LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

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: BG053353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.549	192	197	205	rBV	68162	111965	3.82%	1.068%
2	5.189	299	306	314	rBV	48446	76245	2.60%	0.727%
3	5.671	382	388	395	rBV	241418	407253	13.88%	3.886%
4	5.736	395	399	408	rVB3	13948	34128	1.16%	0.326%
5	6.106	454	462	467	rBV	16807	30307	1.03%	0.289%
6	7.263	651	659	668	rBV	157554	287951	9.81%	2.747%
7	7.627	713	721	726	rBV	37747	61337	2.09%	0.585%
8	7.680	726	730	737	rVB	38273	59073	2.01%	0.564%
9	7.868	754	762	772	rBV2	61971	106190	3.62%	1.013%
10	8.103	793	802	808	rBV	94479	165312	5.63%	1.577%
11	8.156	808	811	817	rVB3	20981	32904	1.12%	0.314%
12	9.266	992	1000	1012	rVB	363078	660766	22.51%	6.304%
13	10.917	1274	1281	1286	rBV	116980	220227	7.50%	2.101%
14	13.084	1643	1650	1660	rBV2	52536	89141	3.04%	0.850%
15	13.349	1684	1695	1704	rBV	942732	1605057	54.69%	15.314%
16	13.566	1726	1732	1738	rBV	197159	289302	9.86%	2.760%
17	14.723	1923	1929	1936	rBV	203188	328888	11.21%	3.138%
18	15.528	2059	2066	2074	rVB	44306	65743	2.24%	0.627%
19	16.063	2151	2157	2166	rVB	43190	64844	2.21%	0.619%
20	16.216	2175	2183	2197	rBV2	798259	1284357	43.76%	12.254%
21	17.473	2391	2397	2403	rBV	290366	447478	15.25%	4.269%
22	18.131	2504	2509	2514	rBV3	36952	46834	1.60%	0.447%
23	20.075	2834	2840	2846	rBV	2196687	2934852	100.00%	28.001%
24	21.755	3119	3126	3135	rVB	335068	538885	18.36%	5.141%
25	25.051	3677	3687	3701	rVB2	186052	532249	18.14%	5.078%

Sum of corrected areas: 10481288

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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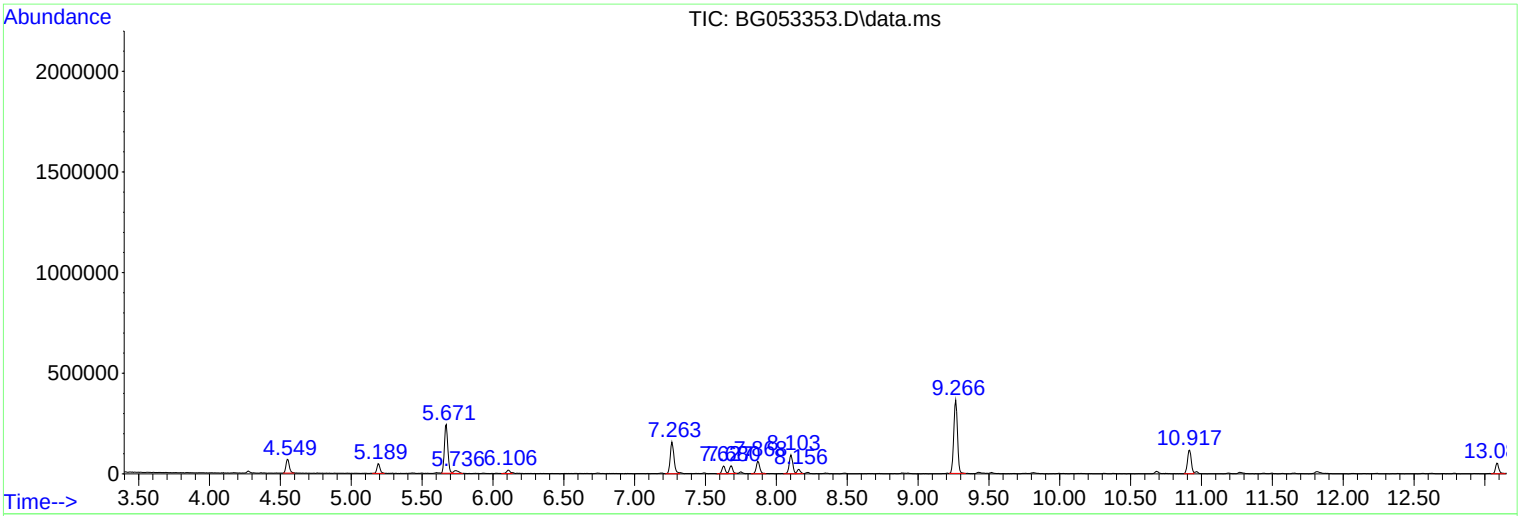
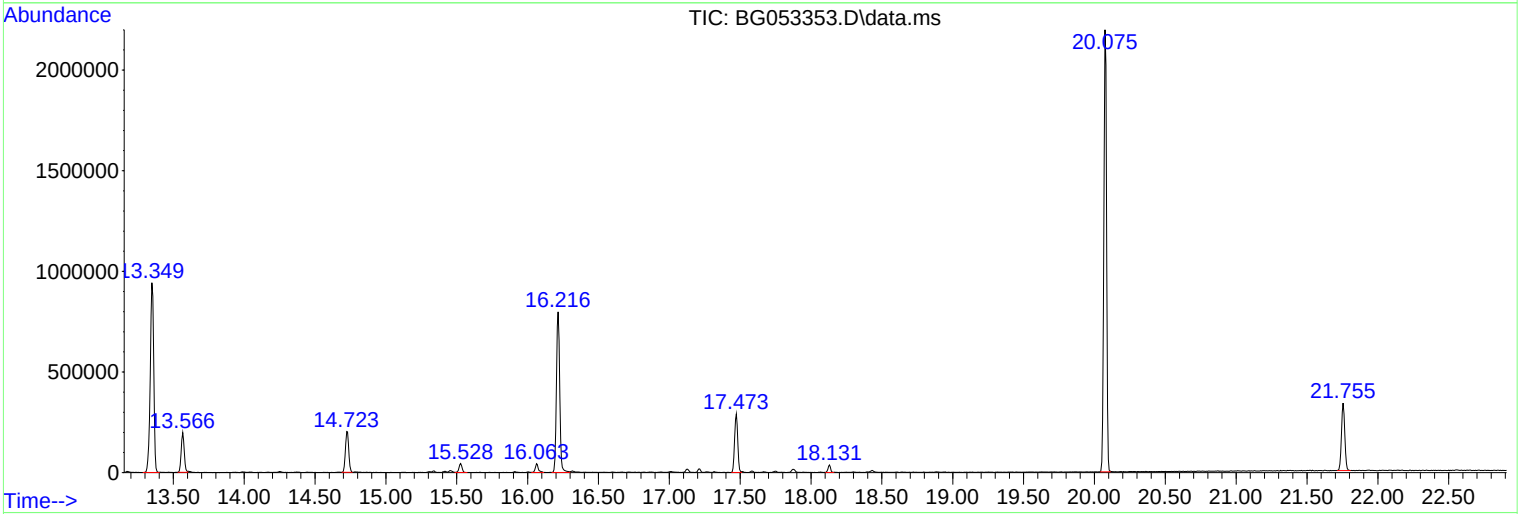
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

