LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053329.D
Acq On : 26 Apr 2022 20:48
Operator : CG/JU
Sample : N2481-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-30

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: BG053329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.553	188	198	202	rBV	68036	121097	4.45%	1.160%
2	4.594	202	205	211	rVB	49964	70289	2.58%	0.673%
3	5.193	301	307	314	rBV	91220	145913	5.36%	1.397%
4	5.669	382	388	400	rBV	311875	521831	19.16%	4.997%
5	7.267	651	660	670	rVB	234013	418395	15.36%	4.006%
6	7.631	716	722	726	rBV	53352	85689	3.15%	0.821%
7	7.684	726	731	739	rVB	55451	89028	3.27%	0.852%
8	7.872	756	763	772	rBV	94801	158863	5.83%	1.521%
9	8.107	792	803	808	rBV	93658	170508	6.26%	1.633%
10	8.160	808	812	819	rVB	66937	106988	3.93%	1.024%
11	9.270	993	1001	1011	rVB	308148	579249	21.26%	5.547%
12	10.915	1274	1281	1295	rVB	120755	222405	8.16%	2.130%
13	13.088	1645	1651	1658	rBV	43358	69671	2.56%	0.667%
14	13.353	1687	1696	1705	rBV	884927	1440095	52.87%	13.789%
15	13.570	1726	1733	1741	rBV	156513	236700	8.69%	2.266%
16	14.727	1924	1930	1938	rVB	212559	338772	12.44%	3.244%
17	15.532	2061	2067	2071	rVB	32211	45951	1.69%	0.440%
18	16.067	2151	2158	2169	rBV	33608	51505	1.89%	0.493%
19	16.214	2177	2183	2197	rBV	740723	1215375	44.62%	11.638%
20	17.471	2391	2397	2403	rBV	286003	451436	16.57%	4.323%
21	18.129	2505	2509	2514	rVB2	46532	55501	2.04%	0.531%
22	20.079	2834	2841	2846	rBV	2045985	2723962	100.00%	26.083%
23	21.753	3120	3126	3135	rVB	336379	564205	20.71%	5.402%
24	25.049	3674	3687	3699	rBV2	184386	559994	20.56%	5.362%

Sum of corrected areas: 10443422

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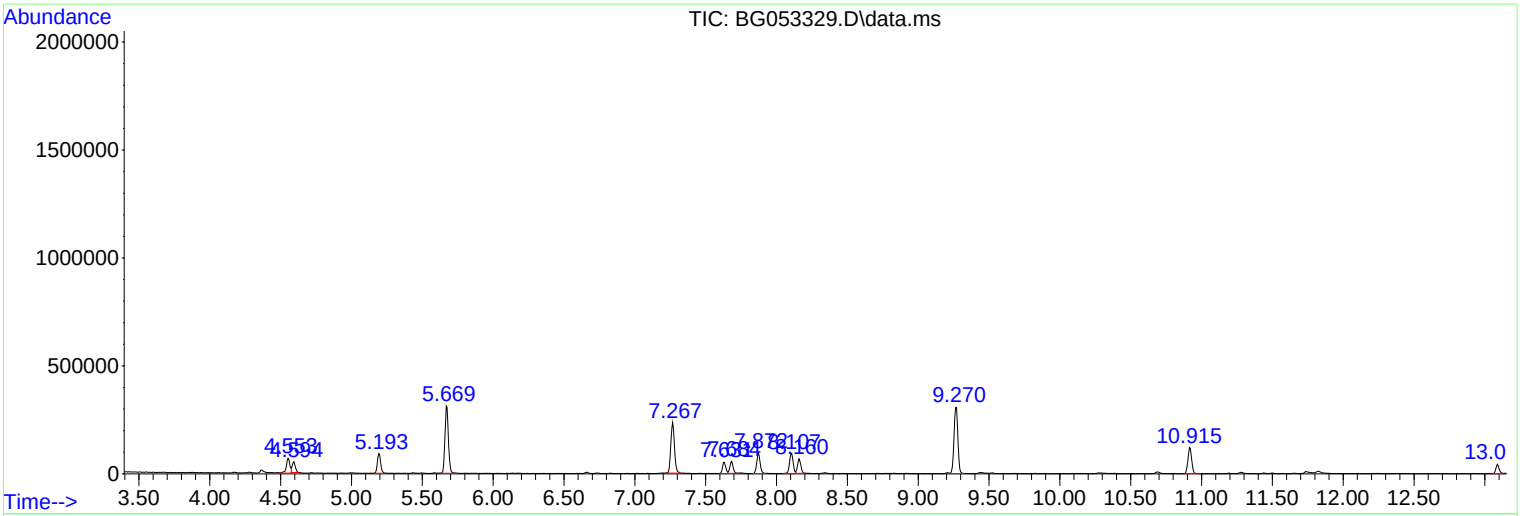
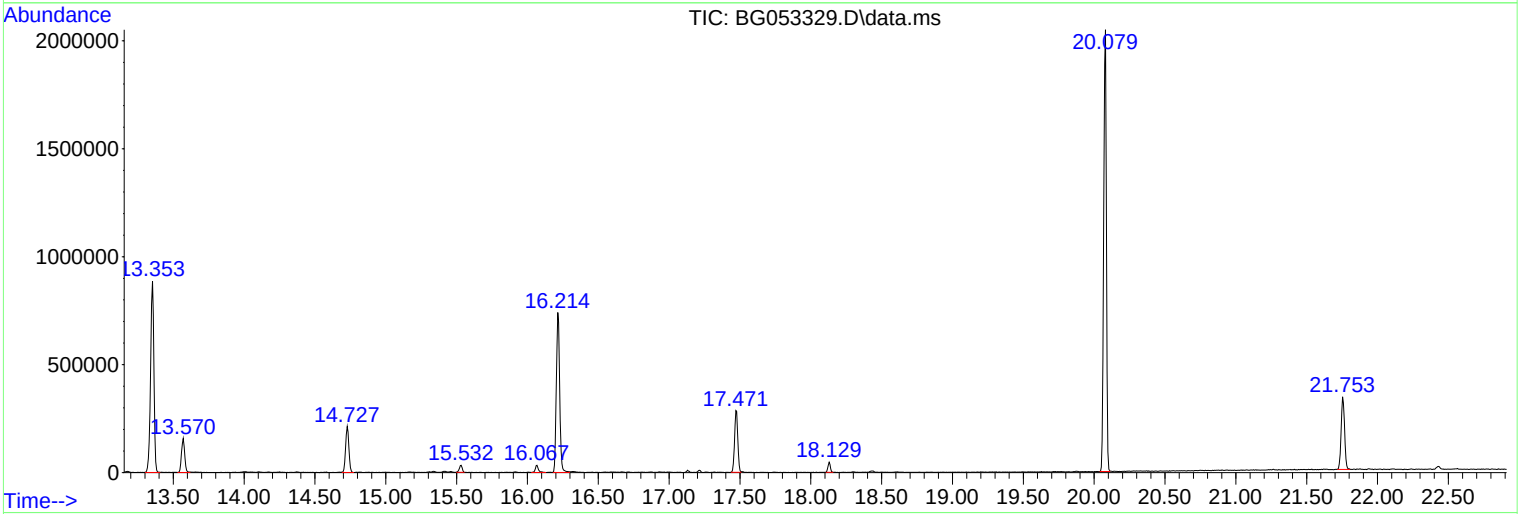
Misc :
ALS Vial : 10 Sample Multiplier: 1

