LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

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_X\METHOD\82X062920W.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	1.276	28	31	40	rVB	320549	326304	4.93%	1.202%
2	2.429	214	220	225	rBV	76419	130659	1.97%	0.481%
3	3.008	305	315	332	rBV	2275159	5044734	76.16%	18.578%
4	4.660	562	586	598	rBV	2100692	6624010	100.00%	24.393%
5	5.087	644	656	679	rBV	1178379	3524631	53.21%	12.980%
6	5.465	707	718	730	rBV	148929	432568	6.53%	1.593%
7	5.629	733	745	761	rVB	259203	712771	10.76%	2.625%
8	6.032	799	811	819	rBV	161968	422793	6.38%	1.557%
9	6.117	819	825	832	rVV2	31884	91041	1.37%	0.335%
10	6.245	832	846	866	rVV3	138805	626490	9.46%	2.307%
11	6.830	931	942	954	rBV	399225	947964	14.31%	3.491%
12	7.958	1120	1127	1144	rVB	58066	116233	1.75%	0.428%
13	8.592	1226	1231	1234	rBV	44220	78358	1.18%	0.289%
14	8.696	1241	1248	1254	rBV	863510	1331206	20.10%	4.902%
15	8.763	1254	1259	1268	rVV2	131756	228156	3.44%	0.840%
16	8.848	1268	1273	1285	rVB	98937	159276	2.40%	0.587%
17	9.421	1358	1367	1373	rBV	314957	458241	6.92%	1.688%
18	10.098	1467	1478	1490	rVV	933293	1405426	21.22%	5.176%
19	10.250	1497	1503	1511	rVV3	36276	72965	1.10%	0.269%
20	10.342	1511	1518	1524	rVV	189416	274178	4.14%	1.010%
21	10.421	1524	1531	1541	rVB2	34914	72135	1.09%	0.266%
22	10.683	1569	1574	1578	rBV	128472	170706	2.58%	0.629%
23	11.122	1639	1646	1651	rBV	835945	1055537	15.94%	3.887%
24	11.793	1745	1756	1759	rVV	48882	74451	1.12%	0.274%
25	11.927	1771	1778	1786	rVB	92416	132747	2.00%	0.489%
26	12.061	1794	1800	1807	rVB	1110512	1434084	21.65%	5.281%
27	12.140	1807	1813	1817	rBV2	63923	120688	1.82%	0.444%
28	12.280	1830	1836	1841	rBV	51190	81152	1.23%	0.299%
29	12.616	1888	1891	1895	rVB	102031	110770	1.67%	0.408%
30	12.805	1913	1922	1926	rVV2	119350	189467	2.86%	0.698%
31	12.945	1938	1945	1949	rBV	280004	348134	5.26%	1.282%
32	13.000	1949	1954	1966	rVB3	88086	155573	2.35%	0.573%
33	13.512	2033	2038	2042	rBV2	91316	132026	1.99%	0.486%
34	13.628	2052	2057	2063	rBV4	45390	69467	1.05%	0.256%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

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_X\METHOD\82X062920W.M
Title : SW846 8260

