LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054591.D
Acq On : 10 Aug 2022 16:48
Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.090	11	17	30	rVB	231354	447113	26.87%	5.920%
2	4.406	237	241	251	rVB	37903	71563	4.30%	0.948%
3	5.058	347	352	361	rVB2	17407	30911	1.86%	0.409%
4	5.463	414	421	430	rBV	58500	107869	6.48%	1.428%
5	5.563	432	438	453	rVB	135354	252748	15.19%	3.347%
6	6.603	610	615	626	rVB	21635	36624	2.20%	0.485%
7	7.179	706	713	723	rBV	88057	168460	10.12%	2.231%
8	7.972	841	848	854	rBV	57624	100648	6.05%	1.333%
9	8.031	854	858	862	rVV	17054	28687	1.72%	0.380%
10	8.090	862	868	876	rVB	76013	134828	8.10%	1.785%
11	8.348	904	912	920	rVB	123662	214834	12.91%	2.845%
12	9.083	1031	1037	1041	rBV2	24258	41369	2.49%	0.548%
13	9.142	1041	1047	1058	rVB	187070	365321	21.95%	4.837%
14	9.606	1121	1126	1133	rBV	11882	19195	1.15%	0.254%
15	9.706	1138	1143	1150	rVB	10852	19157	1.15%	0.254%
16	10.029	1192	1198	1205	rVB	11643	20256	1.22%	0.268%
17	10.176	1214	1223	1233	rBV4	39591	83243	5.00%	1.102%
18	10.787	1319	1327	1331	rBV	76087	144088	8.66%	1.908%
19	10.834	1331	1335	1342	rVB	134508	238244	14.32%	3.155%
20	11.721	1480	1486	1497	rVB3	14365	34888	2.10%	0.462%
21	12.661	1637	1646	1653	rVB3	20748	36910	2.22%	0.489%
22	12.966	1692	1698	1705	rBV4	11274	19673	1.18%	0.260%
23	13.237	1736	1744	1752	rBV	555835	895700	53.83%	11.860%
24	13.466	1777	1783	1795	rVB	168425	274508	16.50%	3.635%
25	14.617	1972	1979	1986	rBV	137177	218728	13.14%	2.896%
26	16.116	2225	2234	2247	rBV2	514135	809636	48.65%	10.720%
27	16.691	2328	2332	2340	rVB2	11717	18199	1.09%	0.241%
28	17.367	2440	2447	2455	rBV	173454	277885	16.70%	3.679%
29	18.019	2554	2558	2563	rVB2	20050	29127	1.75%	0.386%
30	19.976	2884	2891	2896	rBV	1191784	1664048	100.00%	22.034%
31	21.633	3168	3173	3180	rBV2	217658	360125	21.64%	4.768%
32	24.841	3712	3719	3729	rVB2	129645	387682	23.30%	5.133%

Sum of corrected areas: 7552267

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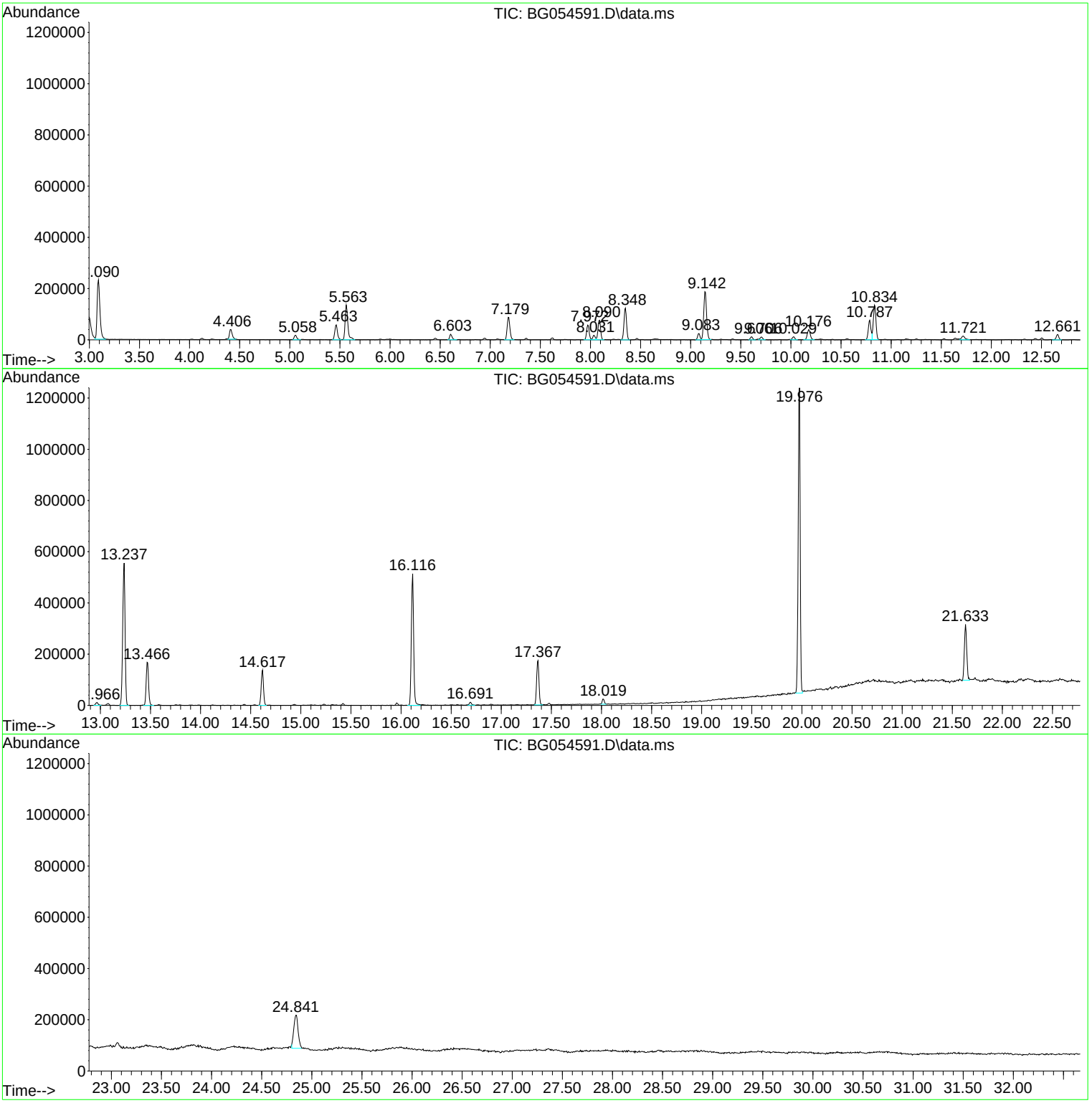
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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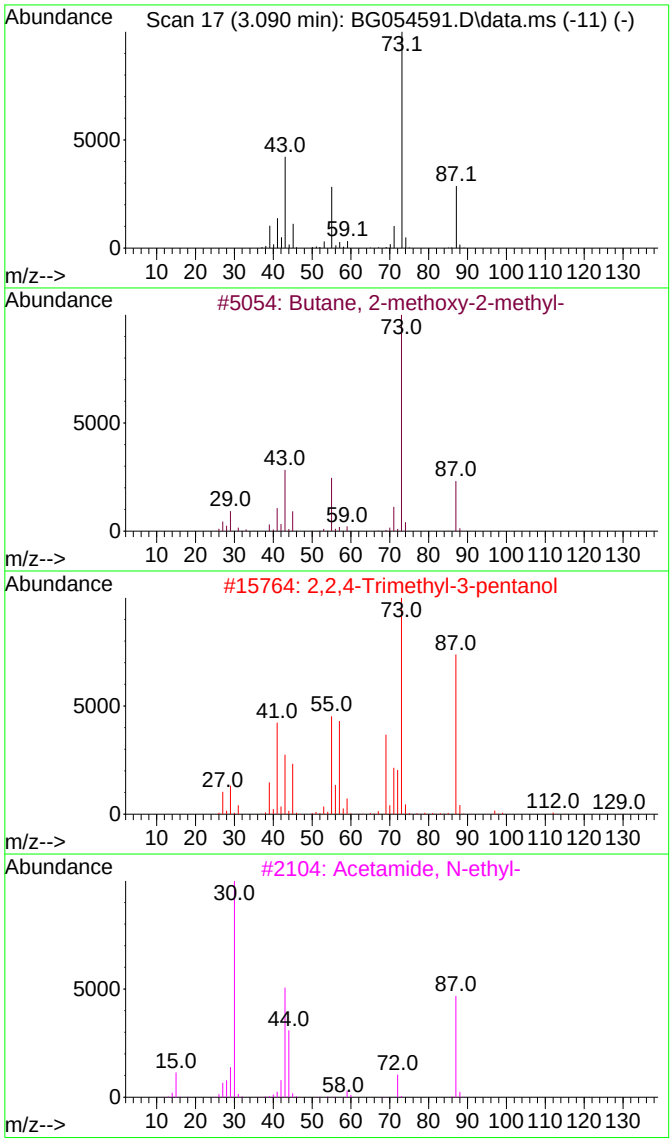
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