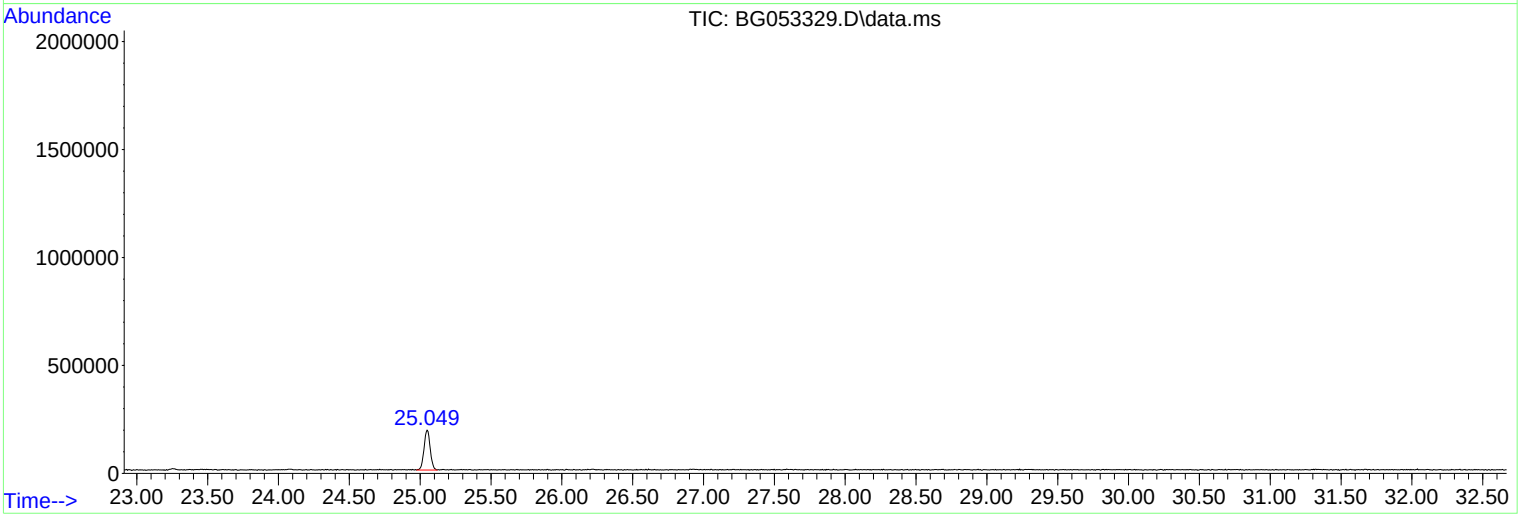
Instrument :
BNA_G
ClientSampleId :
MW-30

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

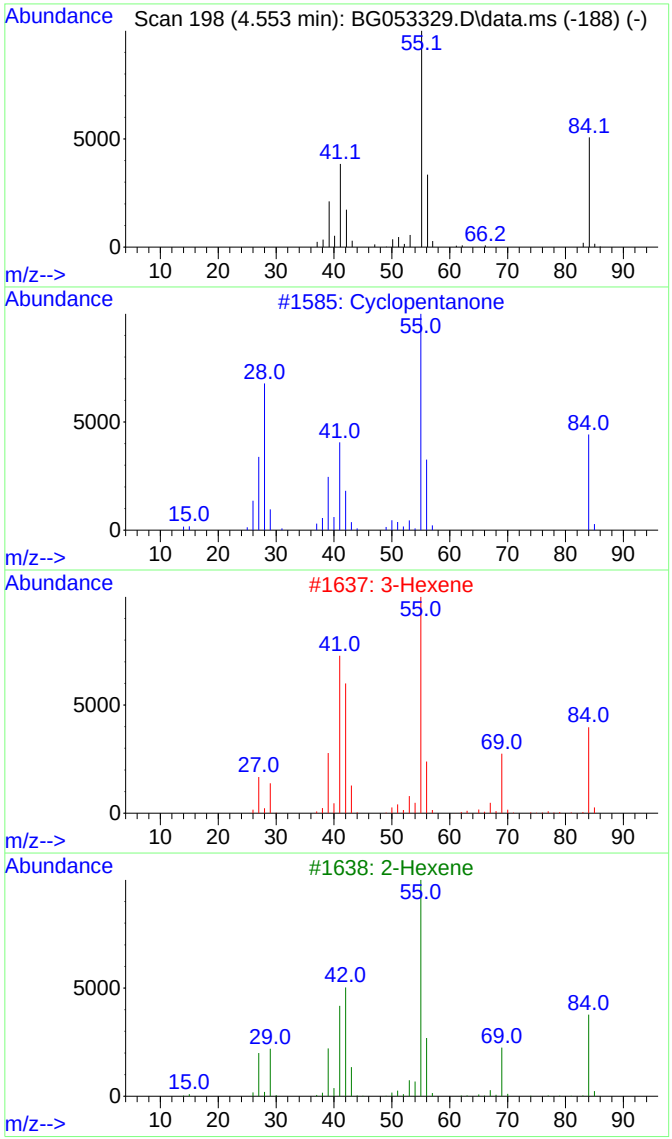
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

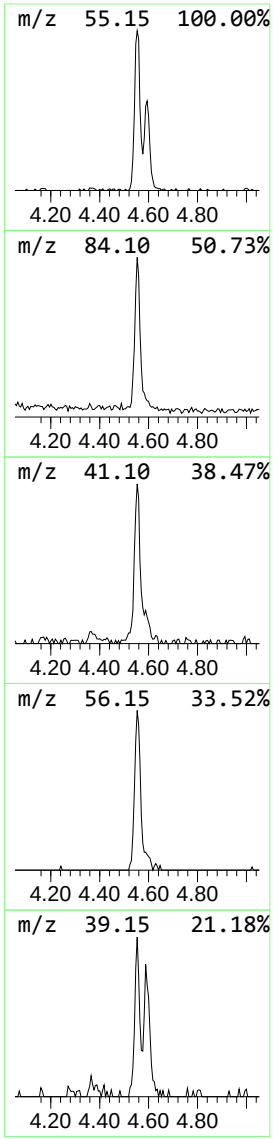
****

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.553	14.20 ng	121097	1,4-Dichlorobenzene-d4	8.101

