LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

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\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029672.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	23	31	44	rBV	501966	1910956	36.43%	3.724%
2	1.368	44	46	50	rVB	53825	65770	1.25%	0.128%
3	1.746	104	108	127	rVB3	69492	154579	2.95%	0.301%
4	2.532	229	237	255	rBV2	39762	204367	3.90%	0.398%
5	4.300	518	527	539	rVB3	18338	54666	1.04%	0.107%
6	4.556	557	569	588	rBV	87801	250207	4.77%	0.488%
7	5.391	695	706	715	rBV	142065	416356	7.94%	0.811%
8	5.556	723	733	751	rVB	259884	751305	14.32%	1.464%
9	5.958	789	799	807	rBV	149342	397694	7.58%	0.775%
10	6.044	807	813	825	rVB2	48892	132665	2.53%	0.259%
11	6.763	920	931	944	rBV	400497	949335	18.10%	1.850%
12	8.653	1234	1241	1247	rBV	785380	1237019	23.58%	2.411%
13	8.720	1247	1252	1259	rVB	549897	828533	15.79%	1.615%
14	10.055	1465	1471	1480	rBV	810331	1072456	20.44%	2.090%
15	10.195	1489	1494	1504	rVB	550079	697482	13.30%	1.359%
16	10.299	1504	1511	1519	rBV	2420805	3303928	62.98%	6.439%
17	10.640	1562	1567	1580	rVB	1500686	2008188	38.28%	3.914%
18	10.964	1613	1620	1625	rVB	75595	98699	1.88%	0.192%
19	11.085	1634	1640	1652	rBV	608195	809513	15.43%	1.578%
20	11.305	1671	1676	1683	rBV	315812	369289	7.04%	0.720%
21	11.378	1683	1688	1696	rVV	1676229	2869555	54.70%	5.593%
22	11.451	1696	1700	1713	rVB	950708	1158042	22.07%	2.257%
23	11.616	1721	1727	1736	rVB	933337	1145271	21.83%	2.232%
24	11.756	1744	1750	1756	rBV	4306416	5246131	100.00%	10.225%
25	11.969	1779	1785	1789	rBV	96448	120986	2.31%	0.236%
26	12.024	1789	1794	1799	rVB	852759	1053433	20.08%	2.053%
27	12.085	1799	1804	1810	rBV	1671787	2133069	40.66%	4.157%
28	12.244	1822	1830	1833	rBV	1441980	1885976	35.95%	3.676%
29	12.317	1838	1842	1852	rVB2	658970	941024	17.94%	1.834%
30	12.408	1852	1857	1862	rBV2	72234	102566	1.96%	0.200%
31	12.463	1862	1866	1872	rVB	211060	262552	5.00%	0.512%
32	12.530	1872	1877	1879	rBV	498869	619560	11.81%	1.208%
33	12.555	1879	1881	1886	rVV	431486	493879	9.41%	0.963%
34	12.616	1886	1891	1894	rVV	794378	944858	18.01%	1.842%
35	12.646	1894	1896	1900	rVB	165423	175999	3.35%	0.343%
36	12.701	1900	1905	1913	rBV2	483752	731188	13.94%	1.425%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

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\82X061822W.M
Title : SW846 8260

37	12.847	1924	1929	1934	rVB	296544	370772	7.07%	0.723%
38	12.920	1934	1941	1945	rBV	575363	732168	13.96%	1.427%
39	12.963	1945	1948	1954	rVB	962035	1108706	21.13%	2.161%
40	13.024	1954	1958	1959	rBV	53591	59051	1.13%	0.115%
41	13.170	1978	1982	1986	rVB	728590	856361	16.32%	1.669%
42	13.256	1992	1996	1998	rBV2	79175	117656	2.24%	0.229%
43	13.292	1998	2002	2007	rVB2	1562332	1998685	38.10%	3.895%
44	13.341	2007	2010	2014	rBV	295269	357288	6.81%	0.696%
45	13.420	2019	2023	2031	rVB	314914	422495	8.05%	0.823%
46	13.506	2031	2037	2040	rBV2	92072	140653	2.68%	0.274%
47	13.548	2040	2044	2047	rVV	244818	347496	6.62%	0.677%
48	13.585	2047	2050	2056	rVV3	226706	421209	8.03%	0.821%
49	13.640	2056	2059	2061	rVV	98896	141726	2.70%	0.276%
50	13.664	2061	2063	2069	rVB2	172074	249728	4.76%	0.487%
51	13.774	2076	2081	2088	rBV	2818076	3659703	69.76%	7.133%
52	13.853	2090	2094	2099	rVB	45122	69744	1.33%	0.136%
53	13.926	2099	2106	2110	rBV2	119192	175236	3.34%	0.342%
54	13.969	2110	2113	2117	rVB	90515	106871	2.04%	0.208%
55	14.079	2126	2131	2135	rBV	151583	186516	3.56%	0.364%
56	14.176	2143	2147	2151	rBV	364907	428334	8.16%	0.835%
57	14.219	2151	2154	2158	rVV3	132370	208599	3.98%	0.407%
58	14.262	2158	2161	2167	rVB	395858	479201	9.13%	0.934%
59	14.323	2167	2171	2176	rBV2	136902	203271	3.87%	0.396%
60	14.371	2176	2179	2183	rVB	116800	135275	2.58%	0.264%
61	14.481	2192	2197	2202	rBV2	92938	136740	2.61%	0.267%
62	14.640	2216	2223	2228	rBV	1121978	1443580	27.52%	2.814%
63	14.780	2240	2246	2251	rBV	707757	856749	16.33%	1.670%
64	14.902	2263	2266	2270	rVB	54839	69537	1.33%	0.136%
65	14.987	2276	2280	2285	rBV	67024	88003	1.68%	0.172%
66	15.487	2356	2362	2372	rVB3	36704	76528	1.46%	0.149%
67	15.615	2378	2383	2386	rBV2	41356	64031	1.22%	0.125%

