LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
Sample : N3481-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

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\82X062822W.M
Title : SW846 8260

Signal : TIC: VX029884.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	22	29	38	rBV	166515	155886	13.18%	1.180%
2	1.368	43	46	52	rVV	163688	165960	14.03%	1.256%
3	1.752	104	109	117	rVB	130803	173730	14.69%	1.315%
4	1.953	138	142	149	rVB	27632	38915	3.29%	0.295%
5	2.343	200	206	209	rBV4	7298	13380	1.13%	0.101%
6	2.386	209	213	221	rVB2	8094	14205	1.20%	0.108%
7	2.782	269	278	282	rBV4	21056	49336	4.17%	0.373%
8	2.825	282	285	289	rVV2	19982	38663	3.27%	0.293%
9	2.867	289	292	303	rVB2	19715	37341	3.16%	0.283%
10	2.971	303	309	320	rVB3	6859	16319	1.38%	0.124%
11	3.105	322	331	346	rVB3	35593	92327	7.81%	0.699%
12	3.446	378	387	394	rBV6	5178	13448	1.14%	0.102%
13	4.312	518	529	537	rVB2	47589	134035	11.33%	1.014%
14	5.391	688	706	714	rBV2	129245	377515	31.92%	2.857%
15	5.477	714	720	725	rVV2	27511	83820	7.09%	0.634%
16	5.556	725	733	757	rVB	234672	696989	58.94%	5.275%
17	5.842	769	780	789	rVB5	5482	16916	1.43%	0.128%
18	5.964	789	800	807	rVV	146505	384975	32.56%	2.914%
19	6.044	807	813	824	rVV2	56142	148736	12.58%	1.126%
20	6.165	826	833	838	rVV6	9163	28504	2.41%	0.216%
21	6.257	841	848	857	rVV5	16583	52834	4.47%	0.400%
22	6.354	857	864	874	rVB6	10349	30085	2.54%	0.228%
23	6.763	920	931	942	rBV	364888	886545	74.97%	6.710%
24	7.379	1022	1032	1042	rVB4	33392	92754	7.84%	0.702%
25	7.891	1113	1116	1123	rVV7	6573	12723	1.08%	0.096%
26	7.982	1123	1131	1139	rVB3	8291	17382	1.47%	0.132%
27	8.110	1145	1152	1156	rBV2	19980	45211	3.82%	0.342%
28	8.147	1156	1158	1163	rVB2	13249	16416	1.39%	0.124%
29	8.433	1199	1205	1211	rBV2	15835	26992	2.28%	0.204%
30	8.507	1211	1217	1224	rVB6	9485	17698	1.50%	0.134%
31	8.653	1235	1241	1249	rVV	751399	1182518	100.00%	8.950%
32	8.726	1249	1253	1258	rVB	11156	17721	1.50%	0.134%
33	8.958	1287	1291	1301	rVB4	27728	47942	4.05%	0.363%
34	9.049	1301	1306	1310	rBV2	22013	33404	2.82%	0.253%
35	9.104	1312	1315	1320	rVB2	7577	11893	1.01%	0.090%
36	9.165	1320	1325	1329	rBV2	8247	12627	1.07%	0.096%

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Instrument :
MSVOA_X
ClientSampleId :
MW-16

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

37	9.451	1365	1372	1377	rBV5	6473	14005	1.18%	0.106%
38	10.055	1466	1471	1481	rVB	756370	996674	84.28%	7.543%
39	10.195	1489	1494	1500	rBV	169376	210347	17.79%	1.592%
40	10.305	1506	1512	1516	rVB2	12328	20390	1.72%	0.154%
41	10.646	1563	1568	1576	rVB	17855	25279	2.14%	0.191%
42	10.963	1615	1620	1626	rBV	123259	152982	12.94%	1.158%
43	11.085	1634	1640	1650	rBV	553691	719588	60.85%	5.446%
44	11.305	1671	1676	1684	rVB	230100	278135	23.52%	2.105%
45	11.402	1684	1692	1698	rBV	16469	23554	1.99%	0.178%
46	11.616	1721	1727	1734	rBV	240182	290303	24.55%	2.197%
47	11.756	1745	1750	1756	rVB	277917	347264	29.37%	2.628%
48	11.872	1764	1769	1770	rBV	16508	22456	1.90%	0.170%
49	11.890	1770	1772	1777	rVV	27562	32117	2.72%	0.243%
50	12.024	1788	1794	1799	rVV	787784	946043	80.00%	7.160%
51	12.091	1799	1805	1811	rVV	349452	433645	36.67%	3.282%
52	12.177	1815	1819	1824	rVB	11260	14235	1.20%	0.108%
53	12.244	1824	1830	1837	rBV2	453991	585682	49.53%	4.433%
54	12.317	1837	1842	1851	rVB2	43425	73345	6.20%	0.555%
55	12.408	1851	1857	1861	rBV	36958	47107	3.98%	0.357%
56	12.463	1861	1866	1873	rVB	70796	86773	7.34%	0.657%
57	12.530	1873	1877	1886	rBV	65247	90851	7.68%	0.688%
58	12.616	1886	1891	1894	rBV	186009	226827	19.18%	1.717%
59	12.646	1894	1896	1900	rVV	62315	67557	5.71%	0.511%
60	12.701	1900	1905	1913	rVB2	263051	366500	30.99%	2.774%
61	12.847	1924	1929	1934	rVV2	71576	95540	8.08%	0.723%
62	12.920	1934	1941	1945	rVV	171408	222509	18.82%	1.684%
63	12.963	1945	1948	1954	rVV	132733	155619	13.16%	1.178%
64	13.030	1954	1959	1965	rVB2	12573	20729	1.75%	0.157%
65	13.140	1973	1977	1978	rBV	11107	12097	1.02%	0.092%
66	13.170	1978	1982	1991	rVB	149134	181683	15.36%	1.375%
67	13.292	1991	2002	2007	rBV2	412903	561934	47.52%	4.253%
68	13.347	2007	2011	2014	rBV4	13716	16234	1.37%	0.123%
69	13.426	2019	2024	2031	rVB	49022	67963	5.75%	0.514%
70	13.506	2031	2037	2040	rBV4	11707	17107	1.45%	0.129%
71	13.548	2040	2044	2046	rVV	32991	47346	4.00%	0.358%
72	13.585	2046	2050	2055	rVV3	32622	61337	5.19%	0.464%
73	13.646	2055	2060	2061	rVV3	25174	40302	3.41%	0.305%
74	13.664	2061	2063	2070	rVB2	44269	56105	4.74%	0.425%
75	13.774	2075	2081	2087	rBV	150268	205630	17.39%	1.556%
76	13.926	2102	2106	2110	rBV4	16991	21534	1.82%	0.163%