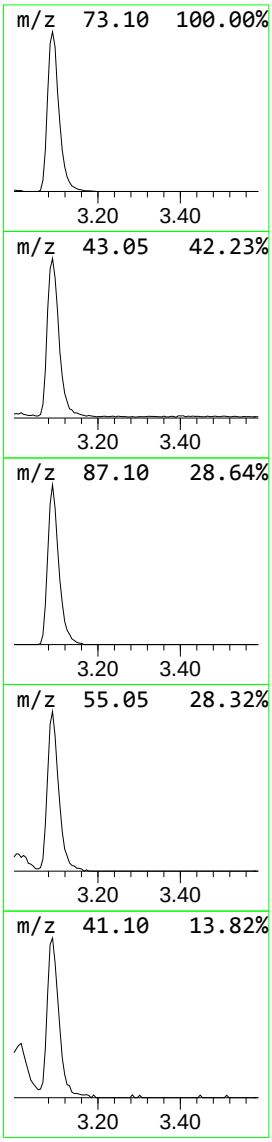
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.090	88.85 ng	447113	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG054591.D
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Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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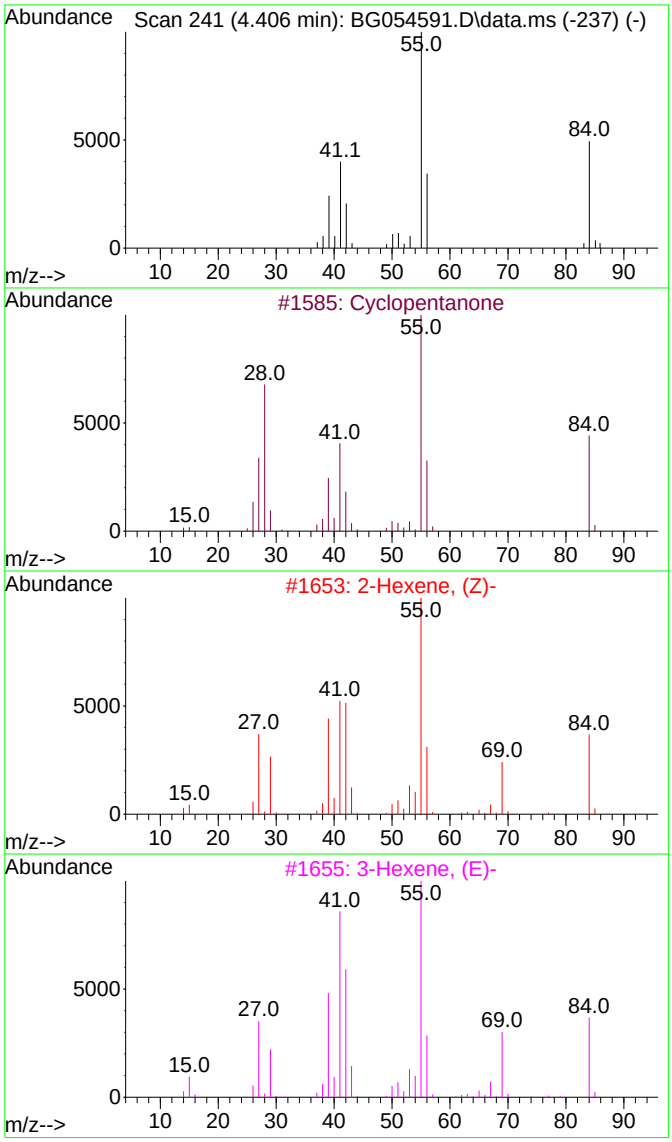
TIC Integration Parameters: LSCINT.P

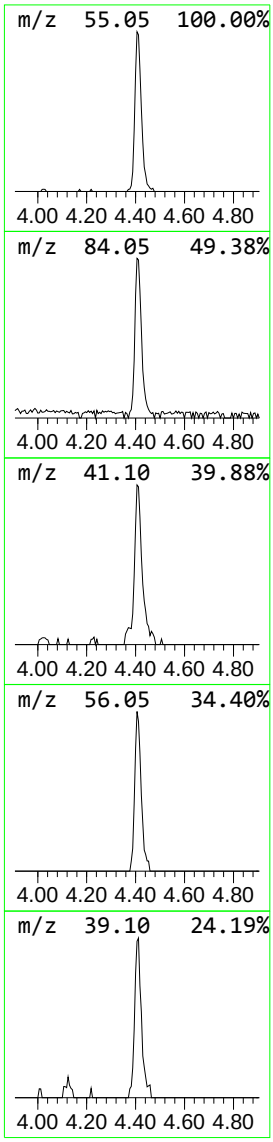
****

Peak Number 2 Cyclopentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.406	14.22 ng	71563	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene, (Z)-	84	C6H12	007688-21-3	59
3	3-Hexene, (E)-	84	C6H12	013269-52-8	59
4	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	53
5	3-Hexene	84	C6H12	000592-47-2	53





