LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052816.D
Acq On : 24 Mar 2022 19:39
Operator : CG/JU
Sample : N2090-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-55

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-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052816.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.072	111	116	124	rBV2	29607	53055	1.61%	0.451%
2	4.167	128	132	145	rVB	46588	83208	2.52%	0.707%
3	5.700	386	393	402	rVB	272896	438861	13.30%	3.729%
4	7.286	657	663	675	rVB	185419	322430	9.77%	2.740%
5	8.143	801	809	815	rBV	102033	174762	5.30%	1.485%
6	8.637	886	893	899	rBV2	42154	69417	2.10%	0.590%
7	9.254	991	998	1001	rBV2	66199	112790	3.42%	0.958%
8	9.301	1001	1006	1020	rVB	406086	772511	23.41%	6.564%
9	9.777	1081	1087	1093	rVB	66621	114699	3.48%	0.975%
10	10.352	1176	1185	1192	rBV3	20235	36294	1.10%	0.308%
11	10.951	1276	1287	1293	rBV	137387	274877	8.33%	2.335%
12	12.273	1505	1512	1518	rVB	20264	35465	1.07%	0.301%
13	13.389	1693	1702	1709	rBV	1128006	1756179	53.23%	14.921%
14	14.764	1929	1936	1942	rVB	245007	396700	12.02%	3.371%
15	16.244	2181	2188	2195	rBV	1162627	1766439	53.54%	15.009%
16	17.507	2395	2403	2413	rVB	367543	595092	18.04%	5.056%
17	18.383	2548	2552	2558	rBV4	21738	35474	1.08%	0.301%
18	20.110	2840	2846	2852	rBV	2440552	3299400	100.00%	28.033%
19	21.425	3065	3070	3075	rBV4	38678	68574	2.08%	0.583%
20	21.790	3125	3132	3141	rBV	407481	689977	20.91%	5.862%
21	25.103	3687	3696	3708	rVB2	225418	673336	20.41%	5.721%

