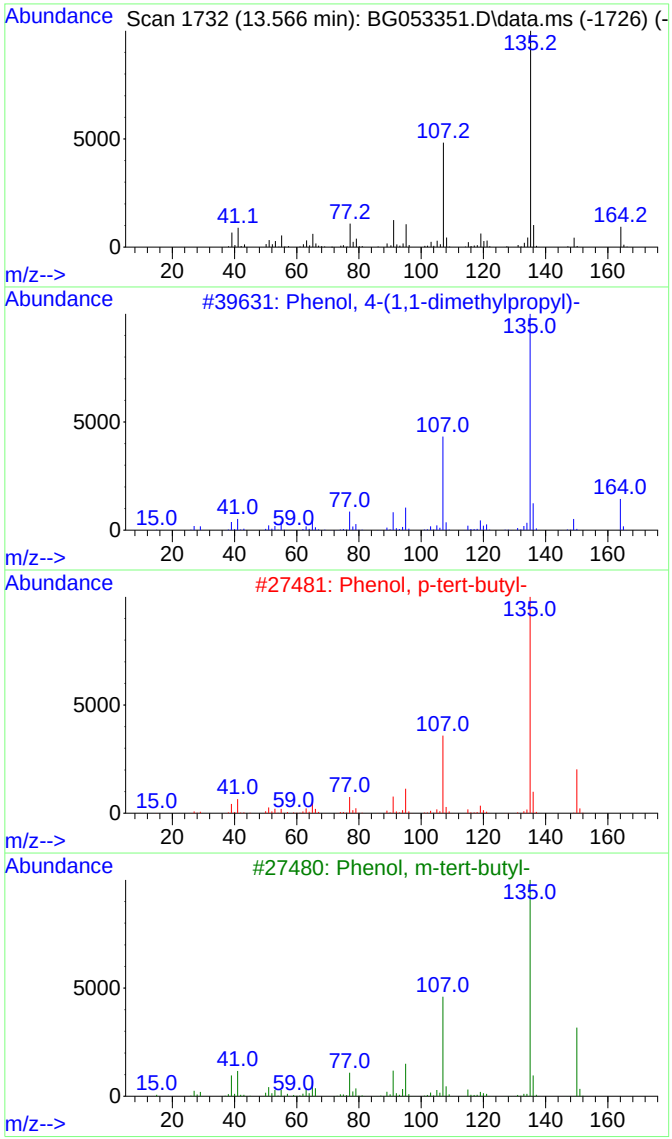
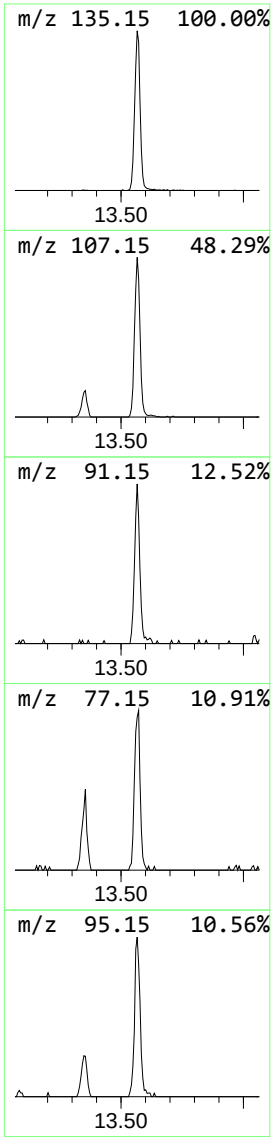
****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.566	18.77 ng	331829	Acenaphthene-d10	14.729

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
4	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64
5	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64