Sum of corrected areas: 51309008

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
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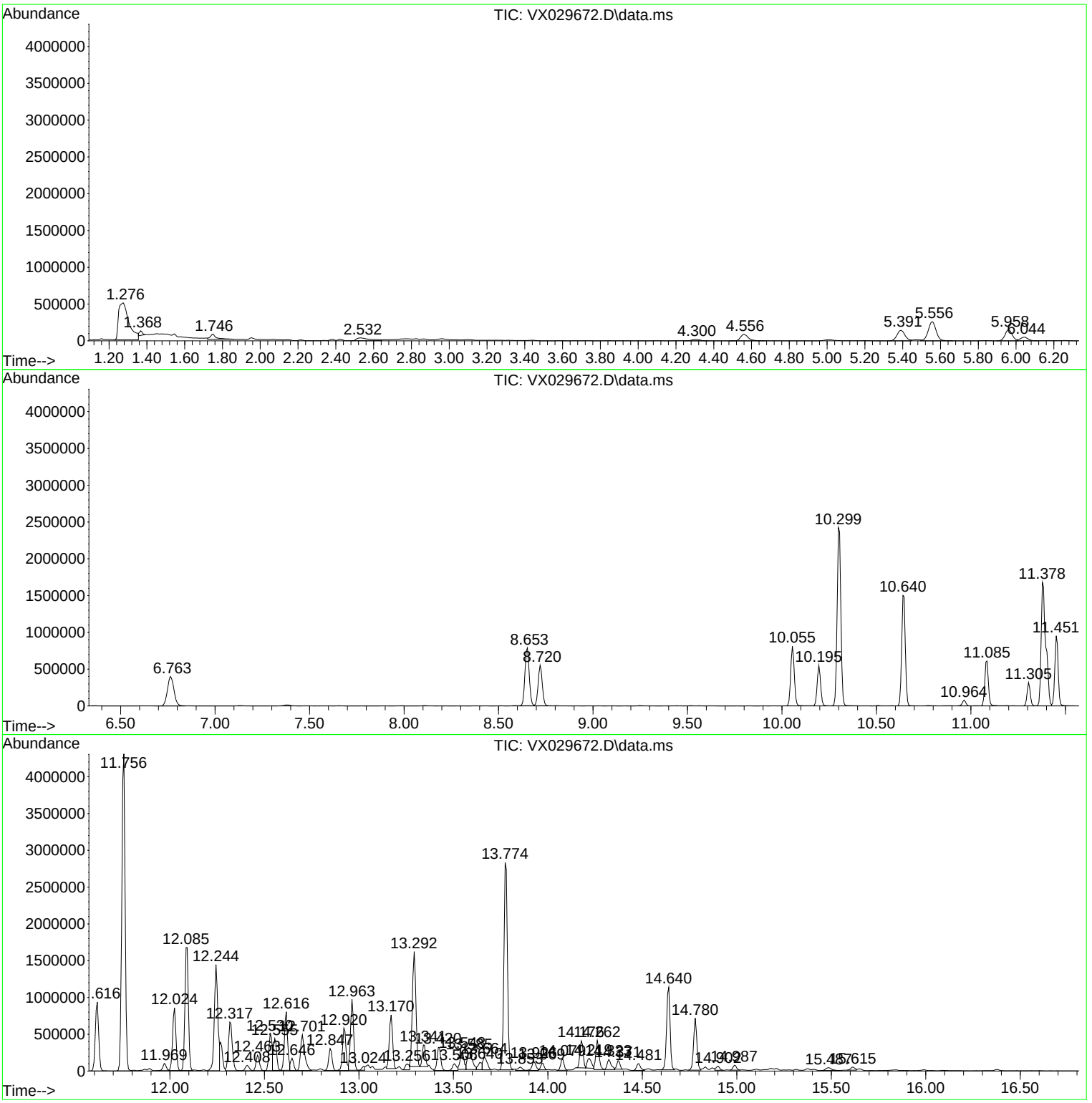
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

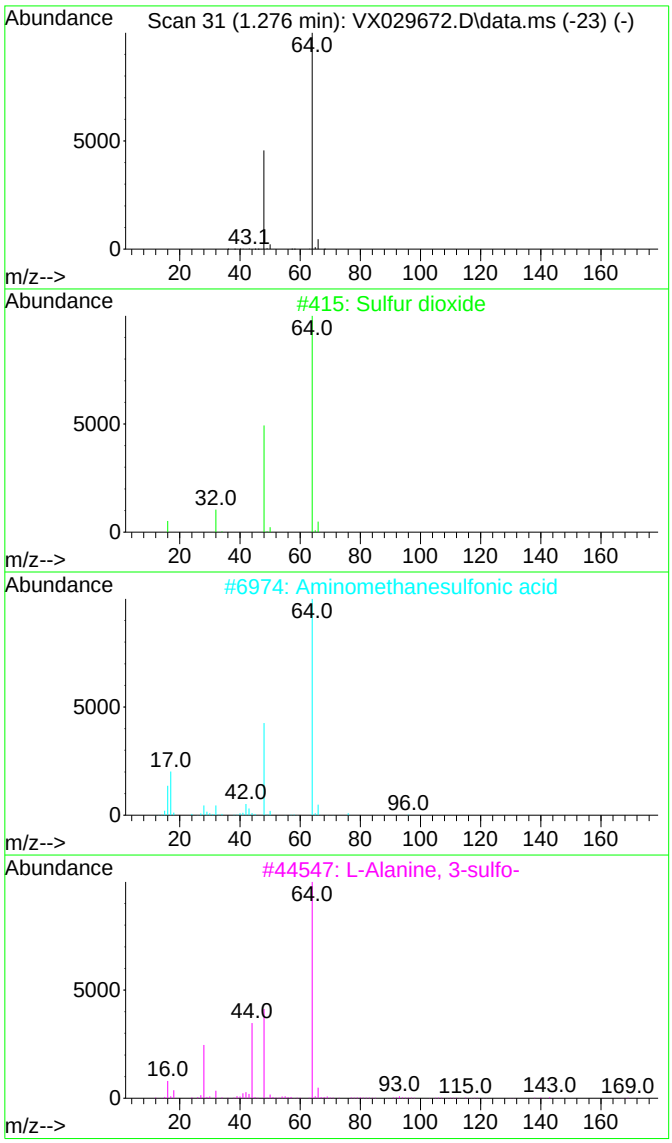
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