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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

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
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Title : SW846 8260

77	13.969	2110	2113	2117	rVB2	13592	15847	1.34%	0.120%
78	14.079	2126	2131	2136	rBV3	15832	21719	1.84%	0.164%
79	14.213	2148	2153	2159	rBV2	17041	28837	2.44%	0.218%
80	14.323	2167	2171	2176	rBV	10974	13116	1.11%	0.099%
81	14.371	2176	2179	2186	rVB2	11362	16008	1.35%	0.121%
82	14.780	2241	2246	2255	rVB	57589	75845	6.41%	0.574%

Sum of corrected areas: 13212445

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Data File : VX029884.D
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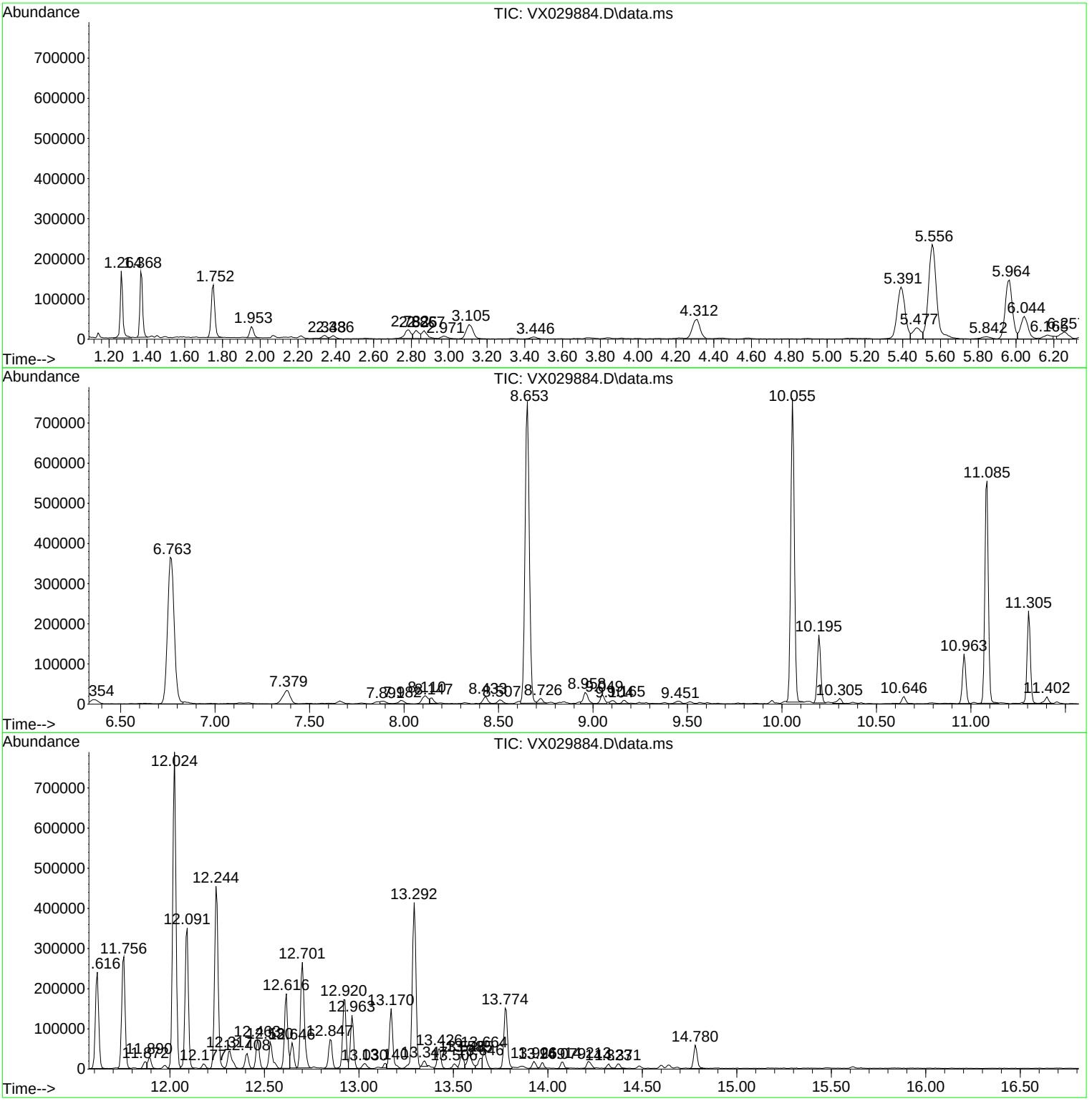
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

