LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053349.D
Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

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: BG053349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.557	193	199	206	rBV	49390	84622	2.93%	0.823%
2	5.191	303	307	313	rBV2	18930	29825	1.03%	0.290%
3	5.673	382	389	398	rBV	252336	423573	14.66%	4.117%
4	7.265	653	660	670	rBV	162072	290534	10.05%	2.824%
5	7.629	715	722	727	rBV2	29404	48706	1.69%	0.473%
6	7.682	727	731	738	rVB	30594	46763	1.62%	0.455%
7	7.870	758	763	774	rBV	44459	78644	2.72%	0.764%
8	8.105	793	803	808	rBV	95158	166750	5.77%	1.621%
9	8.158	808	812	822	rVB	52021	83760	2.90%	0.814%
10	9.268	993	1001	1010	rVB	355915	652693	22.58%	6.344%
11	10.913	1273	1281	1288	rBV	122487	219265	7.59%	2.131%
12	13.086	1645	1651	1662	rBV2	57596	93800	3.25%	0.912%
13	13.351	1686	1696	1707	rBV	952593	1617522	55.96%	15.722%
14	13.568	1726	1733	1739	rBV	159766	251201	8.69%	2.442%
15	14.725	1924	1930	1937	rVB	202445	319275	11.05%	3.103%
16	15.524	2060	2066	2071	rVB	35963	53394	1.85%	0.519%
17	16.065	2152	2158	2167	rBV	36071	52144	1.80%	0.507%
18	16.217	2177	2184	2197	rBV	820898	1307449	45.24%	12.709%
19	17.469	2391	2397	2404	rBV	292230	442052	15.29%	4.297%
20	18.127	2504	2509	2516	rVB2	45690	55816	1.93%	0.543%
21	20.077	2834	2841	2847	rBV	2194577	2890245	100.00%	28.093%
22	21.751	3119	3126	3136	rBV2	308127	539032	18.65%	5.239%
23	25.047	3677	3687	3701	rVB2	188357	540897	18.71%	5.258%

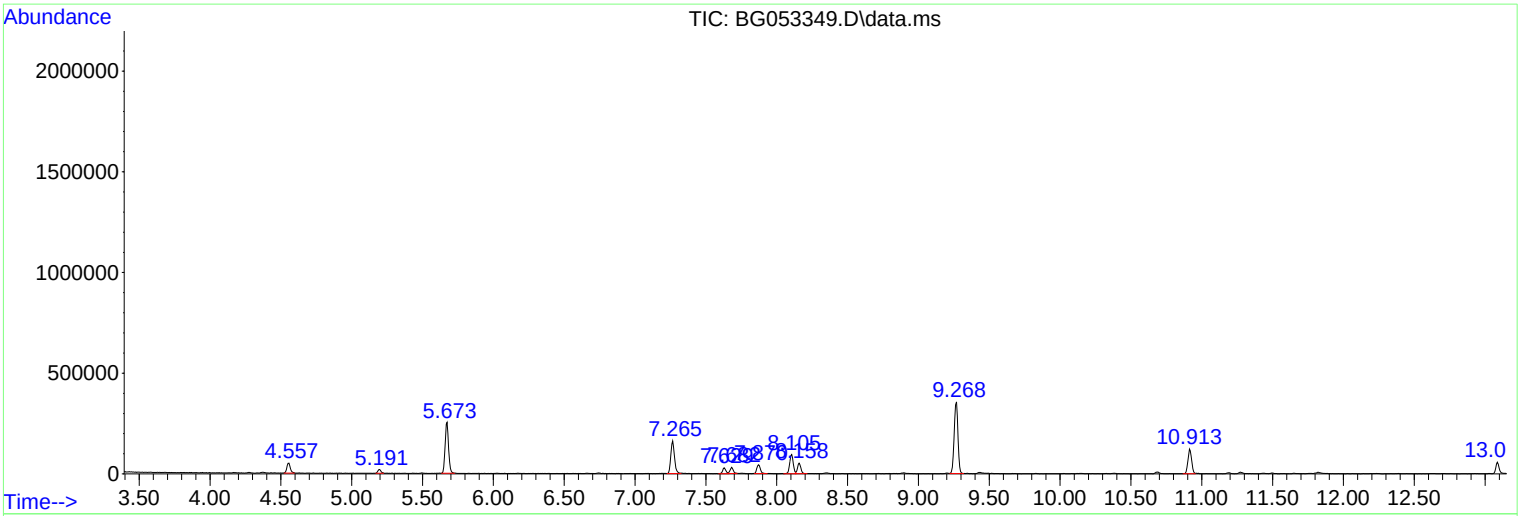
Sum of corrected areas: 10287962

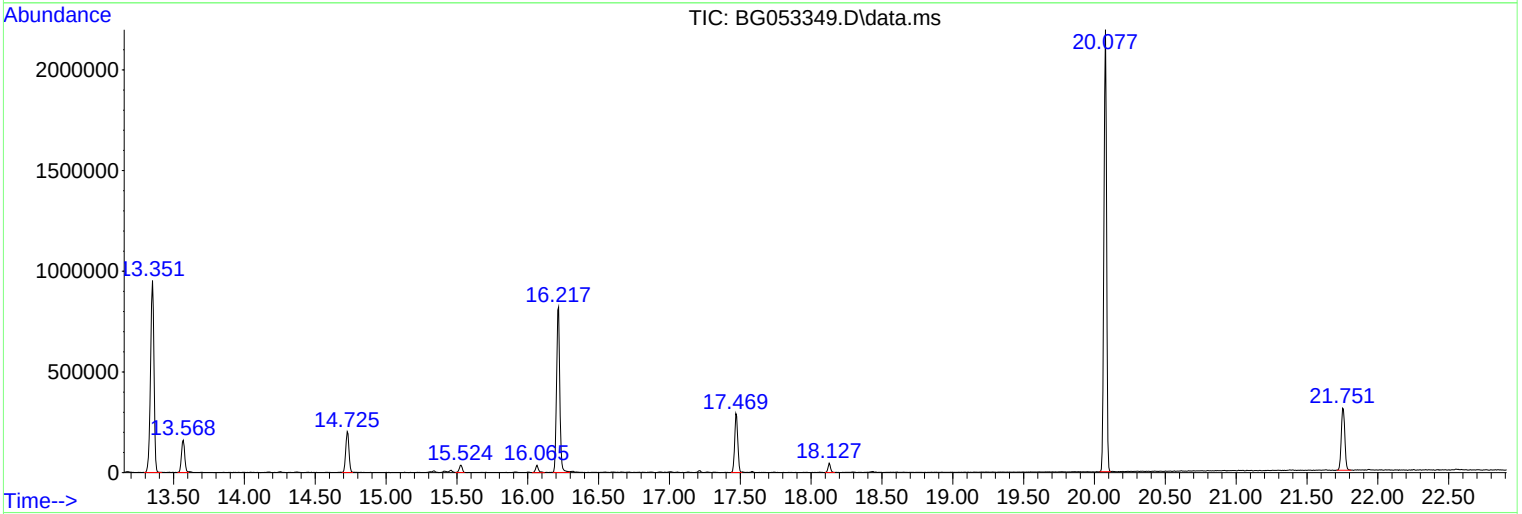
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053349.D
Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