Sum of corrected areas: 11769540

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
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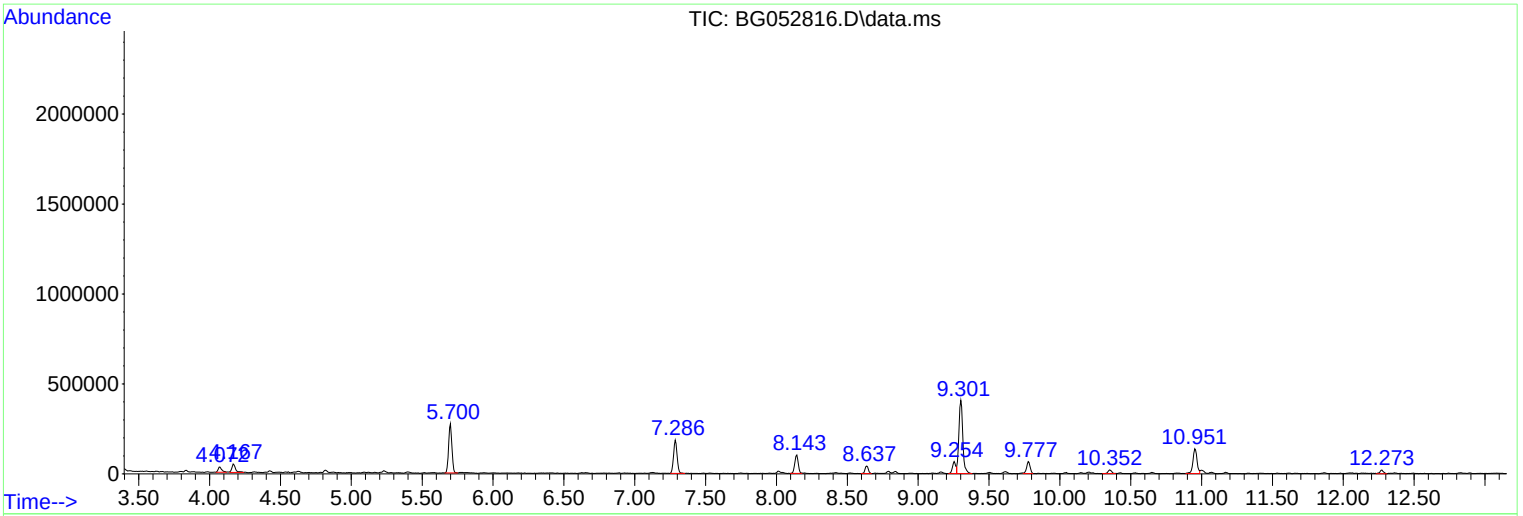
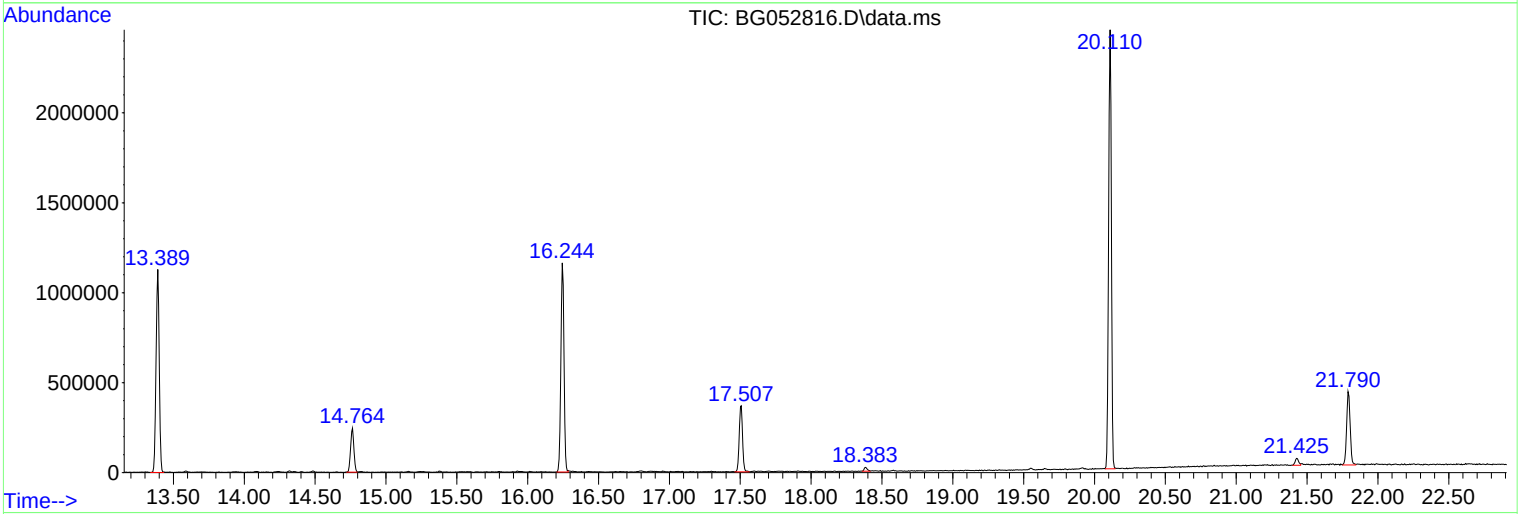
Misc :
ALS Vial : 11 Sample Multiplier: 1