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	86
2	3-Hexene	84	C6H12	000592-47-2	72
3	2-Hexene	84	C6H12	000592-43-8	72
4	2-Amino-oxazole	84	C3H4N2O	004570-45-0	40
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	39





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Data File : BG053329.D
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Operator : CG/JU
Sample : N2481-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-30

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

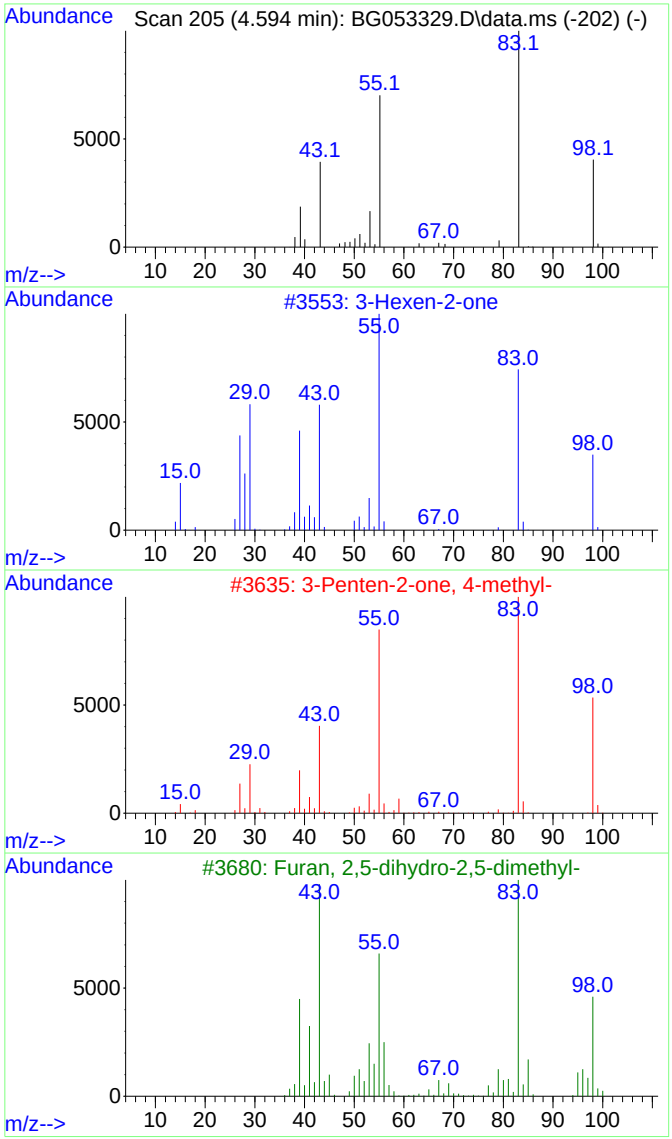
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

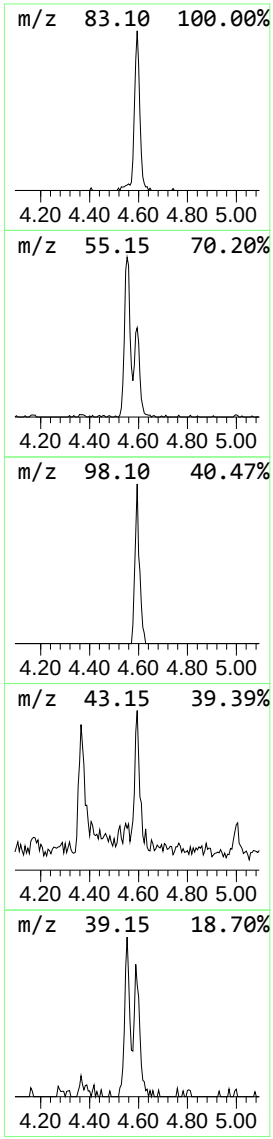
****

Peak Number 2 3-Hexen-2-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.594	8.24 ng	70289	1,4-Dichlorobenzene-d4	8.101

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	83
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	80
3	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	64
4	3-Penten-2-one, 3-methyl-	98	C6H10O	000565-62-8	32
5	2(5H)-Furanone, 5-methyl-	98	C5H6O2	000591-11-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
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Operator : CG/JU
Sample : N2481-10
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
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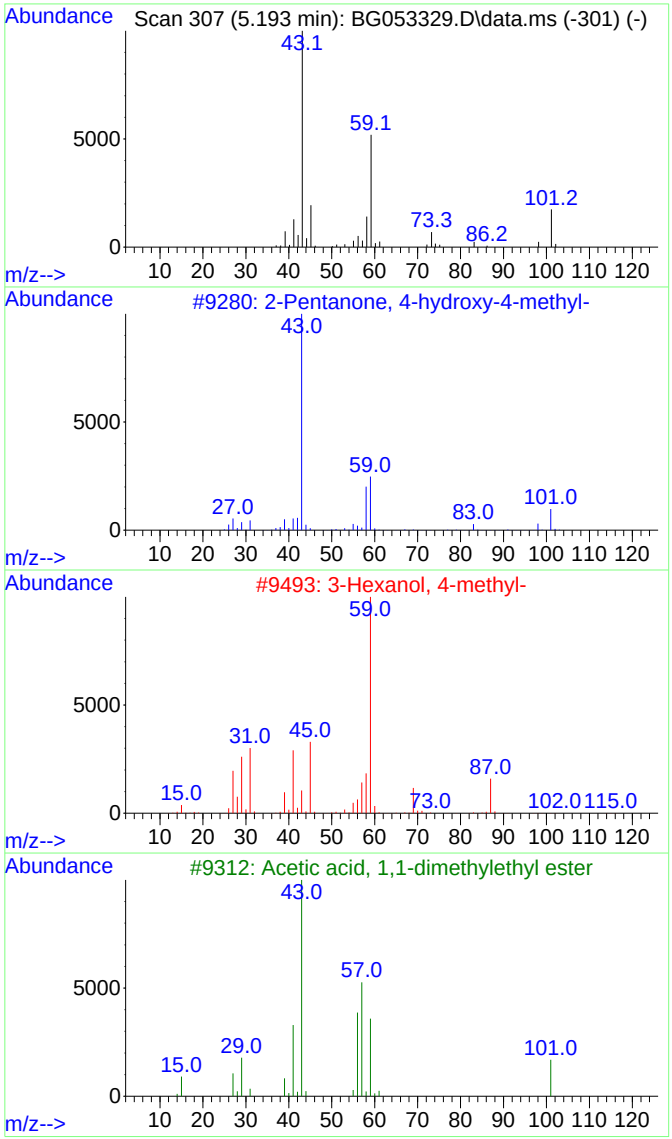
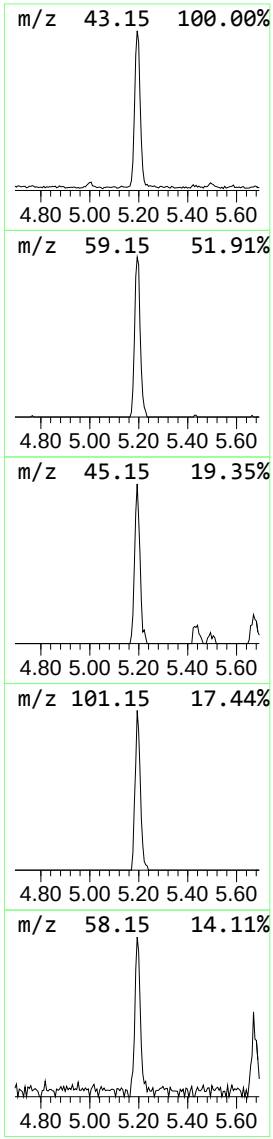
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	17.12 ng	145913	1,4-Dichlorobenzene-d4	8.101