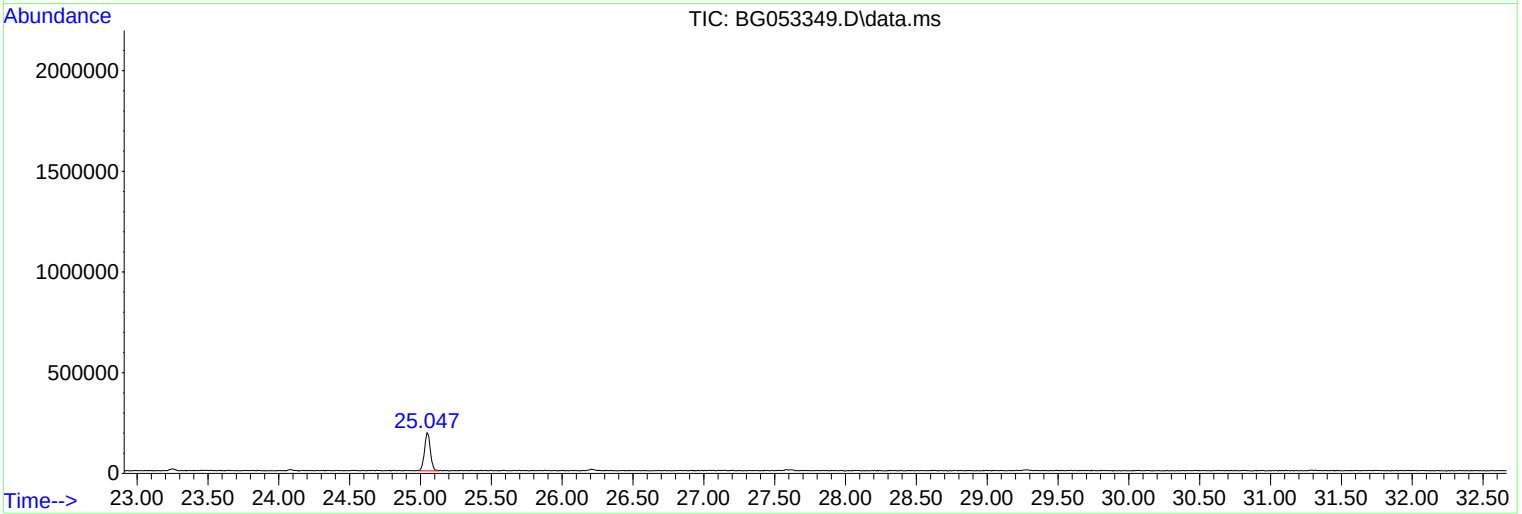
Instrument :
BNA_G
ClientSampleId :
MW-26R

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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Data File : BG053349.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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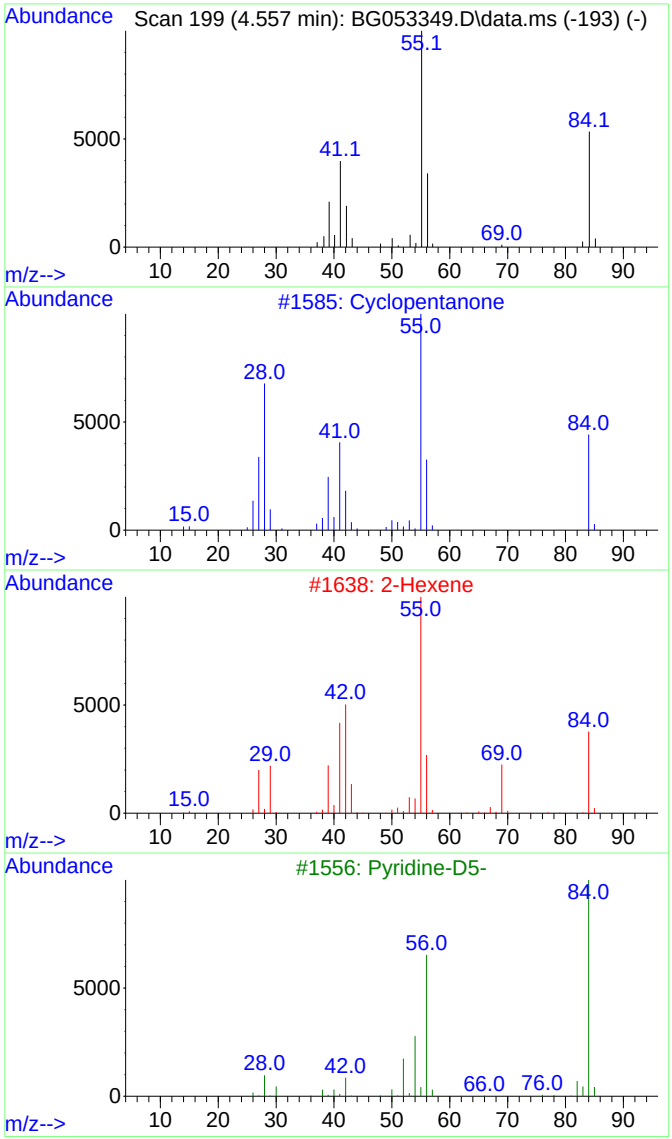
TIC Integration Parameters: LSCINT.P

