LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

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_U\METHOD\82U090619W.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	4.862	1157	1173	1191	rBV	281371	642921	5.98%	2.014%
2	4.961	1191	1204	1232	rVB	348960	788445	7.33%	2.470%
3	5.289	1292	1306	1320	rBV	291207	621974	5.78%	1.949%
4	5.370	1321	1331	1351	rVB2	113767	255936	2.38%	0.802%
5	5.868	1471	1486	1508	rBV	484474	998701	9.29%	3.129%
6	7.546	1994	2008	2021	rBV	1061750	1886748	17.55%	5.911%
7	7.617	2021	2030	2060	rVB	236281	459652	4.27%	1.440%
8	9.070	2470	2482	2509	rBV	738272	1253986	11.66%	3.929%
9	9.231	2521	2532	2551	rVB	143264	240802	2.24%	0.754%
10	9.353	2556	2570	2598	rBV	272077	470832	4.38%	1.475%
11	9.762	2686	2697	2725	rVB	170774	303634	2.82%	0.951%
12	10.289	2843	2861	2890	rBV	818875	1341676	12.48%	4.203%
13	10.662	2964	2977	2996	rBV	94675	214633	2.00%	0.672%
14	10.755	2996	3006	3020	rVB3	65923	123167	1.15%	0.386%
15	11.128	3101	3122	3138	rBV	192250	315796	2.94%	0.989%
16	11.379	3188	3200	3215	rBV	422540	718158	6.68%	2.250%
17	11.463	3215	3226	3243	rVB	1093990	1773305	16.49%	5.556%
18	11.556	3243	3255	3268	rBV2	118907	290170	2.70%	0.909%
19	11.746	3299	3314	3338	rBV	1021358	1606220	14.94%	5.032%
20	11.958	3367	3380	3400	rBV	948814	1502864	13.98%	4.708%
21	12.334	3485	3497	3508	rBV	67461	107806	1.00%	0.338%
22	12.594	3552	3578	3593	rBV2	286952	709174	6.59%	2.222%
23	12.678	3593	3604	3614	rBV	375028	717682	6.67%	2.249%
24	12.945	3678	3687	3698	rBV2	77796	121649	1.13%	0.381%
25	13.106	3728	3737	3746	rVB2	145641	218596	2.03%	0.685%
26	13.170	3746	3757	3778	rVB2	273151	477709	4.44%	1.497%
27	13.276	3780	3790	3804	rVB4	105642	187360	1.74%	0.587%
28	13.376	3808	3821	3835	rBV2	290284	512870	4.77%	1.607%
29	13.723	3914	3929	3953	rBV	6806195	10753735	100.00%	33.692%
30	13.842	3955	3966	3977	rBV	404059	653891	6.08%	2.049%
31	14.858	4271	4282	4311	rBV	588996	1006707	9.36%	3.154%
32	15.044	4329	4340	4358	rBV	381908	641309	5.96%	2.009%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

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_U\METHOD\82U090619W.M
Title : SW846 8260

Sum of corrected areas: 31918108

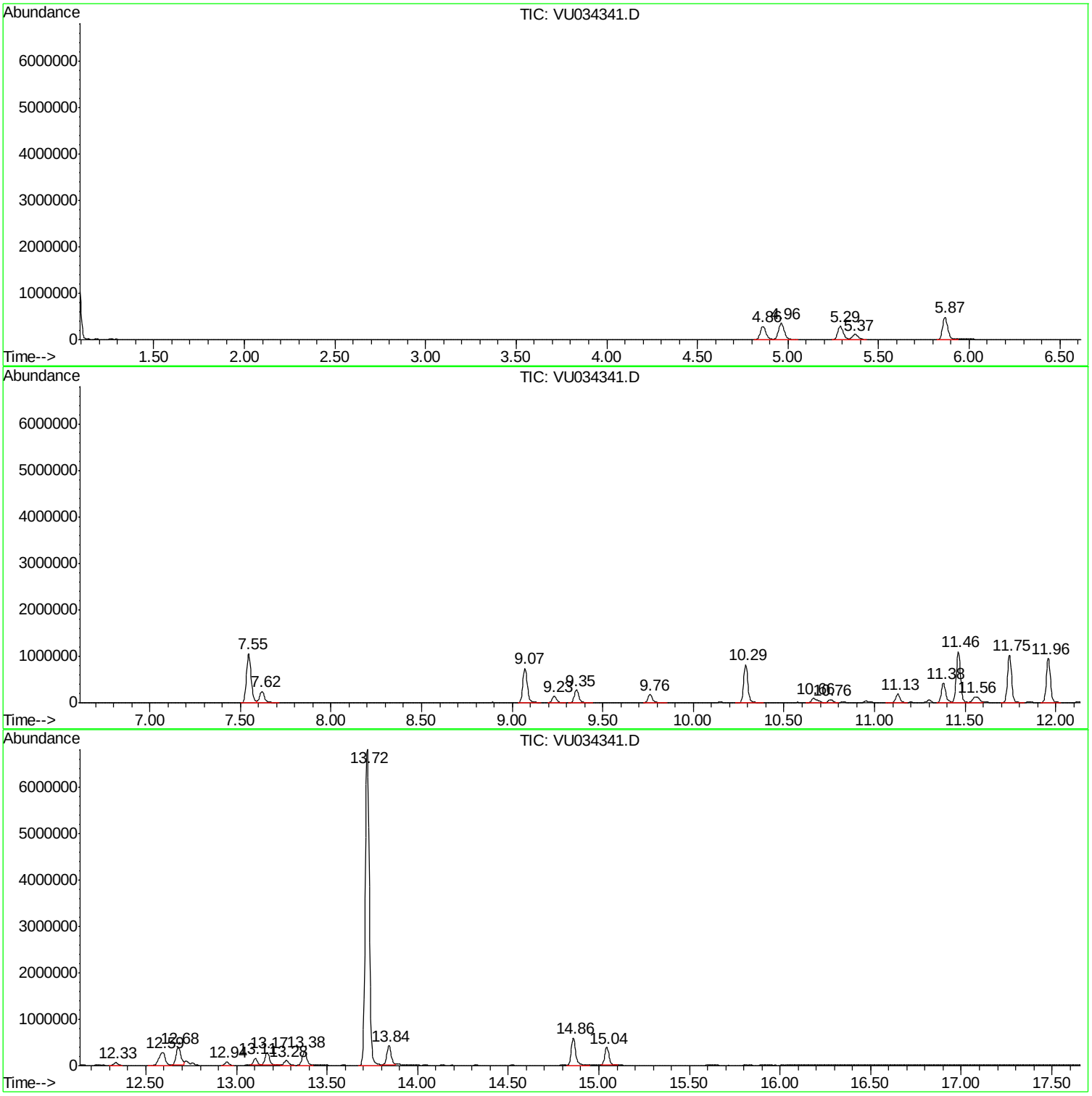
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