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Data File : BG054591.D
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Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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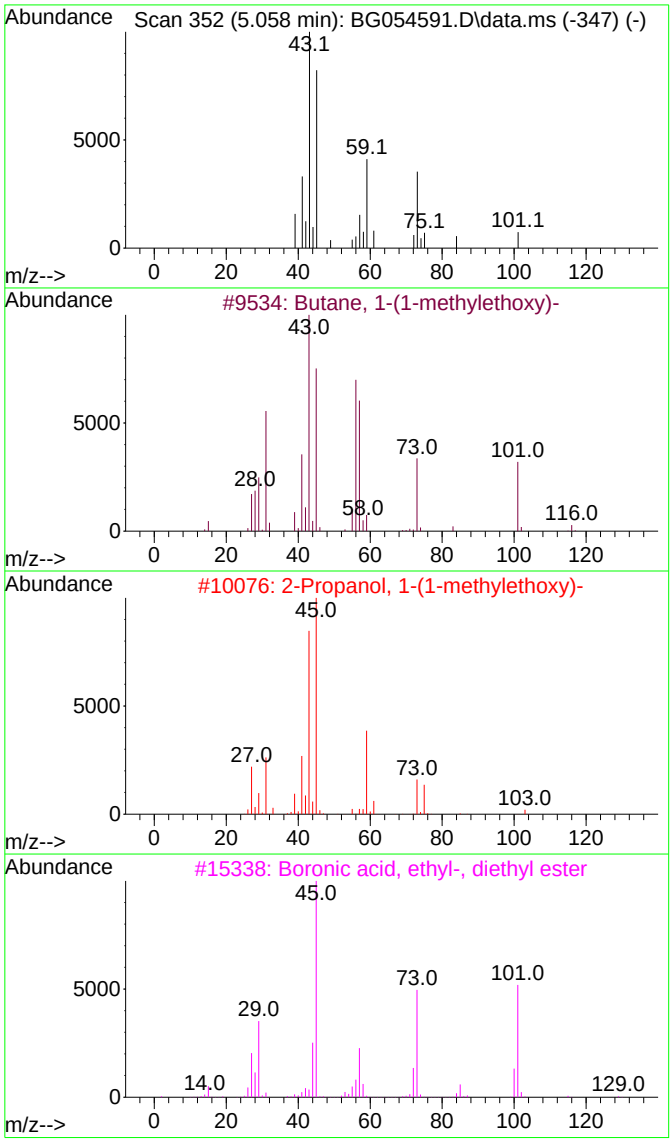
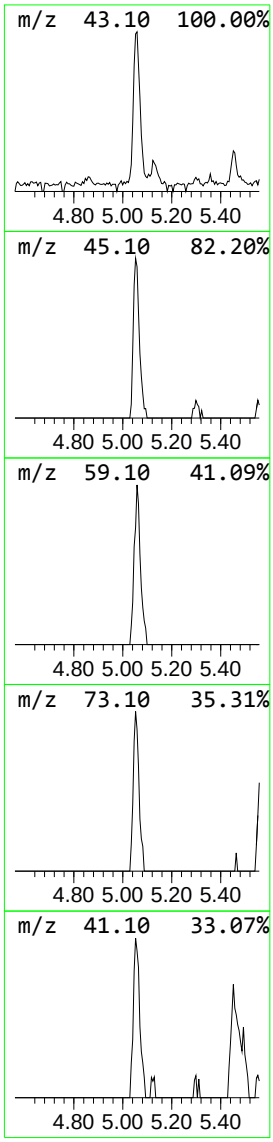
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 1-(1-methylethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.058	6.14 ng	30911	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	50
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
3	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	38
4	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	33
5	2-O-Mesyl arabinose	228	C6H12O7S	1000130-06-0	28





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Operator : CG/JU
Sample : N3971-14
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-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

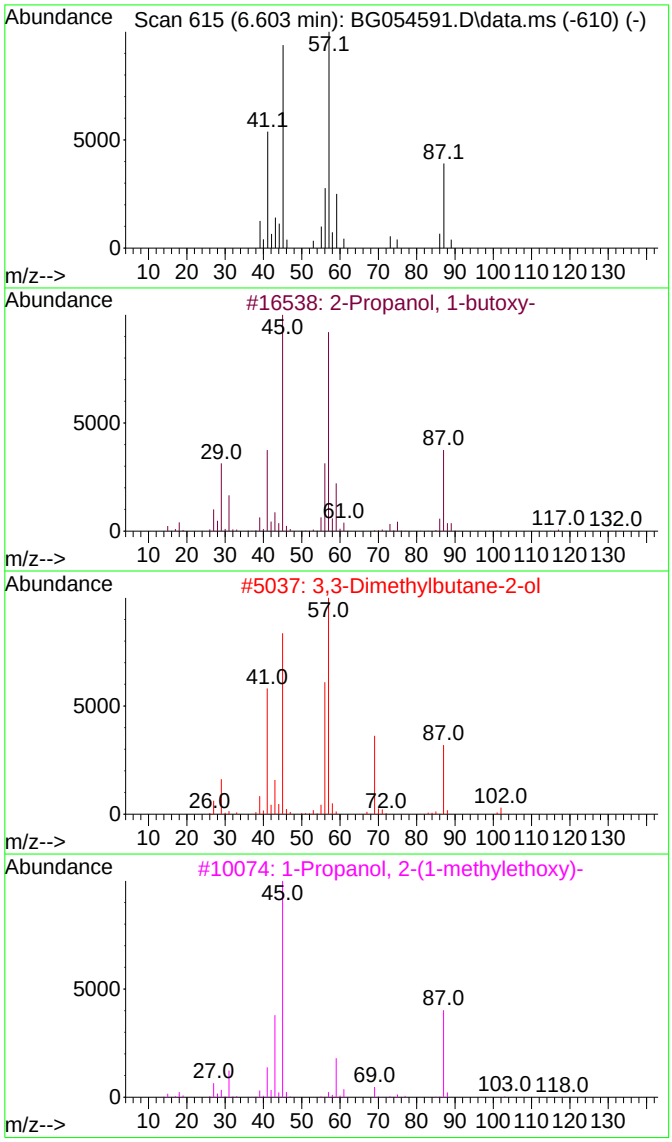
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

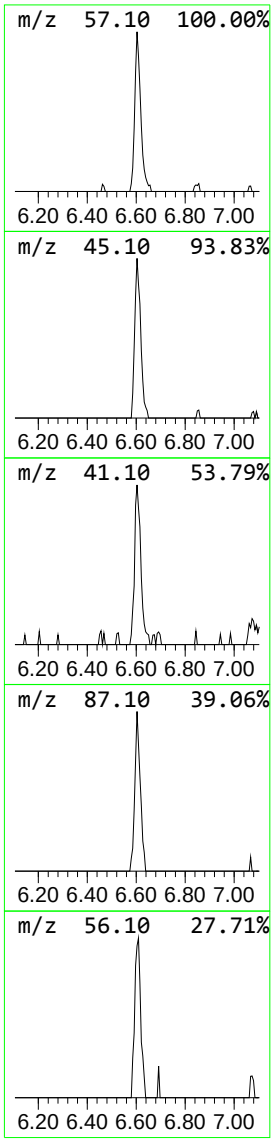
****

Peak Number 5 2-Propanol, 1-butoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.603	7.28 ng	36624	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	38
4	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	36
5	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	33





