LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053350.D
Acq On : 27 Apr 2022 16:48
Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

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: BG053350.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.982	97	101	109	rVB	23956	36253	1.27%	0.337%
2	4.546	191	197	200	rBV2	46655	69835	2.44%	0.649%
3	4.587	200	204	215	rVB	211355	331391	11.57%	3.081%
4	5.192	301	307	314	rVB	159737	244410	8.53%	2.272%
5	5.668	382	388	401	rVB	244102	400285	13.97%	3.722%
6	7.266	650	660	671	rVB	146770	271699	9.49%	2.526%
7	7.630	717	722	726	rBV2	17386	28856	1.01%	0.268%
8	7.683	726	731	736	rVB	20522	32227	1.13%	0.300%
9	7.871	757	763	770	rBV	29211	53193	1.86%	0.495%
10	8.106	796	803	807	rBV	90310	152831	5.34%	1.421%
11	8.158	807	812	821	rVB	77398	123197	4.30%	1.145%
12	9.263	993	1000	1010	rVB	350834	646601	22.57%	6.012%
13	10.914	1272	1281	1291	rBV	118787	217924	7.61%	2.026%
14	11.278	1337	1343	1346	rBV2	35146	62578	2.18%	0.582%
15	11.313	1346	1349	1358	rVB2	35264	57003	1.99%	0.530%
16	11.730	1415	1420	1427	rBV3	18167	42805	1.49%	0.398%
17	13.351	1687	1696	1703	rBV	951642	1528743	53.37%	14.214%
18	13.569	1726	1733	1747	rBV	212960	328074	11.45%	3.050%
19	14.726	1923	1930	1938	rVB	196366	321415	11.22%	2.988%
20	15.525	2060	2066	2076	rVB	39620	59229	2.07%	0.551%
21	16.065	2153	2158	2162	rBV	42226	57746	2.02%	0.537%
22	16.212	2176	2183	2195	rBV	830025	1345252	46.96%	12.508%
23	17.469	2391	2397	2408	rVB	288690	450490	15.73%	4.189%
24	20.078	2834	2841	2847	rBV	2122121	2864401	100.00%	26.632%
25	21.758	3119	3127	3138	rVB	305785	537296	18.76%	4.996%
26	23.267	3373	3384	3390	rBV	9153	29053	1.01%	0.270%
27	25.053	3677	3688	3704	rVB2	138454	421387	14.71%	3.918%
28	25.699	3788	3798	3804	rBV10	14487	41140	1.44%	0.383%

Sum of corrected areas: 10755314

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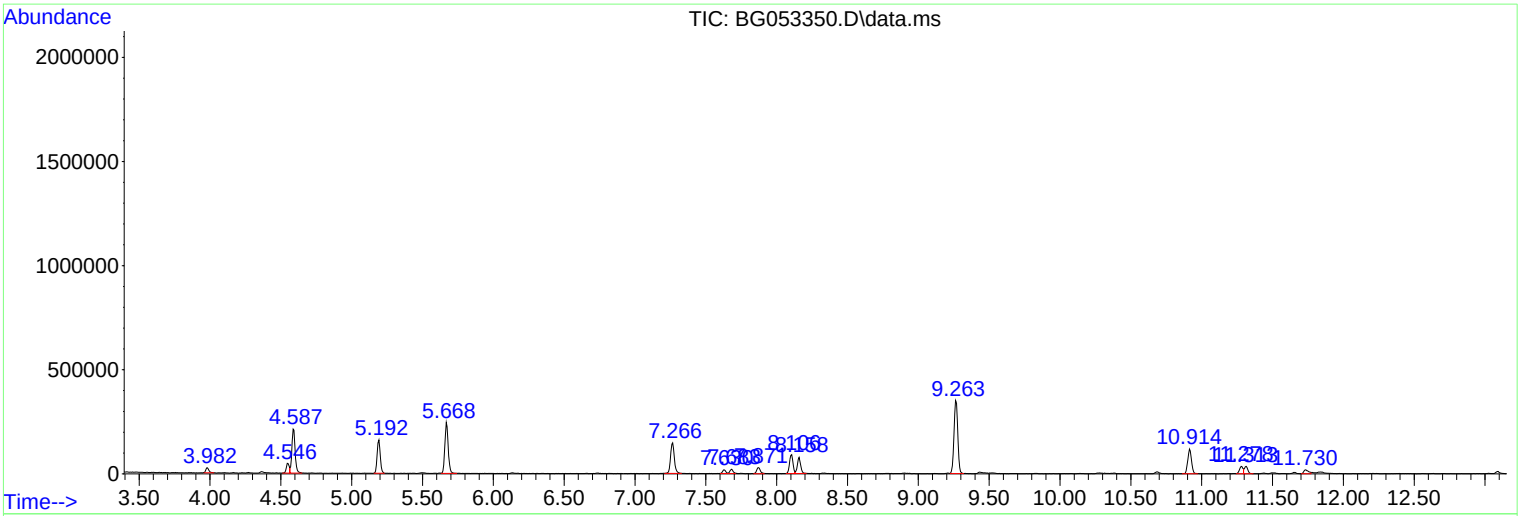
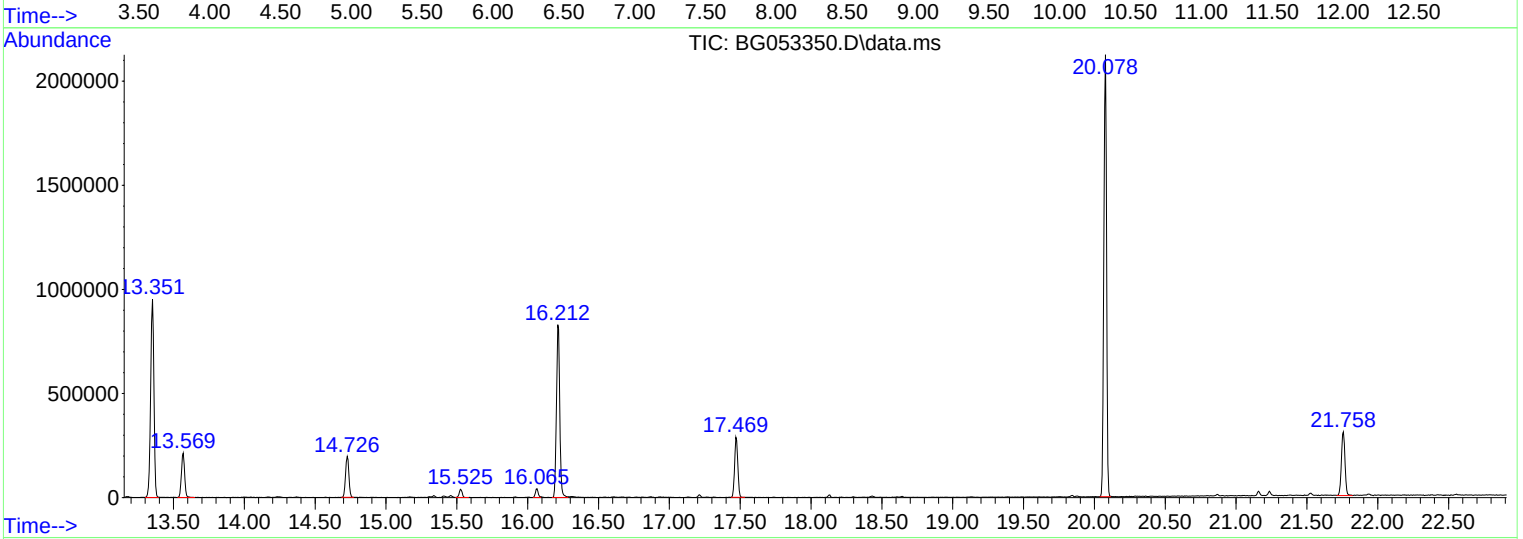
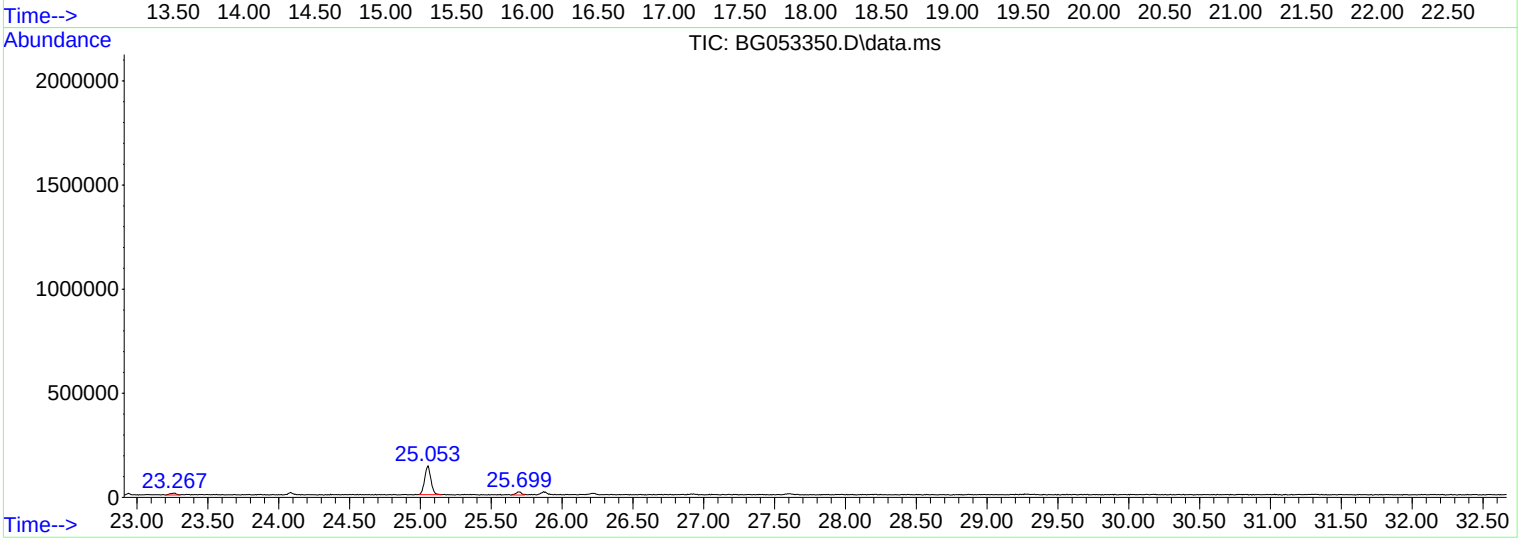
Instrument :
BNA_G
ClientSampleId :
GES-2R

