LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
Data File : BG053365.D
Acq On : 28 Apr 2022 14:11
Operator : CG/JU
Sample : N2482-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

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: BG053365.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	208	rBV	71671	119461	3.42%	0.946%
2	5.188	301	306	313	rVB	29364	45147	1.29%	0.358%
3	5.670	382	388	400	rVB	404142	658637	18.86%	5.217%
4	7.262	652	659	674	rVB	296087	531827	15.23%	4.213%
5	7.626	716	721	726	rBV	40088	64864	1.86%	0.514%
6	7.679	726	730	736	rVB2	42819	63895	1.83%	0.506%
7	7.867	756	762	772	rBV	64746	112307	3.22%	0.890%
8	8.102	795	802	807	rBV	104321	183425	5.25%	1.453%
9	8.155	807	811	818	rVB	47994	79933	2.29%	0.633%
10	9.265	992	1000	1010	rBV	472780	858055	24.57%	6.797%
11	10.910	1271	1280	1287	rBV	133254	242065	6.93%	1.918%
12	11.715	1412	1417	1425	rBV5	22416	45271	1.30%	0.359%
13	13.084	1644	1650	1658	rBV	56547	95253	2.73%	0.755%
14	13.348	1685	1695	1707	rBV	1151972	2008738	57.52%	15.912%
15	13.565	1724	1732	1738	rBV	208137	310952	8.90%	2.463%
16	14.728	1923	1930	1936	rVB	215494	351919	10.08%	2.788%
17	15.527	2060	2066	2073	rVB	44255	64211	1.84%	0.509%
18	16.062	2151	2157	2168	rBV	41461	63557	1.82%	0.503%
19	16.215	2176	2183	2196	rBV	1053485	1666877	47.73%	13.204%
20	17.472	2390	2397	2403	rBV	294208	457725	13.11%	3.626%
21	20.080	2834	2841	2846	rBV	2532616	3492073	100.00%	27.663%
22	21.754	3120	3126	3137	rVB	336503	557233	15.96%	4.414%
23	25.050	3676	3687	3699	rVB3	181996	550268	15.76%	4.359%

Sum of corrected areas: 12623693

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
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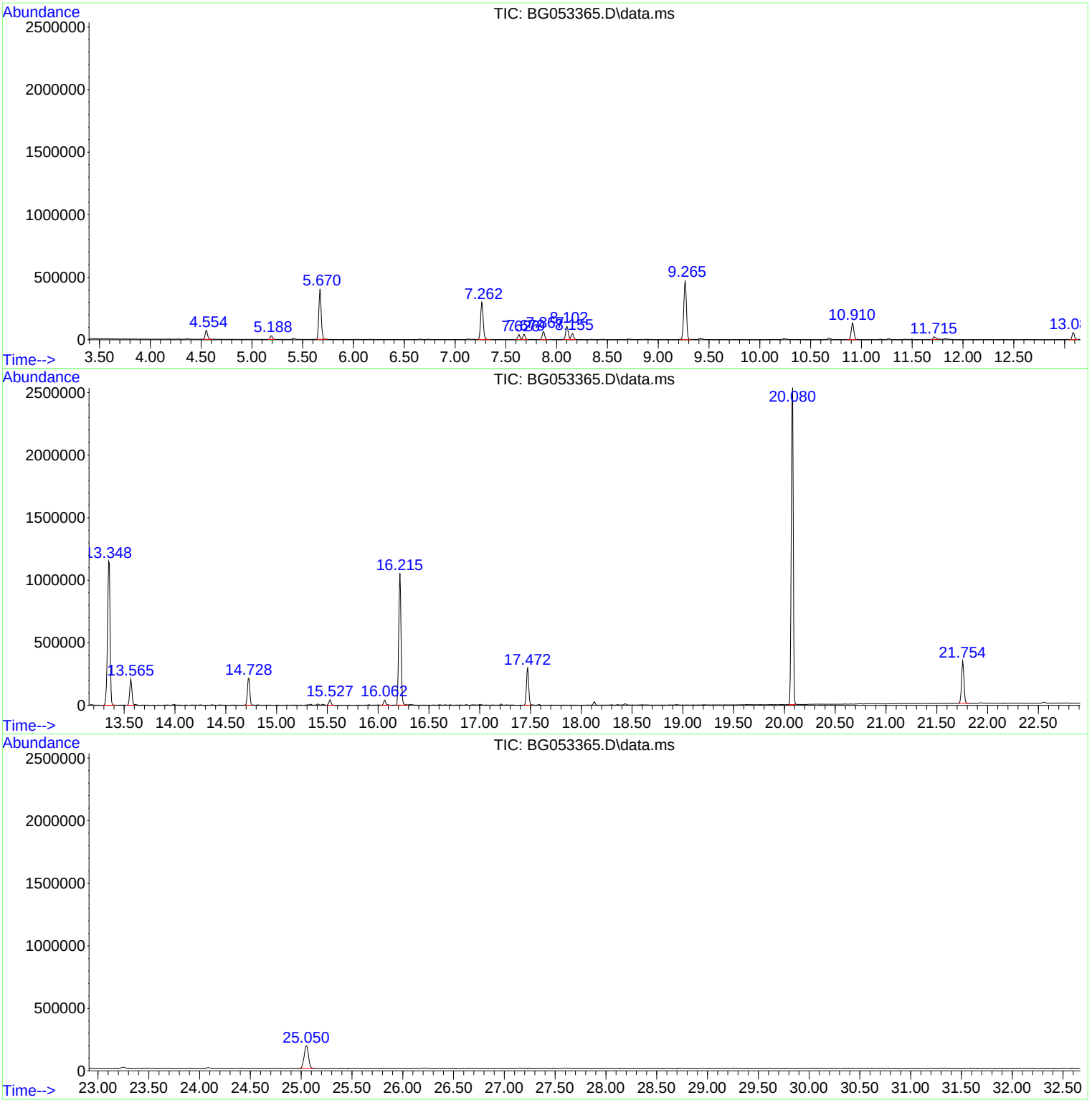
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