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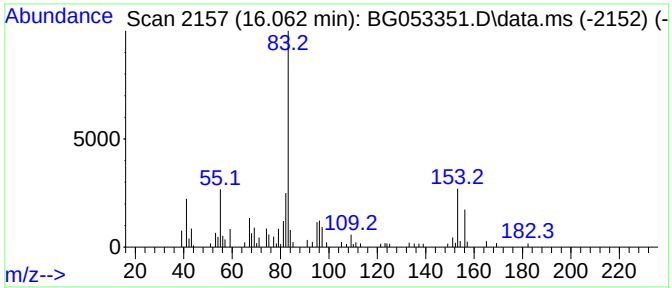
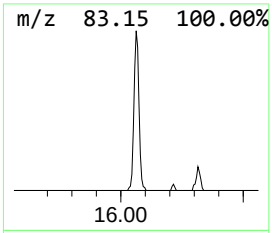
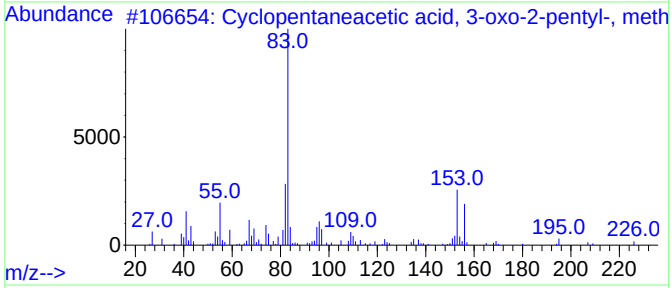
****
Peak Number 9 Cyclopentaneacetic acid, 3-... Concentration Rank 8

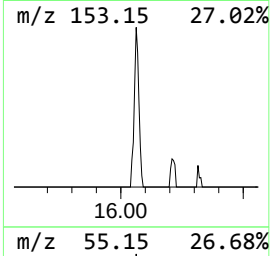
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.062	4.21 ng	74441	Acenaphthene-d10	14.729

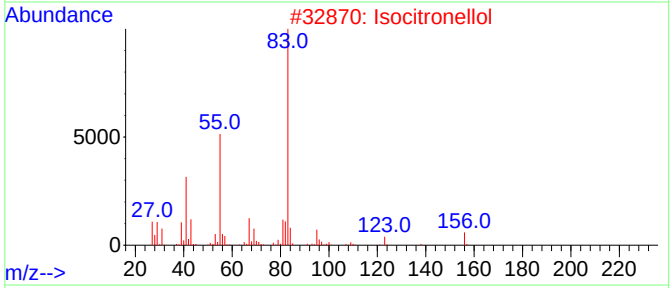
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	90
2	Isocitronellol	156	C10H20O	018479-52-2	53
3	Methyl 5-methyl-3-keto-4-hexenoate	156	C8H12O3	1000427-08-8	50
4	Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	47
5	N-(Piperidin-3-yl)acetamide	142	C7H14N2O	005810-55-9	47

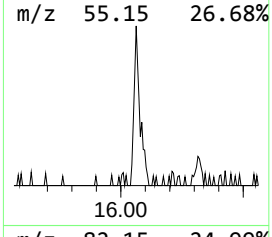


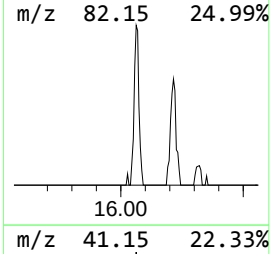


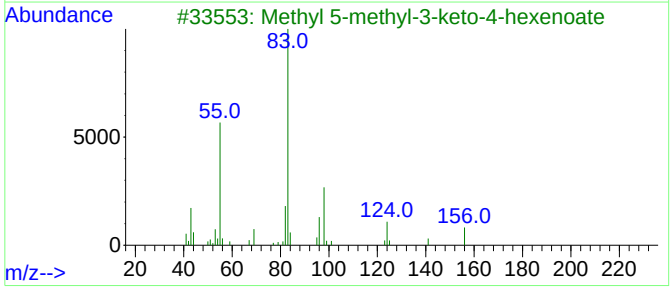


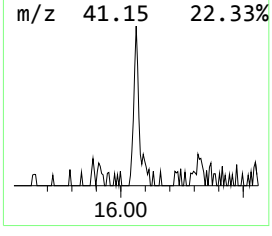












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053351.D
Acq On : 27 Apr 2022 17:27
Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1R