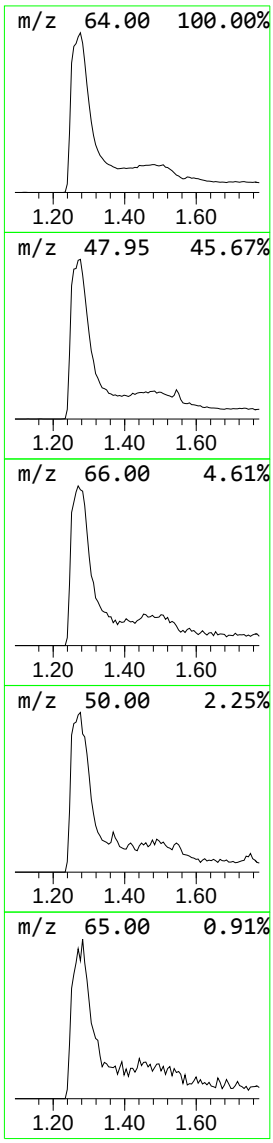
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.276	127.18 ug/l	1910960	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

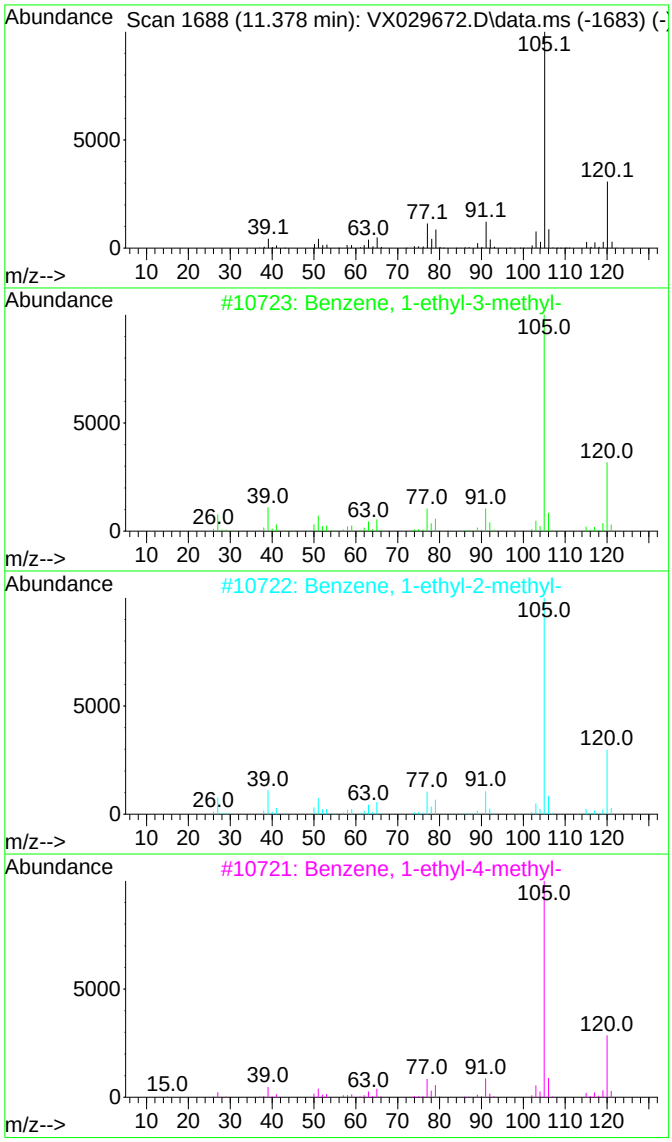
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

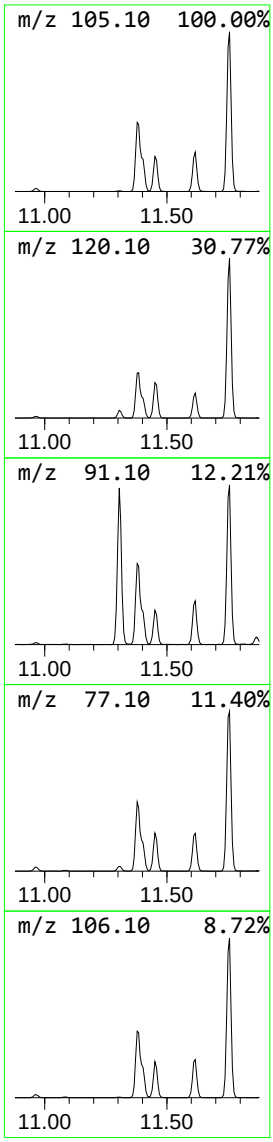
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	136.20 ug/l	2869560	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