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	47
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	38
5	Ethanol, 2-ethoxy-	90	C4H10O2	000110-80-5	37





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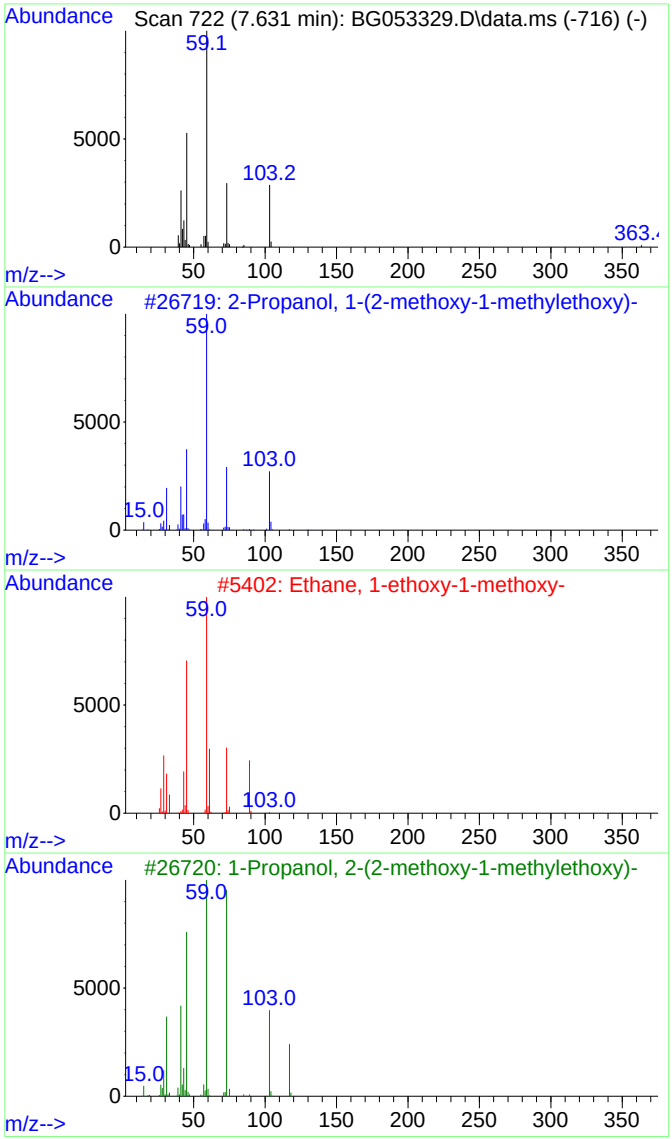
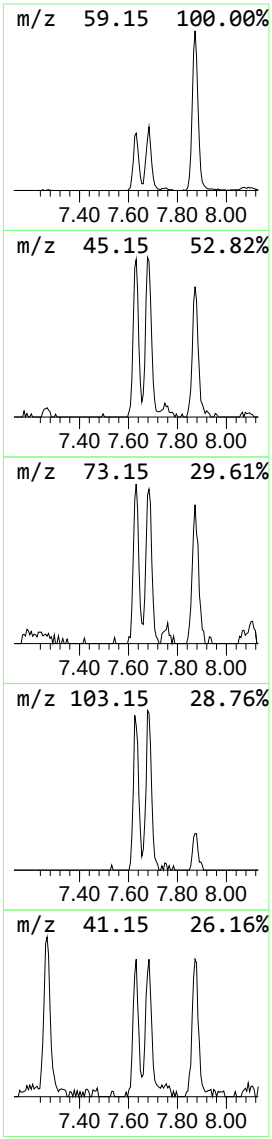
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.631	10.05 ng	85689	1,4-Dichlorobenzene-d4	8.101

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	64
3	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	59
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
5	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	45