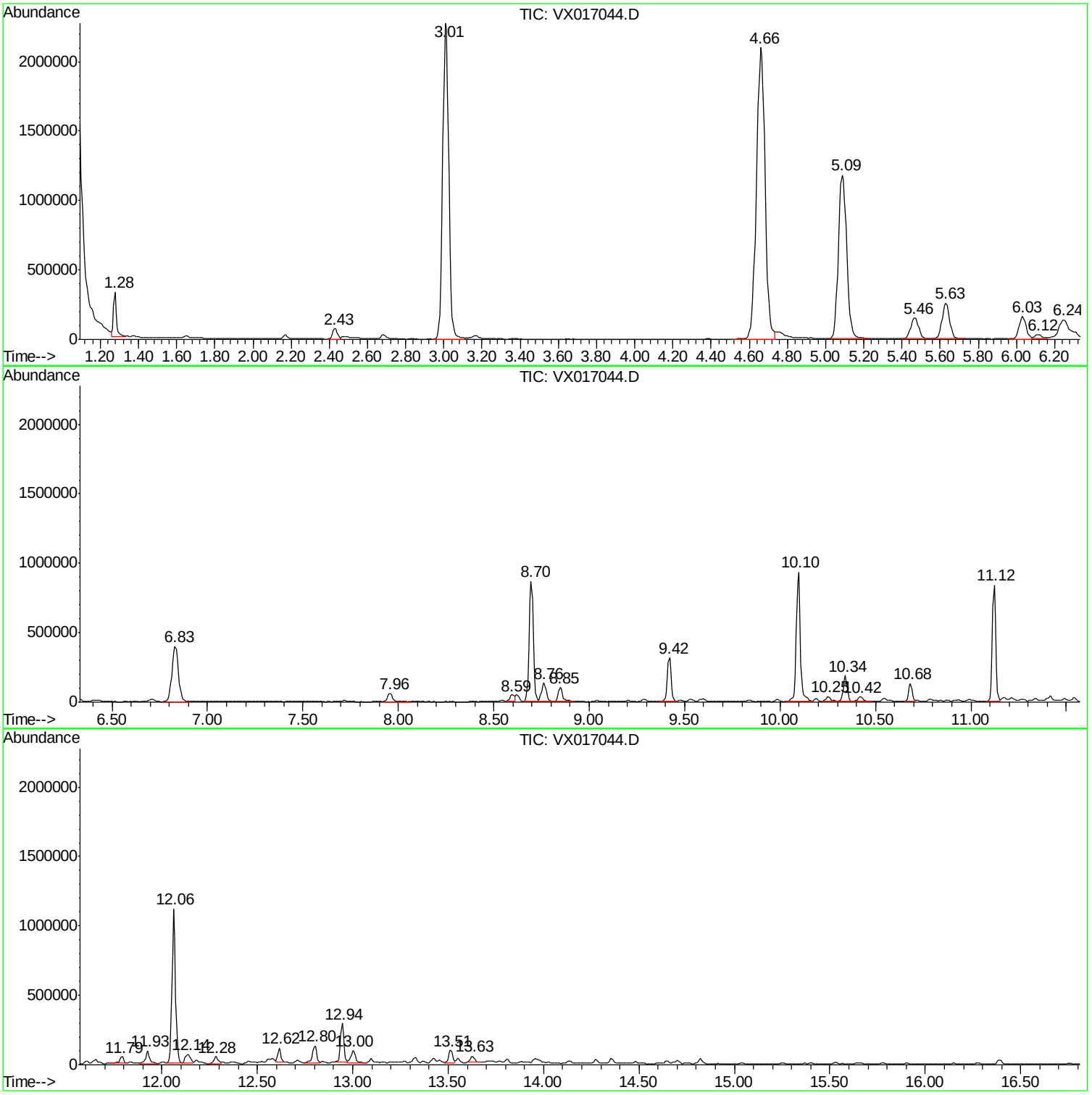
Sum of corrected areas: 27154941

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.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_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

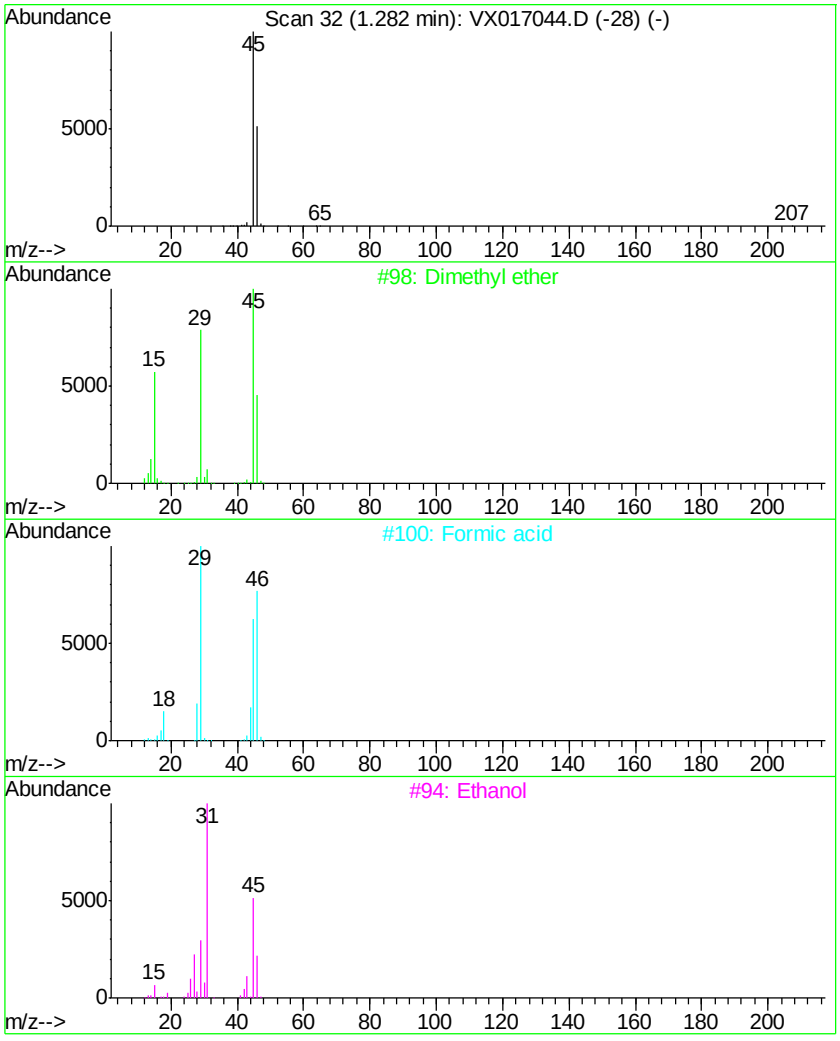
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