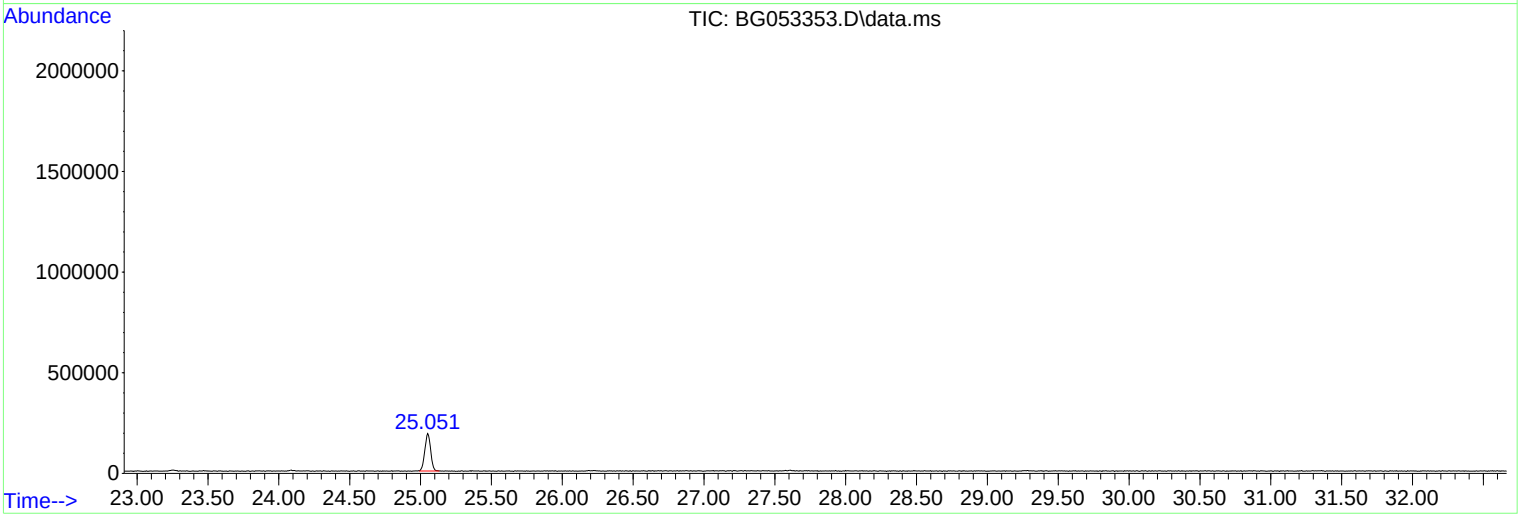
Instrument :
BNA_G
ClientSampleId :
MW-25R

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 : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

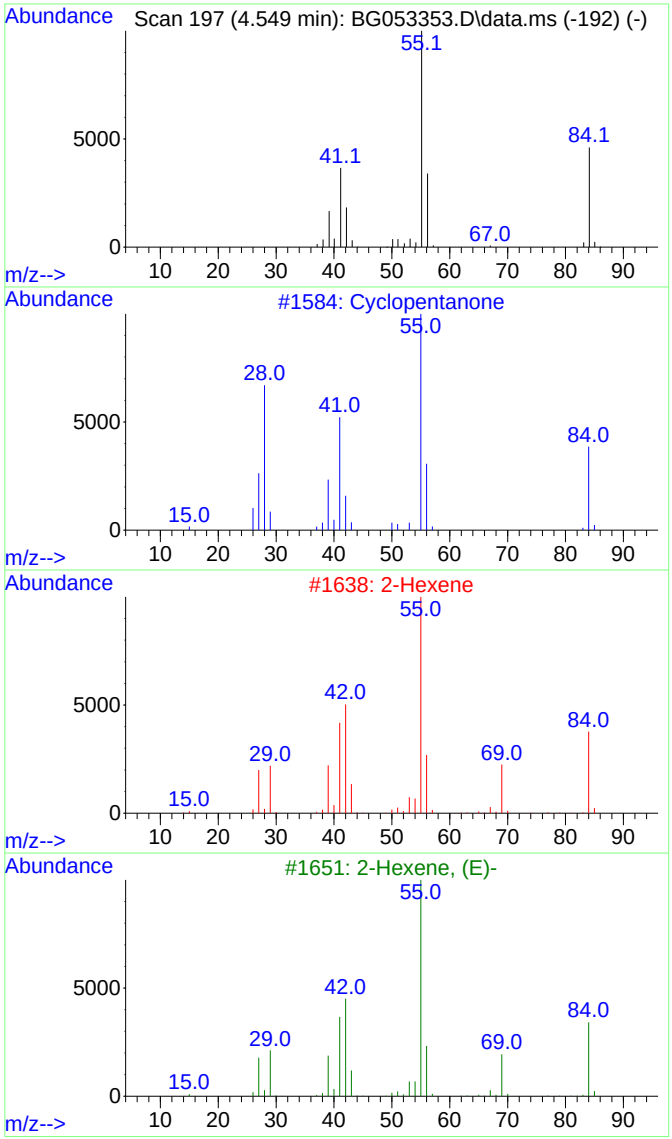
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

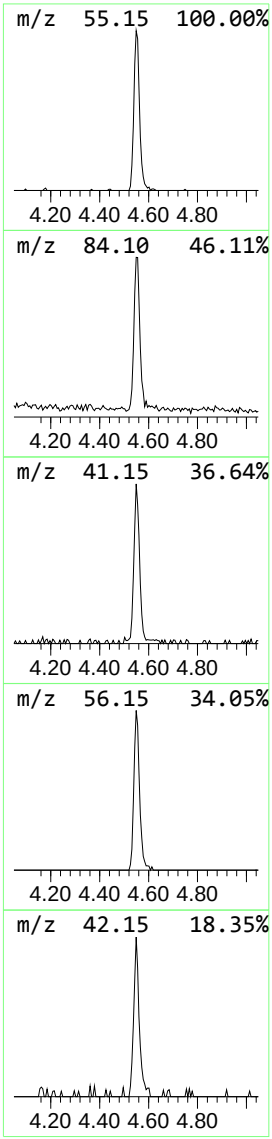
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.549	13.55 ng	111965	1,4-Dichlorobenzene-d4	8.103

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	59
3	2-Hexene, (E)-	84	C6H12	004050-45-7	59
4	1H-Tetrazole, 1-methyl-	84	C2H4N4	016681-77-9	53
5	2(5H)-Furanone	84	C4H4O2	000497-23-4	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

