LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

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:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.821	621	637	661	rVB	488394	1247763	17.00%	2.365%
2	4.085	705	719	742	rVB	75840	215629	2.94%	0.409%
3	5.053	995	1020	1047	rBV2	280663	1032734	14.07%	1.958%
4	6.854	1564	1580	1601	rBV3	26846	76389	1.04%	0.145%
5	7.590	1790	1809	1820	rBV2	1016716	2511083	34.22%	4.760%
6	7.664	1820	1832	1890	rVB	1784008	4676600	63.73%	8.864%
7	8.027	1928	1945	1967	rBV	1013649	2438415	33.23%	4.622%
8	8.587	2103	2119	2167	rVB	2450654	5551934	75.66%	10.524%
9	9.079	2254	2272	2287	rVB8	38667	103017	1.40%	0.195%
10	10.091	2571	2587	2629	rBV	3632764	7338151	100.00%	13.909%
11	11.406	2981	2996	3019	rBV	3167118	5900052	80.40%	11.184%
12	11.622	3052	3063	3071	rBV3	44152	101040	1.38%	0.192%
13	11.943	3145	3163	3179	rBV6	38083	117080	1.60%	0.222%
14	12.249	3247	3258	3270	rVB	317639	514435	7.01%	0.975%
15	12.400	3292	3305	3326	rBV	2543324	4428274	60.35%	8.394%
16	12.590	3351	3364	3377	rVB	346140	581902	7.93%	1.103%
17	13.040	3497	3504	3516	rVB	60093	94008	1.28%	0.178%
18	13.172	3531	3545	3554	rBV4	168753	332204	4.53%	0.630%
19	13.342	3585	3598	3618	rVB	2683467	4588807	62.53%	8.698%
20	13.442	3619	3629	3640	rVV2	94334	153453	2.09%	0.291%
21	13.512	3640	3651	3653	rVV	245967	332544	4.53%	0.630%
22	13.541	3653	3660	3670	rVV	847947	1419312	19.34%	2.690%
23	13.590	3670	3675	3690	rVV4	79984	175266	2.39%	0.332%
24	13.670	3691	3700	3712	rVB	173269	291693	3.98%	0.553%
25	13.889	3757	3768	3777	rBV	516140	813706	11.09%	1.542%
26	13.947	3777	3786	3791	rVV	190276	284642	3.88%	0.540%
27	13.992	3791	3800	3811	rVB2	725868	1215646	16.57%	2.304%
28	14.130	3831	3843	3851	rBV2	117680	198344	2.70%	0.376%
29	14.207	3852	3867	3886	rVB	450239	809930	11.04%	1.535%
30	14.429	3926	3936	3943	rVV4	63543	129837	1.77%	0.246%
31	14.477	3943	3951	3960	rVV3	123386	205742	2.80%	0.390%
32	14.590	3972	3986	3998	rVV3	1062196	2210497	30.12%	4.190%
33	14.654	3999	4006	4015	rVB5	48379	84616	1.15%	0.160%
34	14.741	4023	4033	4043	rVB	267944	425819	5.80%	0.807%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

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:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Title : SW846 8260

35	14.850	4058	4067	4073	rBV3	128978	224872	3.06%	0.426%
36	14.882	4074	4077	4087	rVV3	92643	134072	1.83%	0.254%
37	14.956	4090	4100	4109	rVB3	202887	408938	5.57%	0.775%
38	15.133	4147	4155	4164	rVB	140956	224722	3.06%	0.426%
39	15.188	4165	4172	4180	rVB3	70419	95147	1.30%	0.180%
40	15.262	4181	4195	4201	rBV3	92350	232324	3.17%	0.440%
41	15.483	4258	4264	4275	rVB6	44685	73889	1.01%	0.140%
42	15.612	4300	4304	4314	rVB2	82651	115985	1.58%	0.220%
43	15.911	4384	4397	4412	rBV2	163056	338604	4.61%	0.642%
44	16.348	4521	4533	4551	rBV2	139051	307417	4.19%	0.583%