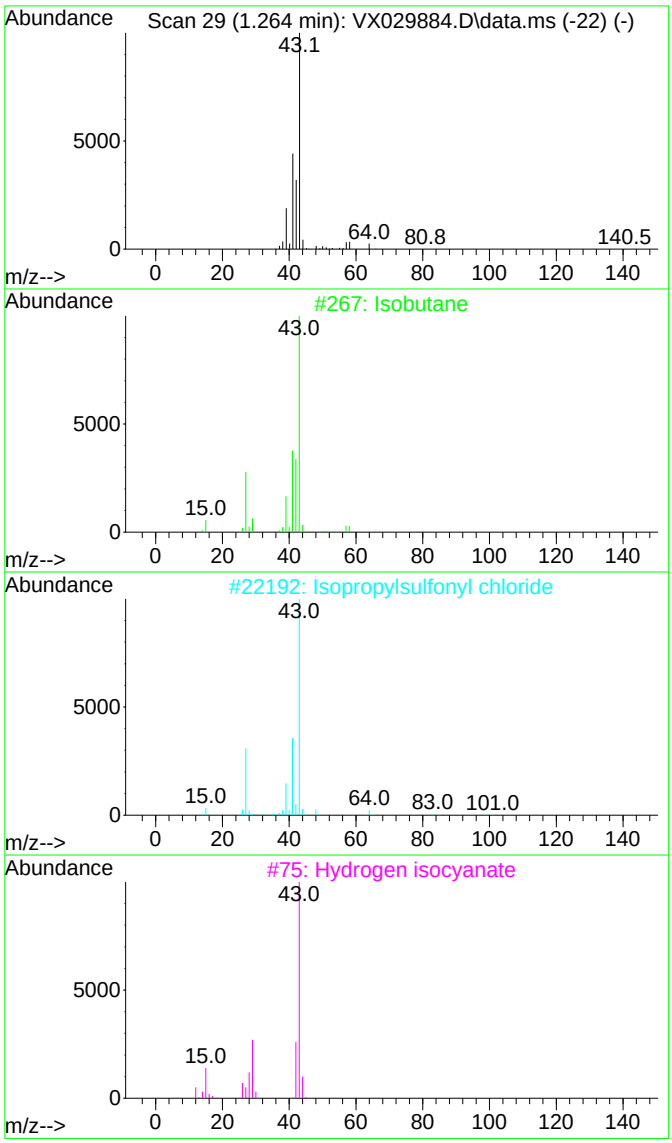
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

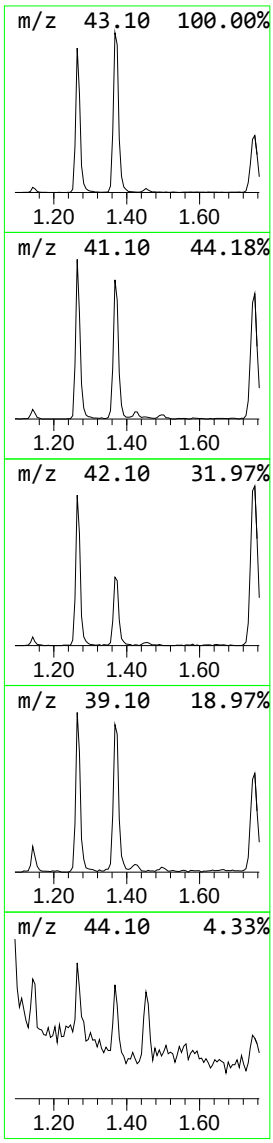
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Isobutane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	11.18 ug/l	155886	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	72
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	28
3	Hydrogen isocyanate	43	CHNO	000075-13-8	4
4	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4
5	Cyclobutylamine	71	C4H9N	002516-34-9	4





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

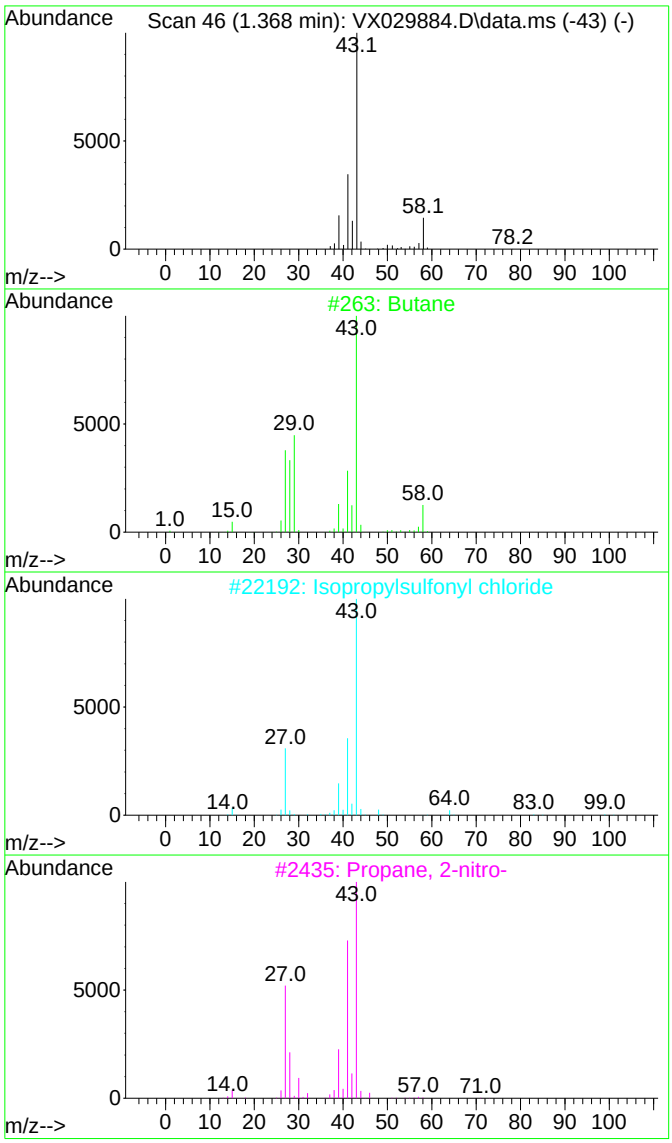
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

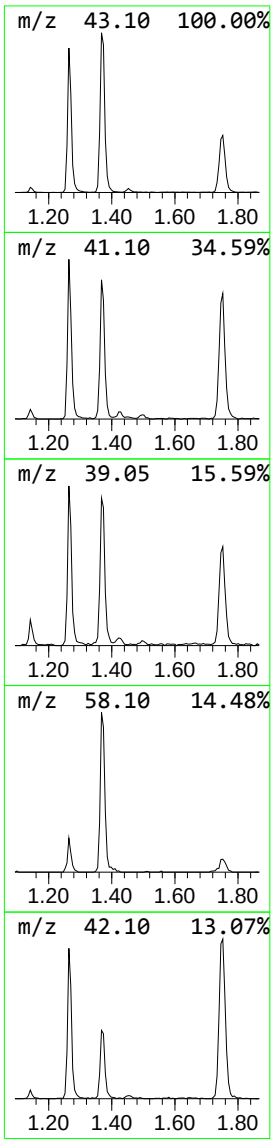
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	11.91 ug/l	165960	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
4	Isobutane	58	C4H10	000075-28-5	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