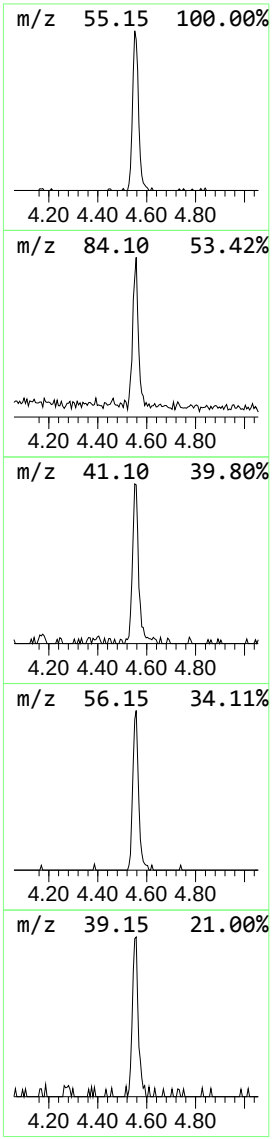
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	10.15 ng	84622	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	90
2	2-Hexene	84	C6H12	000592-43-8	53
3	Pyridine-D5-	84	C5D5N	007291-22-7	47
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	46
5	2-Hexene, (Z)-	84	C6H12	007688-21-3	45





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Data File : BG053349.D
Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

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

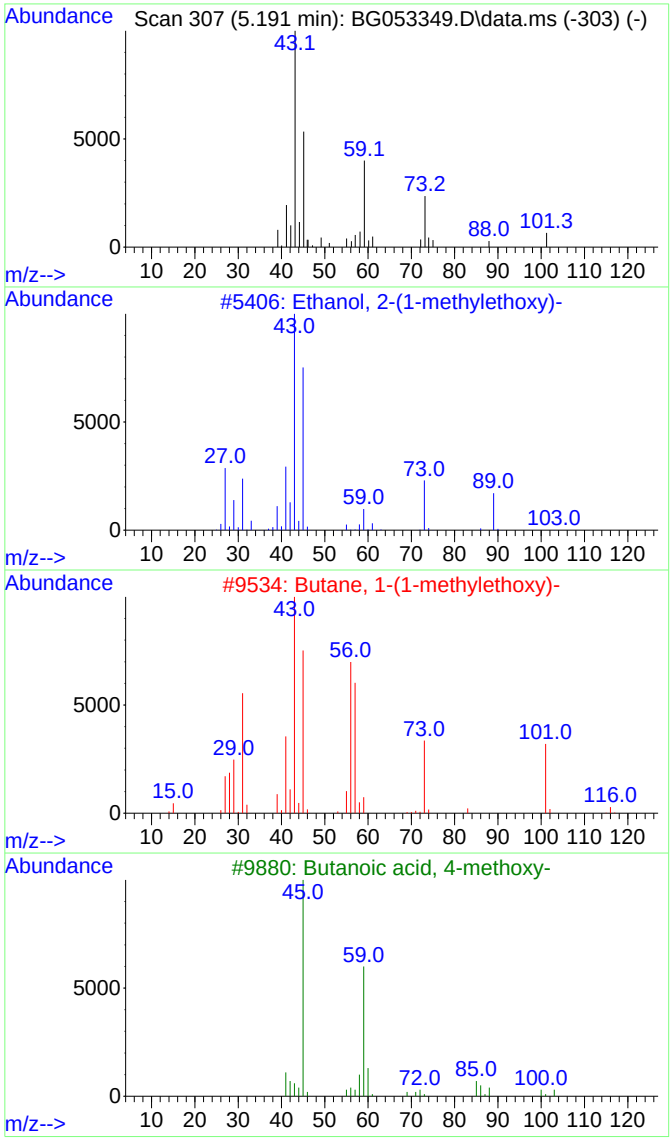
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

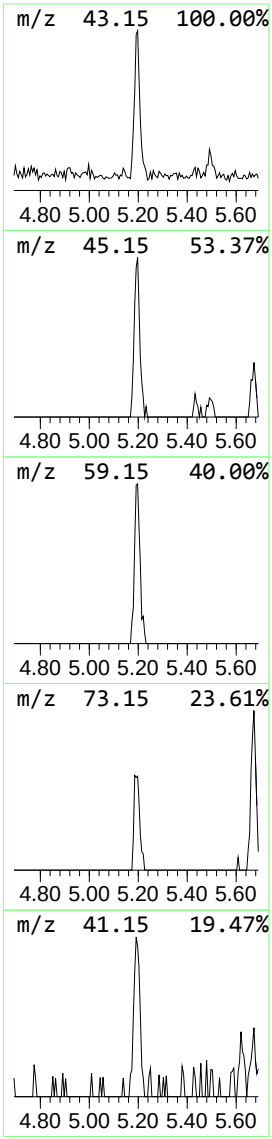
****

Peak Number 2 unknown5.191 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	3.58 ng	29825	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	37
2	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	28
3	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	25
4	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	25
5	Formamide, N-butyl-	101	C5H11NO	000871-71-6	22





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Data File : BG053349.D
Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