Sum of corrected areas: 52756534

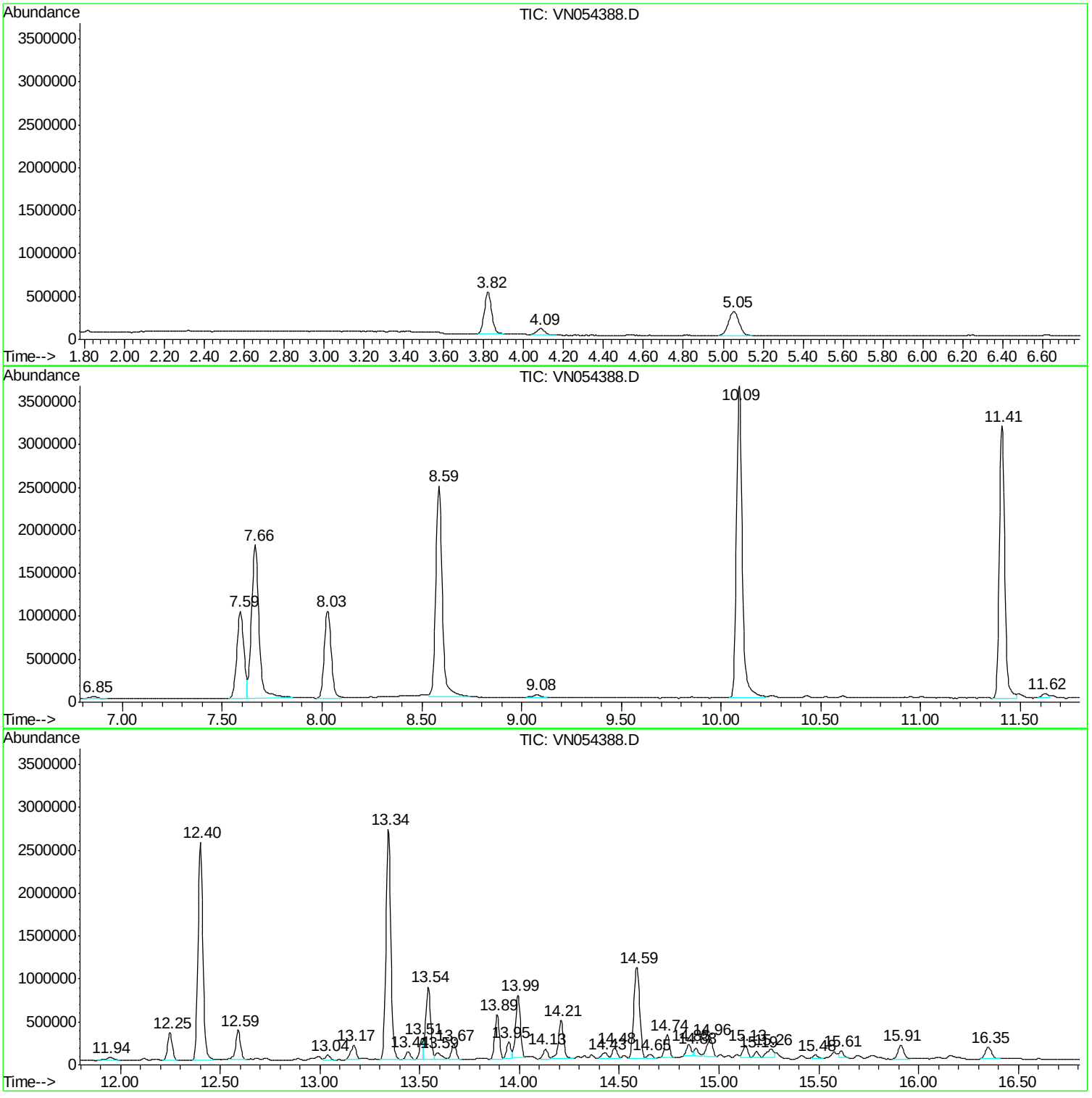
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Quant Title : SW846 8260