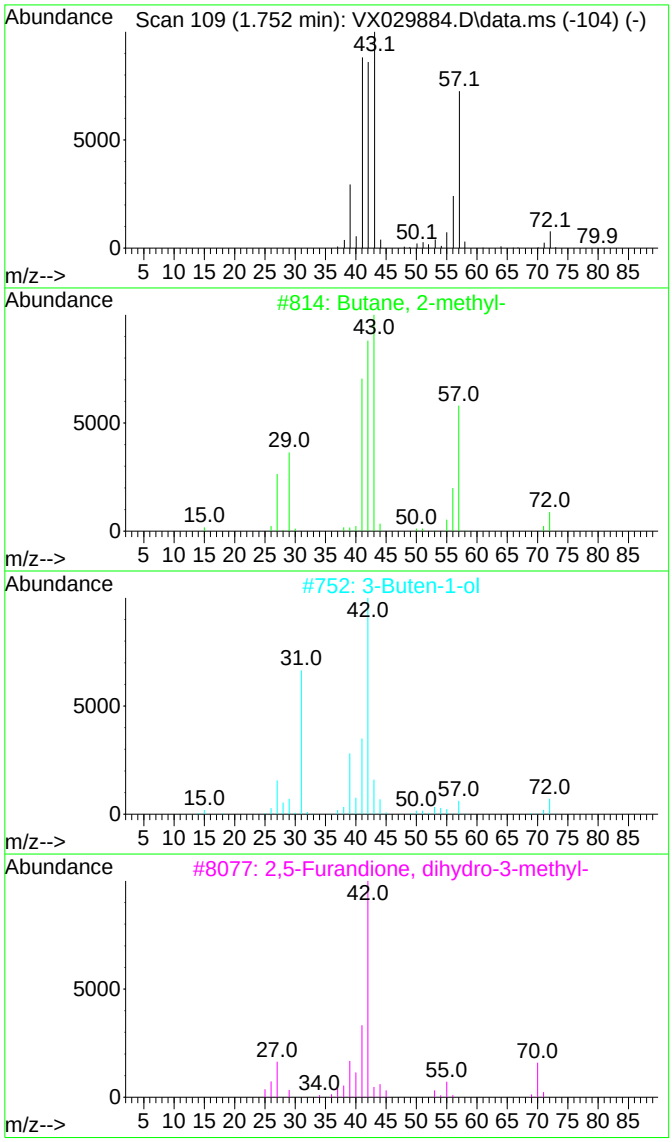
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

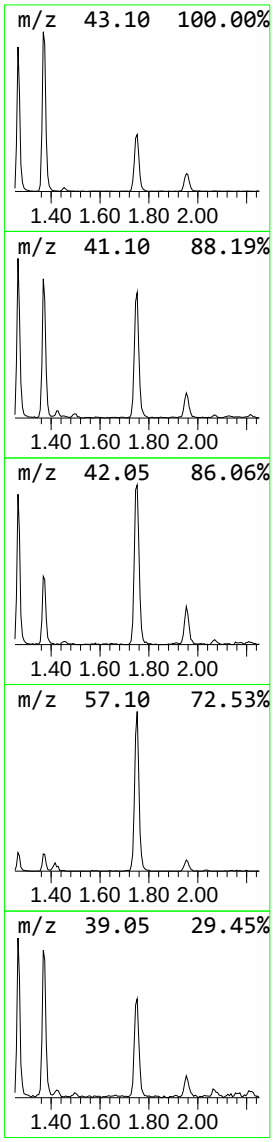
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	12.46 ug/l	173730	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	28
3	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	23
4	1-Butene	56	C4H8	000106-98-9	10
5	Azetidine	57	C3H7N	000503-29-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

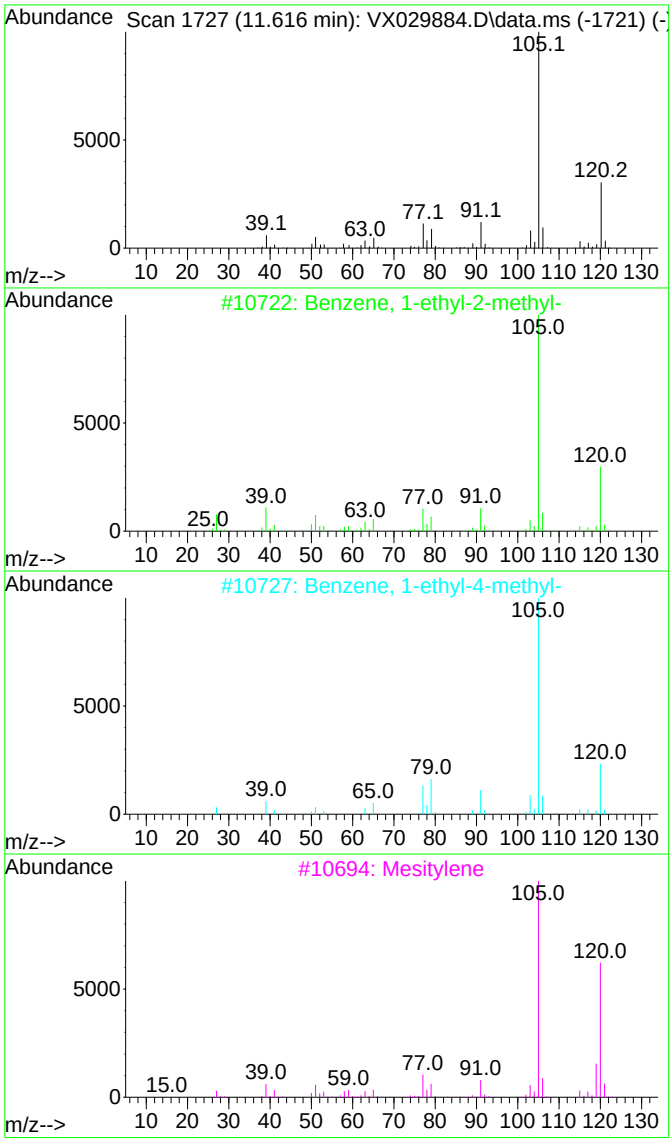
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