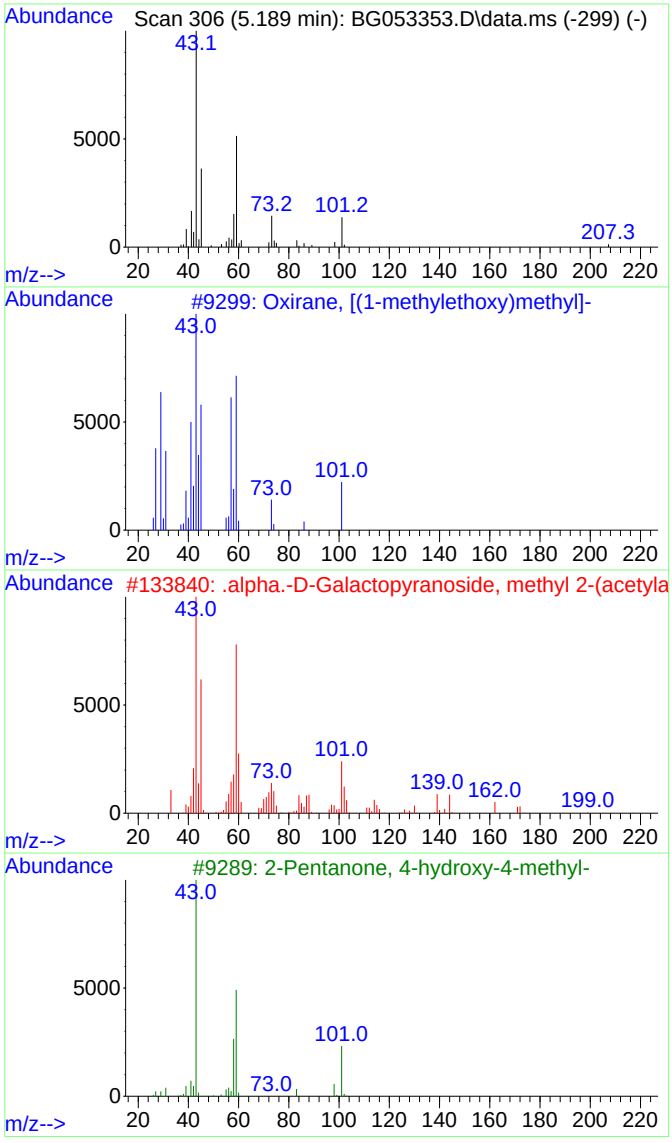
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

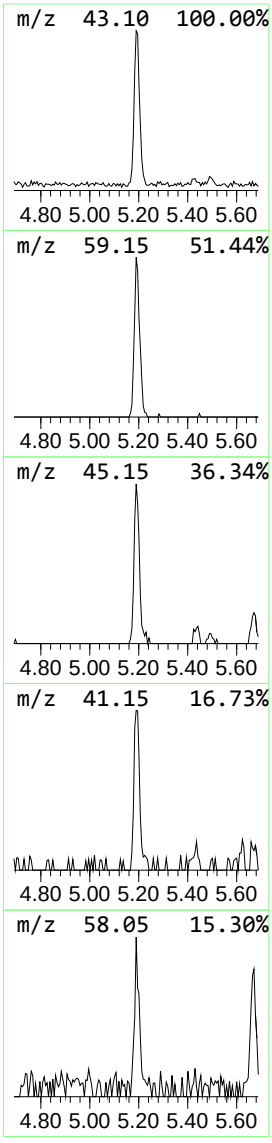
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Oxirane, [(1-methylethoxy)m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.189	9.22 ng	76245	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	50
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	38
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4	Carbonic acid, 2-ethoxyethyl 2,2...	264	C7H11Cl3O4	1000331-44-6	38
5	Silane, trimethyl-	74	C3H10Si	000993-07-7	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

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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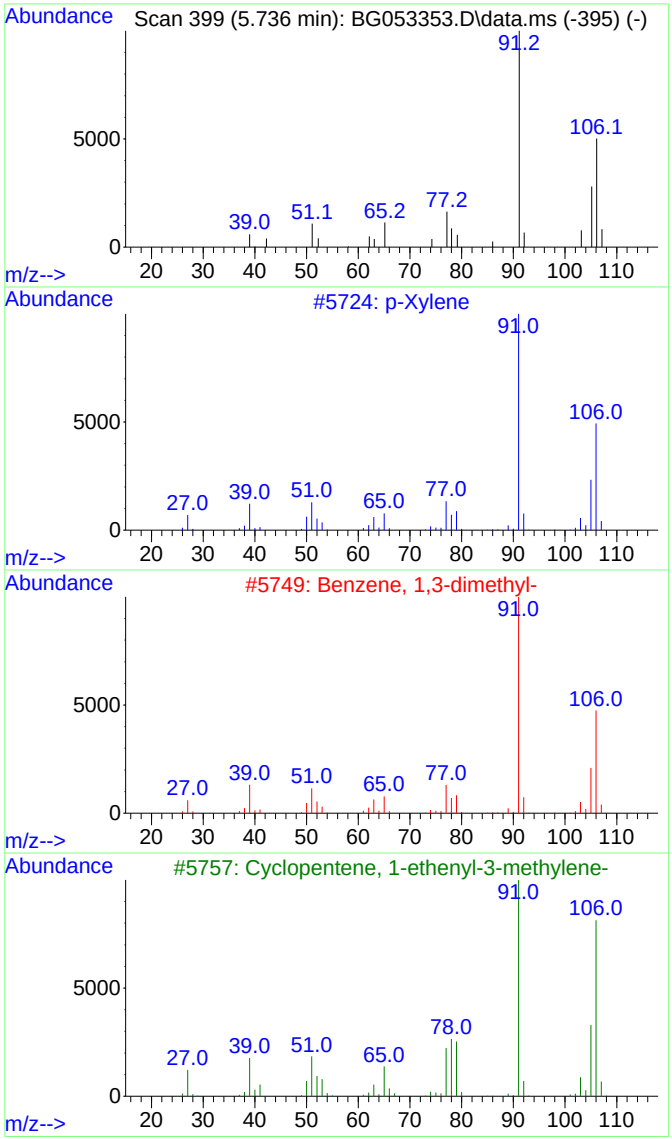
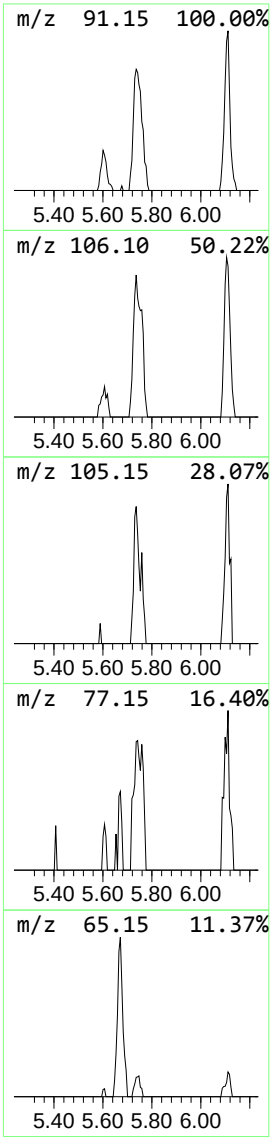
Peak Number 3 p-Xylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.736	4.13 ng	34128	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	91
2	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	91
3	Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	91
4	o-Xylene	106	C8H10	000095-47-6	87
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