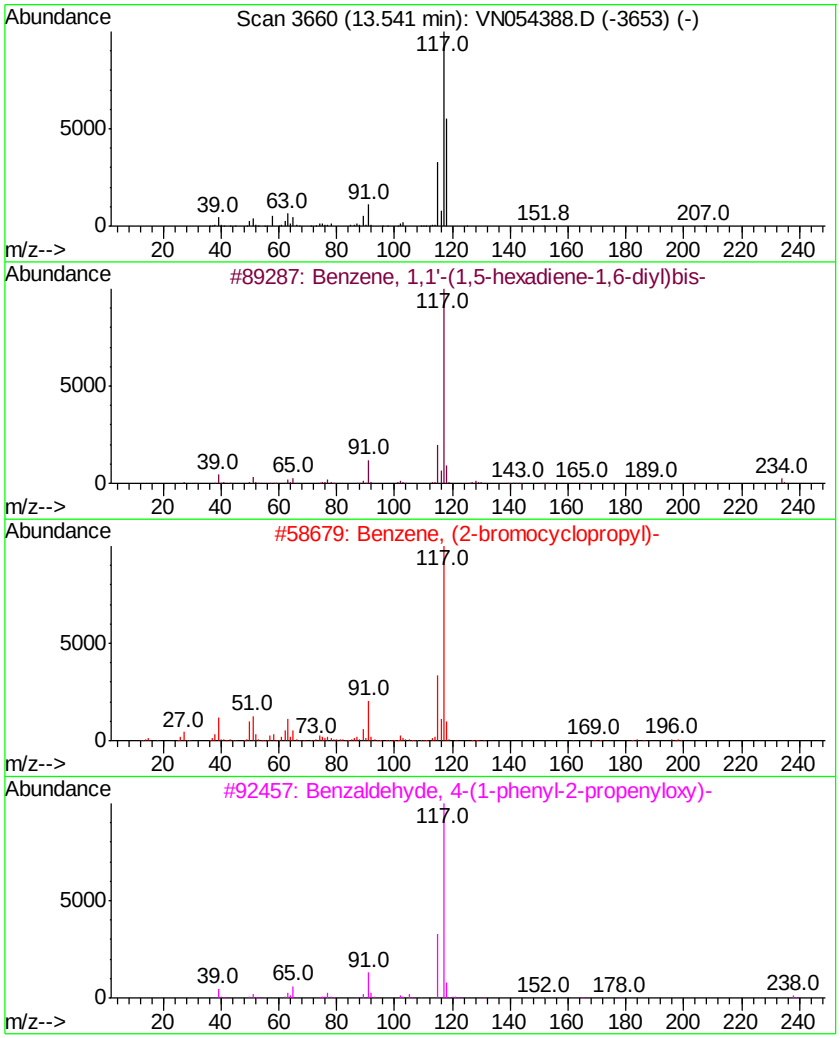
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

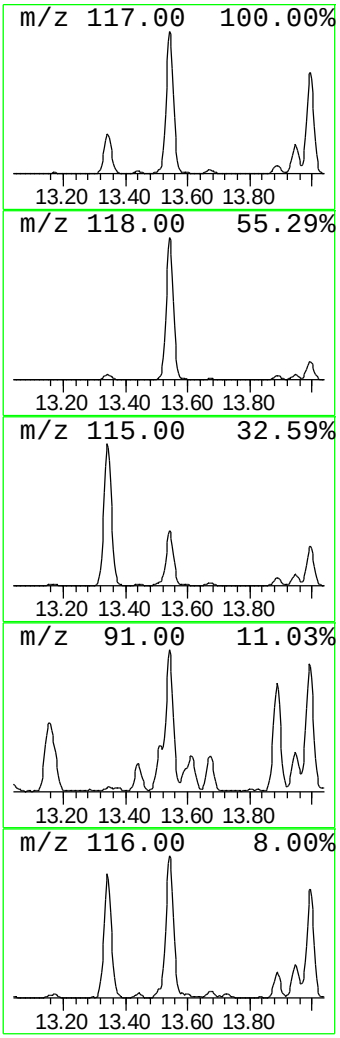
****

Peak Number 1 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	15.46 ug/l	1419310	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
2	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
3	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	36
4	Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	25
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	23