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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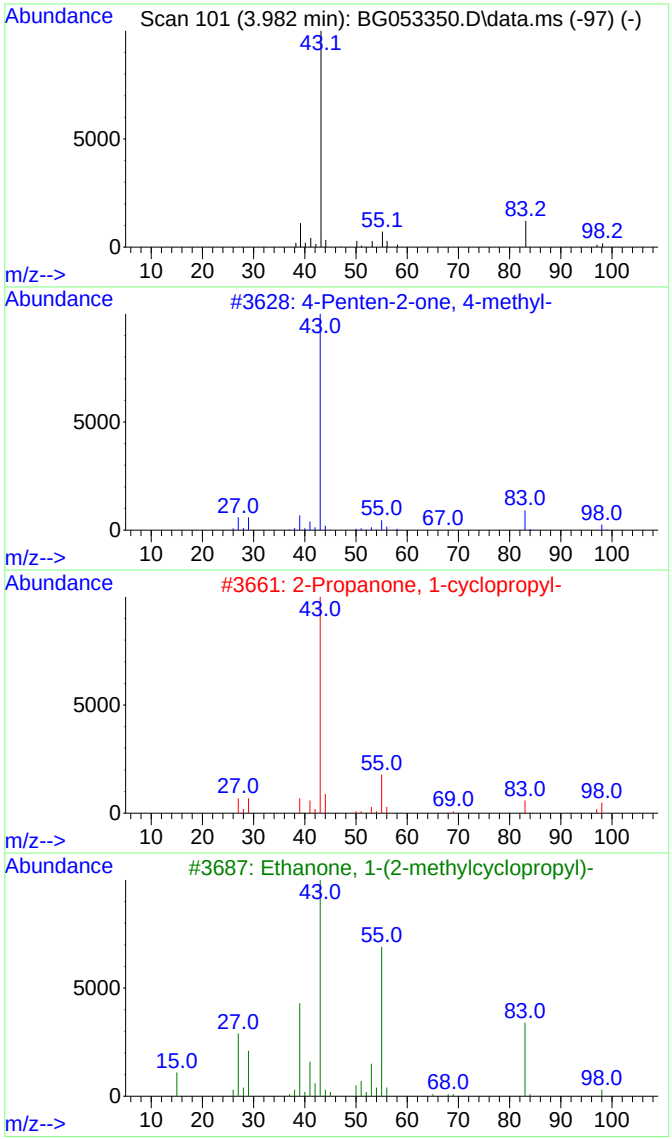
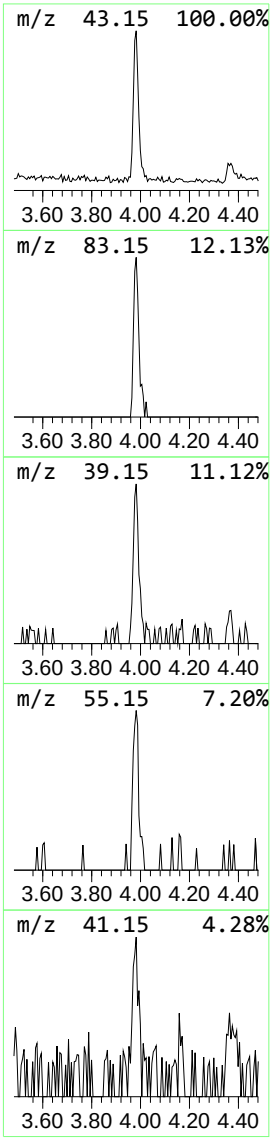
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.982	4.74 ng	36253	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	78
2	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	5
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	4
4	5-Hexen-2-one	98	C6H10O	000109-49-9	4
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	4





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Data File : BG053350.D
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Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