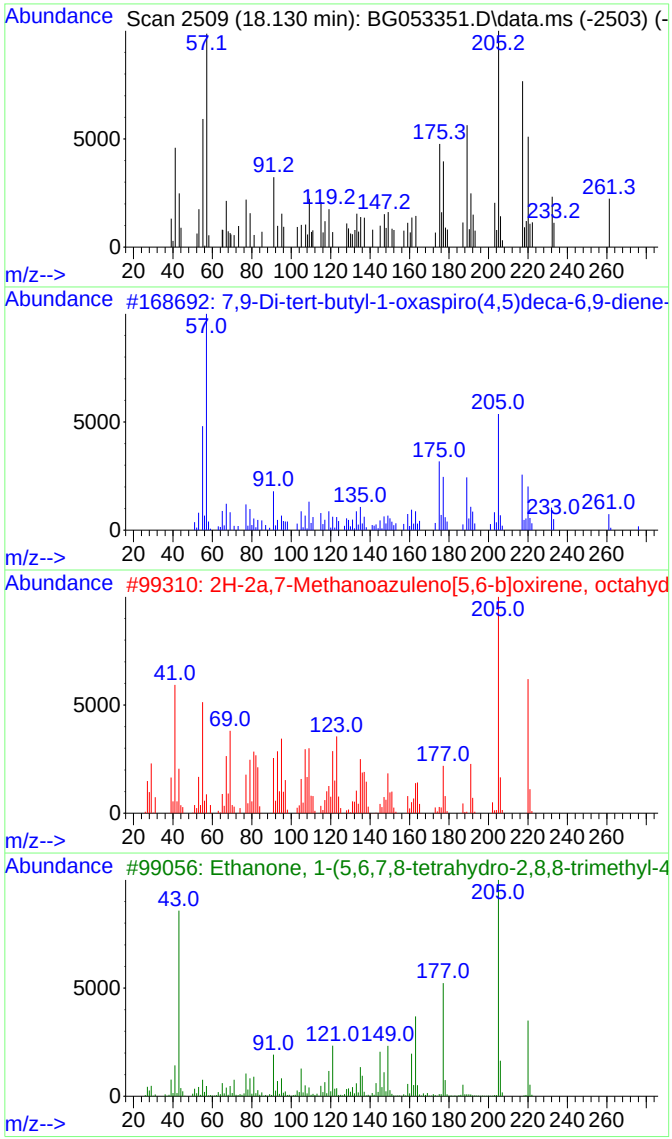
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

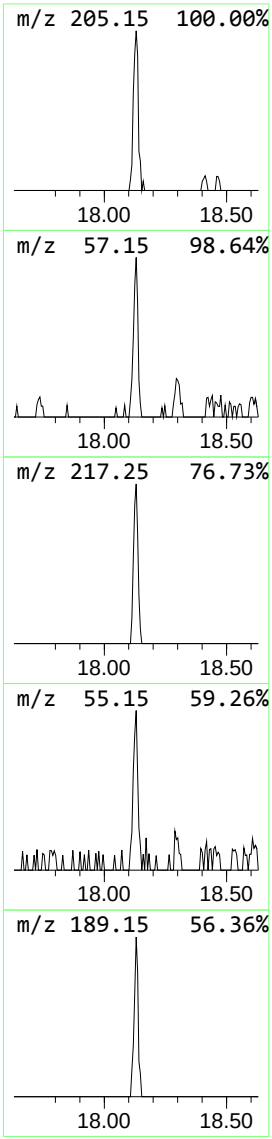
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.130	2.22 ng	51715	Phenanthrene-d10	17.472

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2	2H-2a,7-Methanoazuleno[5,6-b]oxi...	220	C15H24O	029597-36-2	47
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	42
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	41
5	Phenanthrene, 2,3,5-trimethyl-	220	C17H16	003674-73-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053351.D
Acq On : 27 Apr 2022 17:27
Operator : CG/JU
Sample : N2481-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1R

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	4.554	10.8	ng	95298	1	8.103	177118	20.0
unknown5.195	5.195	3.7	ng	32848	1	8.103	177118	20.0
2-Propanol, 1-(...	7.633	4.8	ng	42749	1	8.103	177118	20.0
1-Propanol, 2-(...	7.680	4.9	ng	43578	1	8.103	177118	20.0
2-Propanol, 1-(...	7.868	8.2	ng	72495	1	8.103	177118	20.0
1-Hexanol, 2-et...	8.161	12.1	ng	106704	1	8.103	177118	20.0
3-Hexenoic acid...	13.084	4.9	ng	86357	3	14.729	353667	20.0
Phenol, 4-(1,1-...	13.566	18.8	ng	331829	3	14.729	353667	20.0
Cyclopentaneace...	16.062	4.2	ng	74441	3	14.729	353667	20.0
7,9-Di-tert-but...	18.130	2.2	ng	51715	4	17.472	466487	20.0