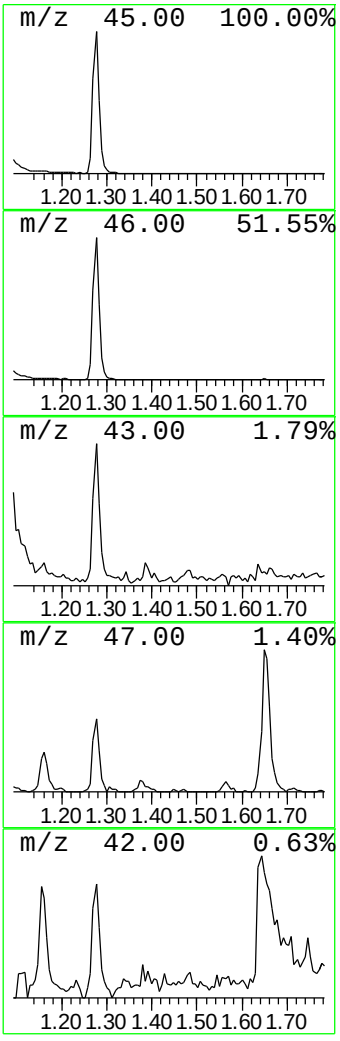
****

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	22.89 ug/l	326304	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	56
2	Formic acid	46	CH2O2	000064-18-6	7
3	Ethanol	46	C2H6O	000064-17-5	7
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

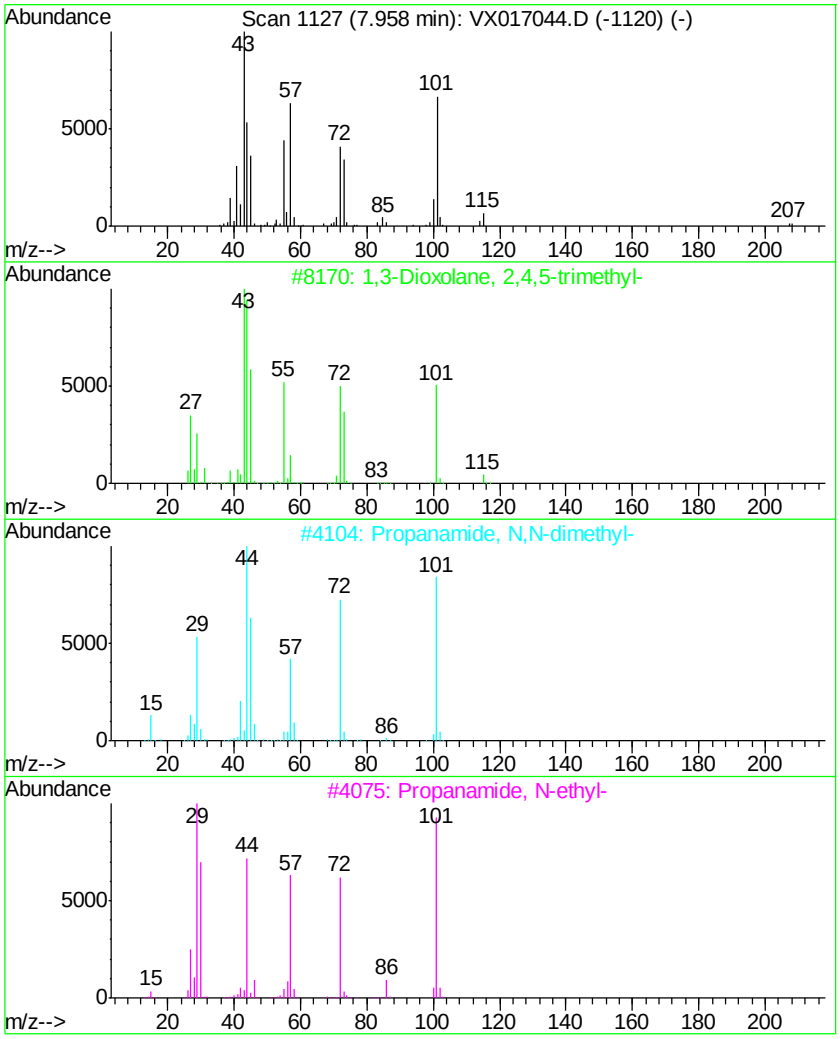
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