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 : BG053365.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

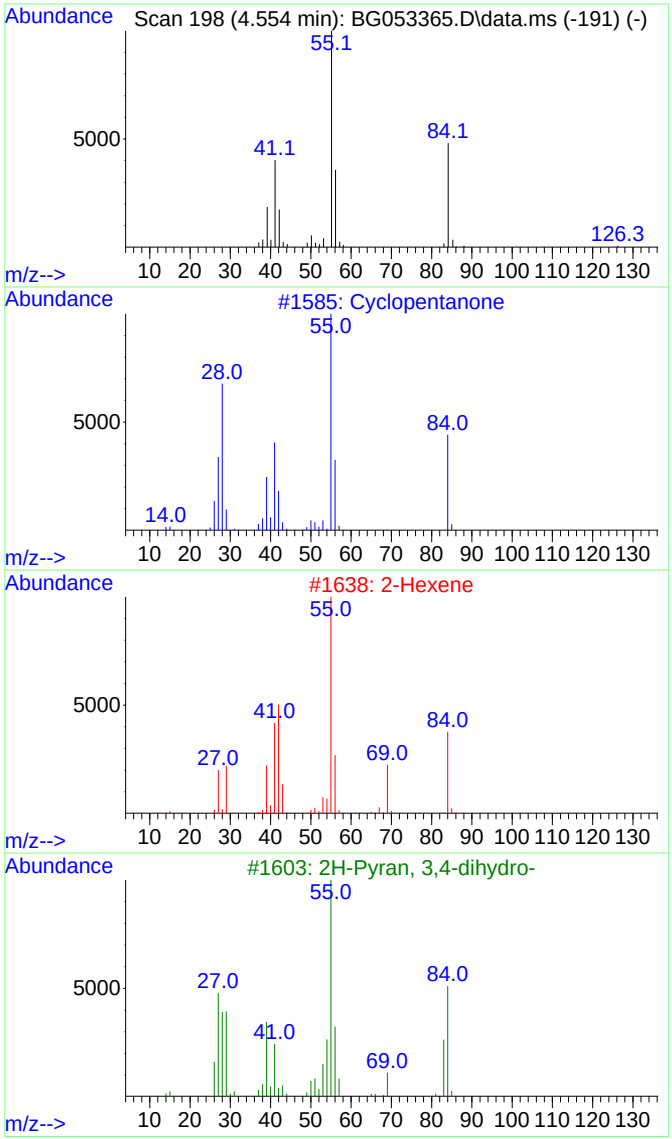
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

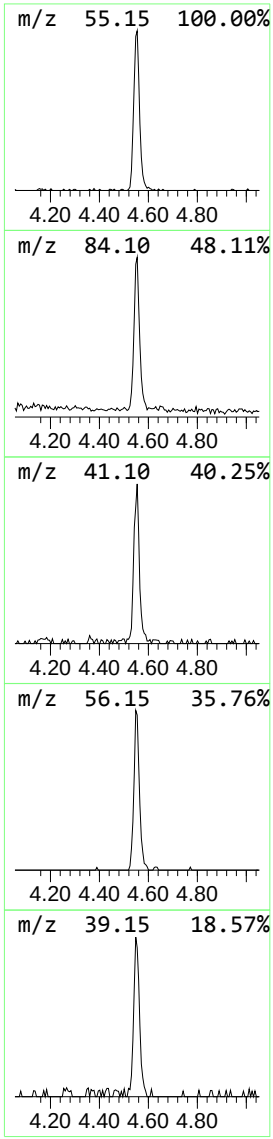
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.554	13.03 ng	119461	1,4-Dichlorobenzene-d4	8.102

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	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	58
4	2-Hexene, (Z)-	84	C6H12	007688-21-3	56
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	53





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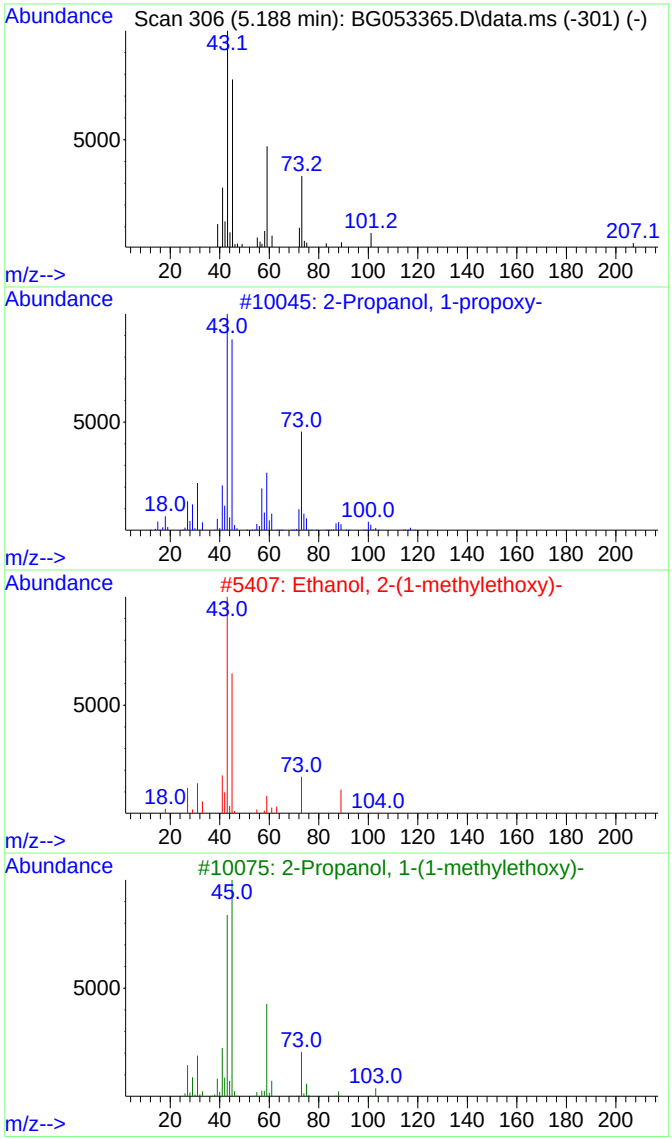
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