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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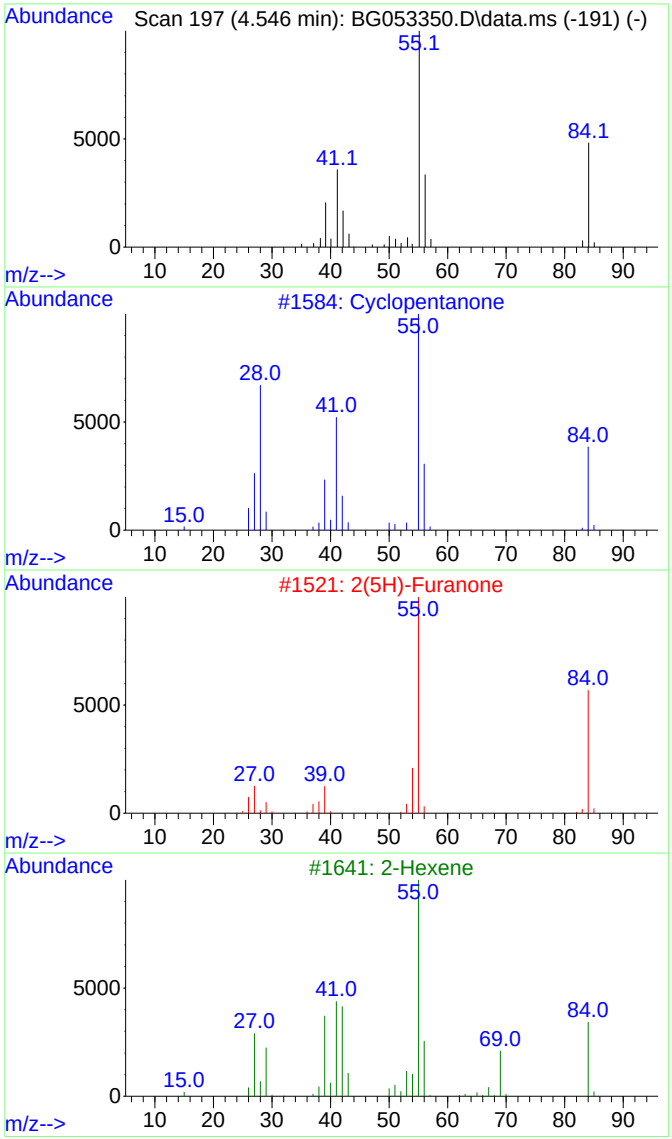
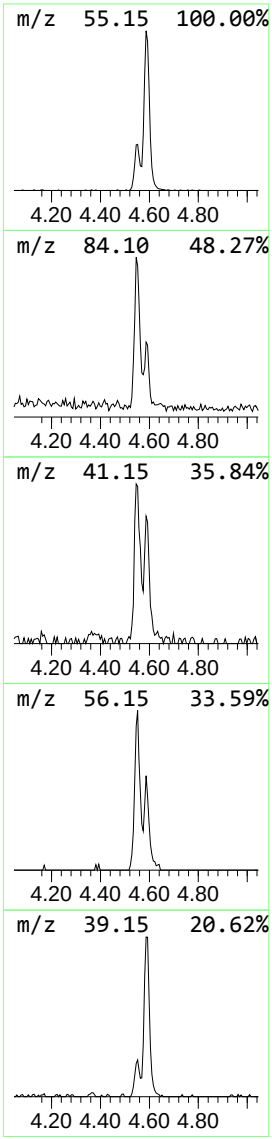
****

Peak Number 2 Cyclopentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.546	9.14 ng	69835	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	87
2	2(5H)-Furanone	84	C4H4O2	000497-23-4	49
3	2-Hexene	84	C6H12	000592-43-8	42
4	3-Hexene, (E)-	84	C6H12	013269-52-8	38
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	38





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Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

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

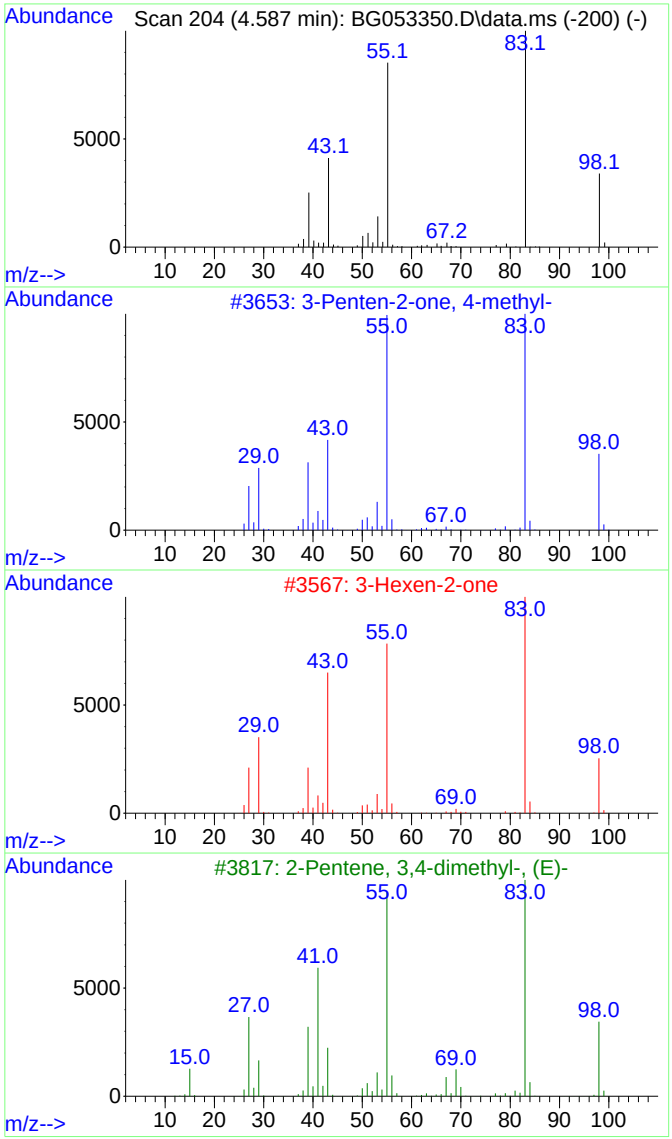
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

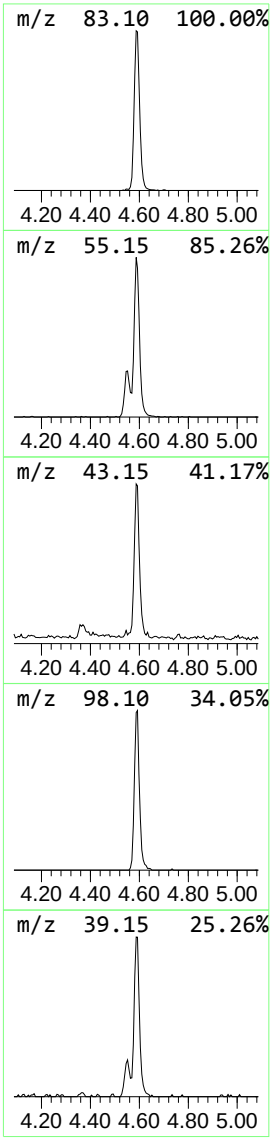
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.587	43.37 ng	331391	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	64





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Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