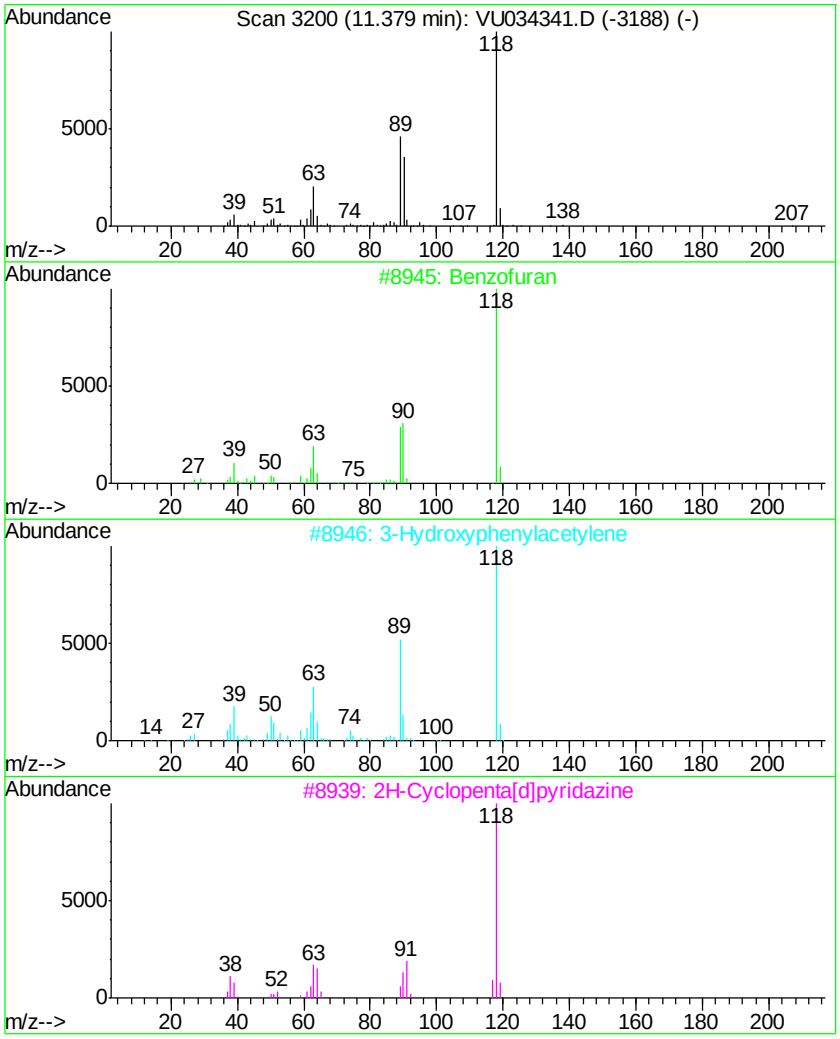
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

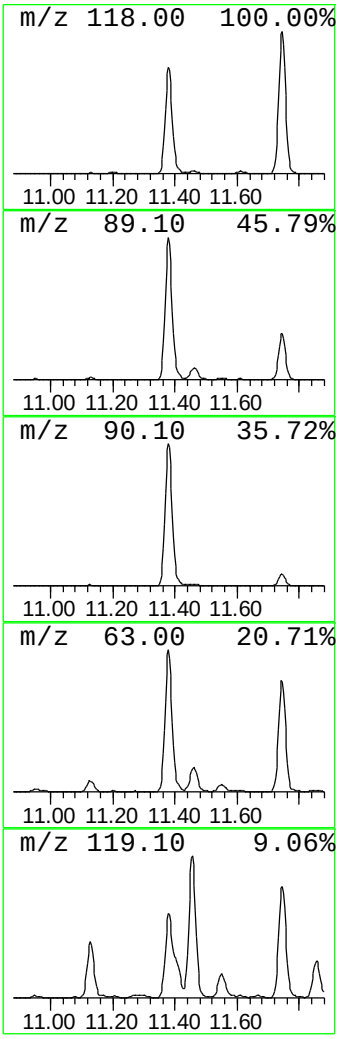
****

Peak Number 1 Benzofuran Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.38	20.25 ug/l	718158	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran	118	C8H6O	000271-89-6	91
2	3-Hydroxyphenylacetylene	118	C8H6O	010401-11-3	86
3	2H-Cyclopenta[d]pyridazine	118	C7H6N2	000270-64-4	53
4	Benzonitrile, 2-amino-	118	C7H6N2	001885-29-6	43
5	1H-Pyrrolo[2,3-b]pyridine	118	C7H6N2	000271-63-6	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