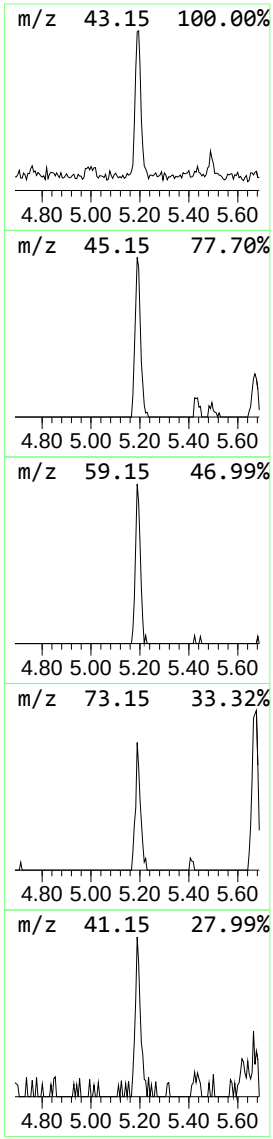
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanol, 1-propoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.188	4.92 ng	45147	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	64
2	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	53
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	2-[2-[2-[2-[2-[2-(2-Methoxyet...	384	C17H36O9	025990-96-9	45
5	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	42





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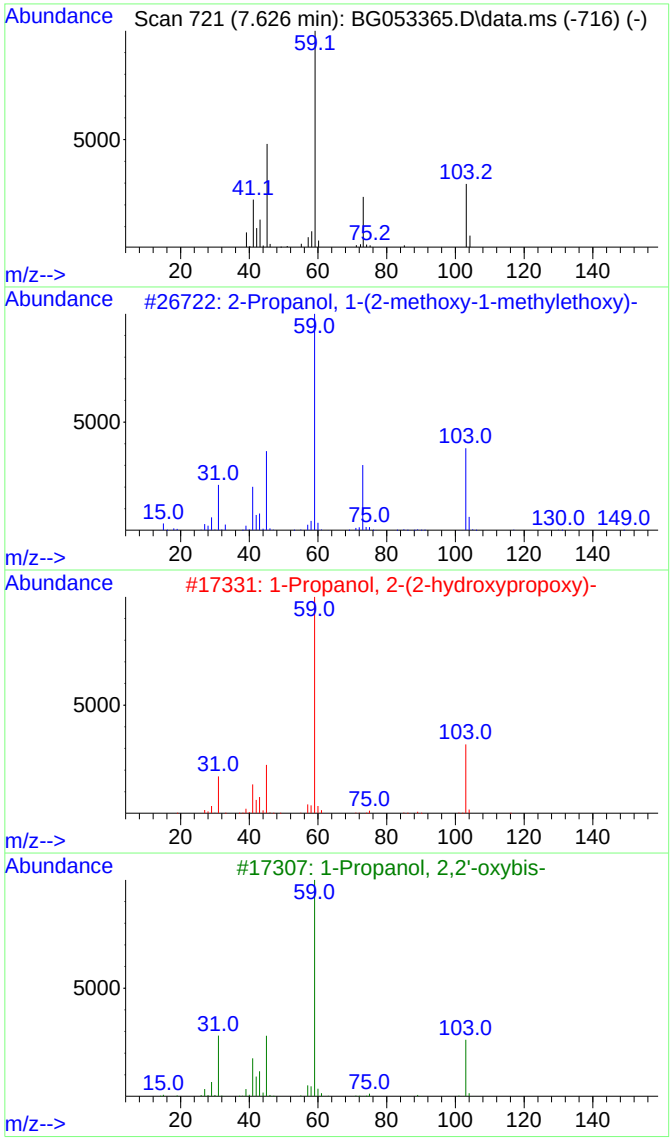
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

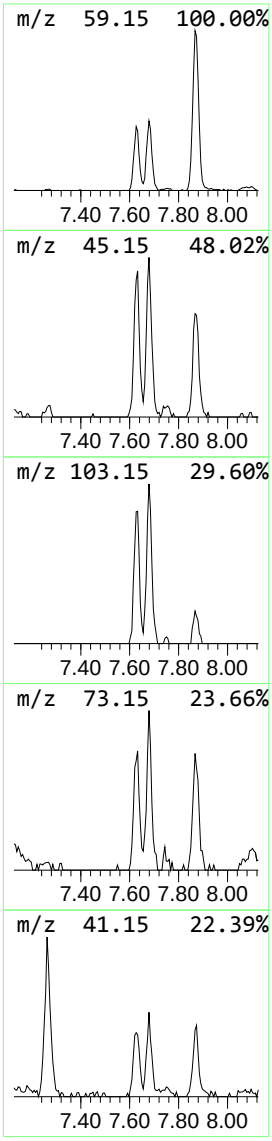
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.626	7.07 ng	64864	1,4-Dichlorobenzene-d4	8.102