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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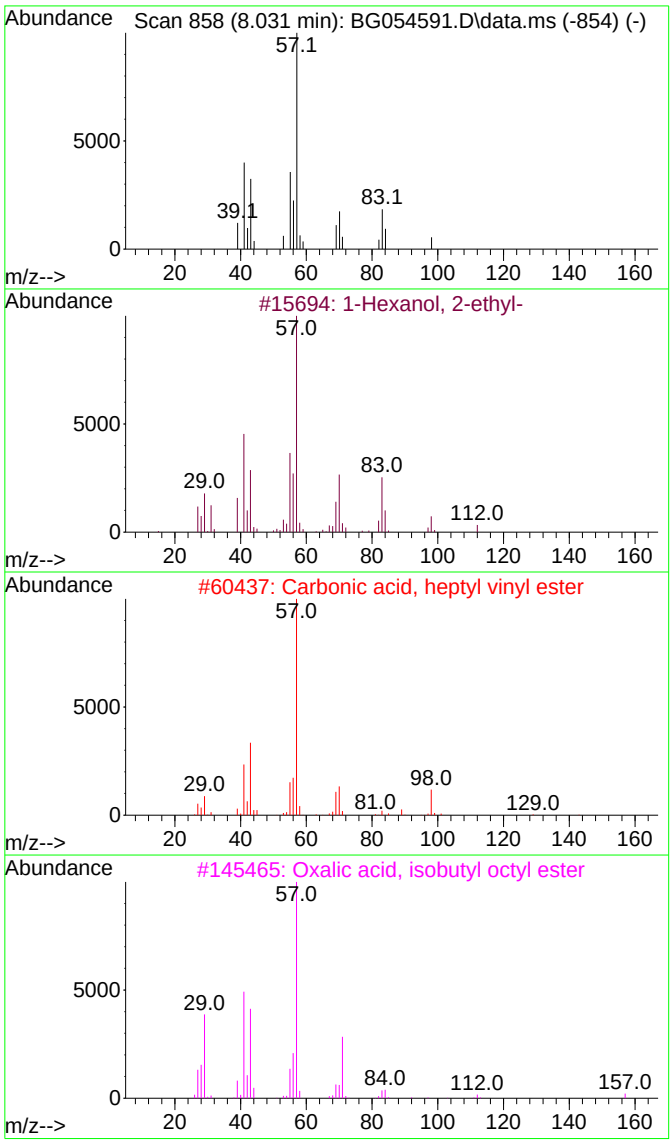
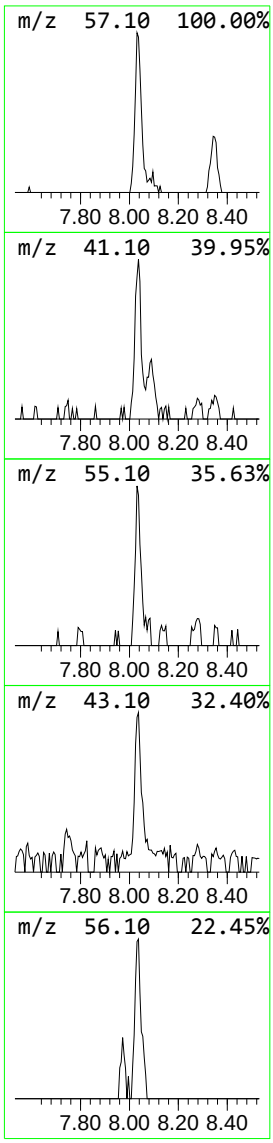
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.031	5.70 ng	28687	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53
3	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	50
4	Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	47
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	38





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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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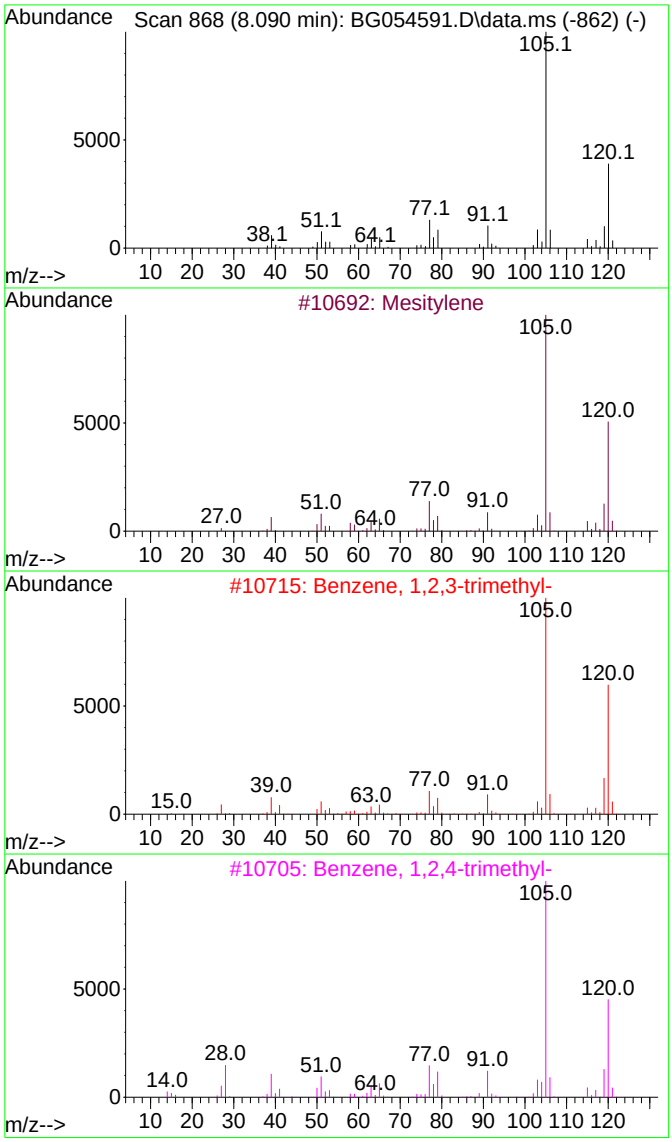
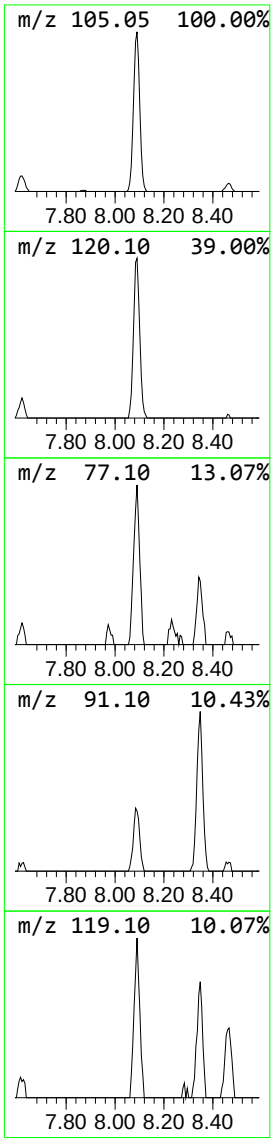
****