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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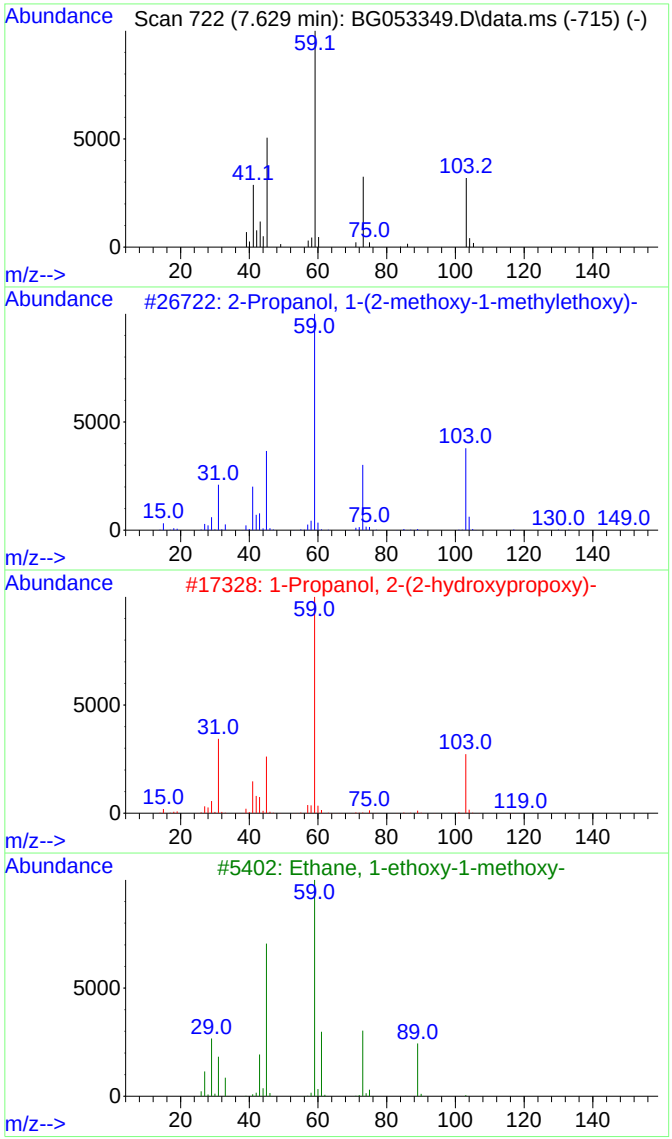
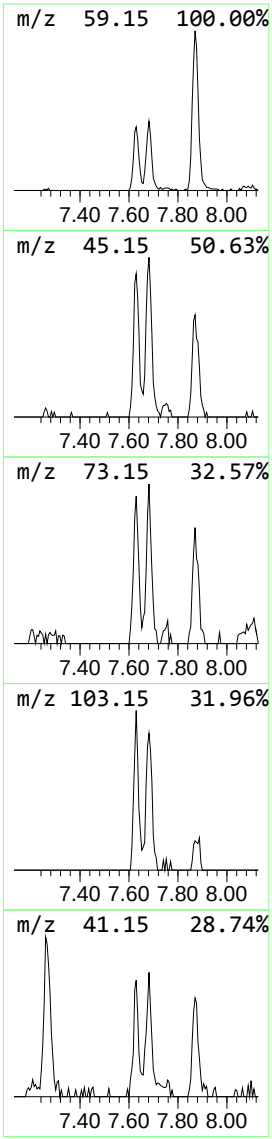
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.629	5.84 ng	48706	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	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
4	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	38
5	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	36





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Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

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

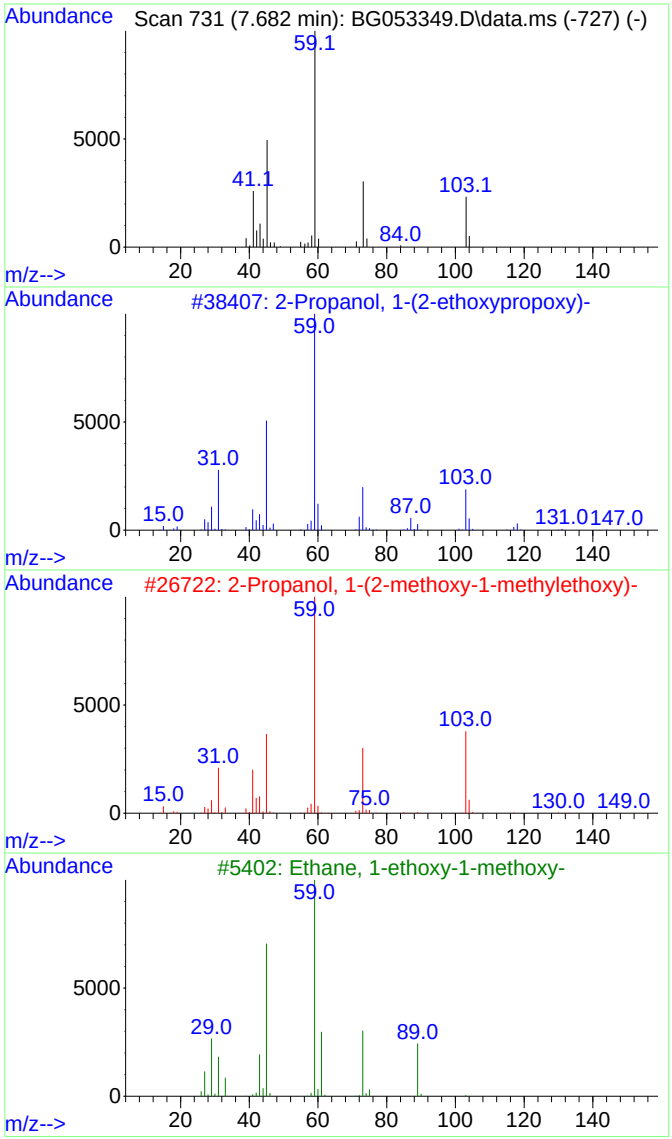
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