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	53
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50





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ALS Vial : 7 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
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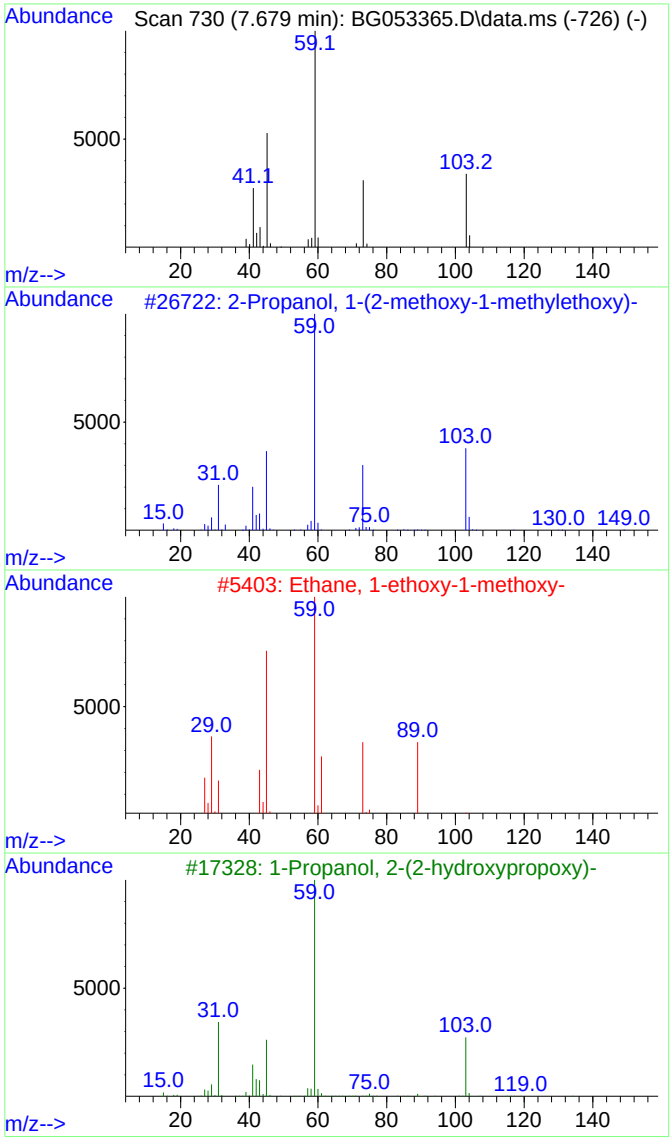
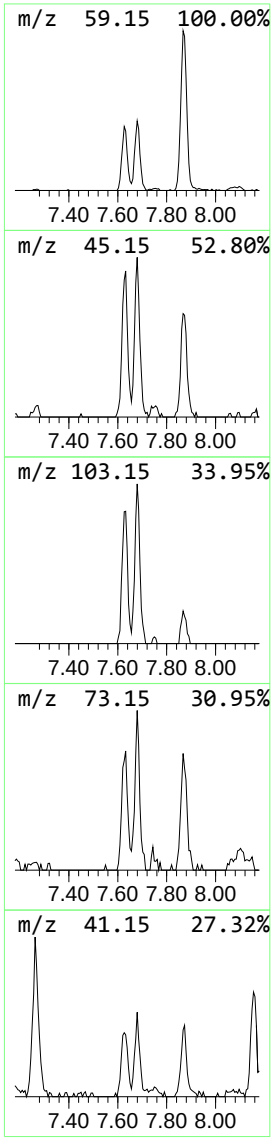
****

Peak Number 4 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.679	6.97 ng	63895	1,4-Dichlorobenzene-d4	8.102

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	59
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	Ethyl ether	74	C4H10O	000060-29-7	38
5	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	36





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Operator : CG/JU
Sample : N2482-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