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

Instrument :
BNA_G
ClientSampleId :
MW-30

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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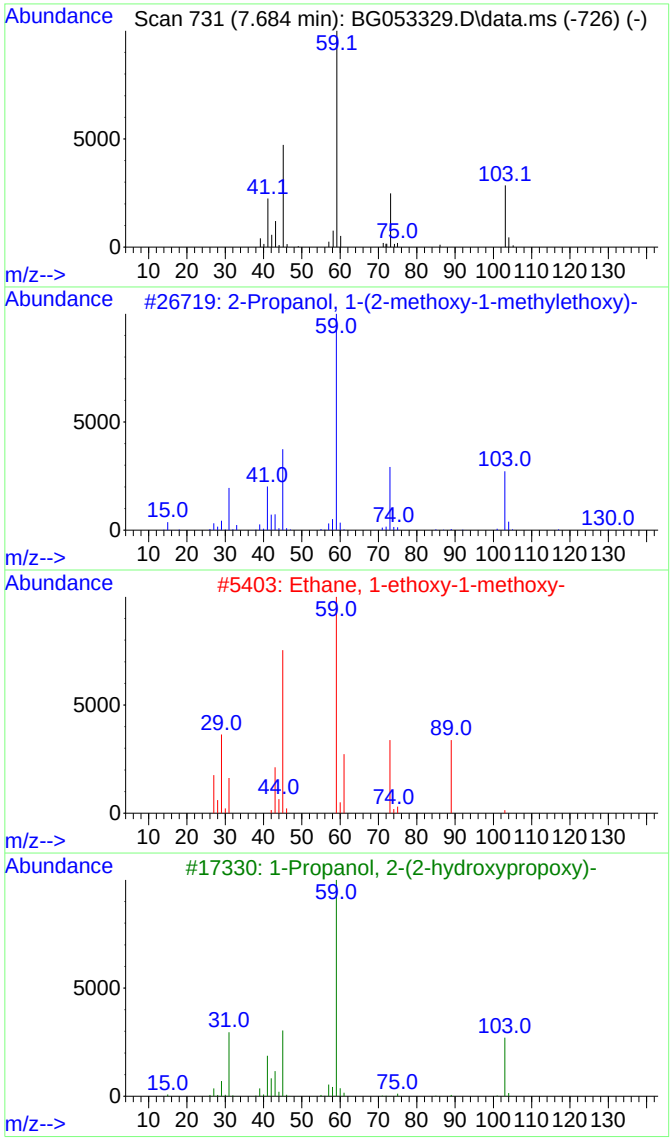
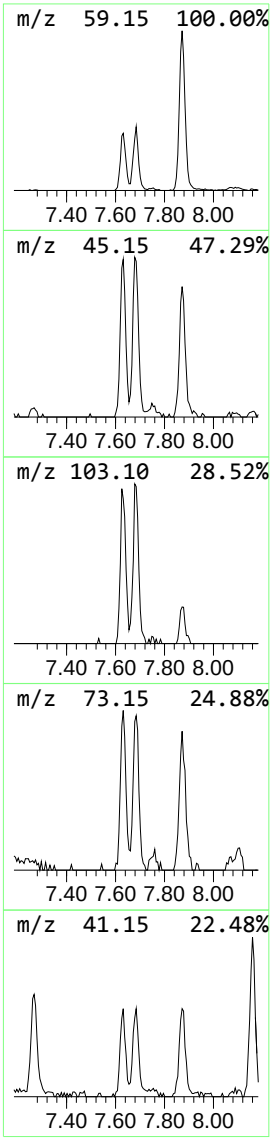
****

Peak Number 5 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.684	10.44 ng	89028	1,4-Dichlorobenzene-d4	8.101

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	42
5	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	39





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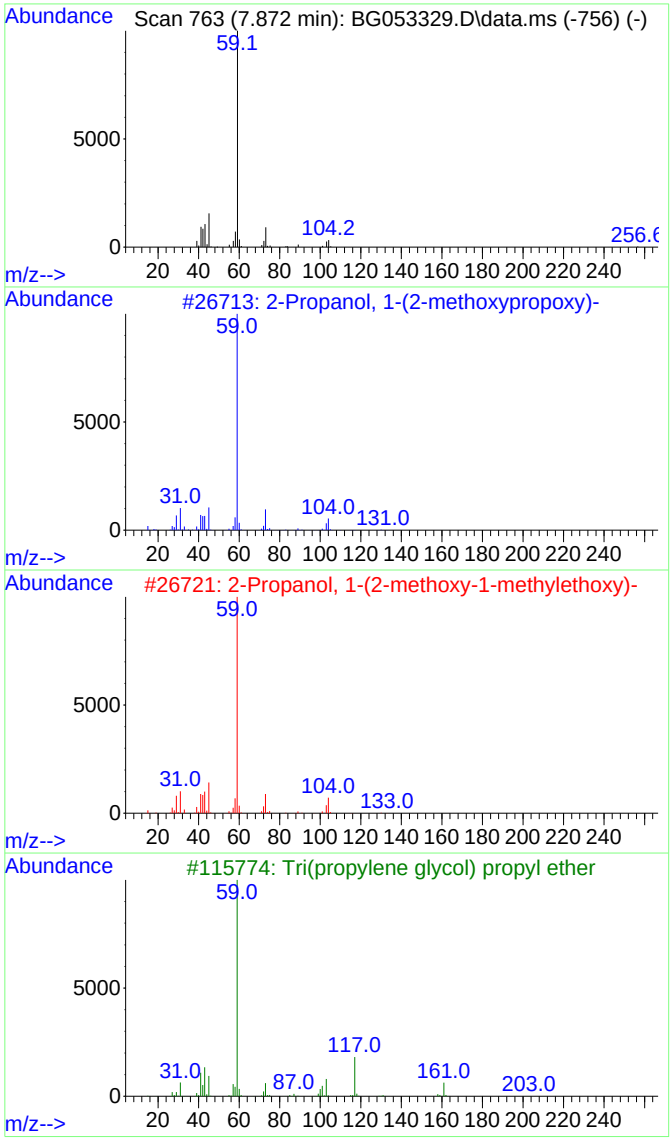
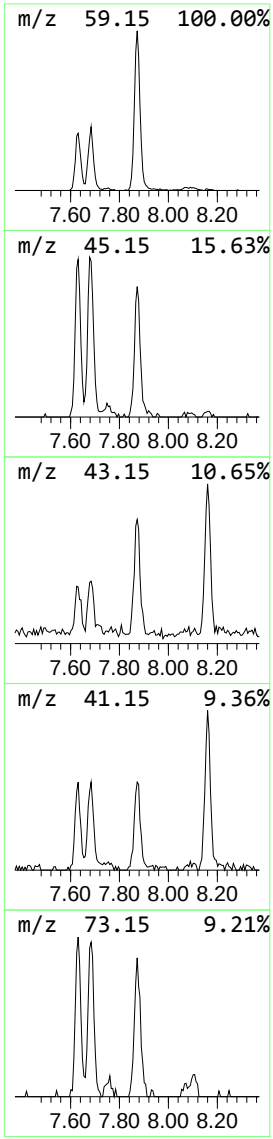
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.872	18.63 ng	158863	1,4-Dichlorobenzene-d4	8.101

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	74
3	Tri(propylene glycol) propyl ether	234	C12H26O4	096077-04-2	64
4	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	64
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64