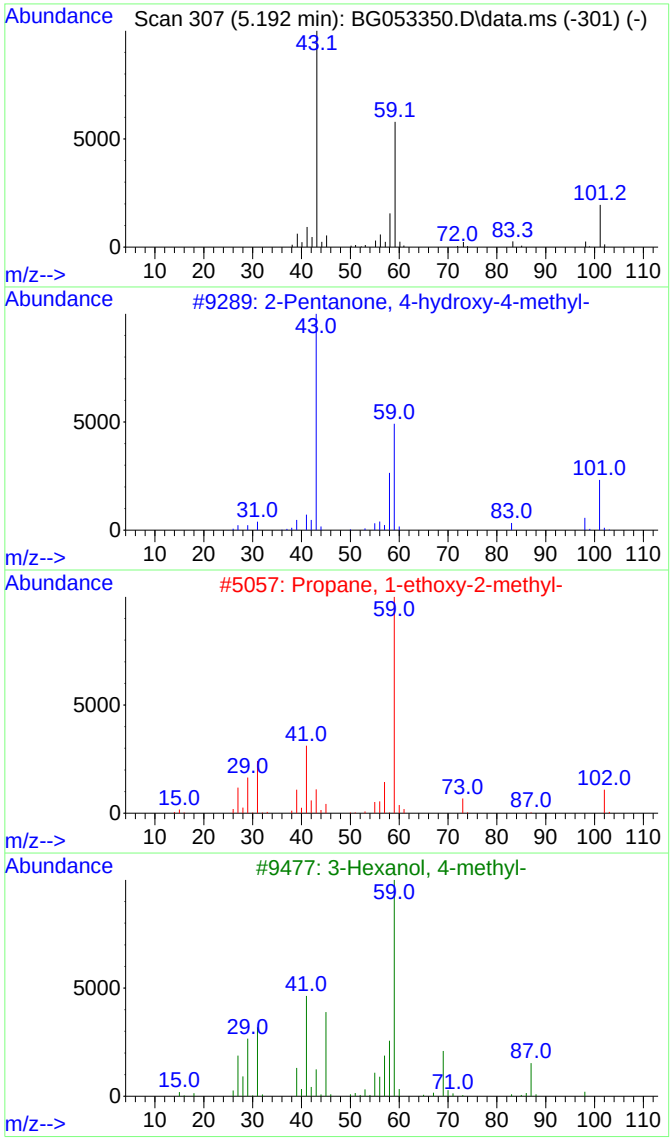
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

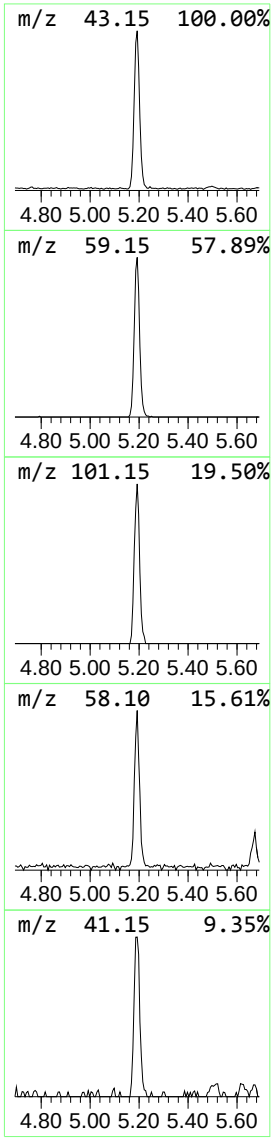
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	31.98 ng	244410	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	25





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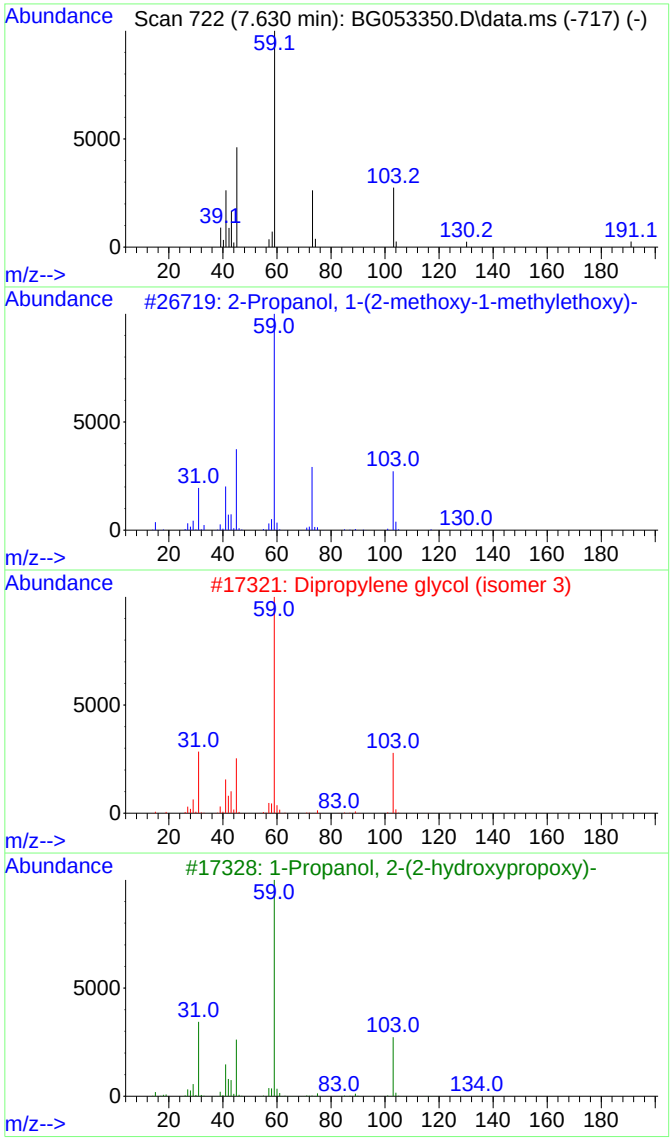
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

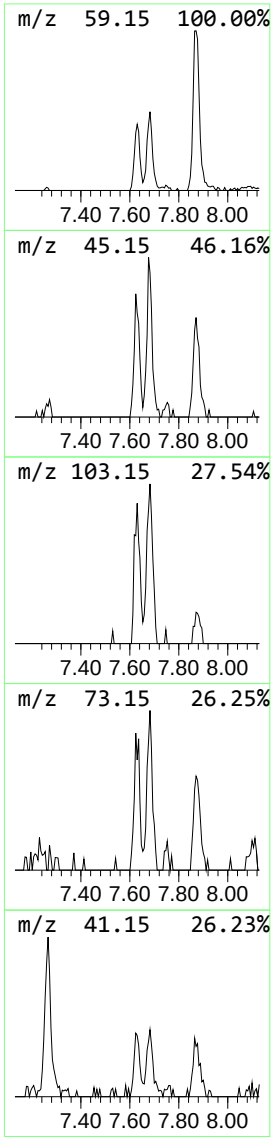
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.630	3.78 ng	28856	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	42
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
4	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	39
5	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	39