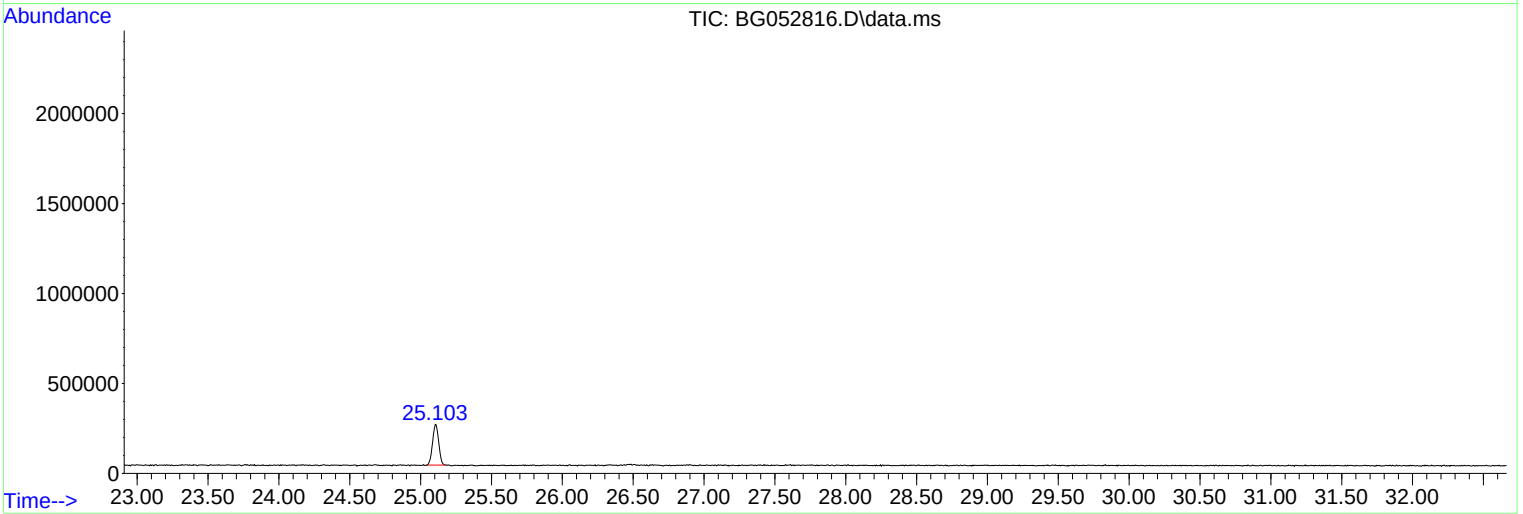
Instrument :
BNA_G
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052816.D
Acq On : 24 Mar 2022 19:39
Operator : CG/JU
Sample : N2090-11
Misc :
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

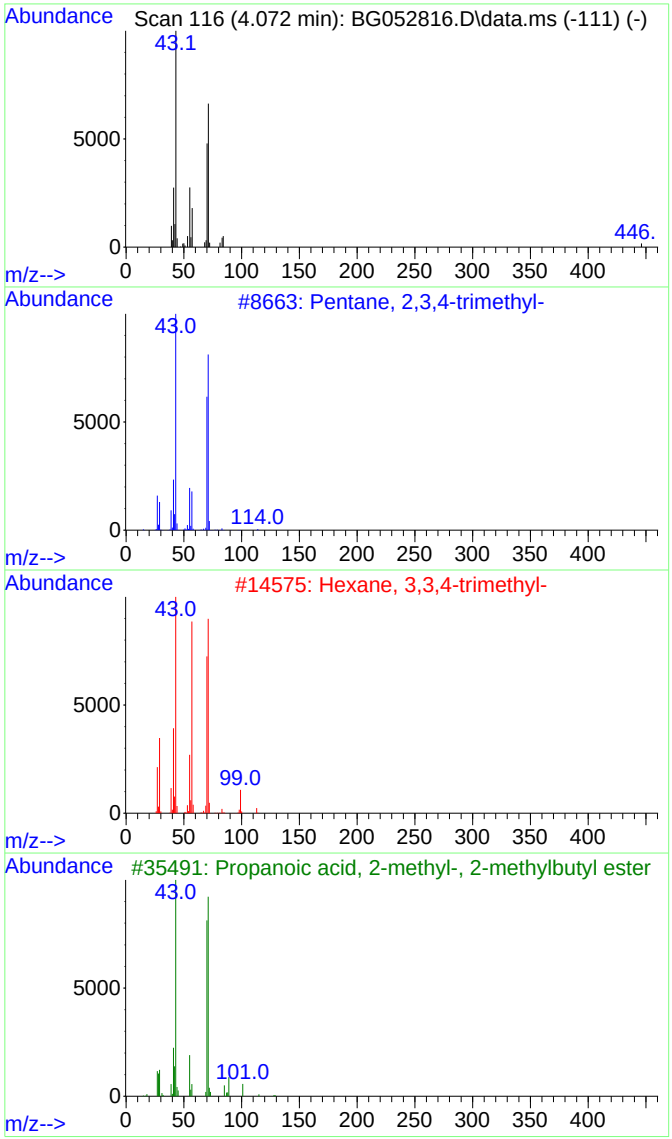
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