Peak Number 7 Mesitylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.090	26.79 ng	134828	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	94
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

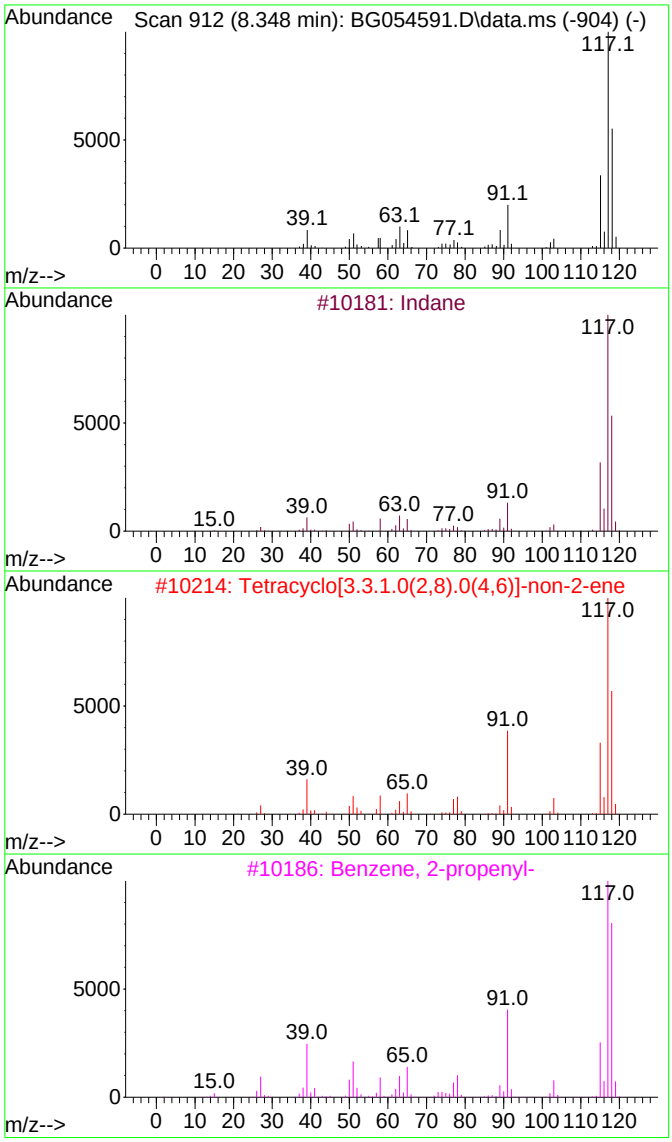
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

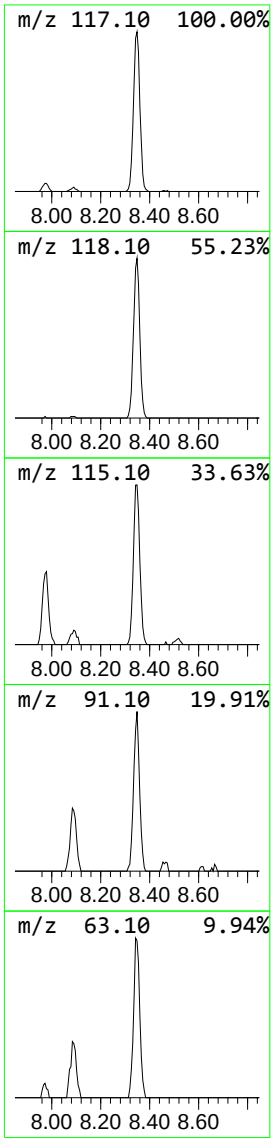
****

Peak Number 8 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.348	42.69 ng	214834	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	74
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	68





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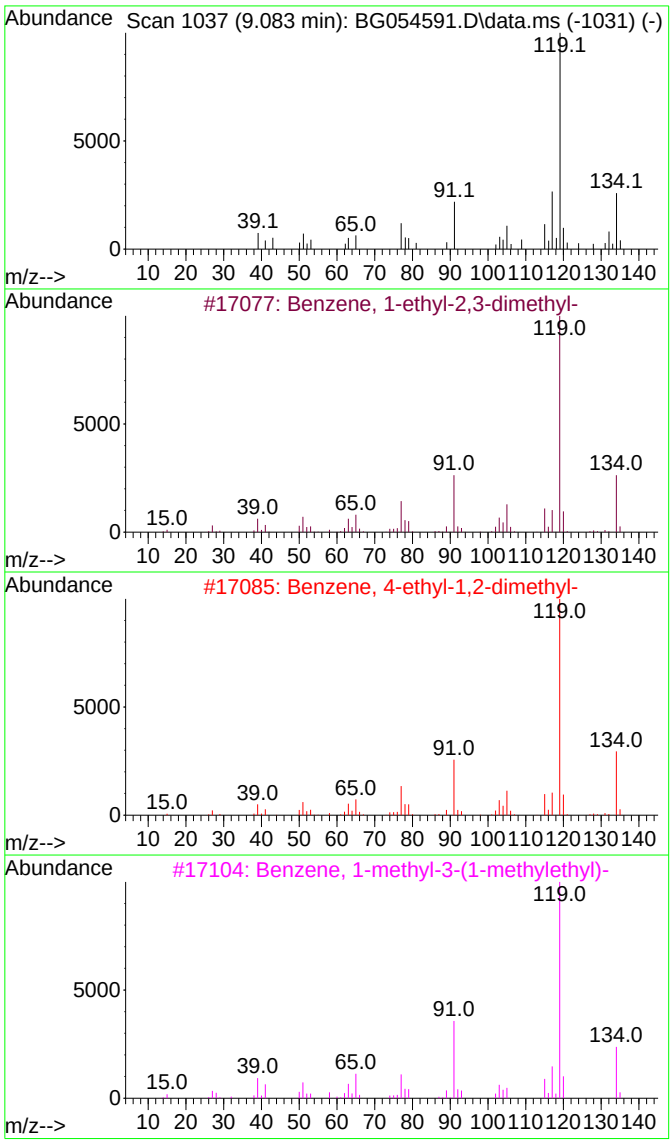
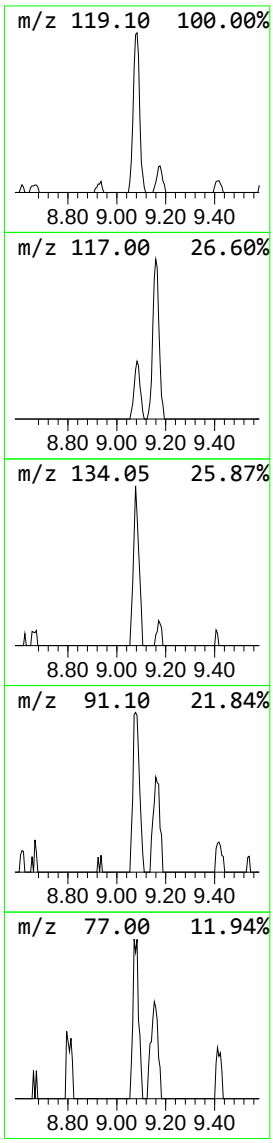
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.083	8.22 ng	41369	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	87
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87
5	p-Cymene	134	C10H14	000099-87-6	87





