LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

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\82X032522W.M
Title : SW846 8260

Signal : TIC: VX027736.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.550	722	732	749	rVB	68234	192300	1.06%	0.188%
2	6.763	922	931	943	rBV	110163	259632	1.43%	0.254%
3	8.653	1235	1241	1246	rVB	214054	349492	1.92%	0.342%
4	8.720	1246	1252	1258	rBV	645161	988651	5.44%	0.967%
5	9.903	1442	1446	1451	rVB	126089	182865	1.01%	0.179%
6	10.061	1467	1472	1477	rVB	215817	309482	1.70%	0.303%
7	10.201	1487	1495	1500	rBV	1824334	2562673	14.11%	2.506%
8	10.305	1503	1512	1518	rVV	4231493	6186595	34.06%	6.050%
9	10.360	1518	1521	1532	rVB	288289	393679	2.17%	0.385%
10	10.591	1552	1559	1563	rBV3	212177	366938	2.02%	0.359%
11	10.646	1563	1568	1576	rVB2	2119439	3421496	18.83%	3.346%
12	10.780	1582	1590	1594	rBV2	445369	675652	3.72%	0.661%
13	10.860	1594	1603	1606	rBV2	397792	674531	3.71%	0.660%
14	10.896	1606	1609	1614	rVB	197252	265352	1.46%	0.259%
15	10.969	1614	1621	1625	rBV	935840	1346329	7.41%	1.317%
16	11.030	1628	1631	1635	rVV	174453	224926	1.24%	0.220%
17	11.085	1635	1640	1643	rVV3	465383	717678	3.95%	0.702%
18	11.110	1643	1644	1651	rVB2	339433	362095	1.99%	0.354%
19	11.195	1651	1658	1660	rBV	349385	507427	2.79%	0.496%
20	11.219	1660	1662	1666	rVB3	174871	201756	1.11%	0.197%
21	11.311	1672	1677	1682	rBV	2744072	3515536	19.35%	3.438%
22	11.390	1684	1690	1697	rVV	8412480	17261514	95.02%	16.879%
23	11.463	1697	1702	1710	rVB	5645894	8291456	45.64%	8.108%
24	11.622	1722	1728	1735	rVB	3163465	4396510	24.20%	4.299%
25	11.719	1741	1744	1746	rVV	581086	657128	3.62%	0.643%
26	11.768	1746	1752	1756	rVV	13009570	18166102	100.00%	17.764%
27	11.811	1756	1759	1762	rVV	421904	498568	2.74%	0.488%
28	11.853	1762	1766	1767	rVV2	218760	313943	1.73%	0.307%
29	11.896	1770	1773	1777	rVV	393947	491009	2.70%	0.480%
30	11.945	1777	1781	1783	rVV	320819	413878	2.28%	0.405%
31	11.975	1783	1786	1790	rVV	467868	599741	3.30%	0.586%
32	12.024	1790	1794	1800	rVV4	352455	844182	4.65%	0.825%
33	12.091	1800	1805	1810	rVV	3201552	4559935	25.10%	4.459%
34	12.134	1810	1812	1816	rVV	203861	222306	1.22%	0.217%
35	12.177	1816	1819	1826	rVB3	273845	382427	2.11%	0.374%
36	12.250	1826	1831	1838	rBV3	4607356	6927913	38.14%	6.774%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

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\82X032522W.M
Title : SW846 8260

37	12.323	1838	1843	1849	rVB2	2276956	3401201	18.72%	3.326%
38	12.420	1849	1859	1863	rBV2	1627400	2425076	13.35%	2.371%
39	12.469	1863	1867	1873	rVB	410983	614203	3.38%	0.601%
40	12.536	1873	1878	1880	rBV	670099	932806	5.13%	0.912%
41	12.561	1880	1882	1885	rVV	608755	604038	3.33%	0.591%
42	12.616	1887	1891	1895	rVB	1418766	1574462	8.67%	1.540%
43	12.707	1900	1906	1918	rVB5	196497	570807	3.14%	0.558%
44	12.890	1933	1936	1939	rBV3	153227	236281	1.30%	0.231%
45	12.926	1939	1942	1945	rVV	290466	349476	1.92%	0.342%
46	12.969	1945	1949	1955	rVB	440711	648173	3.57%	0.634%
47	13.292	1992	2002	2007	rBV3	308827	594727	3.27%	0.582%
48	13.347	2007	2011	2014	rVB2	166538	199671	1.10%	0.195%
49	13.426	2020	2024	2033	rVB	258712	377380	2.08%	0.369%
50	13.780	2072	2082	2089	rVB	1615737	2004809	11.04%	1.960%