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

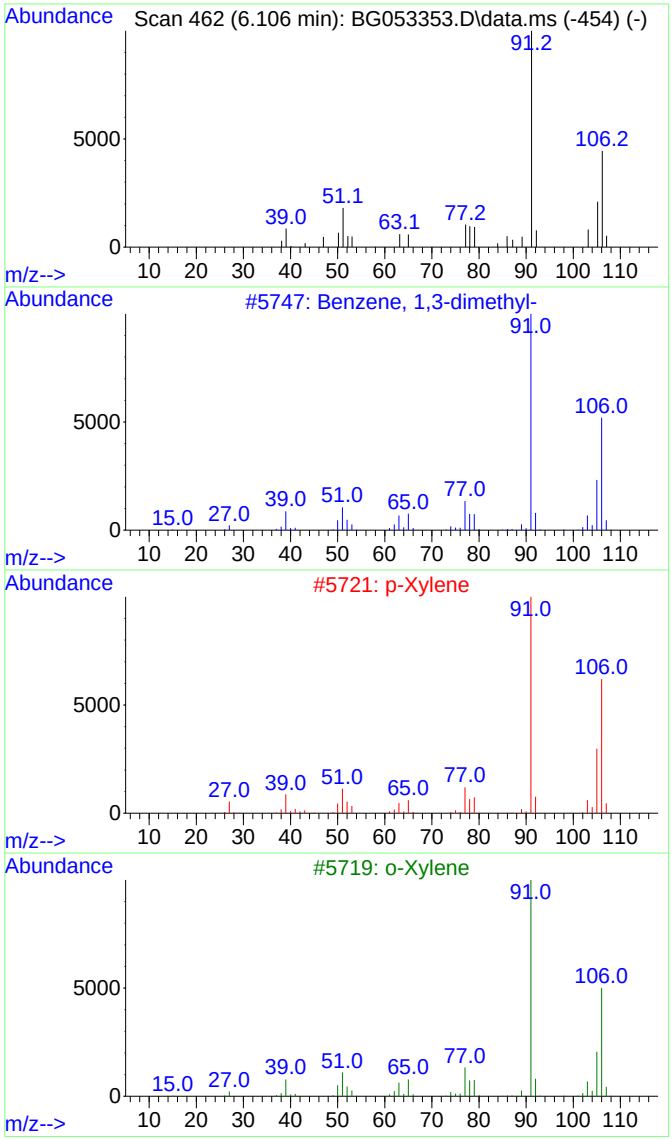
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

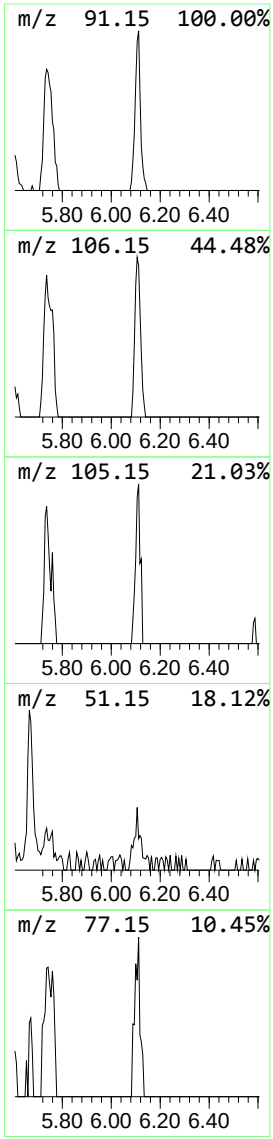
****

Peak Number 4 Benzene, 1,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.106	3.67 ng	30307	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	90
2	p-Xylene	106	C8H10	000106-42-3	90
3	o-Xylene	106	C8H10	000095-47-6	90
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87
5	Ethylbenzene	106	C8H10	000100-41-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

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

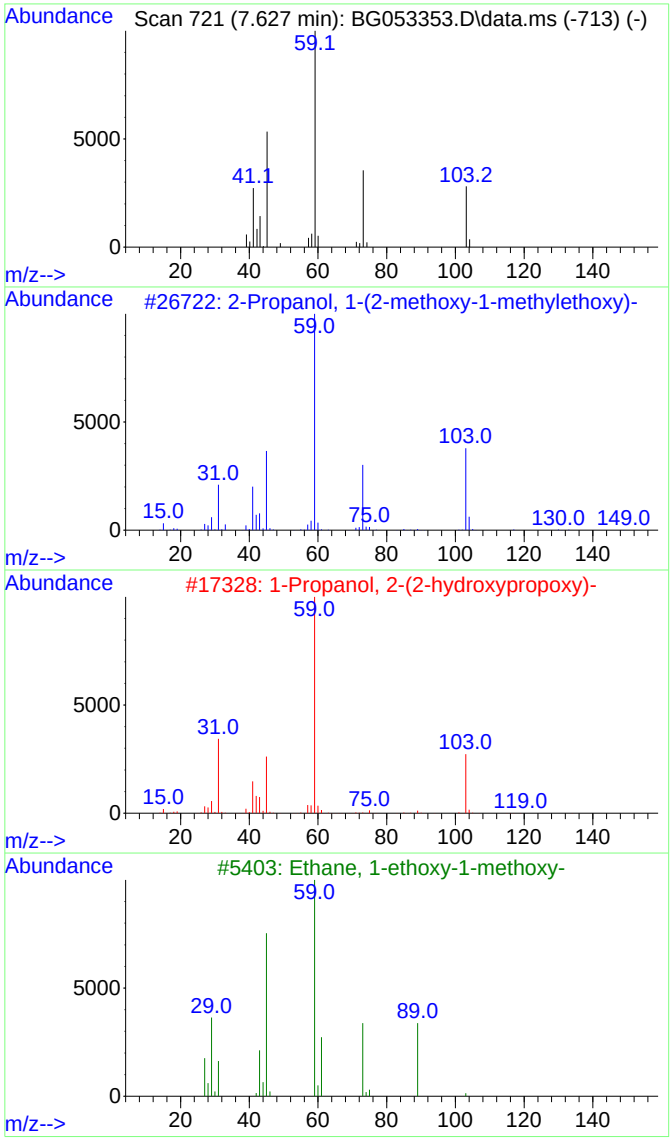
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

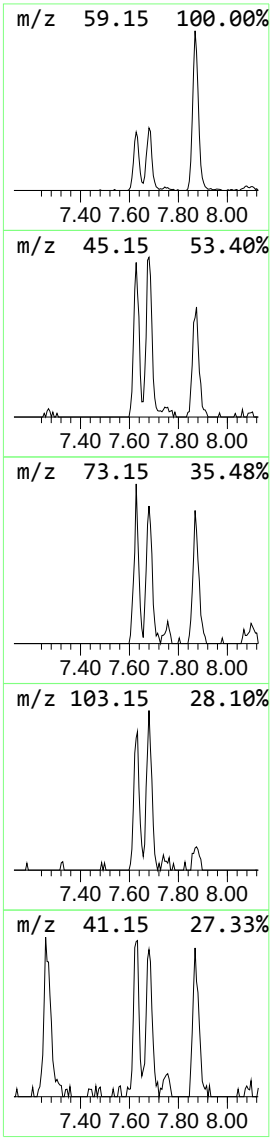
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.627	7.42 ng	61337	1,4-Dichlorobenzene-d4	8.103