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Data File : BG054591.D
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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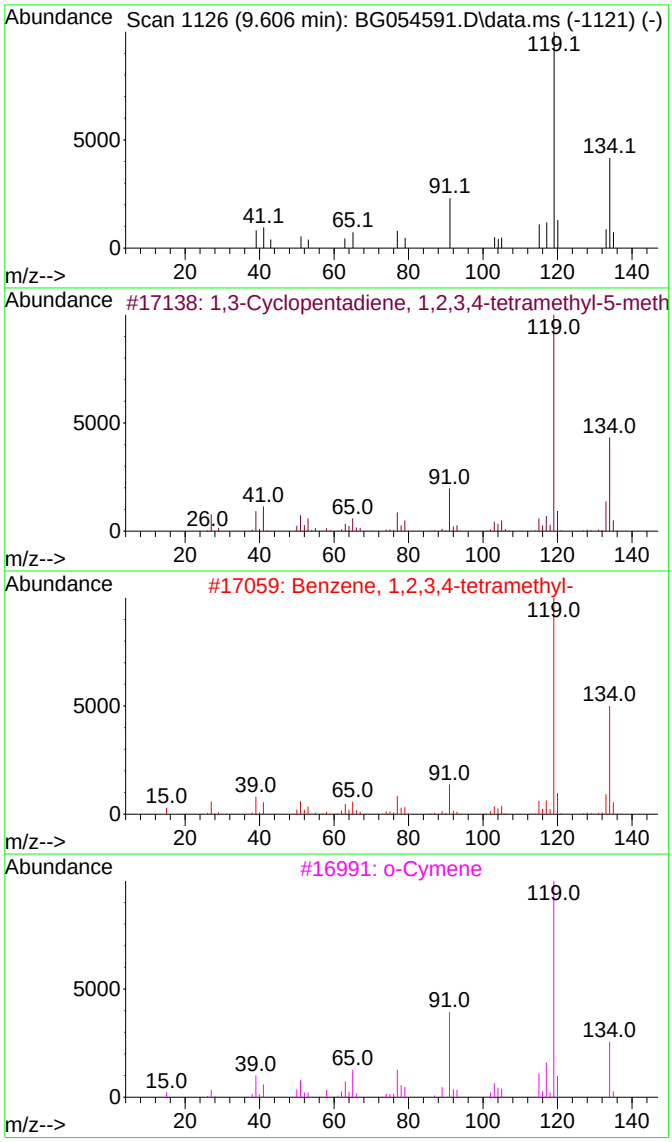
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

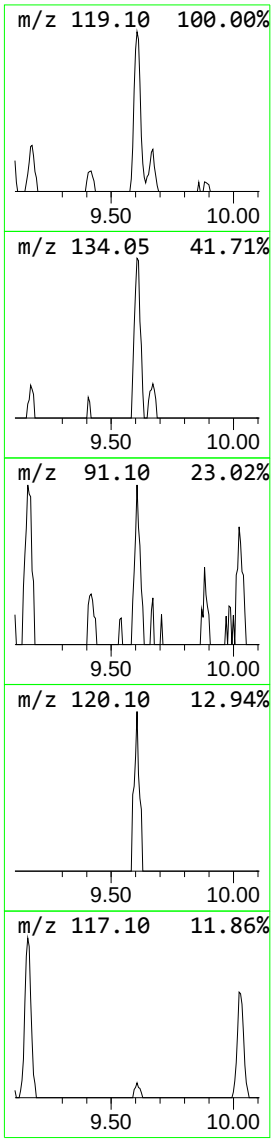
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,3-Cyclopentadiene, 1,2,3,... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.606	2.66 ng	19195	Naphthalene-d8	10.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	91
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
3	o-Cymene	134	C10H14	000527-84-4	91
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91





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Data File : BG054591.D
Acq On : 10 Aug 2022 16:48
Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

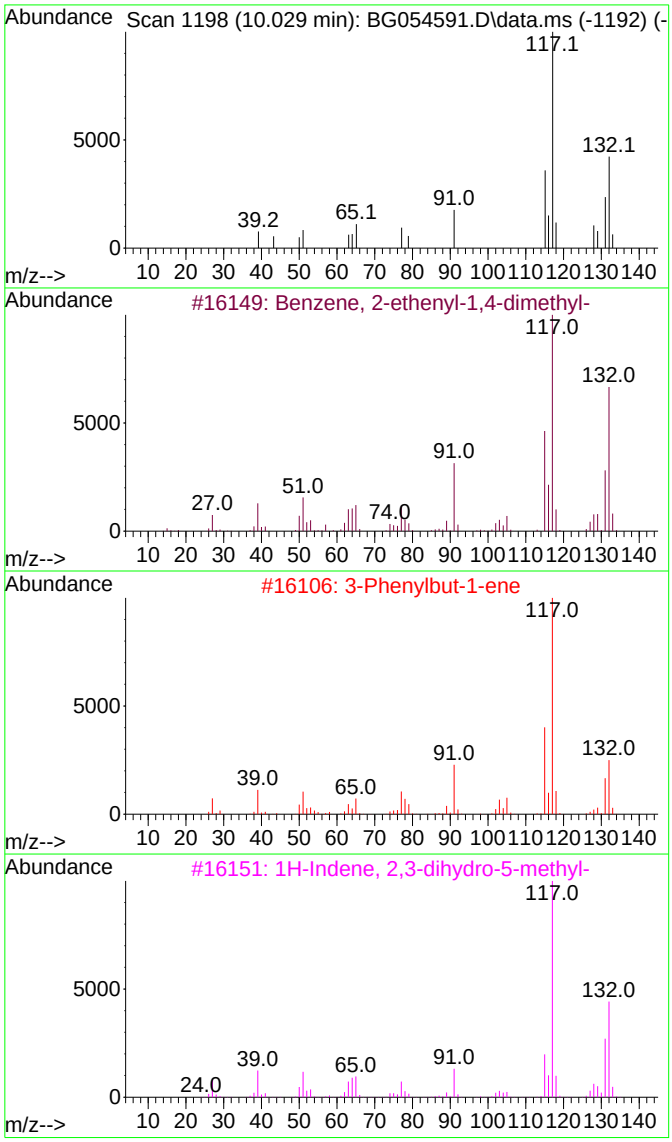
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