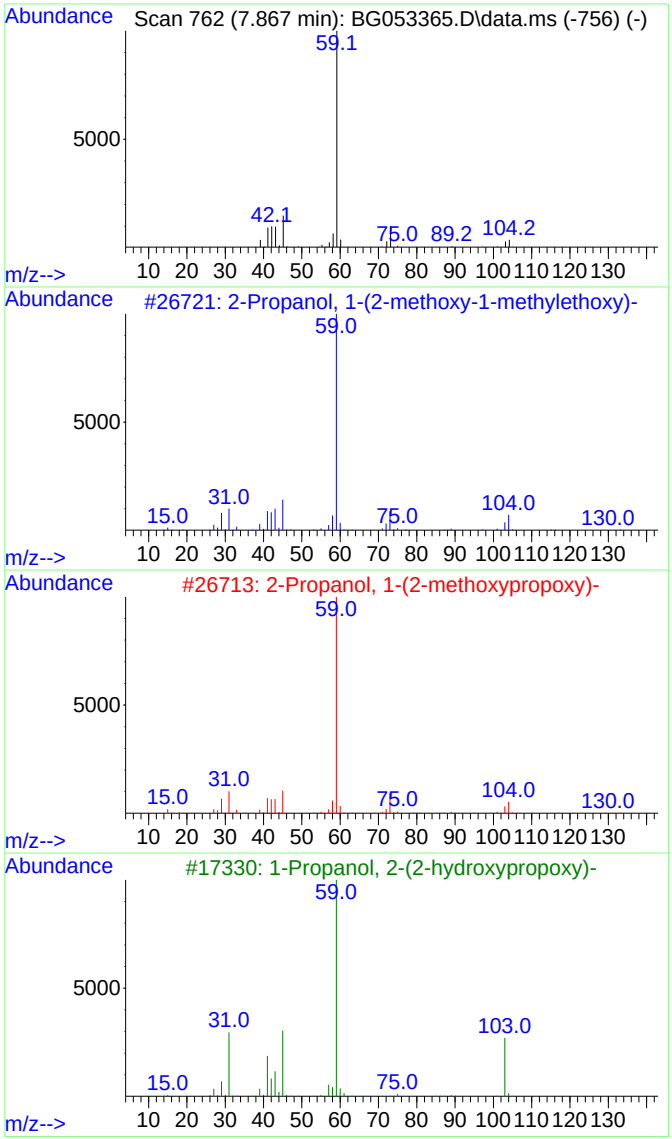
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

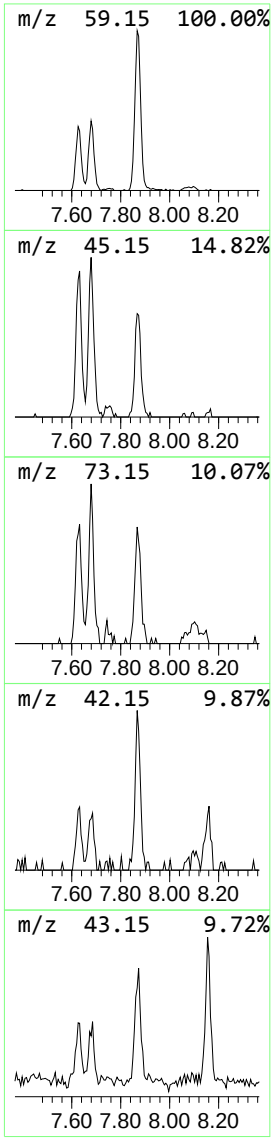
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.867	12.25 ng	112307	1,4-Dichlorobenzene-d4	8.102

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	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50
5	Tetraglyme	222	C10H22O5	000143-24-8	45





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Sample : N2482-10
Misc :
ALS Vial : 7 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

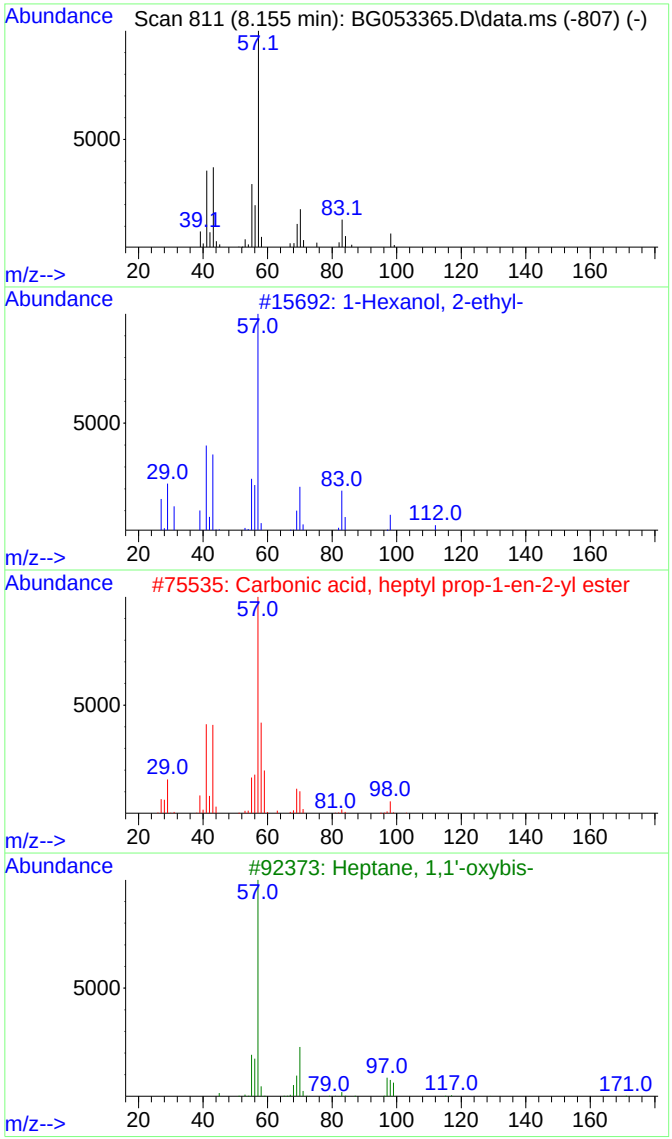
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