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

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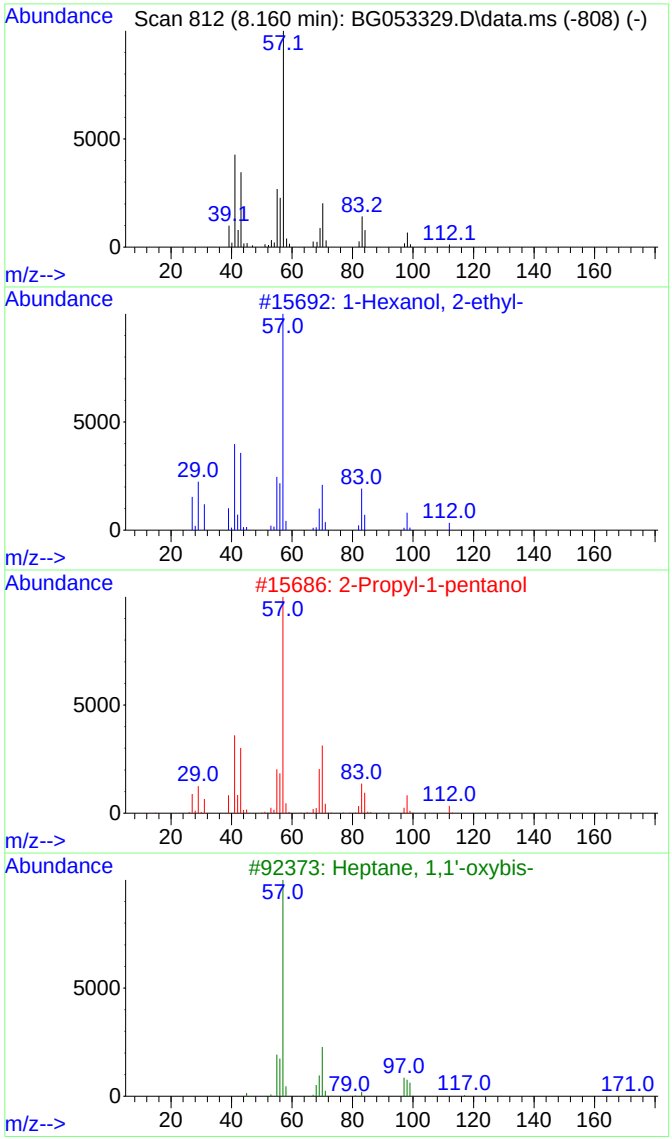
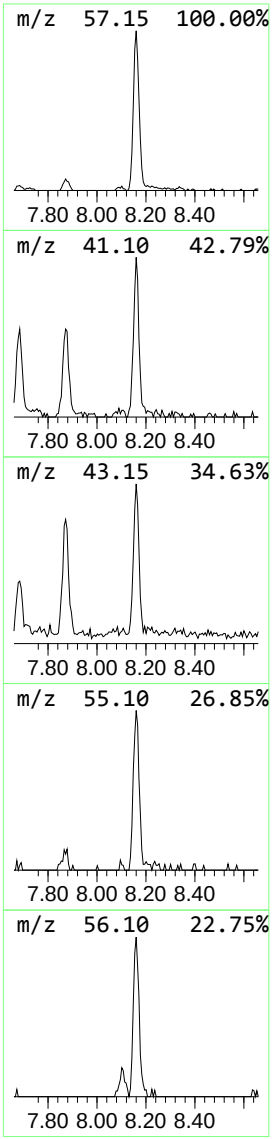
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.160	12.55 ng	106988	1,4-Dichlorobenzene-d4	8.101

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	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4	2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	59
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53





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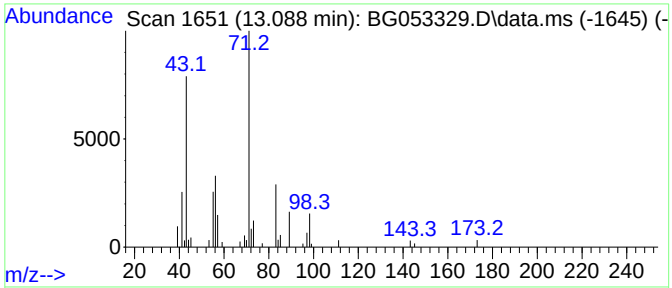
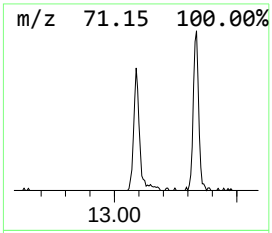
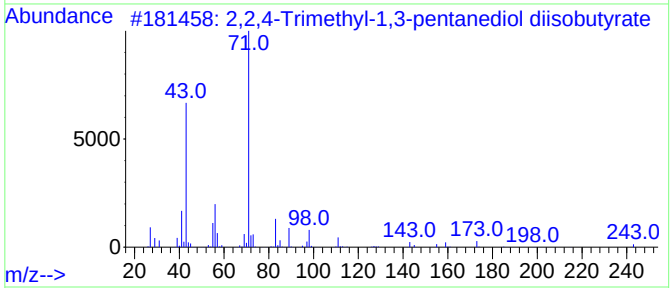
****
Peak Number 8 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 9

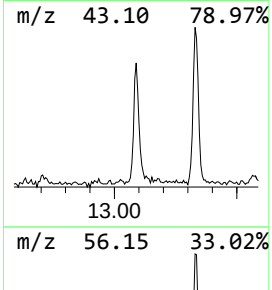
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.089	4.11 ng	69671	Acenaphthene-d10	14.727

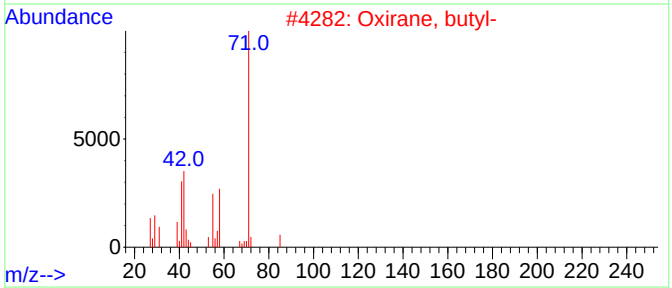
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2	Oxirane, butyl-	100	C6H12O	001436-34-6	47
3	Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	43
4	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	38
5	Allyl 2-ethyl butyrate	156	C9H16O2	007493-69-8	38

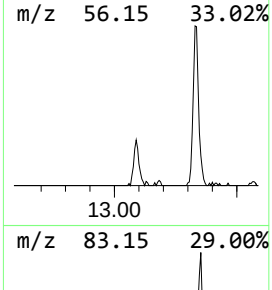


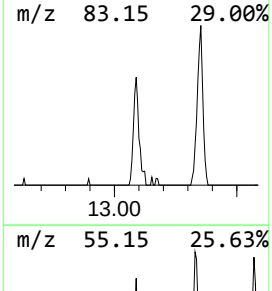


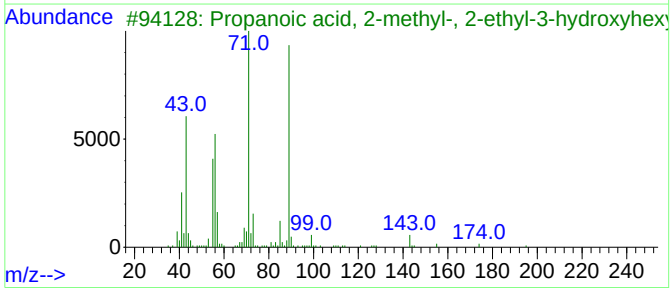


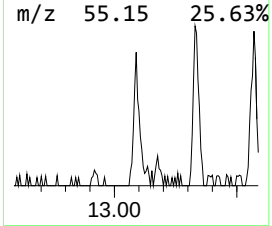












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053329.D
Acq On : 26 Apr 2022 20:48
Operator : CG/JU
Sample : N2481-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-30

