LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053356.D
Acq On : 28 Apr 2022 1:57
Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COP-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: BG053356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.270	144	150	157	rVB2	25567	42382	1.36%	0.343%
2	5.192	302	307	315	rVB	23115	36988	1.19%	0.300%
3	5.668	382	388	395	rBV	447080	730764	23.44%	5.922%
4	5.738	395	400	410	rVB3	22054	51806	1.66%	0.420%
5	6.108	457	463	473	rBV	23063	40973	1.31%	0.332%
6	7.266	652	660	667	rBV	352455	622971	19.98%	5.049%
7	7.630	716	722	726	rBV	30035	48606	1.56%	0.394%
8	7.683	726	731	737	rVB	30771	47279	1.52%	0.383%
9	7.871	756	763	773	rBV	51118	87209	2.80%	0.707%
10	8.106	794	803	808	rBV	99149	178633	5.73%	1.448%
11	8.158	808	812	817	rVB2	33998	57441	1.84%	0.466%
12	9.269	993	1001	1013	rVB	473528	874287	28.05%	7.085%
13	10.914	1273	1281	1287	rBV	128441	236810	7.60%	1.919%
14	13.087	1644	1651	1660	rBV	32043	52519	1.68%	0.426%
15	13.351	1687	1696	1703	rBV	1280157	2035980	65.31%	16.500%
16	13.569	1724	1733	1739	rBV	236470	376445	12.08%	3.051%
17	14.726	1924	1930	1938	rVB	218420	344462	11.05%	2.792%
18	16.065	2154	2158	2167	rVB3	21411	33667	1.08%	0.273%
19	16.218	2177	2184	2195	rBV	988268	1619925	51.96%	13.128%
20	17.469	2392	2397	2403	rBV	273901	428793	13.75%	3.475%
21	18.127	2504	2509	2515	rVB2	78743	106047	3.40%	0.859%
22	19.290	2700	2707	2713	rVB2	61479	85339	2.74%	0.692%
23	20.078	2835	2841	2850	rVB	2379532	3117404	100.00%	25.264%
24	21.382	3058	3063	3072	rBV5	23800	53759	1.72%	0.436%
25	21.758	3120	3127	3133	rVB2	289071	501535	16.09%	4.064%
26	25.053	3677	3688	3700	rVB	177848	527419	16.92%	4.274%