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Quant Title : SW846 8260

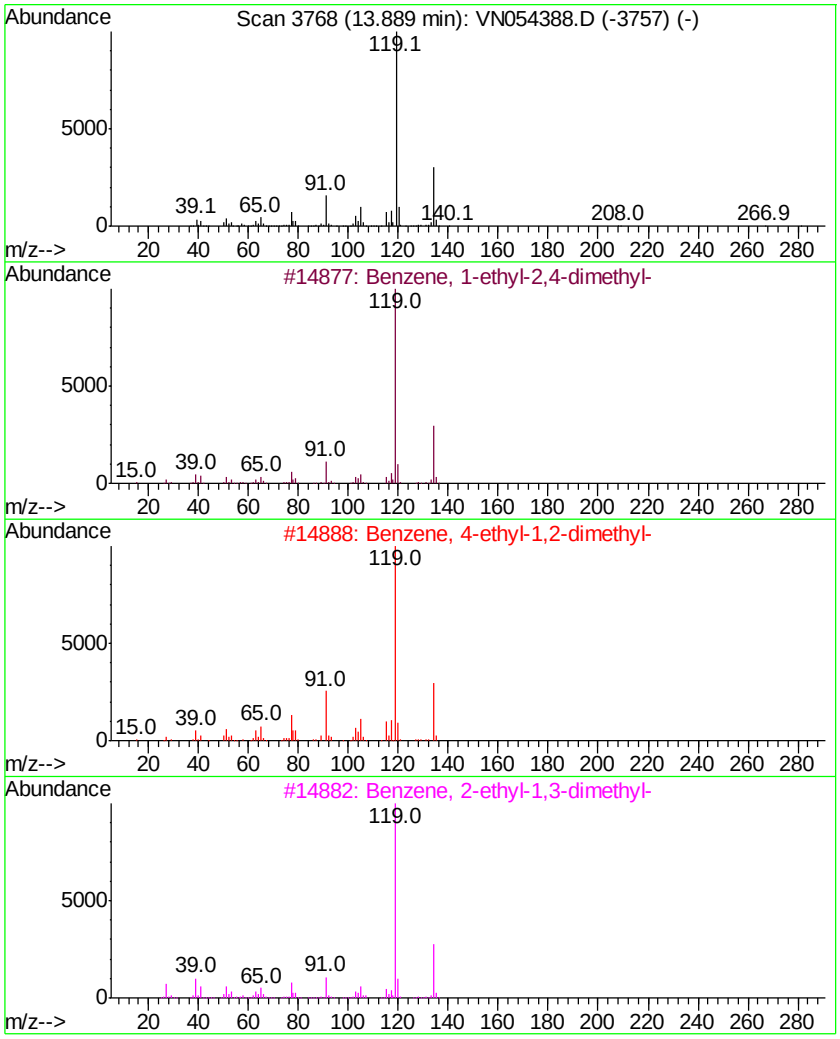
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

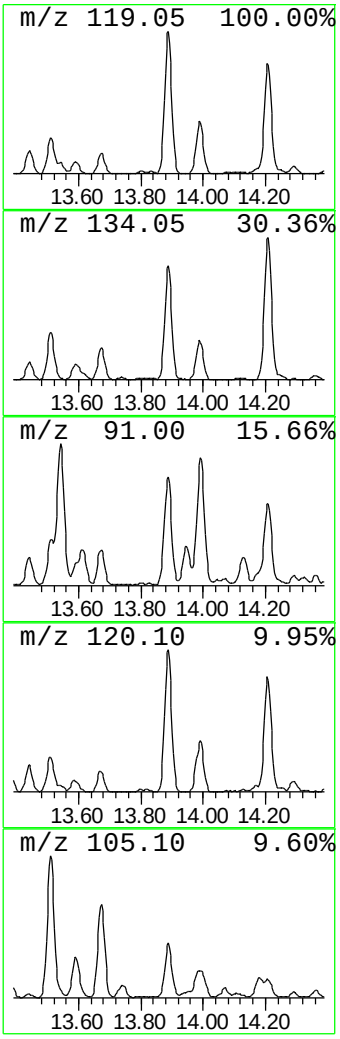
****

Peak Number 2 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	8.87 ug/l	813706	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Quant Title : SW846 8260