Sum of corrected areas: 102264807

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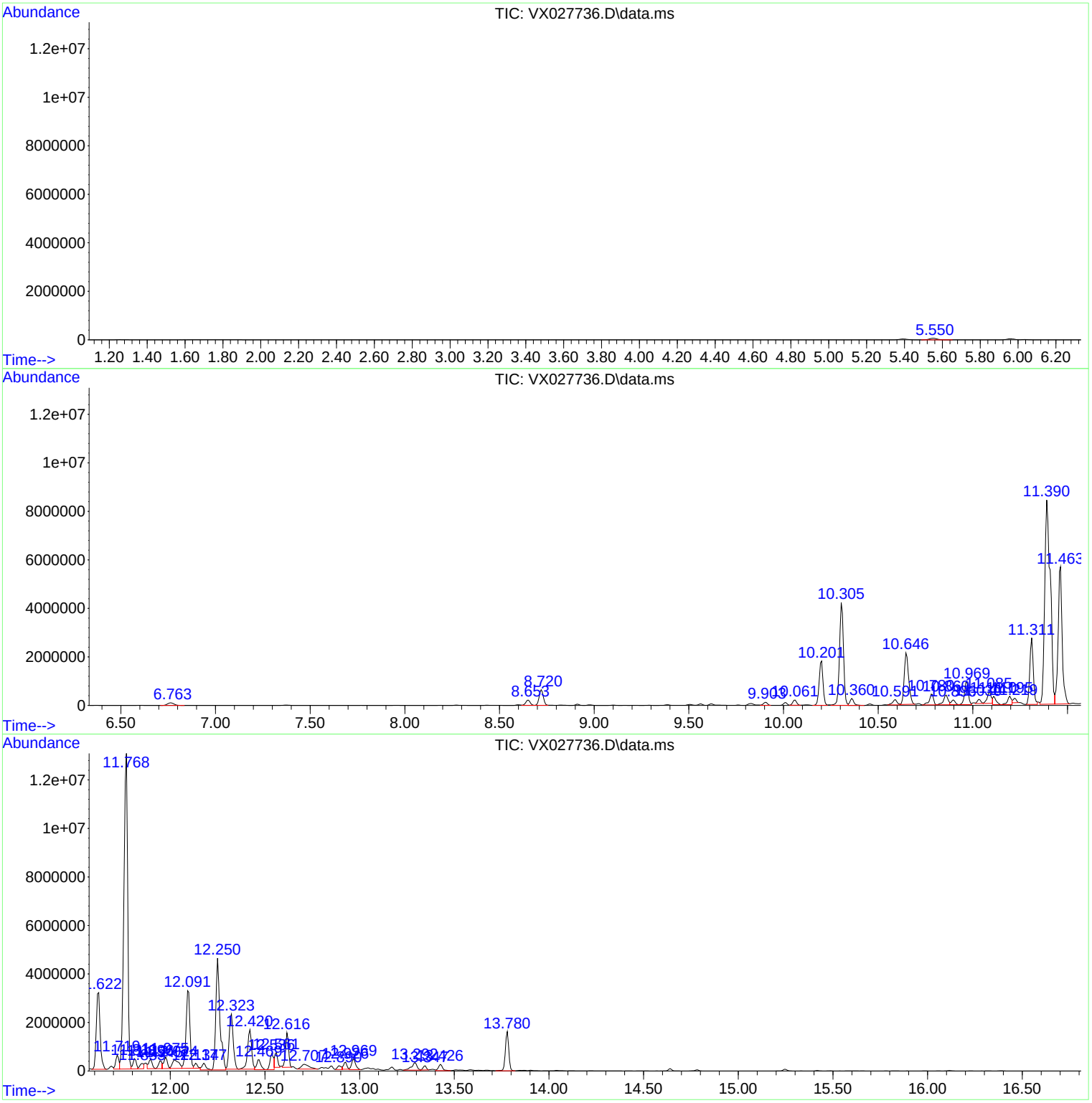
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

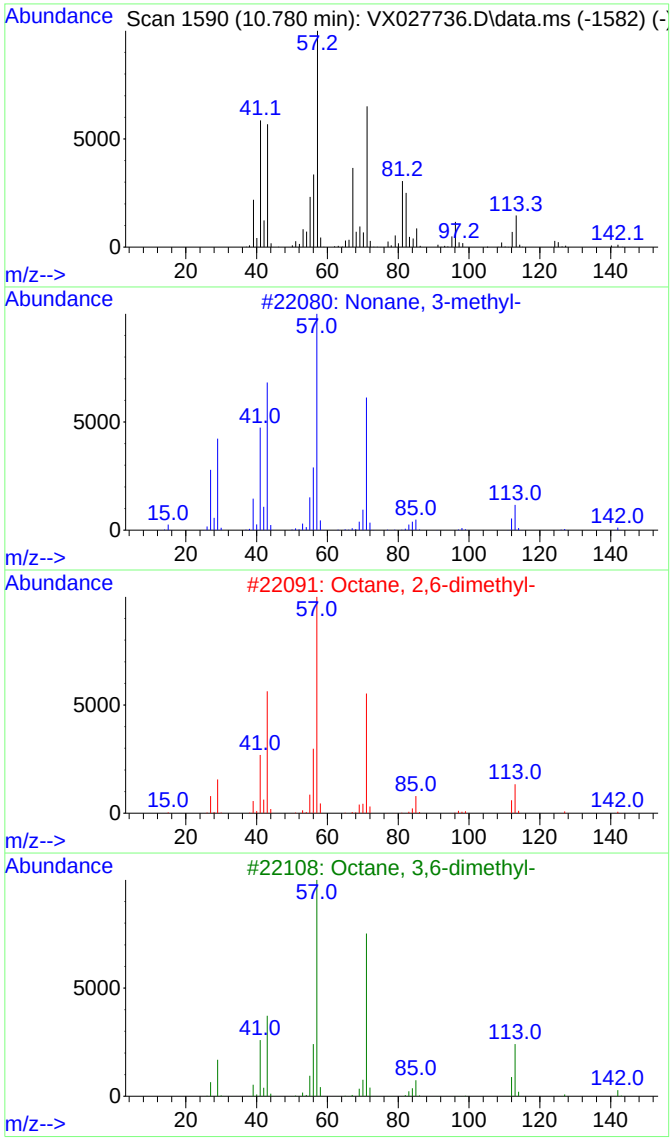
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