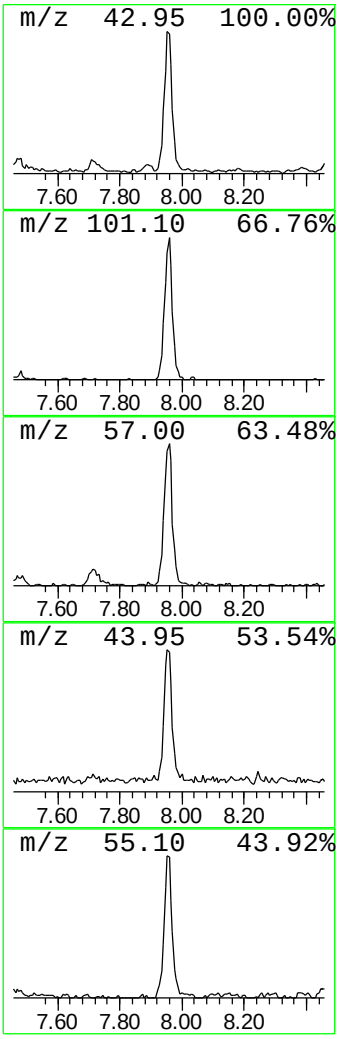
****

Peak Number 4 1,3-Dioxolane, 2,4,5-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	6.13 ug/l	116233	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,4,5-trimethyl-	116	C6H12O2	003299-32-9	78
2	Propanamide, N,N-dimethyl-	101	C5H11NO	000758-96-3	64
3	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	53
4	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	47
5	3(2H)-Furanone, dihydro-2-methyl-	100	C5H8O2	003188-00-9	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

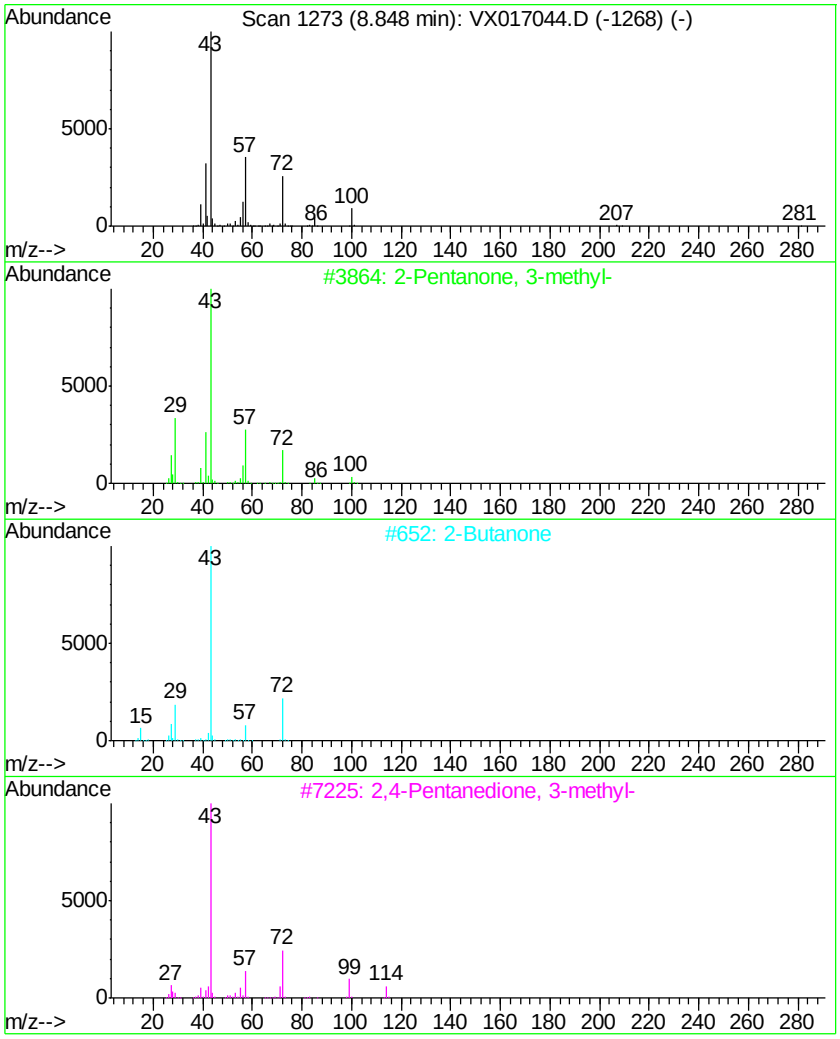
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