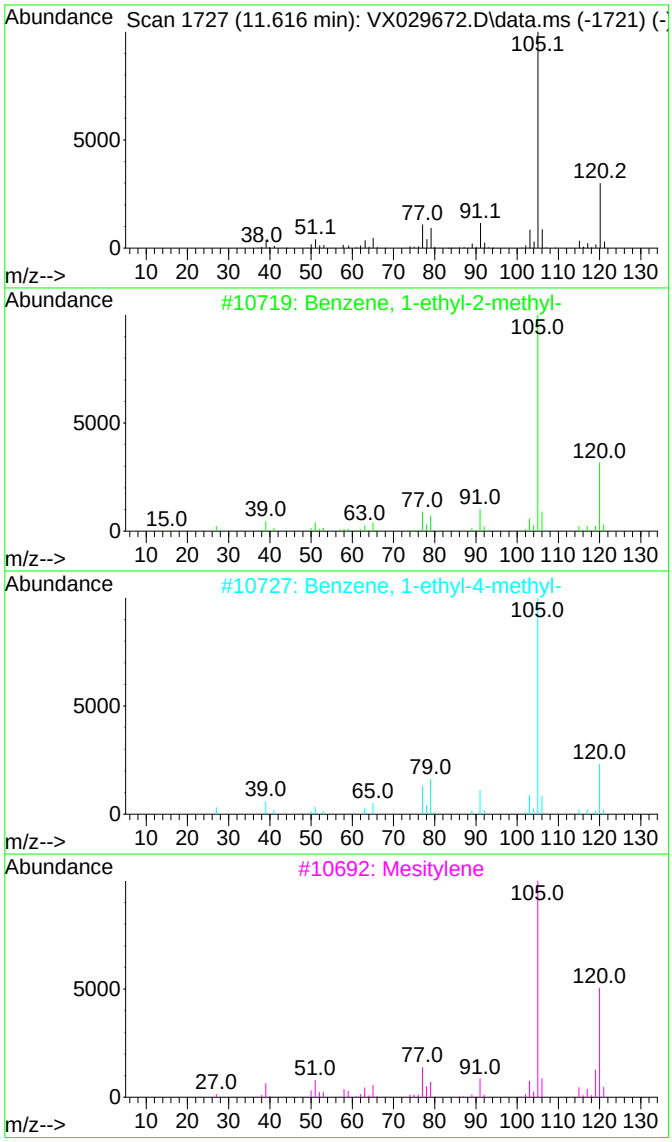
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

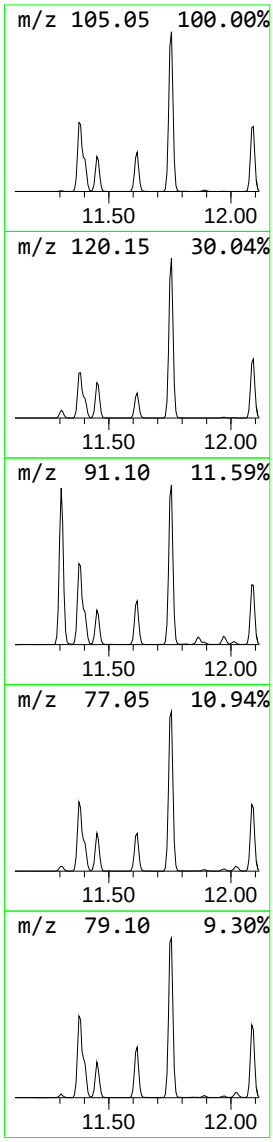
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	54.36 ug/l	1145270	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

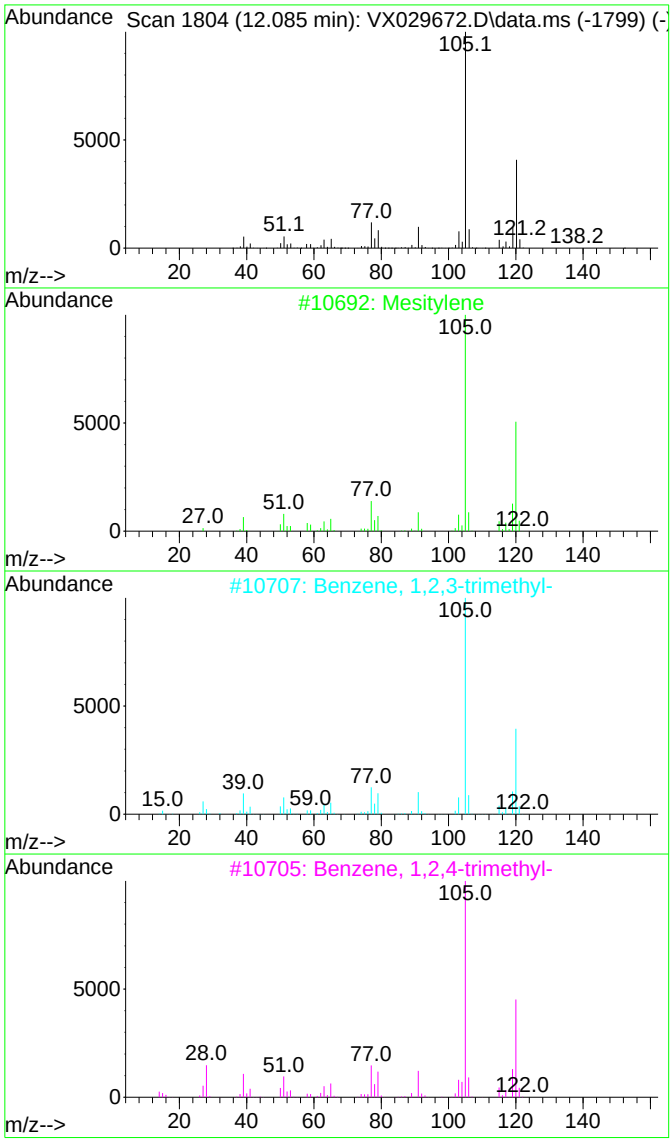
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