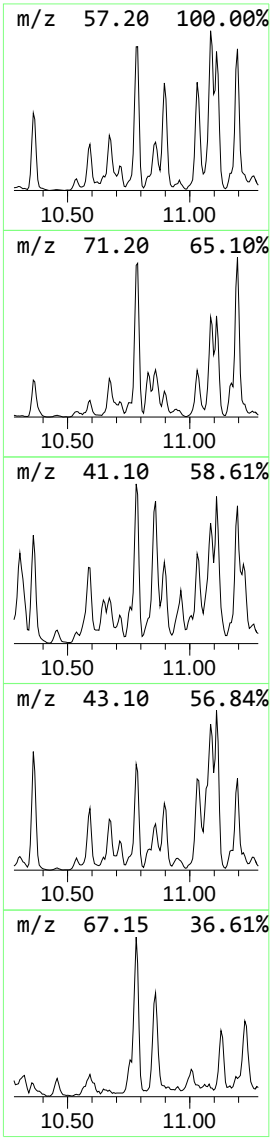
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Nonane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	109.16 ug/l	675652	Chlorobenzene-d5	10.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	60
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	60
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53
4	3-Bromooctane	192	C8H17Br	000999-64-4	46
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

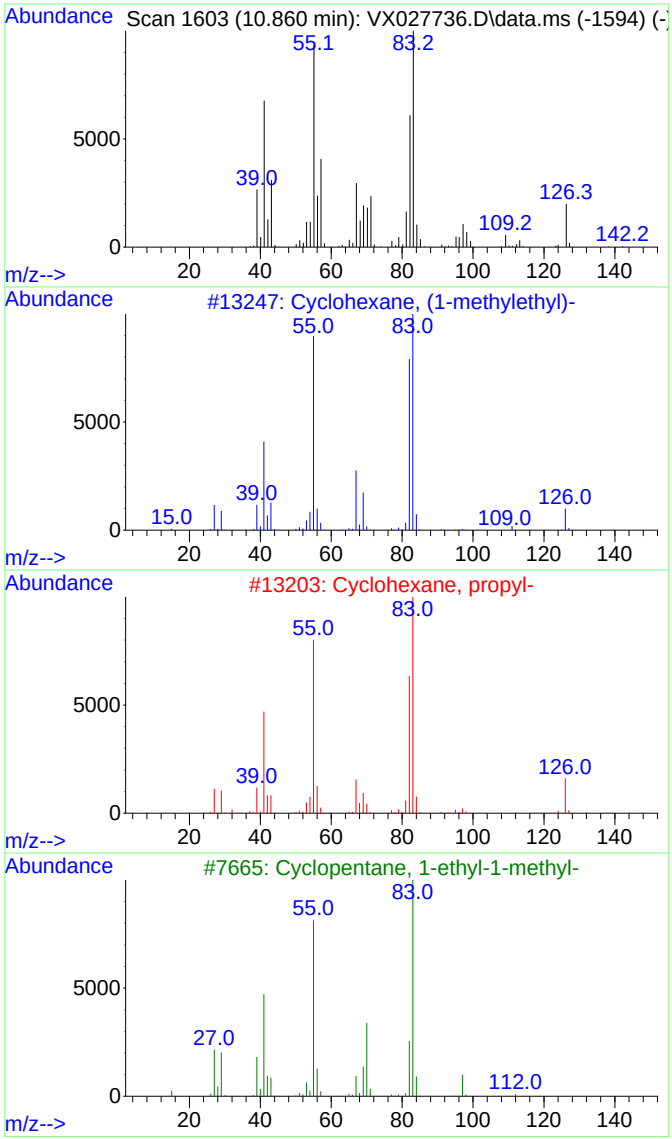
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

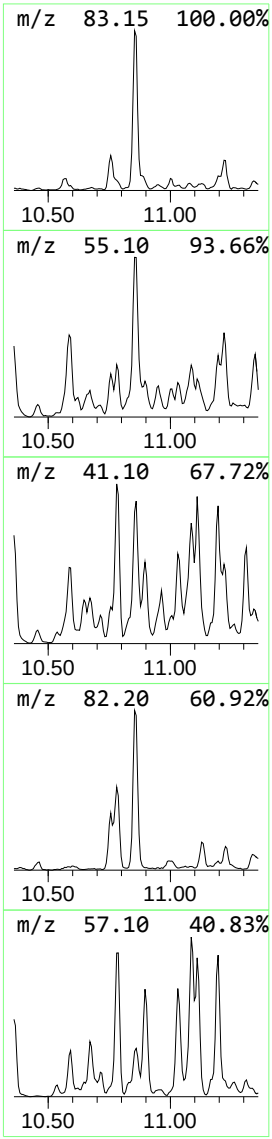
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, (1-methylethyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	108.98 ug/l	674531	Chlorobenzene-d5	10.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	74
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	64
3	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	58
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	43
5	trans-7-Oxabicyclo[4.3.0]nonane	126	C8H14O	027345-70-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