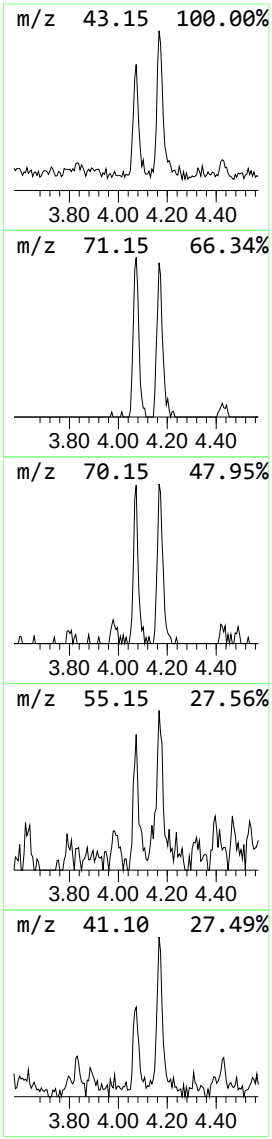
****

Peak Number 1 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.072	6.07 ng	53055	1,4-Dichlorobenzene-d4	8.143

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	72
2	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
3	Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	56
4	Pentane, 3-ethyl-	100	C7H16	000617-78-7	50
5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
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Acq On : 24 Mar 2022 19:39
Operator : CG/JU
Sample : N2090-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-55

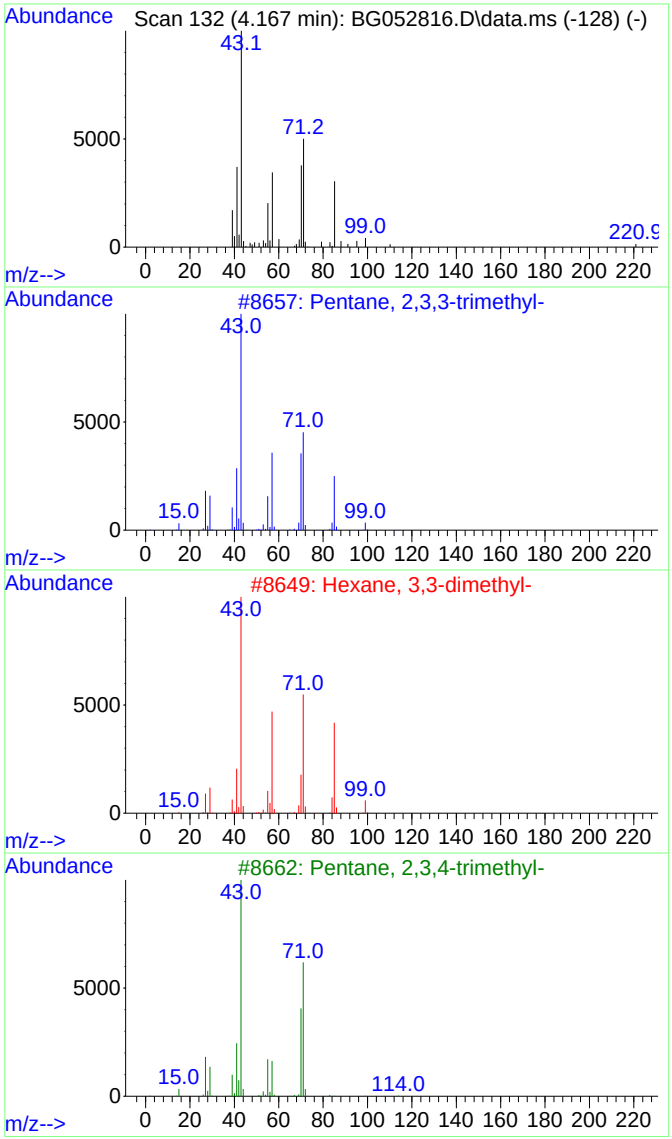
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