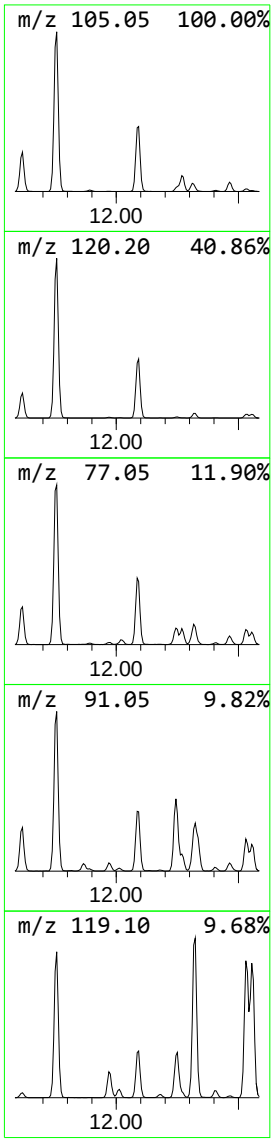
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	101.24 ug/l	2133070	1,4-Dichlorobenzene-d4	12.024

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	95
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	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

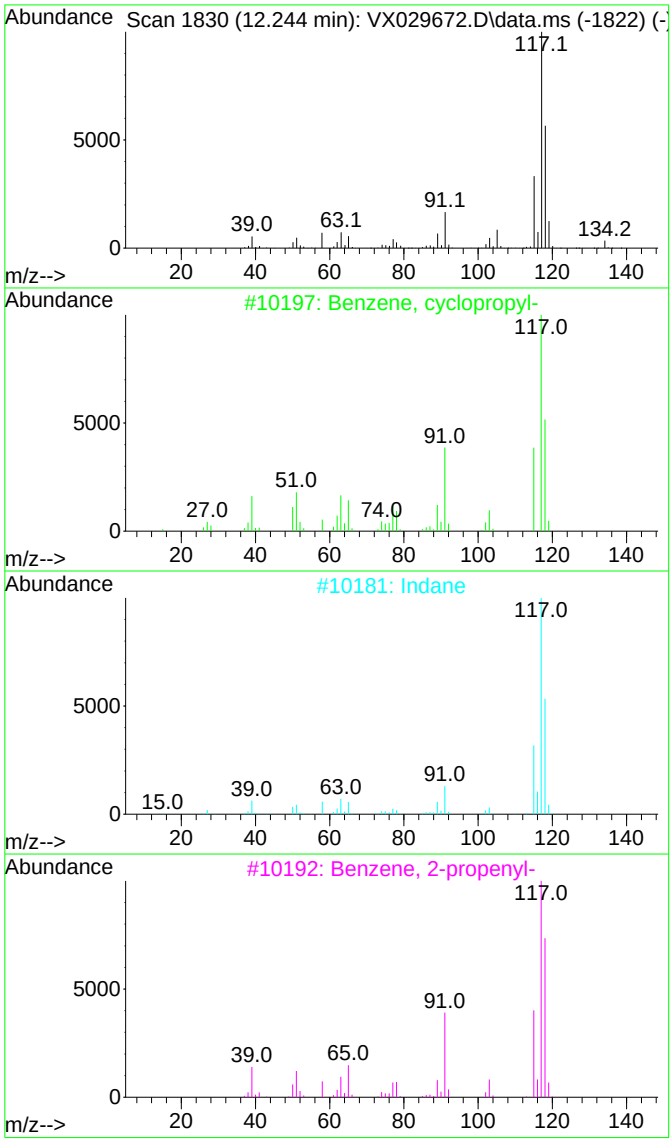
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

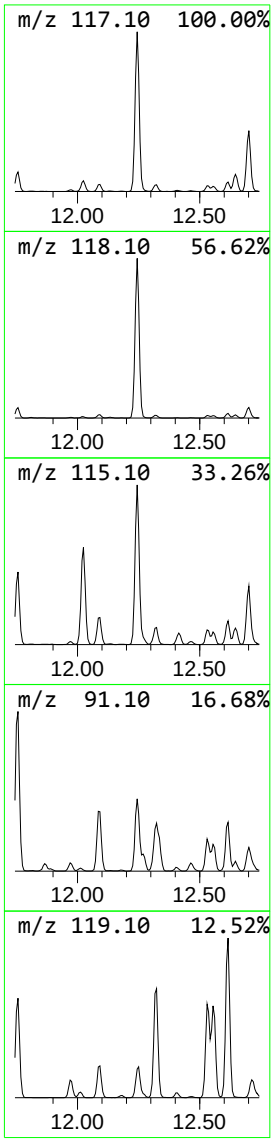
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	89.52 ug/l	1885980	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2	Indane	118	C9H10	000496-11-7	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53
5	Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50





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Data File : VX029672.D
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Operator : JC/MD
Sample : N3398-08
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

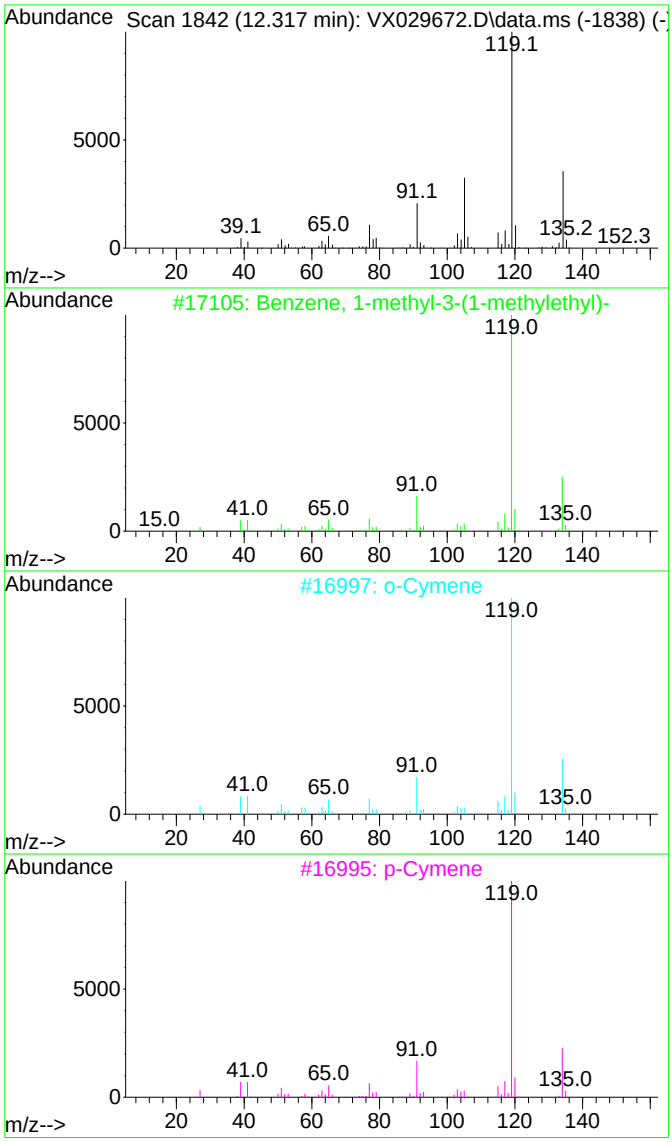
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