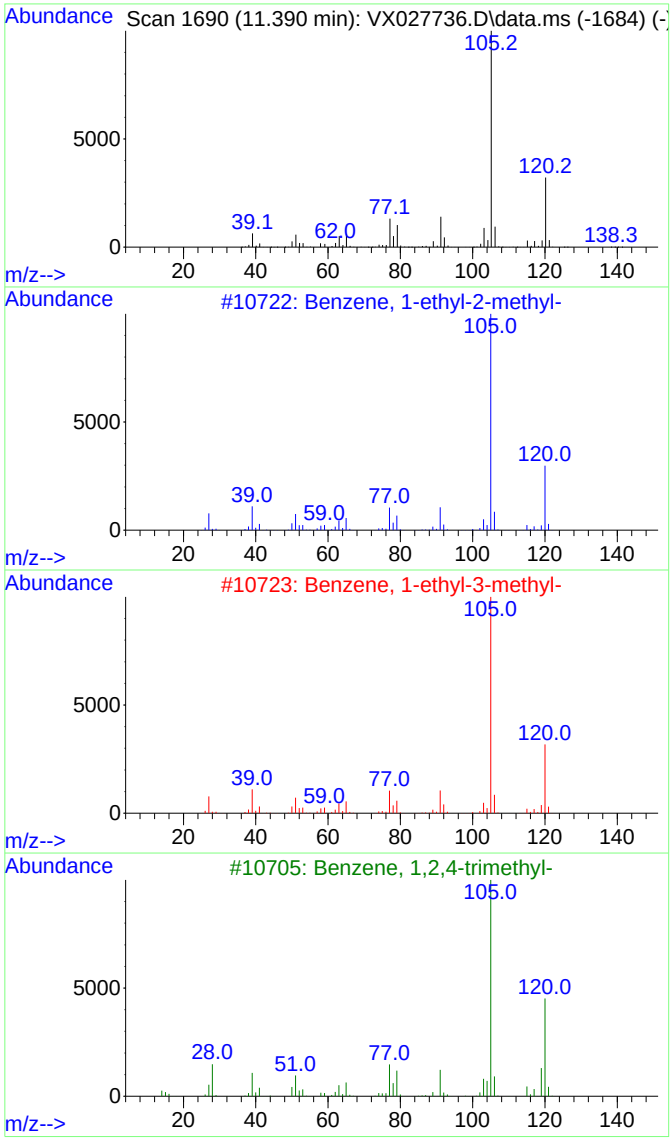
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

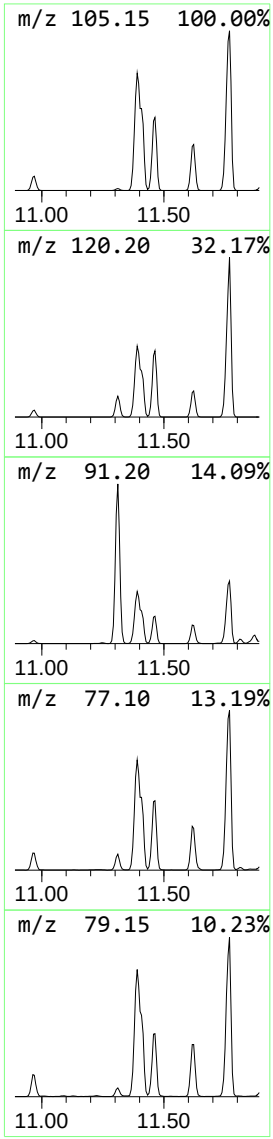
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.390	1022.38 ug/l	17261500	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

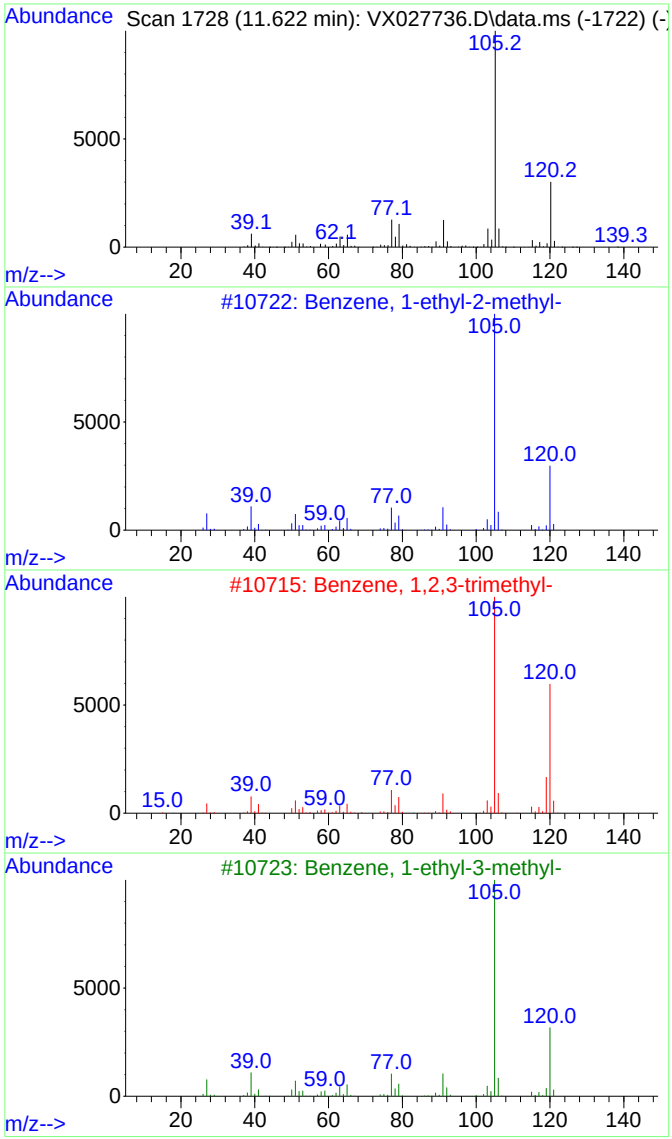
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