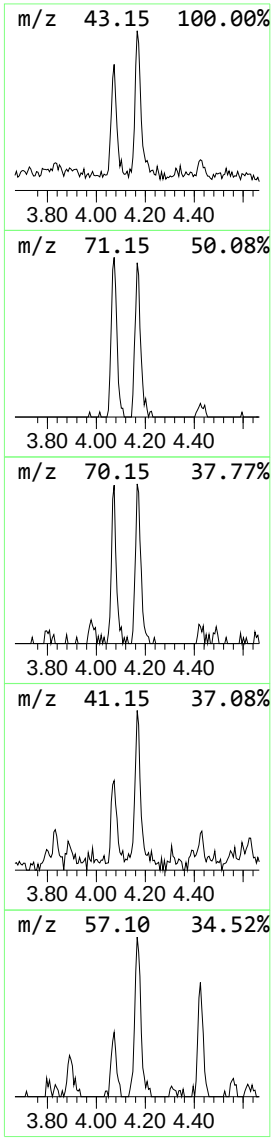
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.167	9.52 ng	83208	1,4-Dichlorobenzene-d4	8.143

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	56
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50
4	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	47
5	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052816.D
Acq On : 24 Mar 2022 19:39
Operator : CG/JU
Sample : N2090-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

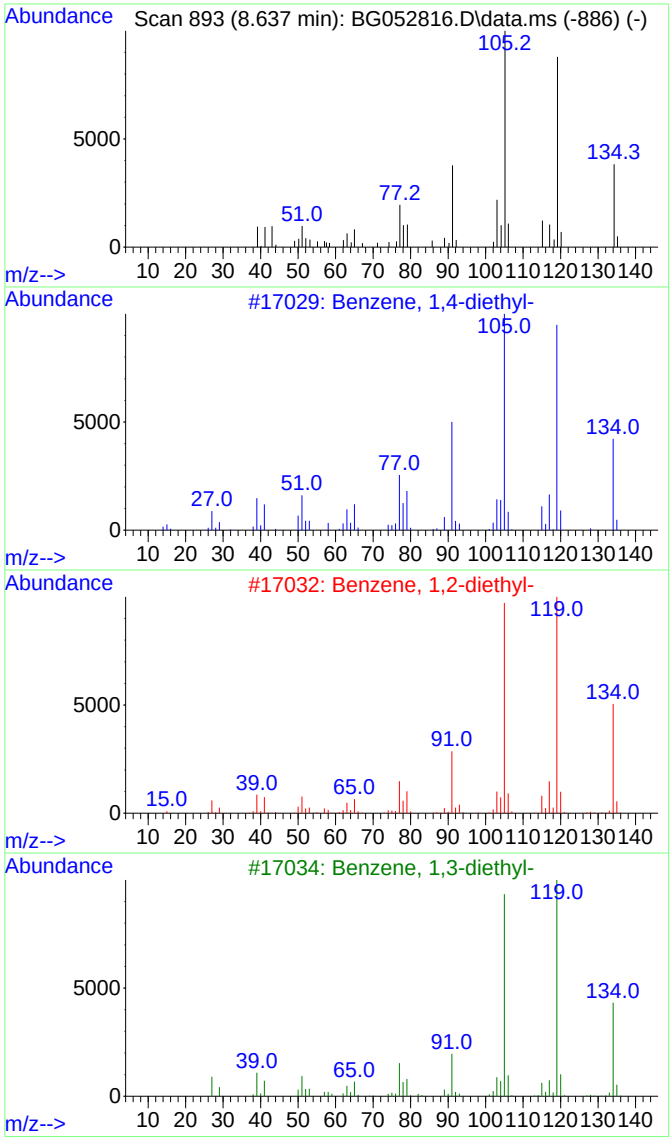
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

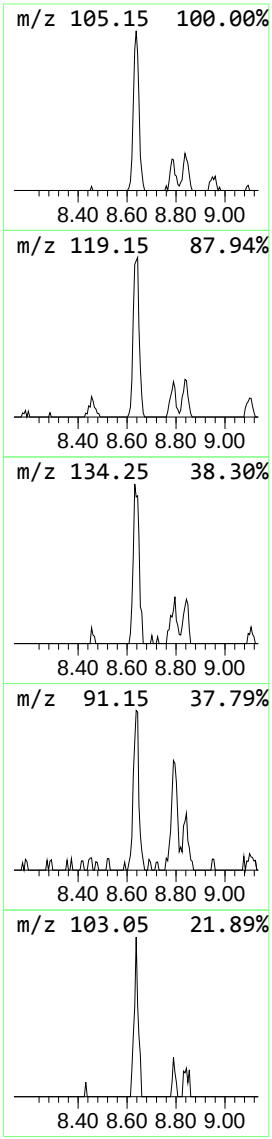
****

Peak Number 3 Benzene, 1,4-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.637	7.94 ng	69417	1,4-Dichlorobenzene-d4	8.143