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Sample : N2481-06
Misc :
ALS Vial : 12 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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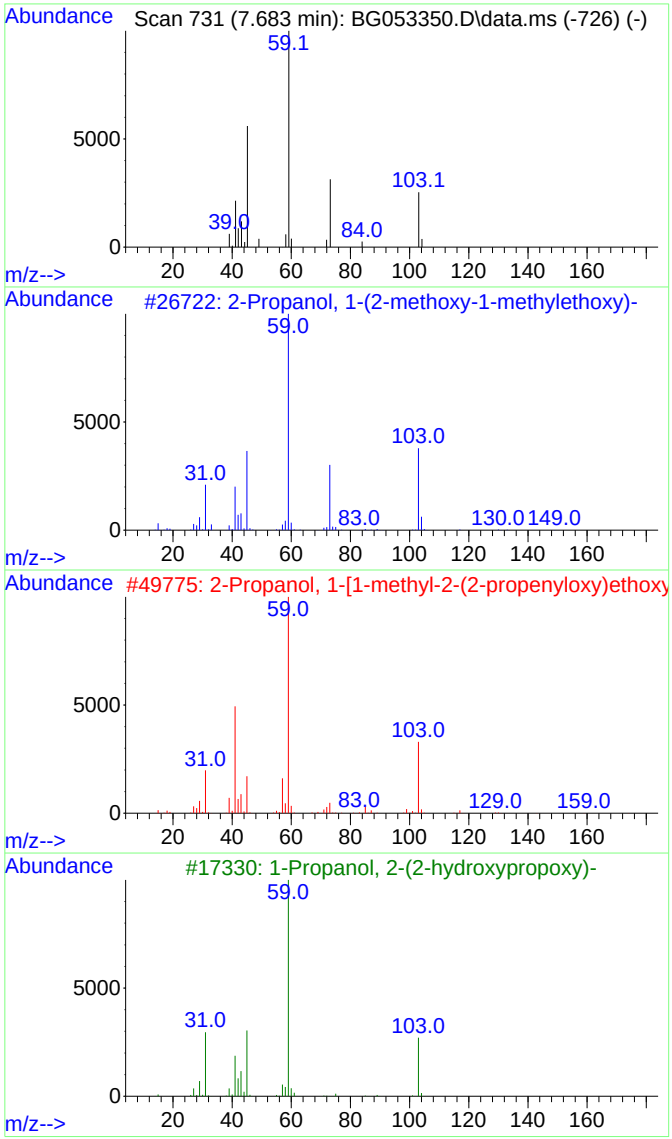
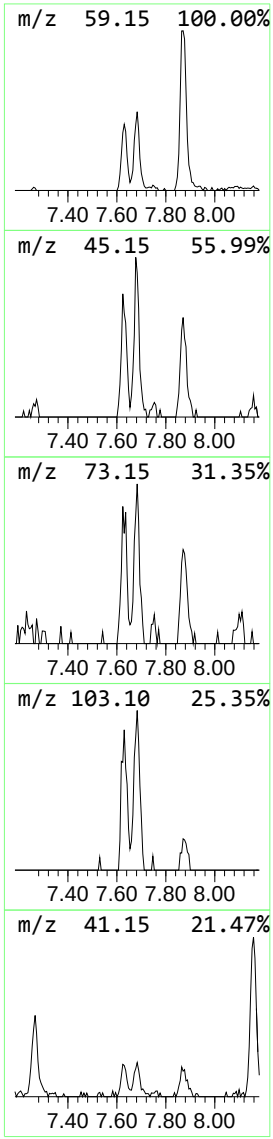
****

Peak Number 6 unknown7.683 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.683	4.22 ng	32227	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	42
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	36





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Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

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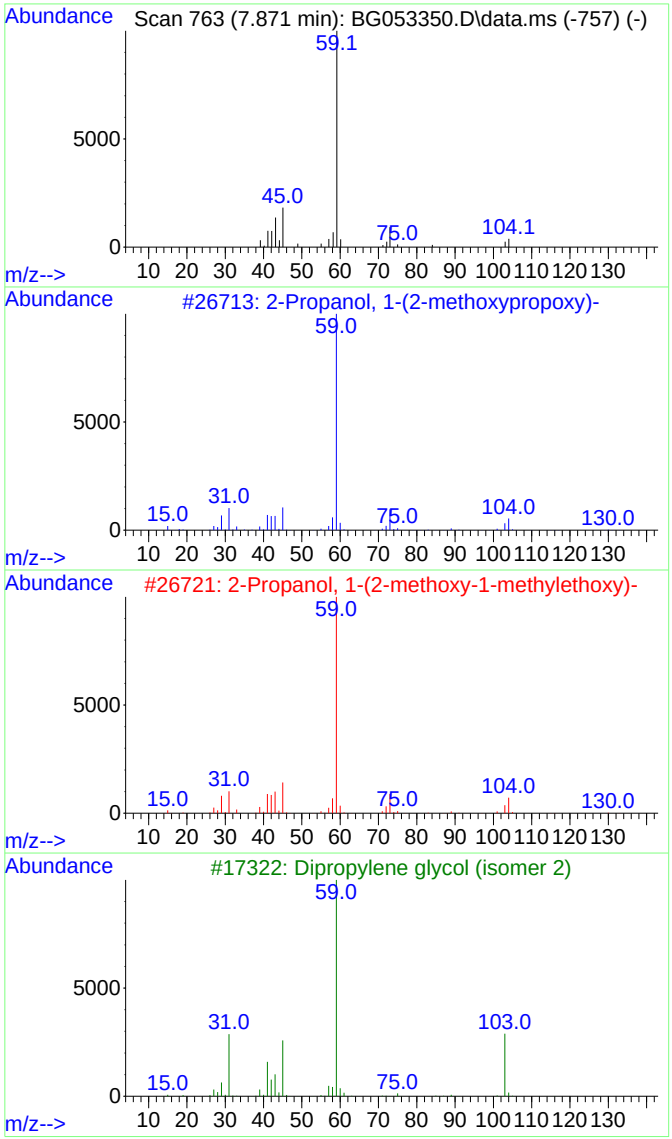
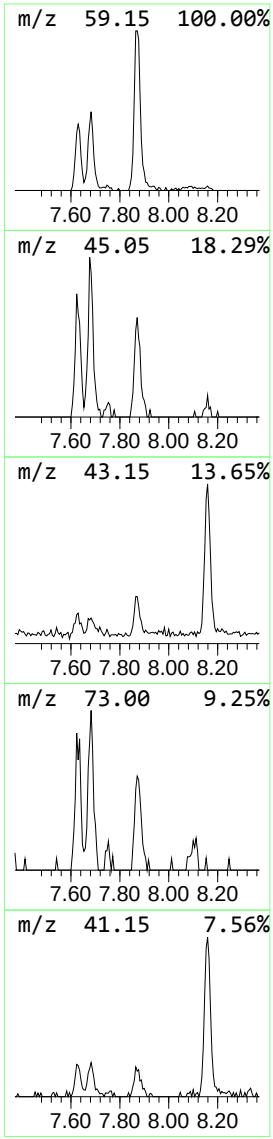
****

Peak Number 7 2-Propanol, 1-(2-methoxypro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.871	6.96 ng	53193	1,4-Dichlorobenzene-d4	8.106

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	78
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64





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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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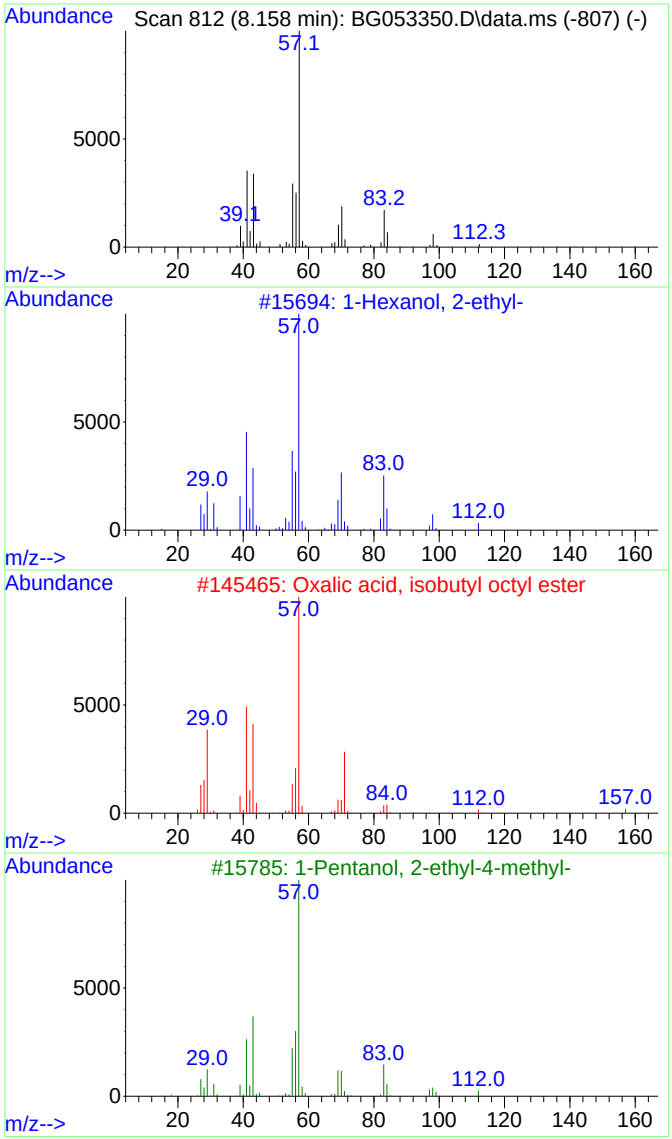
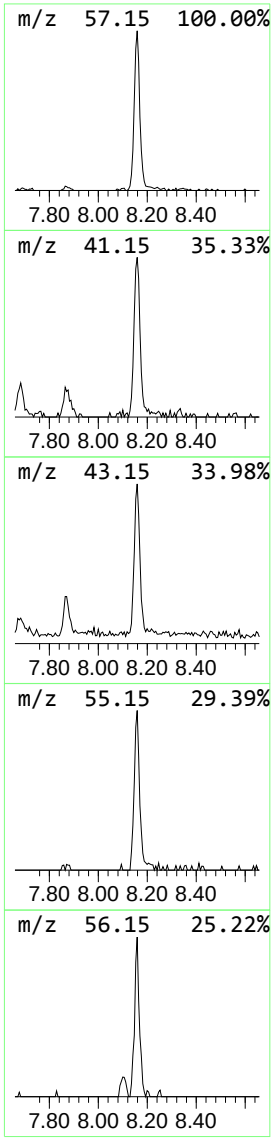
****