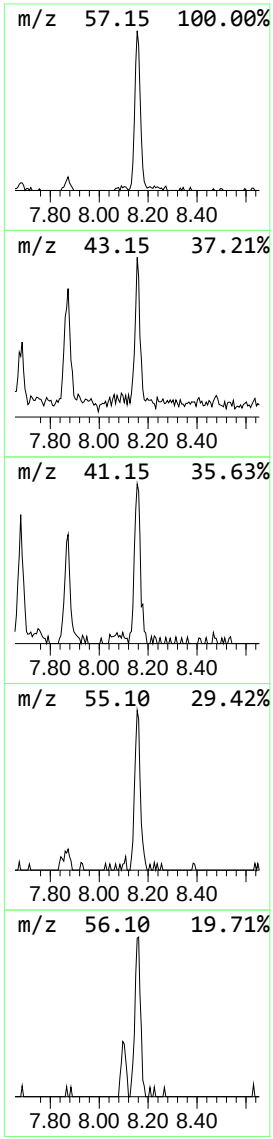
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.155	8.72 ng	79933	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
4	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53





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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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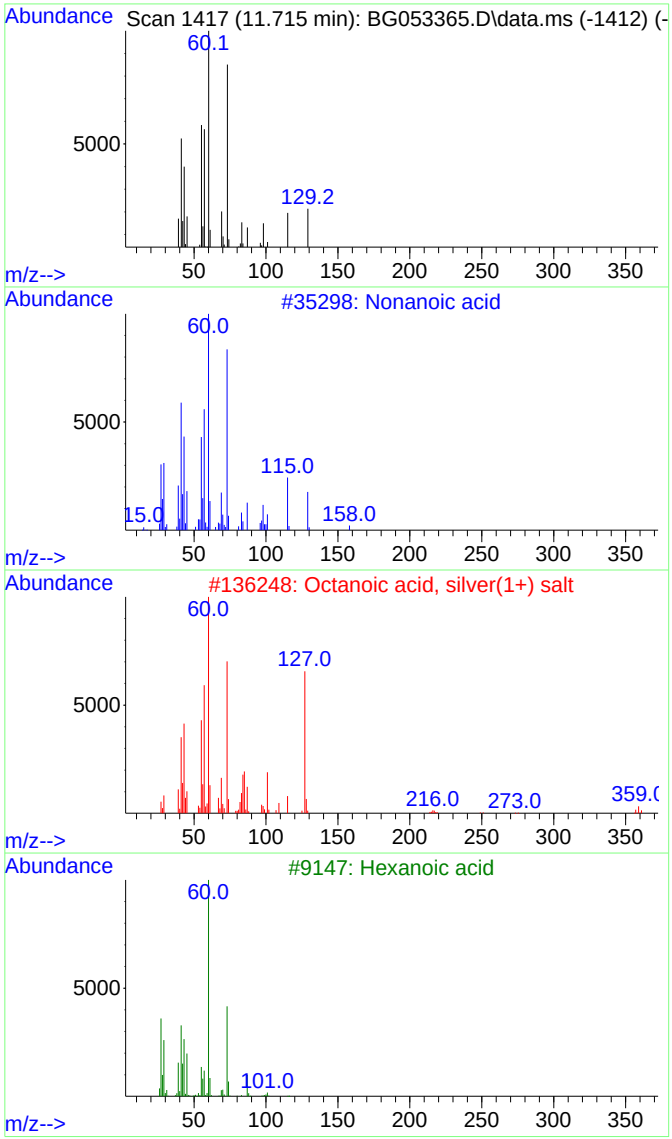
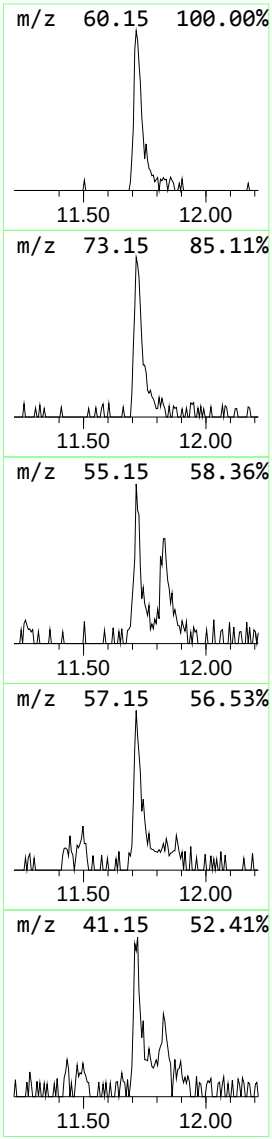
****

Peak Number 7 Nonanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.715	3.74 ng	45271	Naphthalene-d8	10.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	86
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	50
3	Hexanoic acid	116	C6H12O2	000142-62-1	50
4	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43