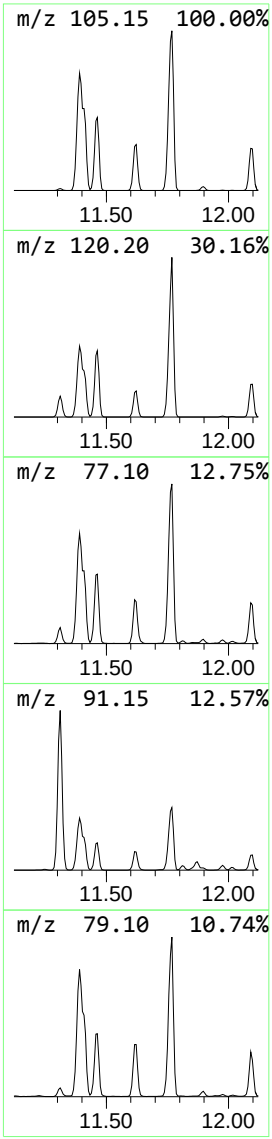
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.622	260.40 ug/l	4396510	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

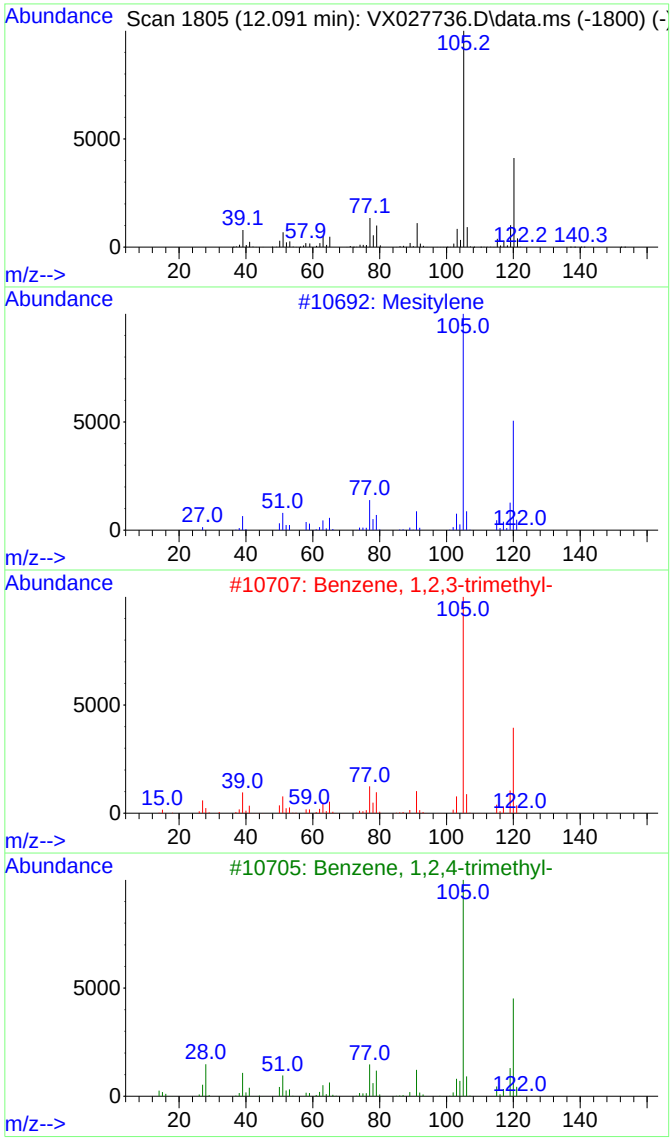
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

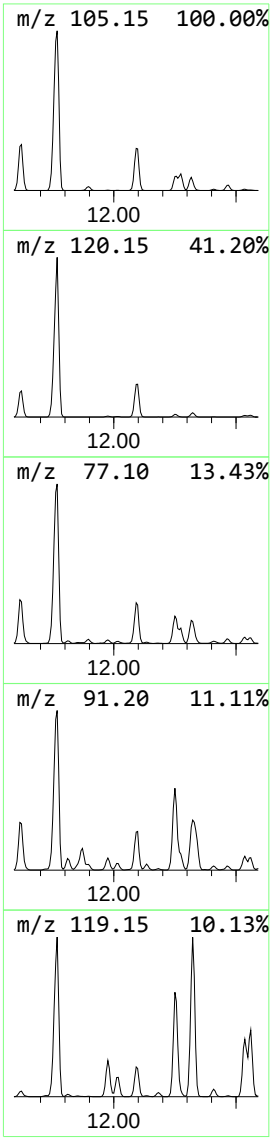
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	270.08 ug/l	4559940	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