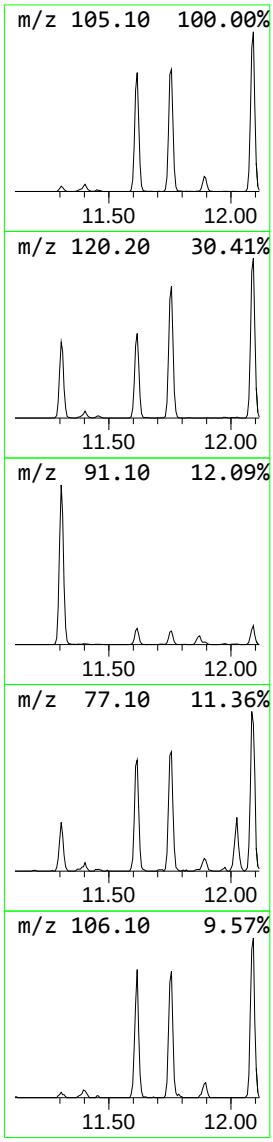
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	15.34 ug/l	290303	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	95
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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Instrument :
MSVOA_X
ClientSampleId :
MW-16

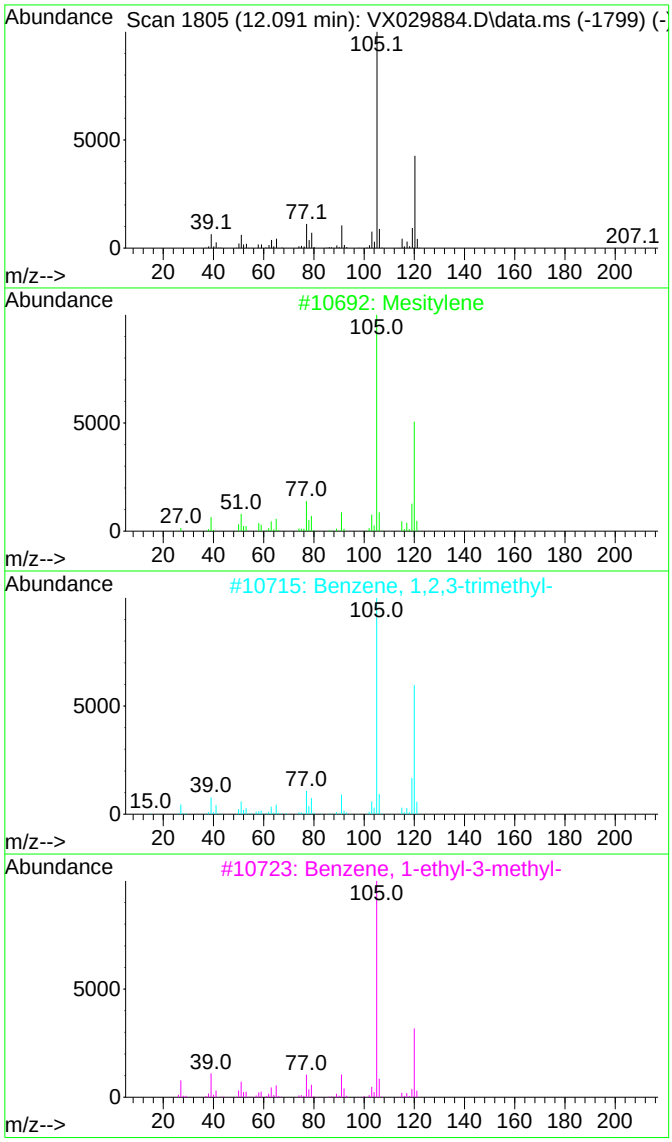
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

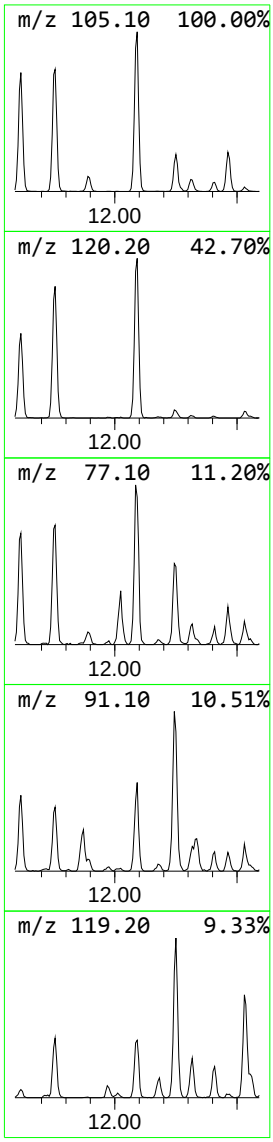
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	22.92 ug/l	433645	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-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