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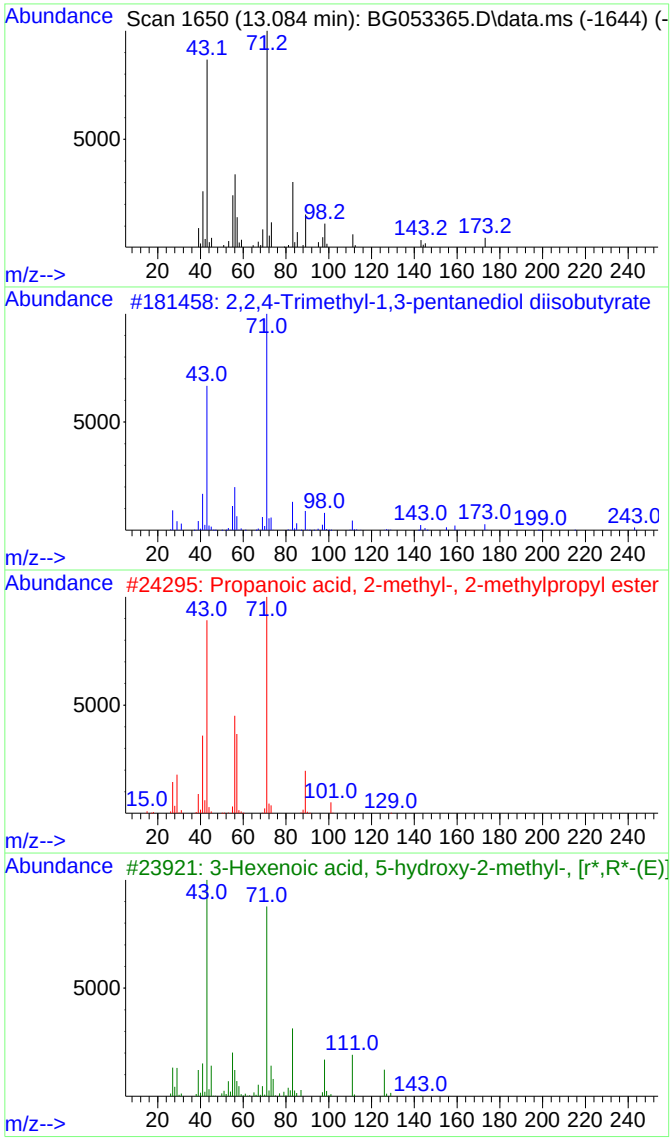
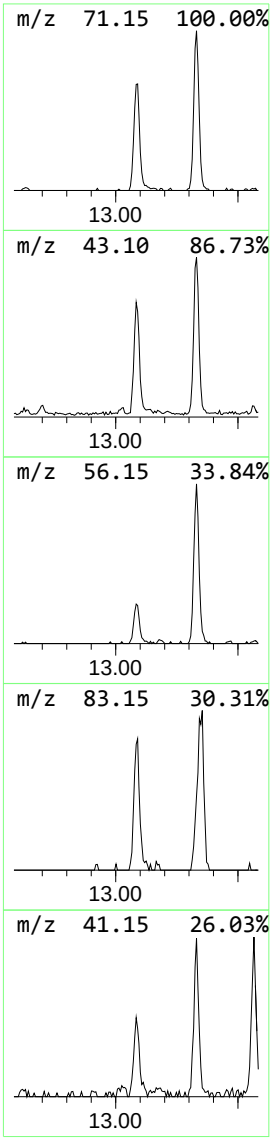
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.084	5.41 ng	95253	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	83
2	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
3	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	50
4	Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	47
5	Cyclohexanecarboxylic acid, 2-te...	212	C12H20O3	1000279-85-7	40





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

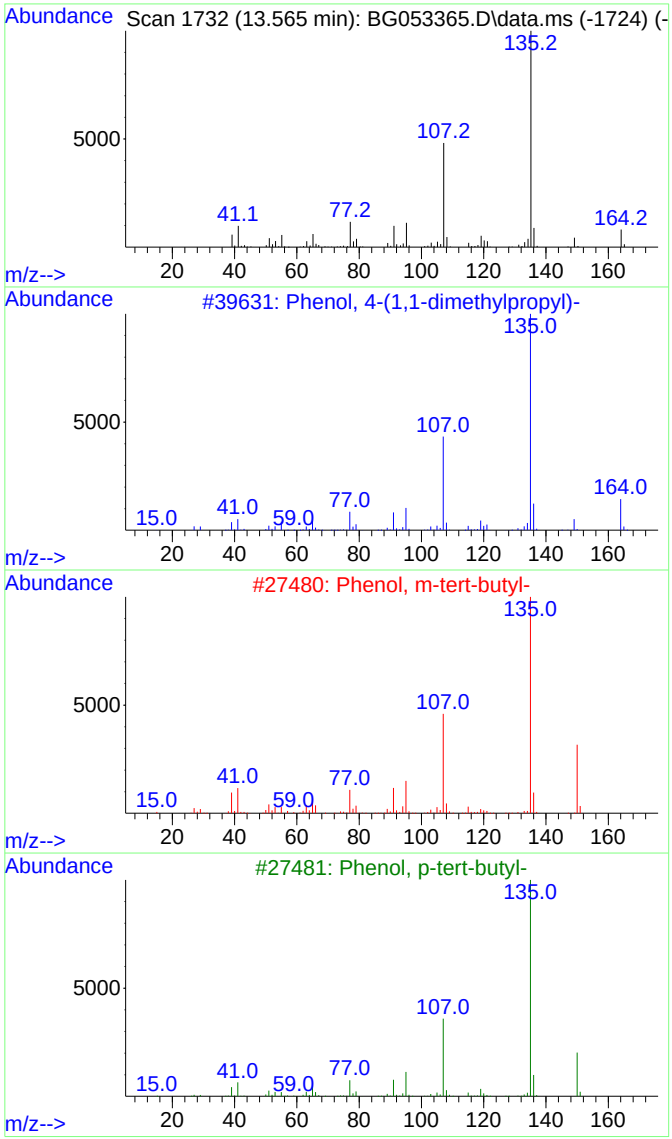
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