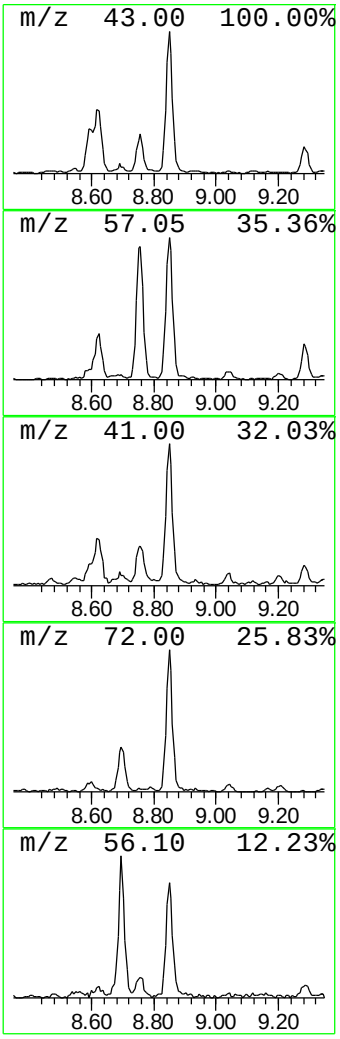
****

Peak Number 5 2-Pentanone, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.85	5.67 ug/l	159276	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	90
2	2-Butanone	72	C4H8O	000078-93-3	47
3	2,4-Pentanedione, 3-methyl-	114	C6H10O2	000815-57-6	42
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	37
5	2,3-Pentanedione	100	C5H8O2	000600-14-6	27





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

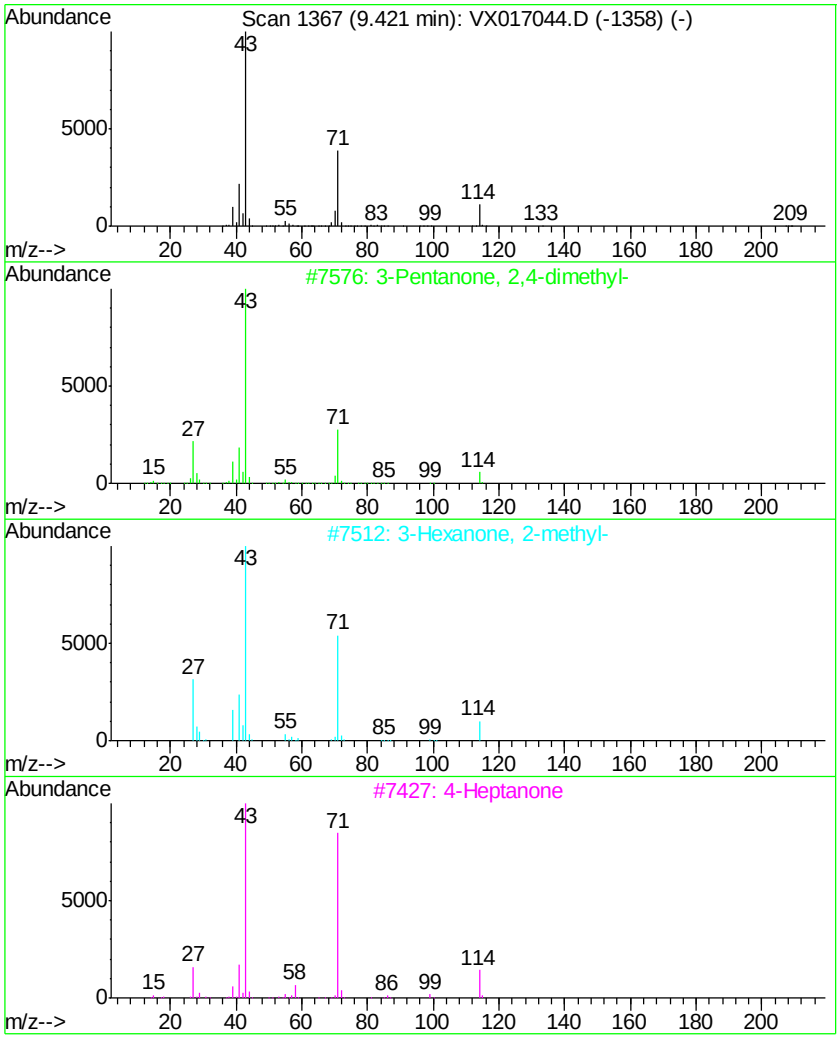
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

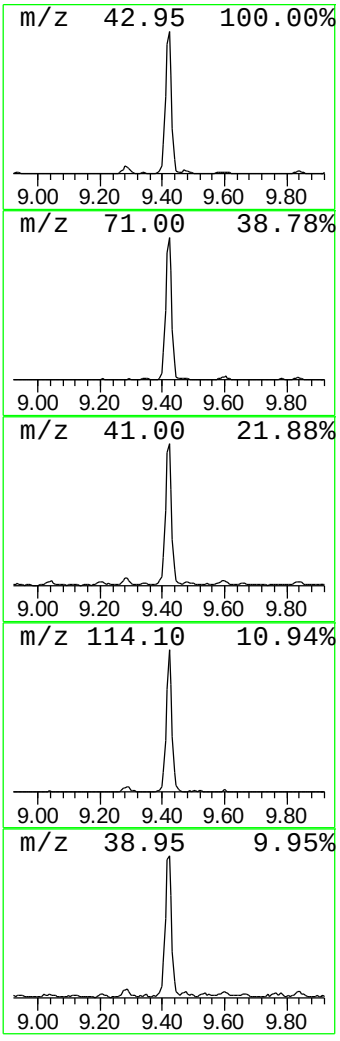
****

Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	16.30 ug/l	458241	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3	4-Heptanone	114	C7H14O	000123-19-3	72
4	Pyrrolidine	71	C4H9N	000123-75-1	53
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	46