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	45
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	45
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	40
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
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Misc :
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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
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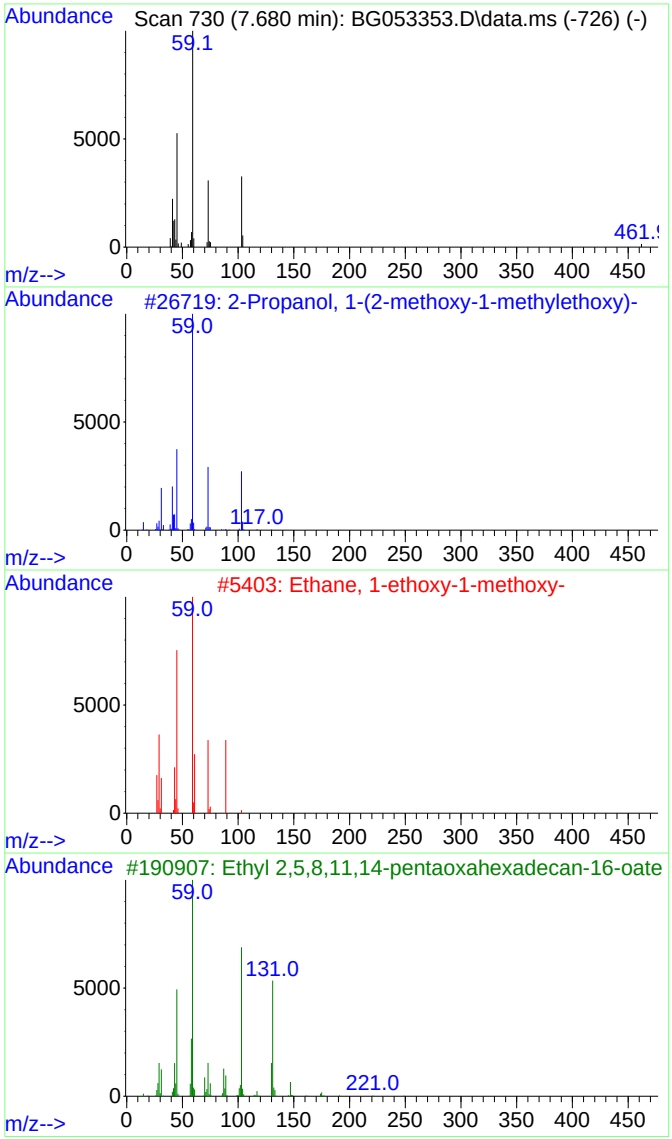
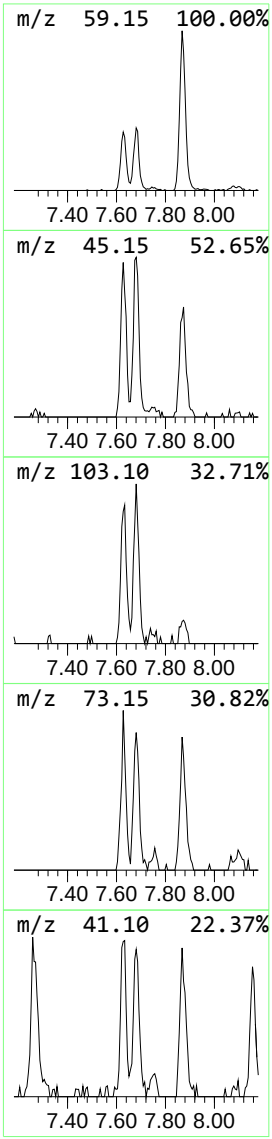
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.680	7.15 ng	59073	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	Ethyl 2,5,8,11,14-pentaoxahexade...	294	C13H26O7	1000366-80-7	56
4	Ethyl 2,5,8,11,14,17-hexaoxanona...	338	C15H30O8	1000366-80-6	56
5	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

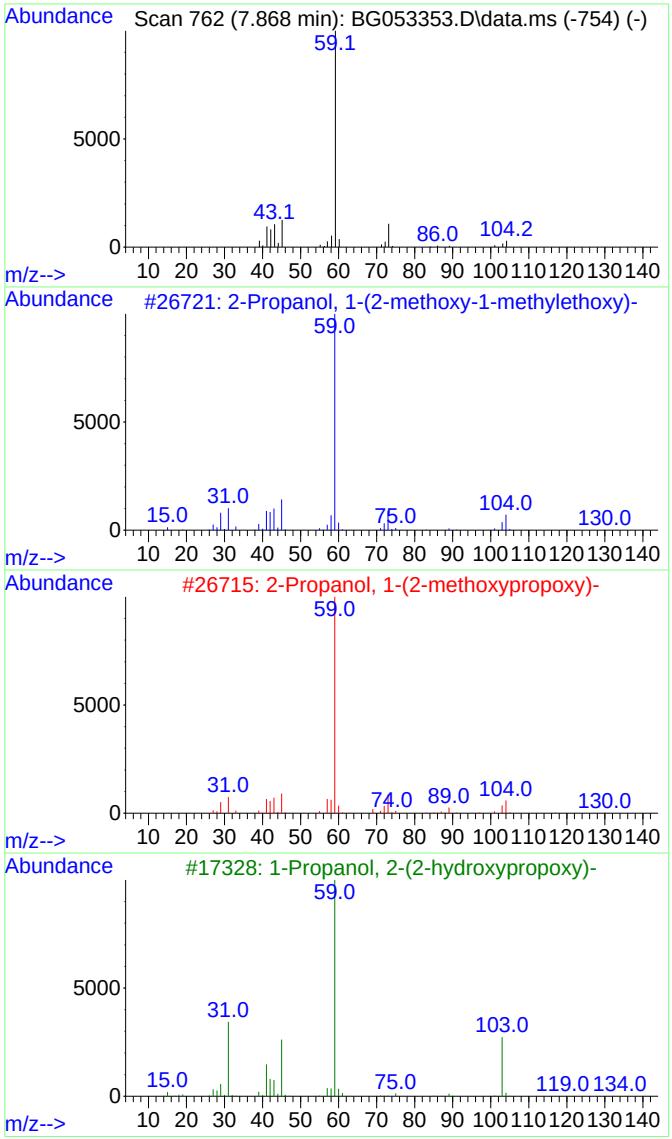
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