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	16.12 ng	123197	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	74
2	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50





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Instrument :
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ClientSampleId :
GES-2R

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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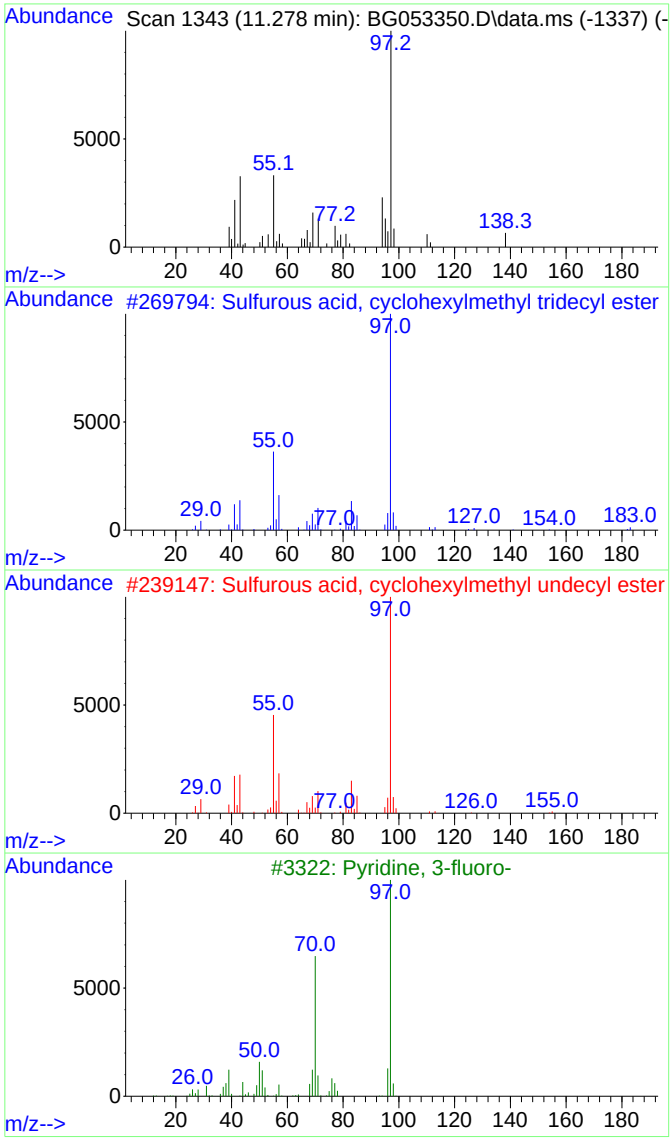
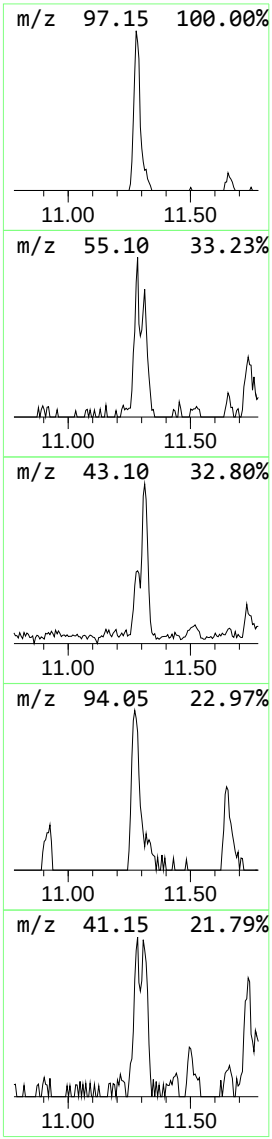
****
Peak Number 9 Sulfurous acid, cyclohexylm... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.278	5.74 ng	62578	Naphthalene-d8	10.914

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	50
2	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	50
3	Pyridine, 3-fluoro-	97	C5H4FN	000372-47-4	42
4	Bis(2-isopropyl-5-methylcyclohex...	372	C21H41O3P	1000510-36-9	40
5	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053350.D
Acq On : 27 Apr 2022 16:48
Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

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

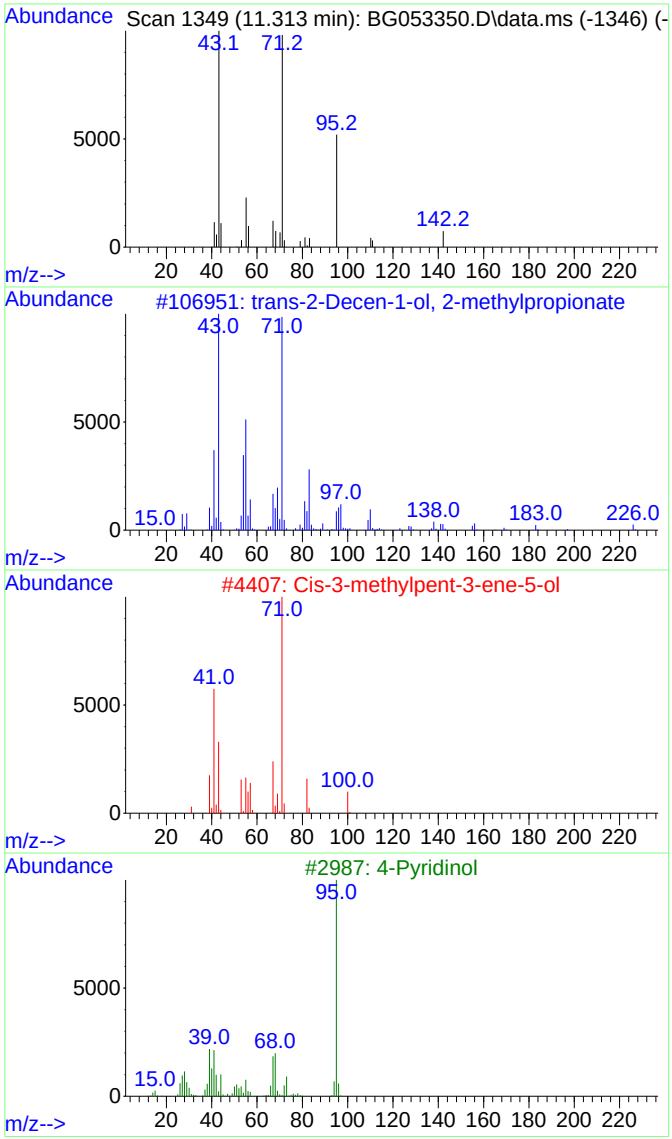
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