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

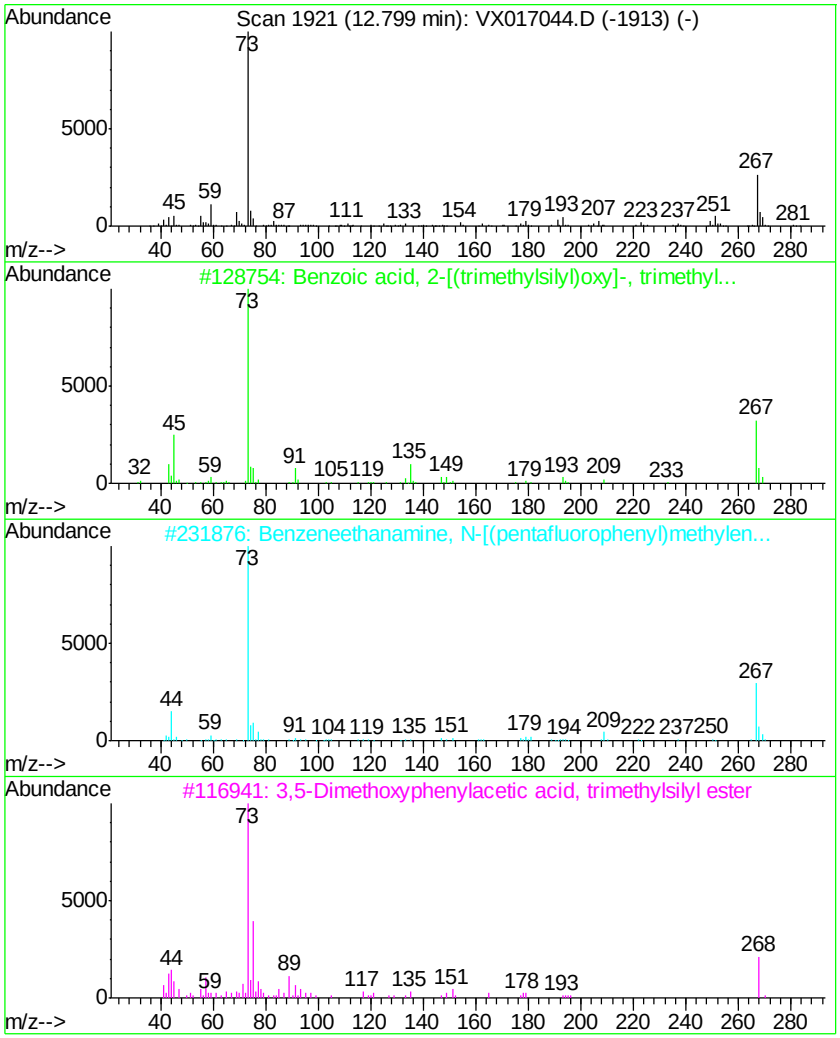
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

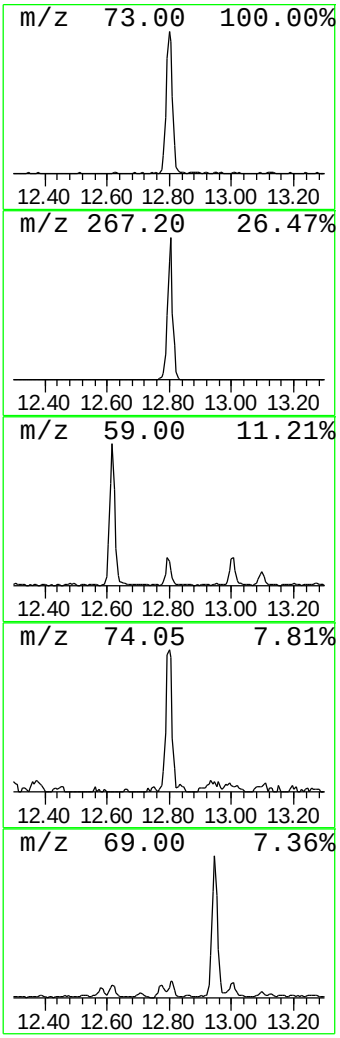
****

Peak Number 7 Benzoic acid, 2-[(trimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	6.61 ug/l	189467	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	59
2	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	45
3	3,5-Dimethoxyphenylacetic acid, ...	268	C13H20O4Si	1000071-82-4	27
4	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	25
5	1-(3-Chlorophenyl)piperazine, 4-...	268	C13H21ClN2Si	1000373-99-3	18