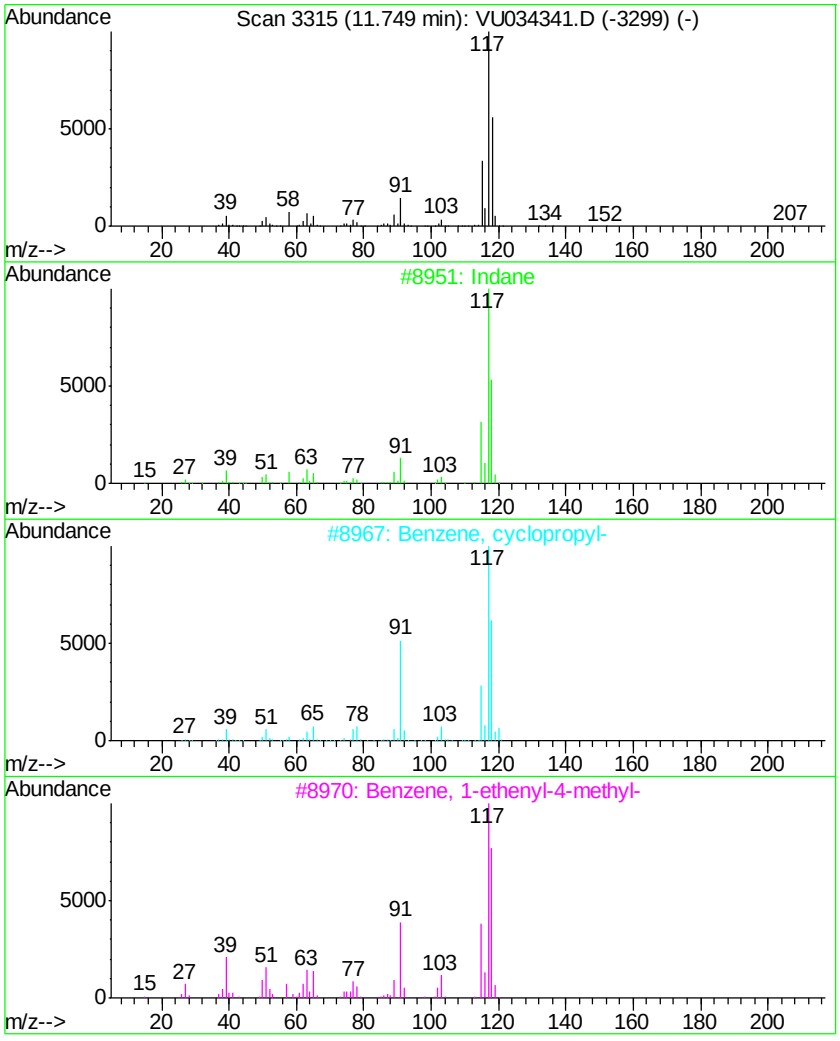
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

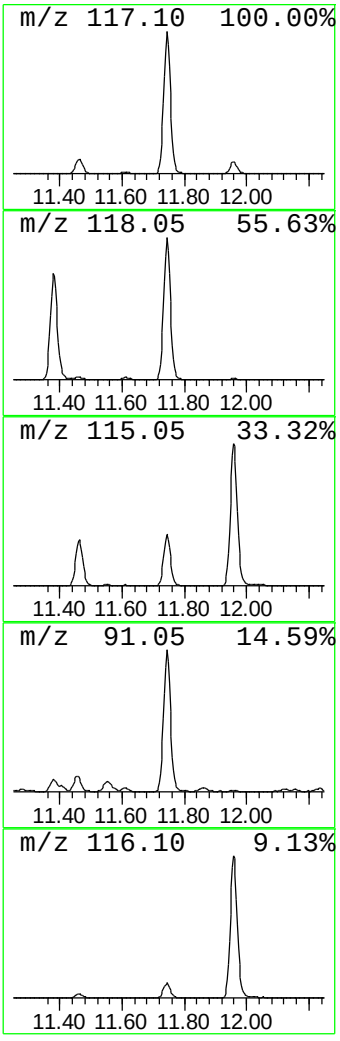
****

Peak Number 2 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	45.29 ug/l	1606220	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	74
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