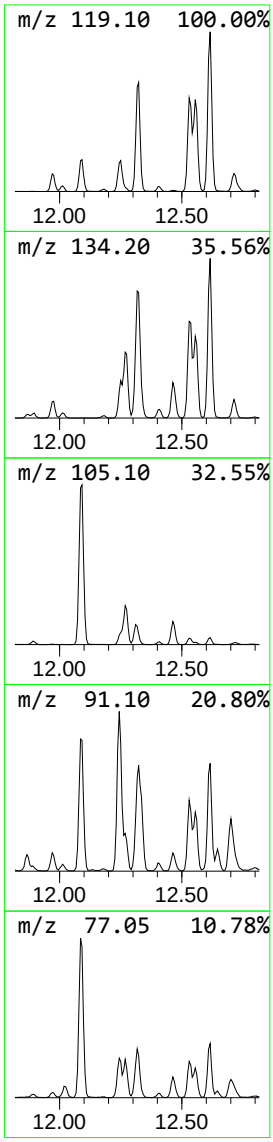
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-methyl-3-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	44.66 ug/l	941024	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	p-Cymene	134	C10H14	000099-87-6	94
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

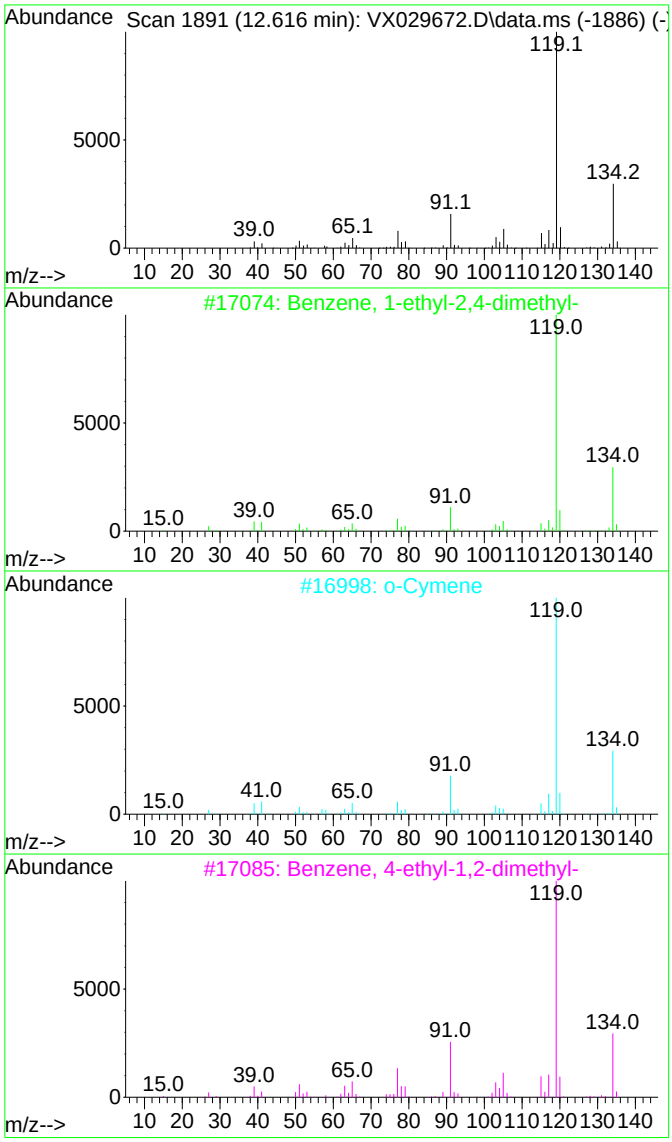
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

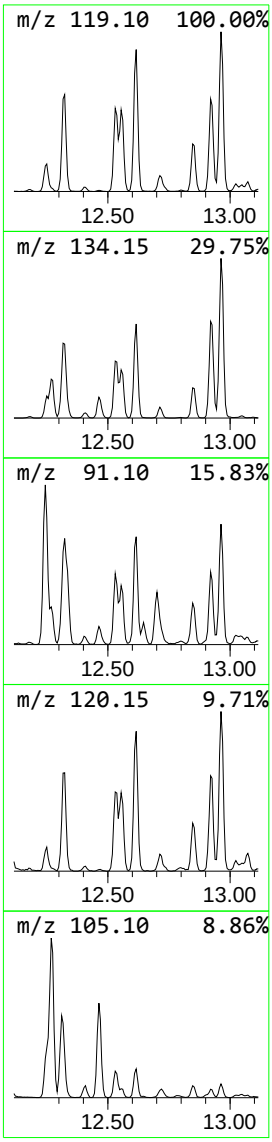
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	44.85 ug/l	944858	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	o-Cymene	134	C10H14	000527-84-4	97
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