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

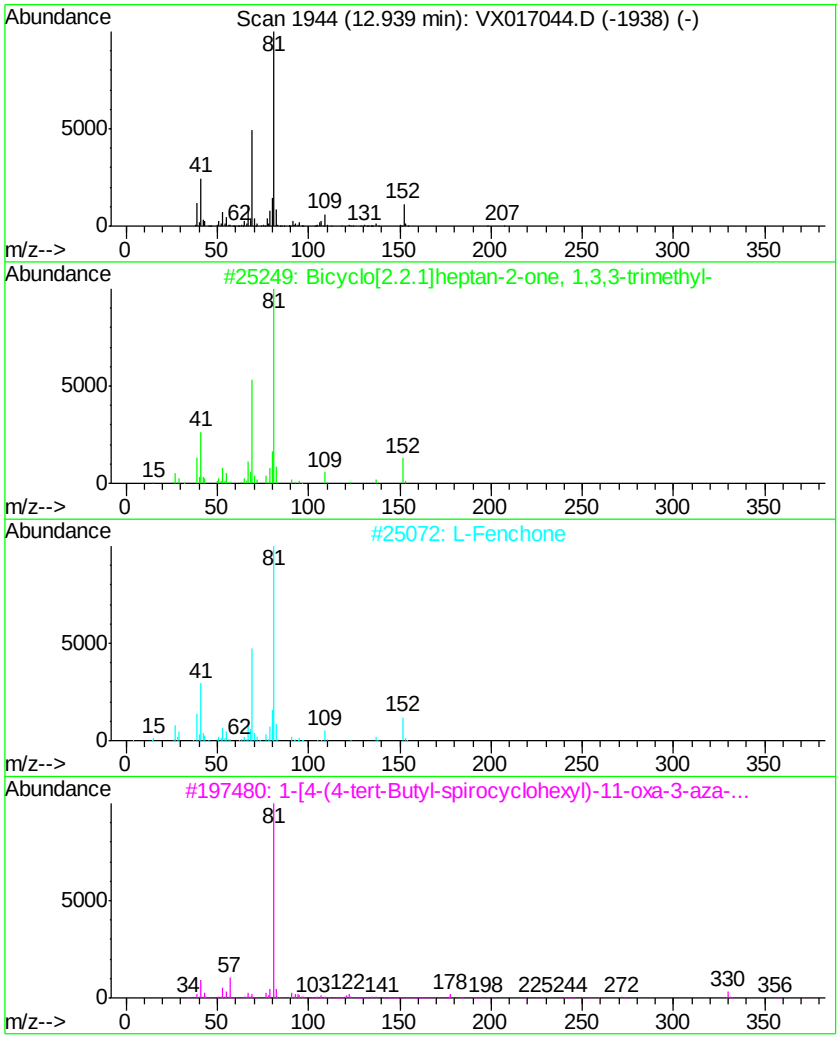
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

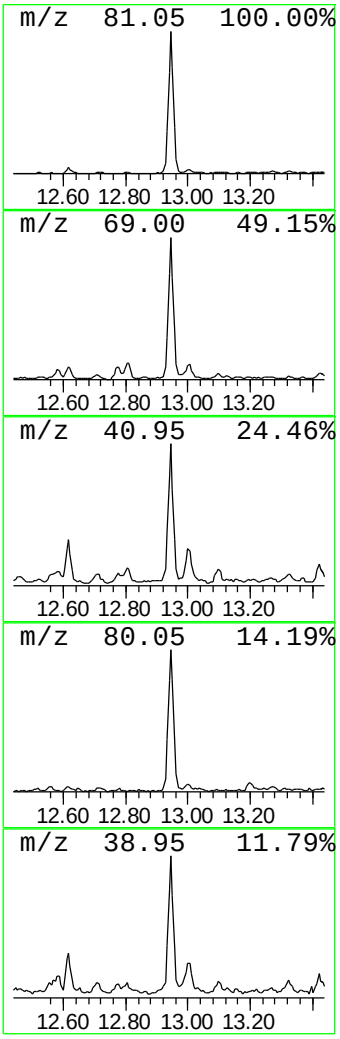
****

Peak Number 8 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	12.14 ug/l	348134	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	95
3	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	50
4	D-Fenchone	152	C10H16O	004695-62-9	46
5	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