Sum of corrected areas: 12339443

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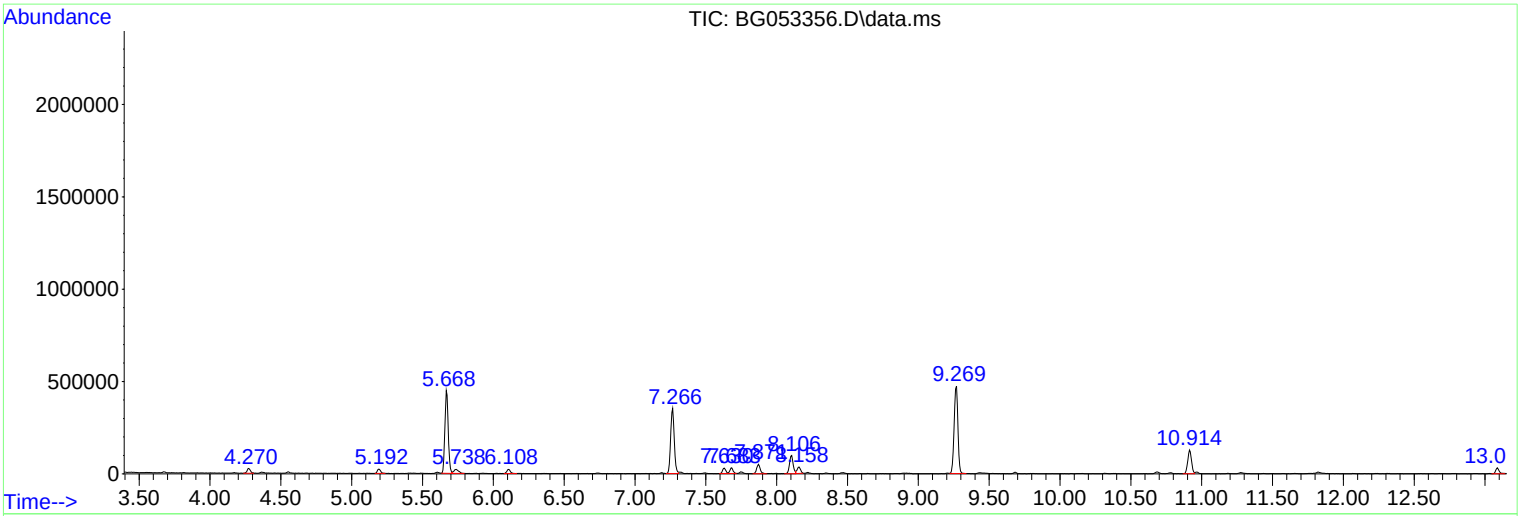
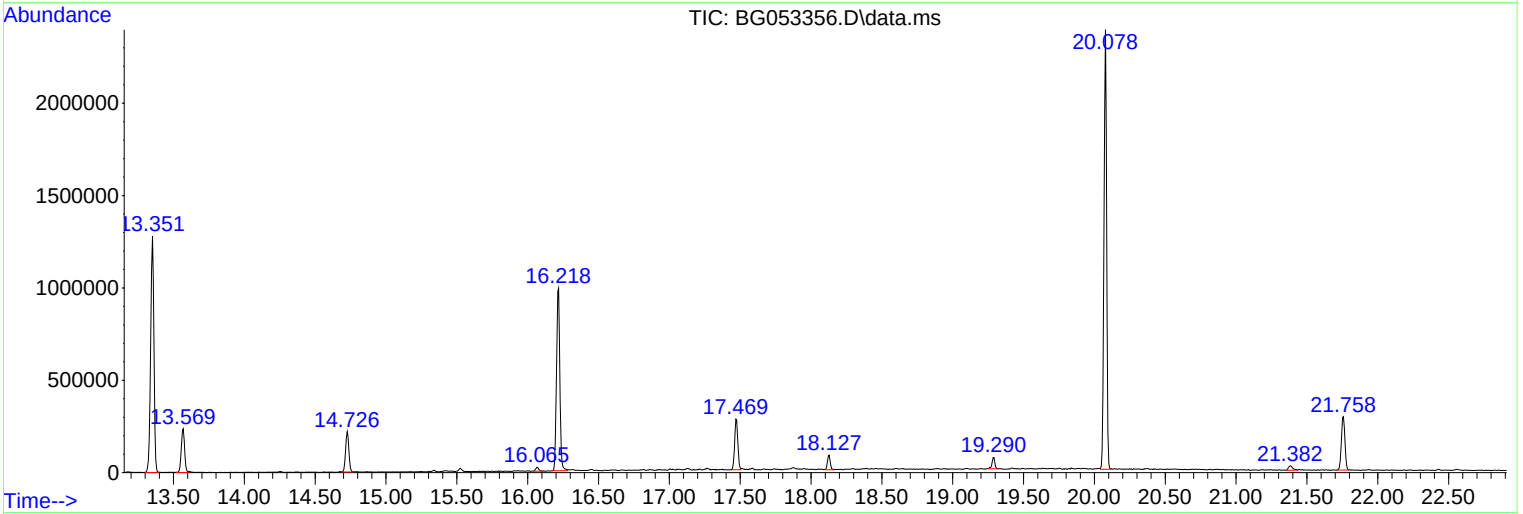
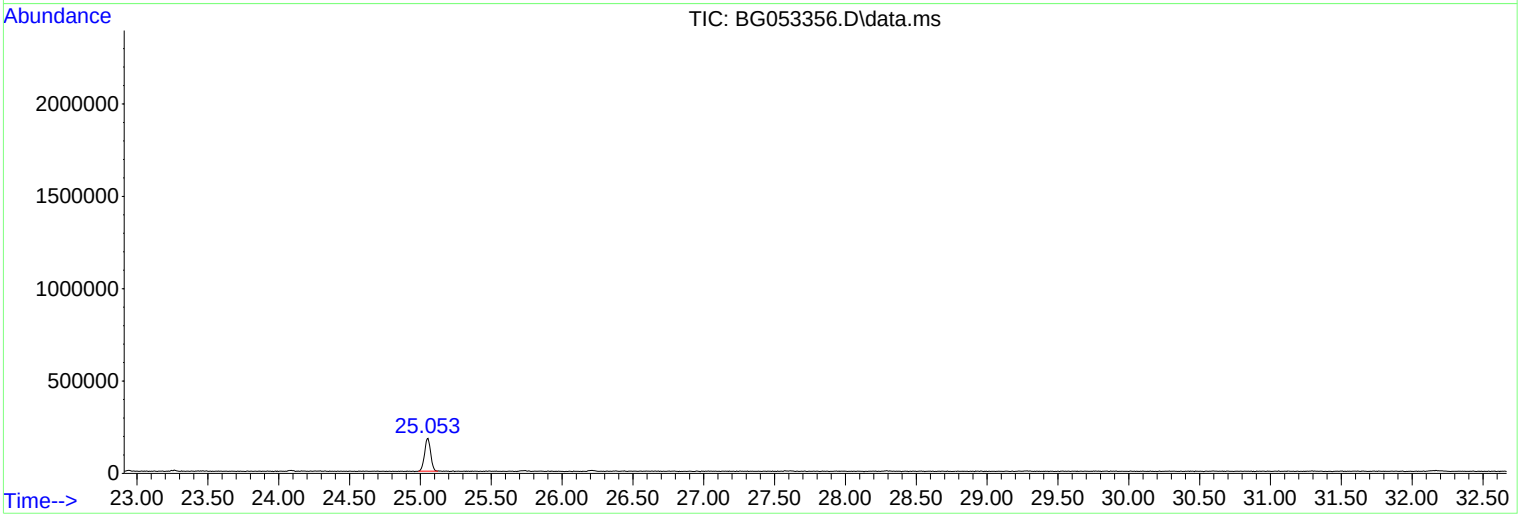
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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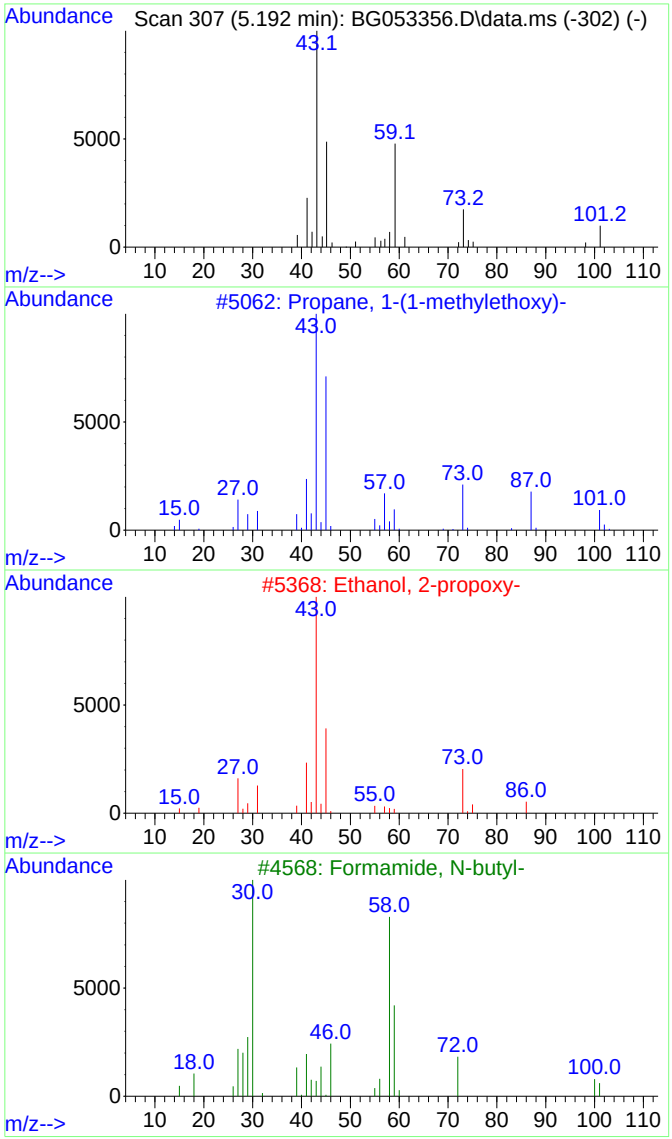
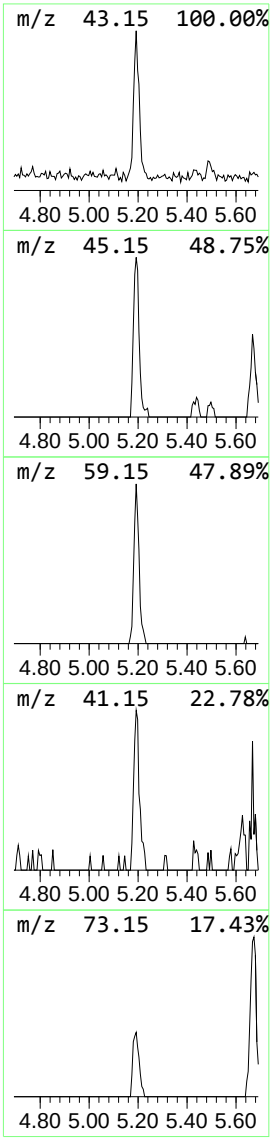
****

Peak Number 2 unknown5.192 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	4.14 ng	36988	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40
2	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	27
3	Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9





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Data File : BG053356.D
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Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-1R