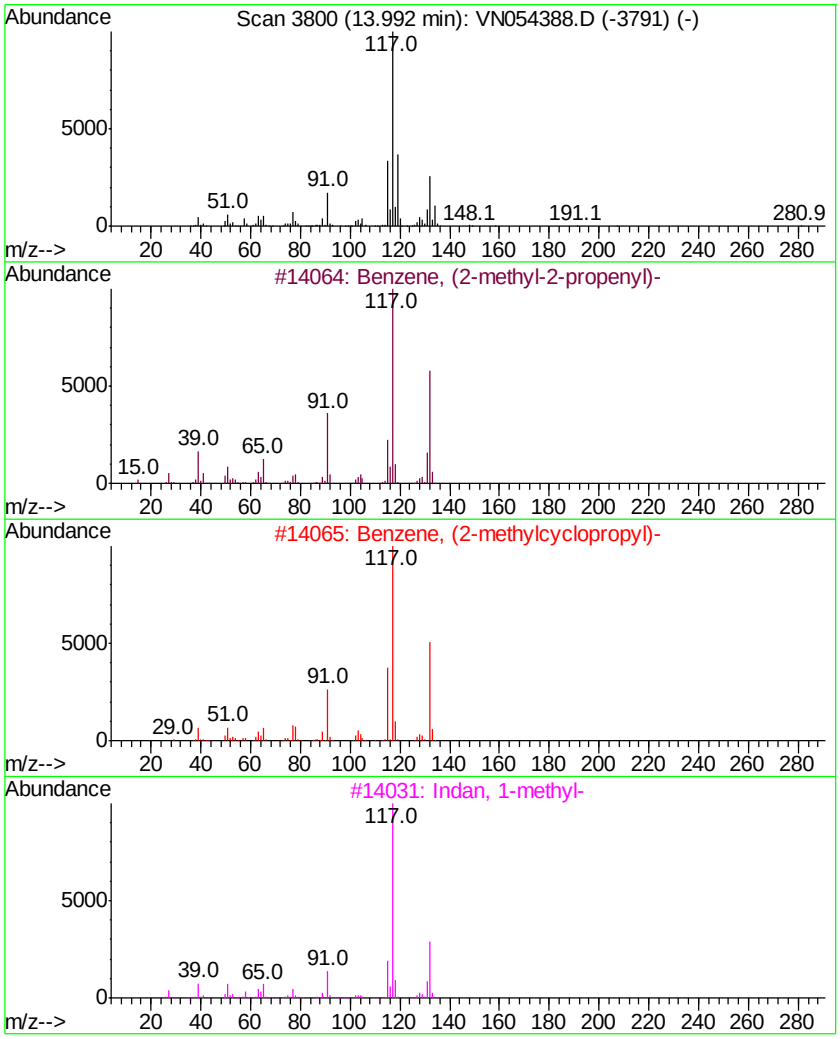
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

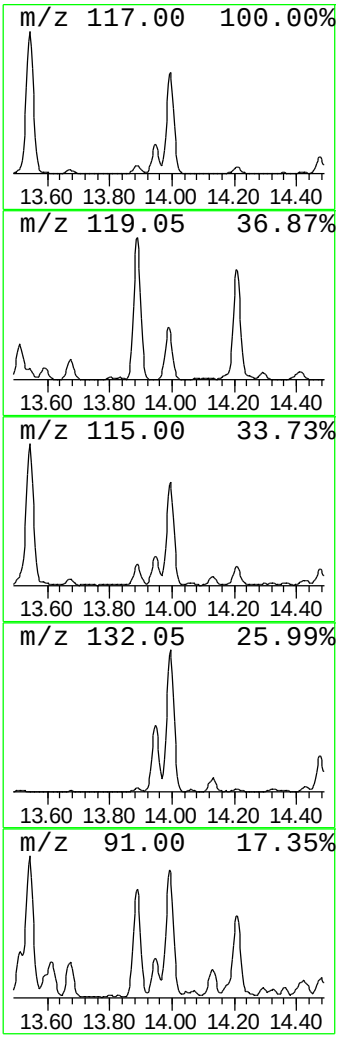
****

Peak Number 3 Benzene, (2-methyl-2-propen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	13.25 ug/l	1215650	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	72
2	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	70
3	Indan, 1-methyl-	132	C10H12	000767-58-8	70
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	68
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Quant Title : SW846 8260