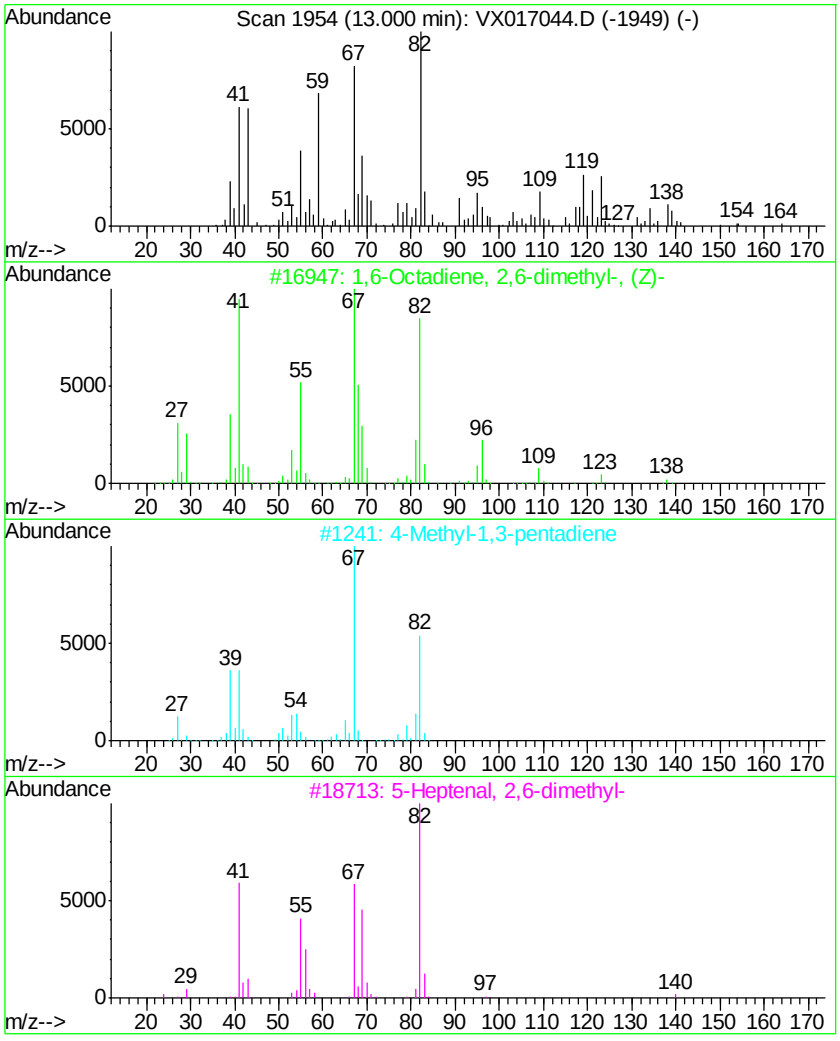
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

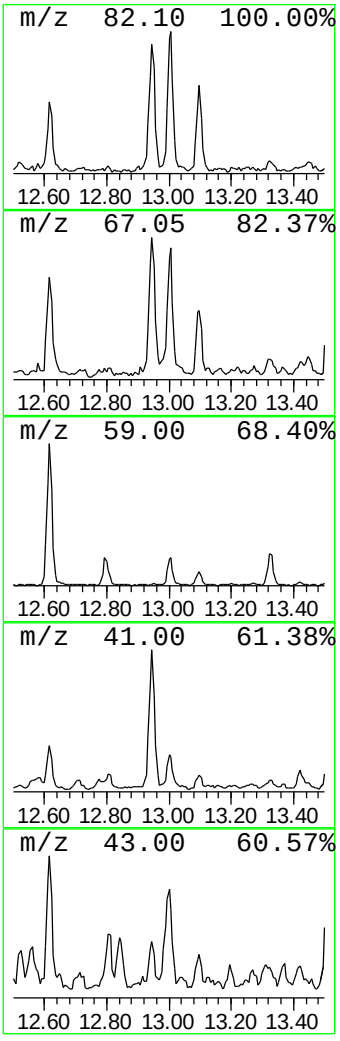
****

Peak Number 9 unknown13.00 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	5.42 ug/l	155573	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Octadiene, 2,6-dimethyl-, (Z)-	138	C10H18	006874-34-6	49
2	4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	46
3	5-Heptenal, 2,6-dimethyl-	140	C9H16O	000106-72-9	46
4	2-Hexyne	82	C6H10	000764-35-2	46
5	7-Methylbicyclo[4.2.0]octane	124	C9H16	1000210-90-2	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX063020\
Data File : VX017044.D
Acq On : 30 Jun 2020 14:53
Operator : JC/SP
Sample : L3146-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200624026-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.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
Dimethyl ether	1.28	22.9	ug/l	326304	1	5.63	712771	50.0
1,3-Dioxolane, 2,...	7.96	6.1	ug/l	116233	2	6.83	947964	50.0
2-Pentanone, 3-me...	8.85	5.7	ug/l	159276	3	10.10	1405430	50.0
3-Pentanone, 2,4-...	9.42	16.3	ug/l	458241	3	10.10	1405430	50.0
Benzoic acid, 2-[...	12.80	6.6	ug/l	189467	4	12.06	1434080	50.0
Bicyclo[2.2.1]hep...	12.94	12.1	ug/l	348134	4	12.06	1434080	50.0
unknown13.00	13.00	5.4	ug/l	155573	4	12.06	1434080	50.0