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

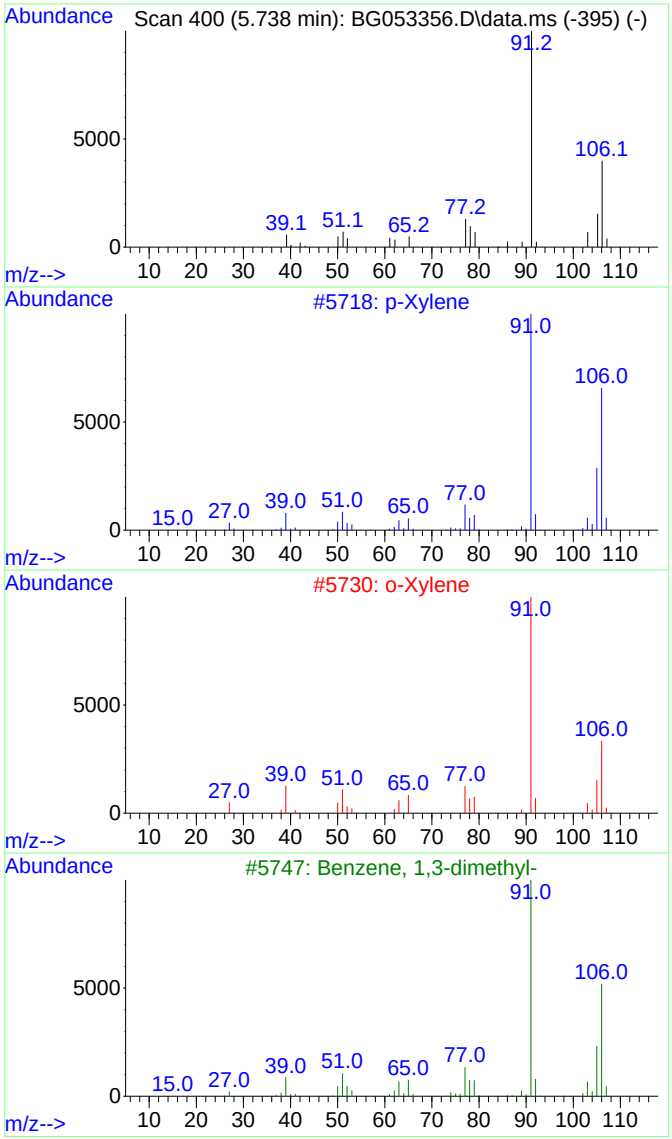
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

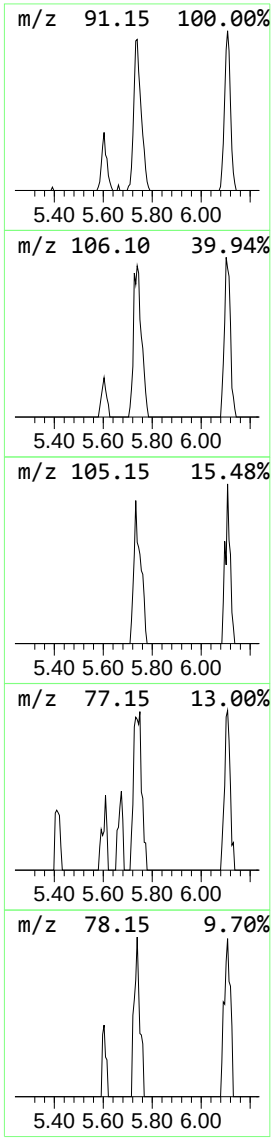
****

Peak Number 3 p-Xylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.738	5.80 ng	51806	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	87
2	o-Xylene	106	C8H10	000095-47-6	87
3	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	83
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	80
5	Ethylbenzene	106	C8H10	000100-41-4	80





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Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-1R

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

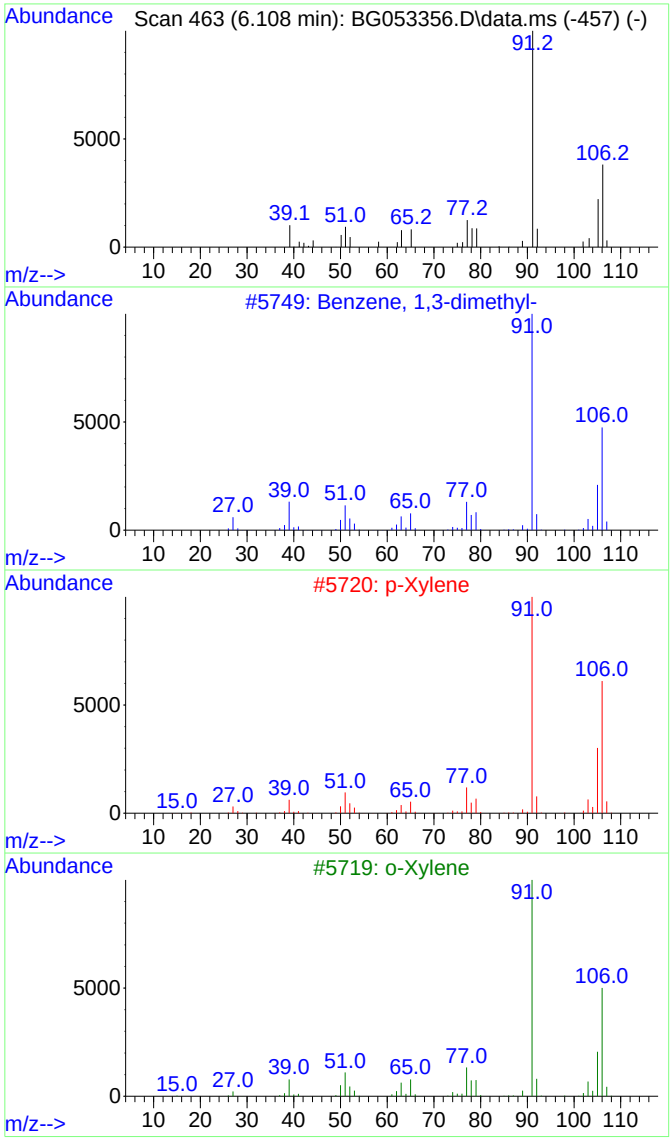
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

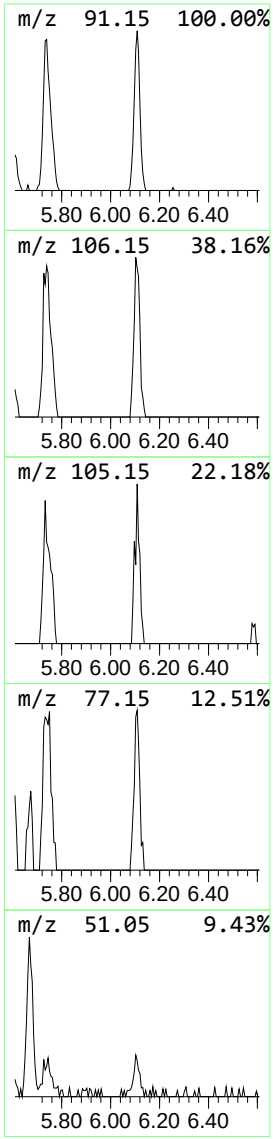
****

Peak Number 4 Benzene, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.108	4.59 ng	40973	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	94
2	p-Xylene	106	C8H10	000106-42-3	91
3	o-Xylene	106	C8H10	000095-47-6	91
4	Ethylbenzene	106	C8H10	000100-41-4	87
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	74