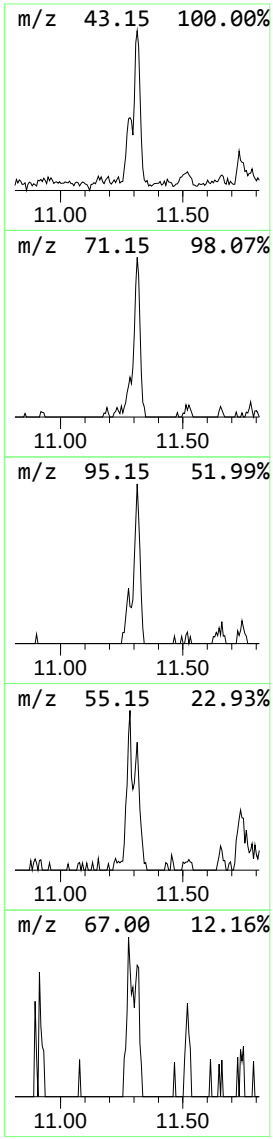
****

Peak Number 10 unknown11.313 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.313	5.23 ng	57003	Naphthalene-d8	10.914

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Decen-1-ol, 2-methylprop...	226	C14H26O2	1010447-32-4	28
2	Cis-3-methylpent-3-ene-5-ol	100	C6H12O	030804-75-2	23
3	4-Pyridinol	95	C5H5NO	000626-64-2	9
4	3-Pyridinol	95	C5H5NO	000109-00-2	9
5	6-Hepten-1-ol, 2-methyl-	128	C8H16O	1000132-12-0	9





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Data File : BG053350.D
Acq On : 27 Apr 2022 16:48
Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

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

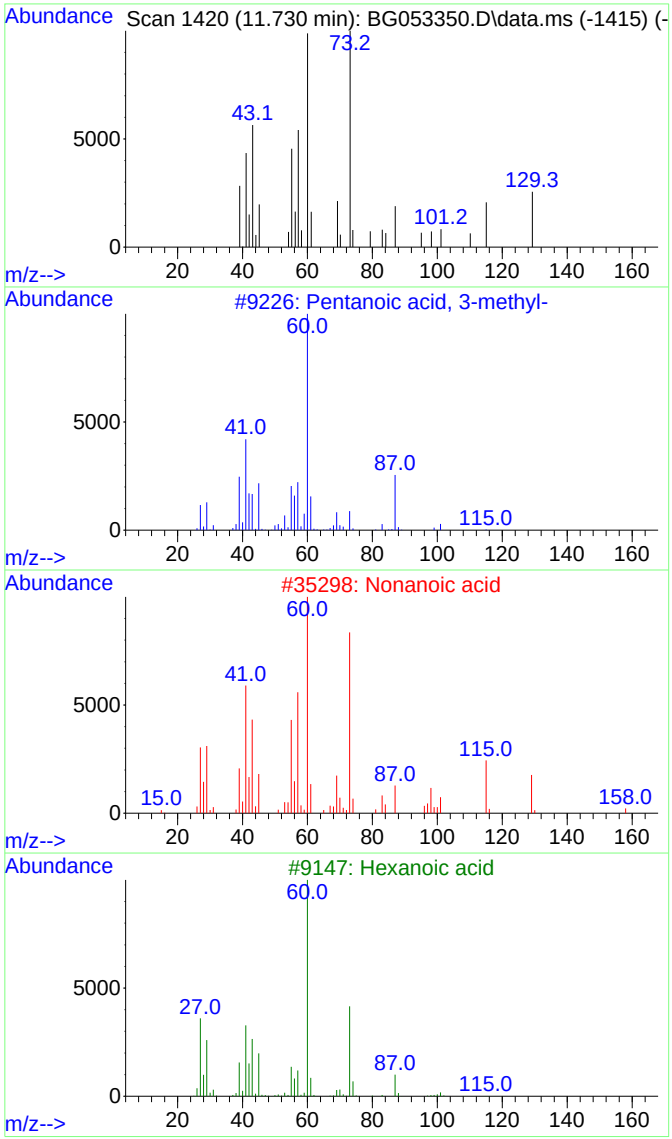
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

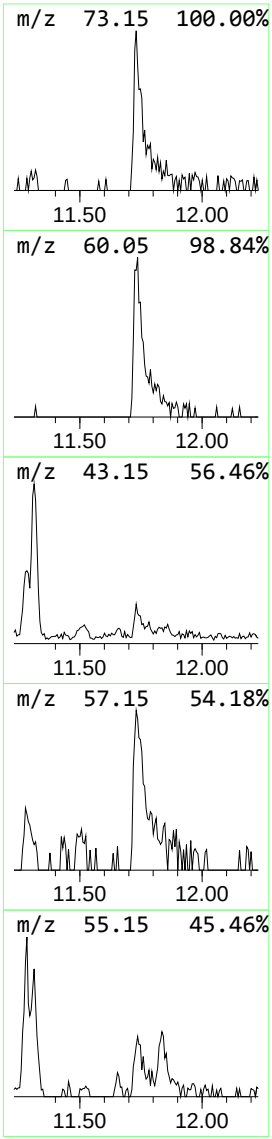
****

Peak Number 11 Pentanoic acid, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.730	3.93 ng	42805	Naphthalene-d8	10.914

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	50
2	Nonanoic acid	158	C9H18O2	000112-05-0	50
3	Hexanoic acid	116	C6H12O2	000142-62-1	40
4	Pentanoic acid	102	C5H10O2	000109-52-4	38
5	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053350.D
Acq On : 27 Apr 2022 16:48
Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

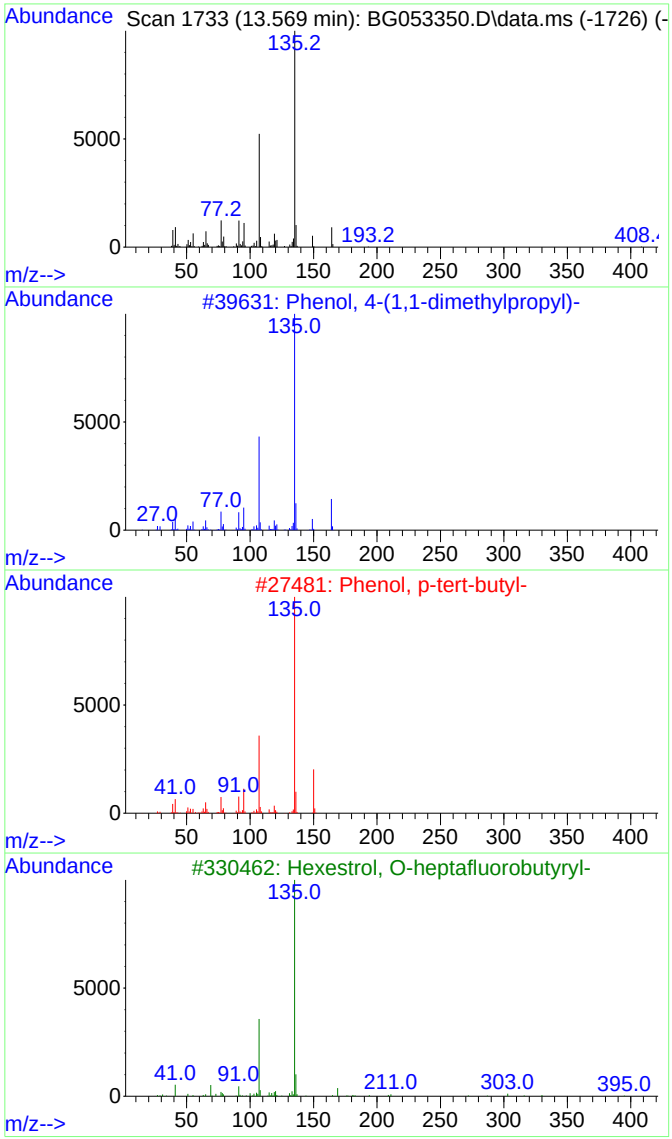
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