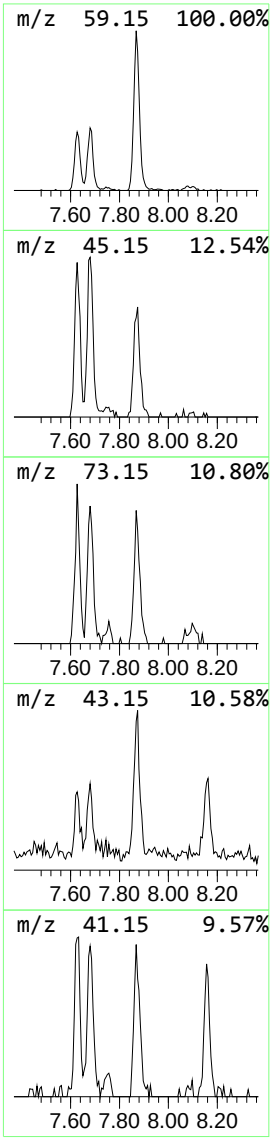
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.868	12.85 ng	106190	1,4-Dichlorobenzene-d4	8.103

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	64
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	59
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43





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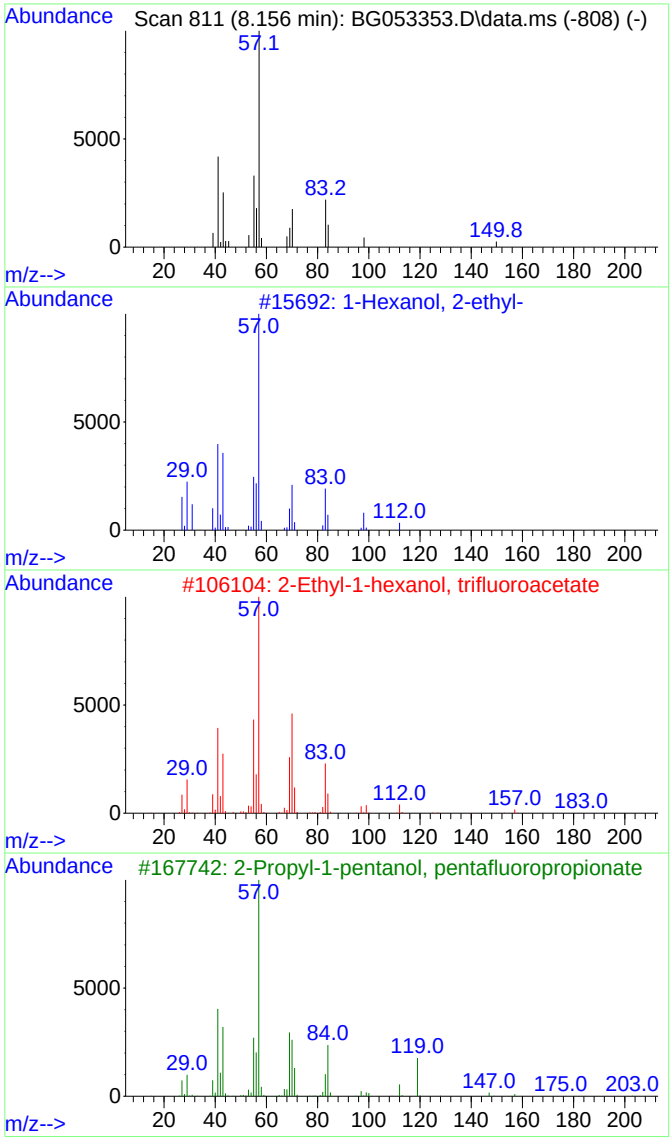
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

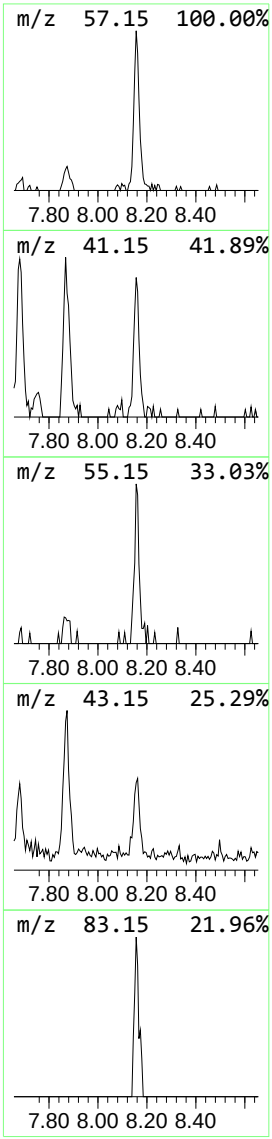
****

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.156	3.98 ng	32904	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	42
3	2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	40
4	2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	38
5	Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

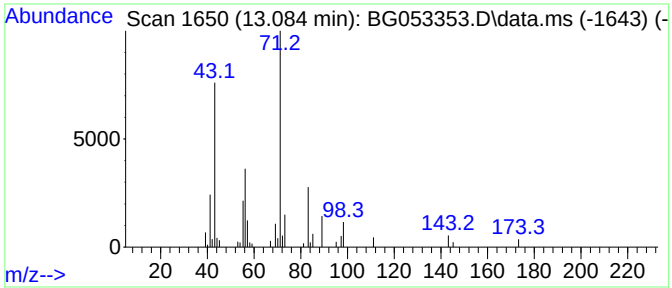
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

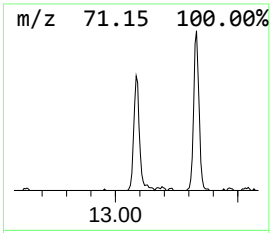
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

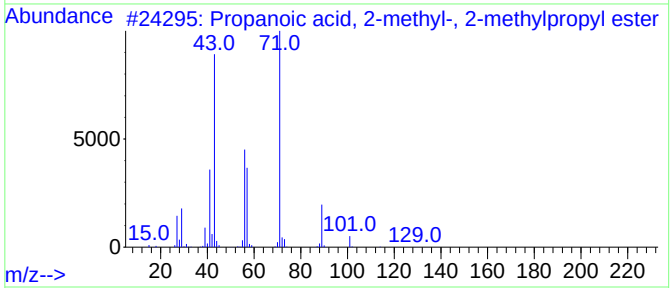
****
Peak Number 9 Propanoic acid, 2-methyl-, ... Concentration Rank 7

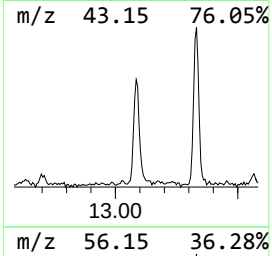
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.085	5.42 ng	89141	Acenaphthene-d10	14.723

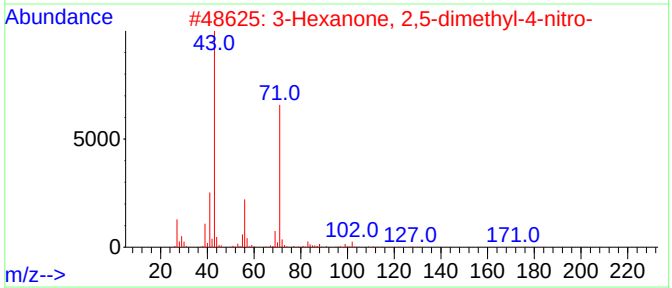
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
2	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
3	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	43
4	Cyclohexanecarboxylic acid, 2-te...	212	C12H20O3	1000279-85-7	40
5	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	40