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	95
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	90
4	o-Cymene	134	C10H14	000527-84-4	76
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052816.D
Acq On : 24 Mar 2022 19:39
Operator : CG/JU
Sample : N2090-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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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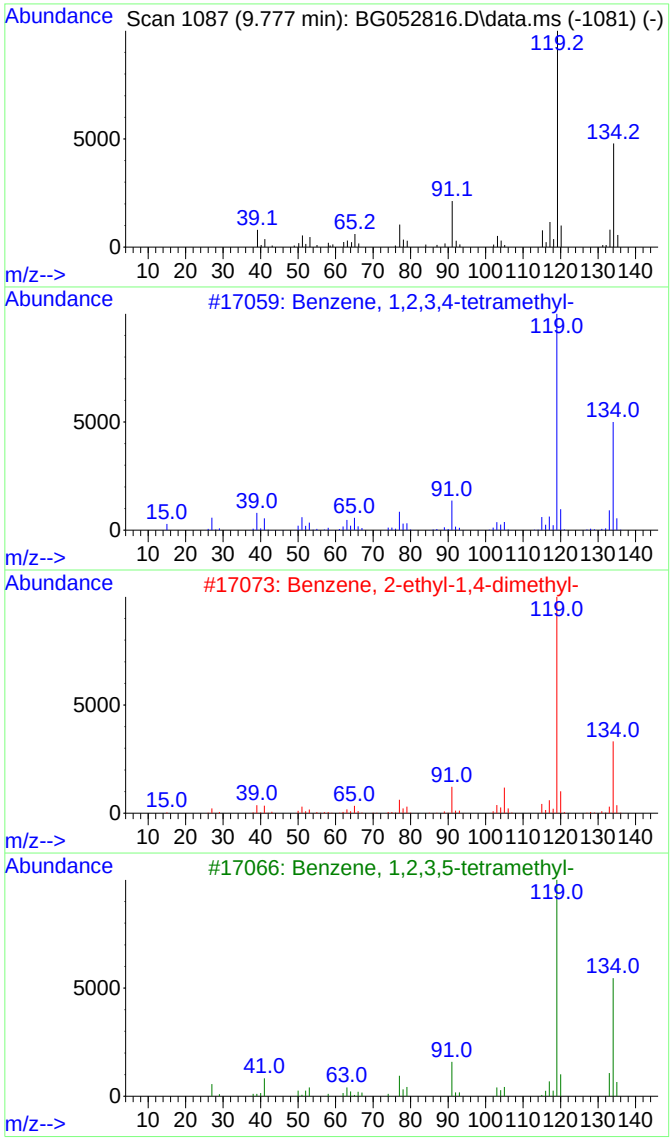
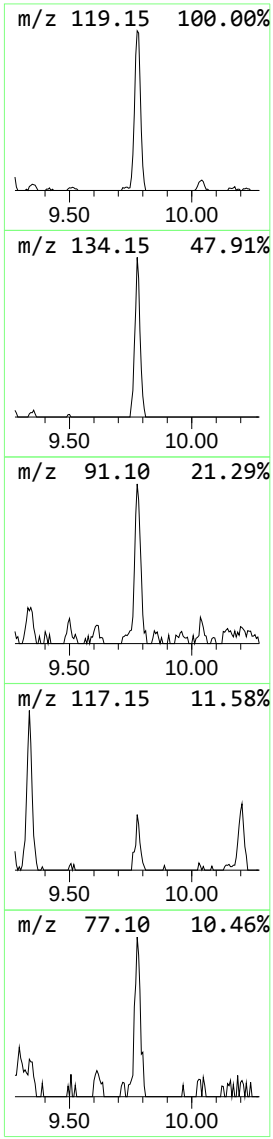
Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.777	8.35 ng	114699	Naphthalene-d8	10.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	93