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Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-1R

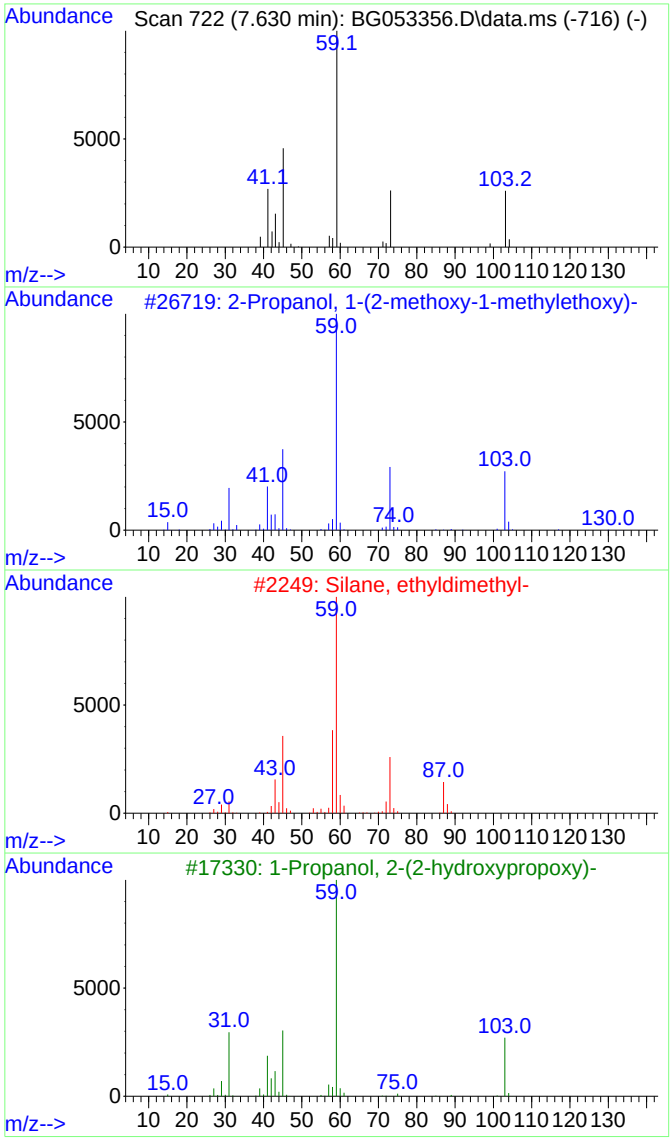
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

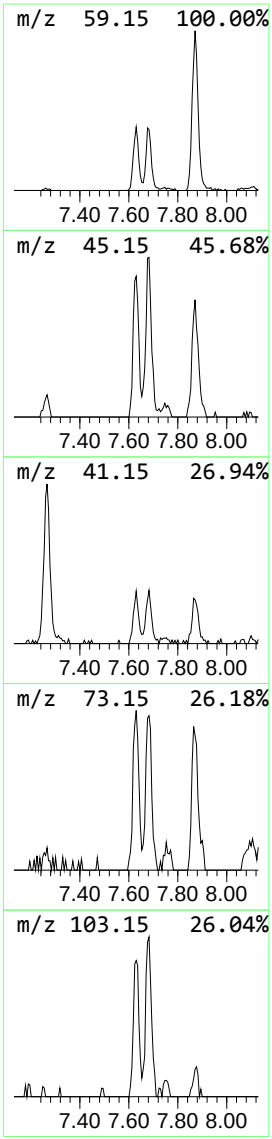
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.630	5.44 ng	48606	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	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	39
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	36
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	33
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	33





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Sample : N2482-04
Misc :
ALS Vial : 18 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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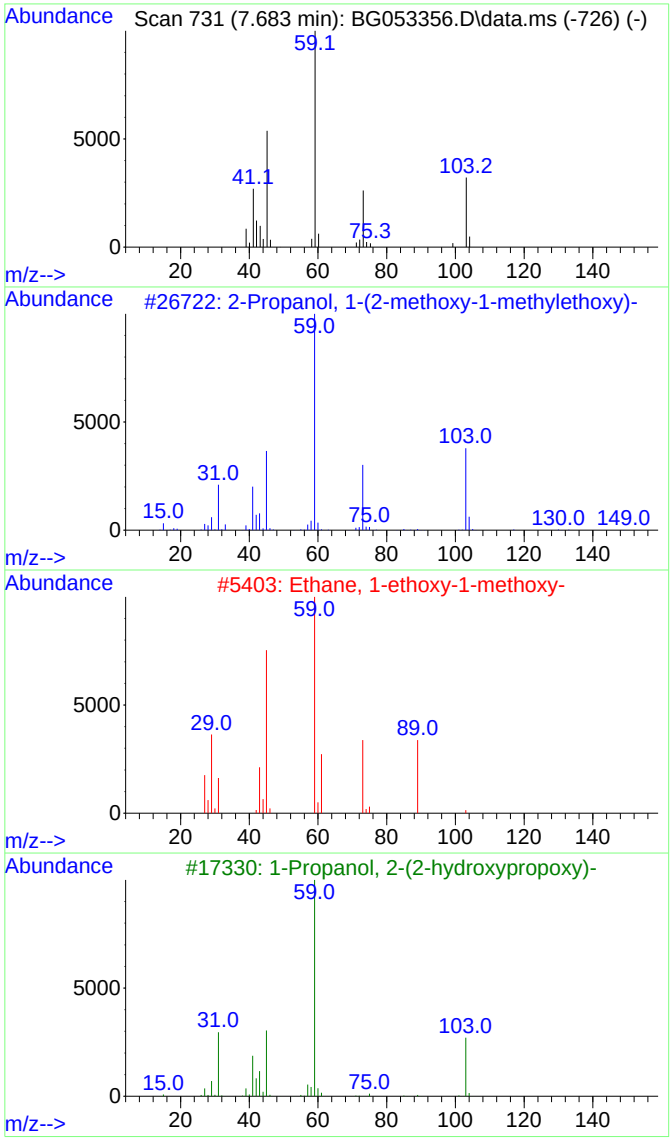
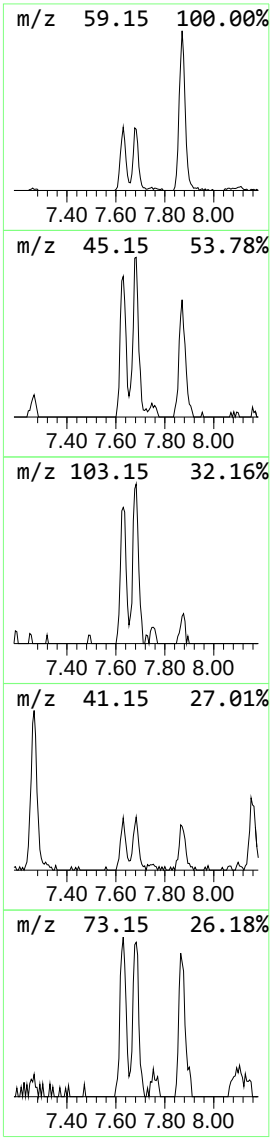
****