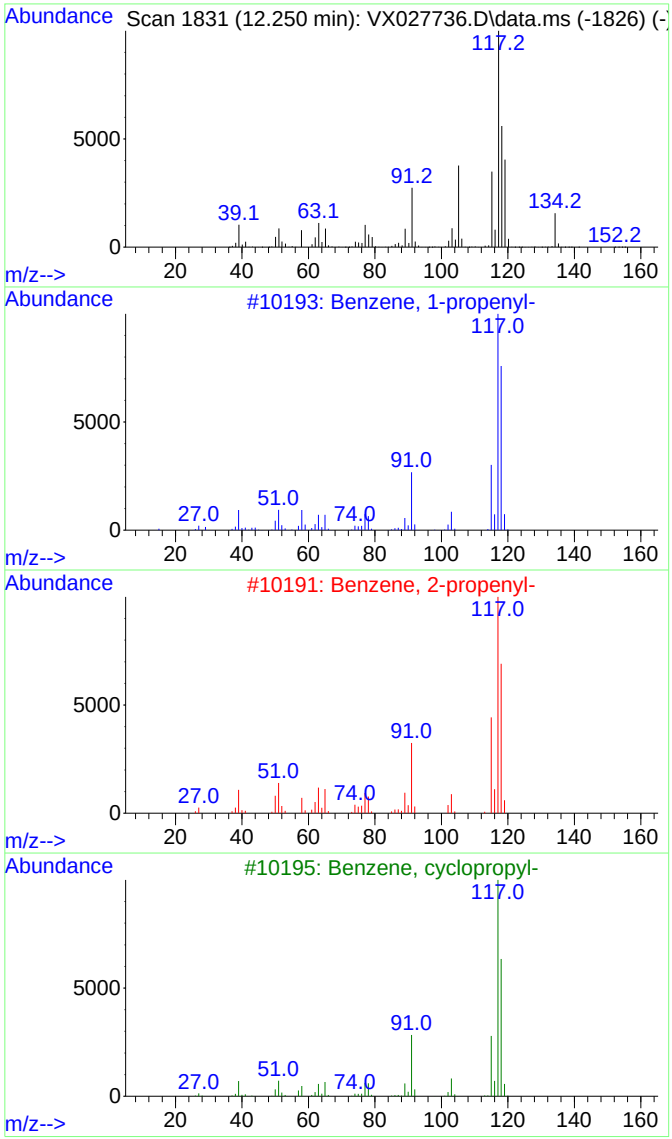
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

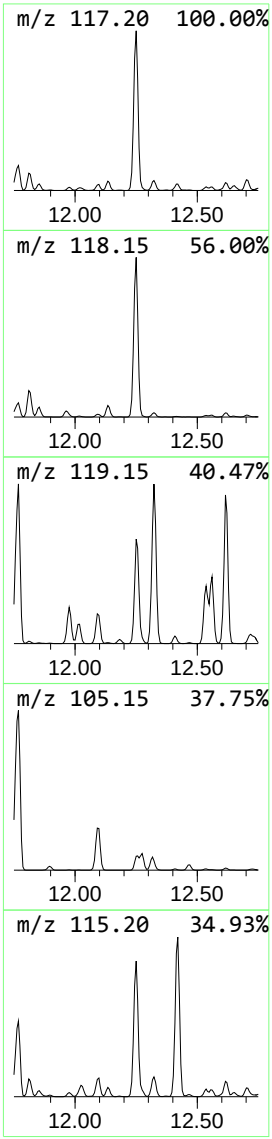
****

Peak Number 6 Benzene, 1-propenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	410.33 ug/l	6927910	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	87
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	55
4	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	52
5	Deltacyclene	118	C9H10	007785-10-6	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
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Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

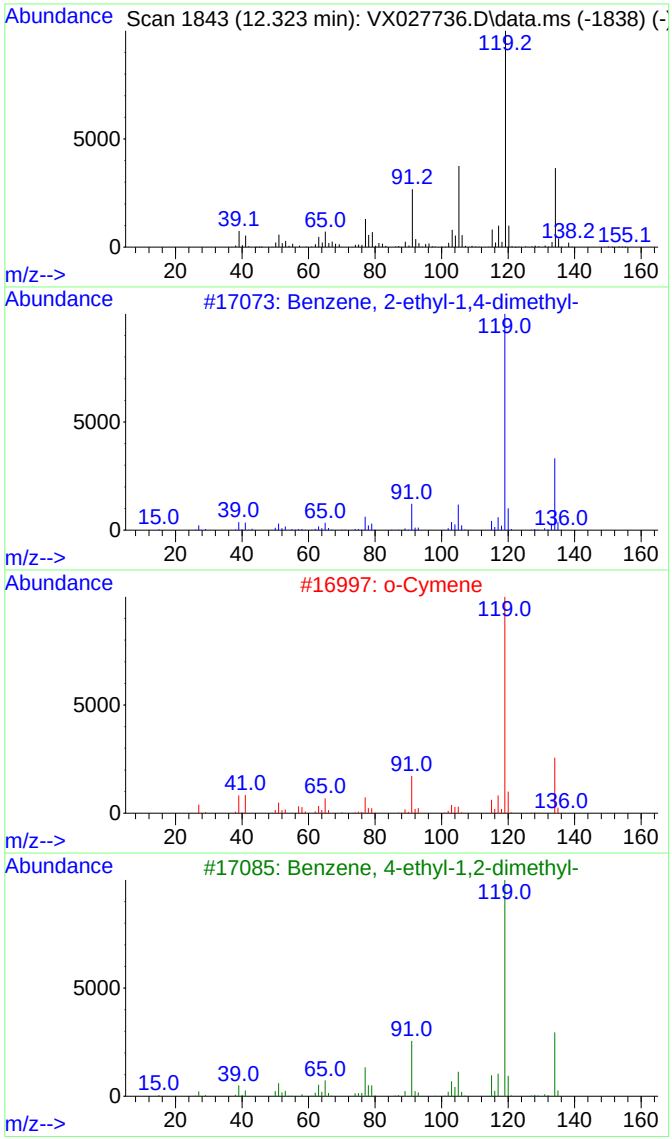
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