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

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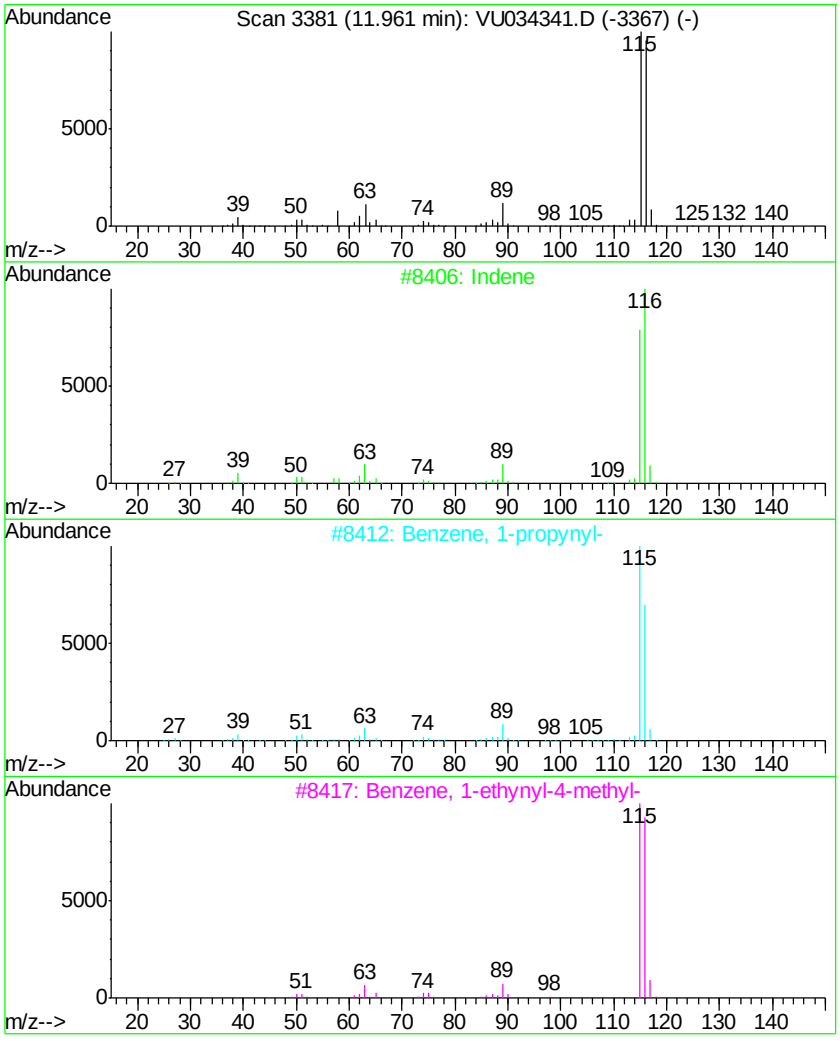
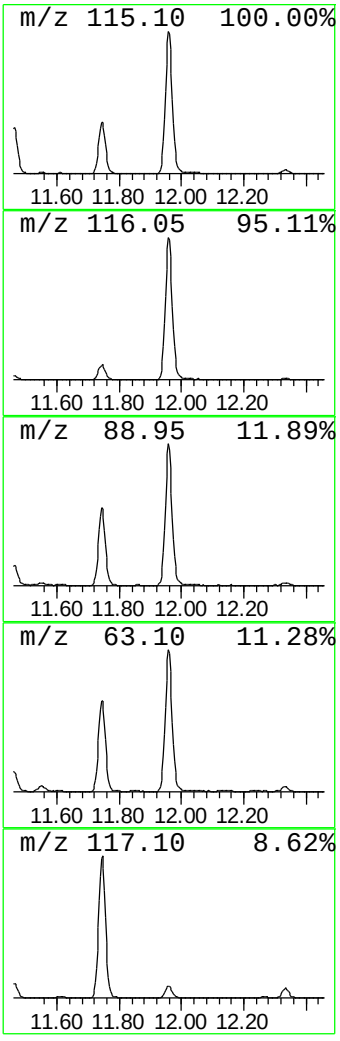
Peak Number 3 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	42.37 ug/l	1502860	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	90





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

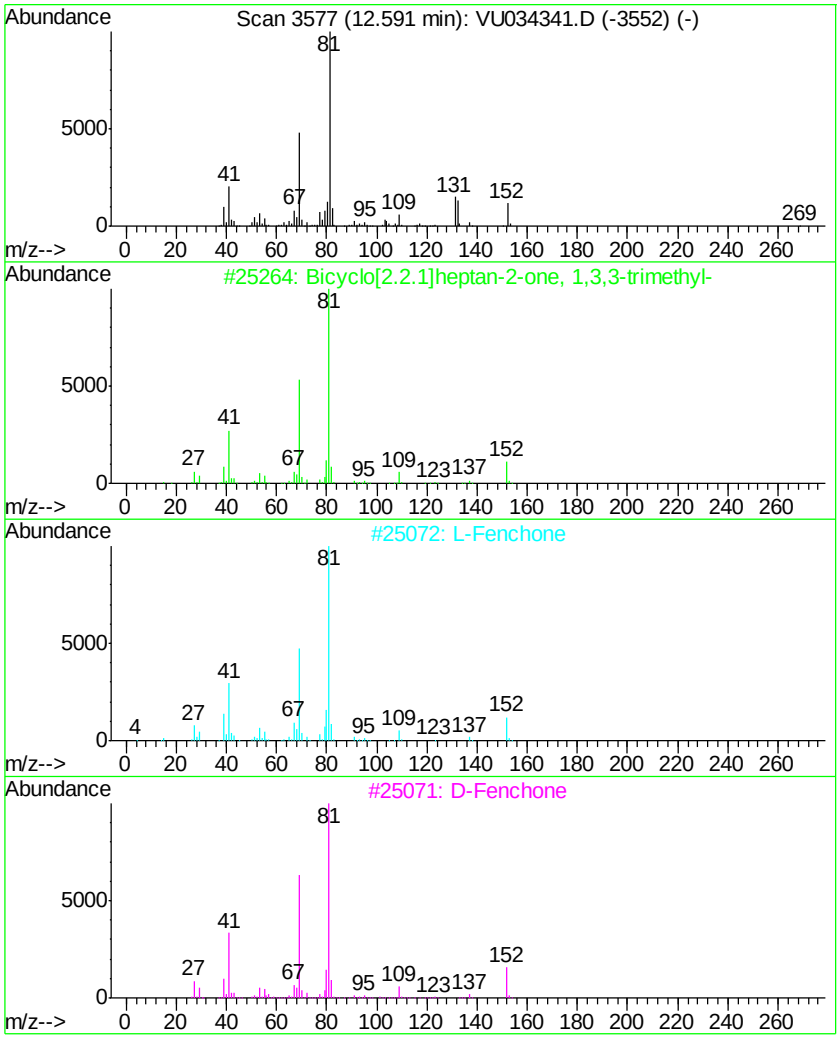
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