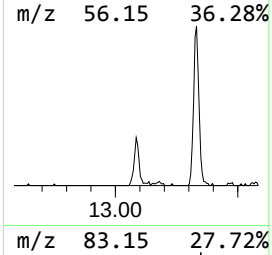


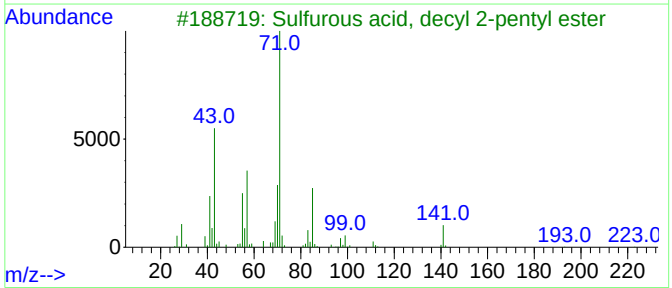


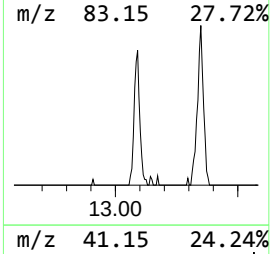


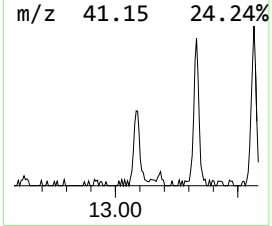












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

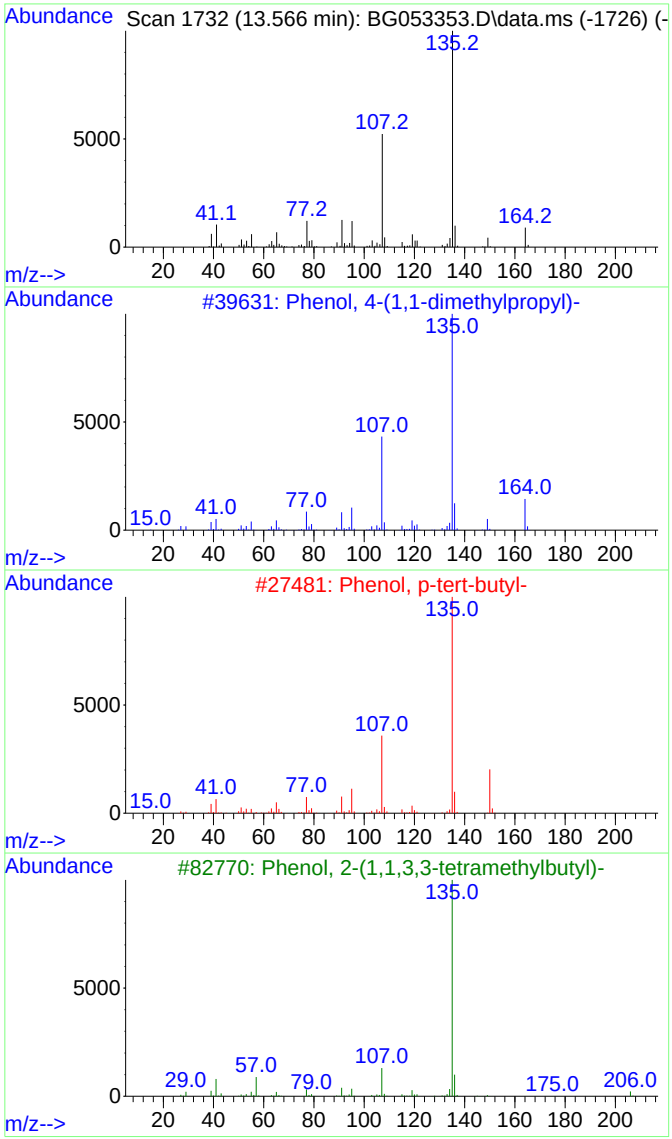
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

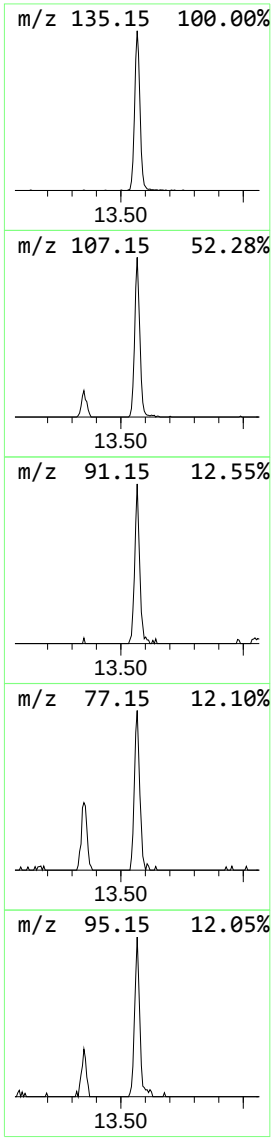
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.566	17.59 ng	289302	Acenaphthene-d10	14.723

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

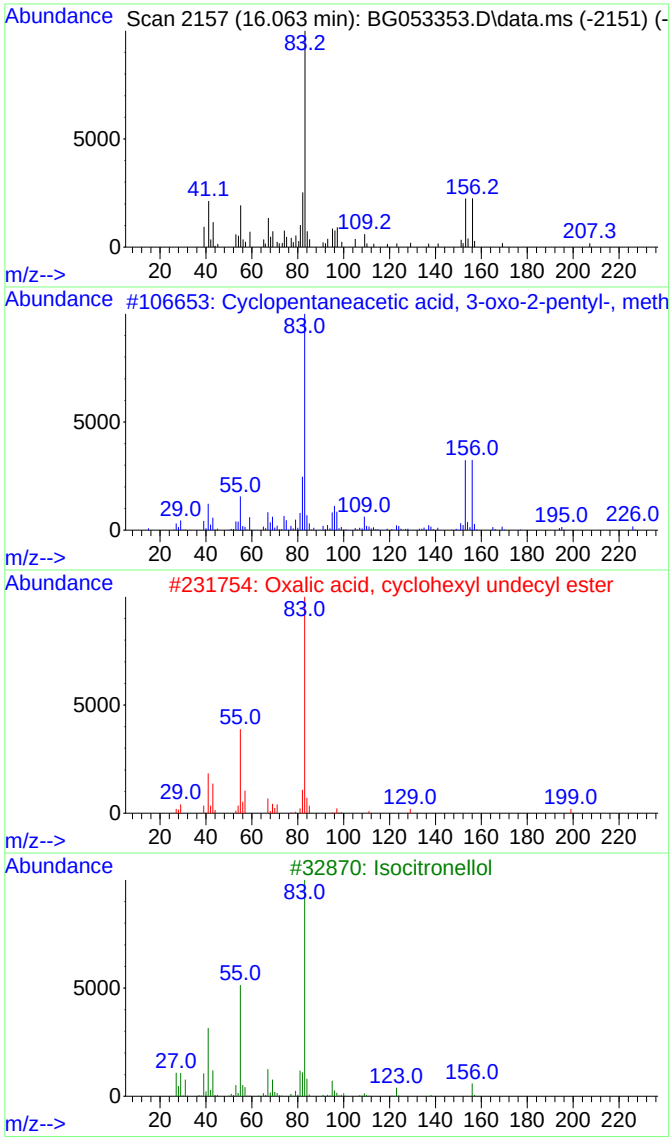
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