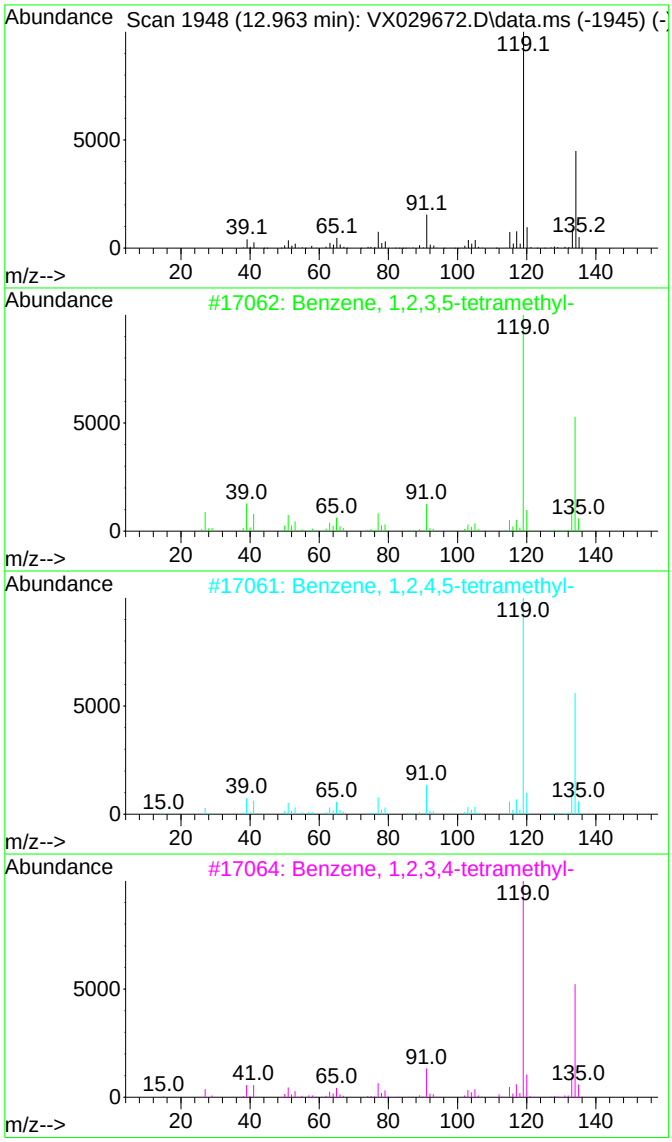
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

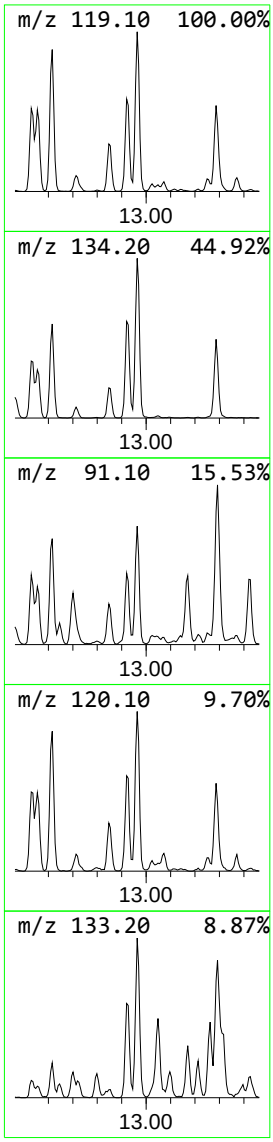
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	52.62 ug/l	1108710	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

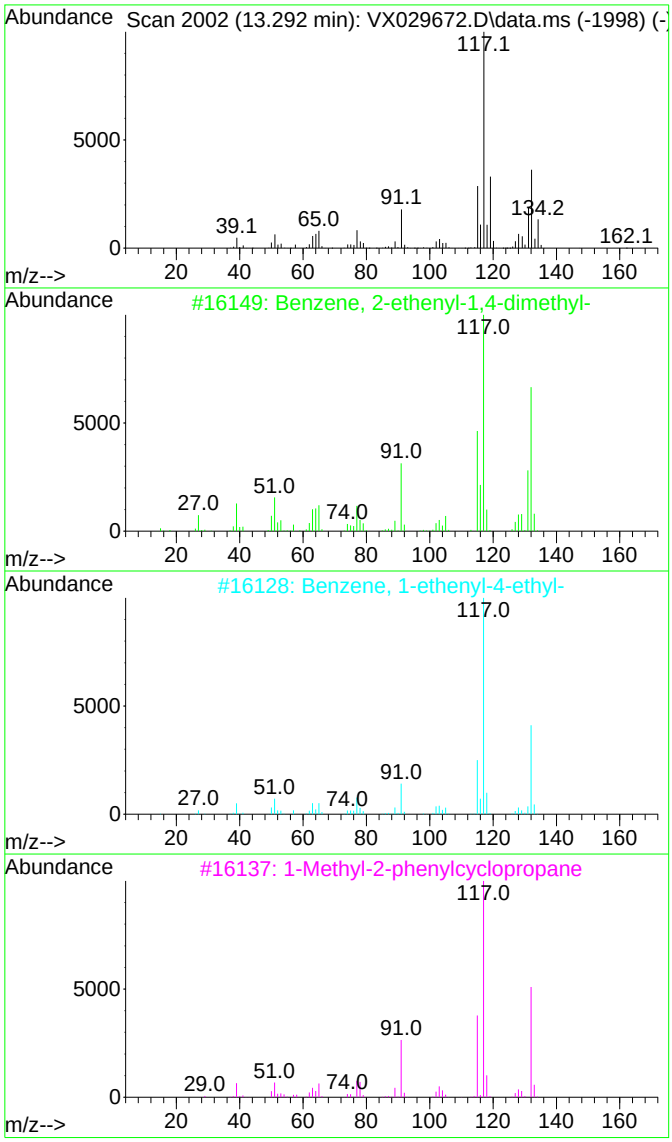
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