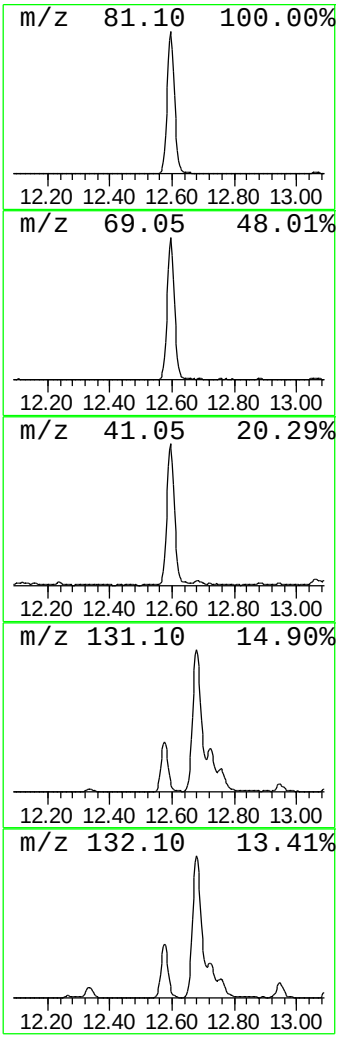
****

Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	20.00 ug/l	709174	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	94
2	L-Fenchone	152	C10H16O	007787-20-4	94
3	D-Fenchone	152	C10H16O	004695-62-9	93
4	2-Furanacetaldehyde, .alpha.-pro...	152	C9H12O2	031681-26-2	40
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	33





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

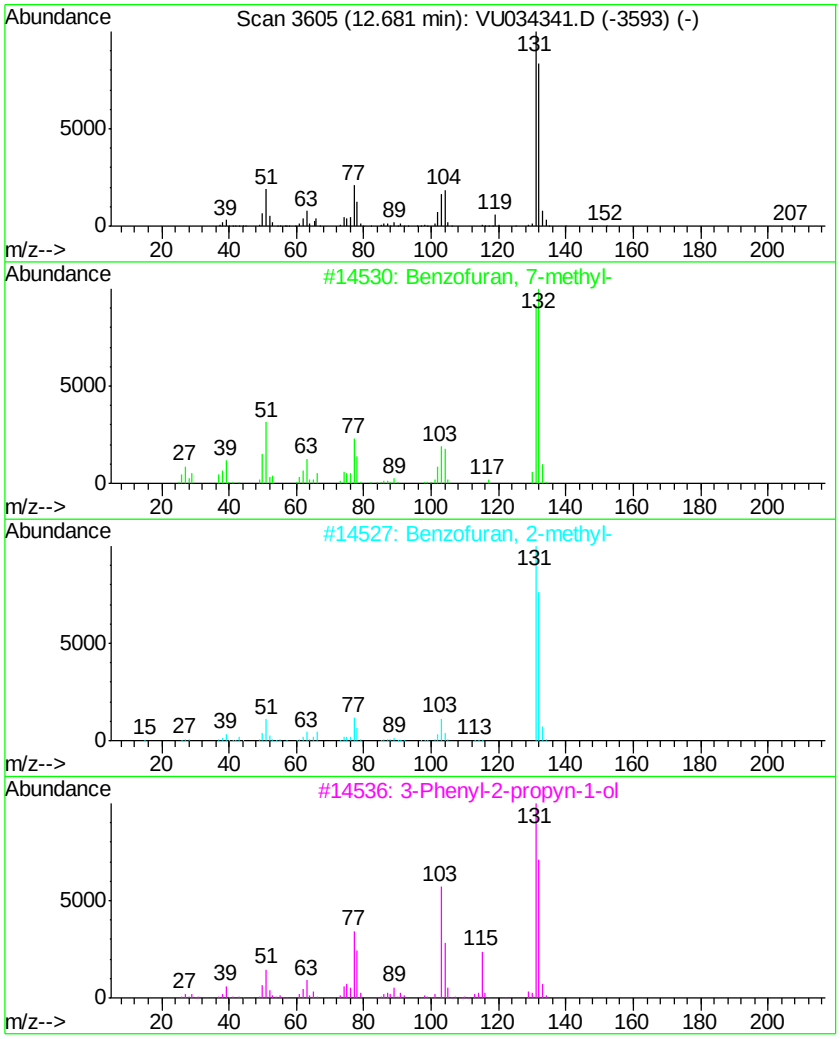
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

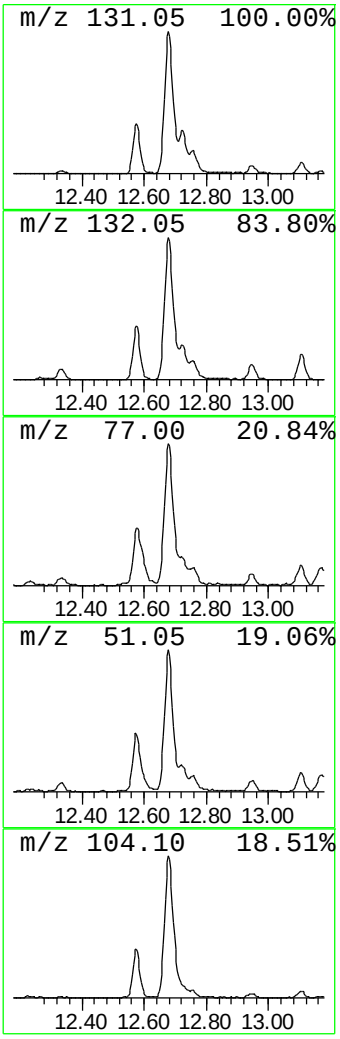
****

Peak Number 5 Benzofuran, 7-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	20.24 ug/l	717682	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	95
2	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	91
3	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	90
4	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	87
5	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	87





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Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