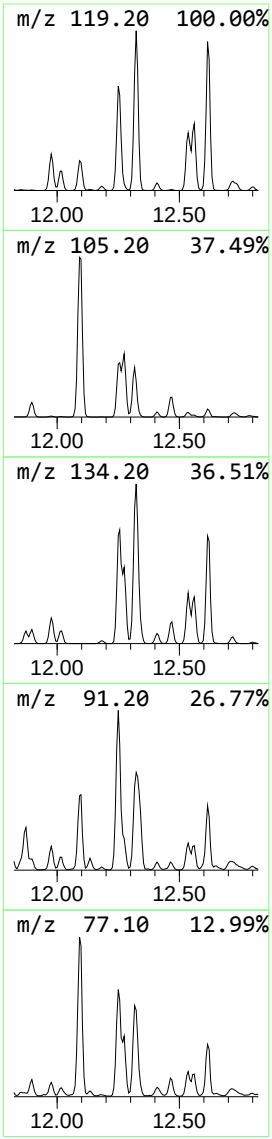
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.323	201.45 ug/l	3401200	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
2	o-Cymene	134	C10H14	000527-84-4	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
4	p-Cymene	134	C10H14	000099-87-6	93
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

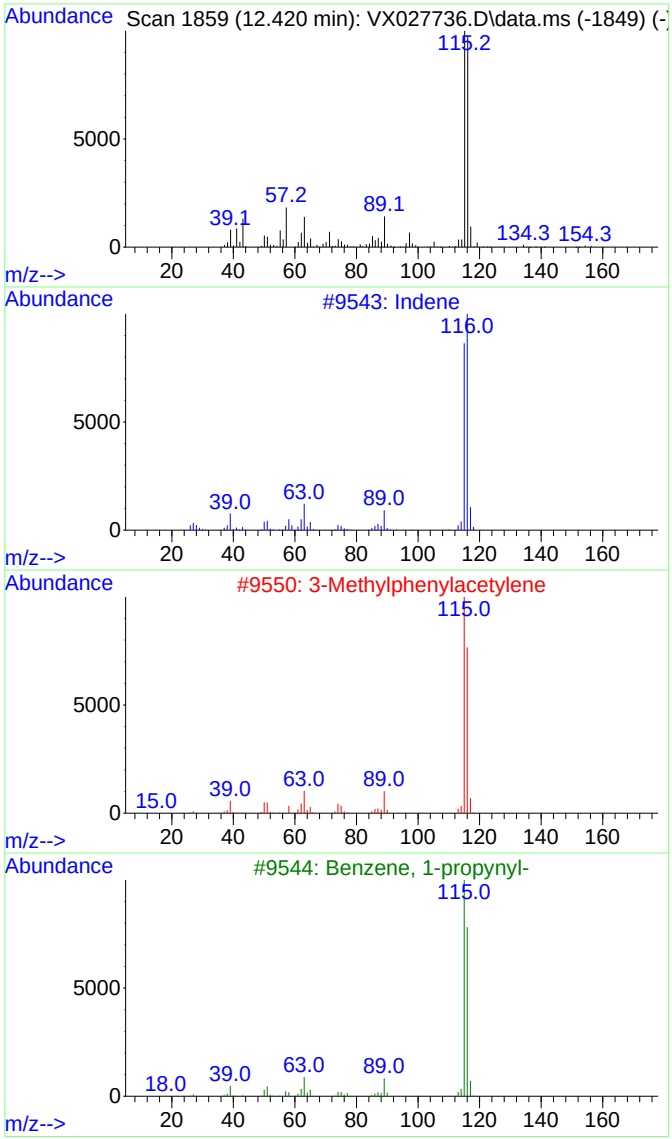
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