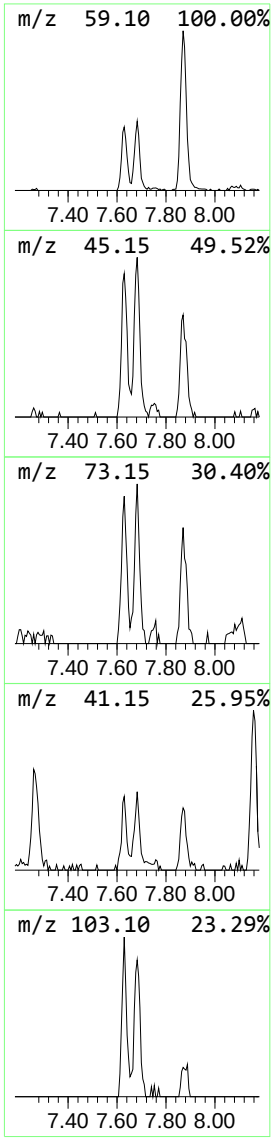
****

Peak Number 4 2-Propanol, 1-(2-ethoxyprop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.682	5.61 ng	46763	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	78
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	56
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
4	Ethyl ether	74	C4H10O	000060-29-7	45
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

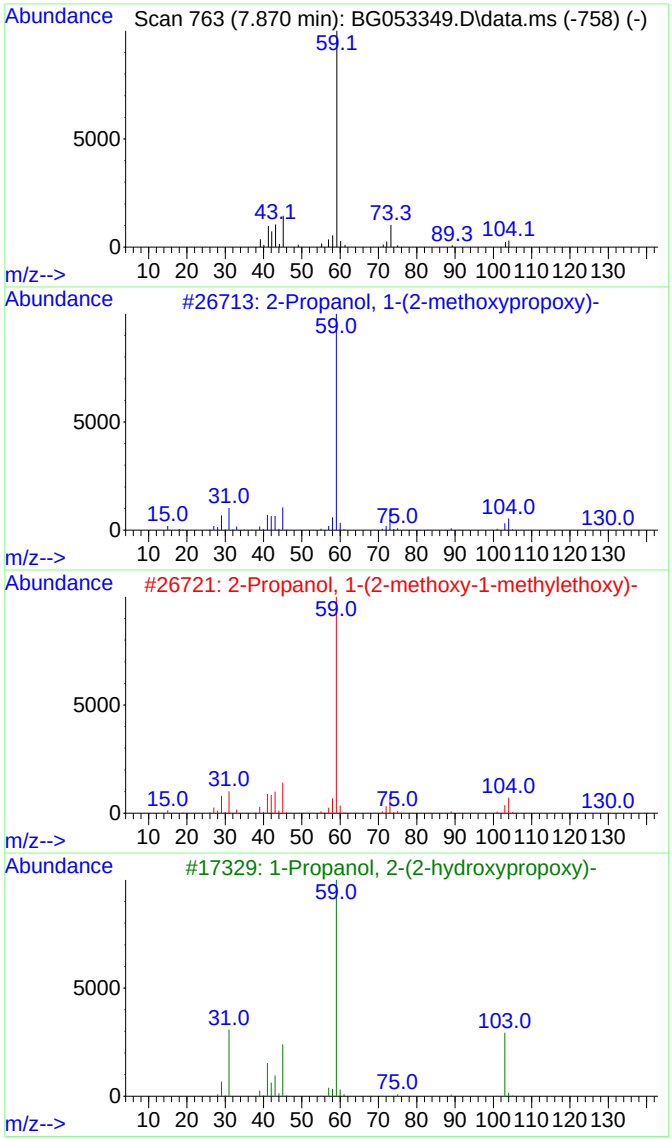
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

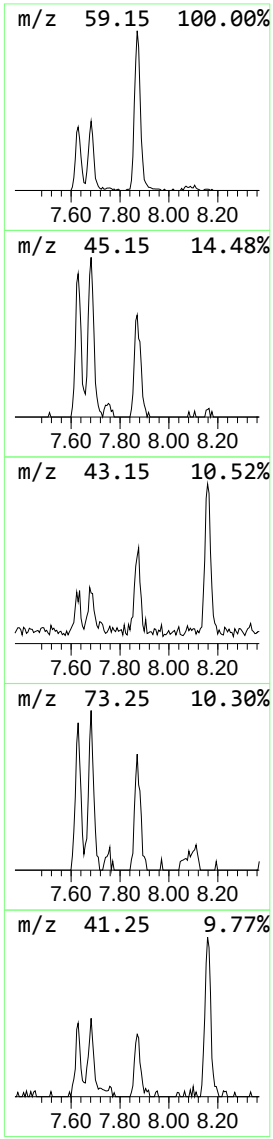
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.870	9.43 ng	78644	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4	Butane, 2-methoxy-	88	C5H12O	006795-87-5	43
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43





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Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

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

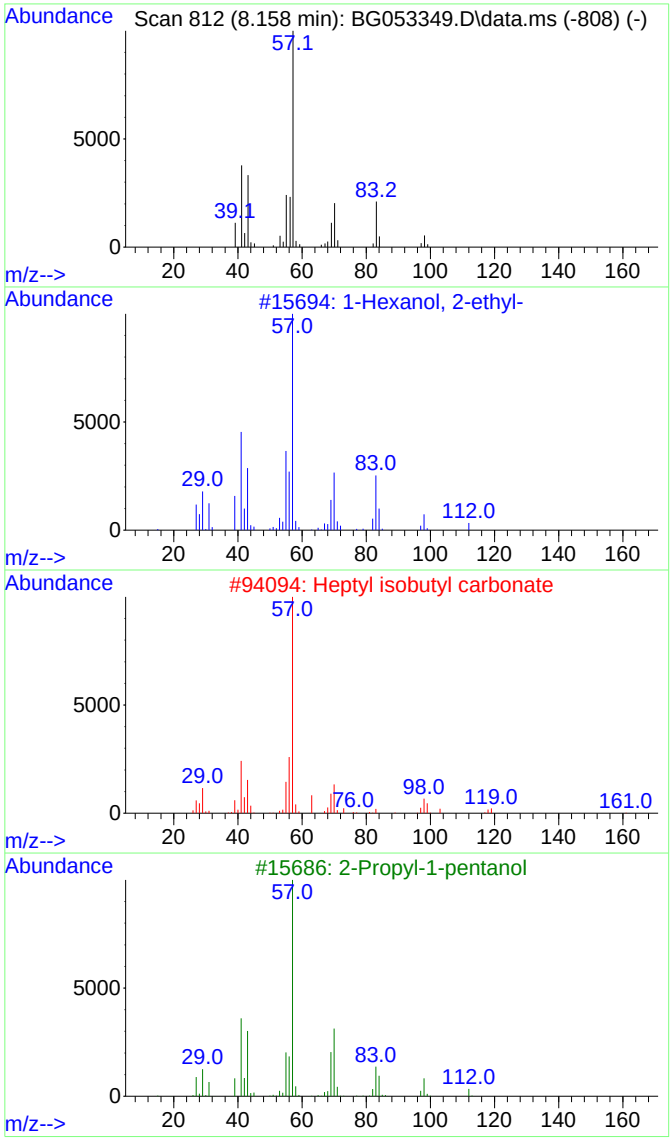
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