Peak Number 6 unknown7.683 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.683	5.29 ng	47279	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	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	45
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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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
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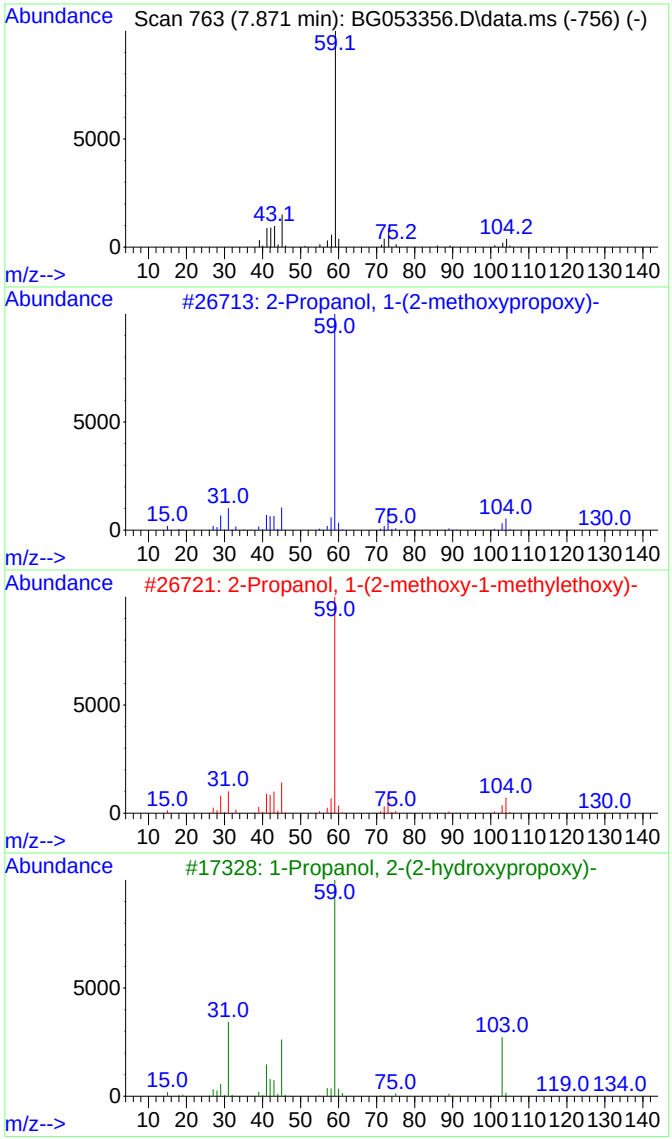
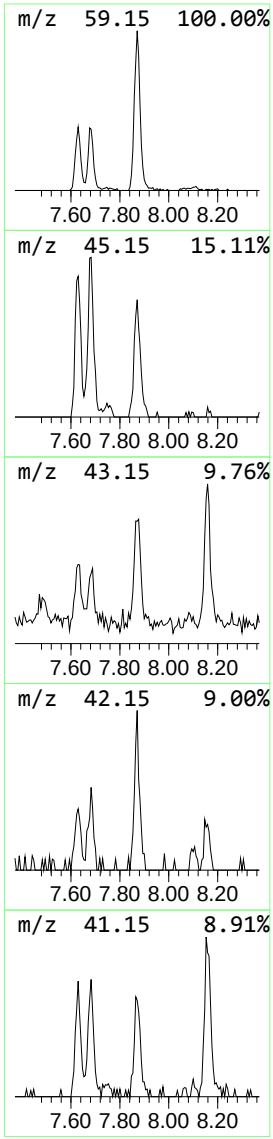
****
Peak Number 7 2-Propanol, 1-(2-methoxypro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.871	9.76 ng	87209	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	83
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	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

TIC Library : C:\Database\NIST20.L
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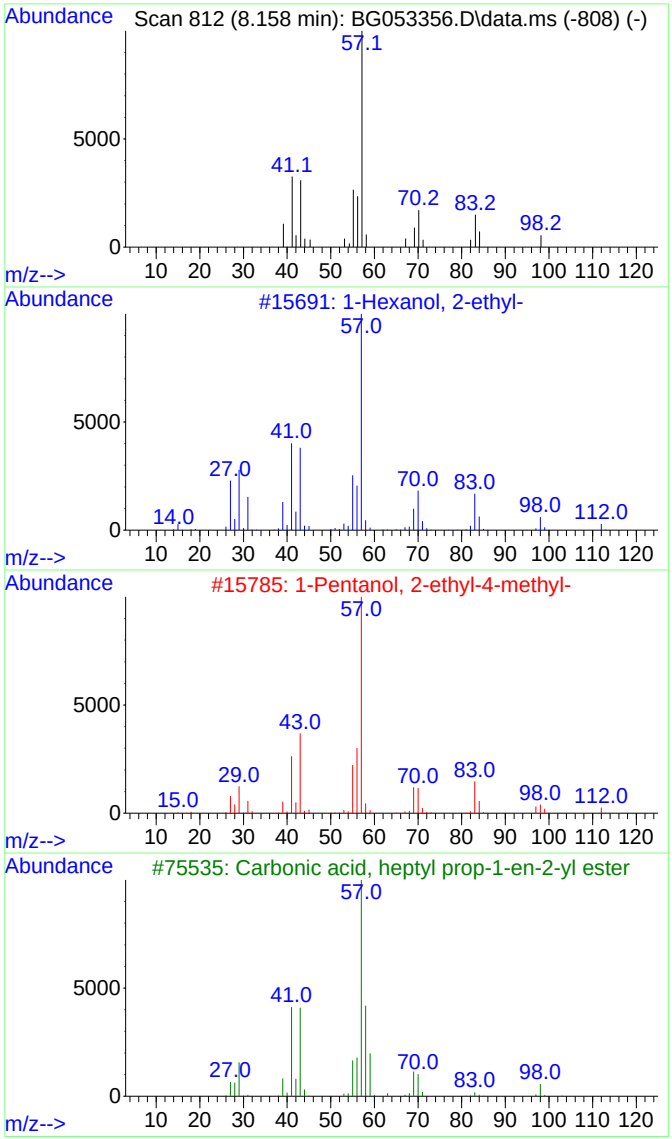
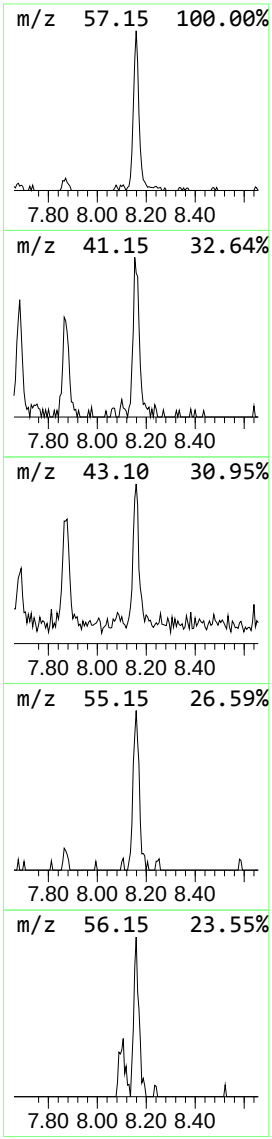
****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	6.43 ng	57441	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	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	50
4	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	38
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	32