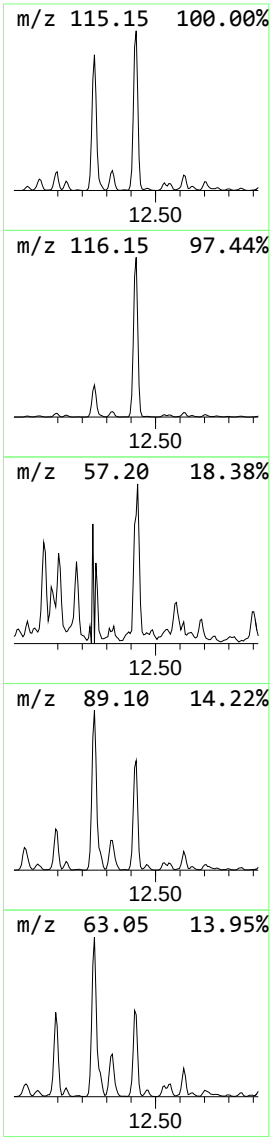
****

Peak Number 8 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.420	143.63 ug/l	2425080	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	94
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

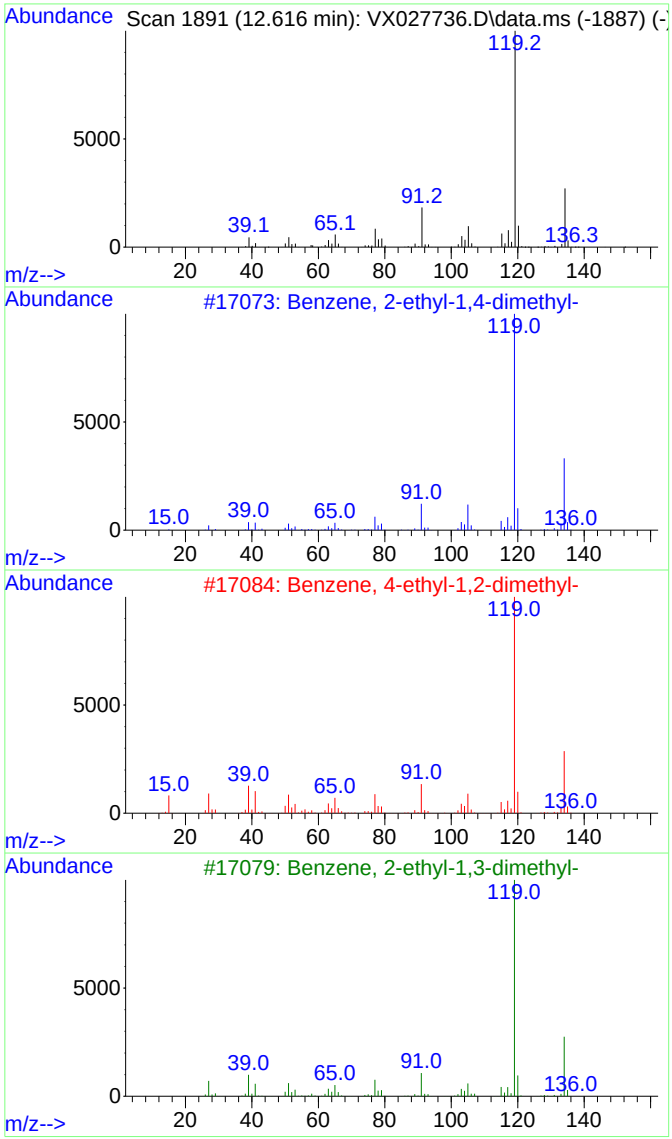
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

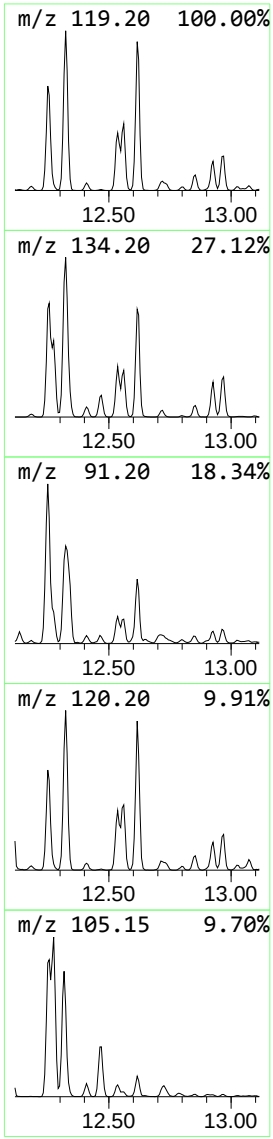
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	93.25 ug/l	1574460	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032622\
Data File : VX027736.D
Acq On : 26 Mar 2022 18:48
Operator : JC/MD
Sample : N2084-01
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BLDG-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Nonane, 3-methyl-	10.781	109.2	ug/l	675652	3	10.061	309482	50.0
Cyclohexane, (1...	10.860	109.0	ug/l	674531	3	10.061	309482	50.0
Benzene, 1-ethy...	11.390	1022.4	ug/l	17261500	4	12.030	844182	50.0
Benzene, 1,2,3-...	11.622	260.4	ug/l	4396510	4	12.030	844182	50.0
Benzene, 1,2,4-...	12.091	270.1	ug/l	4559940	4	12.030	844182	50.0
Benzene, 1-prop...	12.250	410.3	ug/l	6927910	4	12.030	844182	50.0
Benzene, 2-ethy...	12.323	201.4	ug/l	3401200	4	12.030	844182	50.0
Indene	12.420	143.6	ug/l	2425080	4	12.030	844182	50.0
Benzene, 4-ethy...	12.616	93.3	ug/l	1574460	4	12.030	844182	50.0