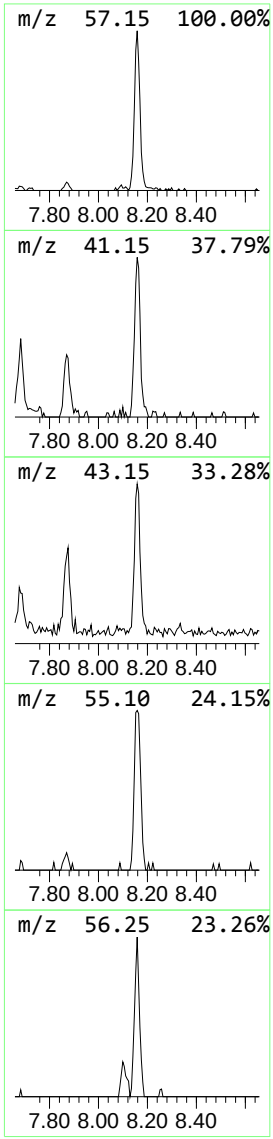
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	10.05 ng	83760	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	56
2	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42





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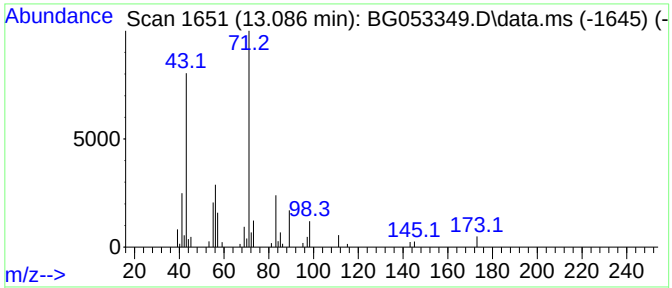
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

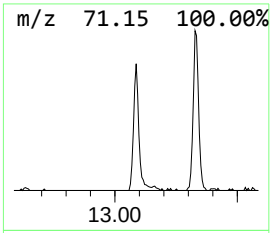
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

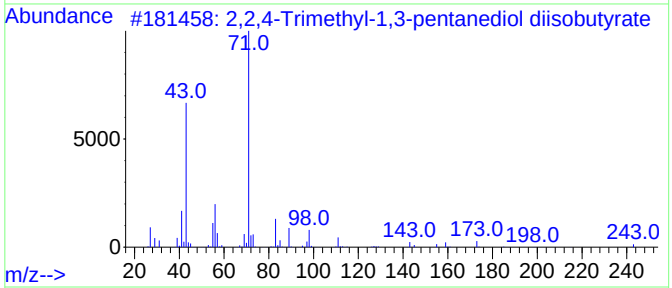
****
Peak Number 7 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 5

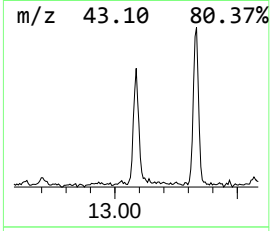
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	5.88 ng	93800	Acenaphthene-d10	14.725

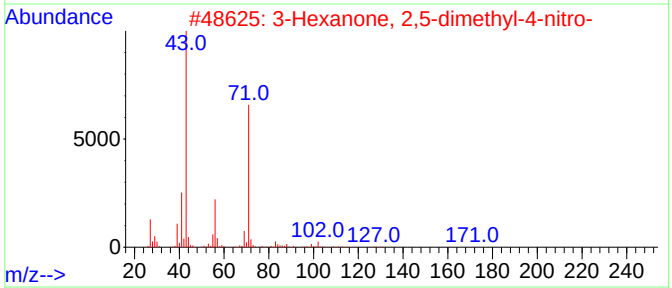
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	90
2	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
3	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	43
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	43
5	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	42

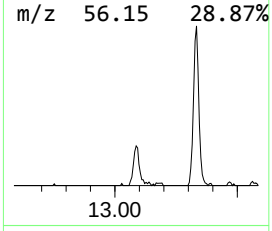


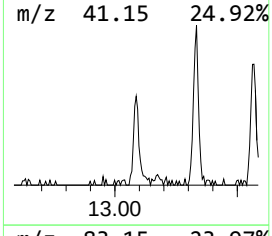


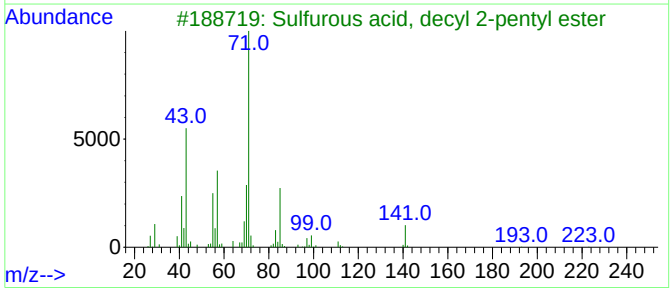


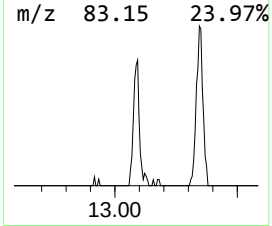












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Acq On : 27 Apr 2022 16:10
Operator : CG/JU
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Misc :
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Instrument :
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ClientSampleId :
MW-26R