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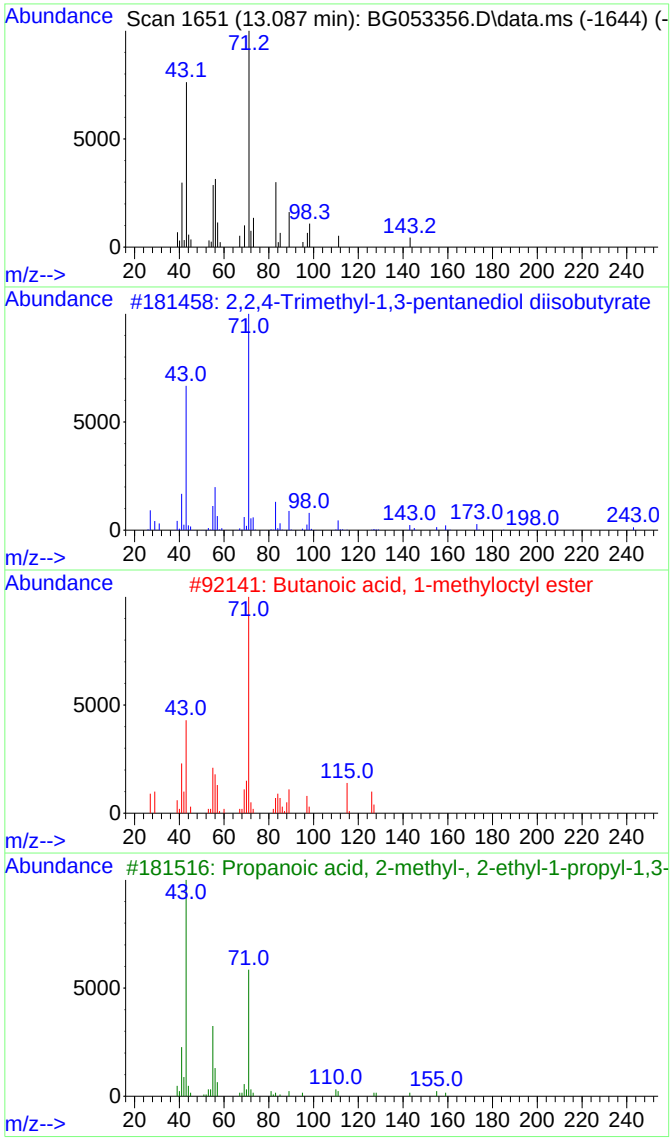
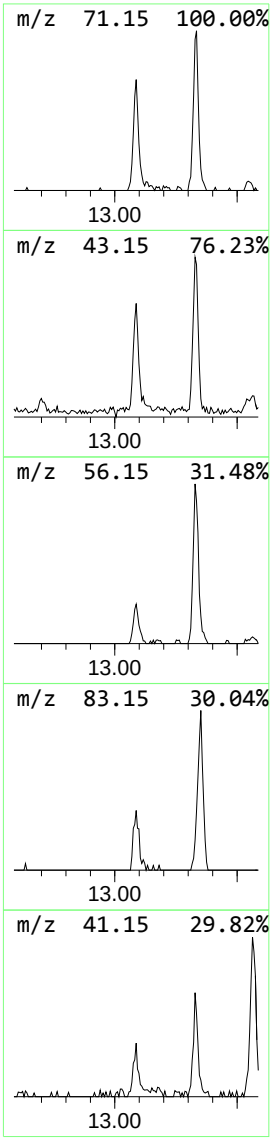
****

Peak Number 9 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.087	3.05 ng	52519	Acenaphthene-d10	14.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	78
2	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	53
3	Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	47
4	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
5	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42





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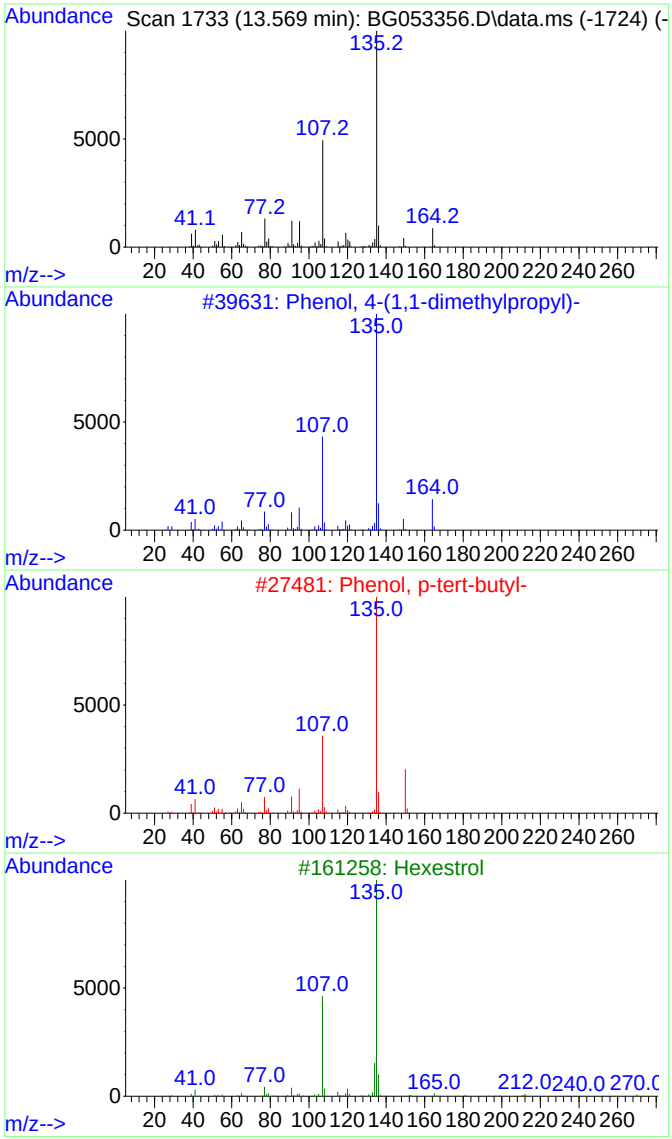
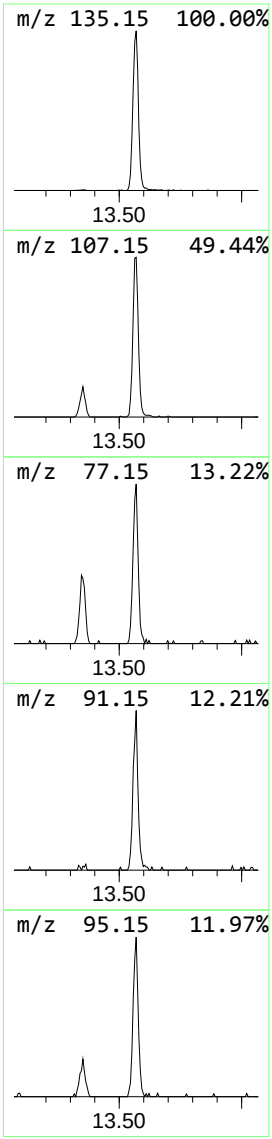
****
Peak Number 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.569	21.86 ng	376445	Acenaphthene-d10	14.726