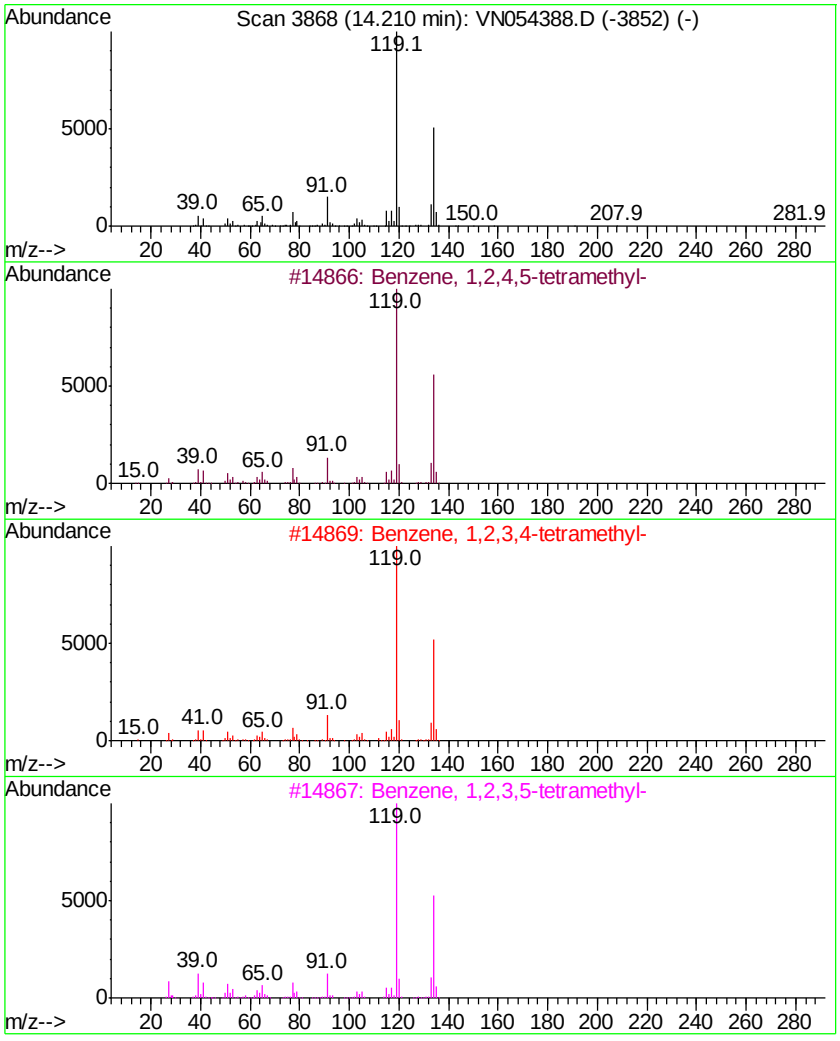
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

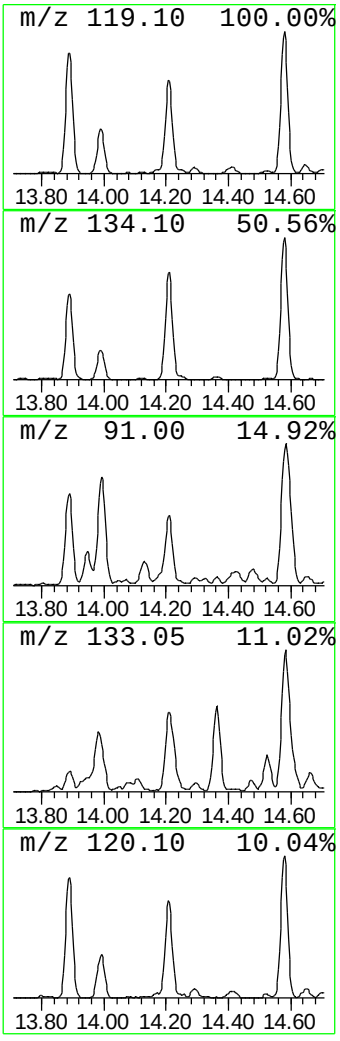
****

Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	8.83 ug/l	809930	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

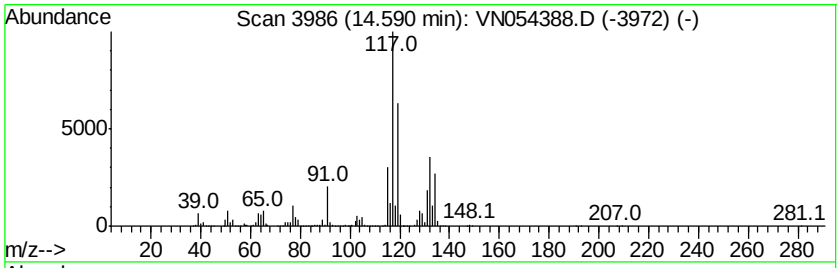
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Quant Title : SW846 8260

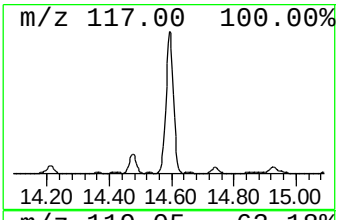
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