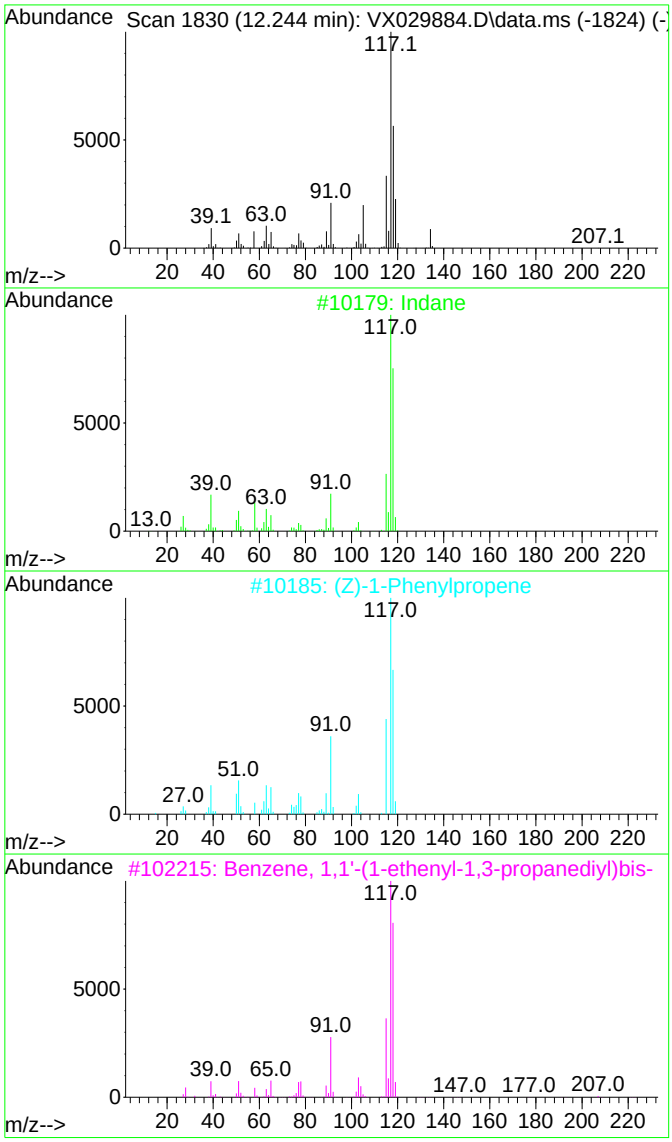
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

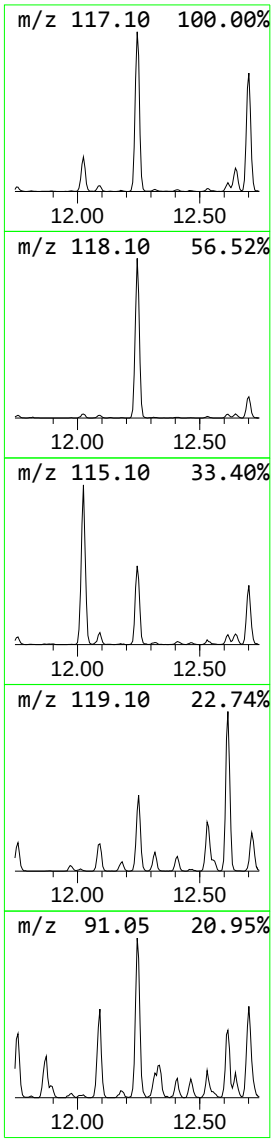
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	30.95 ug/l	585682	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	70
2	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70
3	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	64
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	62
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
Sample : N3481-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

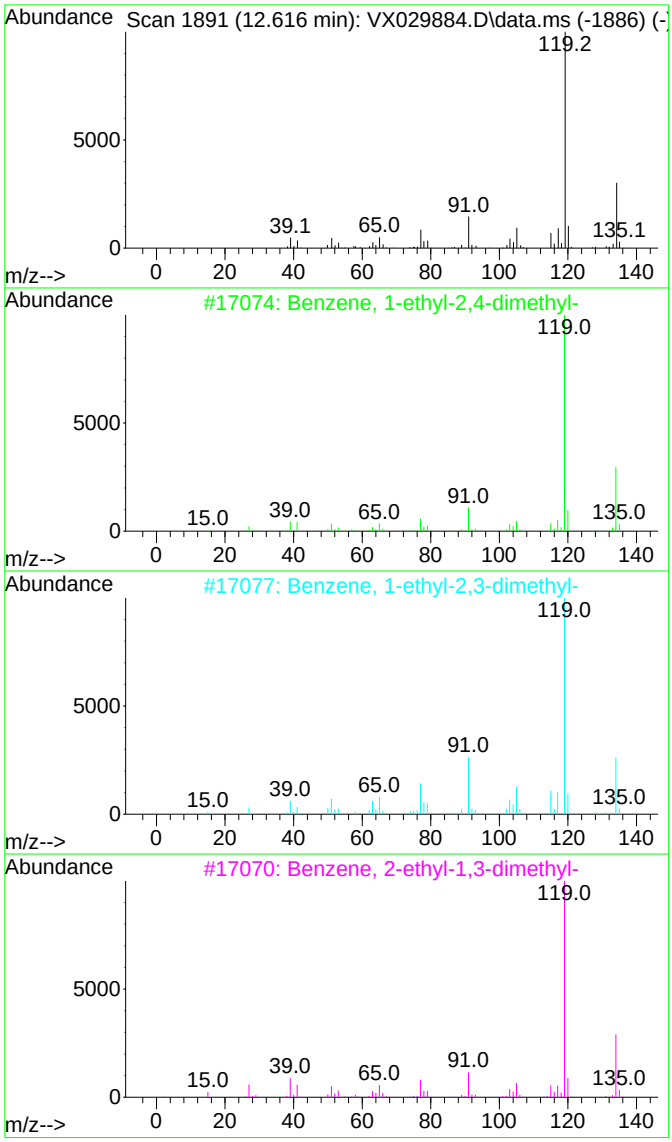
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

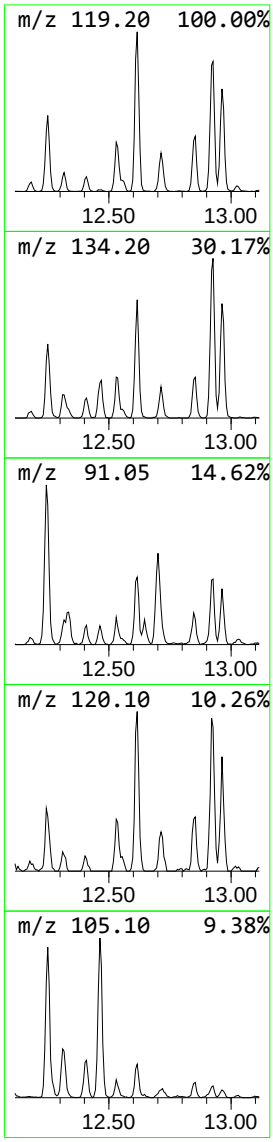
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	11.99 ug/l	226827	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	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
Sample : N3481-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