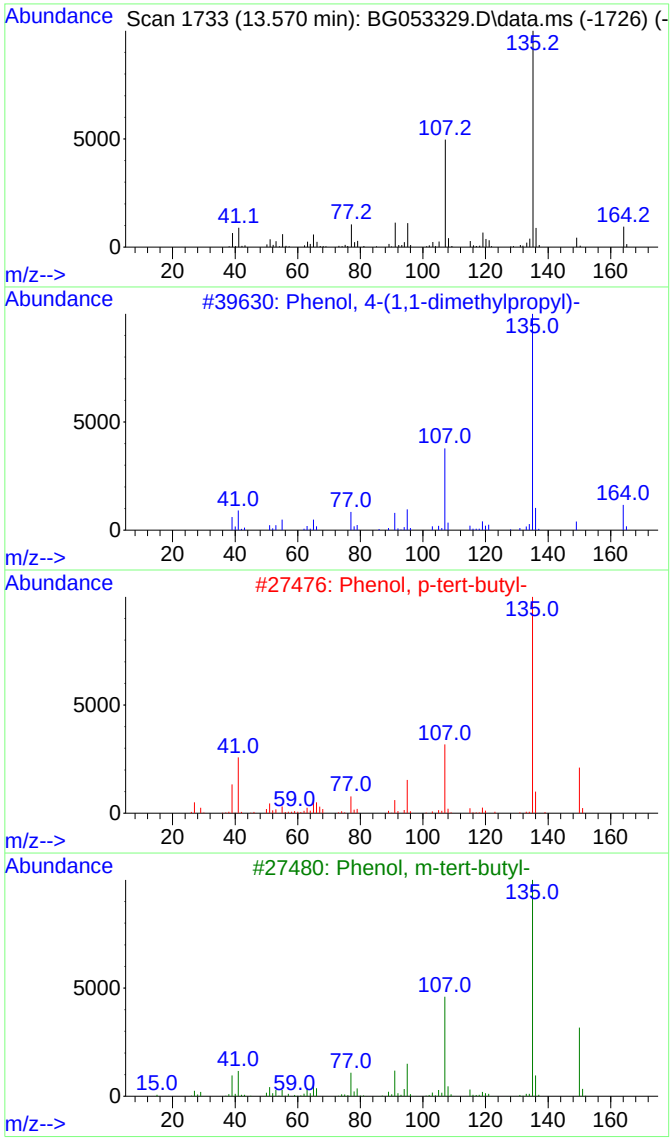
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

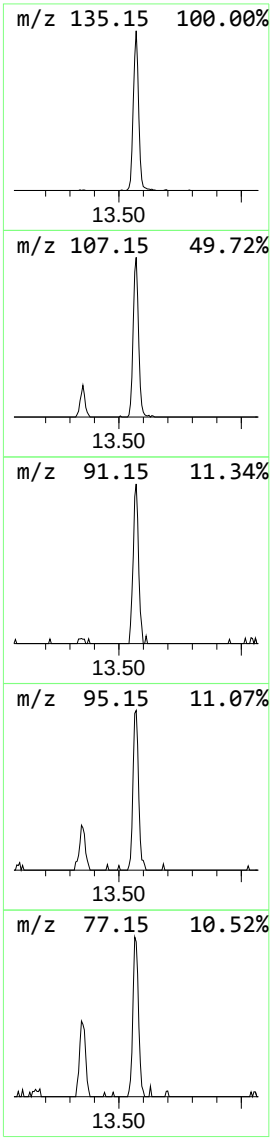
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 4-(1,1-dimethylprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.570	13.97 ng	236700	Acenaphthene-d10	14.727

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	74
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
4	Hexestrol	270	C18H22O2	000084-16-2	64
5	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64





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Operator : CG/JU
Sample : N2481-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-30

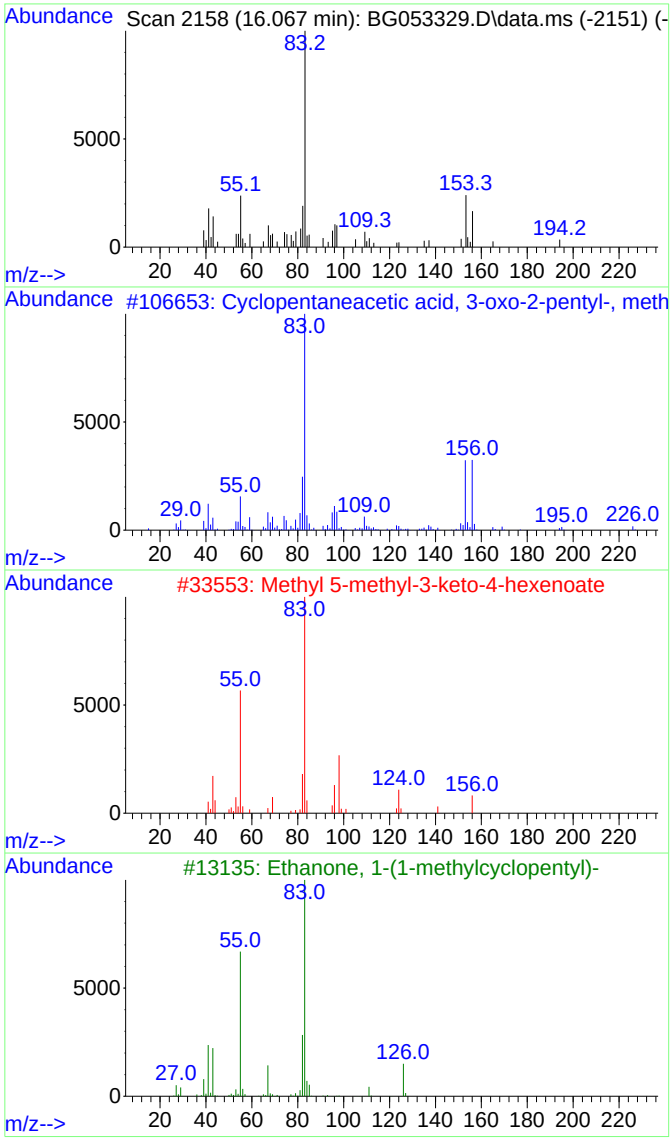
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