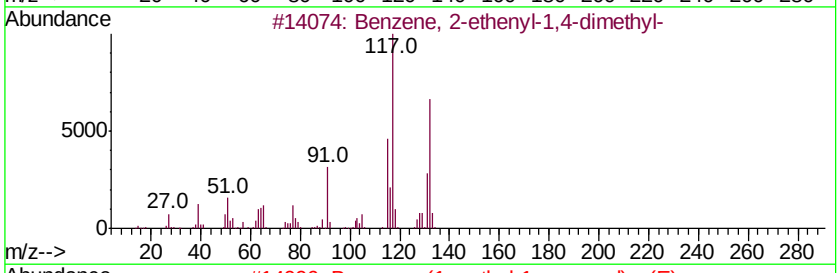
****
Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 1

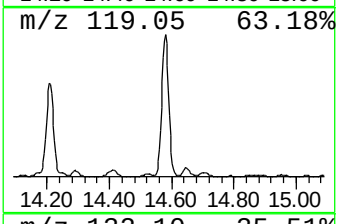
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	24.09 ug/l	2210500	1,4-Dichlorobenzene-d4	13.34

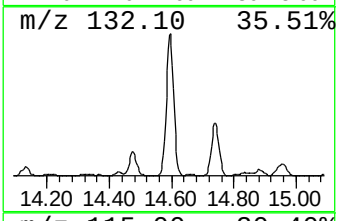
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
3	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	70
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	64

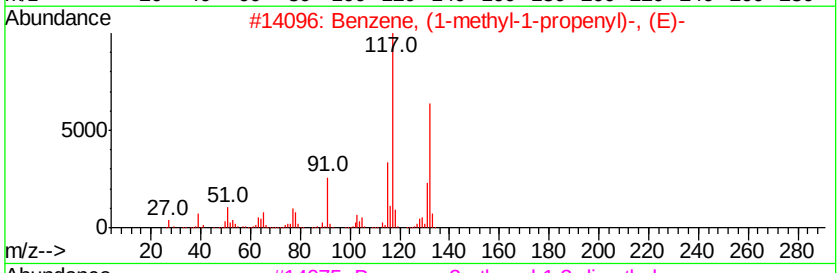


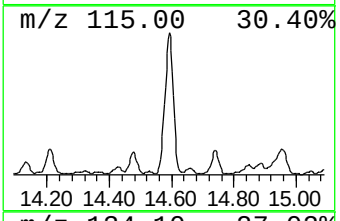


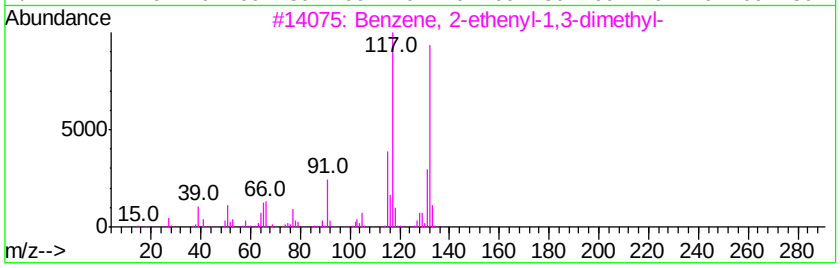


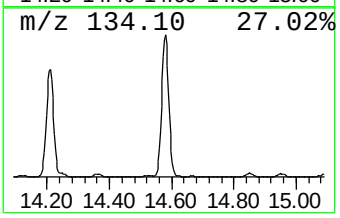












Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031819\
Data File : VN054388.D
Acq On : 18 Mar 2019 12:37
Operator : JC/SP
Sample : K1960-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : DUP-031519-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031219W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, 1,1'-(1,...	13.54	15.5	ug/l	1419310	4	13.34	4588810	50.0
Benzene, 1-ethyl-...	13.89	8.9	ug/l	813706	4	13.34	4588810	50.0
Benzene, (2-methy...	13.99	13.3	ug/l	1215650	4	13.34	4588810	50.0
Benzene, 1,2,4,5-...	14.21	8.8	ug/l	809930	4	13.34	4588810	50.0
Benzene, 2-etheny...	14.59	24.1	ug/l	2210500	4	13.34	4588810	50.0