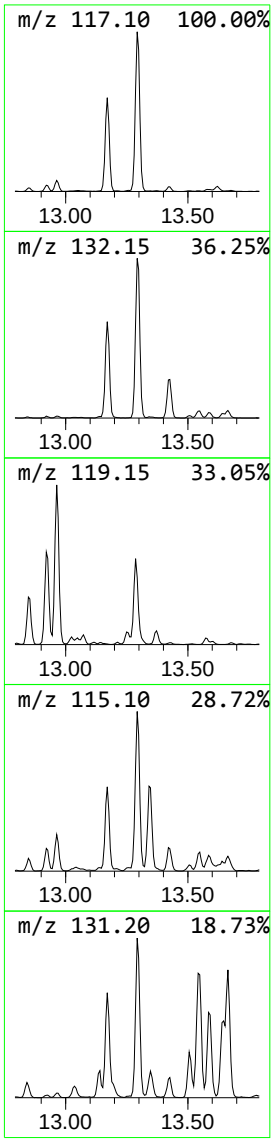
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	94.87 ug/l	1998690	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	92
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

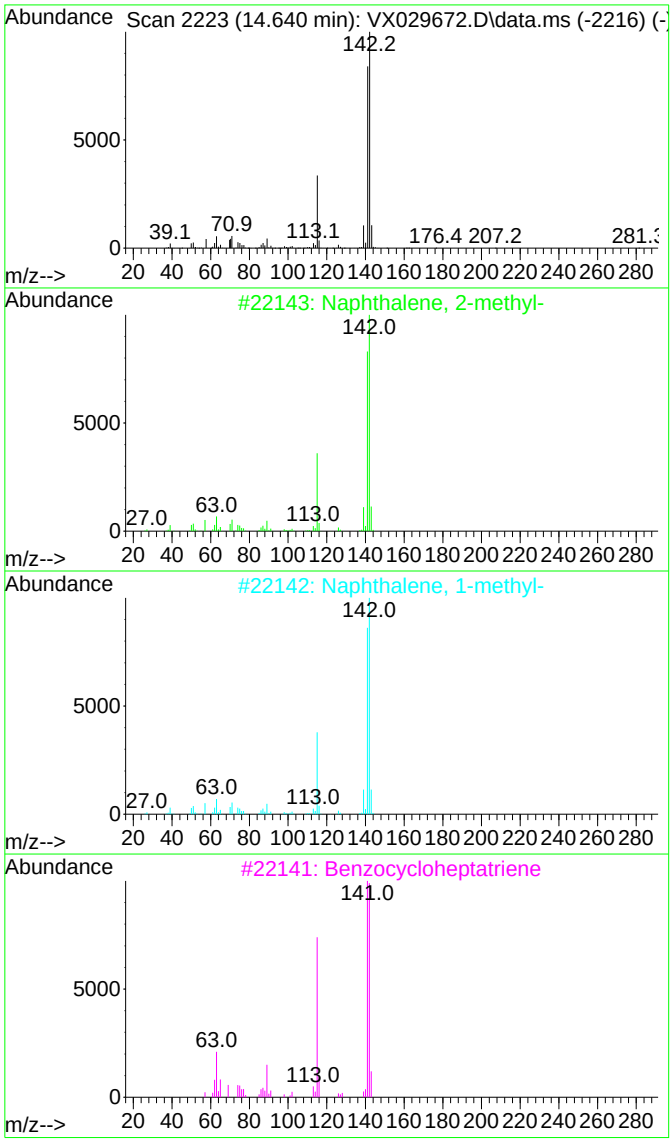
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

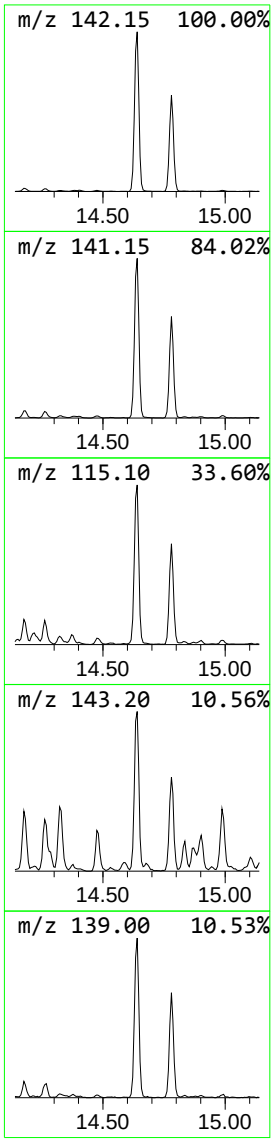
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	68.52 ug/l	1443580	1,4-Dichlorobenzene-d4	12.024

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	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029672.D
Acq On : 21 Jun 2022 19:16
Operator : JC/MD
Sample : N3398-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-520

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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
Sulfur dioxide	1.276	127.2	ug/l	1910960	1	5.556	751305	50.0
Benzene, 1-ethy...	11.378	136.2	ug/l	2869560	4	12.024	1053430	50.0
Benzene, 1-ethy...	11.616	54.4	ug/l	1145270	4	12.024	1053430	50.0
Benzene, 1,2,3-...	12.085	101.2	ug/l	2133070	4	12.024	1053430	50.0
Benzene, cyclop...	12.244	89.5	ug/l	1885980	4	12.024	1053430	50.0
Benzene, 1-meth...	12.317	44.7	ug/l	941024	4	12.024	1053430	50.0
Benzene, 1-ethy...	12.616	44.9	ug/l	944858	4	12.024	1053430	50.0
Benzene, 1,2,3,...	12.963	52.6	ug/l	1108710	4	12.024	1053430	50.0
Benzene, 2-ethe...	13.292	94.9	ug/l	1998690	4	12.024	1053430	50.0
Naphthalene, 2-...	14.640	68.5	ug/l	1443580	4	12.024	1053430	50.0