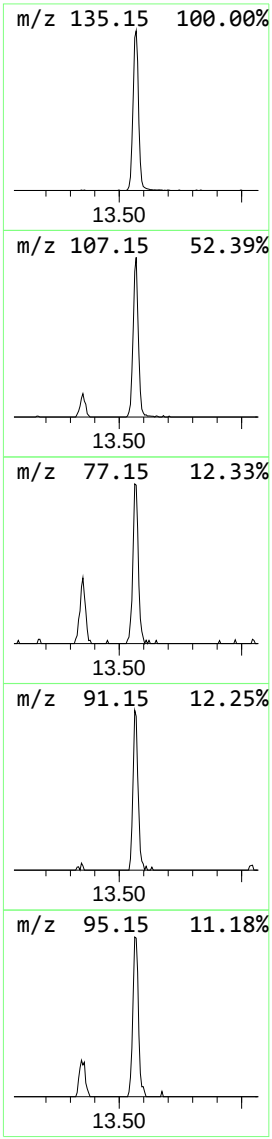
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Phenol, 4-(1,1-dimethylprop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.569	20.41 ng	328074	Acenaphthene-d10	14.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	64
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	64





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Data File : BG053350.D
Acq On : 27 Apr 2022 16:48
Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

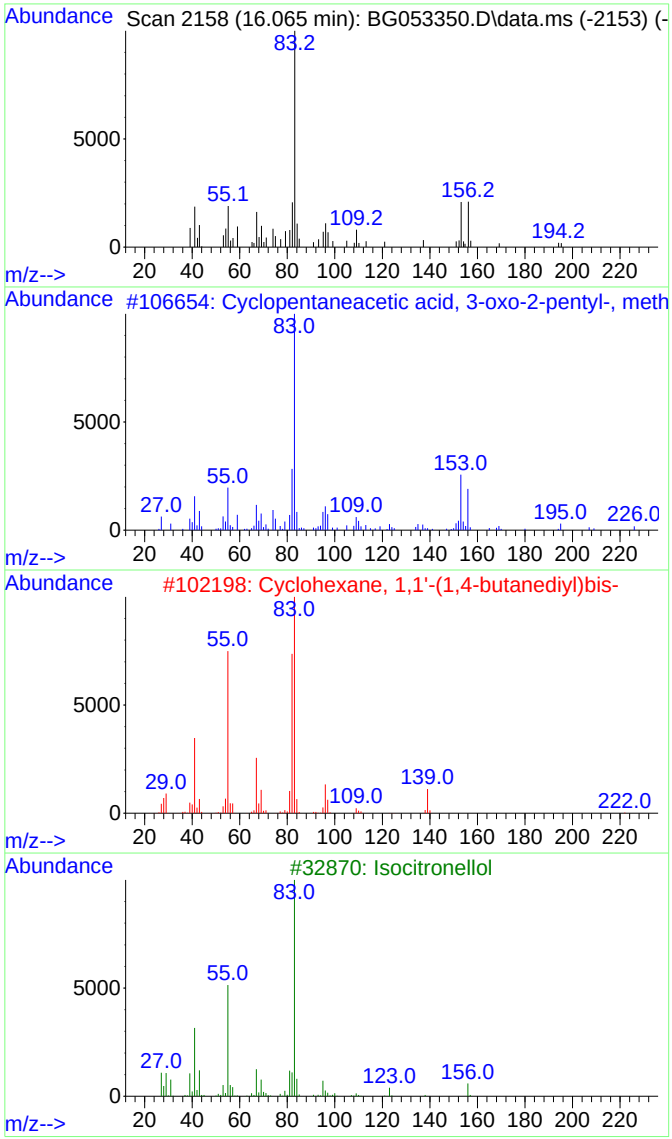
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

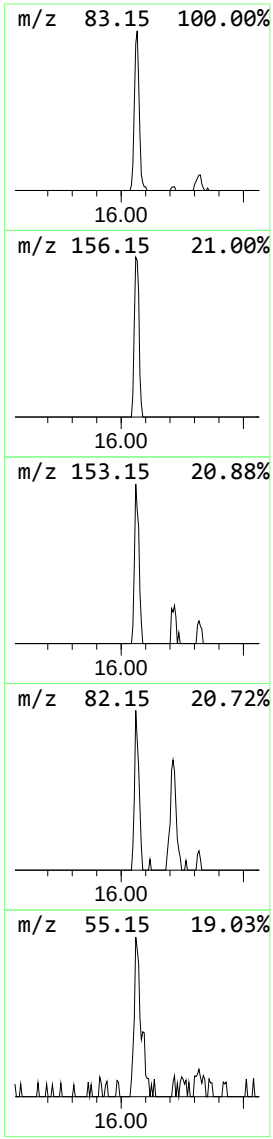
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Cyclopentaneacetic acid, 3-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.065	3.59 ng	57746	Acenaphthene-d10	14.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	78
2	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	43
3	Isocitronellol	156	C10H20O	018479-52-2	42
4	Prop-2-ynyl (E)-2-methylbut-2-en...	138	C8H10O2	1000373-72-5	38
5	Cyclohexane, butyl-	140	C10H20	001678-93-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053350.D
Acq On : 27 Apr 2022 16:48
Operator : CG/JU
Sample : N2481-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-2R

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
4-Penten-2-one,...	3.982	4.7	ng	36253	1	8.106	152831	20.0
Cyclopentanone	4.546	9.1	ng	69835	1	8.106	152831	20.0
3-Penten-2-one,...	4.587	43.4	ng	331391	1	8.106	152831	20.0
2-Pentanone, 4-...	5.192	32.0	ng	244410	1	8.106	152831	20.0
2-Propanol, 1-(...	7.630	3.8	ng	28856	1	8.106	152831	20.0
unknown7.683	7.683	4.2	ng	32227	1	8.106	152831	20.0
2-Propanol, 1-(...	7.871	7.0	ng	53193	1	8.106	152831	20.0
1-Hexanol, 2-et...	8.158	16.1	ng	123197	1	8.106	152831	20.0
Sulfurous acid,...	11.278	5.7	ng	62578	2	10.914	217924	20.0
unknown11.313	11.313	5.2	ng	57003	2	10.914	217924	20.0
Pentanoic acid,...	11.730	3.9	ng	42805	2	10.914	217924	20.0
Phenol, 4-(1,1-...	13.569	20.4	ng	328074	3	14.726	321415	20.0
Cyclopentaneace...	16.065	3.6	ng	57746	3	14.726	321415	20.0