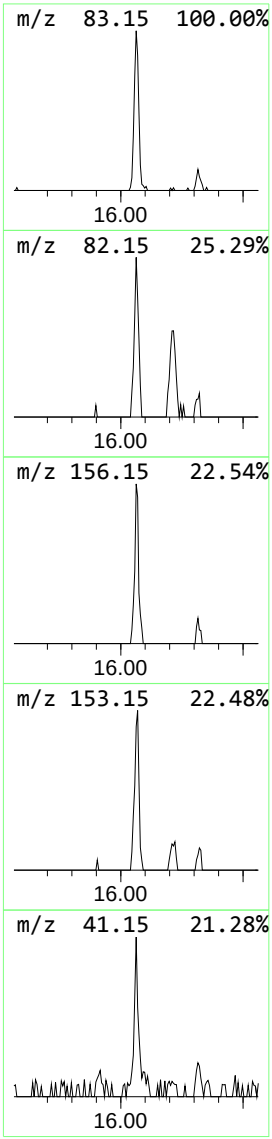
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Cyclopentaneacetic acid, 3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.063	3.94 ng	64844	Acenaphthene-d10	14.723

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	90
2	Oxalic acid, cyclohexyl undecyl ...	326	C19H34O4	1000309-31-3	43
3	Isocitronellol	156	C10H20O	018479-52-2	42
4	2-Nonen-4-one, 2-methyl-	154	C10H18O	002903-23-3	38
5	1,5-Dicyano-2,4-dimethyl-2,4-dia...	152	C7H12N4	1010289-23-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

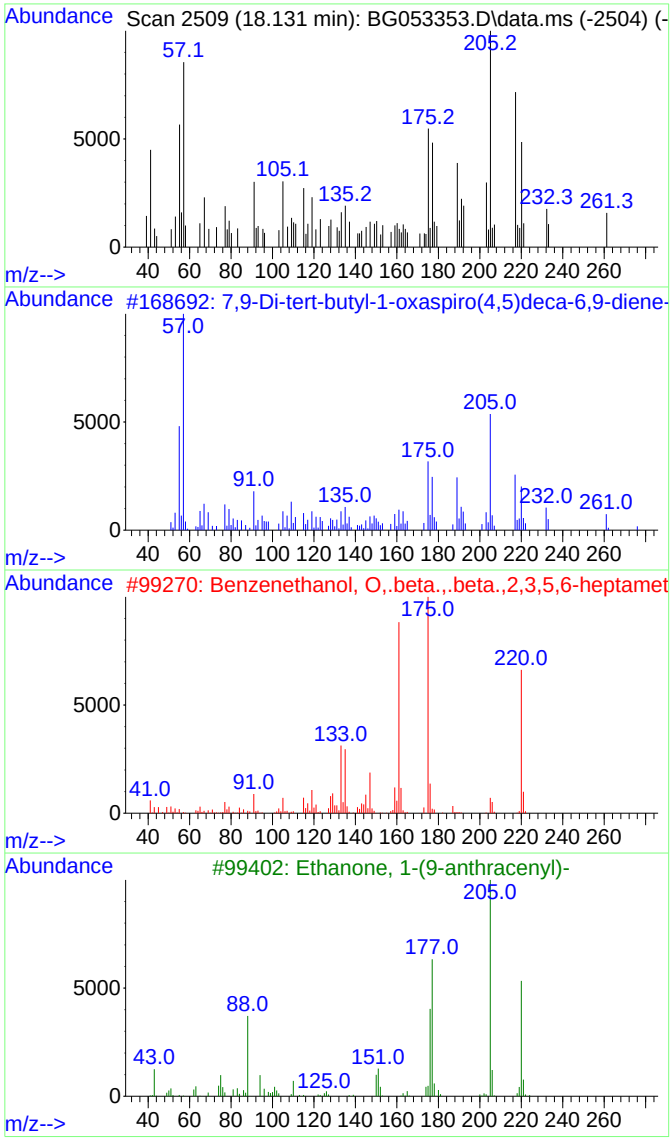
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

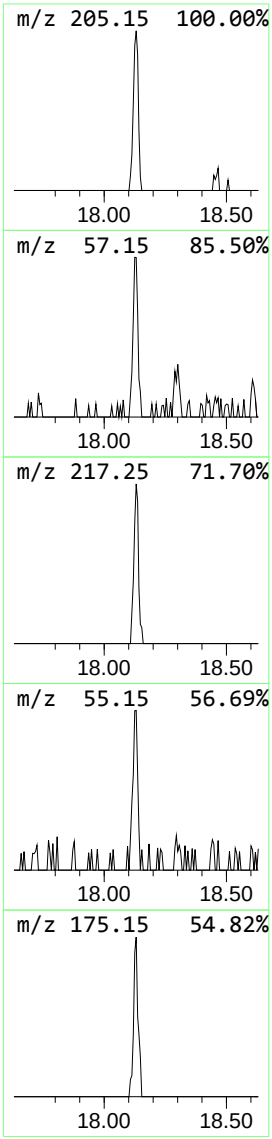
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.131	2.09 ng	46834	Phenanthrene-d10	17.473

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	87
2	Benzenethanol, O,.beta.,.beta.,2...	220	C15H24O	1010128-94-8	53
3	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	50
4	3,5-Cyclohexadiene-1,2-dione, 3,...	220	C14H20O2	003383-21-9	38
5	1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053353.D
Acq On : 27 Apr 2022 18:45
Operator : CG/JU
Sample : N2482-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

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	4.549	13.6	ng	111965	1	8.103	165312	20.0
Oxirane, [(1-me...	5.189	9.2	ng	76245	1	8.103	165312	20.0
p-Xylene	5.736	4.1	ng	34128	1	8.103	165312	20.0
Benzene, 1,3-di...	6.106	3.7	ng	30307	1	8.103	165312	20.0
2-Propanol, 1-(...	7.627	7.4	ng	61337	1	8.103	165312	20.0
Ethane, 1-ethox...	7.680	7.2	ng	59073	1	8.103	165312	20.0
2-Propanol, 1-(...	7.868	12.9	ng	106190	1	8.103	165312	20.0
1-Hexanol, 2-et...	8.156	4.0	ng	32904	1	8.103	165312	20.0
Propanoic acid,...	13.085	5.4	ng	89141	3	14.723	328888	20.0
Phenol, 4-(1,1-...	13.566	17.6	ng	289302	3	14.723	328888	20.0
Cyclopentaneace...	16.063	3.9	ng	64844	3	14.723	328888	20.0
7,9-Di-tert-but...	18.131	2.1	ng	46834	4	17.473	447478	20.0