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	Hexestrol	270	C18H22O2	000084-16-2	72
4	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	72
5	4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	64





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Data File : BG053356.D
Acq On : 28 Apr 2022 1:57
Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-1R

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

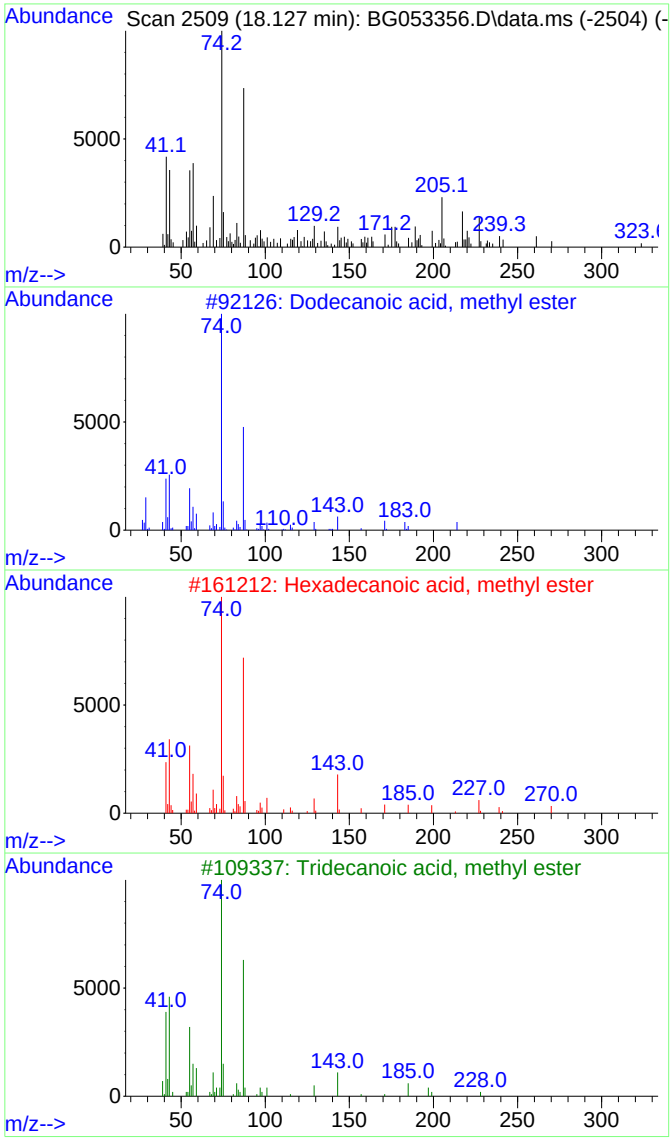
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

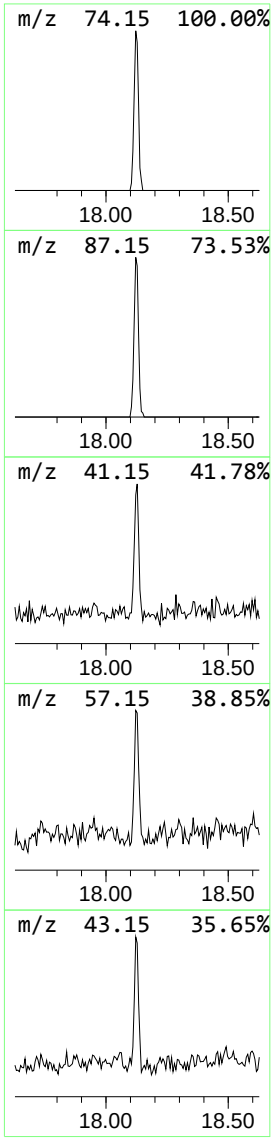
****

Peak Number 11 Dodecanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	4.95 ng	106047	Phenanthrene-d10	17.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	70
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	62
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	53
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053356.D
Acq On : 28 Apr 2022 1:57
Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-1R

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

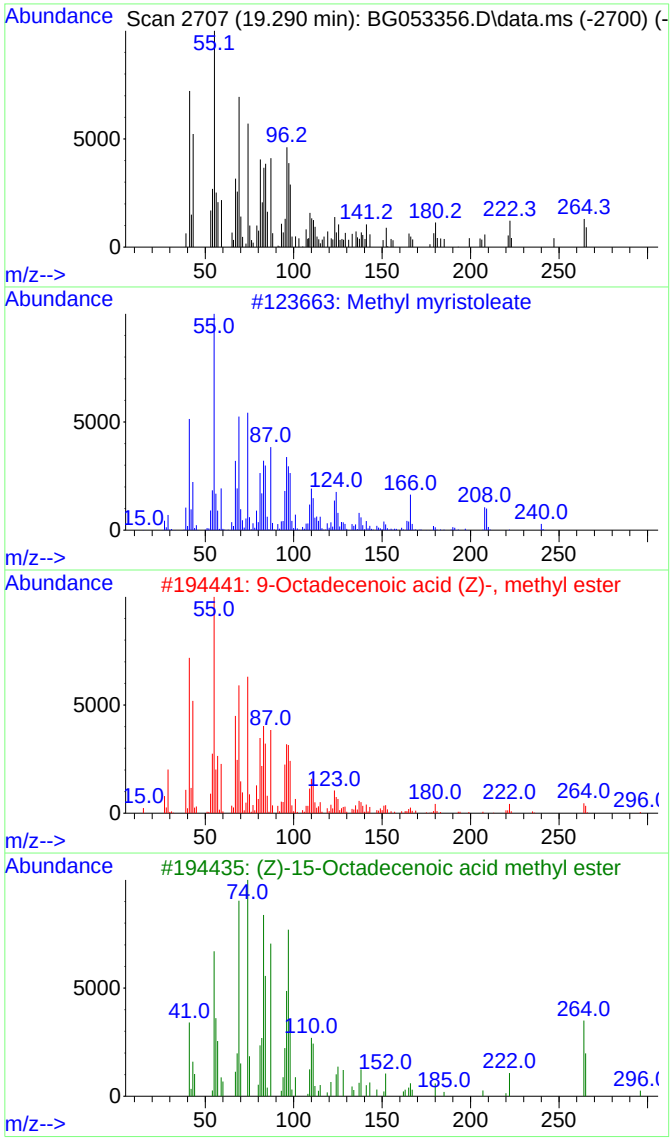
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