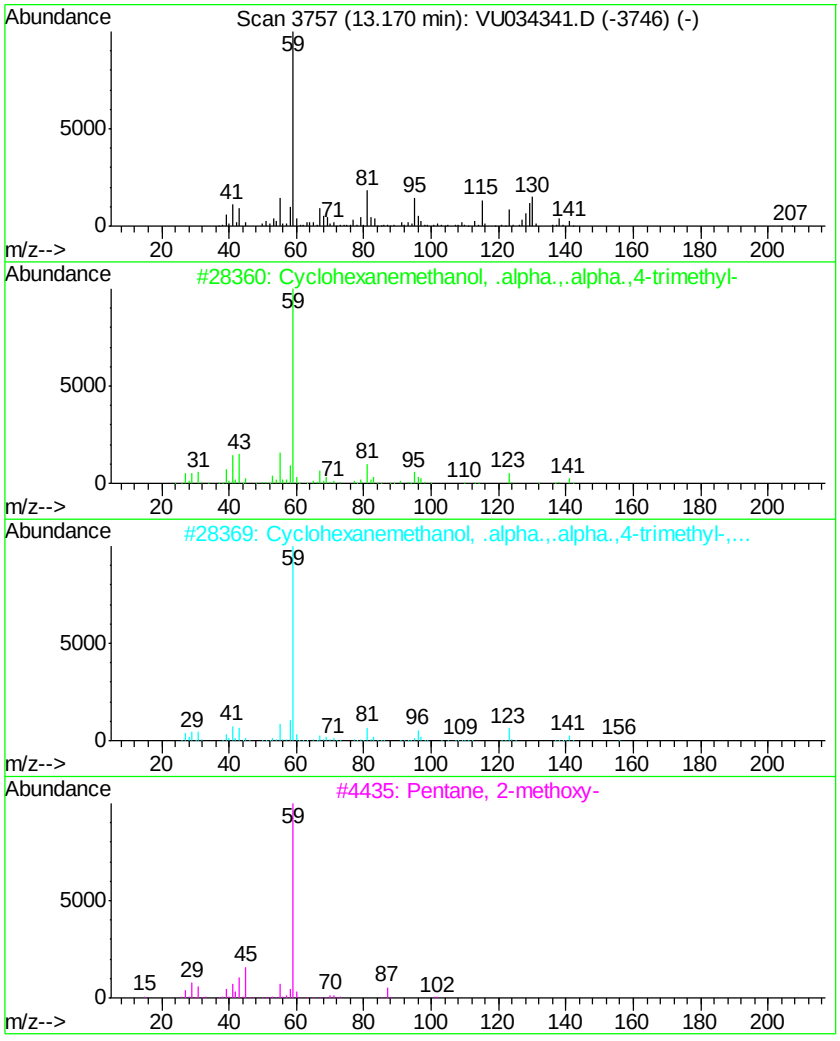
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

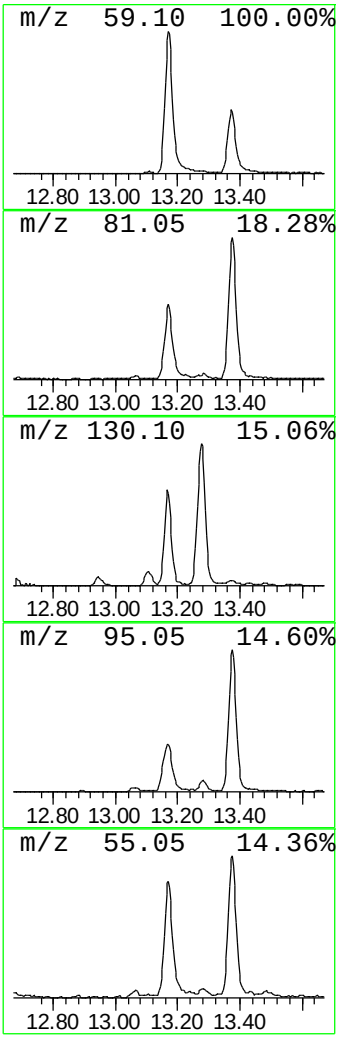
****

Peak Number 6 Cyclohexanemethanol, .alpha... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	13.47 ug/l	477709	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	53
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	50
3	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	38
4	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	38
5	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

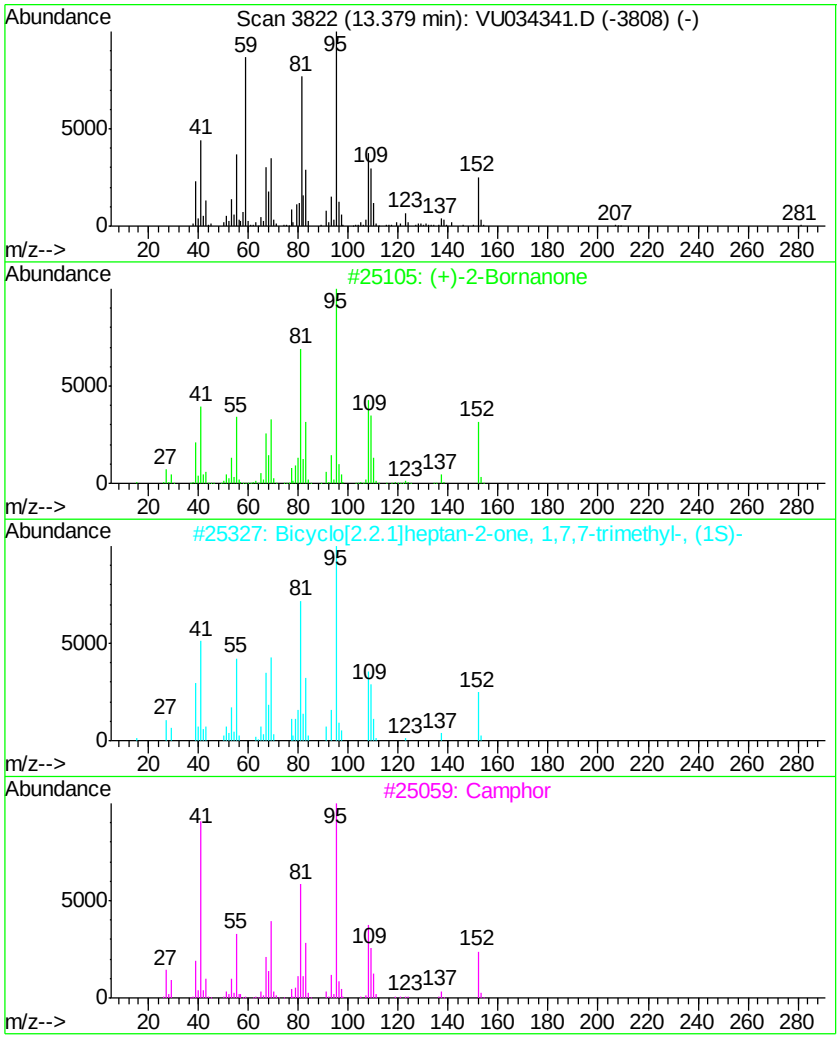
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