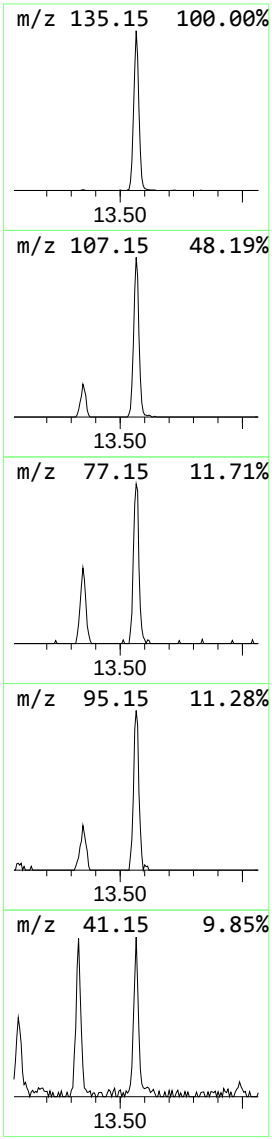
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.565	17.67 ng	310952	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	78
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
4	Hexestrol	270	C18H22O2	000084-16-2	64
5	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64





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Misc :
ALS Vial : 7 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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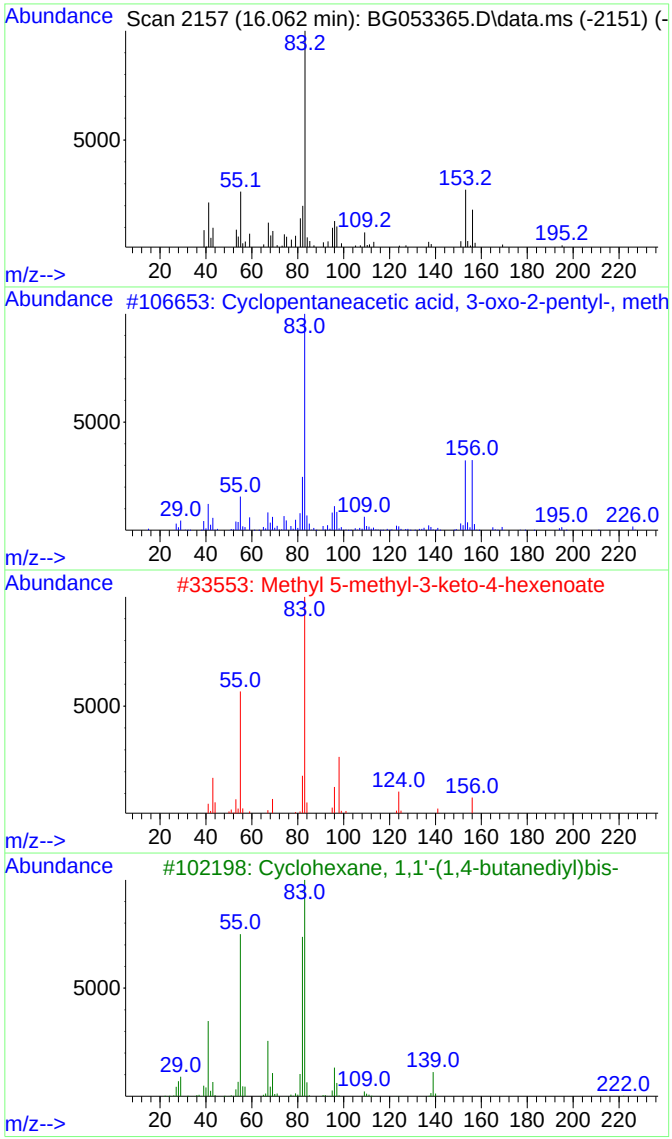
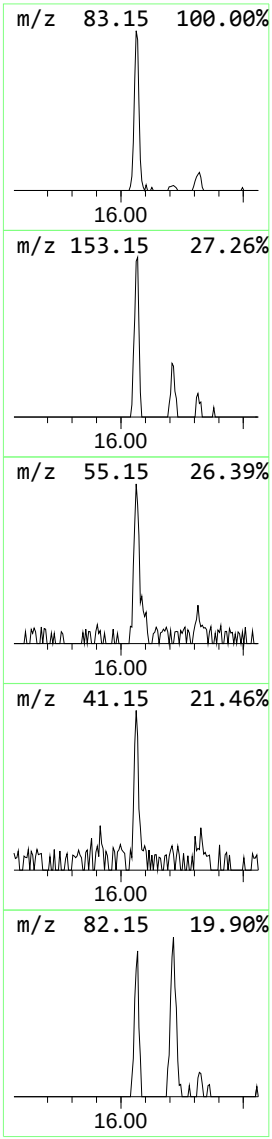
****
Peak Number 10 Cyclopentaneacetic acid, 3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.062	3.61 ng	63557	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	83
2	Methyl 5-methyl-3-keto-4-hexenoate	156	C8H12O3	1000427-08-8	50
3	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	43
4	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	43
5	Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
Data File : BG053365.D
Acq On : 28 Apr 2022 14:11
Operator : CG/JU
Sample : N2482-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

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	13.0	ng	119461	1	8.102	183425	20.0
2-Propanol, 1-p...	5.188	4.9	ng	45147	1	8.102	183425	20.0
2-Propanol, 1-(...	7.626	7.1	ng	64864	1	8.102	183425	20.0
Ethane, 1-ethox...	7.679	7.0	ng	63895	1	8.102	183425	20.0
2-Propanol, 1-(...	7.867	12.3	ng	112307	1	8.102	183425	20.0
1-Hexanol, 2-et...	8.155	8.7	ng	79933	1	8.102	183425	20.0
Nonanoic acid	11.715	3.7	ng	45271	2	10.910	242065	20.0
2,2,4-Trimethyl...	13.084	5.4	ng	95253	3	14.728	351919	20.0
Phenol, 4-(1,1-...	13.565	17.7	ng	310952	3	14.728	351919	20.0
Cyclopentaneace...	16.062	3.6	ng	63557	3	14.728	351919	20.0