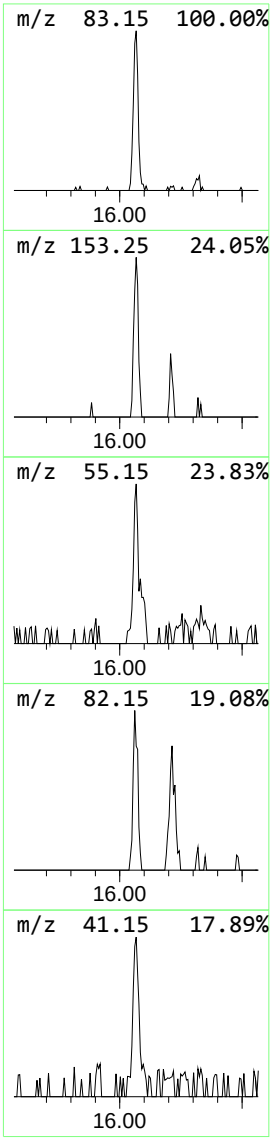
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopentaneacetic acid, 3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.067	3.04 ng	51505	Acenaphthene-d10	14.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	78
2	Methyl 5-methyl-3-keto-4-hexenoate	156	C8H12O3	1000427-08-8	50
3	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	47
4	6-Hydroxy-10a-methyl-4,7-dimethy...	376	C20H24O7	1798297-60-5	43
5	2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	43





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Data File : BG053329.D
Acq On : 26 Apr 2022 20:48
Operator : CG/JU
Sample : N2481-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-30

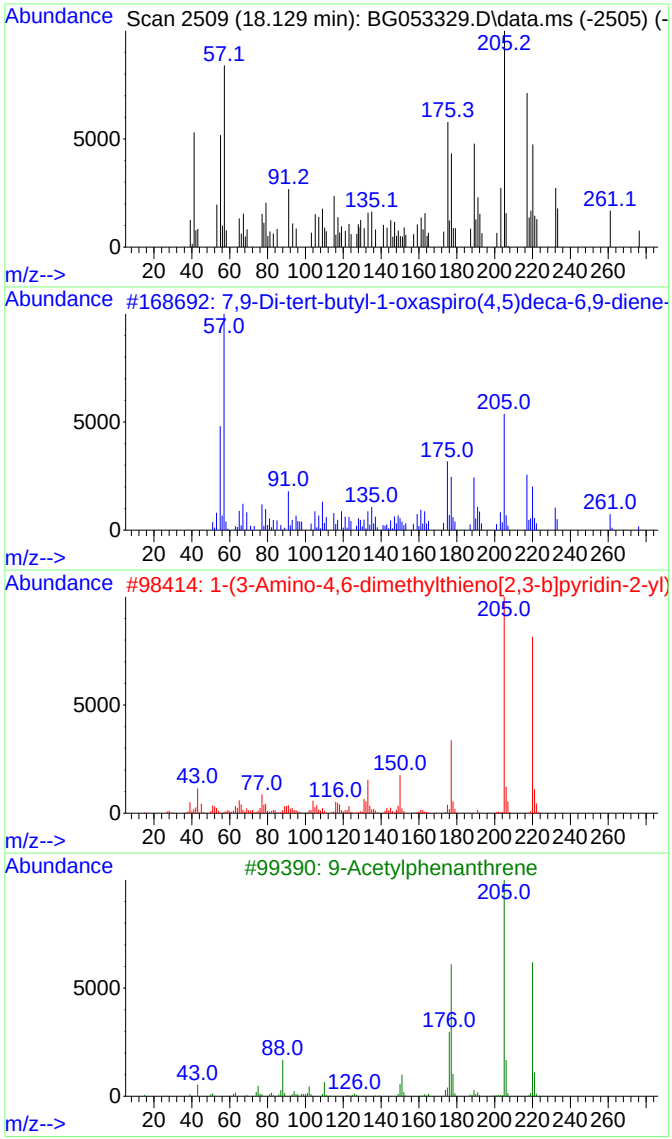
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

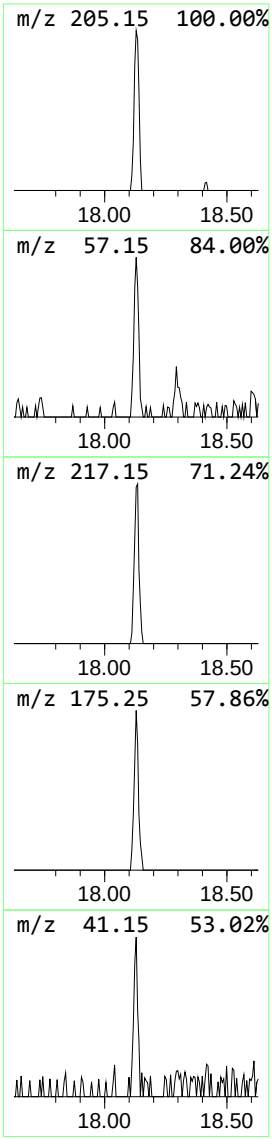
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.129	2.46 ng	55501	Phenanthrene-d10	17.477

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45
3	9-Acetylphenanthrene	220	C16H12O	002039-77-2	43
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42
5	1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053329.D
Acq On : 26 Apr 2022 20:48
Operator : CG/JU
Sample : N2481-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-30

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	4.553	14.2	ng	121097	1	8.101	170508	20.0
3-Hexen-2-one	4.594	8.2	ng	70289	1	8.101	170508	20.0
2-Pentanone, 4-...	5.193	17.1	ng	145913	1	8.101	170508	20.0
2-Propanol, 1-(...	7.631	10.1	ng	85689	1	8.101	170508	20.0
Ethane, 1-ethox...	7.684	10.4	ng	89028	1	8.101	170508	20.0
2-Propanol, 1-(...	7.872	18.6	ng	158863	1	8.101	170508	20.0
1-Hexanol, 2-et...	8.160	12.6	ng	106988	1	8.101	170508	20.0
2,2,4-Trimethyl...	13.089	4.1	ng	69671	3	14.727	338772	20.0
Phenol, 4-(1,1-...	13.570	14.0	ng	236700	3	14.727	338772	20.0
Cyclopentaneace...	16.067	3.0	ng	51505	3	14.727	338772	20.0
7,9-Di-tert-but...	18.129	2.5	ng	55501	4	17.477	451436	20.0