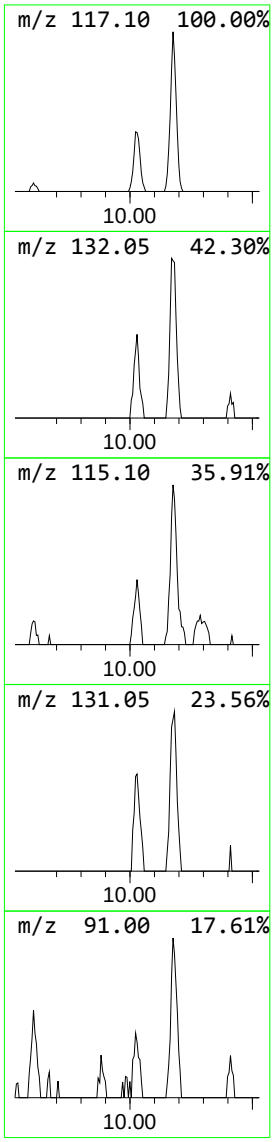
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.029	2.81 ng	20256	Naphthalene-d8	10.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054591.D
Acq On : 10 Aug 2022 16:48
Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

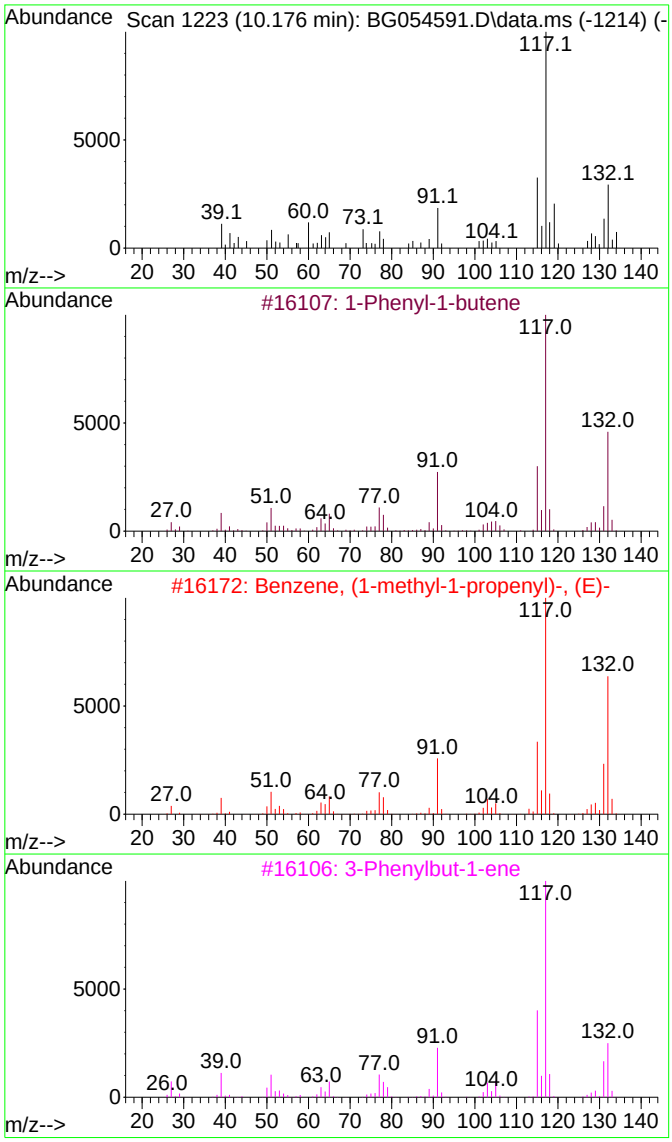
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

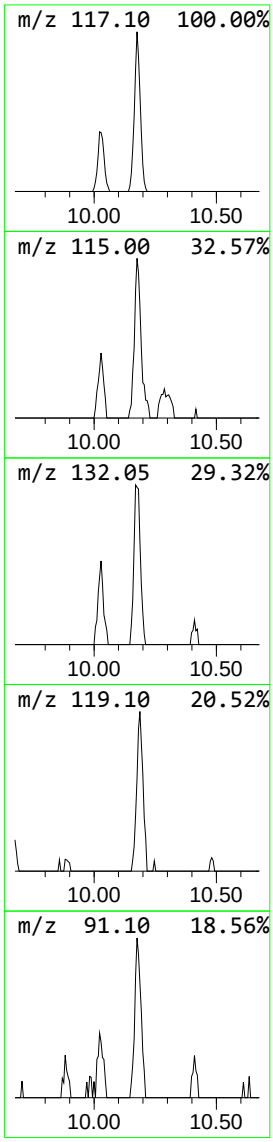
****

Peak Number 12 1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.176	11.55 ng	83243	Naphthalene-d8	10.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76
5	Indan, 1-methyl-	132	C10H12	000767-58-8	74





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Data File : BG054591.D
Acq On : 10 Aug 2022 16:48
Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

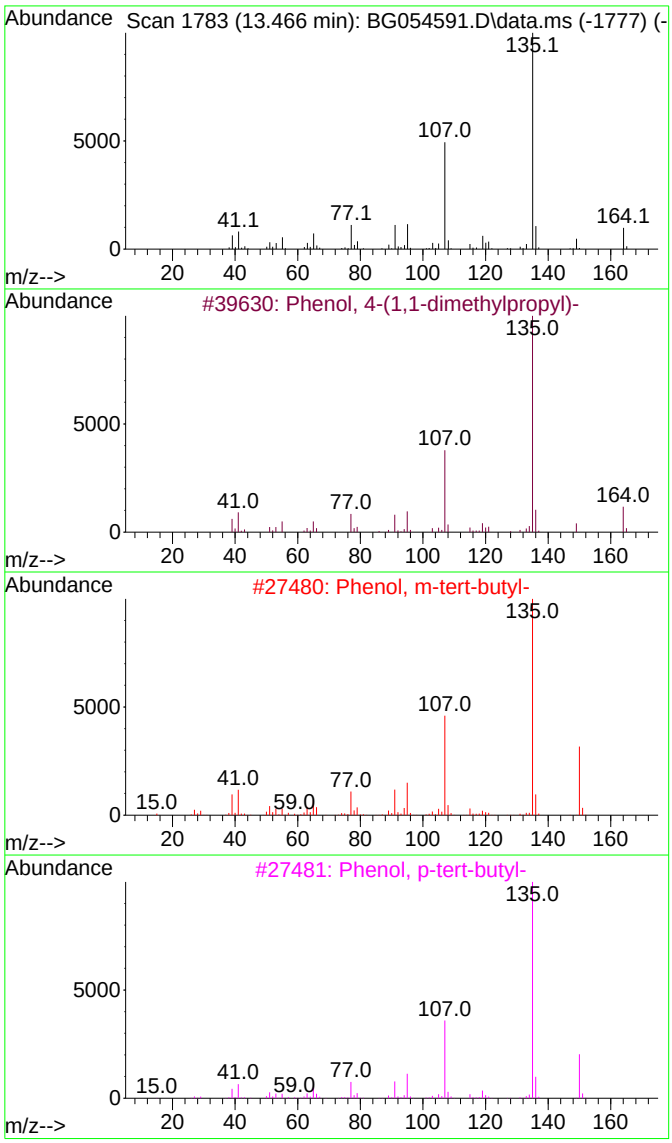
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