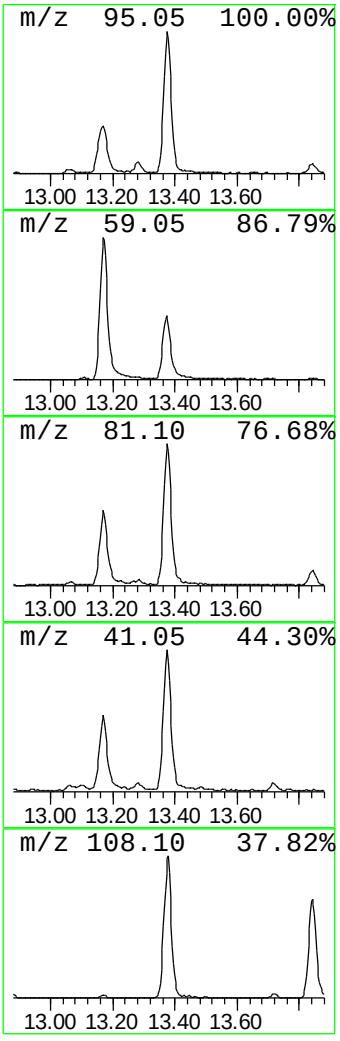
****

Peak Number 7 (+)-2-Bornanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	14.46 ug/l	512870	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
2	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
3	Camphor	152	C10H16O	000076-22-2	96
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	42
5	2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	41





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

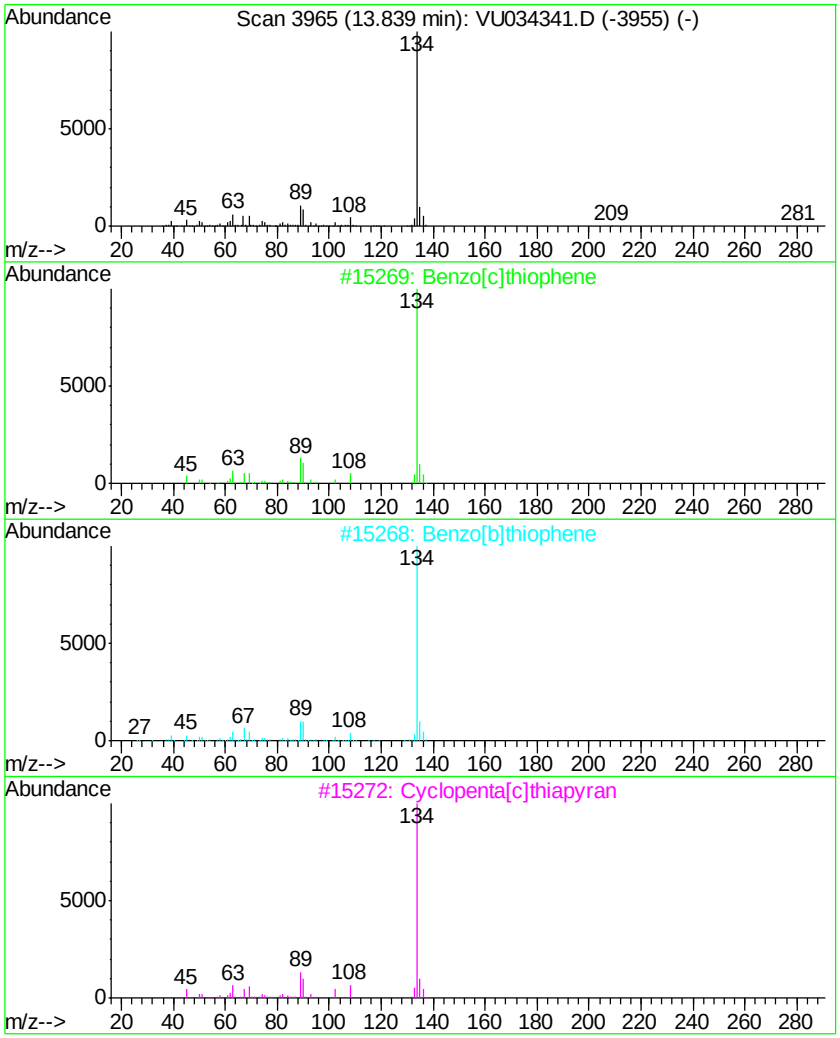
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

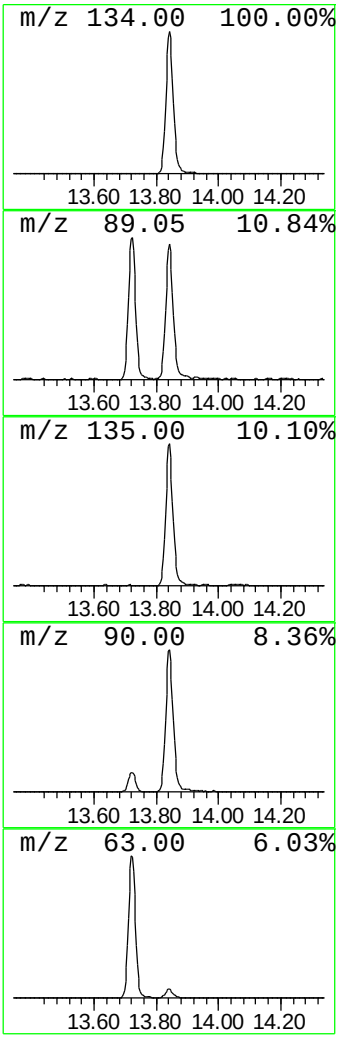
****

Peak Number 8 Benzo[c]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	18.44 ug/l	653891	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2	Benzo[b]thiophene	134	C8H6S	000095-15-8	95
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
4	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5	Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