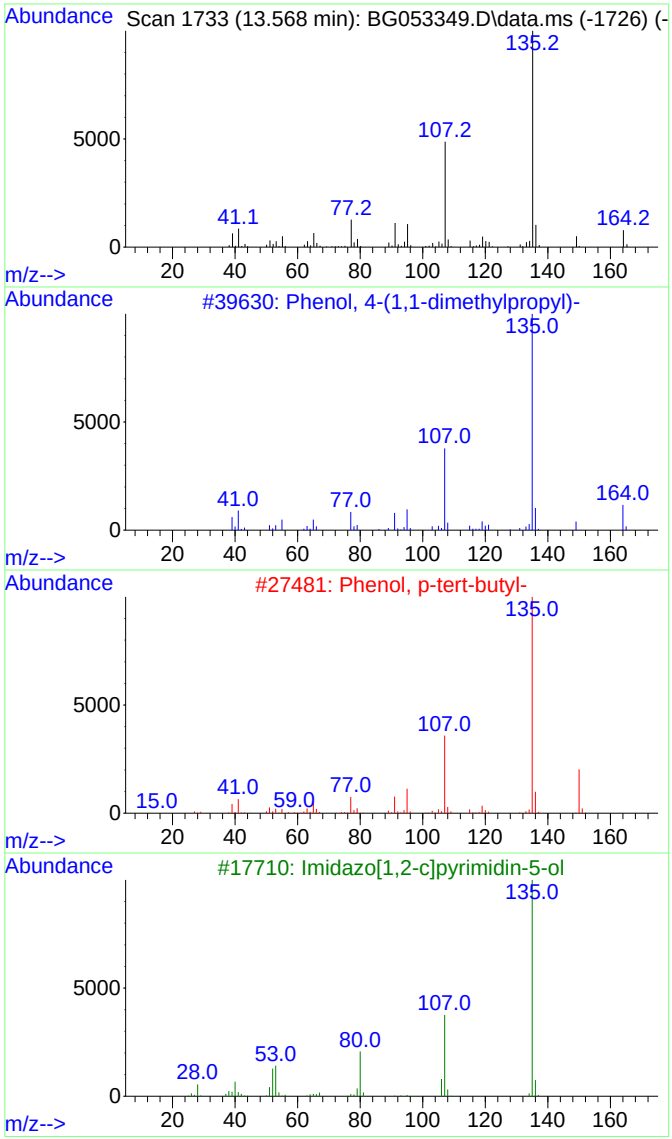
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

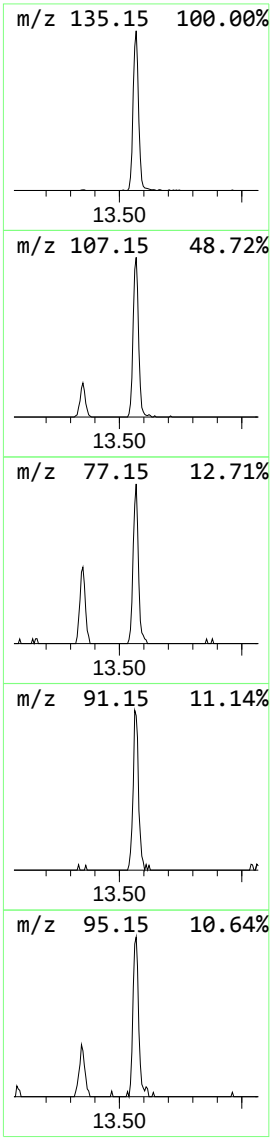
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	15.74 ng	251201	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	59
4	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	59
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053349.D
Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

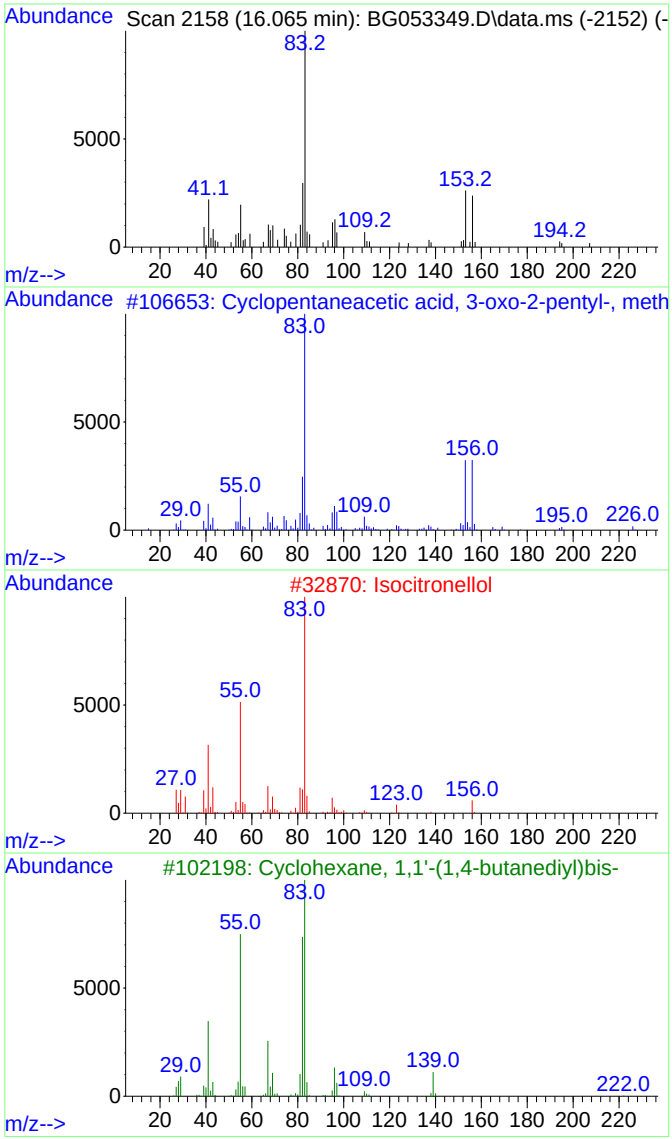
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