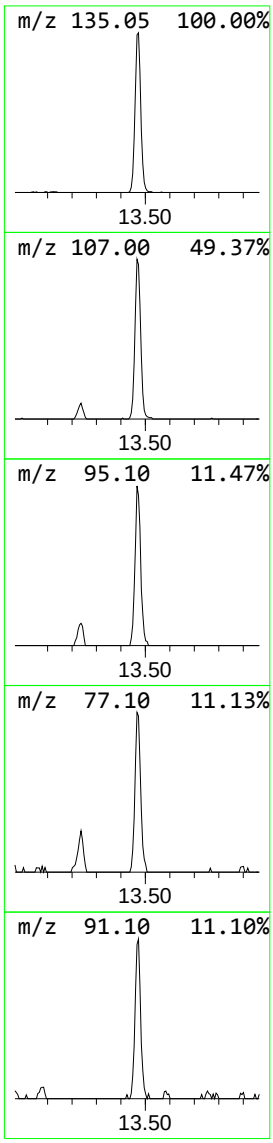
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Phenol, 4-(1,1-dimethylprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.466	25.10 ng	274508	Acenaphthene-d10	14.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	64





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Data File : BG054591.D
Acq On : 10 Aug 2022 16:48
Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

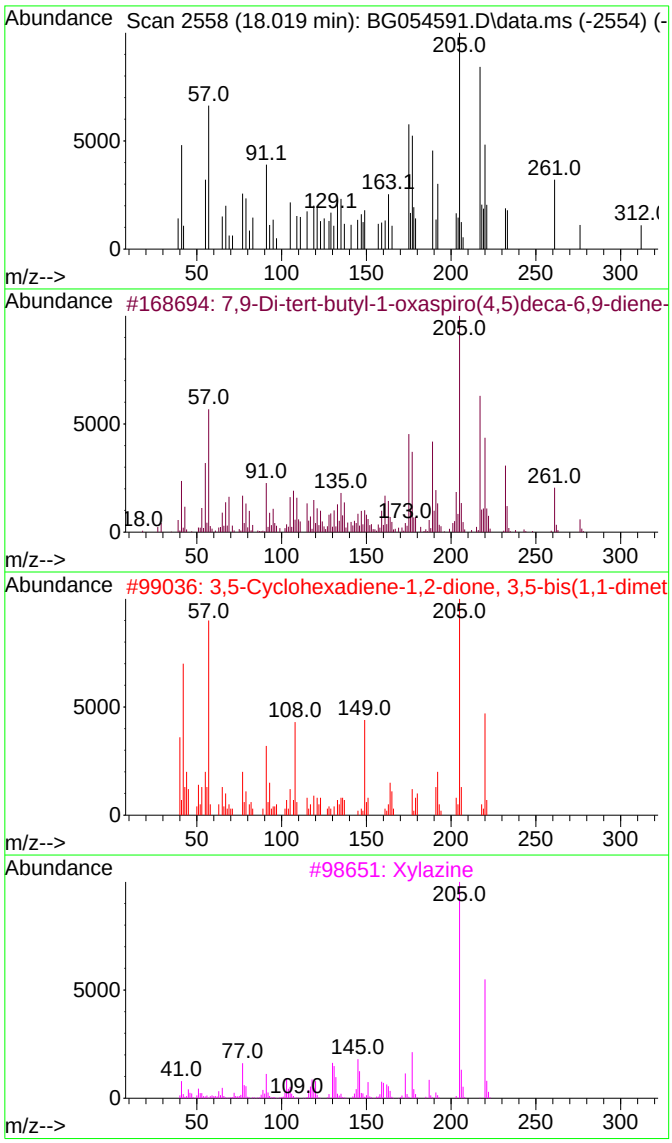
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

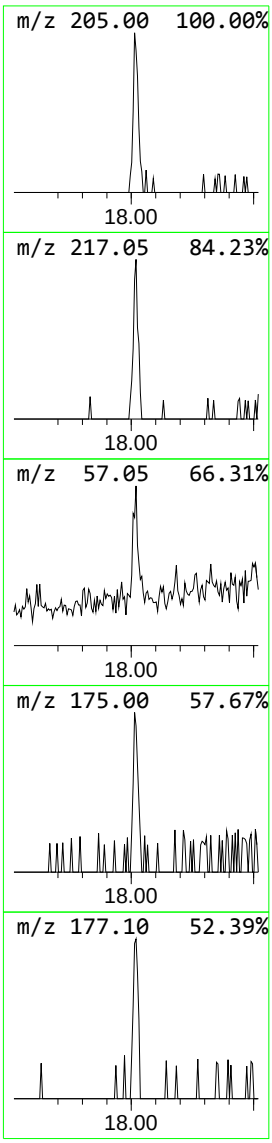
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.019	2.10 ng	29127	Phenanthrene-d10	17.367

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	70
2	3,5-Cyclohexadiene-1,2-dione, 3,...	220	C14H20O2	003383-21-9	30
3	Xylazine	220	C12H16N2S	007361-61-7	25
4	2-(3,3-Dimethylbut-1-ynyl)thieno...	220	C12H12S2	1010250-48-5	18
5	Benzenethanol, O,.beta.,.beta.,2...	220	C15H24O	1010128-94-8	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054591.D
Acq On : 10 Aug 2022 16:48
Operator : CG/JU
Sample : N3971-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
Butane, 2-metho...	3.090	88.8	ng	447113	1	7.972	100648	20.0
Cyclopentanone	4.406	14.2	ng	71563	1	7.972	100648	20.0
Butane, 1-(1-me...	5.058	6.1	ng	30911	1	7.972	100648	20.0
2-Propanol, 1-b...	6.603	7.3	ng	36624	1	7.972	100648	20.0
1-Hexanol, 2-et...	8.031	5.7	ng	28687	1	7.972	100648	20.0
Mesitylene	8.090	26.8	ng	134828	1	7.972	100648	20.0
Indane	8.348	42.7	ng	214834	1	7.972	100648	20.0
Benzene, 1-ethy...	9.083	8.2	ng	41369	1	7.972	100648	20.0
1,3-Cyclopentad...	9.606	2.7	ng	19195	2	10.787	144088	20.0
Benzene, 2-ethe...	10.029	2.8	ng	20256	2	10.787	144088	20.0
1-Phenyl-1-butene	10.176	11.6	ng	83243	2	10.787	144088	20.0
Phenol, 4-(1,1-...	13.466	25.1	ng	274508	3	14.618	218728	20.0
7,9-Di-tert-but...	18.019	2.1	ng	29127	4	17.367	277885	20.0