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Operator : CG/JU
Sample : N2090-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

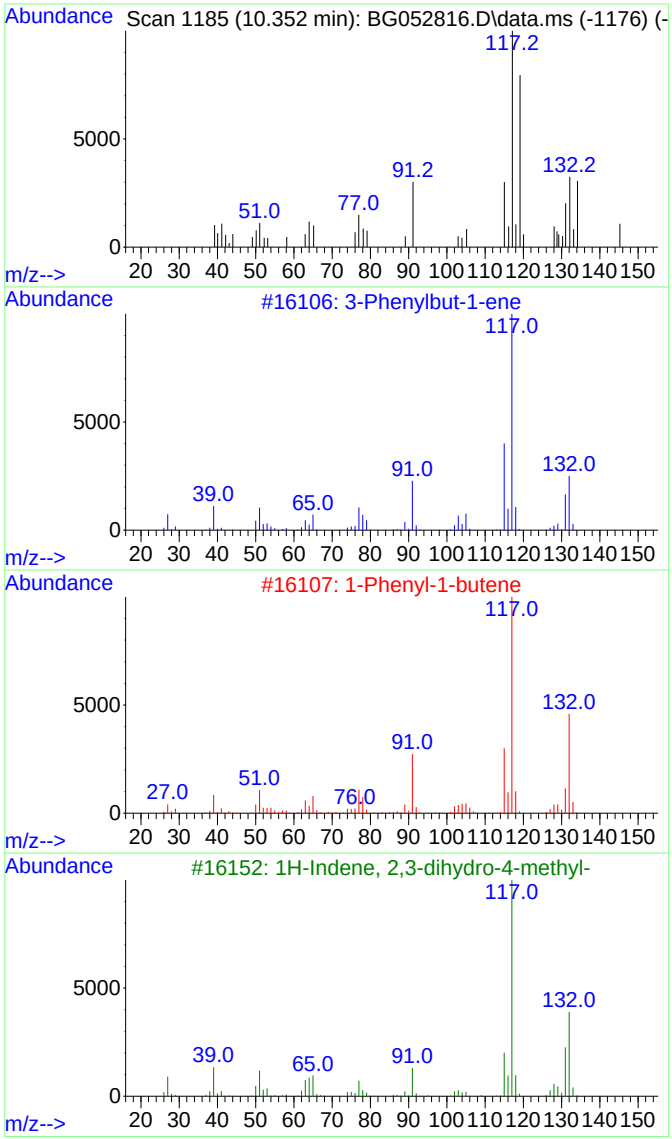
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

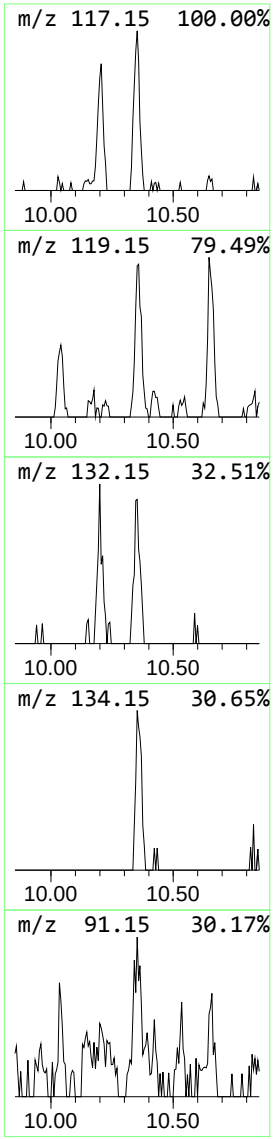
****

Peak Number 5 3-Phenylbut-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.352	2.64 ng	36294	Naphthalene-d8	10.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	50
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	46
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	45
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	45
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	43