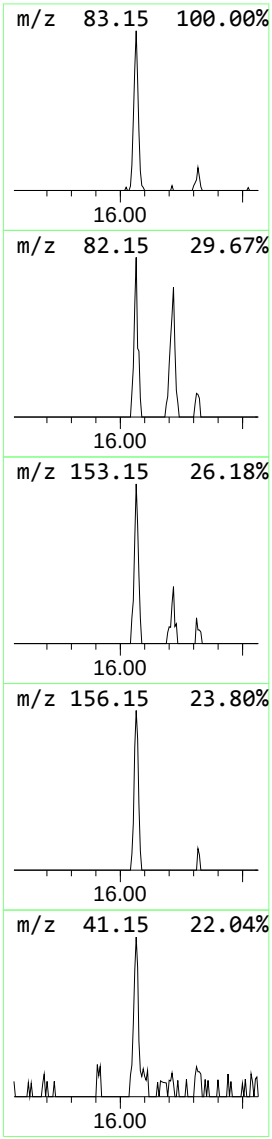
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.065	3.27 ng	52144	Acenaphthene-d10	14.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	86
2	Isocitronellol	156	C10H20O	018479-52-2	53
3	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	43
4	Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	38
5	Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053349.D
Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

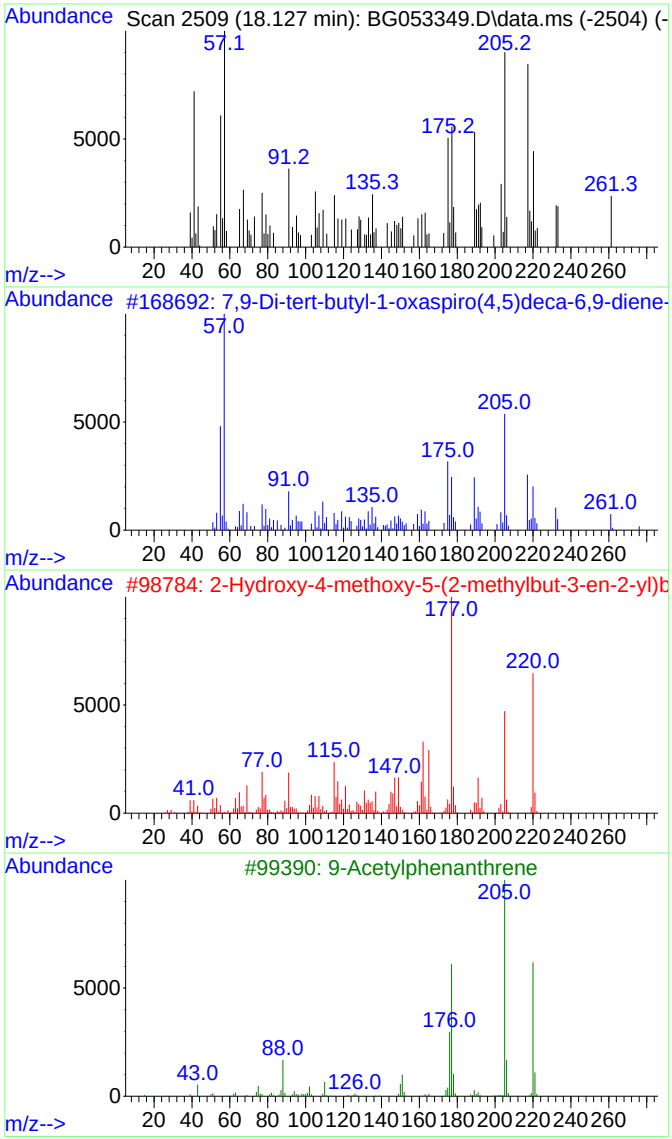
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

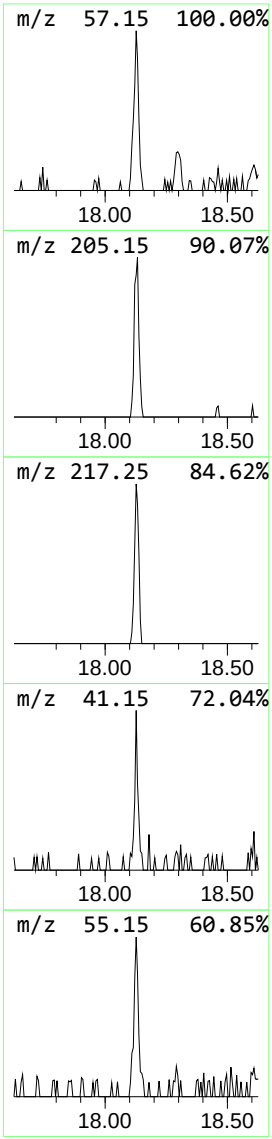
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	2.53 ng	55816	Phenanthrene-d10	17.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	83
2	2-Hydroxy-4-methoxy-5-(2-methylb...	220	C13H16O3	2108511-28-8	45
3	9-Acetylphenanthrene	220	C16H12O	002039-77-2	38
4	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	38
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053349.D
Acq On : 27 Apr 2022 16:10
Operator : CG/JU
Sample : N2481-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-26R

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	4.557	10.2	ng	84622	1	8.105	166750	20.0
unknown5.191	5.191	3.6	ng	29825	1	8.105	166750	20.0
2-Propanol, 1-(...	7.629	5.8	ng	48706	1	8.105	166750	20.0
2-Propanol, 1-(...	7.682	5.6	ng	46763	1	8.105	166750	20.0
2-Propanol, 1-(...	7.870	9.4	ng	78644	1	8.105	166750	20.0
1-Hexanol, 2-et...	8.158	10.1	ng	83760	1	8.105	166750	20.0
2,2,4-Trimethyl...	13.086	5.9	ng	93800	3	14.725	319275	20.0
Phenol, 4-(1,1-...	13.568	15.7	ng	251201	3	14.725	319275	20.0
Cyclopentaneace...	16.065	3.3	ng	52144	3	14.725	319275	20.0
7,9-Di-tert-but...	18.127	2.5	ng	55816	4	17.469	442052	20.0