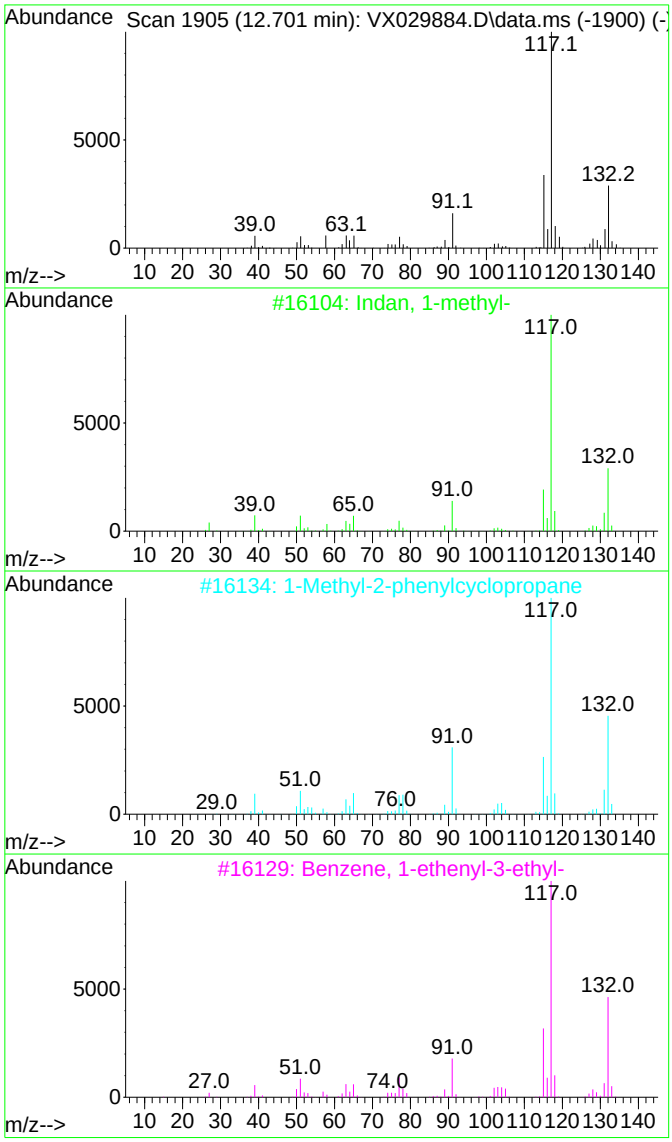
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

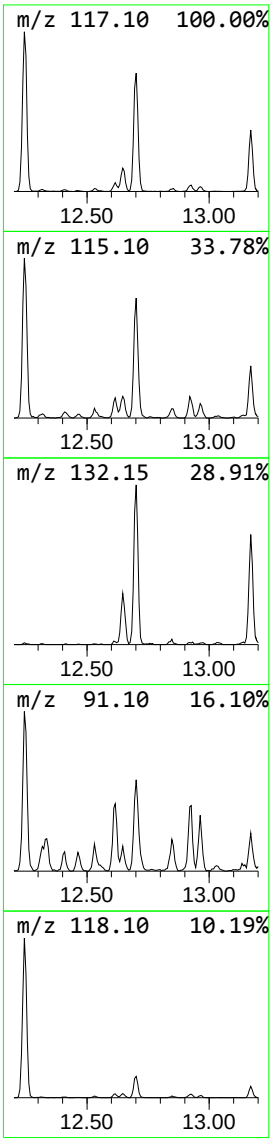
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	19.37 ug/l	366500	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	90
2	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
Sample : N3481-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

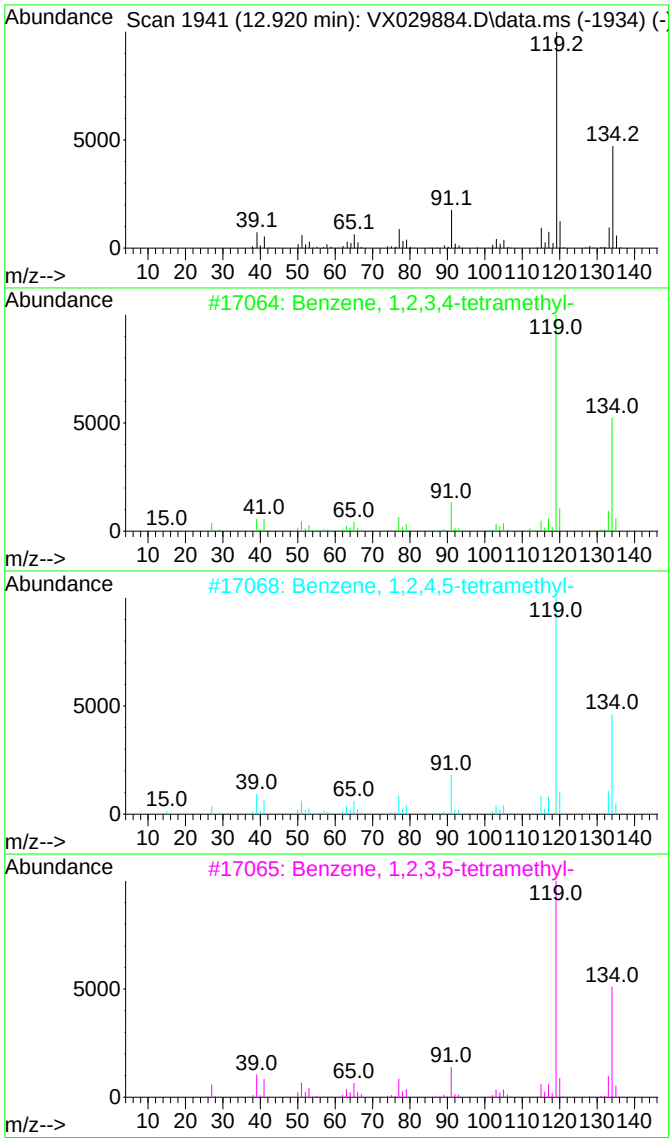
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