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

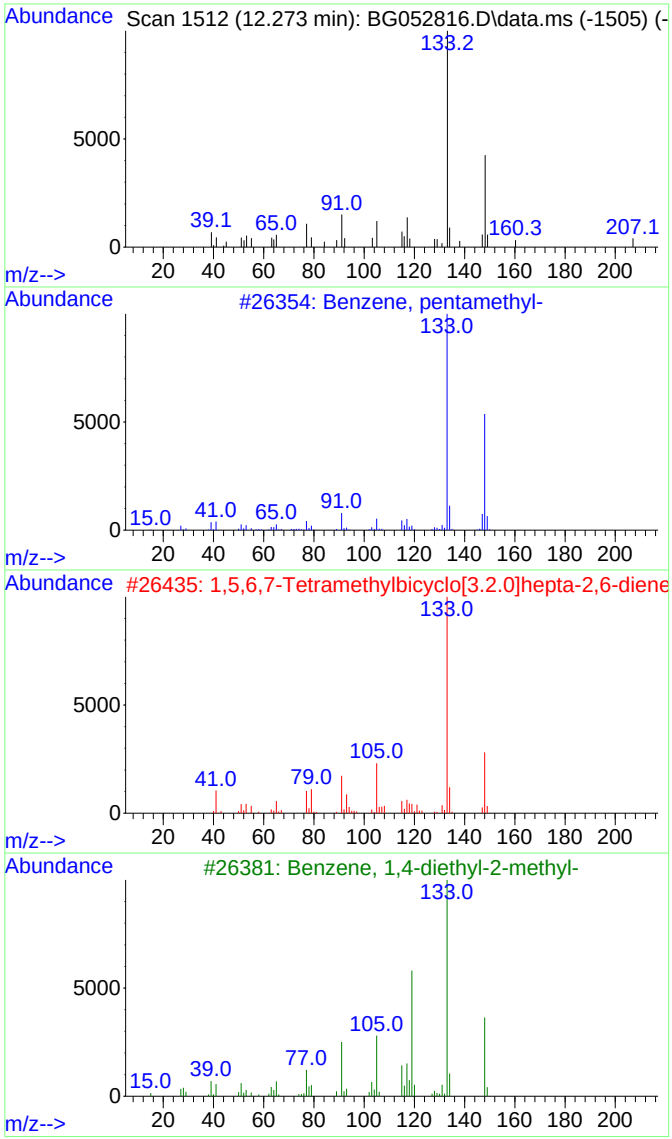
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

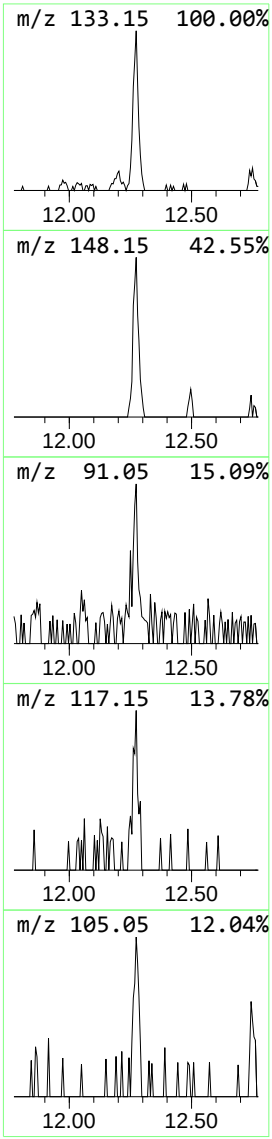
****

Peak Number 6 Benzene, pentamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.273	2.58 ng	35465	Naphthalene-d8	10.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, pentamethyl-	148	C11H16	000700-12-9	90
2	1,5,6,7-Tetramethylbicyclo[3.2.0...	148	C11H16	134329-46-7	83
3	Benzene, 1,4-diethyl-2-methyl-	148	C11H16	013632-94-5	80
4	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	72
5	Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	017851-27-3	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
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Acq On : 24 Mar 2022 19:39
Operator : CG/JU
Sample : N2090-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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
Pentane, 2,3,4-...	4.072	6.1	ng	53055	1	8.143	174762	20.0
Pentane, 2,3,3-...	4.167	9.5	ng	83208	1	8.143	174762	20.0
Benzene, 1,4-di...	8.637	7.9	ng	69417	1	8.143	174762	20.0
Benzene, 1,2,3,...	9.777	8.3	ng	114699	2	10.951	274877	20.0
3-Phenylbut-1-ene	10.352	2.6	ng	36294	2	10.951	274877	20.0
Benzene, pentam...	12.273	2.6	ng	35465	2	10.951	274877	20.0