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

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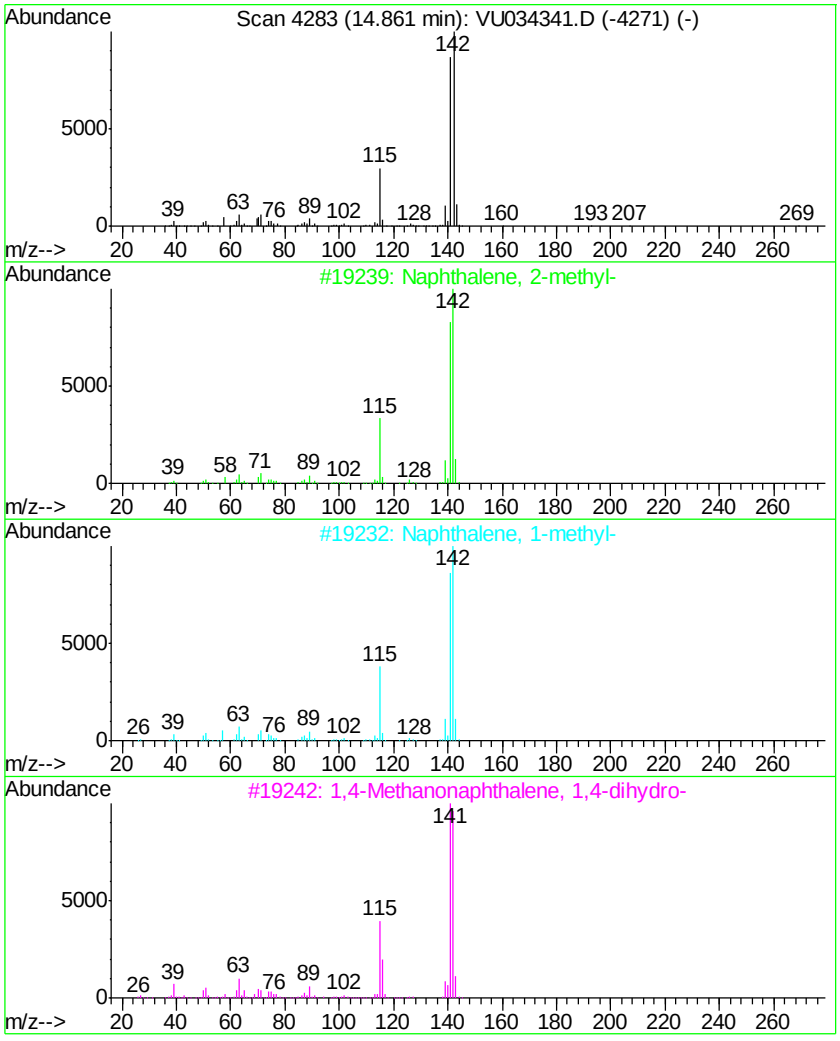
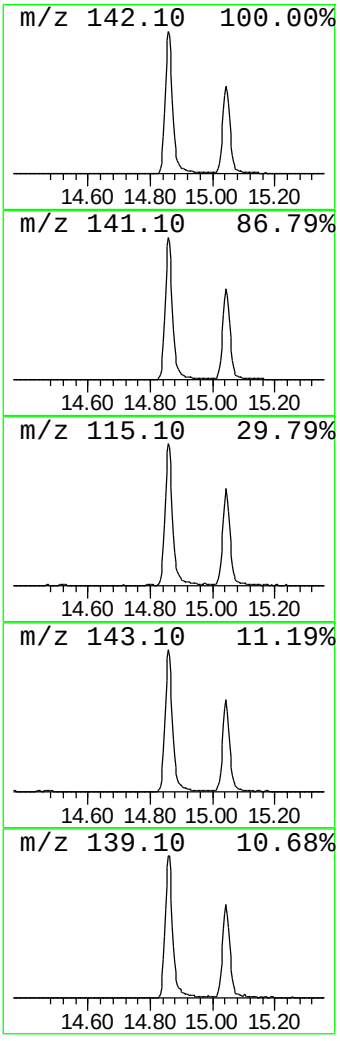
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	28.39 ug/l	1006710	1,4-Dichlorobenzene-d4	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Naphthalene, 1-(2-hydroxypropyl)	186	C13H14O	027653-13-0	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090719\
Data File : VU034341.D
Acq On : 06 Sep 2019 19:17
Operator : JC/SP
Sample : K4689-01 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-1A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.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
Benzofuran	11.38	20.3	ug/l	718158	4	11.46	1773310	50.0
Indane	11.75	45.3	ug/l	1606220	4	11.46	1773310	50.0
Indene	11.96	42.4	ug/l	1502860	4	11.46	1773310	50.0
Bicyclo[2.2.1]hep...	12.59	20.0	ug/l	709174	4	11.46	1773310	50.0
Benzofuran, 7-met...	12.68	20.2	ug/l	717682	4	11.46	1773310	50.0
Cyclohexanemethan...	13.17	13.5	ug/l	477709	4	11.46	1773310	50.0
(+)-2-Bornanone	13.38	14.5	ug/l	512870	4	11.46	1773310	50.0
Benzo[c]thiophene	13.84	18.4	ug/l	653891	4	11.46	1773310	50.0
Naphthalene, 1-me...	14.86	28.4	ug/l	1006710	4	11.46	1773310	50.0