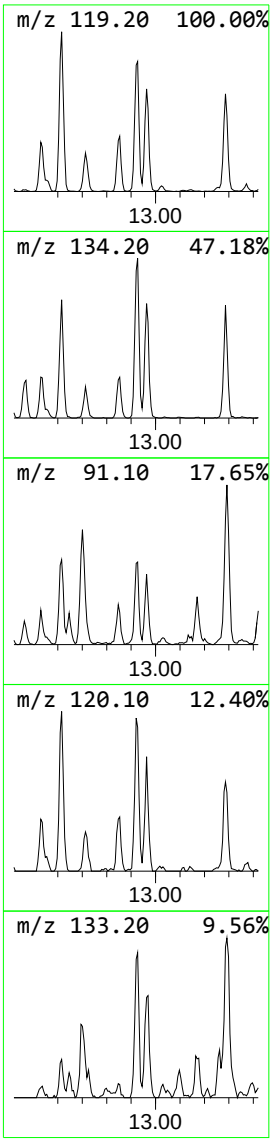
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	11.76 ug/l	222509	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





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Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
Sample : N3481-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

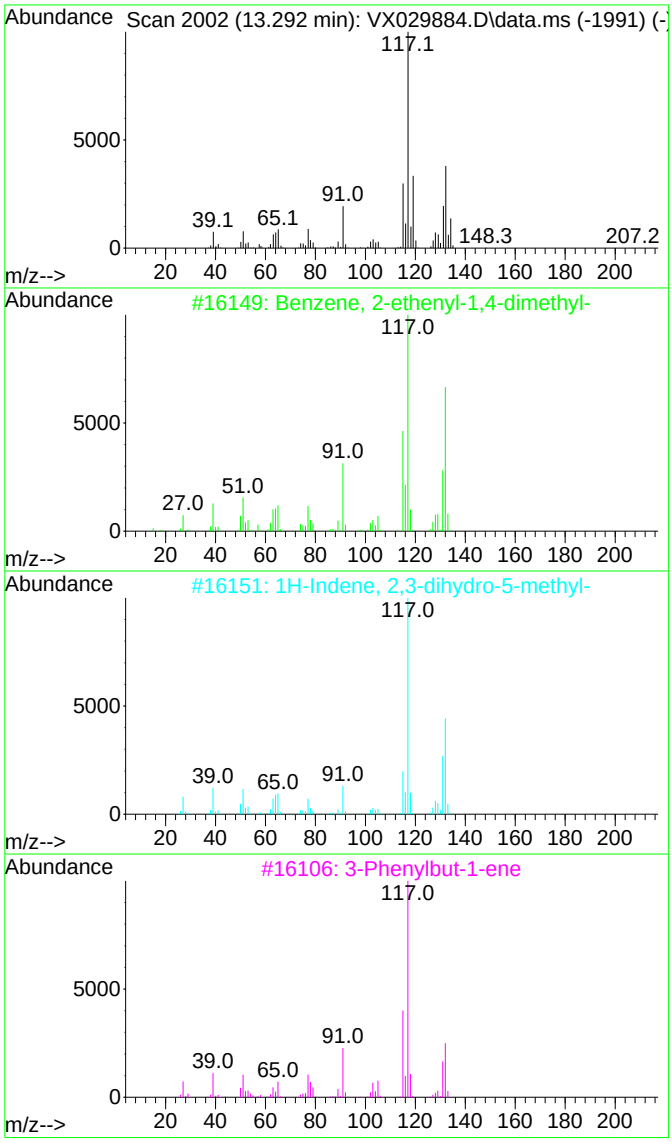
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

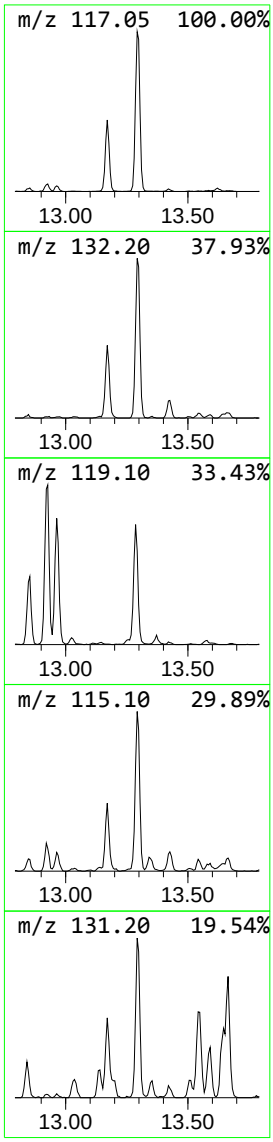
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	29.70 ug/l	561934	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	96
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	83
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
Data File : VX029884.D
Acq On : 30 Jun 2022 01:20
Operator : JC/MD
Sample : N3481-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.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
Isobutane	1.264	11.2	ug/l	155886	1	5.556	696989	50.0
Butane	1.368	11.9	ug/l	165960	1	5.556	696989	50.0
Butane, 2-methyl-	1.752	12.5	ug/l	173730	1	5.556	696989	50.0
Benzene, 1-ethy...	11.616	15.3	ug/l	290303	4	12.024	946043	50.0
Benzene, 1,2,3-...	12.091	22.9	ug/l	433645	4	12.024	946043	50.0
Indane	12.244	30.9	ug/l	585682	4	12.024	946043	50.0
Benzene, 1-ethy...	12.616	12.0	ug/l	226827	4	12.024	946043	50.0
Indan, 1-methyl-	12.701	19.4	ug/l	366500	4	12.024	946043	50.0
Benzene, 1,2,3,...	12.920	11.8	ug/l	222509	4	12.024	946043	50.0
Benzene, 2-ethe...	13.292	29.7	ug/l	561934	4	12.024	946043	50.0