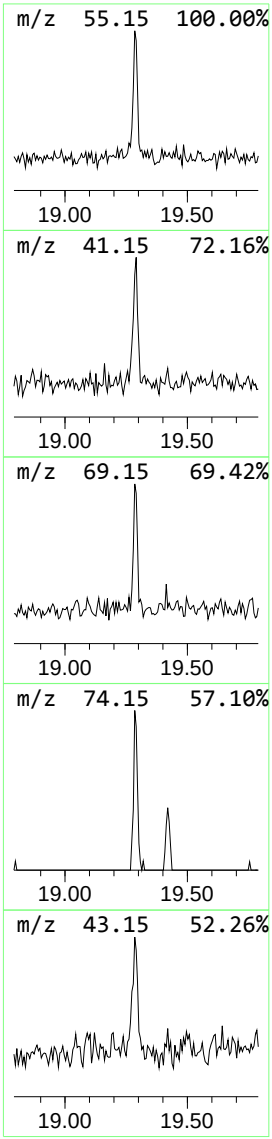
****

Peak Number 12 Methyl myristoleate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.290	3.98 ng	85339	Phenanthrene-d10	17.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl myristoleate	240	C15H28O2	056219-06-8	80
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	80
3	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	72
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	64
5	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053356.D
Acq On : 28 Apr 2022 1:57
Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-1R

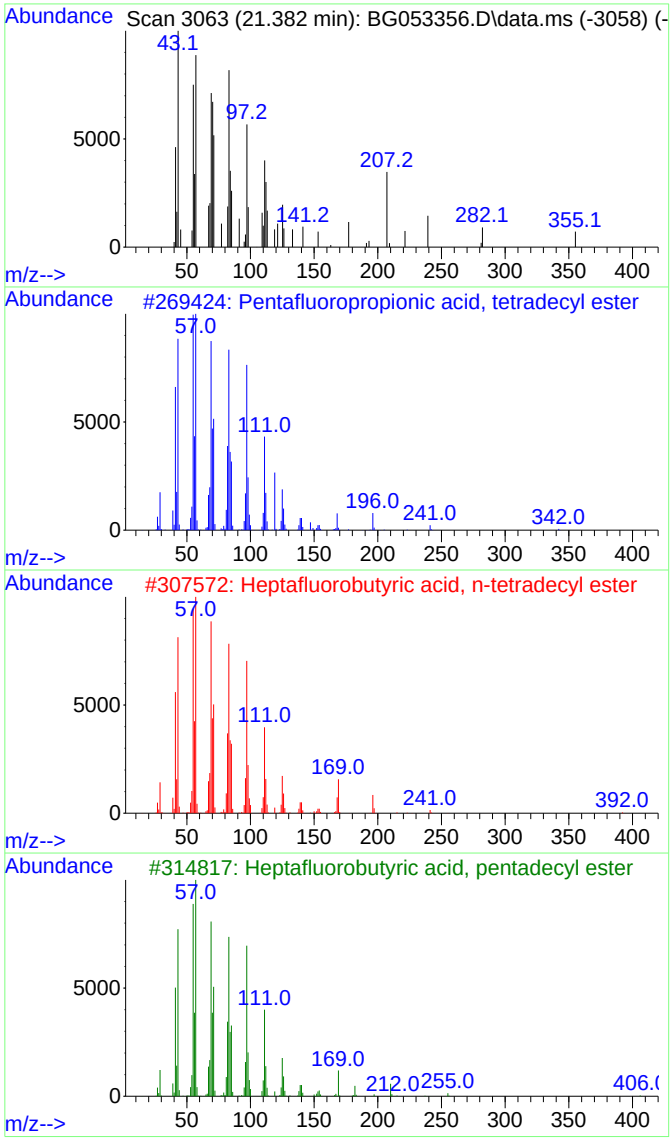
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

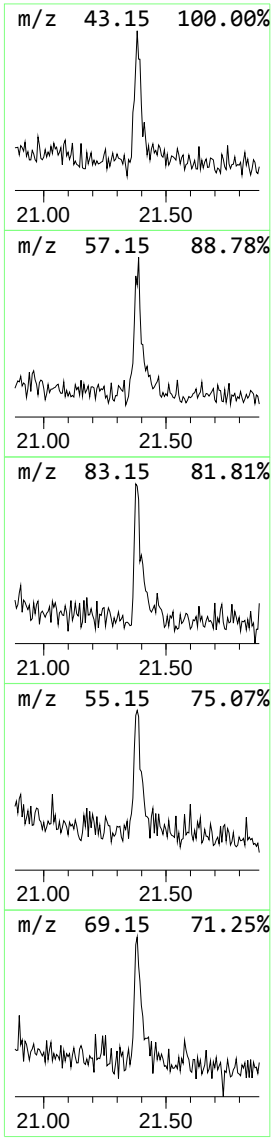
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Pentafluoropropionic acid, ... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.382	2.14 ng	53759	Chrysene-d12	21.758

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	83
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5	1-Tetracosene	336	C24H48	010192-32-2	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053356.D
Acq On : 28 Apr 2022 1:57
Operator : CG/JU
Sample : N2482-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-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
unknown5.192	5.192	4.1	ng	36988	1	8.106	178633	20.0
p-Xylene	5.738	5.8	ng	51806	1	8.106	178633	20.0
Benzene, 1,3-di...	6.108	4.6	ng	40973	1	8.106	178633	20.0
2-Propanol, 1-(...	7.630	5.4	ng	48606	1	8.106	178633	20.0
unknown7.683	7.683	5.3	ng	47279	1	8.106	178633	20.0
2-Propanol, 1-(...	7.871	9.8	ng	87209	1	8.106	178633	20.0
1-Hexanol, 2-et...	8.158	6.4	ng	57441	1	8.106	178633	20.0
2,2,4-Trimethyl...	13.087	3.0	ng	52519	3	14.726	344462	20.0
Phenol, 4-(1,1-...	13.569	21.9	ng	376445	3	14.726	344462	20.0
Dodecanoic acid...	18.127	5.0	ng	106047	4	17.469	428793	20.0
Methyl myristol...	19.290	4.0	ng	85339	4	17.469	428793	20.0
Pentafluoroprop...	21.382	2.1	ng	53759	5	21.758	501535	20.0